wwPDB EM Validation Summary Report (i)

Mar 10, 2026 – 02:58 AM UTC

PDB ID	:	9GM8 / pdb_00009gm8
EMDB ID	:	EMD-51444
Title	:	MukBEF in a nucleotide-bound state with open neck gate
Authors	:	Burmann, F.; Lowe, J.
Deposited on	:	2024-08-28
Resolution	:	3.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

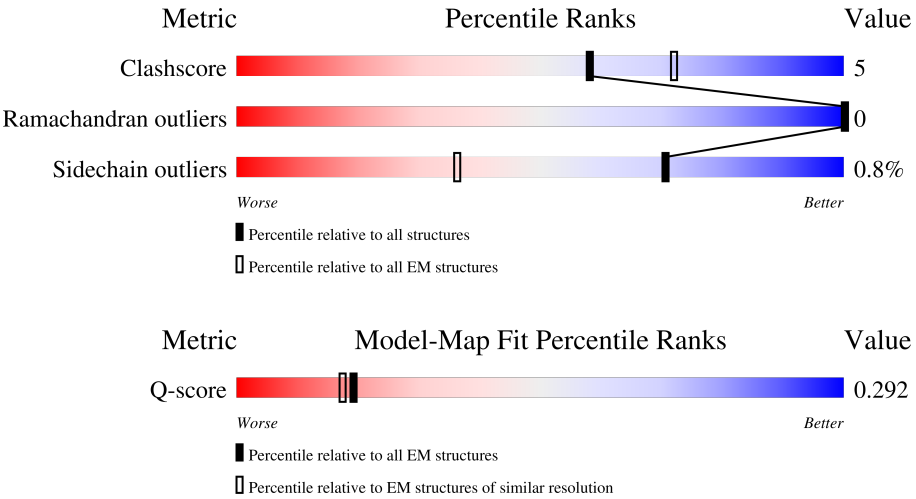
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.90 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	8855 (3.40 - 4.40)

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 <=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	C	440	88% 11%
1	D	440	60% 5% 34%
2	E	240	69% 18% 12%
2	F	240	69% 13% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	78	65% 26% 8%
3	I	78	76% 15% 8%
4	A	1482	68% 7% 25%
4	B	1482	66% 11% 23%

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
3	4HH	G	36	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 56889 atoms, of which 28315 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 Chromosome partition protein MukF.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	440	Total	C	H	N	O	S	0	0
			6982	2218	3451	614	686	13		
1	D	290	Total	C	H	N	O	S	0	0
			4567	1444	2260	402	451	10		

- Molecule 2 is a protein called Chromosome partition protein MukE.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	212	Total	C	H	N	O	S	0	0
			3441	1090	1719	301	322	9		
2	F	198	Total	C	H	N	O	S	0	0
			3246	1029	1627	284	298	8		

- Molecule 3 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms							AltConf	Trace
3	G	72	Total	C	H	N	O	P	S	0	0
			1147	360	564	87	133	1	2		
3	I	72	Total	C	H	N	O	P	S	0	0
			1147	360	564	87	133	1	2		

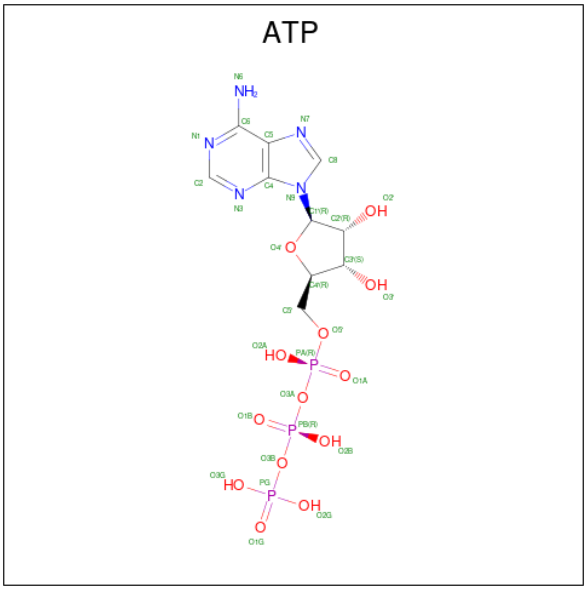
- Molecule 4 is a protein called Chromosome partition protein MukB.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	A	1109	Total	C	H	N	O	S	0	0
			17804	5514	8885	1659	1715	31		
4	B	1148	Total	C	H	N	O	S	0	0
			18467	5712	9221	1720	1780	34		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Mg 1 1	0
5	B	1	Total Mg 1 1	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



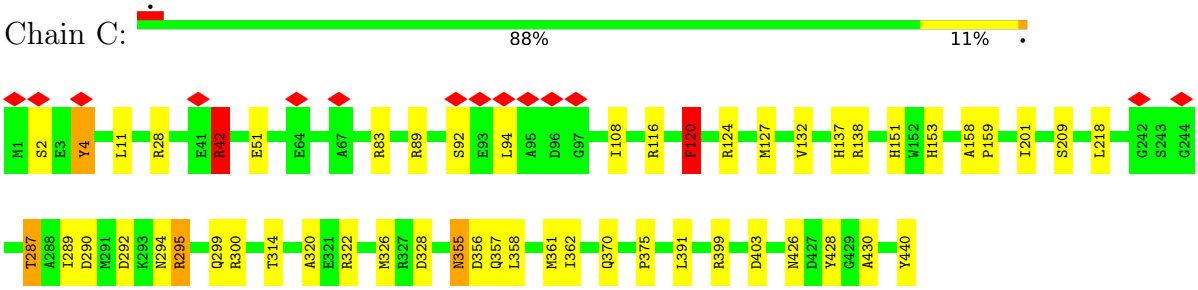
Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
6	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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.

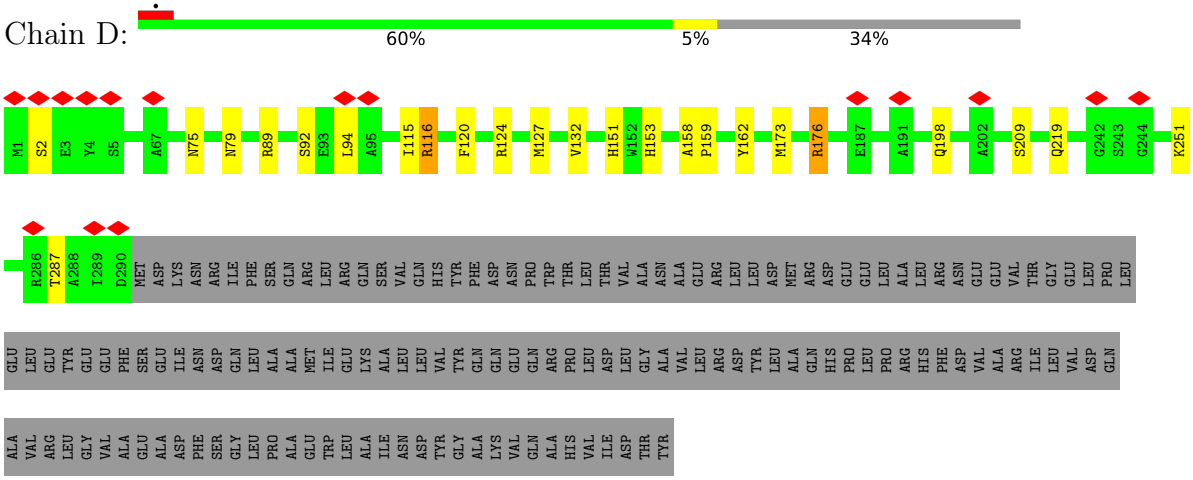
• Molecule 1: Chromosome partition protein MukF

Chain C:



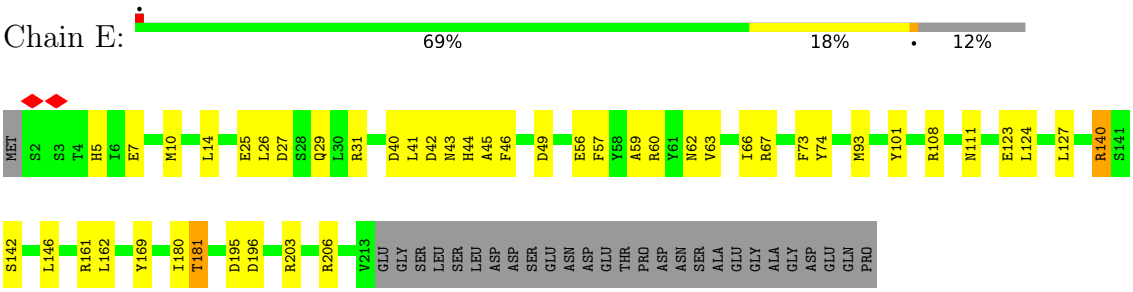
• Molecule 1: Chromosome partition protein MukF

Chain D:



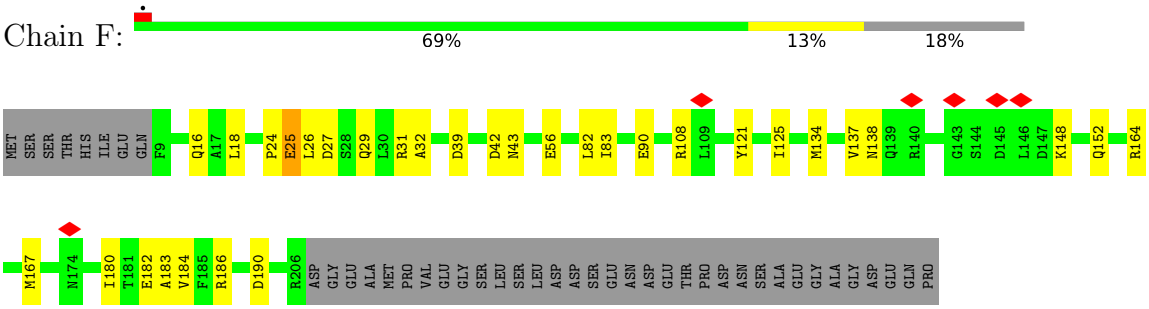
• Molecule 2: Chromosome partition protein MukE

Chain E:



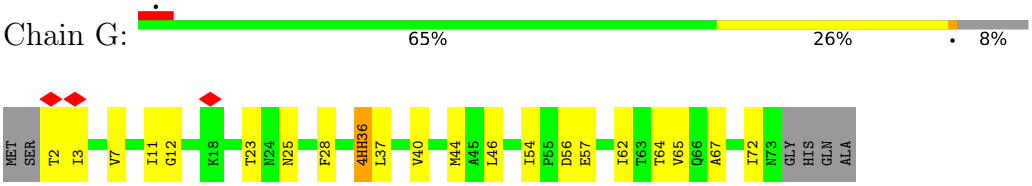
• Molecule 2: Chromosome partition protein MukE

Chain F:



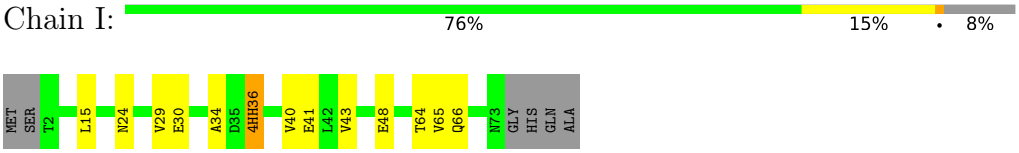
• Molecule 3: Acyl carrier protein

Chain G:



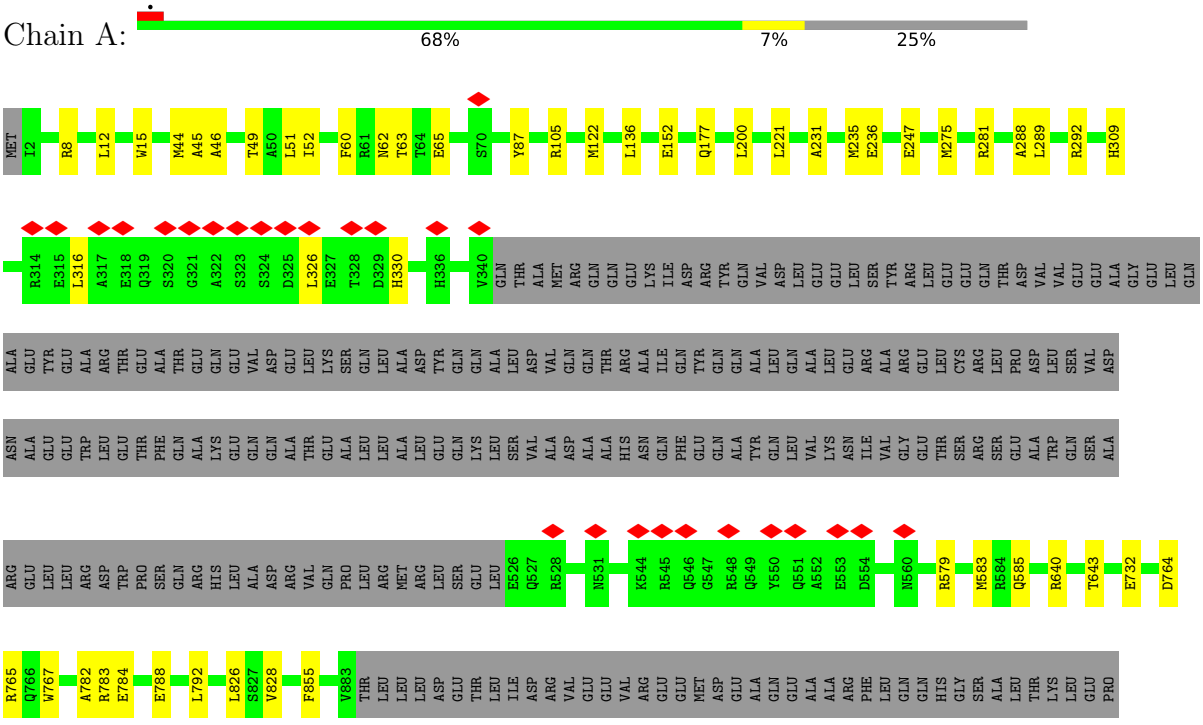
• Molecule 3: Acyl carrier protein

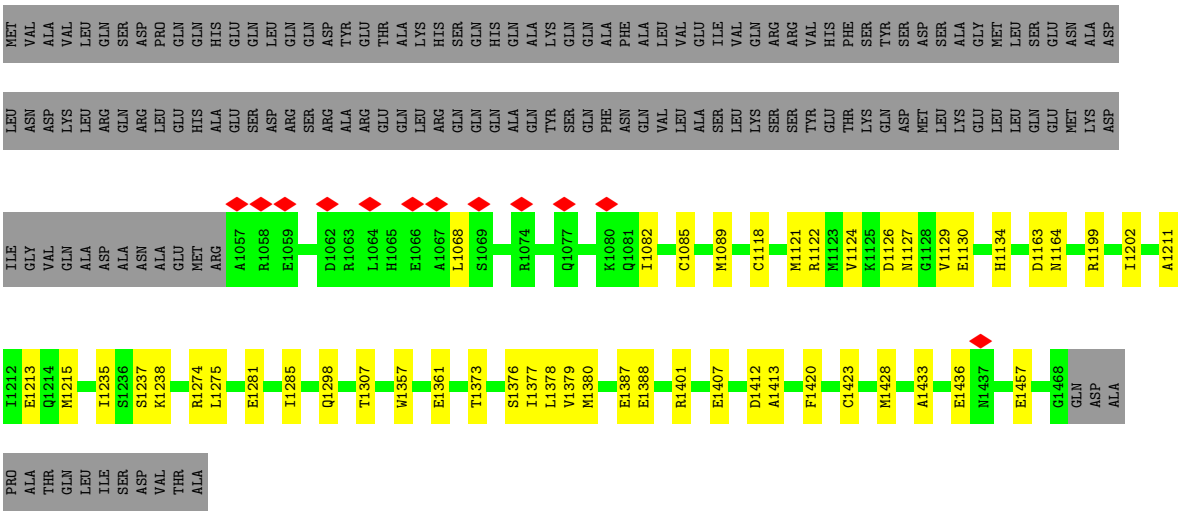
Chain I:



• Molecule 4: Chromosome partition protein MukB

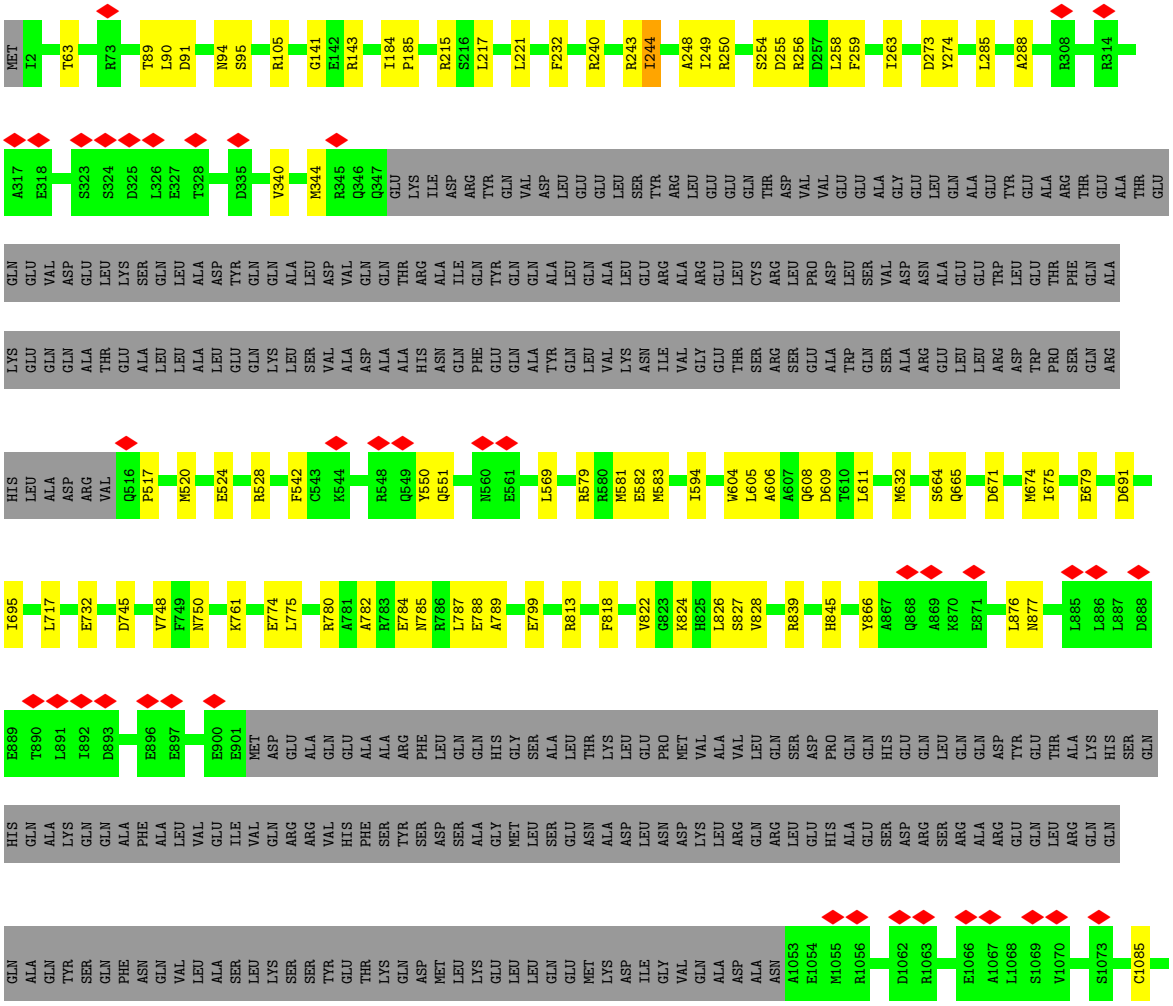
Chain A:

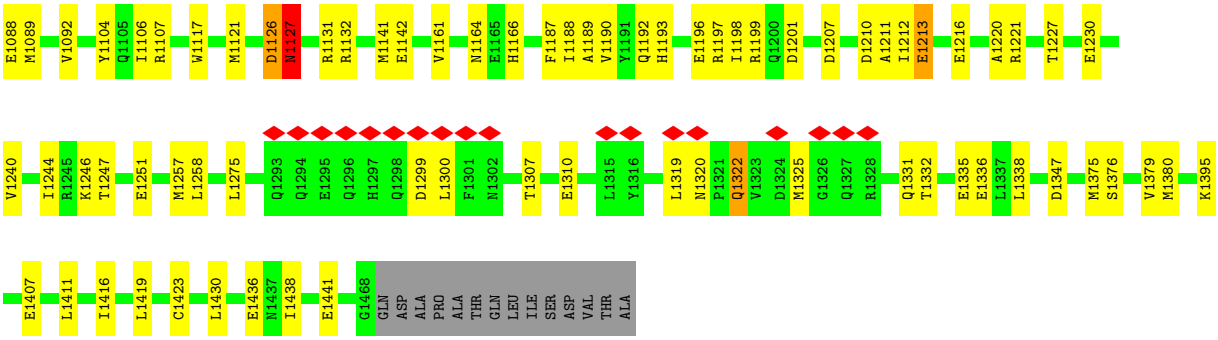




• Molecule 4: Chromosome partition protein MukB

Chain B:




E1088 M1089 V1092 Y1104 Q1105 I1106 R1107 W1117 M1121 D1126 N1127 R1131 R1132 M1141 E1142 V1161 N1164 E1165 H1166 F1187 I1188 A1189 V1190 Y1191 Q1192 H1193 E1196 R1197 I1198 R1199 Q1200 D1201 D1207 D1210 A1211 I1212 E1213 E1216 A1220 R1221 T1227 E1230
V1240 I1244 R1245 K1246 T1247 E1251 M1257 L1258 L1275 Q1293 Q1294 E1295 Q1296 H1297 Q1298 D1299 L1300 F1301 N1302 T1307 E1310 L1315 Y1316 L1319 N1320 P1321 Q1322 V1323 D1324 M1325 G1326 Q1327 R1328 Q1331 T1332 E1335 E1336 L1337 L1338 D1347 M1375 S1376 V1379 M1380 K1395
E1407 L1411 I1416 L1419 C1423 L1430 E1436 N1437 I1438 E1441 G1468 GLN ASP ALA PRO ALA THR GLN LEU ILE SER ASP VAL THR ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34436	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.020	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	460.97998, 460.97998, 460.97998	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4775, 1.4775, 1.4775	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, 4HH

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	C	0.77	5/3592 (0.1%)	1.24	16/4862 (0.3%)
1	D	0.68	0/2343	1.23	7/3165 (0.2%)
2	E	1.50	19/1753 (1.1%)	1.68	43/2361 (1.8%)
2	F	0.77	8/1648 (0.5%)	0.88	8/2218 (0.4%)
3	G	0.12	0/558	0.28	0/754
3	I	0.12	0/558	0.27	0/754
4	A	0.21	0/9041	0.56	0/12174
4	B	0.72	30/9369 (0.3%)	0.86	46/12614 (0.4%)
All	All	0.68	62/28862 (0.2%)	0.93	120/38902 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	8
1	D	0	5
2	E	0	3
All	All	0	16

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	ARG	C-N	-24.32	1.03	1.33
4	B	1193	HIS	CE1-NE2	-8.83	1.23	1.32
2	E	44	HIS	CE1-NE2	-8.78	1.23	1.32
4	B	1166	HIS	CE1-NE2	-8.77	1.23	1.32
4	B	1166	HIS	CD2-NE2	-8.07	1.28	1.37

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	295	ARG	CA-C-N	22.16	147.92	120.88
1	C	295	ARG	C-N-CA	22.16	147.92	120.88
2	F	82	LEU	CA-C-N	9.48	129.42	122.59
2	F	82	LEU	C-N-CA	9.48	129.42	122.59
1	D	176	ARG	CB-CG-CD	8.66	131.22	111.30

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	120	PHE	Sidechain
1	C	28	ARG	Sidechain
1	C	4	TYR	Sidechain
1	C	42	ARG	Sidechain
1	C	89	ARG	Sidechain

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	C	3531	3451	3450	24	0
1	D	2307	2260	2260	7	0
2	E	1722	1719	1718	15	0
2	F	1619	1627	1626	20	0
3	G	583	564	563	25	0
3	I	583	564	563	10	0
4	A	8919	8885	8881	82	0
4	B	9246	9221	9217	114	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	31	12	12	0	0
6	B	31	12	12	0	0
All	All	28574	28315	28302	266	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 5.

The worst 5 of 266 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:36:4HH:CL3	3:G:40:VAL:HG21	1.87	1.04
4:B:1127:ASN:O	4:B:1127:ASN:ND2	1.91	1.02
3:I:48:GLU:OE1	4:B:1107:ARG:NE	2.04	0.90
3:G:36:4HH:SU	4:A:292:ARG:HD3	2.14	0.87
4:B:665:GLN:NE2	4:B:671:ASP:OD2	2.11	0.84

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	C	438/440 (100%)	425 (97%)	13 (3%)	0	100	100
1	D	288/440 (66%)	281 (98%)	7 (2%)	0	100	100
2	E	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
2	F	196/240 (82%)	191 (97%)	5 (3%)	0	100	100
3	G	69/78 (88%)	68 (99%)	1 (1%)	0	100	100
3	I	69/78 (88%)	66 (96%)	3 (4%)	0	100	100
4	A	1103/1482 (74%)	1069 (97%)	34 (3%)	0	100	100
4	B	1142/1482 (77%)	1101 (96%)	41 (4%)	0	100	100
All	All	3515/4480 (78%)	3407 (97%)	108 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	C	376/376 (100%)	367 (98%)	9 (2%)	43	63
1	D	247/376 (66%)	240 (97%)	7 (3%)	38	59
2	E	189/212 (89%)	185 (98%)	4 (2%)	47	65
2	F	177/212 (84%)	175 (99%)	2 (1%)	65	74
3	G	62/66 (94%)	62 (100%)	0	100	100
3	I	62/66 (94%)	62 (100%)	0	100	100
4	A	957/1281 (75%)	956 (100%)	1 (0%)	88	89
4	B	994/1281 (78%)	992 (100%)	2 (0%)	87	87
All	All	3064/3870 (79%)	3039 (99%)	25 (1%)	70	77

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	152	GLN
4	B	1213	GLU
1	D	287	THR
4	B	1127	ASN
1	D	2	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	1342	ASN
4	B	1437	ASN
1	D	269	GLN
4	A	634	GLN
4	A	589	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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
3	4HH	G	36	3	22,26,27	0.45	0	27,35,37	3.17	4 (14%)
3	4HH	I	36	3	22,26,27	0.46	0	27,35,37	1.75	3 (11%)

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
3	4HH	G	36	3	-	5/33/35/37	-
3	4HH	I	36	3	-	7/33/35/37	-

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	36	4HH	O1P-P-OG	11.99	161.90	107.57
3	G	36	4HH	OG-P-O2P	-8.71	74.41	108.94
3	G	36	4HH	P-OG-CB	6.31	157.53	121.35
3	I	36	4HH	P-OG-CB	-5.46	90.04	121.35
3	I	36	4HH	O1P-P-OG	4.80	129.31	107.57

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	36	4HH	CB-OG-P-O3P
3	I	36	4HH	N-CA-CB-OG
3	I	36	4HH	CB-OG-P-O1P
3	I	36	4HH	CO-CP-CQ-NR
3	G	36	4HH	ON-CL3-CM-OM

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	36	4HH	14	0
3	I	36	4HH	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
6	ATP	B	1502	5	32,33,33	0.57	1 (3%)	48,52,52	0.74	2 (4%)
6	ATP	A	1502	5	32,33,33	0.57	1 (3%)	48,52,52	0.75	2 (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
6	ATP	B	1502	5	-	2/22/38/38	0/3/3/3
6	ATP	A	1502	5	-	2/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1502	ATP	PB-O3B	-2.35	1.57	1.59
6	B	1502	ATP	PB-O3B	-2.14	1.57	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1502	ATP	O2'-C2'-C3'	-2.34	104.33	111.82
6	B	1502	ATP	O2'-C2'-C3'	-2.21	104.72	111.82
6	B	1502	ATP	O3'-C3'-C2'	-2.16	104.89	111.82
6	A	1502	ATP	O3'-C3'-C2'	-2.07	105.19	111.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

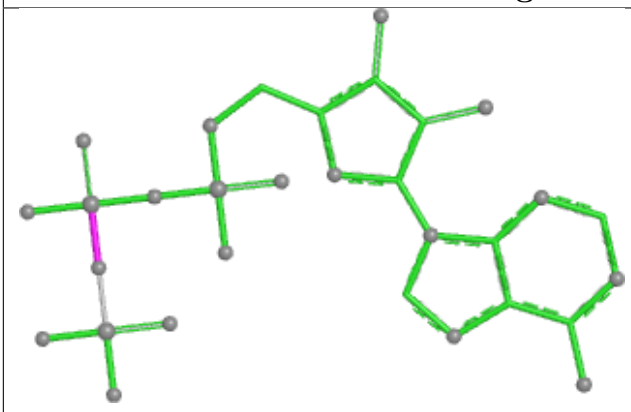
Mol	Chain	Res	Type	Atoms
6	A	1502	ATP	PA-O3A-PB-O2B
6	B	1502	ATP	PA-O3A-PB-O1B
6	B	1502	ATP	PA-O3A-PB-O2B
6	A	1502	ATP	PA-O3A-PB-O1B

There are no ring outliers.

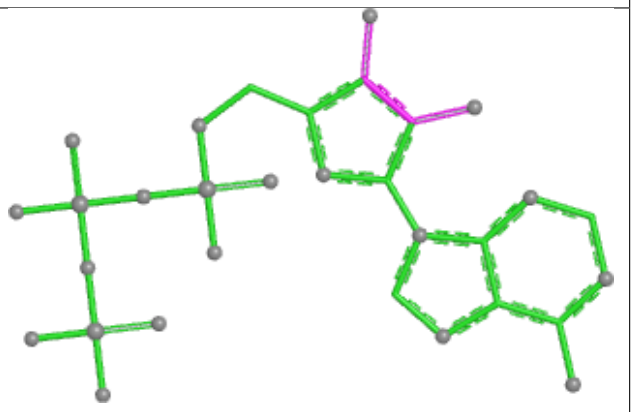
No monomer is involved in short contacts.

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 then 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.

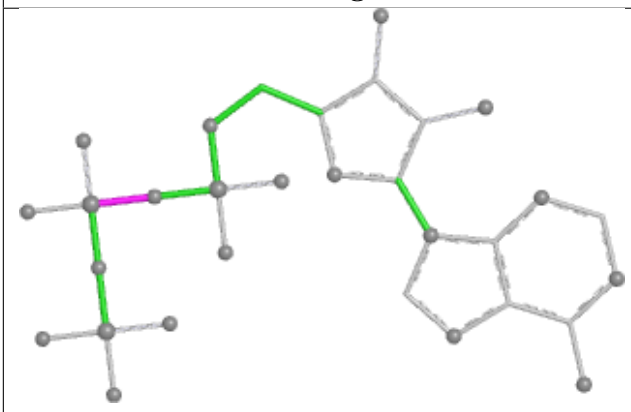
Ligand ATP B 1502



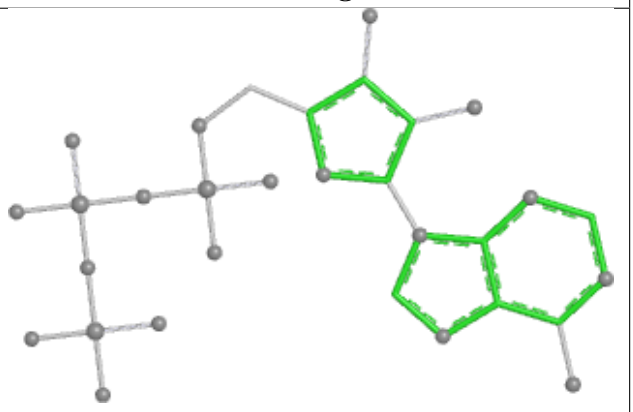
Bond lengths



Bond angles

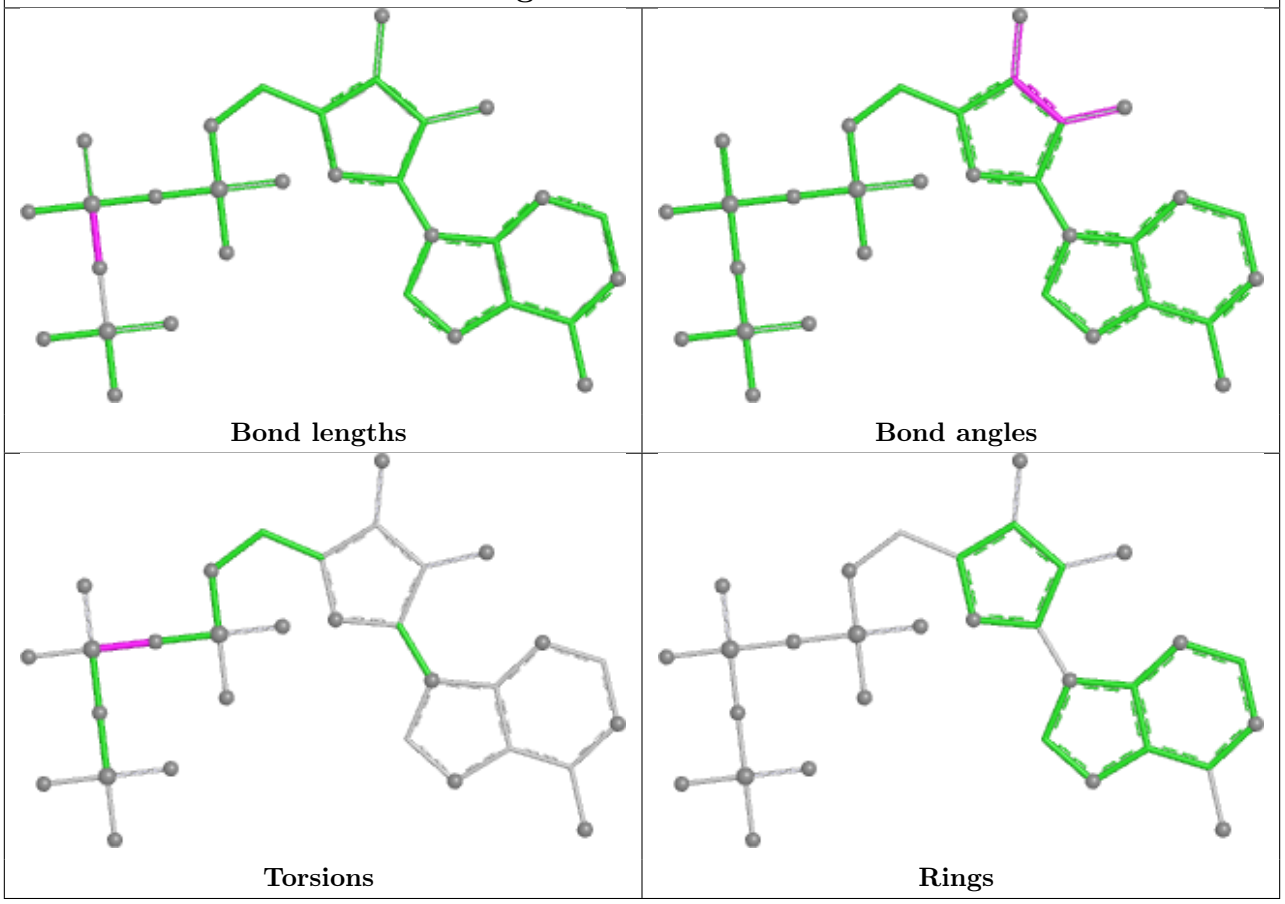


Torsions



Rings

Ligand ATP A 1502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	295:ARG	C	296:ILE	N	1.04

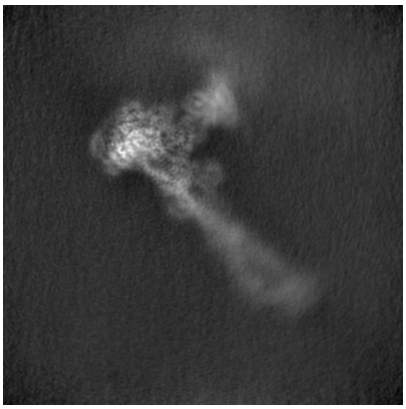
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51444. These allow visual inspection of the internal detail of the map and identification of artifacts.

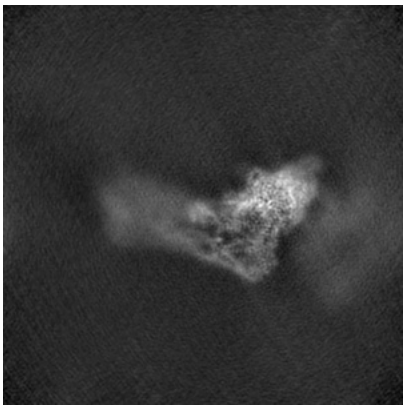
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

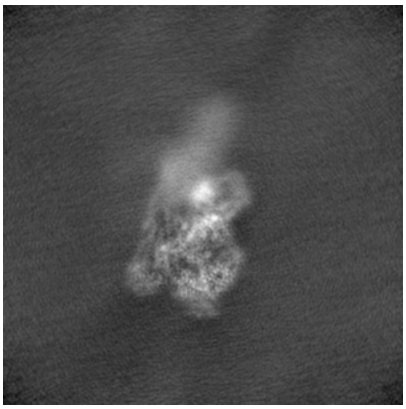
6.1.1 Primary map



X

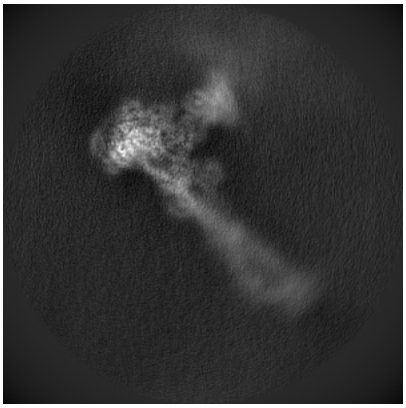


Y

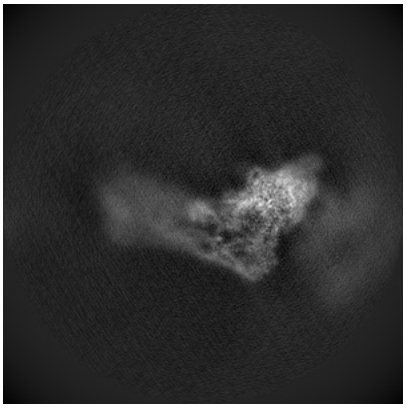


Z

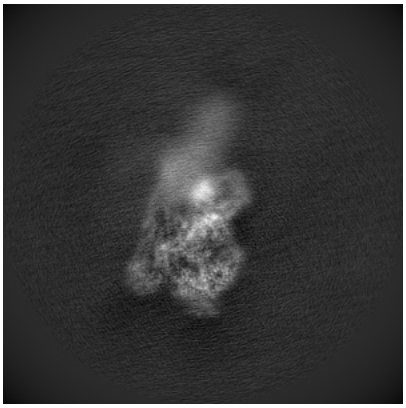
6.1.2 Raw map



X



Y

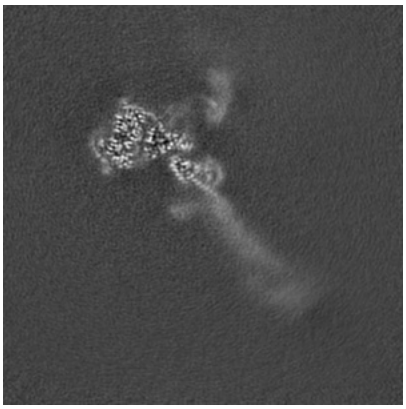


Z

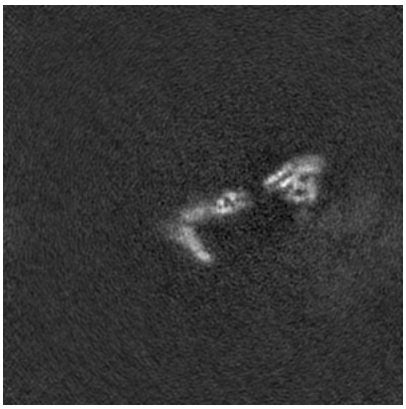
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

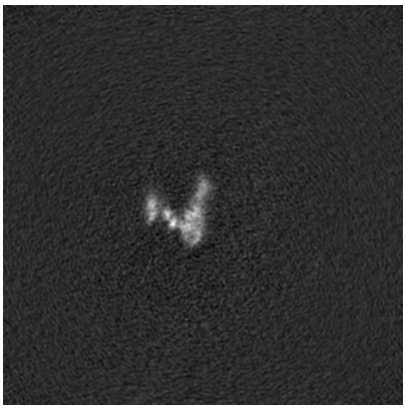
6.2.1 Primary map



X Index: 156

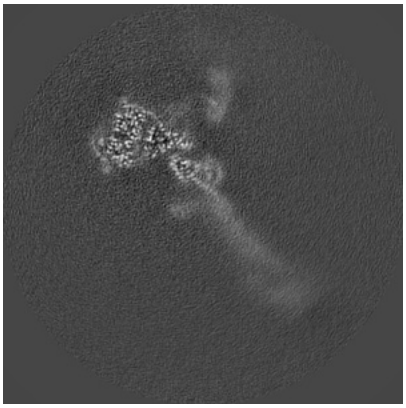


Y Index: 156

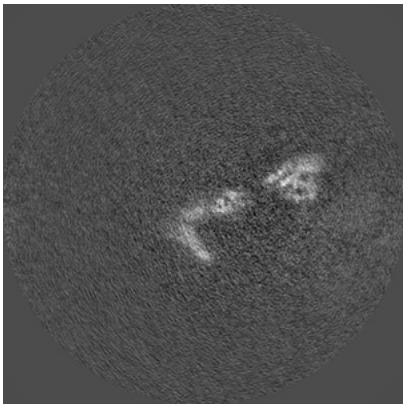


Z Index: 156

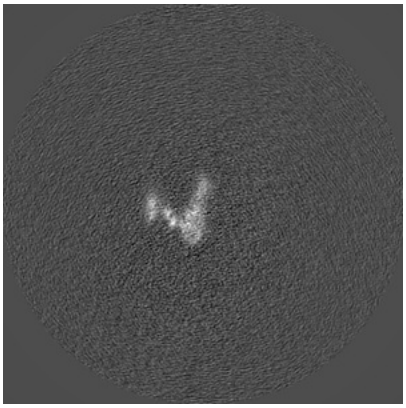
6.2.2 Raw map



X Index: 156



Y Index: 156

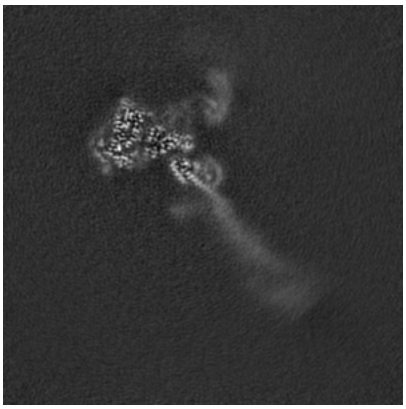


Z Index: 156

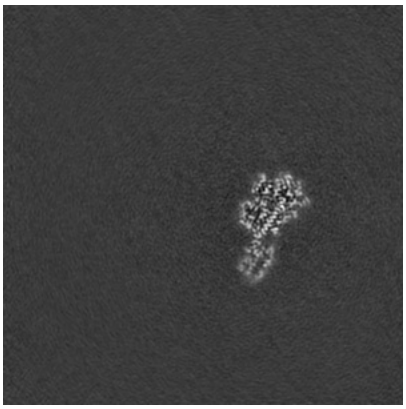
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

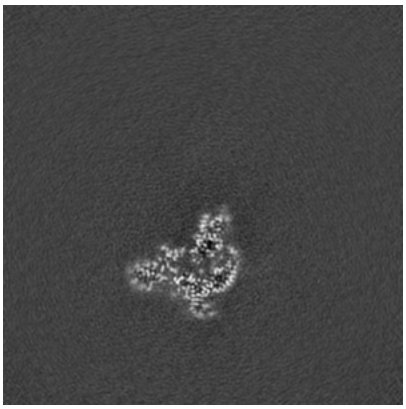
6.3.1 Primary map



X Index: 157

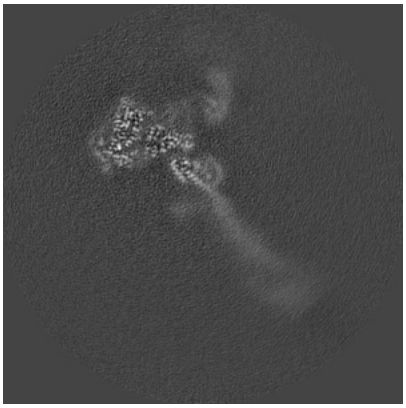


Y Index: 96

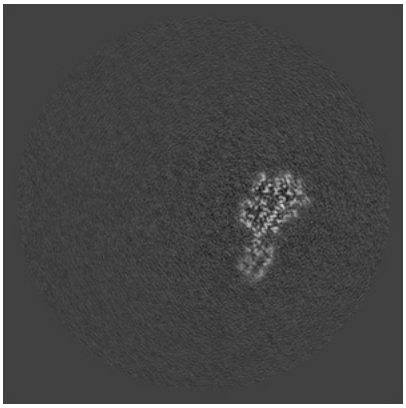


Z Index: 202

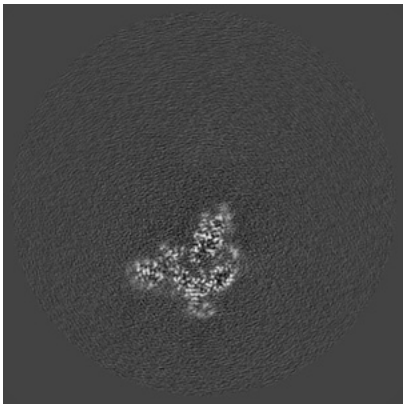
6.3.2 Raw map



X Index: 157



Y Index: 96

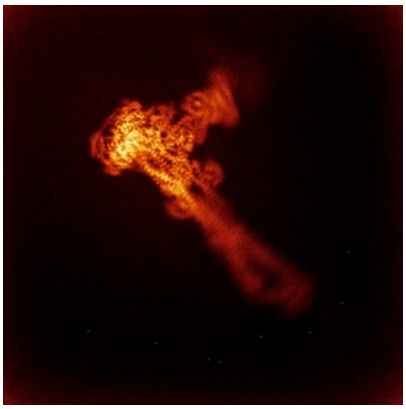


Z Index: 203

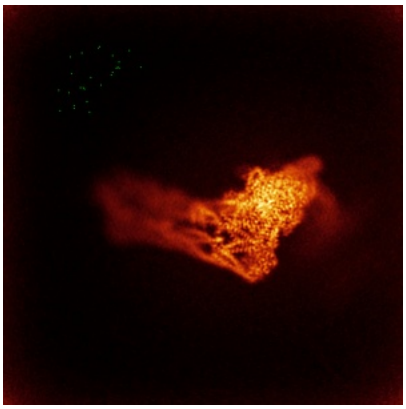
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

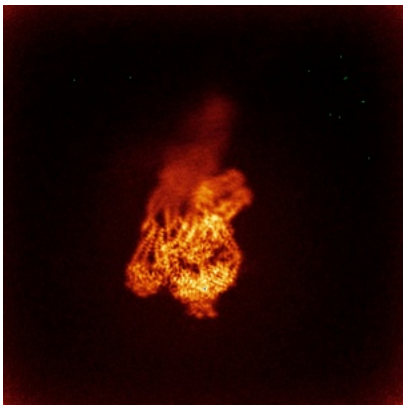
6.4.1 Primary map



X

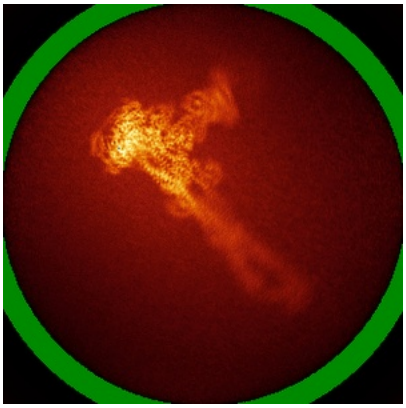


Y

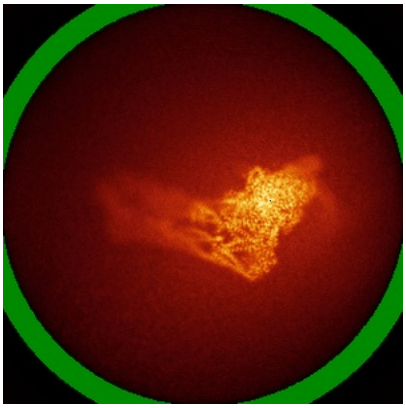


Z

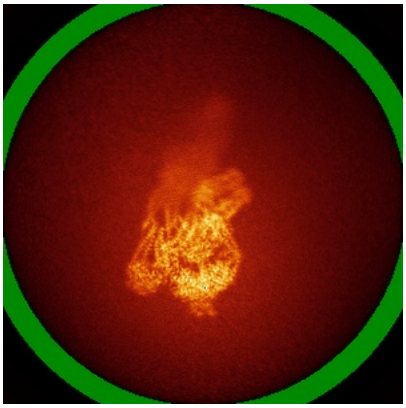
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

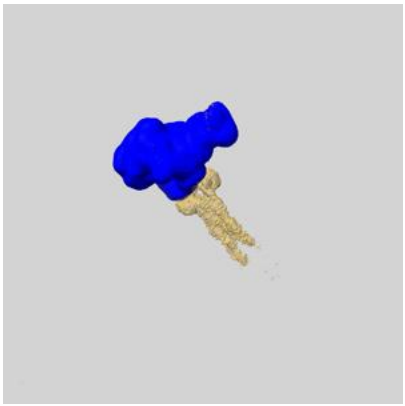
6.6 Mask visualisation (i)

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

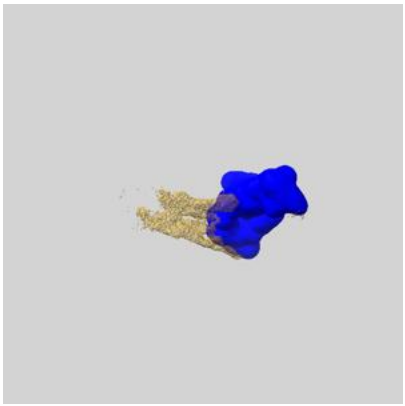
A mask typically either:

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

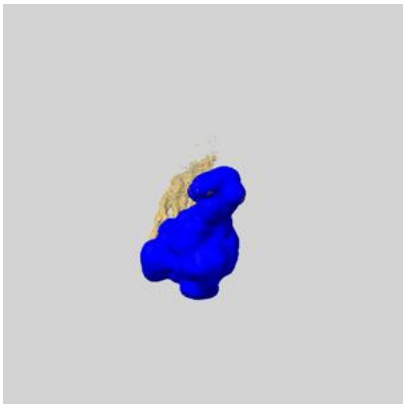
6.6.1 emd_51444_msk_1.map (i)



X



Y

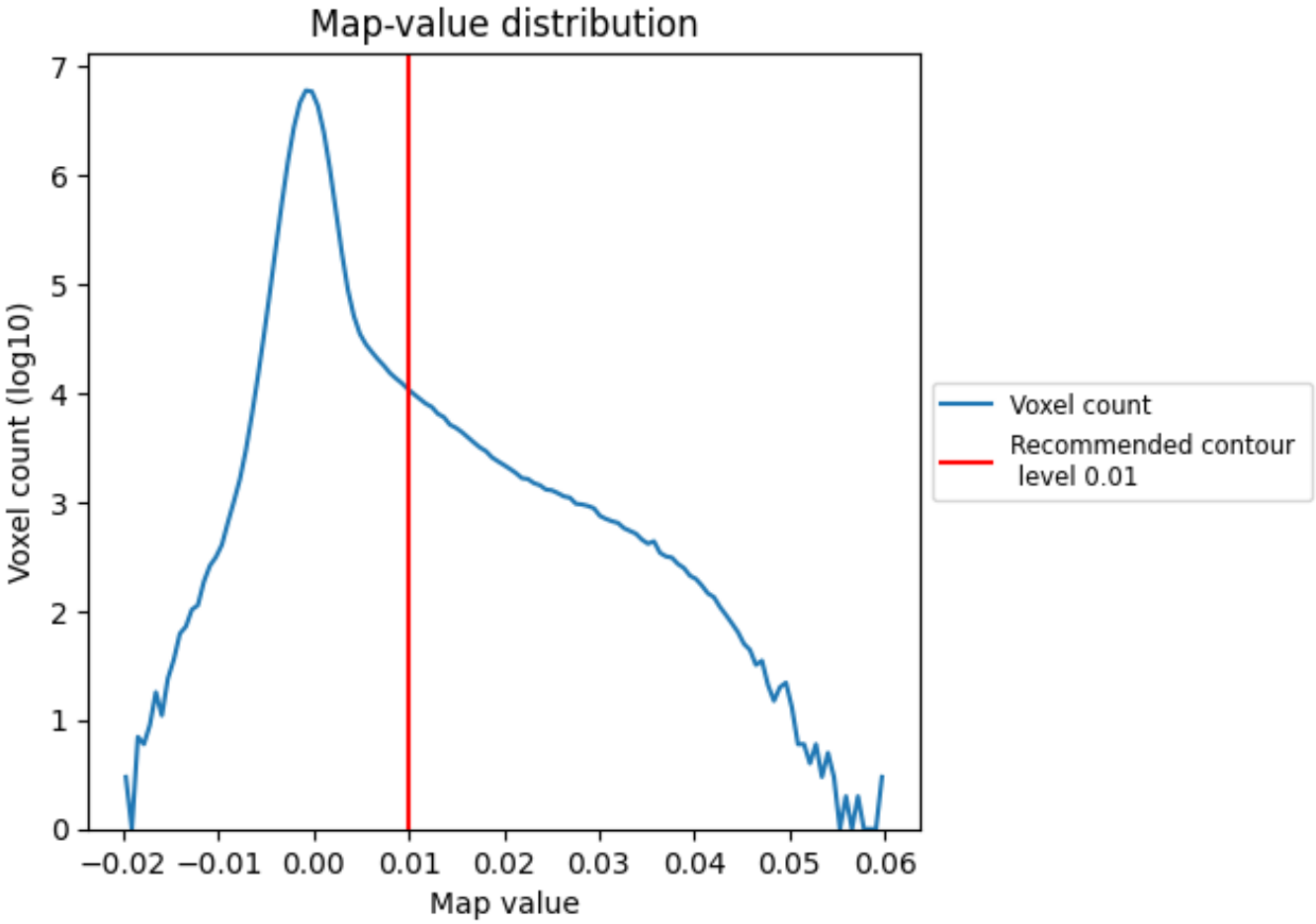


Z

7 Map analysis

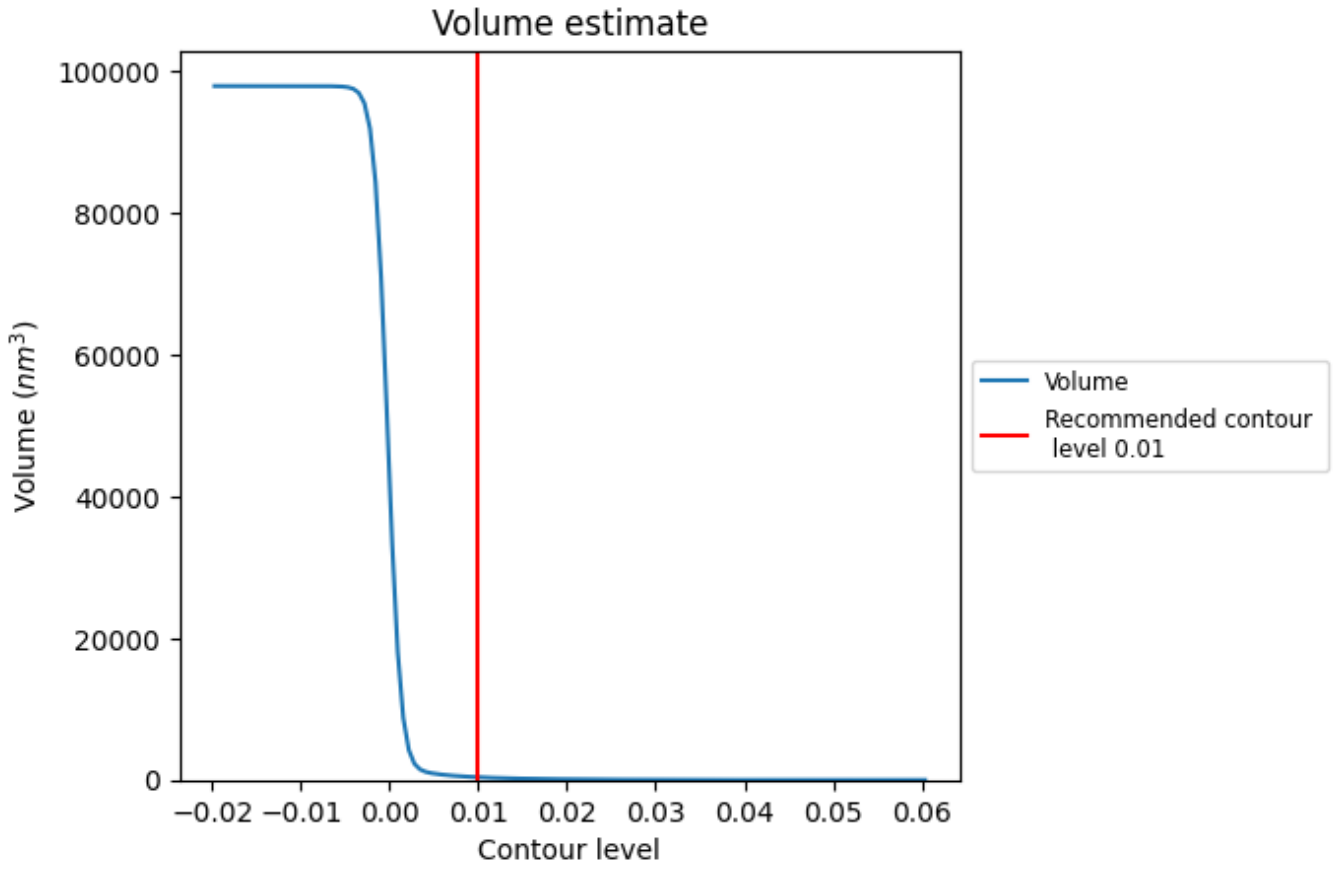
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

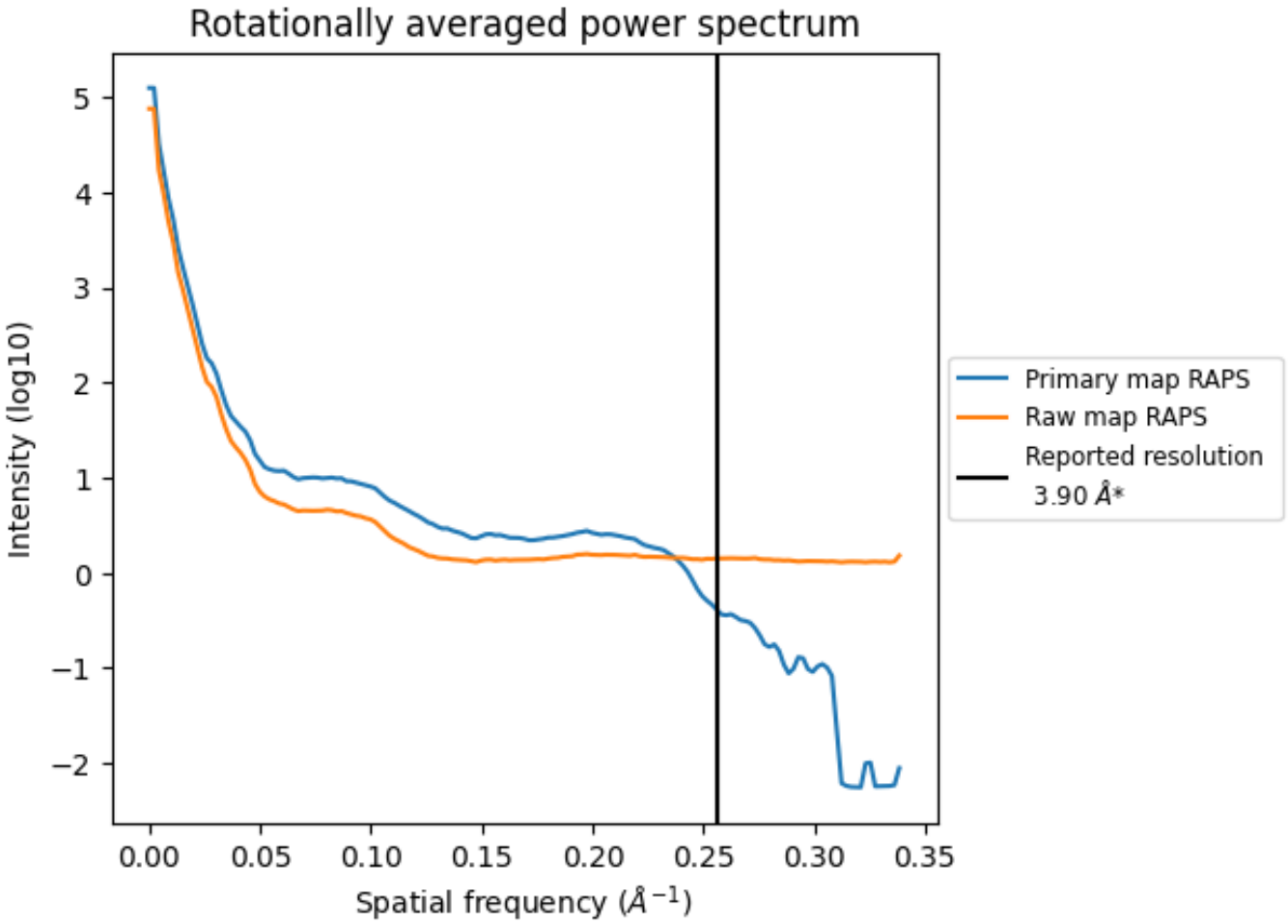
7.2 Volume estimate (i)



The volume at the recommended contour level is 385 nm^3; this corresponds to an approximate mass of 348 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 (i)

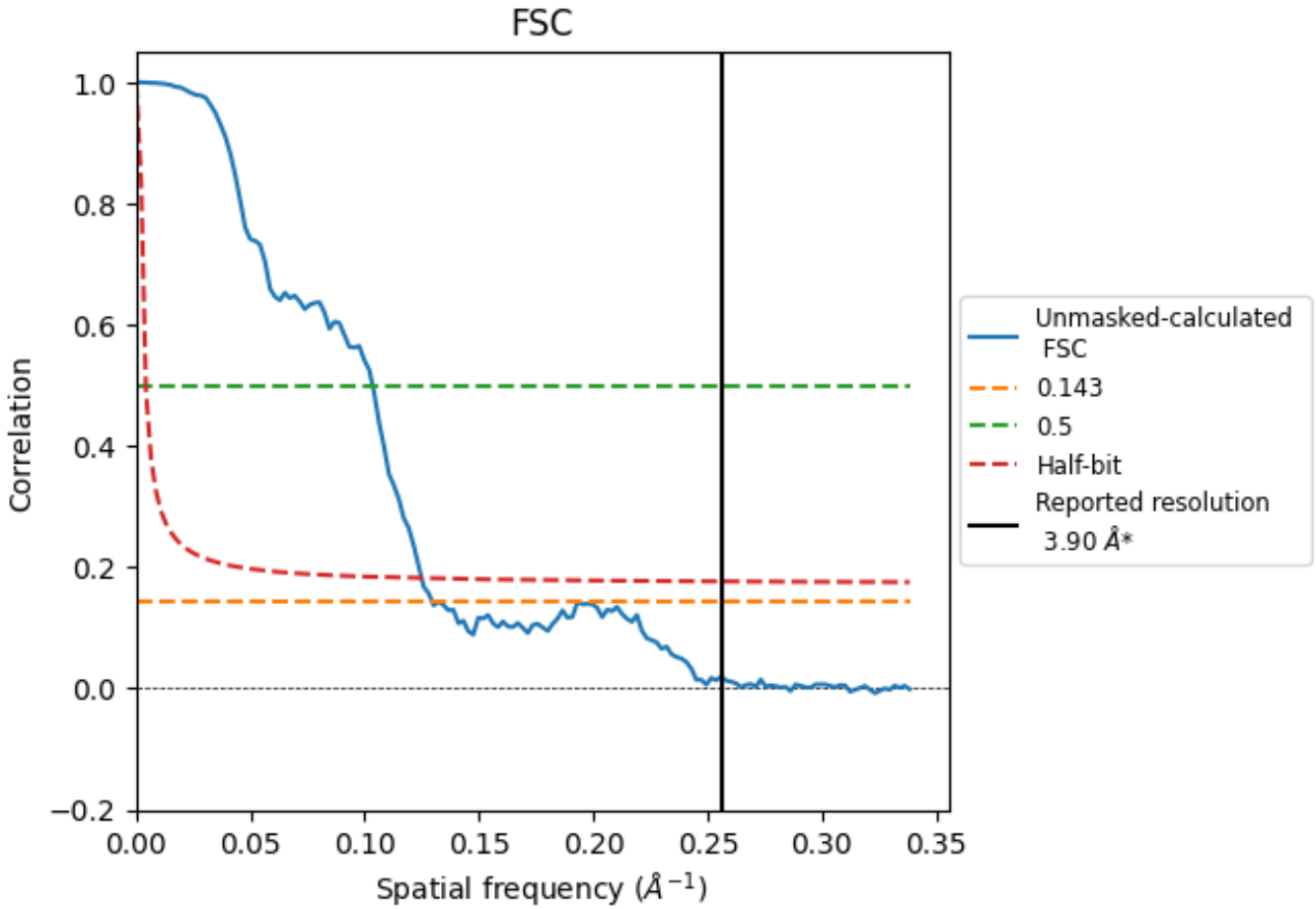


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.72	9.67	8.01

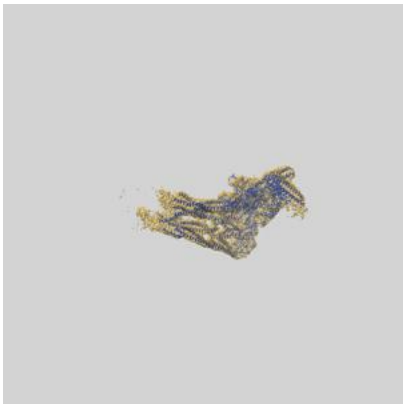
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.72 differs from the reported value 3.9 by more than 10 %

9 Map-model fit

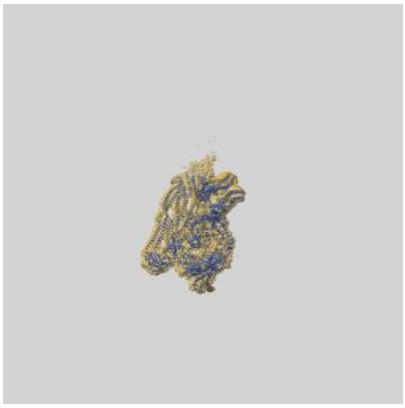
This section contains information regarding the fit between EMDB map EMD-51444 and PDB model 9GM8. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay

X



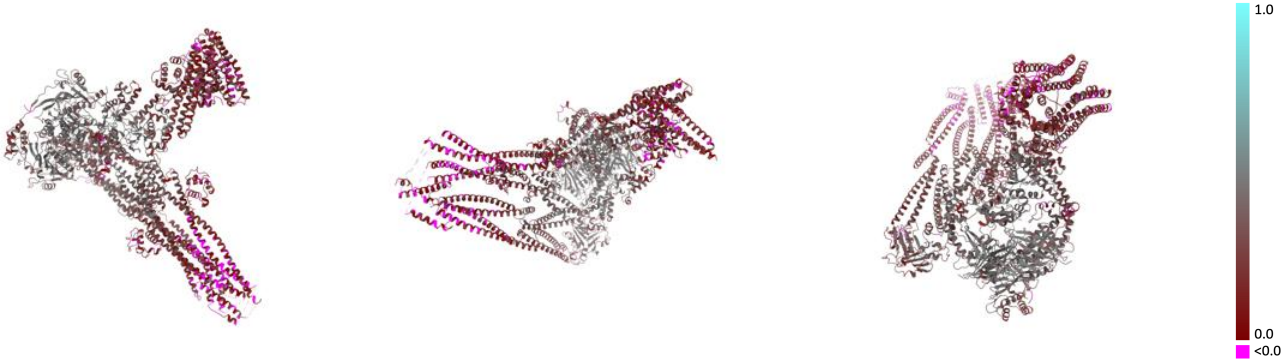
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

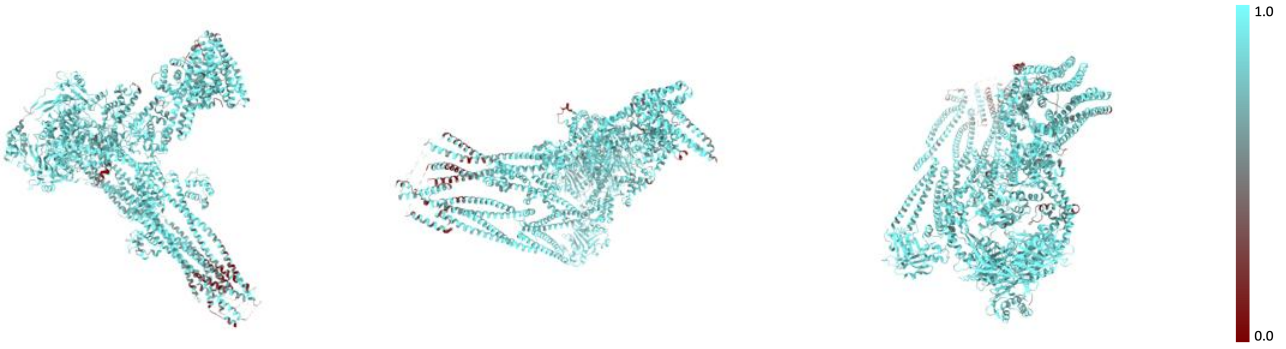
9.2 Q-score mapped to coordinate model



X Y Z

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

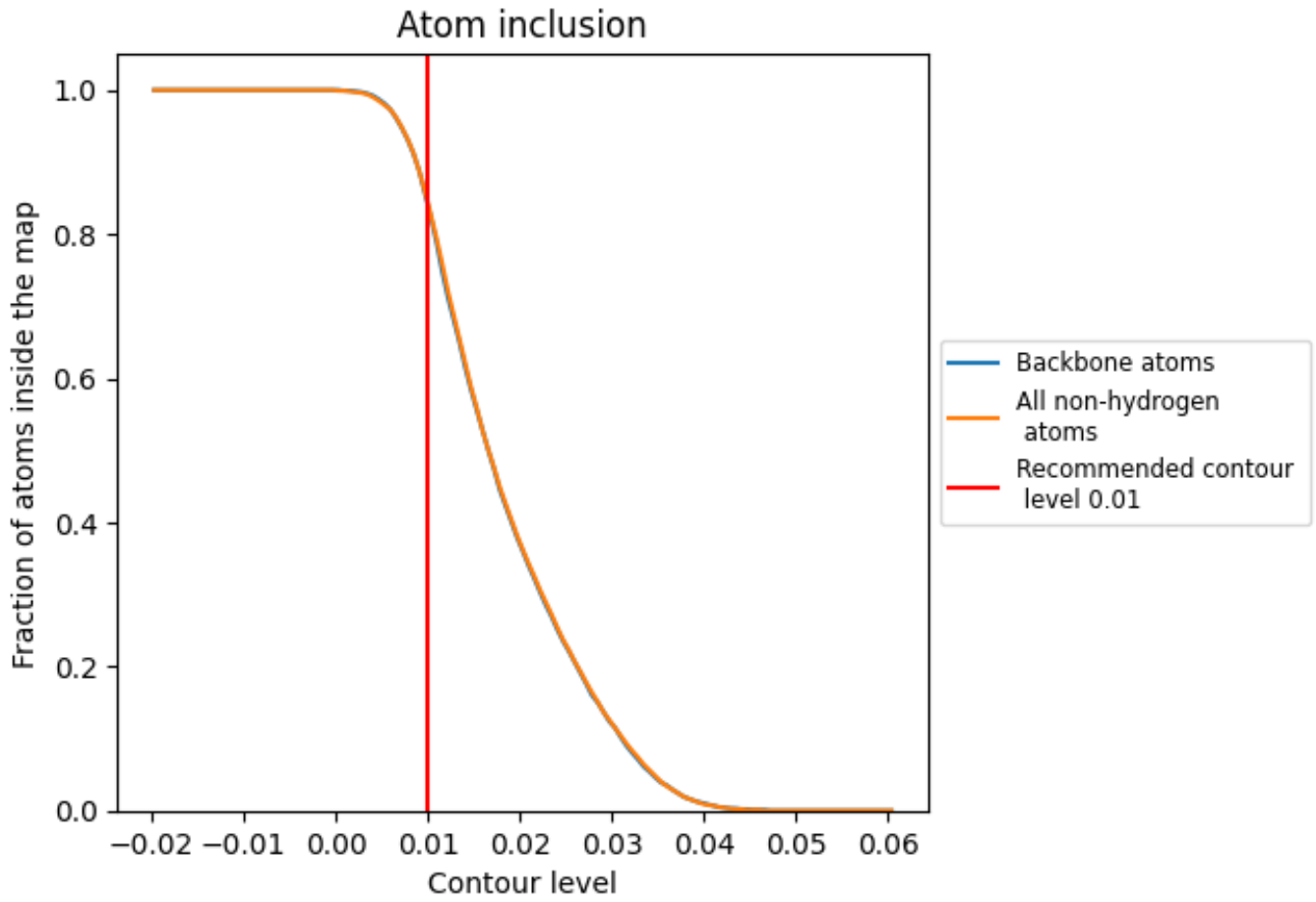
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8440	0.2920
A	0.8700	0.3150
B	0.8490	0.3080
C	0.8330	0.2300
D	0.8300	0.1680
E	0.8890	0.3940
F	0.8770	0.3820
G	0.8410	0.1530
I	0.8170	0.1550