



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 03:37 AM UTC

PDB ID : 7TLJ / pdb_00007tlj
EMDB ID : EMD-25989
Title : Rhodobacter sphaeroides Mitochondrial respiratory chain complex
Authors : Xia, D.; Zhou, F.; Esser, L.; Huang, R.
Deposited on : 2022-01-18
Resolution : 2.91 Å(reported)

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:

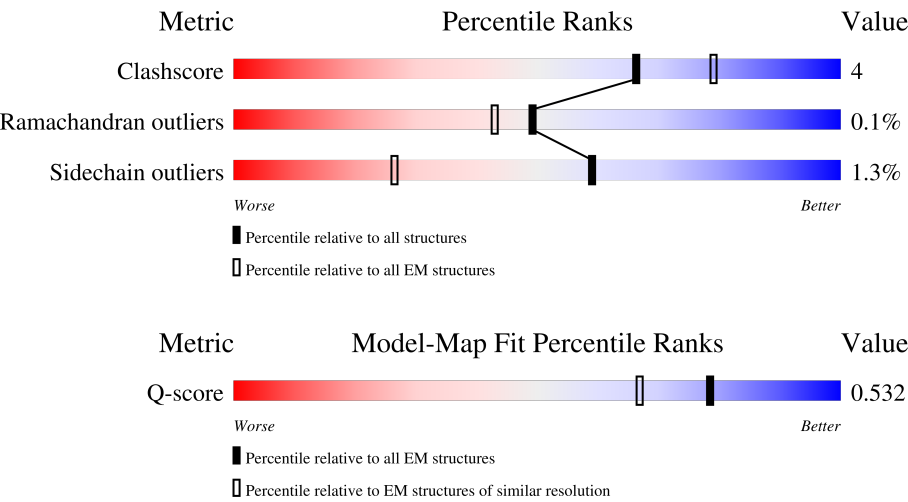
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 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	12972 (2.41 - 3.41)

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	445	89% 8% .
1	E	445	87% 9% .
2	B	272	87% 7% 6%
2	F	272	86% 8% 6%

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Mol	Chain	Length	Quality of chain
3	C	187	86% 10% .
3	G	187	84% 11% ..
4	D	124	17% . 81%
4	H	124	19% . 81%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28105 atoms, of which 13863 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 b.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	428	Total	C	H	N	O	S	0	0
			6850	2319	3415	545	556	15		
1	E	428	Total	C	H	N	O	S	0	0
			6851	2319	3416	545	556	15		

- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	256	Total	C	H	N	O	S	0	0
			3794	1240	1841	326	374	13		
2	F	256	Total	C	H	N	O	S	0	0
			3794	1240	1841	326	374	13		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	98	PRO	ALA	conflict	UNP Q02760
B	264	GLY	-	expression tag	UNP Q02760
B	265	THR	-	expression tag	UNP Q02760
B	266	GLY	-	expression tag	UNP Q02760
B	267	HIS	-	expression tag	UNP Q02760
B	268	HIS	-	expression tag	UNP Q02760
B	269	HIS	-	expression tag	UNP Q02760
B	270	HIS	-	expression tag	UNP Q02760
B	271	HIS	-	expression tag	UNP Q02760
B	272	HIS	-	expression tag	UNP Q02760
F	98	PRO	ALA	conflict	UNP Q02760
F	264	GLY	-	expression tag	UNP Q02760
F	265	THR	-	expression tag	UNP Q02760
F	266	GLY	-	expression tag	UNP Q02760
F	267	HIS	-	expression tag	UNP Q02760
F	268	HIS	-	expression tag	UNP Q02760
F	269	HIS	-	expression tag	UNP Q02760

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Chain	Residue	Modelled	Actual	Comment	Reference
F	270	HIS	-	expression tag	UNP Q02760
F	271	HIS	-	expression tag	UNP Q02760
F	272	HIS	-	expression tag	UNP Q02760

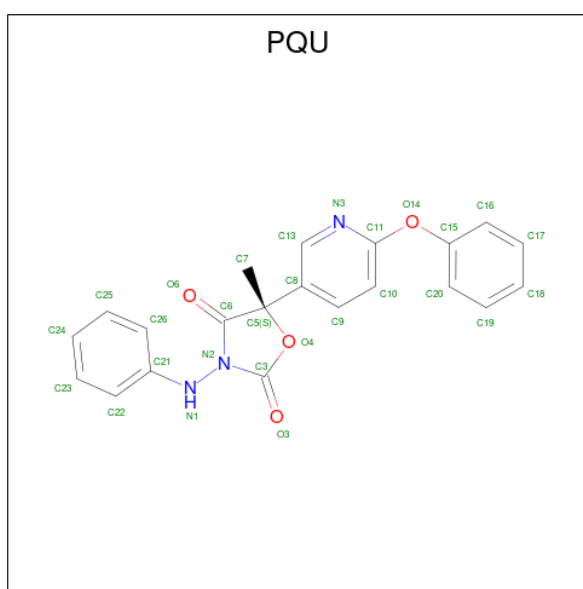
- | Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|-----------|----------|----------|--------|---------|-------|
| 3 | C | 179 | Total
2648 | C
845 | H
1307 | N
237 | O
253 | S
6 | 0 | 0 |
| 3 | G | 179 | Total
2648 | C
845 | H
1307 | N
237 | O
253 | S
6 | 0 | 0 |

- | Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|---------|---------|---------|-------|
| 4 | D | 24 | Total
378 | C
127 | H
192 | N
32 | O
27 | 0 | 0 |
| 4 | H | 24 | Total
378 | C
127 | H
192 | N
32 | O
27 | 0 | 0 |

- # HEM
-
- The diagram shows the chemical structure of the HEM molecule, which is a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure is labeled with atom names (C1A, C2A, etc.) and includes thermal ellipsoids at the 50% probability level. The molecule is a complex macrocycle with various substituents, including two carboxylic acid groups (O1A, O2A, O1D, O2D) and several methyl groups (CMA, CMB, CMC, CMD). The central iron atom is coordinated by four nitrogen atoms (N1, N2, N3, N4) in a square planar geometry. The bond lengths and angles are provided in the table below.
- | Bond | Length (Å) |
|-------|------------|
| Fe-N1 | 2.000 |
| Fe-N2 | 2.000 |
| Fe-N3 | 2.000 |
| Fe-N4 | 2.000 |
- The structure is a complex macrocycle with various substituents, including two carboxylic acid groups (O1A, O2A, O1D, O2D) and several methyl groups (CMA, CMB, CMC, CMD). The central iron atom is coordinated by four nitrogen atoms (N1, N2, N3, N4) in a square planar geometry. The bond lengths and angles are provided in the table below.

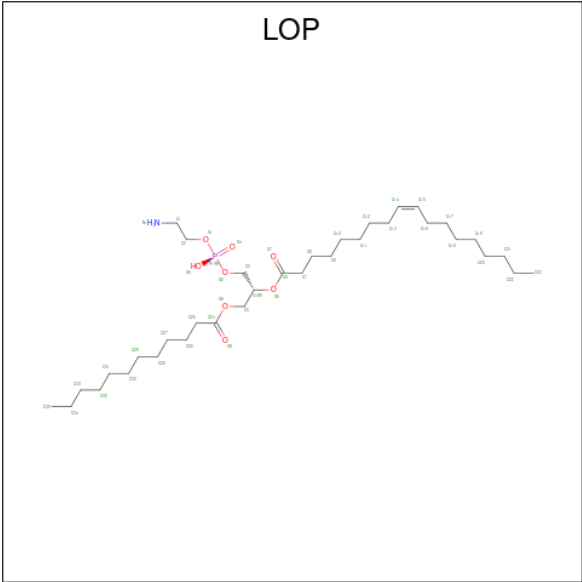
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
5	A	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
5	E	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	
5	E	1	Total	C	Fe	H	N	O	0
			73	34	1	30	4	4	

- Molecule 6 is (5S)-3-anilino-5-methyl-5-(6-phenoxy pyridin-3-yl)-1,3-oxazolidine-2,4-dione (CCD ID: PQU) (formula: C₂₁H₁₇N₃O₄) (labeled as "Ligand of Interest" by depositor).



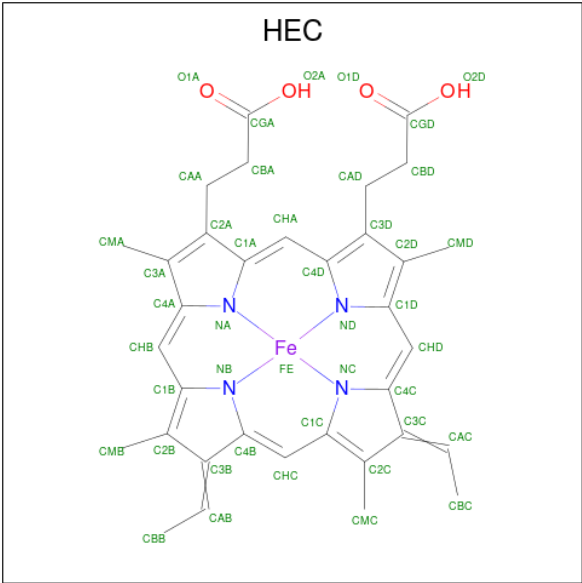
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	H	N	O	0
			45	21	17	3	4	
6	E	1	Total	C	H	N	O	0
			45	21	17	3	4	

- Molecule 7 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (CCD ID: LOP) (formula: C₃₅H₆₈NO₈P).



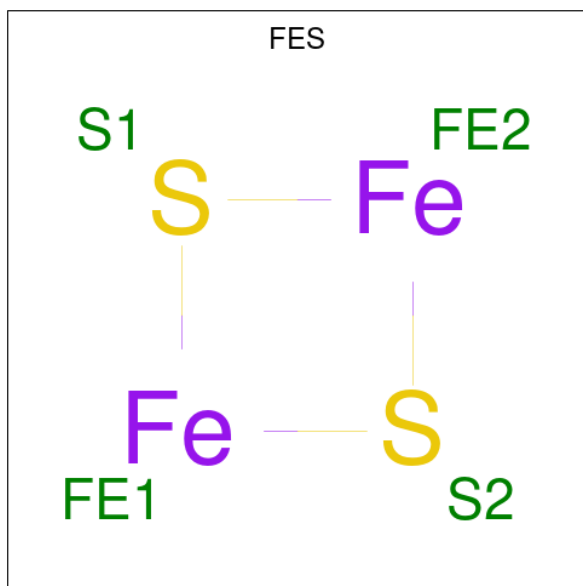
Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total	C	H	N	O	P	0
			112	35	67	1	8	1	
7	E	1	Total	C	H	N	O	P	0
			112	35	67	1	8	1	

- Molecule 8 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						AltConf
8	B	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	
8	F	1	Total	C	Fe	H	N	O	0
			75	34	1	32	4	4	

- Molecule 9 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

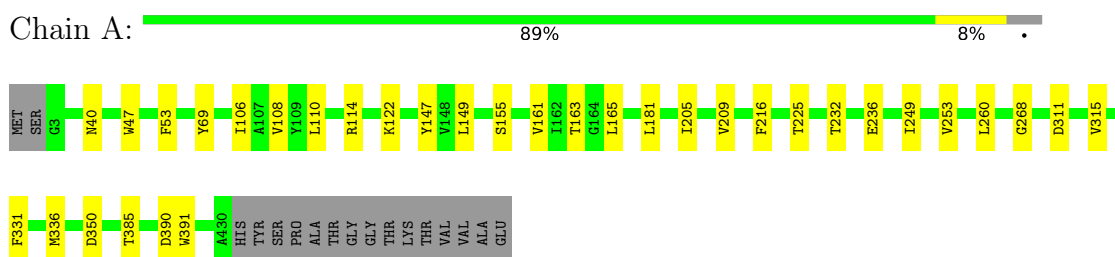


Mol	Chain	Residues	Atoms			AltConf
9	C	1	Total	Fe	S	0
			4	2	2	
9	G	1	Total	Fe	S	0
			4	2	2	

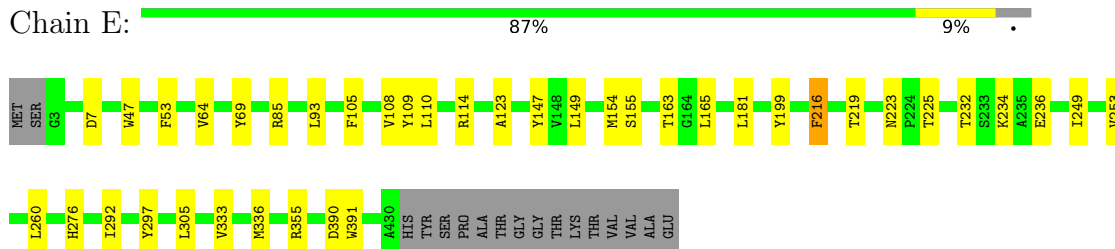
3 Residue-property plots [i](#)

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.

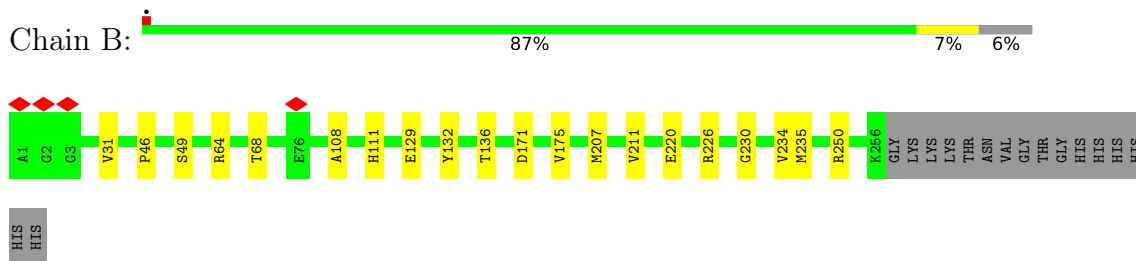
• Molecule 1: Cytochrome b



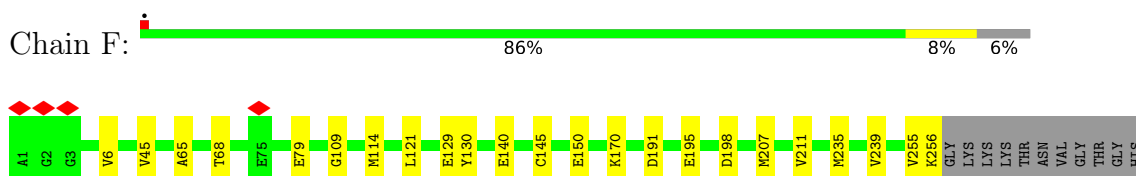
• Molecule 1: Cytochrome b



• Molecule 2: Cytochrome c1

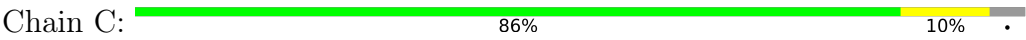


• Molecule 2: Cytochrome c1

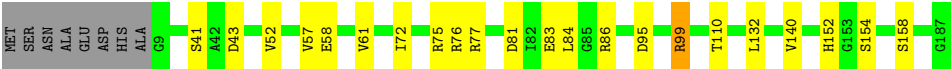
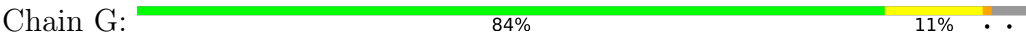


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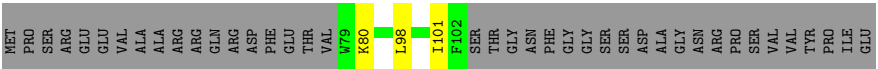
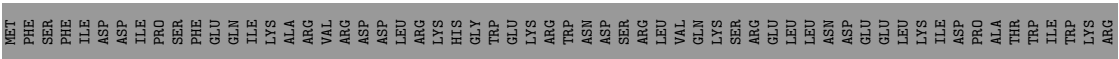
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



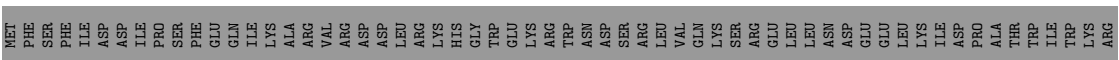
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



- Molecule 4: 14 kDa peptide of ubiquinol-cytochrome c2 oxidoreductase complex



- Molecule 4: 14 kDa peptide of ubiquinol-cytochrome c2 oxidoreductase complex



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	725256	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 ($e^-/\text{\AA}^2$)	54.5	Depositor
Minimum defocus (nm)	836	Depositor
Maximum defocus (nm)	3434	Depositor
Magnification	60241	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	11.122	Depositor
Minimum map value	-3.397	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.277	Depositor
Recommended contour level	1.7	Depositor
Map size (Å)	318.72, 318.72, 318.72	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: PQU, FES, LOP, HEC, HEM

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	0/3565	0.31	0/4891
1	E	0.20	0/3565	0.32	0/4891
2	B	0.18	0/2010	0.28	0/2733
2	F	0.22	0/2010	0.46	0/2733
3	C	0.14	0/1371	0.25	0/1868
3	G	0.20	0/1371	0.44	0/1868
4	D	0.13	0/191	0.22	0/256
4	H	0.11	0/191	0.20	0/256
All	All	0.19	0/14274	0.34	0/19496

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	3435	3415	3420	18	0
1	E	3435	3416	3420	28	0
2	B	1953	1841	1848	15	0
2	F	1953	1841	1848	15	0
3	C	1341	1307	1307	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1341	1307	1307	10	0
4	D	186	192	192	4	0
4	H	186	192	192	4	0
5	A	86	60	60	5	0
5	E	86	60	60	7	0
6	A	28	17	0	0	0
6	E	28	17	0	0	0
7	A	45	67	67	1	0
7	E	45	67	67	0	0
8	B	43	32	30	2	0
8	F	43	32	30	3	0
9	C	4	0	0	0	0
9	G	4	0	0	1	0
All	All	14242	13863	13848	109	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 4.

All (109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:ASN:OD1	1:E:225:THR:OG1	2.02	0.78
3:G:41:SER:OG	3:G:43:ASP:OD1	2.05	0.75
2:B:207:MET:O	2:B:211:VAL:HG23	1.88	0.74
3:C:75:ARG:NH1	3:C:81:ASP:OD2	2.21	0.74
2:F:130:TYR:OH	8:F:1001:HEC:O2A	2.07	0.73
8:B:1001:HEC:HBC3	8:B:1001:HEC:HMC1	1.69	0.73
1:A:147:TYR:O	1:A:155:SER:OG	2.06	0.72
1:A:163:THR:HG21	1:A:181:LEU:HD21	1.72	0.72
8:F:1001:HEC:HMB3	8:F:1001:HEC:HBB3	1.72	0.72
1:E:232:THR:OG1	1:E:236:GLU:OE1	2.07	0.71
3:G:95:ASP:OD2	3:G:99:ARG:NH1	2.24	0.70
5:E:1001:HEM:HBC2	5:E:1001:HEM:HMC1	1.73	0.70
2:B:235:MET:HE2	4:H:98:LEU:HD22	1.74	0.69
1:E:147:TYR:O	1:E:155:SER:OG	2.10	0.69
4:D:98:LEU:HD22	2:F:235:MET:HE2	1.76	0.68
1:E:163:THR:HG21	1:E:181:LEU:HD21	1.75	0.68
1:E:123:ALA:O	1:E:355:ARG:NH1	2.28	0.67
1:A:232:THR:OG1	1:A:236:GLU:OE2	2.13	0.66
1:E:69:TYR:OH	1:E:149:LEU:O	2.14	0.65
5:A:1002:HEM:HMB1	5:A:1002:HEM:HBB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1001:HEC:HMB3	8:B:1001:HEC:HBB3	1.78	0.64
3:G:75:ARG:NH2	3:G:81:ASP:OD2	2.29	0.64
3:G:58:GLU:O	3:G:61:VAL:HG12	1.97	0.64
5:A:1002:HEM:HMC2	5:A:1002:HEM:HBC2	1.81	0.63
3:C:77:ARG:NH2	3:C:111:ASP:OD1	2.32	0.63
2:B:220:GLU:OE2	2:B:226:ARG:NE	2.32	0.62
1:E:85:ARG:NH2	2:F:45:VAL:HG22	2.14	0.62
5:A:1001:HEM:HBC2	5:A:1001:HEM:HMC1	1.81	0.61
1:A:114:ARG:NH1	5:A:1002:HEM:O2A	2.33	0.60
1:E:114:ARG:NH1	5:E:1002:HEM:O2A	2.34	0.60
1:E:64:VAL:HG11	1:E:93:LEU:HD13	1.84	0.60
2:F:235:MET:HE3	2:F:235:MET:HA	1.84	0.59
5:E:1002:HEM:HMC2	5:E:1002:HEM:HBC2	1.83	0.59
3:G:77:ARG:NH1	3:G:158:SER:O	2.35	0.59
3:C:96:THR:O	3:C:109:ALA:N	2.36	0.58
1:A:40:ASN:ND2	1:A:225:THR:OG1	2.36	0.58
2:F:79:GLU:N	2:F:79:GLU:OE1	2.37	0.58
1:E:53:PHE:CE2	1:E:260:LEU:HD21	2.38	0.58
1:A:53:PHE:CE2	1:A:260:LEU:HD21	2.39	0.58
1:A:47:TRP:CZ2	1:A:110:LEU:HD13	2.40	0.57
3:G:154:SER:OG	9:G:1001:FES:S1	2.51	0.57
1:E:165:LEU:CD2	1:E:305:LEU:HD11	2.35	0.56
2:F:65:ALA:O	2:F:68:THR:OG1	2.24	0.56
3:C:162:ILE:HG22	3:C:170:ASN:OD1	2.06	0.56
1:E:47:TRP:CZ2	1:E:110:LEU:HD13	2.41	0.55
3:C:57:VAL:O	3:C:76:ARG:NH2	2.39	0.55
1:E:305:LEU:HD12	1:E:336:MET:SD	2.46	0.55
1:A:69:TYR:OH	1:A:149:LEU:O	2.17	0.55
1:E:199:TYR:CZ	5:E:1001:HEM:HBC1	2.41	0.55
3:C:79:GLU:N	3:C:79:GLU:OE1	2.40	0.55
2:B:171:ASP:OD1	2:B:175:VAL:N	2.41	0.54
1:E:154:MET:HE1	1:E:292:ILE:HA	1.90	0.54
1:A:122:LYS:NZ	1:A:350:ASP:OD2	2.30	0.53
3:G:132:LEU:HD12	3:G:152:HIS:CE1	2.44	0.52
3:G:57:VAL:O	3:G:76:ARG:NH2	2.43	0.51
1:E:199:TYR:CE2	5:E:1001:HEM:HBC1	2.46	0.51
2:F:121:LEU:HD13	2:F:121:LEU:O	2.11	0.51
1:A:390:ASP:OD1	1:A:391:TRP:N	2.43	0.50
1:E:163:THR:HG21	1:E:181:LEU:CD2	2.41	0.50
4:H:98:LEU:O	4:H:98:LEU:HD23	2.11	0.50
2:B:132:TYR:O	2:B:136:THR:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:LEU:HD21	1:E:305:LEU:HD11	1.94	0.50
1:E:390:ASP:OD1	1:E:391:TRP:N	2.43	0.50
1:A:165:LEU:HD13	1:A:336:MET:HE1	1.93	0.49
3:C:117:ASP:N	3:C:117:ASP:OD1	2.43	0.49
1:E:105:PHE:HA	1:E:108:VAL:HG22	1.94	0.49
4:D:101:ILE:HG22	4:D:101:ILE:O	2.13	0.49
3:C:118:GLU:N	3:C:118:GLU:OE2	2.46	0.48
1:A:163:THR:HG21	1:A:181:LEU:CD2	2.41	0.48
2:F:255:VAL:HG23	2:F:256:LYS:H	1.78	0.48
1:A:161:VAL:HG13	3:G:132:LEU:HD13	1.95	0.47
1:A:315:VAL:HG22	1:A:331:PHE:CD1	2.50	0.47
4:D:98:LEU:CD2	2:F:235:MET:HE2	2.44	0.47
2:B:31:VAL:CG1	2:B:211:VAL:HG22	2.45	0.47
2:B:46:PRO:O	2:B:49:SER:OG	2.25	0.47
5:E:1001:HEM:HBC2	5:E:1001:HEM:CMC	2.41	0.47
2:F:129:GLU:OE1	2:F:129:GLU:N	2.46	0.47
5:E:1002:HEM:HMB1	5:E:1002:HEM:HBB2	1.97	0.46
3:C:94:VAL:HB	3:C:162:ILE:HG23	1.99	0.45
4:D:98:LEU:HD23	4:D:98:LEU:O	2.17	0.45
2:F:207:MET:O	2:F:211:VAL:HG23	2.17	0.45
1:E:154:MET:HE3	1:E:276:HIS:CD2	2.51	0.45
2:B:235:MET:HE2	4:H:98:LEU:CD2	2.45	0.44
1:E:249:ILE:O	1:E:253:VAL:HG23	2.17	0.44
2:B:129:GLU:OE1	2:B:129:GLU:N	2.48	0.44
2:B:31:VAL:HG13	2:B:211:VAL:HG22	2.00	0.44
1:E:7:ASP:OD1	1:E:234:LYS:NZ	2.21	0.44
1:E:216:PHE:HA	1:E:219:THR:HG22	1.99	0.44
2:F:6:VAL:HG21	2:F:109:GLY:O	2.18	0.43
1:E:109:TYR:OH	1:E:297:TYR:O	2.35	0.43
1:A:249:ILE:O	1:A:253:VAL:HG23	2.19	0.43
2:F:198:ASP:OD1	2:F:198:ASP:N	2.45	0.43
2:F:255:VAL:HG23	2:F:256:LYS:N	2.34	0.43
5:A:1001:HEM:HMB1	5:A:1001:HEM:HBB2	2.01	0.42
1:A:268:GLY:O	2:B:226:ARG:NH1	2.52	0.42
1:E:64:VAL:CG1	1:E:93:LEU:HD13	2.49	0.42
2:B:64:ARG:O	2:B:68:THR:HG23	2.19	0.42
3:C:58:GLU:O	3:C:61:VAL:HG12	2.20	0.41
3:C:67:PHE:HB3	3:C:72:ILE:HD12	2.02	0.41
1:E:154:MET:HE3	1:E:276:HIS:CG	2.56	0.41
2:B:108:ALA:O	2:B:111:HIS:NE2	2.54	0.41
8:F:1001:HEC:CMC	8:F:1001:HEC:HBC3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:HD12	7:A:1004:LOP:H351	2.03	0.41
1:E:165:LEU:HD22	1:E:333:VAL:HG22	2.03	0.40
1:A:205:ILE:O	1:A:209:VAL:HG23	2.21	0.40
2:F:150:GLU:OE1	2:F:150:GLU:N	2.52	0.40
2:B:230:GLY:O	2:B:234:VAL:HG23	2.21	0.40
2:B:235:MET:HE2	4:H:98:LEU:HD13	2.02	0.40
3:G:83:GLU:OE1	3:G:84:LEU:N	2.54	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	426/445 (96%)	422 (99%)	4 (1%)	0	100	100
1	E	426/445 (96%)	418 (98%)	8 (2%)	0	100	100
2	B	254/272 (93%)	246 (97%)	8 (3%)	0	100	100
2	F	254/272 (93%)	241 (95%)	13 (5%)	0	100	100
3	C	177/187 (95%)	170 (96%)	7 (4%)	0	100	100
3	G	177/187 (95%)	163 (92%)	13 (7%)	1 (1%)	21	50
4	D	22/124 (18%)	21 (96%)	1 (4%)	0	100	100
4	H	22/124 (18%)	22 (100%)	0	0	100	100
All	All	1758/2056 (86%)	1703 (97%)	54 (3%)	1 (0%)	49	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	140	VAL

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	353/366 (96%)	349 (99%)	4 (1%)	65	86
1	E	353/366 (96%)	352 (100%)	1 (0%)	86	95
2	B	203/216 (94%)	202 (100%)	1 (0%)	81	93
2	F	203/216 (94%)	196 (97%)	7 (3%)	32	65
3	C	138/144 (96%)	138 (100%)	0	100	100
3	G	138/144 (96%)	133 (96%)	5 (4%)	31	63
4	D	15/105 (14%)	14 (93%)	1 (7%)	15	41
4	H	15/105 (14%)	15 (100%)	0	100	100
All	All	1418/1662 (85%)	1399 (99%)	19 (1%)	59	84

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	VAL
1	A	216	PHE
1	A	311	ASP
1	A	385	THR
2	B	250	ARG
4	D	80	LYS
1	E	216	PHE
2	F	114	MET
2	F	140	GLU
2	F	145	CYS
2	F	170	LYS
2	F	191	ASP
2	F	195	GLU
2	F	239	VAL
3	G	52	VAL
3	G	72	ILE
3	G	86	ARG
3	G	99	ARG
3	G	110	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	217	HIS
1	A	223	ASN
2	B	62	GLN
1	E	88	ASN
2	F	123	ASN
2	F	157	ASN
2	F	161	GLN
2	F	200	HIS
2	F	228	GLN
2	F	248	ASN
3	G	92	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](#)

12 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
8	HEC	B	1001	2	46,50,50	1.83	6 (13%)	58,82,82	1.82	4 (6%)
5	HEM	A	1001	1	50,50,50	1.34	8 (16%)	67,82,82	1.04	1 (1%)
5	HEM	A	1002	1	50,50,50	1.38	6 (12%)	67,82,82	1.00	4 (5%)
6	PQU	A	1003	-	30,31,31	0.85	2 (6%)	36,44,44	1.34	6 (16%)
5	HEM	E	1002	1	50,50,50	1.33	6 (12%)	67,82,82	1.00	4 (5%)
7	LOP	A	1004	-	44,44,44	1.51	4 (9%)	47,49,49	1.32	8 (17%)
5	HEM	E	1001	1	50,50,50	1.34	8 (16%)	67,82,82	1.02	0
8	HEC	F	1001	2	46,50,50	1.82	5 (10%)	58,82,82	1.82	5 (8%)
7	LOP	E	1004	-	44,44,44	1.51	3 (6%)	47,49,49	1.48	9 (19%)
9	FES	G	1001	3	0,4,4	-	-	-	-	-
6	PQU	E	1003	-	30,31,31	0.86	2 (6%)	36,44,44	1.29	4 (11%)
9	FES	C	1001	3	0,4,4	-	-	-	-	-

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
8	HEC	B	1001	2	-	4/14/54/54	-
5	HEM	A	1001	1	-	3/14/54/54	-
5	HEM	A	1002	1	-	1/14/54/54	-
6	PQU	A	1003	-	-	0/14/33/33	0/4/4/4
5	HEM	E	1002	1	-	3/14/54/54	-
7	LOP	A	1004	-	-	18/48/48/48	-
5	HEM	E	1001	1	-	3/14/54/54	-
8	HEC	F	1001	2	-	4/14/54/54	-
7	LOP	E	1004	-	-	24/48/48/48	-
9	FES	G	1001	3	-	-	0/1/1/1
6	PQU	E	1003	-	-	0/14/33/33	0/4/4/4
9	FES	C	1001	3	-	-	0/1/1/1

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1004	LOP	P1-O4	6.24	1.72	1.50
7	E	1004	LOP	P1-O4	6.23	1.72	1.50
8	B	1001	HEC	CAC-C3C	6.17	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	1001	HEC	CAC-C3C	6.15	1.55	1.35
8	F	1001	HEC	CAB-C3B	6.00	1.54	1.35
8	B	1001	HEC	CAB-C3B	6.00	1.54	1.35
8	B	1001	HEC	C3D-C2D	5.54	1.53	1.38
8	F	1001	HEC	C3D-C2D	5.46	1.53	1.38
5	A	1002	HEM	FE-NC	3.86	2.07	1.95
5	A	1002	HEM	FE-NB	3.80	2.06	1.94
5	E	1002	HEM	FE-NB	3.60	2.06	1.94
7	A	1004	LOP	P1-O3	3.57	1.71	1.55
7	E	1004	LOP	P1-O3	3.56	1.71	1.55
5	E	1001	HEM	FE-NB	3.42	2.05	1.94
7	E	1004	LOP	P1-O1	3.42	1.72	1.59
7	A	1004	LOP	P1-O1	3.38	1.72	1.59
5	A	1001	HEM	FE-NB	3.33	2.05	1.94
5	A	1002	HEM	CAB-C3B	2.95	1.55	1.47
5	E	1002	HEM	CAB-C3B	2.93	1.55	1.47
5	E	1001	HEM	CAB-C3B	2.91	1.55	1.47
5	A	1001	HEM	CAB-C3B	2.90	1.55	1.47
5	A	1001	HEM	FE-NA	2.90	2.04	1.95
5	E	1001	HEM	FE-NA	2.90	2.04	1.95
5	A	1002	HEM	CAC-C3C	2.87	1.55	1.47
5	E	1002	HEM	CAC-C3C	2.82	1.54	1.47
5	A	1001	HEM	CAC-C3C	2.80	1.54	1.47
5	E	1001	HEM	CAC-C3C	2.79	1.54	1.47
5	E	1002	HEM	FE-NC	2.67	2.04	1.95
5	A	1001	HEM	FE-ND	2.37	2.02	1.94
5	E	1001	HEM	FE-ND	2.25	2.01	1.94
8	F	1001	HEC	C3B-C2B	-2.23	1.33	1.41
6	E	1003	PQU	C3-N2	-2.21	1.38	1.43
6	A	1003	PQU	C3-N2	-2.21	1.38	1.43
8	B	1001	HEC	C3B-C2B	-2.21	1.33	1.41
5	A	1002	HEM	CMC-C2C	2.16	1.55	1.50
6	E	1003	PQU	C21-N1	2.14	1.44	1.41
6	A	1003	PQU	C21-N1	2.11	1.44	1.41
8	B	1001	HEC	CMC-C2C	2.08	1.55	1.50
7	A	1004	LOP	O5-C6	-2.08	1.28	1.34
8	F	1001	HEC	C3C-C2C	-2.07	1.34	1.41
5	A	1001	HEM	CMB-C2B	2.06	1.55	1.50
5	E	1002	HEM	CMC-C2C	2.05	1.55	1.50
5	A	1001	HEM	CMC-C2C	2.05	1.55	1.50
5	E	1001	HEM	CMC-C2C	2.04	1.54	1.50
5	E	1001	HEM	CMB-C2B	2.04	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1002	HEM	CMB-C2B	2.03	1.54	1.50
5	E	1001	HEM	C2A-C3A	-2.03	1.33	1.38
5	A	1002	HEM	CMB-C2B	2.03	1.54	1.50
5	A	1001	HEM	C2A-C3A	-2.03	1.33	1.38
8	B	1001	HEC	C3C-C2C	-2.01	1.34	1.41

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1001	HEC	CBB-CAB-C3B	-9.12	109.20	127.43
8	F	1001	HEC	CBB-CAB-C3B	-8.77	109.90	127.43
8	F	1001	HEC	CBC-CAC-C3C	-6.78	113.89	127.43
8	B	1001	HEC	CBC-CAC-C3C	-6.47	114.50	127.43
7	E	1004	LOP	O5-C6-C7	4.53	121.28	111.48
6	A	1003	PQU	C15-O14-C11	3.72	128.99	119.06
6	E	1003	PQU	C15-O14-C11	3.69	128.93	119.06
8	B	1001	HEC	C4D-ND-C1D	3.36	111.30	105.82
6	A	1003	PQU	C13-N3-C11	3.20	119.63	116.72
8	F	1001	HEC	C4D-ND-C1D	3.20	111.03	105.82
6	E	1003	PQU	C13-N3-C11	3.16	119.59	116.72
7	A	1004	LOP	O5-C6-C7	3.12	118.23	111.48
7	E	1004	LOP	O6-C5-C4	3.08	117.28	108.40
7	E	1004	LOP	O6-C24-C25	2.99	120.94	111.83
7	A	1004	LOP	C5-C4-C3	2.99	118.75	111.78
7	E	1004	LOP	O5-C6-O7	-2.72	117.34	123.70
7	A	1004	LOP	O6-C24-C25	2.71	120.09	111.83
7	E	1004	LOP	C4-O5-C6	2.68	124.21	117.80
6	E	1003	PQU	O4-C3-O3	2.50	125.54	122.54
7	A	1004	LOP	O6-C5-C4	2.47	115.53	108.40
6	A	1003	PQU	O4-C3-O3	2.45	125.48	122.54
7	E	1004	LOP	O1-P1-O4	2.44	118.59	108.94
7	A	1004	LOP	O1-C2-C1	2.39	117.90	109.17
6	A	1003	PQU	C21-N1-N2	2.36	120.57	116.20
6	E	1003	PQU	O3-C3-N2	2.31	127.84	119.95
6	A	1003	PQU	O3-C3-N2	2.30	127.83	119.95
5	A	1002	HEM	C4D-ND-C1D	2.30	107.93	105.21
8	F	1001	HEC	C2A-C1A-NA	-2.28	108.12	110.32
7	E	1004	LOP	O1-C2-C1	2.24	117.36	109.17
5	A	1002	HEM	CAD-CBD-CGD	-2.21	107.81	113.67
7	A	1004	LOP	O1-P1-O4	2.19	117.63	108.94
8	B	1001	HEC	C2A-C1A-NA	-2.17	108.23	110.32
7	A	1004	LOP	O3-P1-O1	2.17	117.39	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1002	HEM	C4D-ND-C1D	2.15	107.75	105.21
5	A	1002	HEM	C3D-C4D-ND	-2.11	107.86	110.17
5	E	1002	HEM	CAD-CBD-CGD	-2.10	108.09	113.67
5	A	1001	HEM	C1B-NB-C4B	2.10	107.69	105.21
5	A	1002	HEM	C2A-C1A-NA	-2.09	107.83	110.15
7	E	1004	LOP	O3-P1-O1	2.07	116.94	107.57
5	E	1002	HEM	C2A-C1A-NA	-2.06	107.86	110.15
7	E	1004	LOP	O2-P1-O4	-2.03	100.88	108.94
7	A	1004	LOP	O3-P1-O2	-2.03	98.38	107.57
6	A	1003	PQU	O6-C6-N2	2.02	127.31	124.43
5	E	1002	HEM	C3D-C4D-ND	-2.01	107.96	110.17
8	F	1001	HEC	CAA-CBA-CGA	-2.00	108.35	113.67

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1004	LOP	C2-O1-P1-O2
7	A	1004	LOP	C2-O1-P1-O3
7	E	1004	LOP	C2-O1-P1-O2
7	E	1004	LOP	C2-O1-P1-O3
7	E	1004	LOP	C3-O2-P1-O1
7	E	1004	LOP	C3-O2-P1-O3
7	E	1004	LOP	C3-O2-P1-O4
7	E	1004	LOP	O7-C6-O5-C4
7	E	1004	LOP	C7-C6-O5-C4
8	B	1001	HEC	C2B-C3B-CAB-CBB
8	B	1001	HEC	C4B-C3B-CAB-CBB
8	B	1001	HEC	C2C-C3C-CAC-CBC
8	B	1001	HEC	C4C-C3C-CAC-CBC
8	F	1001	HEC	C2B-C3B-CAB-CBB
8	F	1001	HEC	C4B-C3B-CAB-CBB
8	F	1001	HEC	C2C-C3C-CAC-CBC
8	F	1001	HEC	C4C-C3C-CAC-CBC
7	E	1004	LOP	C30-C31-C32-C33
7	A	1004	LOP	C9-C10-C11-C12
7	A	1004	LOP	C11-C10-C9-C8
7	E	1004	LOP	C24-C25-C26-C27
5	E	1002	HEM	C2A-CAA-CBA-CGA
7	E	1004	LOP	C7-C8-C9-C10
7	A	1004	LOP	C27-C28-C29-C30
7	A	1004	LOP	O2-C3-C4-O5

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Mol	Chain	Res	Type	Atoms
7	E	1004	LOP	C20-C21-C22-C23
7	E	1004	LOP	C15-C16-C17-C18
7	E	1004	LOP	C28-C29-C30-C31
7	E	1004	LOP	C10-C11-C12-C13
7	A	1004	LOP	O2-C3-C4-C5
7	A	1004	LOP	C30-C31-C32-C33
7	E	1004	LOP	C13-C14-C15-C16
7	A	1004	LOP	C3-C4-C5-O6
7	E	1004	LOP	C3-C4-C5-O6
7	E	1004	LOP	C26-C27-C28-C29
7	A	1004	LOP	C7-C8-C9-C10
7	E	1004	LOP	C16-C17-C18-C19
7	E	1004	LOP	C9-C10-C11-C12
5	E	1001	HEM	C3D-CAD-CBD-CGD
7	E	1004	LOP	O5-C4-C5-O6
5	A	1002	HEM	C2A-CAA-CBA-CGA
7	A	1004	LOP	O7-C6-O5-C4
7	A	1004	LOP	C16-C17-C18-C19
7	A	1004	LOP	C3-O2-P1-O1
5	A	1001	HEM	C3D-CAD-CBD-CGD
7	A	1004	LOP	O5-C4-C5-O6
5	E	1001	HEM	CAD-CBD-CGD-O1D
5	A	1001	HEM	CAD-CBD-CGD-O1D
7	E	1004	LOP	C32-C33-C34-C35
5	E	1001	HEM	CAD-CBD-CGD-O2D
5	A	1001	HEM	CAD-CBD-CGD-O2D
7	A	1004	LOP	C12-C13-C14-C15
7	A	1004	LOP	C14-C15-C16-C17
7	E	1004	LOP	O6-C24-C25-C26
7	E	1004	LOP	O8-C24-C25-C26
7	A	1004	LOP	O6-C24-C25-C26
5	E	1002	HEM	CAA-CBA-CGA-O2A
7	A	1004	LOP	O8-C24-C25-C26
7	E	1004	LOP	O2-C3-C4-C5
5	E	1002	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

8 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1001	HEC	2	0
5	A	1001	HEM	2	0

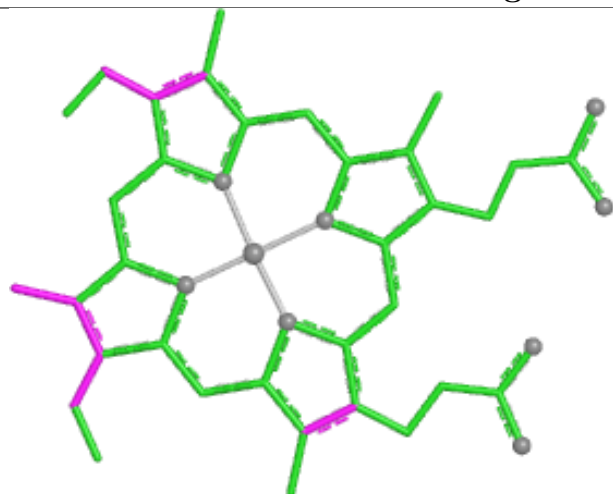
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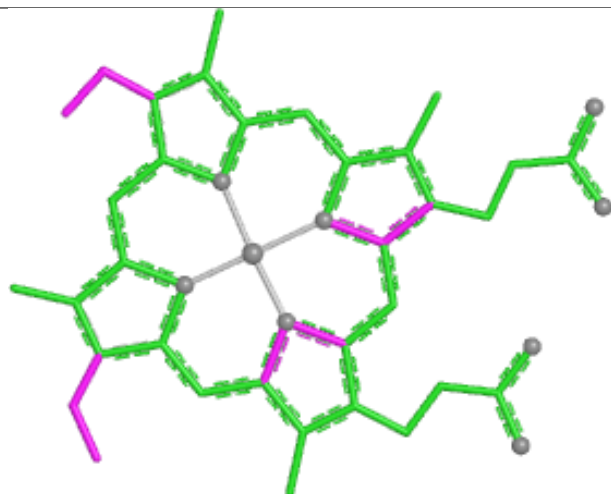
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1002	HEM	3	0
5	E	1002	HEM	3	0
7	A	1004	LOP	1	0
5	E	1001	HEM	4	0
8	F	1001	HEC	3	0
9	G	1001	FES	1	0

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

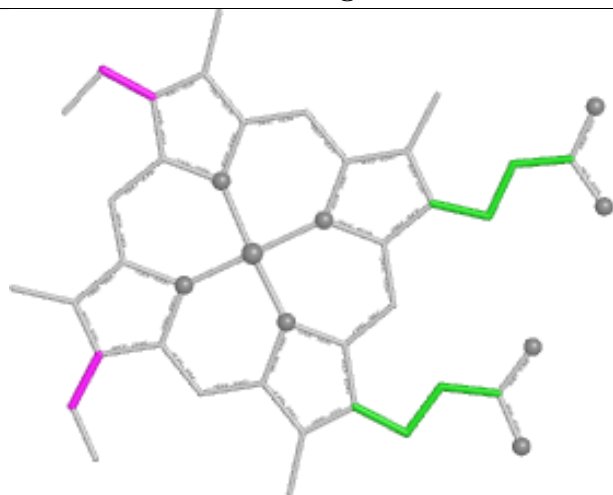
Ligand HEC B 1001



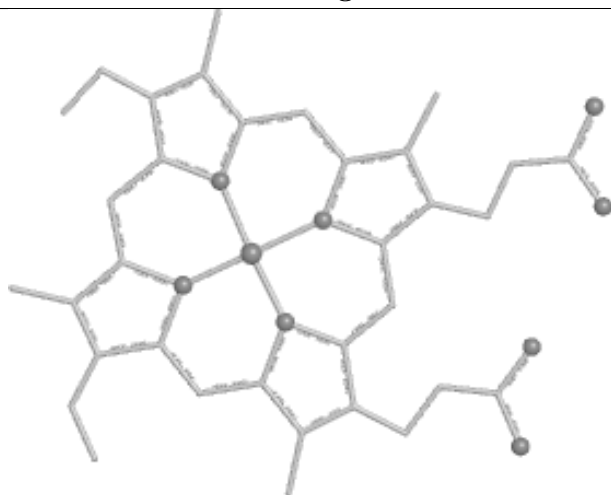
Bond lengths



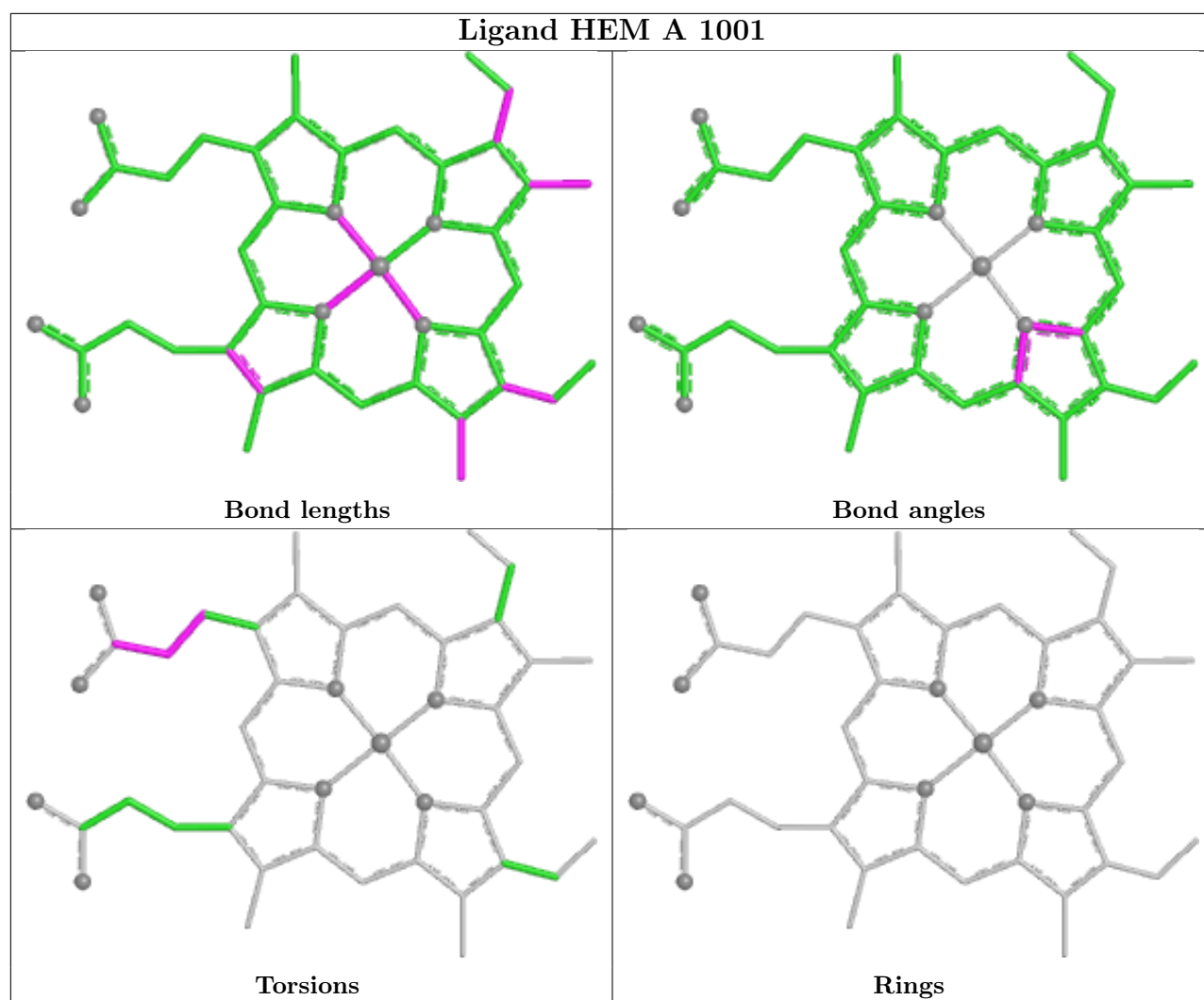
Bond angles

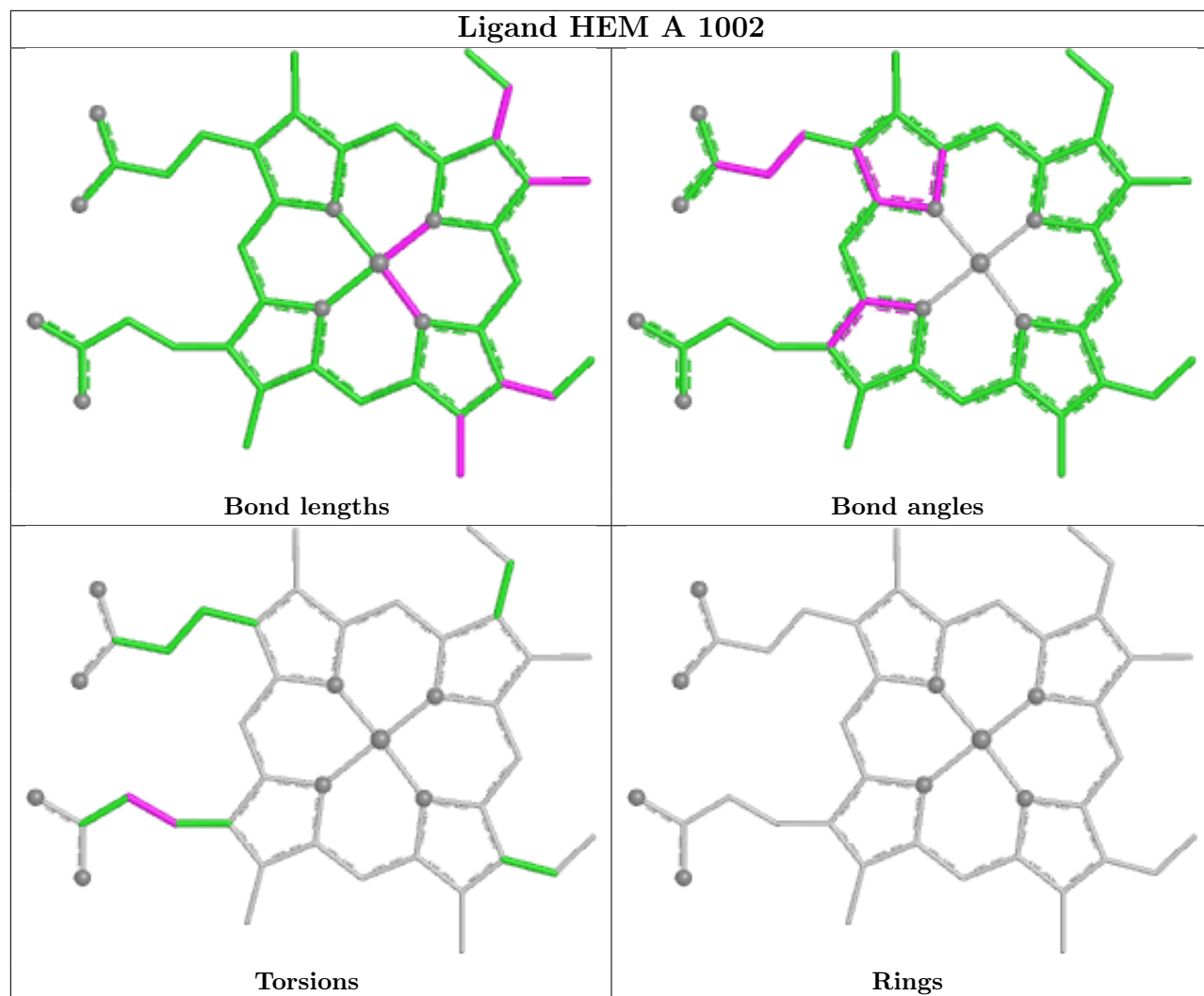


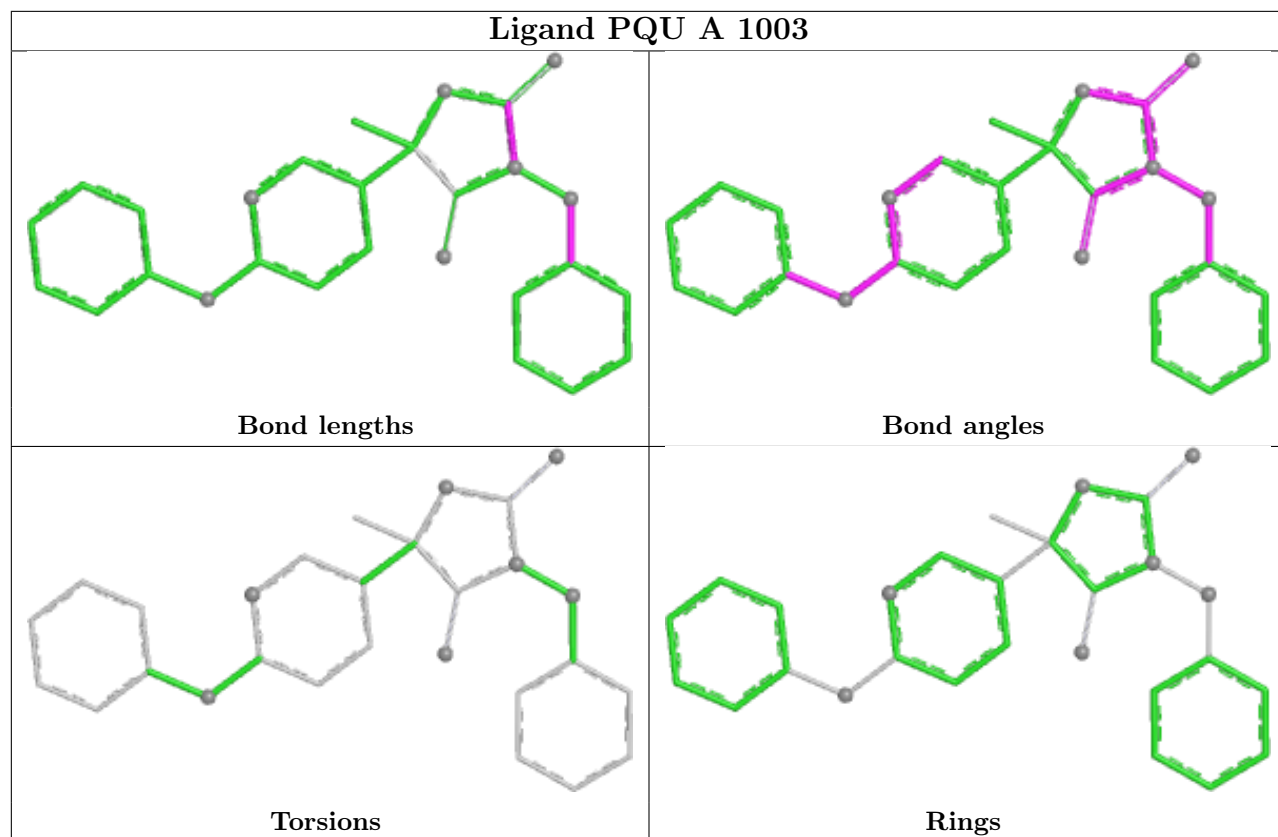
Torsions

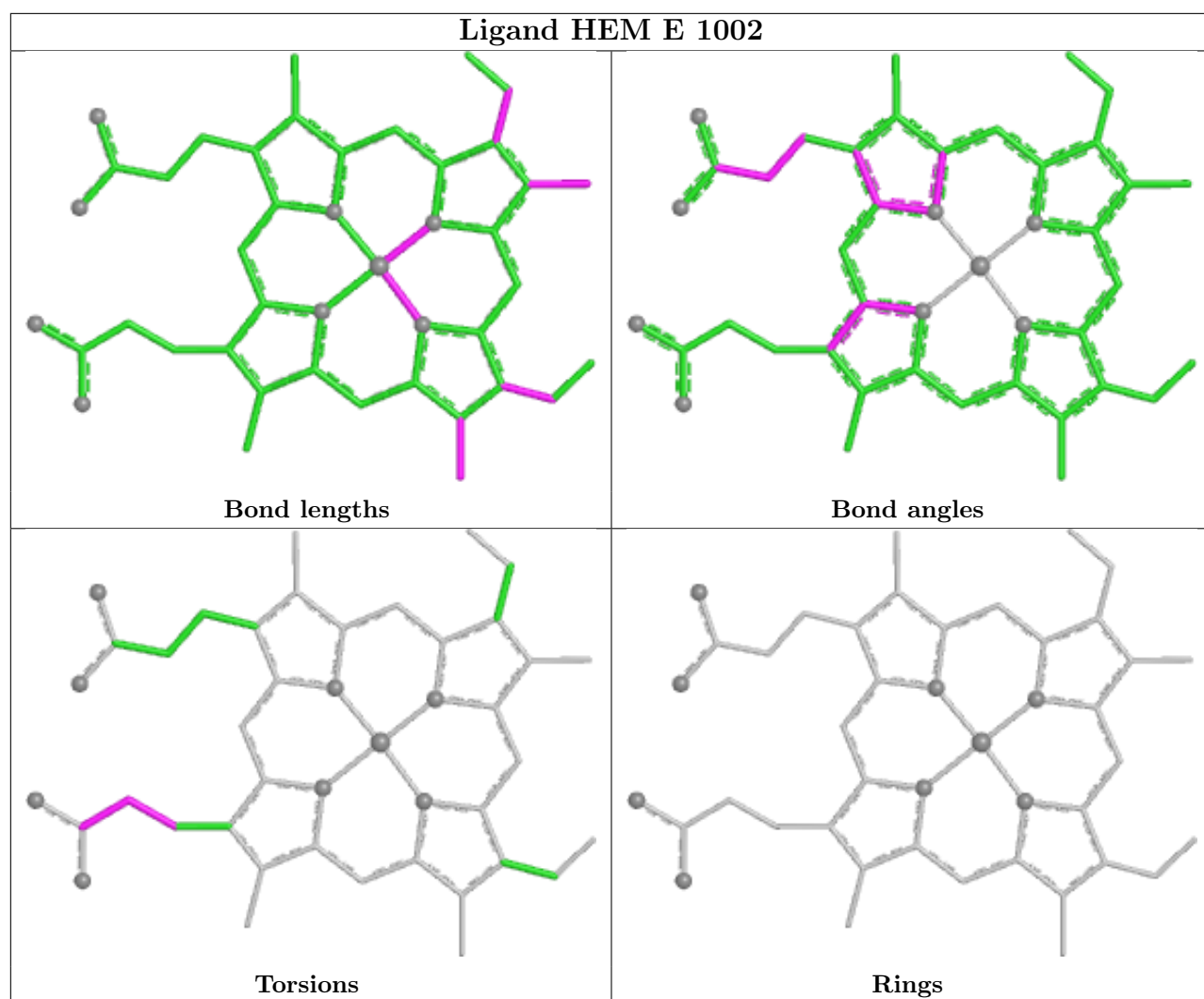


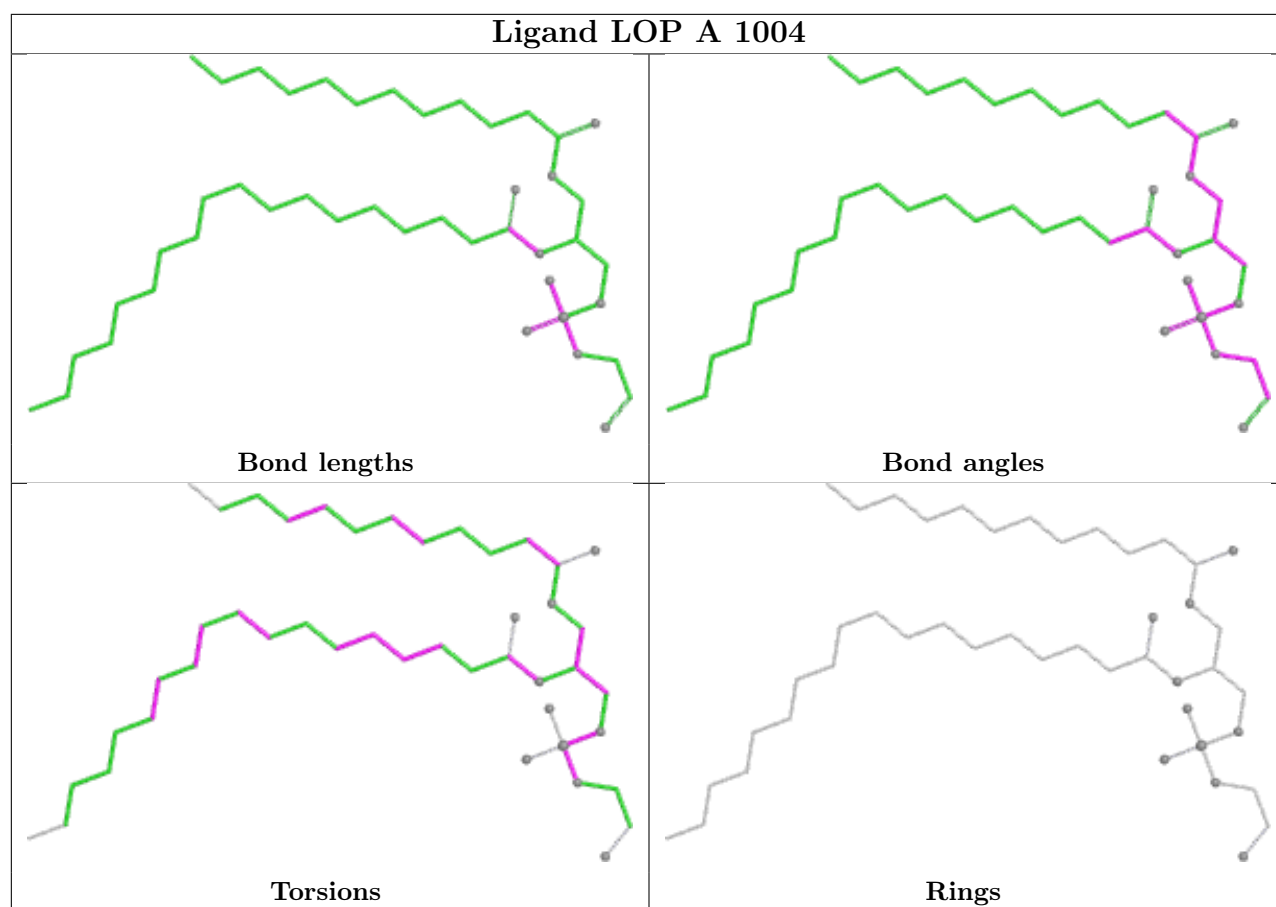
Rings

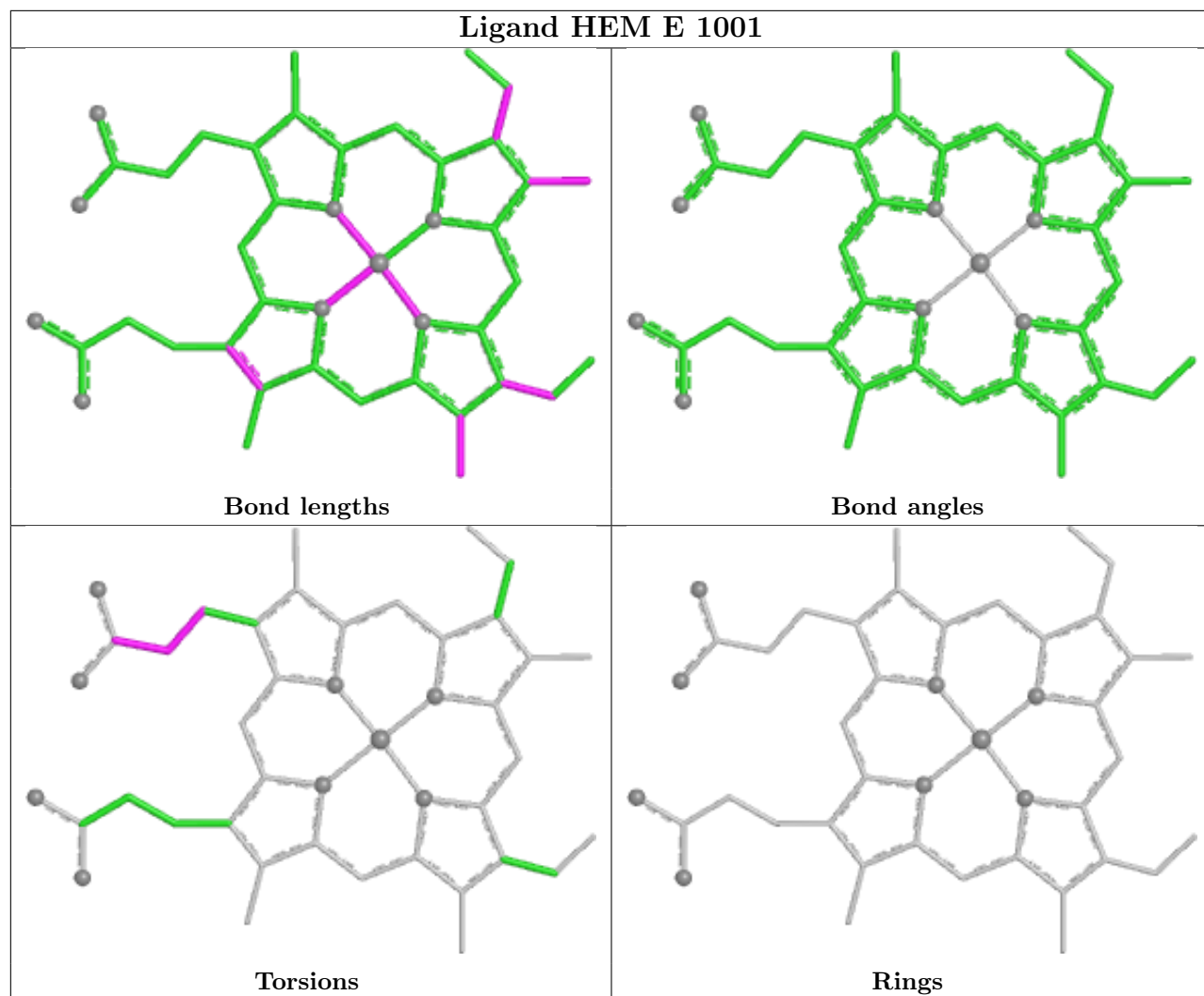


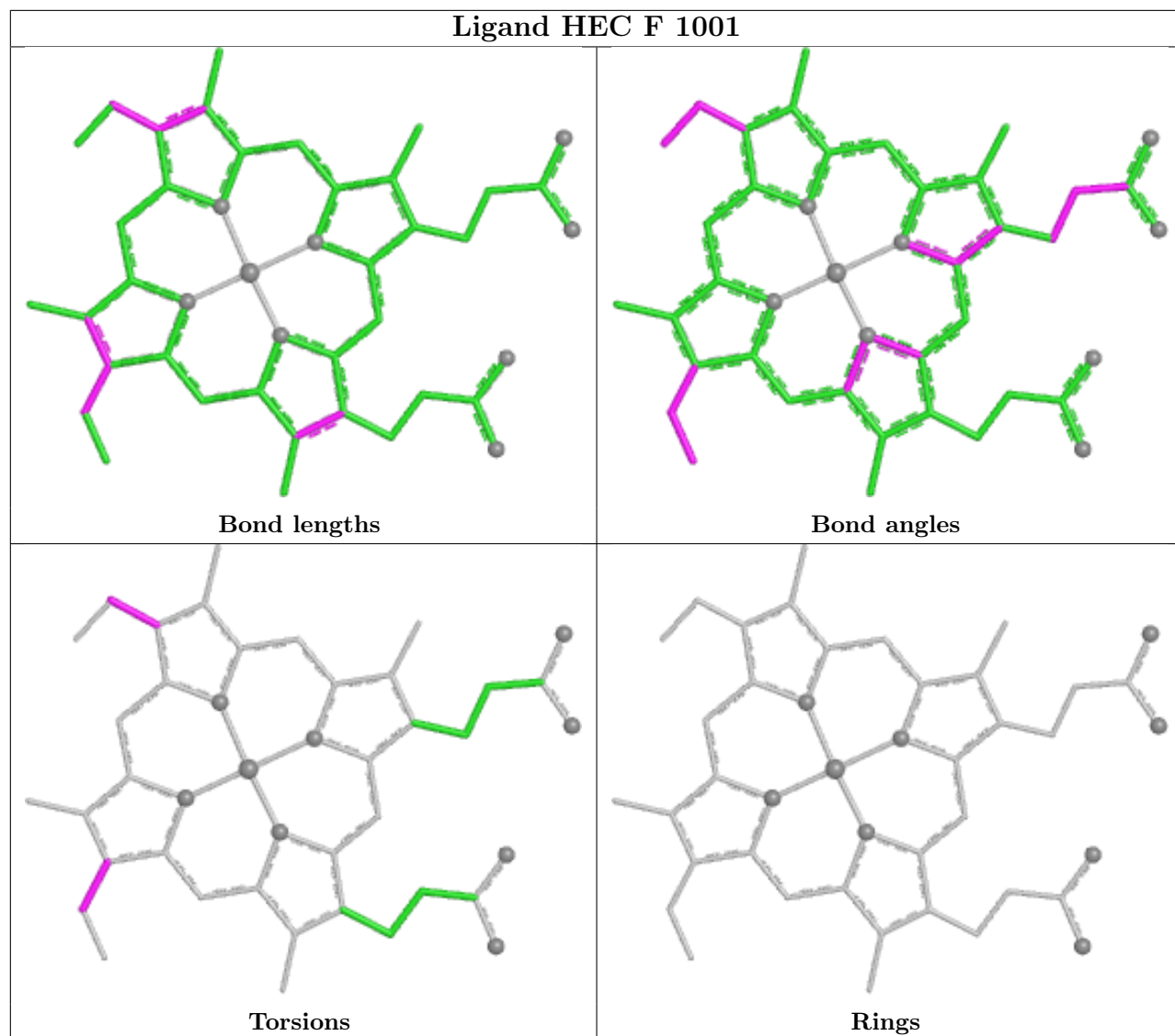


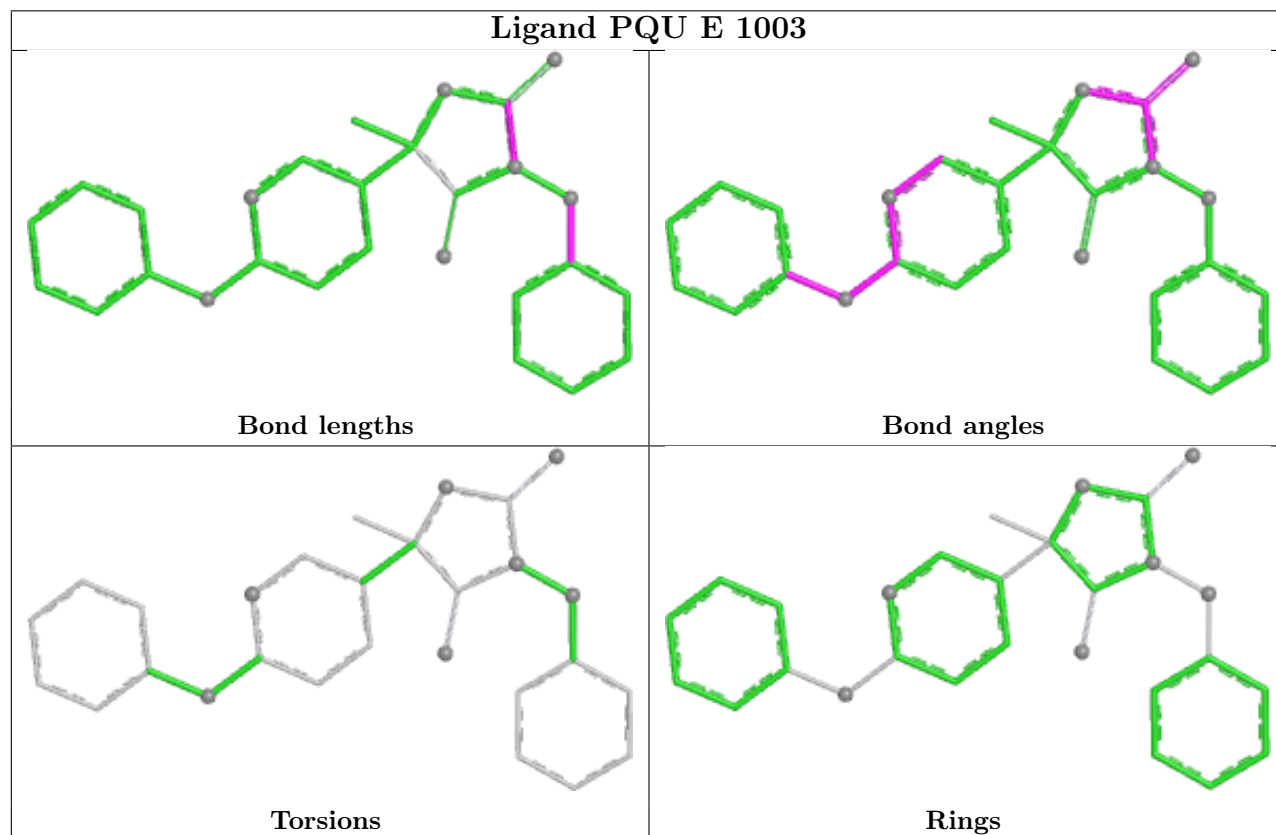
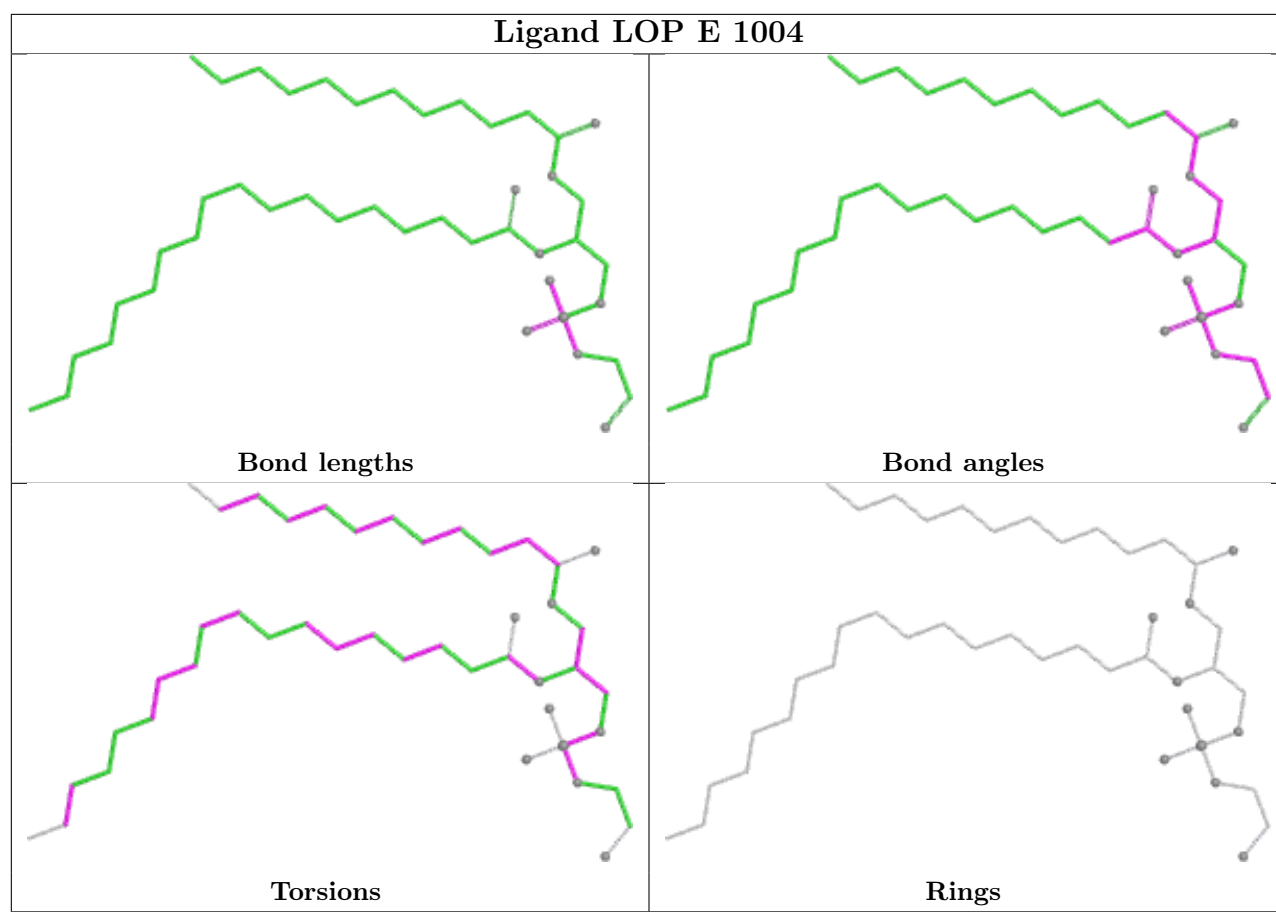












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

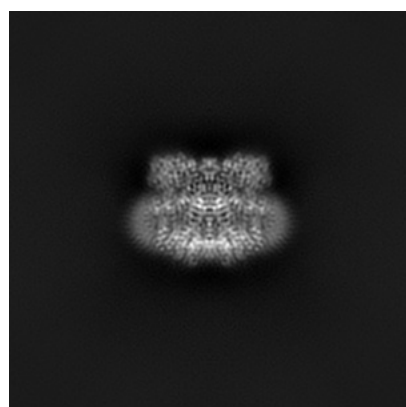
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25989. These allow visual inspection of the internal detail of the map and identification of artifacts.

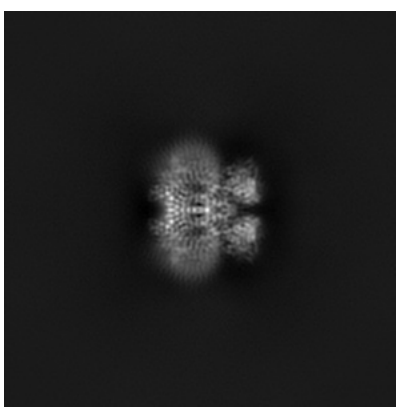
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

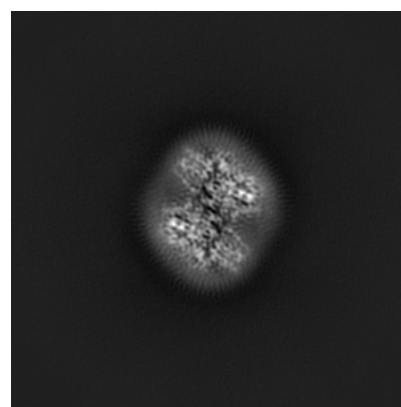
6.1.1 Primary map



X



Y

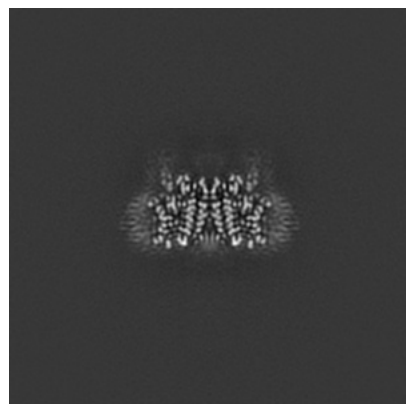


Z

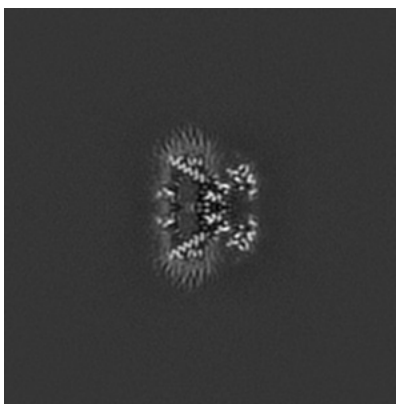
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

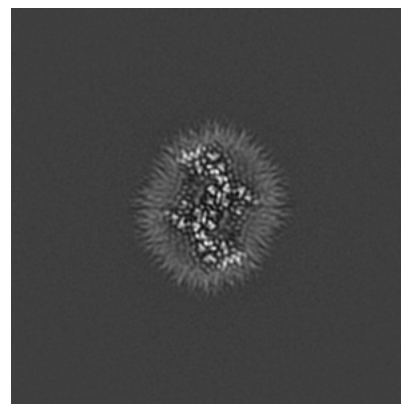
6.2.1 Primary map



X Index: 192



Y Index: 192

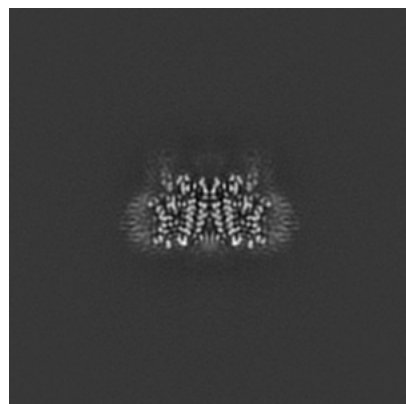


Z Index: 192

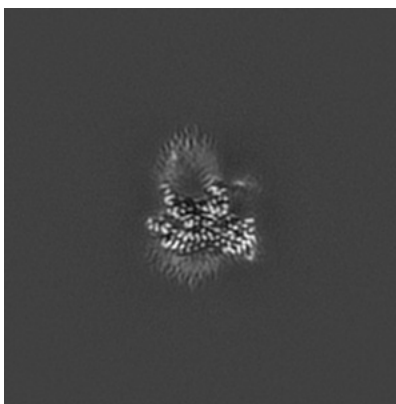
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

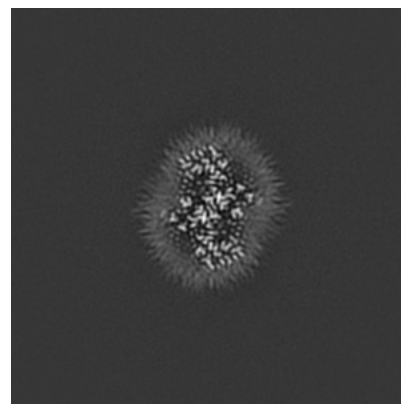
6.3.1 Primary map



X Index: 192



Y Index: 177

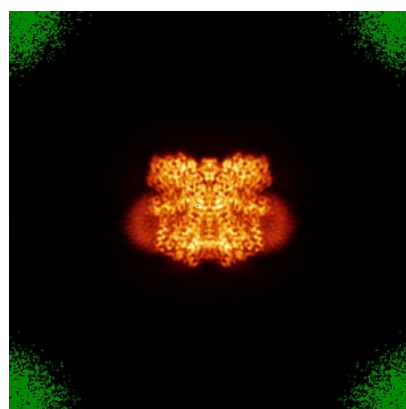


Z Index: 195

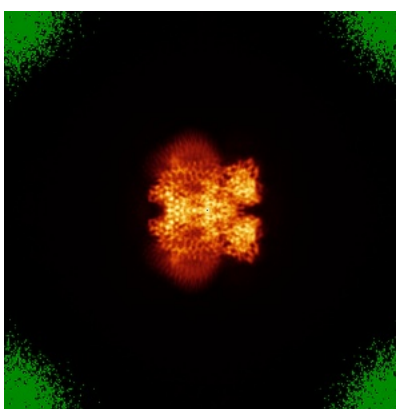
The images above show the largest variance slices of the map in three orthogonal directions.

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

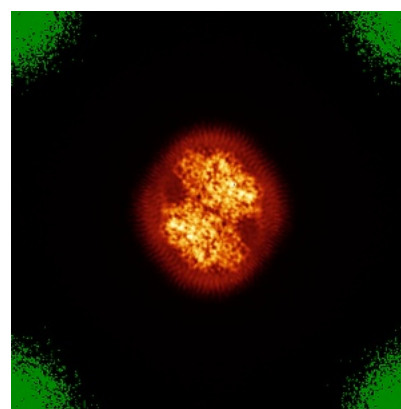
6.4.1 Primary map



X



Y

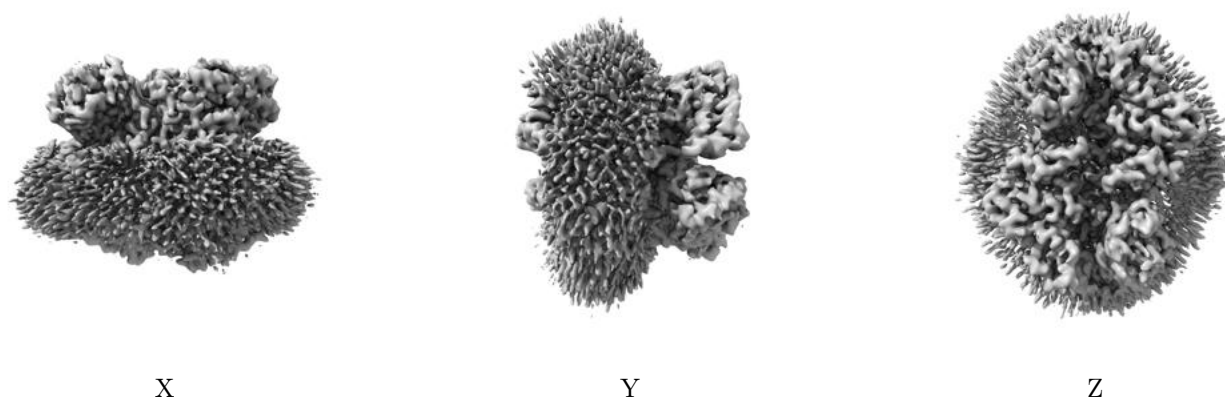


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

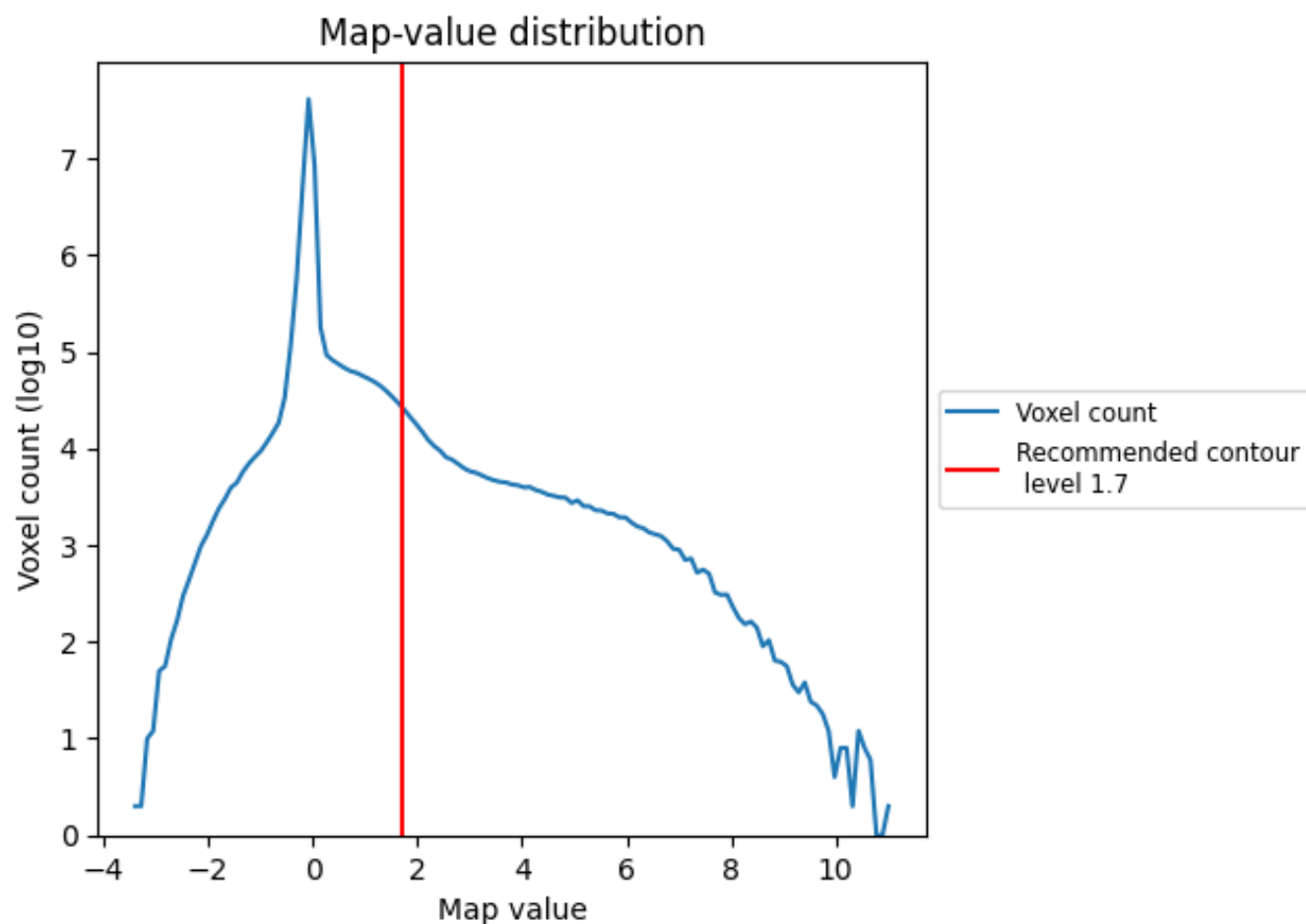
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

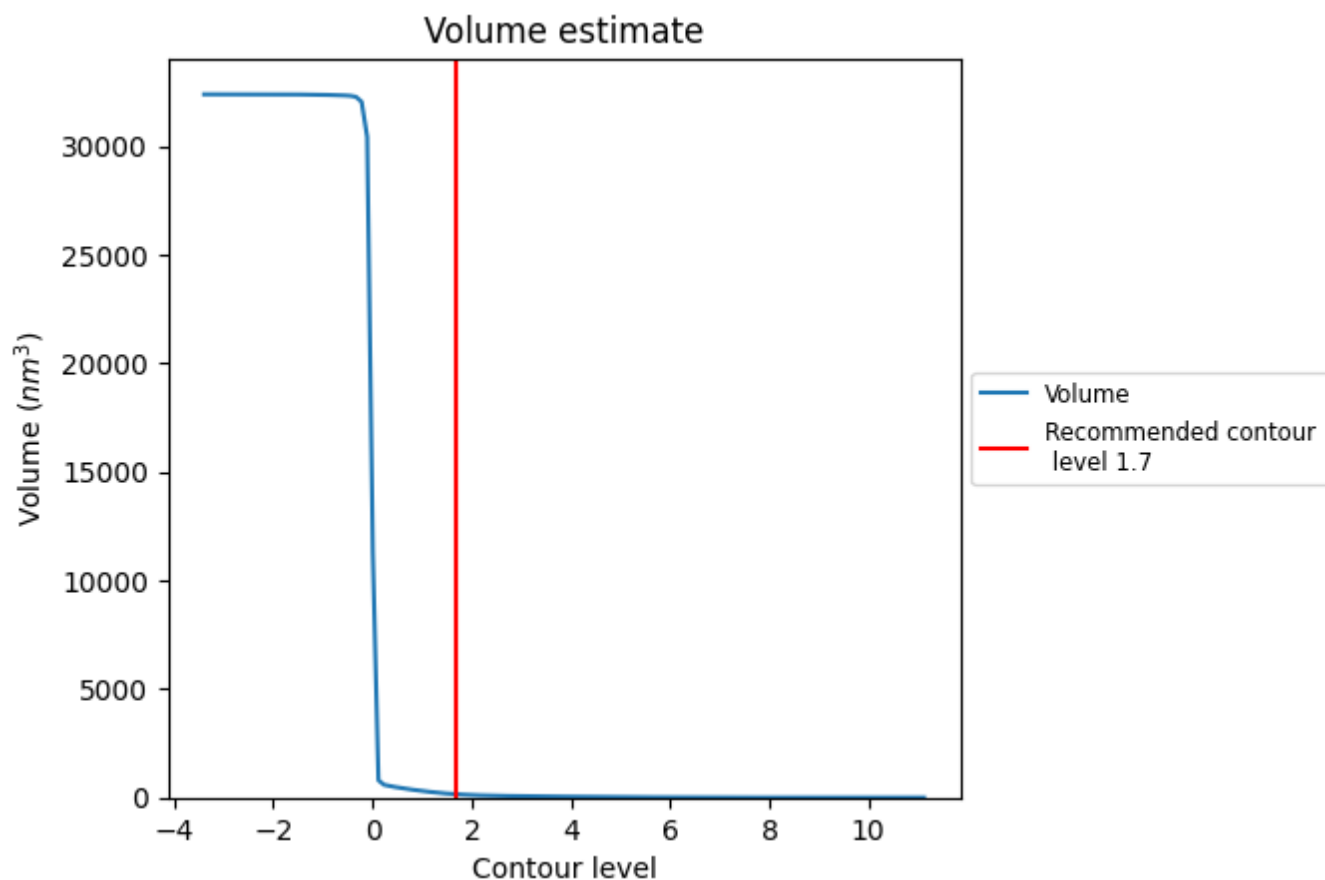
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

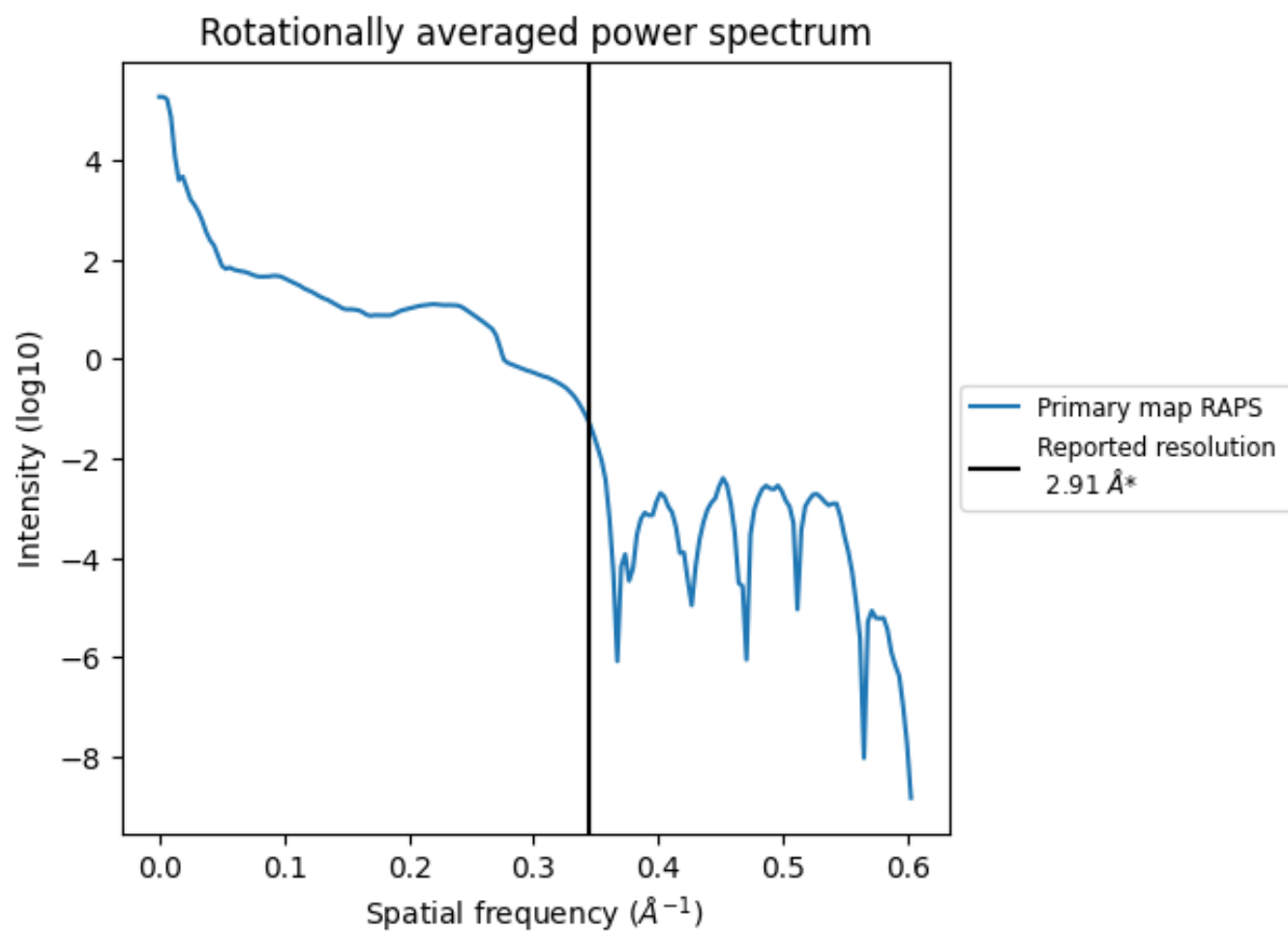
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 151 nm³; this corresponds to an approximate mass of 137 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 0.344 Å⁻¹

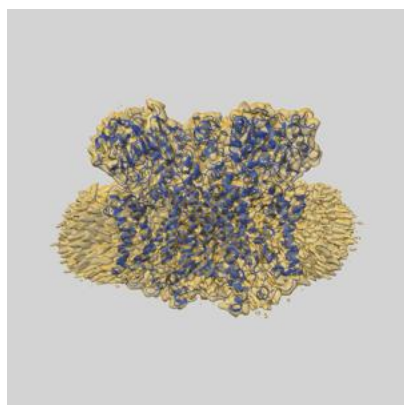
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

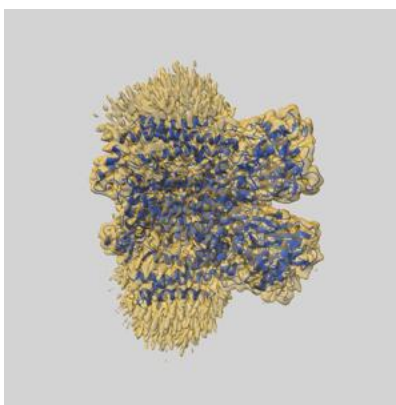
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25989 and PDB model 7TLJ. Per-residue inclusion information can be found in section [3](#) on page [9](#).

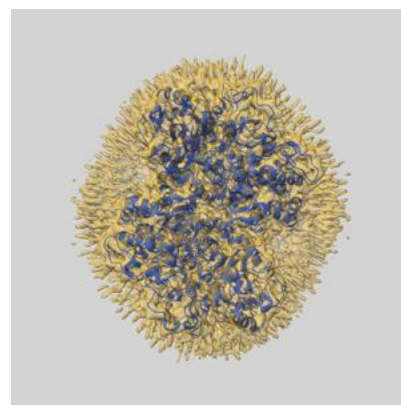
9.1 Map-model overlay [i](#)



X



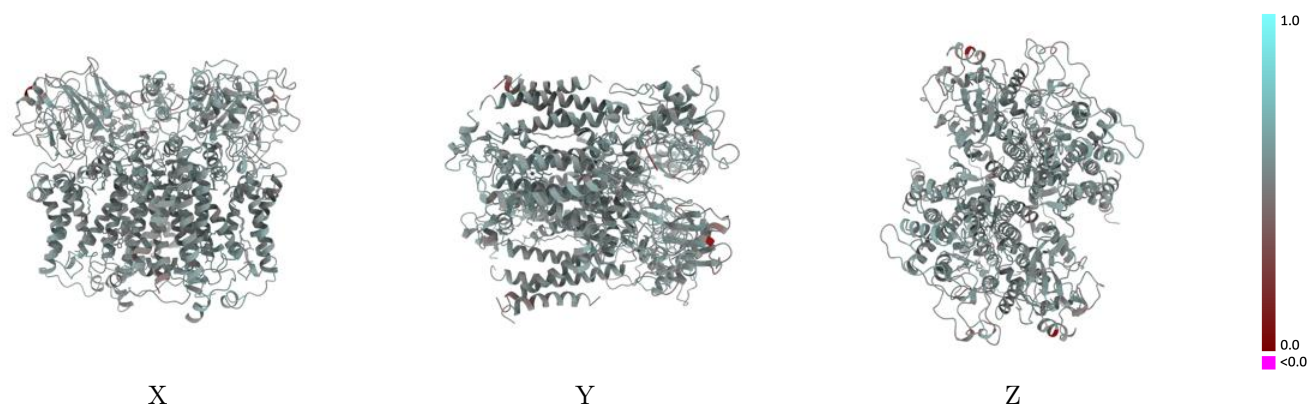
Y



Z

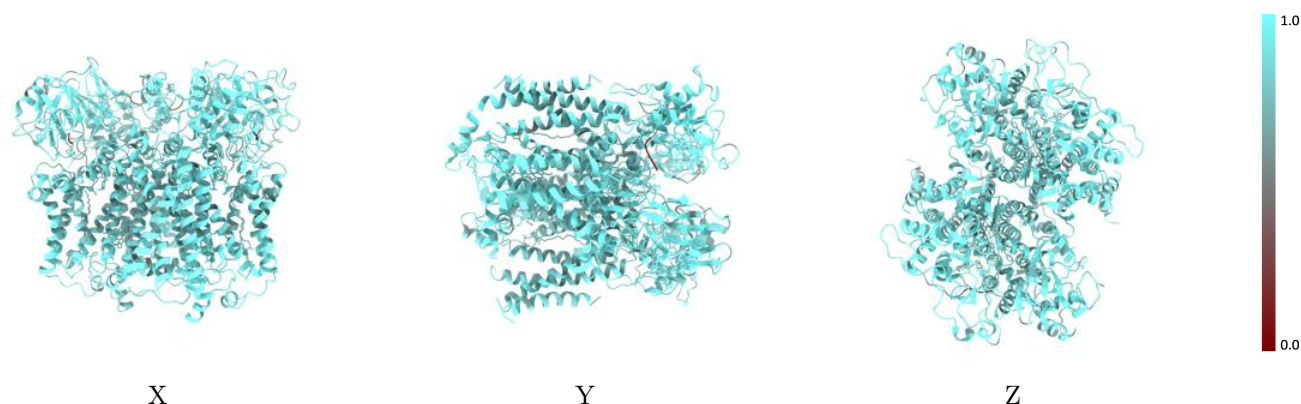
The images above show the 3D surface view of the map at the recommended contour level 1.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



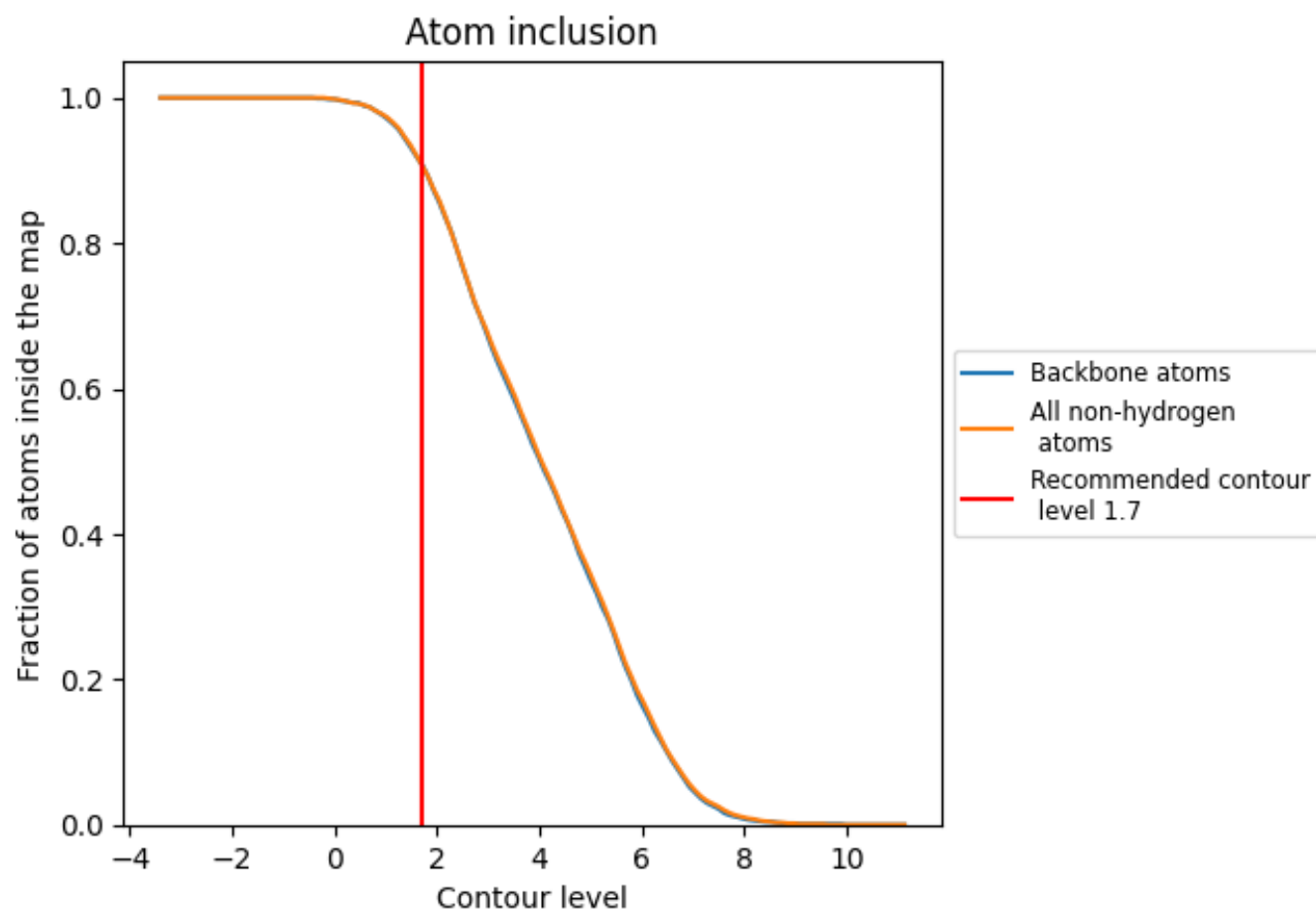
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (1.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9080	0.5320
A	0.9160	0.5430
B	0.9180	0.5290
C	0.8970	0.5130
D	0.8880	0.5000
E	0.9130	0.5430
F	0.9130	0.5250
G	0.8900	0.5140
H	0.8880	0.4980

1.0

0.0

<0.0