Full wwPDB EM Validation Report ⓘ

May 26, 2025 – 01:16 PM EDT

PDB ID	:	8VVN / pdb_00008vvn
EMDB ID	:	EMD-43563
Title	:	Cryo-EM structure of a type I ZorAB complex from Shewanella sp. strain ANA-3
Authors	:	Deme, J.C.; Lea, S.M.
Deposited on	:	2024-01-31
Resolution	:	2.20 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:

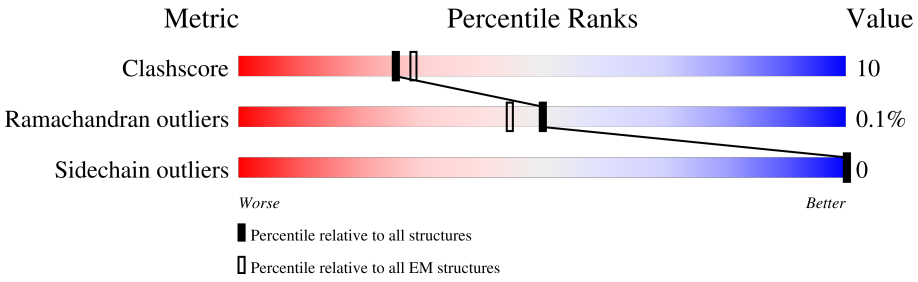
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.20 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	282	60% 20% 20%
1	B	282	56% 24% 20%
2	C	696	6% 25% 8% 67%
2	D	696	11% 24% 9% 67%
2	E	696	11% 24% 9% 67%
2	F	696	6% 26% 8% 67%
2	G	696	9% 26% 7% 67%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12935 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 Chemotaxis protein MotB-related protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	225	Total	C	N	O	S	0	0
			1821	1154	316	349	2		
1	A	226	Total	C	N	O	S	0	0
			1831	1159	316	354	2		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	244	GLU	-	expression tag	UNP A0L1T5
B	245	ASN	-	expression tag	UNP A0L1T5
B	246	LEU	-	expression tag	UNP A0L1T5
B	247	TYR	-	expression tag	UNP A0L1T5
B	248	PHE	-	expression tag	UNP A0L1T5
B	249	GLN	-	expression tag	UNP A0L1T5
B	250	GLY	-	expression tag	UNP A0L1T5
B	251	GLN	-	expression tag	UNP A0L1T5
B	252	PHE	-	expression tag	UNP A0L1T5
B	253	GLY	-	expression tag	UNP A0L1T5
B	254	SER	-	expression tag	UNP A0L1T5
B	255	TRP	-	expression tag	UNP A0L1T5
B	256	SER	-	expression tag	UNP A0L1T5
B	257	HIS	-	expression tag	UNP A0L1T5
B	258	PRO	-	expression tag	UNP A0L1T5
B	259	GLN	-	expression tag	UNP A0L1T5
B	260	PHE	-	expression tag	UNP A0L1T5
B	261	GLU	-	expression tag	UNP A0L1T5
B	262	LYS	-	expression tag	UNP A0L1T5
B	263	GLY	-	expression tag	UNP A0L1T5
B	264	GLY	-	expression tag	UNP A0L1T5
B	265	GLY	-	expression tag	UNP A0L1T5
B	266	SER	-	expression tag	UNP A0L1T5
B	267	GLY	-	expression tag	UNP A0L1T5
B	268	GLY	-	expression tag	UNP A0L1T5
B	269	GLY	-	expression tag	UNP A0L1T5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	270	SER	-	expression tag	UNP A0L1T5
B	271	GLY	-	expression tag	UNP A0L1T5
B	272	GLY	-	expression tag	UNP A0L1T5
B	273	GLY	-	expression tag	UNP A0L1T5
B	274	SER	-	expression tag	UNP A0L1T5
B	275	TRP	-	expression tag	UNP A0L1T5
B	276	SER	-	expression tag	UNP A0L1T5
B	277	HIS	-	expression tag	UNP A0L1T5
B	278	PRO	-	expression tag	UNP A0L1T5
B	279	GLN	-	expression tag	UNP A0L1T5
B	280	PHE	-	expression tag	UNP A0L1T5
B	281	GLU	-	expression tag	UNP A0L1T5
B	282	LYS	-	expression tag	UNP A0L1T5
A	244	GLU	-	expression tag	UNP A0L1T5
A	245	ASN	-	expression tag	UNP A0L1T5
A	246	LEU	-	expression tag	UNP A0L1T5
A	247	TYR	-	expression tag	UNP A0L1T5
A	248	PHE	-	expression tag	UNP A0L1T5
A	249	GLN	-	expression tag	UNP A0L1T5
A	250	GLY	-	expression tag	UNP A0L1T5
A	251	GLN	-	expression tag	UNP A0L1T5
A	252	PHE	-	expression tag	UNP A0L1T5
A	253	GLY	-	expression tag	UNP A0L1T5
A	254	SER	-	expression tag	UNP A0L1T5
A	255	TRP	-	expression tag	UNP A0L1T5
A	256	SER	-	expression tag	UNP A0L1T5
A	257	HIS	-	expression tag	UNP A0L1T5
A	258	PRO	-	expression tag	UNP A0L1T5
A	259	GLN	-	expression tag	UNP A0L1T5
A	260	PHE	-	expression tag	UNP A0L1T5
A	261	GLU	-	expression tag	UNP A0L1T5
A	262	LYS	-	expression tag	UNP A0L1T5
A	263	GLY	-	expression tag	UNP A0L1T5
A	264	GLY	-	expression tag	UNP A0L1T5
A	265	GLY	-	expression tag	UNP A0L1T5
A	266	SER	-	expression tag	UNP A0L1T5
A	267	GLY	-	expression tag	UNP A0L1T5
A	268	GLY	-	expression tag	UNP A0L1T5
A	269	GLY	-	expression tag	UNP A0L1T5
A	270	SER	-	expression tag	UNP A0L1T5
A	271	GLY	-	expression tag	UNP A0L1T5
A	272	GLY	-	expression tag	UNP A0L1T5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	273	GLY	-	expression tag	UNP A0L1T5
A	274	SER	-	expression tag	UNP A0L1T5
A	275	TRP	-	expression tag	UNP A0L1T5
A	276	SER	-	expression tag	UNP A0L1T5
A	277	HIS	-	expression tag	UNP A0L1T5
A	278	PRO	-	expression tag	UNP A0L1T5
A	279	GLN	-	expression tag	UNP A0L1T5
A	280	PHE	-	expression tag	UNP A0L1T5
A	281	GLU	-	expression tag	UNP A0L1T5
A	282	LYS	-	expression tag	UNP A0L1T5

- Molecule 2 is a protein called MotA/TolQ/ExbB proton channel domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	232	Total	C	N	O	S	0	0
			1830	1200	296	330	4		
2	D	231	Total	C	N	O	S	0	0
			1821	1195	295	327	4		
2	E	232	Total	C	N	O	S	0	0
			1830	1200	296	330	4		
2	F	232	Total	C	N	O	S	0	0
			1830	1200	296	330	4		
2	G	232	Total	C	N	O	S	0	0
			1830	1200	296	330	4		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	D	1	Total	Na	0
			1	1	
3	F	1	Total	Na	0
			1	1	

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	B	24	Total	O	0
			24	24	
4	A	26	Total	O	0
			26	26	

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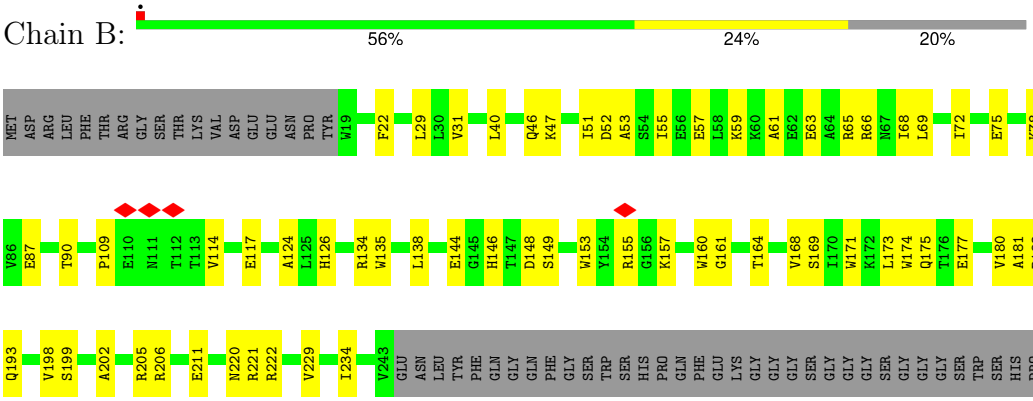
Mol	Chain	Residues	Atoms	AltConf
4	C	23	Total O 23 23	0
4	D	14	Total O 14 14	0
4	E	16	Total O 16 16	0
4	F	20	Total O 20 20	0
4	G	17	Total O 17 17	0

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.

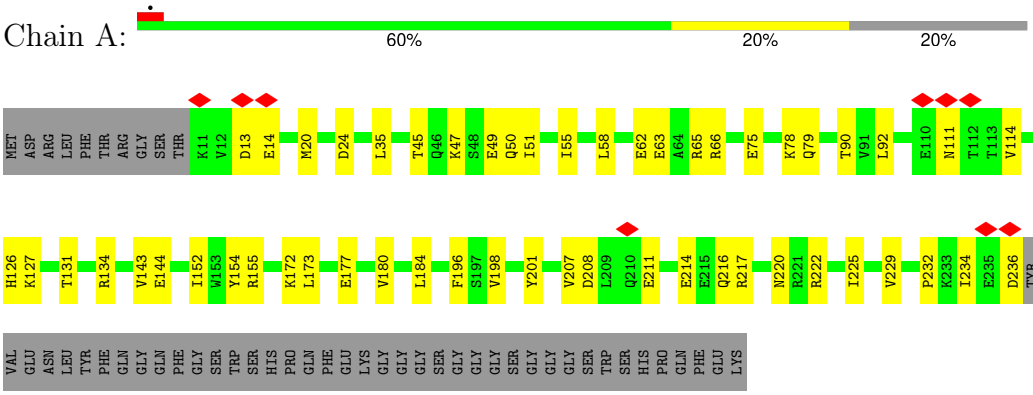
• Molecule 1: Chemotaxis protein MotB-related protein

Chain B:



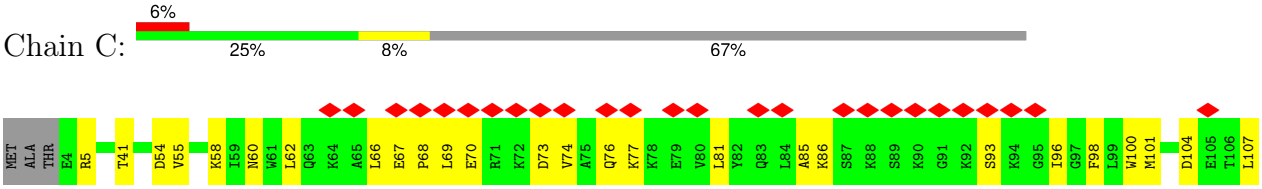
• Molecule 1: Chemotaxis protein MotB-related protein

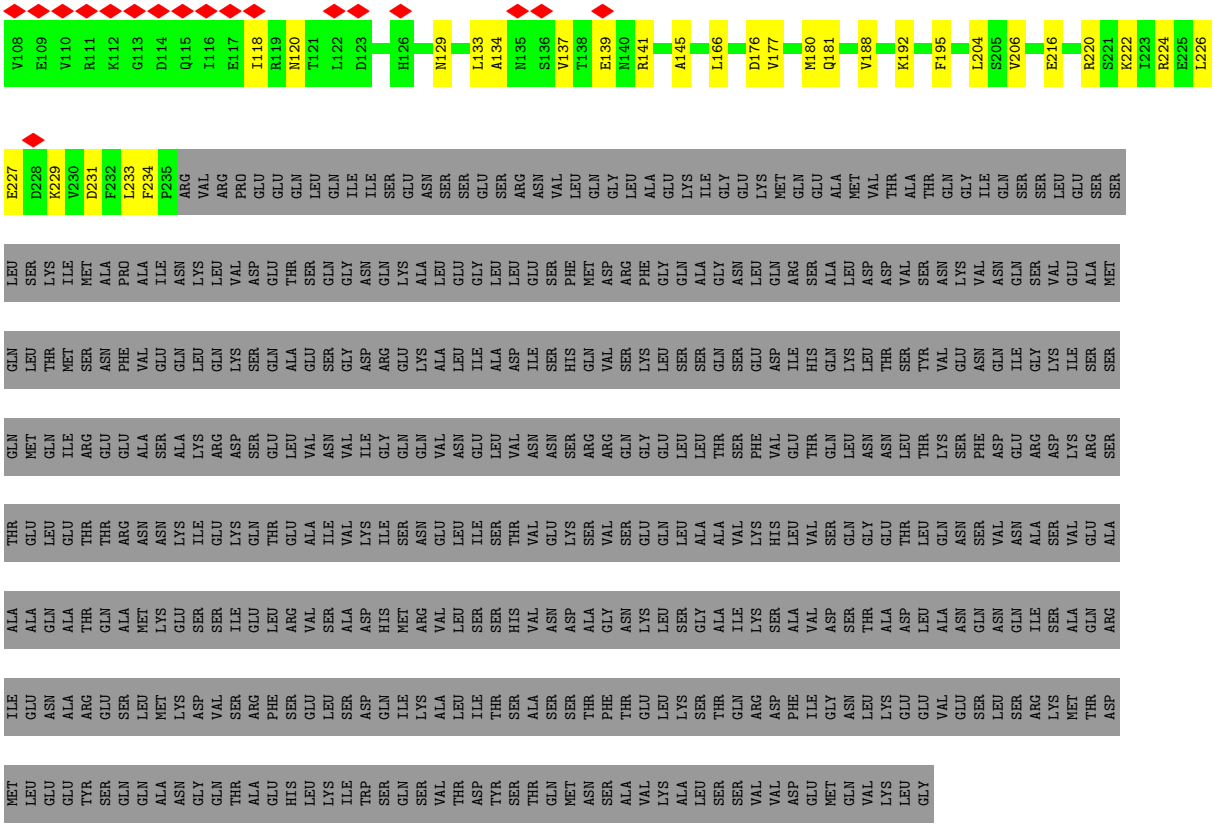
Chain A:



• Molecule 2: MotA/TolQ/ExbB proton channel domain-containing protein

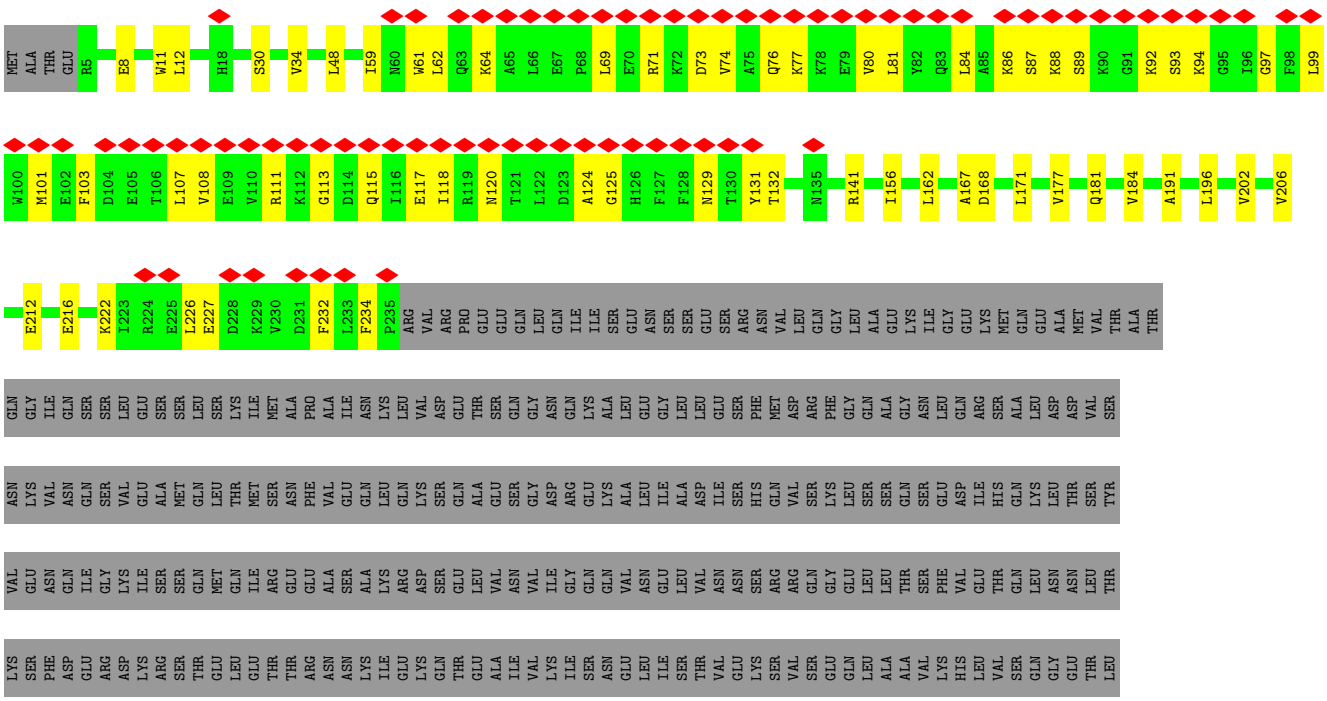
Chain C:

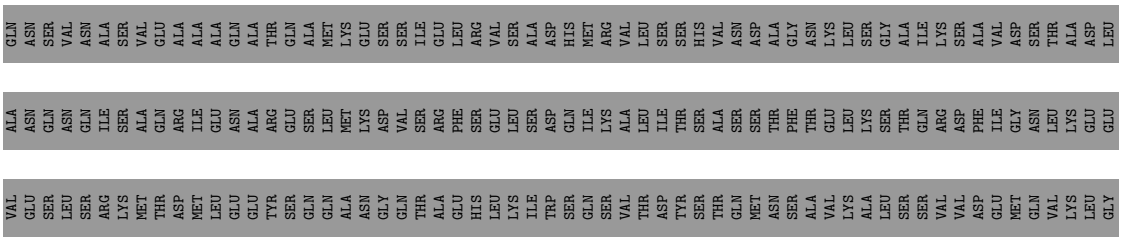




• Molecule 2: MotA/TolQ/ExbB proton channel domain-containing protein

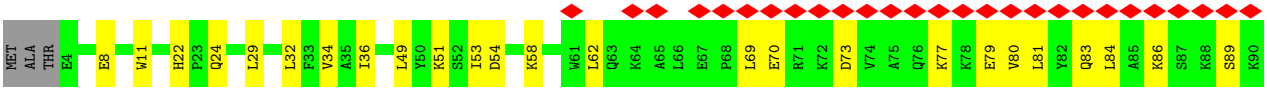
Chain D:

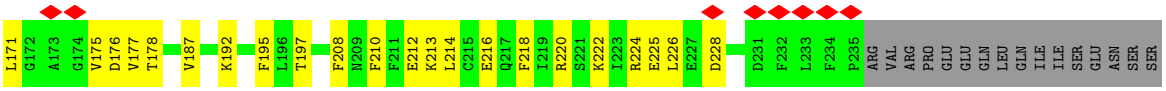




• Molecule 2: MotA/TolQ/ExbB proton channel domain-containing protein

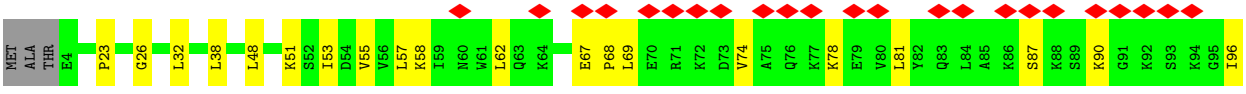
Chain E:

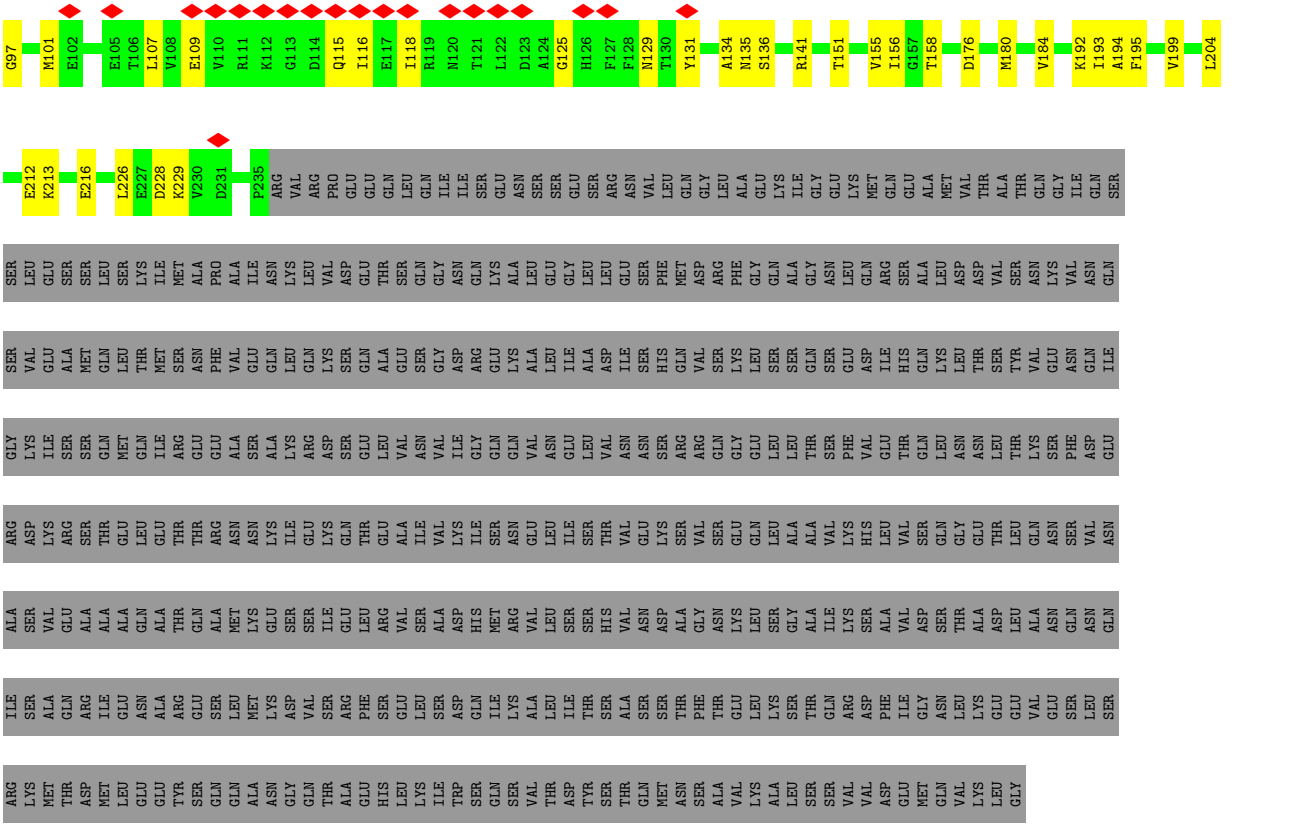




• Molecule 2: MotA/TolQ/ExbB proton channel domain-containing protein

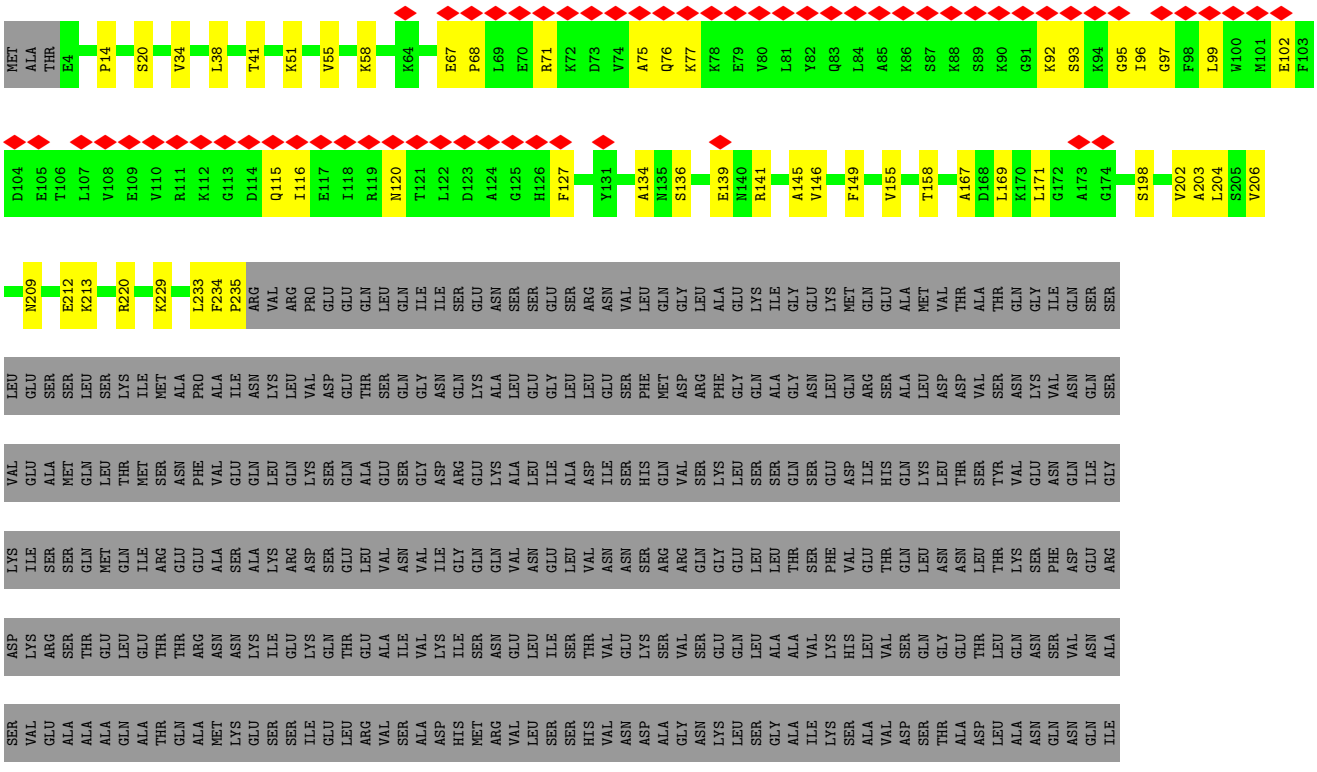
Chain F:





• Molecule 2: MotA/TolQ/ExbB proton channel domain-containing protein

Chain G:



SER ALA GLN ARG ILE GLU ASN ALA ARG GLU SER LEU MET LYS ASP VAL SER ARG PHE SER GLU LEU SER ASP GLN ILE LYS ALA LEU ILE THR SER ALA SER SER THR PHE THR GLU LEU LYS SER THR GLN ARG ASP PHE ILE GLY ASN LEU LYS GLU GLU VAL GLU SER LEU SER ARG

LYS MET THR ASP MET LEU GLU GLU TYR SER GLN GLN ALA ASN GLY GLN THR ALA GLU HIS LEU LYS ILE TRP SER GLN SER VAL THR ASP TYR SER THR GLN MET ASN SER ALA VAL LYS ALA LEU SER SER VAL VAL ASP GLU MET GLN VAL LYS LEU GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	587313	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 ($e^-/Å^2$)	54.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	76.768	Depositor
Minimum map value	-45.719	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.061	Depositor
Recommended contour level	7.8	Depositor
Map size (Å)	347.04, 347.04, 347.04	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.723, 0.723, 0.723	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.18	0/1861	0.36	0/2520
1	B	0.18	0/1850	0.34	0/2503
2	C	0.15	0/1867	0.29	0/2526
2	D	0.16	0/1858	0.35	0/2514
2	E	0.15	0/1867	0.31	0/2526
2	F	0.17	0/1867	0.31	0/2526
2	G	0.16	0/1867	0.31	0/2526
All	All	0.16	0/13037	0.33	0/17641

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	1831	0	1847	42	0
1	B	1821	0	1848	55	0
2	C	1830	0	1882	40	0
2	D	1821	0	1874	46	0
2	E	1830	0	1882	49	0
2	F	1830	0	1879	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1830	0	1882	35	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
4	A	26	0	0	1	0
4	B	24	0	0	0	0
4	C	23	0	0	0	0
4	D	14	0	0	0	0
4	E	16	0	0	0	0
4	F	20	0	0	0	0
4	G	17	0	0	1	0
All	All	12935	0	13094	259	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 10.

All (259) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:141:ARG:NH1	2:F:216:GLU:OE1	2.10	0.84
2:E:69:LEU:HD21	2:E:77:LYS:HG2	1.63	0.79
2:F:87:SER:O	2:F:90:LYS:NZ	2.15	0.77
2:C:120:ASN:ND2	2:C:234:PHE:O	2.18	0.77
1:B:63:GLU:OE2	1:B:66:ARG:NH2	2.21	0.74
2:G:92:LYS:HZ1	2:G:97:GLY:H	1.37	0.71
2:C:231:ASP:HB3	2:D:93:SER:HB3	1.74	0.70
2:D:69:LEU:HD12	2:D:77:LYS:HE2	1.73	0.69
2:G:120:ASN:ND2	2:G:234:PHE:O	2.25	0.69
2:C:62:LEU:HD23	2:C:226:LEU:HD11	1.75	0.69
2:E:62:LEU:HD22	2:E:226:LEU:HD11	1.75	0.68
2:F:62:LEU:HD22	2:F:226:LEU:HD11	1.74	0.68
2:D:216:GLU:OE1	2:E:141:ARG:NE	2.24	0.68
2:G:41:THR:HG21	2:G:204:LEU:HD22	1.76	0.67
1:A:14:GLU:OE2	2:C:141:ARG:NE	2.27	0.66
2:E:51:LYS:NZ	2:E:136:SER:O	2.28	0.66
2:C:5:ARG:NH2	2:D:168:ASP:OD2	2.29	0.66
2:G:14:PRO:HG3	2:G:34:VAL:HG11	1.77	0.66
2:D:71:ARG:NH1	2:D:232:PHE:O	2.29	0.65
2:D:184:VAL:HG12	2:E:171:LEU:HD21	1.79	0.65
2:F:38:LEU:HD23	2:F:204:LEU:HD11	1.80	0.64
1:B:109:PRO:HD2	1:B:114:VAL:HG11	1.81	0.63
1:A:92:LEU:HB3	1:A:225:ILE:HB	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:VAL:HA	1:B:117:GLU:HB2	1.81	0.62
1:A:214:GLU:OE1	1:A:217:ARG:NH2	2.33	0.61
1:A:50:GLN:HG2	1:A:236:ASP:HB2	1.83	0.61
2:G:71:ARG:HH12	2:G:235:PRO:HD3	1.65	0.61
2:E:77:LYS:HA	2:E:80:VAL:HG12	1.83	0.61
1:A:63:GLU:OE1	1:A:66:ARG:NH1	2.33	0.61
2:G:202:VAL:O	2:G:206:VAL:HG23	2.01	0.60
2:G:209:ASN:OD1	2:G:213:LYS:NZ	2.34	0.60
2:D:181:GLN:NE2	2:E:175:VAL:O	2.28	0.60
2:G:158:THR:OG1	2:G:198:SER:OG	2.20	0.60
2:D:61:TRP:CG	2:D:88:LYS:HZ1	2.19	0.60
2:G:102:GLU:HG3	2:G:127:PHE:HE1	1.67	0.60
2:C:224:ARG:NH1	2:C:227:GLU:OE2	2.34	0.60
2:C:229:LYS:HE2	2:C:233:LEU:HD11	1.85	0.59
2:F:74:VAL:HG12	2:F:118:ILE:HD13	1.83	0.59
1:A:58:LEU:HB2	1:A:232:PRO:HG3	1.82	0.59
1:A:152:ILE:HD12	1:A:154:TYR:HB2	1.84	0.59
2:E:69:LEU:HD11	2:E:77:LYS:HE3	1.84	0.59
2:F:228:ASP:OD1	2:F:229:LYS:N	2.36	0.58
1:B:68:ILE:O	1:B:72:ILE:HG13	2.03	0.58
1:A:51:ILE:O	1:A:55:ILE:HG13	2.04	0.58
1:B:146:HIS:CE1	1:B:205:ARG:HB2	2.39	0.58
2:D:73:ASP:OD1	2:D:76:GLN:NE2	2.37	0.57
2:E:192:LYS:HD3	2:G:167:ALA:HB2	1.86	0.57
2:F:141:ARG:NH2	2:G:212:GLU:OE1	2.36	0.57
2:D:107:LEU:HD22	2:D:234:PHE:HZ	1.69	0.57
1:B:46:GLN:HE22	2:E:177:VAL:HG11	1.70	0.57
2:G:220:ARG:HG3	2:G:220:ARG:HH11	1.70	0.56
2:D:62:LEU:HD12	2:D:226:LEU:HD11	1.87	0.56
2:C:58:LYS:HE3	2:C:96:ILE:HB	1.87	0.56
2:C:86:LYS:HZ2	2:C:101:MET:HE3	1.71	0.56
2:E:86:LYS:HG2	2:E:101:MET:HE1	1.87	0.56
1:A:20:MET:HG2	2:F:155:VAL:HG21	1.87	0.56
2:F:55:VAL:HA	2:F:58:LYS:HE2	1.88	0.55
2:C:104:ASP:HA	2:C:107:LEU:HD13	1.89	0.55
2:C:216:GLU:HG2	2:C:220:ARG:HE	1.71	0.55
2:C:227:GLU:HG3	2:D:94:LYS:NZ	2.21	0.55
2:D:59:ILE:HG21	2:D:222:LYS:HB3	1.88	0.55
2:E:176:ASP:OD2	2:E:178:THR:OG1	2.25	0.55
1:B:68:ILE:HG13	1:B:134:ARG:HD3	1.89	0.54
2:C:54:ASP:OD1	2:C:55:VAL:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:212:GLU:OE2	2:E:213:LYS:NZ	2.41	0.54
2:F:55:VAL:HG11	2:F:134:ALA:HB2	1.90	0.54
1:B:205:ARG:O	1:B:222:ARG:NH2	2.40	0.54
2:C:177:VAL:O	2:C:181:GLN:HG3	2.07	0.54
2:E:169:LEU:HD11	2:E:187:VAL:HG21	1.89	0.54
2:F:67:GLU:HG2	2:F:68:PRO:HD3	1.89	0.53
2:D:48:LEU:HD21	2:D:212:GLU:HA	1.88	0.53
2:D:61:TRP:HD1	2:D:64:LYS:HE3	1.73	0.53
1:A:92:LEU:HD23	1:A:225:ILE:HD12	1.91	0.53
2:E:79:GLU:O	2:E:83:GLN:NE2	2.41	0.53
2:D:77:LYS:HA	2:D:80:VAL:HG12	1.90	0.53
2:E:89:SER:HB2	2:E:97:GLY:HA3	1.91	0.53
1:B:65:ARG:NE	1:B:90:THR:HG22	2.24	0.52
2:D:86:LYS:HD3	2:D:89:SER:O	2.08	0.52
1:B:234:ILE:HD13	1:A:58:LEU:HD23	1.91	0.52
2:C:67:GLU:HB3	2:C:68:PRO:HD3	1.92	0.52
1:A:24:ASP:HB2	2:F:155:VAL:HG22	1.90	0.52
2:C:69:LEU:HD11	2:C:77:LYS:HG2	1.90	0.52
1:B:29:LEU:HG	2:E:195:PHE:CZ	2.45	0.52
1:B:31:VAL:HG11	2:D:191:ALA:HB2	1.91	0.52
1:A:131:THR:O	1:A:134:ARG:HG3	2.09	0.52
2:C:227:GLU:HG3	2:D:94:LYS:HZ1	1.75	0.51
1:B:53:ALA:O	1:B:57:GLU:HG2	2.10	0.51
2:D:120:ASN:HB3	2:D:234:PHE:CE2	2.45	0.51
1:A:45:THR:O	1:A:49:GLU:HG3	2.11	0.51
1:B:144:GLU:HG2	1:B:199:SER:HB2	1.92	0.51
2:D:84:LEU:HA	2:D:87:SER:OG	2.10	0.51
2:G:55:VAL:HG11	2:G:134:ALA:HB2	1.93	0.51
2:D:12:LEU:HG	2:E:164:LEU:HD21	1.92	0.51
2:E:81:LEU:HD12	2:E:84:LEU:HD11	1.91	0.50
2:C:41:THR:HG21	2:C:204:LEU:HD22	1.93	0.50
2:E:216:GLU:OE1	2:G:141:ARG:NH2	2.41	0.50
2:E:8:GLU:O	2:E:11:TRP:NE1	2.38	0.50
2:F:125:GLY:O	2:F:129:ASN:ND2	2.44	0.50
2:G:51:LYS:HD3	2:G:136:SER:OG	2.11	0.50
2:C:73:ASP:HA	2:C:76:GLN:NE2	2.27	0.50
1:B:126:HIS:CE1	1:B:180:VAL:HB	2.47	0.50
2:C:70:GLU:H	2:C:73:ASP:HB3	1.77	0.50
2:D:8:GLU:HB2	2:D:11:TRP:CE2	2.47	0.50
2:E:54:ASP:O	2:E:58:LYS:HG3	2.12	0.50
2:F:58:LYS:HB3	2:F:96:ILE:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:213:LYS:HE2	2:G:145:ALA:HB2	1.94	0.49
2:D:81:LEU:HA	2:D:84:LEU:HG	1.94	0.49
1:B:160:TRP:CD1	1:A:172:LYS:HD3	2.47	0.49
1:B:46:GLN:HE21	2:D:177:VAL:HG11	1.77	0.49
1:B:206:ARG:NH1	1:B:211:GLU:OE1	2.43	0.49
1:A:144:GLU:HG2	1:A:201:TYR:HE2	1.76	0.49
1:B:189:ASN:OD1	1:B:193:GLN:HG2	2.13	0.49
2:E:112:LYS:HB2	2:E:115:GLN:HB2	1.95	0.49
2:F:78:LYS:HE2	2:F:107:LEU:HD12	1.95	0.49
1:B:171:TRP:CE2	1:B:175:GLN:NE2	2.80	0.49
1:B:55:ILE:HD12	1:A:234:ILE:HG12	1.95	0.48
2:F:26:GLY:HA2	2:F:193:ILE:HD11	1.95	0.48
2:F:158:THR:HG23	2:F:194:ALA:HB1	1.95	0.48
2:E:222:LYS:O	2:E:226:LEU:N	2.42	0.48
2:F:176:ASP:O	2:F:180:MET:HG3	2.14	0.48
1:B:126:HIS:NE2	1:B:182:PRO:O	2.47	0.48
1:B:171:TRP:NE1	1:B:175:GLN:NE2	2.60	0.48
1:A:65:ARG:HH21	1:A:229:VAL:N	2.12	0.48
2:E:137:VAL:HG23	2:E:138:THR:HG23	1.95	0.48
1:A:65:ARG:HD3	1:A:90:THR:HA	1.96	0.48
1:B:168:VAL:HG22	1:B:198:VAL:HG11	1.95	0.47
2:E:160:MET:O	2:E:164:LEU:HG	2.13	0.47
1:B:46:GLN:NE2	2:E:177:VAL:HG11	2.29	0.47
1:B:155:ARG:CZ	1:A:155:ARG:HD2	2.43	0.47
1:B:52:ASP:OD2	1:A:47:LYS:NZ	2.25	0.47
1:B:138:LEU:O	1:B:189:ASN:HB2	2.14	0.47
2:E:99:LEU:HD11	2:E:127:PHE:O	2.14	0.47
2:E:115:GLN:O	2:E:117:GLU:HG2	2.13	0.47
1:A:111:ASN:HD21	1:A:114:VAL:HG23	1.79	0.47
2:C:93:SER:HA	2:C:98:PHE:CD2	2.50	0.47
2:D:99:LEU:HD21	2:D:132:THR:HG23	1.96	0.47
2:D:125:GLY:HA2	2:D:227:GLU:OE2	2.15	0.47
2:E:146:VAL:HB	2:E:208:PHE:CE2	2.50	0.47
1:B:135:TRP:HA	1:B:138:LEU:HD12	1.97	0.47
2:C:176:ASP:OD1	2:C:177:VAL:N	2.48	0.47
2:C:188:VAL:HG11	2:D:171:LEU:HD12	1.95	0.47
2:D:73:ASP:HA	2:D:76:GLN:NE2	2.31	0.46
2:F:78:LYS:HD2	2:F:118:ILE:HG12	1.96	0.46
2:G:229:LYS:HE3	2:G:233:LEU:HD11	1.96	0.46
1:A:184:LEU:HD22	1:A:196:PHE:CZ	2.51	0.46
2:F:131:TYR:O	2:F:135:ASN:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:THR:O	1:B:168:VAL:HG23	2.15	0.46
2:G:92:LYS:NZ	2:G:97:GLY:H	2.10	0.46
1:B:51:ILE:O	1:B:55:ILE:HG12	2.16	0.46
1:A:211:GLU:OE1	1:A:217:ARG:HG2	2.16	0.46
1:B:149:SER:OG	1:B:211:GLU:OE1	2.34	0.46
1:B:148:ASP:OD2	1:B:221:ARG:NH1	2.49	0.45
2:F:195:PHE:O	2:F:199:VAL:HG23	2.17	0.45
1:B:160:TRP:HA	1:B:202:ALA:HB2	1.99	0.45
2:D:196:LEU:N	2:E:163:GLN:HE21	2.15	0.45
2:D:74:VAL:HG11	2:D:117:GLU:HA	1.99	0.45
2:D:111:ARG:NH2	2:D:115:GLN:O	2.50	0.45
2:F:51:LYS:HE3	2:F:136:SER:HB2	1.98	0.45
2:G:38:LEU:HD12	2:G:204:LEU:HD11	1.97	0.45
1:A:119:ARG:O	1:A:123:ILE:HG13	2.17	0.44
2:F:115:GLN:HA	2:F:115:GLN:OE1	2.18	0.44
2:G:58:LYS:CG	2:G:96:ILE:HB	2.48	0.44
1:B:155:ARG:NH2	1:A:155:ARG:HD2	2.33	0.44
2:E:51:LYS:HZ1	2:E:137:VAL:HG12	1.83	0.44
1:A:126:HIS:CE1	1:A:180:VAL:HB	2.53	0.44
2:D:74:VAL:HG22	2:D:118:ILE:HG22	2.00	0.44
1:B:40:LEU:HG	2:G:171:LEU:HD21	2.00	0.44
2:E:22:HIS:NE2	2:E:24:GLN:OE1	2.51	0.44
2:F:23:PRO:HG3	2:F:32:LEU:HD23	1.99	0.44
2:G:75:ALA:HB1	2:G:116:ILE:HB	2.00	0.44
1:A:20:MET:HE3	2:F:151:THR:HG22	2.00	0.44
2:G:58:LYS:HG2	2:G:96:ILE:HB	1.99	0.44
2:C:107:LEU:HB3	2:C:118:ILE:HD11	1.99	0.43
2:F:48:LEU:HD21	2:F:212:GLU:HA	2.00	0.43
2:E:224:ARG:HH12	2:G:136:SER:HB2	1.83	0.43
1:A:75:GLU:OE2	1:A:127:LYS:HD2	2.18	0.43
2:G:95:GLY:O	2:G:99:LEU:HG	2.18	0.43
1:B:69:LEU:HB3	1:B:85:ILE:HG12	2.00	0.43
1:B:169:SER:O	1:B:173:LEU:HD13	2.19	0.43
1:A:65:ARG:HH21	1:A:229:VAL:H	1.66	0.43
1:A:79:GLN:OE1	1:A:120:LEU:HD13	2.19	0.43
2:F:67:GLU:CG	2:F:68:PRO:HD3	2.48	0.43
1:B:149:SER:HG	1:B:211:GLU:CD	2.25	0.43
1:B:189:ASN:HD21	1:B:193:GLN:HE21	1.66	0.43
2:E:218:PHE:CZ	2:E:222:LYS:HE2	2.54	0.43
1:B:47:LYS:O	1:B:51:ILE:HG13	2.18	0.43
1:B:75:GLU:OE1	1:B:124:ALA:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LYS:HB3	1:B:161:GLY:HA3	2.01	0.43
1:A:13:ASP:OD1	2:D:141:ARG:NH2	2.32	0.43
2:D:129:ASN:HD21	2:D:131:TYR:HE1	1.64	0.43
2:E:125:GLY:O	2:E:129:ASN:ND2	2.51	0.43
1:B:173:LEU:HA	1:B:177:GLU:OE1	2.19	0.43
2:C:60:ASN:OD1	2:C:222:LYS:NZ	2.49	0.43
2:E:11:TRP:H	2:E:11:TRP:CD1	2.37	0.43
2:G:146:VAL:HA	2:G:149:PHE:CD2	2.54	0.43
1:B:59:LYS:HZ2	1:B:59:LYS:HG3	1.61	0.43
2:E:220:ARG:NH1	2:G:139:GLU:OE1	2.51	0.43
2:E:49:LEU:O	2:E:53:ILE:HG12	2.19	0.42
1:B:174:TRP:HB3	1:B:184:LEU:HD12	2.00	0.42
2:C:81:LEU:O	2:C:85:ALA:N	2.43	0.42
2:C:206:VAL:HB	2:D:156:ILE:HD11	2.01	0.42
2:D:103:PHE:CZ	2:D:124:ALA:HB2	2.54	0.42
1:B:81:ILE:HG12	1:B:117:GLU:OE2	2.19	0.42
2:C:139:GLU:O	2:C:139:GLU:HG2	2.19	0.42
2:F:69:LEU:HD21	2:F:81:LEU:HD11	2.02	0.42
2:F:156:ILE:HD11	2:G:203:ALA:HA	2.01	0.42
2:F:158:THR:HA	2:F:194:ALA:HA	2.01	0.42
1:B:22:PHE:CD2	2:G:155:VAL:HG21	2.55	0.42
2:D:89:SER:HA	2:D:92:LYS:HE2	2.02	0.42
2:E:222:LYS:HA	2:E:225:GLU:HB3	2.02	0.42
1:A:118:VAL:HG12	1:A:173:LEU:HD22	2.01	0.42
2:D:61:TRP:HA	2:D:64:LYS:HG3	2.02	0.42
2:E:34:VAL:HG23	2:E:197:THR:HG22	2.01	0.42
2:E:70:GLU:HG2	2:E:73:ASP:CG	2.45	0.42
2:F:53:ILE:O	2:F:57:LEU:HG	2.20	0.42
1:A:35:LEU:HD22	2:F:184:VAL:HG13	2.00	0.42
2:E:29:LEU:HD11	2:E:160:MET:HE2	2.00	0.42
1:B:181:ALA:HB3	1:B:182:PRO:HD3	2.02	0.41
1:A:75:GLU:HA	1:A:78:LYS:NZ	2.35	0.41
2:C:192:LYS:HD2	2:D:167:ALA:HA	2.02	0.41
2:E:228:ASP:HA	2:G:93:SER:HB3	2.02	0.41
2:G:67:GLU:HB3	2:G:68:PRO:HD3	2.02	0.41
2:C:222:LYS:HE3	2:C:222:LYS:HB3	1.90	0.41
2:E:32:LEU:O	2:E:36:ILE:HG13	2.20	0.41
1:B:47:LYS:HB2	1:B:47:LYS:HE2	1.93	0.41
1:B:75:GLU:HA	1:B:78:LYS:NZ	2.35	0.41
2:C:195:PHE:CZ	2:D:162:LEU:HD23	2.55	0.41
2:F:97:GLY:O	2:F:101:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:TRP:CZ3	1:B:155:ARG:HA	2.55	0.41
1:B:211:GLU:HG3	1:B:220:ASN:ND2	2.36	0.41
2:C:145:ALA:HB2	2:F:213:LYS:HE2	2.02	0.41
2:E:62:LEU:CD2	2:E:226:LEU:HD11	2.48	0.41
1:B:61:ALA:HB1	1:B:229:VAL:HB	2.02	0.41
2:C:70:GLU:O	2:C:74:VAL:HG23	2.21	0.41
2:G:76:GLN:NE2	2:G:77:LYS:HE3	2.35	0.41
1:B:87:GLU:O	1:B:90:THR:OG1	2.26	0.41
2:C:66:LEU:O	2:C:229:LYS:NZ	2.30	0.41
2:D:202:VAL:O	2:D:206:VAL:HG23	2.21	0.41
2:G:20:SER:OG	4:G:701:HOH:O	2.21	0.41
2:G:169:LEU:HD23	2:G:169:LEU:HA	1.89	0.41
1:A:65:ARG:NH2	4:A:302:HOH:O	2.33	0.41
2:C:180:MET:HE3	2:C:180:MET:HB3	1.89	0.41
2:D:108:VAL:O	2:D:118:ILE:HD11	2.21	0.41
2:E:210:PHE:CZ	2:E:214:LEU:HD22	2.55	0.41
1:A:143:VAL:HB	1:A:198:VAL:HG22	2.03	0.40
2:C:129:ASN:O	2:C:133:LEU:HB2	2.22	0.40
1:A:58:LEU:O	1:A:62:GLU:HG3	2.21	0.40
1:A:173:LEU:HG	1:A:177:GLU:OE2	2.20	0.40
1:A:207:VAL:HG13	1:A:222:ARG:CZ	2.51	0.40
1:A:208:ASP:OD2	1:A:216:GLN:HB3	2.21	0.40
2:D:30:SER:O	2:D:34:VAL:HG23	2.21	0.40
2:D:97:GLY:O	2:D:101:MET:HG2	2.21	0.40
2:F:109:GLU:OE2	2:F:116:ILE:HG23	2.22	0.40
1:A:211:GLU:OE2	1:A:220:ASN:ND2	2.54	0.40
2:C:85:ALA:HB2	2:C:100:TRP:HD1	1.87	0.40
2:C:134:ALA:HB1	2:C:137:VAL:HB	2.03	0.40
2:C:166:LEU:O	2:F:192:LYS:HE2	2.22	0.40
2:E:213:LYS:HE3	2:G:141:ARG:HG2	2.03	0.40
2:D:111:ARG:NH2	2:D:113:GLY:O	2.55	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	224/282 (79%)	213 (95%)	11 (5%)	0	100	100
1	B	223/282 (79%)	215 (96%)	8 (4%)	0	100	100
2	C	230/696 (33%)	227 (99%)	3 (1%)	0	100	100
2	D	229/696 (33%)	218 (95%)	11 (5%)	0	100	100
2	E	230/696 (33%)	226 (98%)	4 (2%)	0	100	100
2	F	230/696 (33%)	222 (96%)	8 (4%)	0	100	100
2	G	230/696 (33%)	225 (98%)	4 (2%)	1 (0%)	30	34
All	All	1596/4044 (40%)	1546 (97%)	49 (3%)	1 (0%)	50	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	115	GLN

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	A	203/246 (82%)	203 (100%)	0	100	100
1	B	201/246 (82%)	201 (100%)	0	100	100
2	C	198/607 (33%)	198 (100%)	0	100	100
2	D	197/607 (32%)	197 (100%)	0	100	100
2	E	198/607 (33%)	198 (100%)	0	100	100
2	F	198/607 (33%)	198 (100%)	0	100	100
2	G	198/607 (33%)	198 (100%)	0	100	100
All	All	1393/3527 (40%)	1393 (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 (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	B	46	GLN
1	B	79	GLN
1	B	193	GLN
1	B	210	GLN
1	A	67	ASN
1	A	82	HIS
1	A	159	ASN
2	D	18	HIS
2	D	63	GLN
2	E	60	ASN
2	E	83	GLN
2	E	135	ASN
2	E	163	GLN
2	F	163	GLN
2	F	189	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

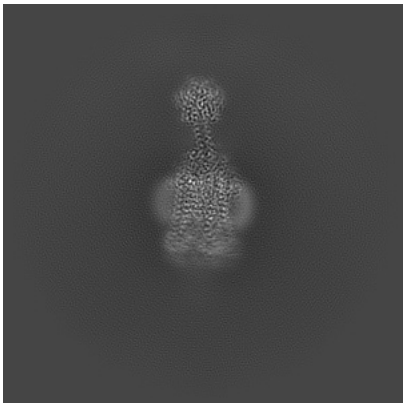
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43563. These allow visual inspection of the internal detail of the map and identification of artifacts.

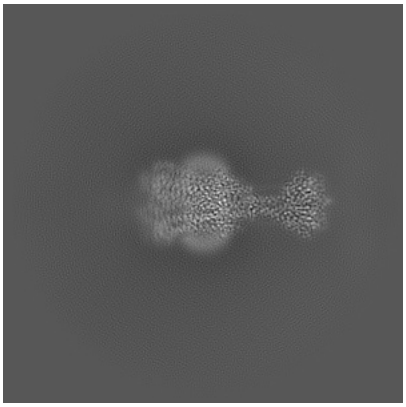
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

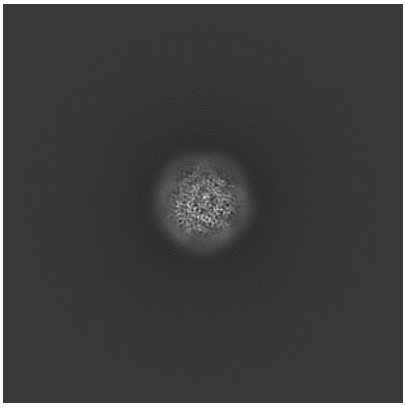
6.1.1 Primary map



X



Y

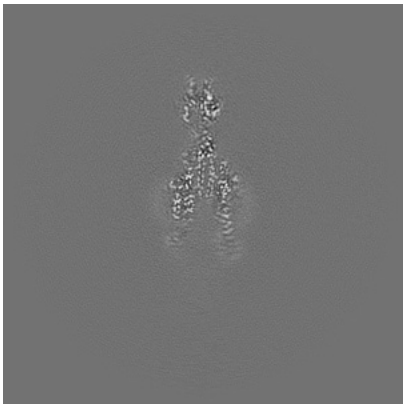


Z

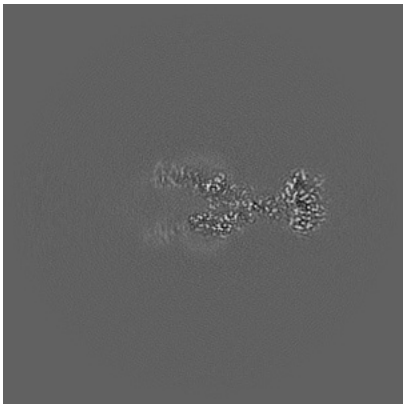
The images above show the map projected in three orthogonal directions.

6.2 Central slices

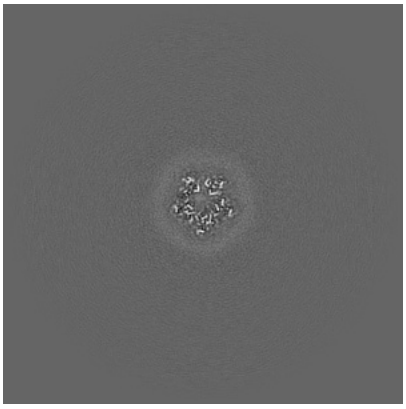
6.2.1 Primary map



X Index: 240



Y Index: 240

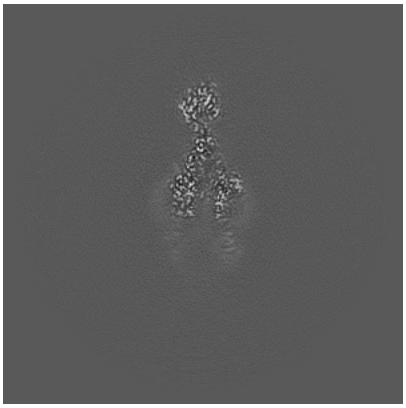


Z Index: 240

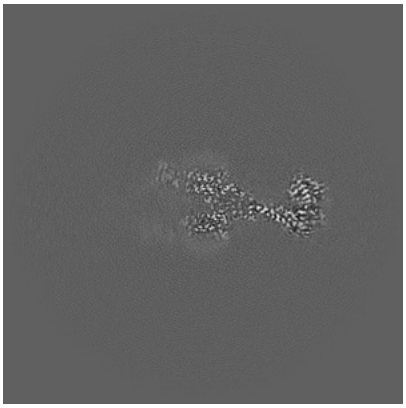
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

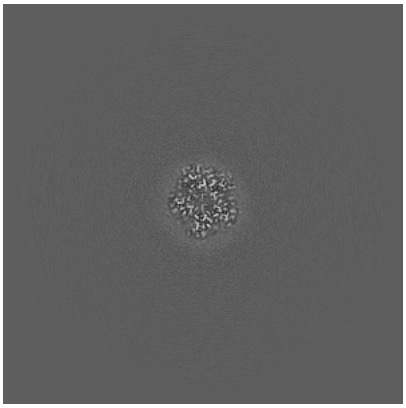
6.3.1 Primary map



X Index: 234



Y Index: 233

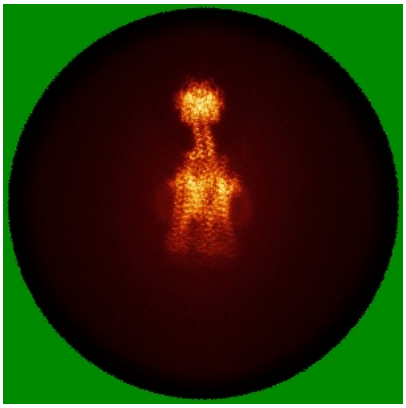


Z Index: 260

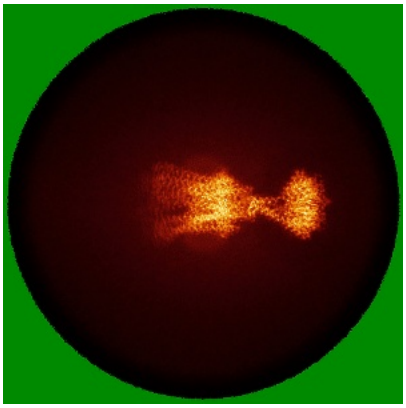
The images above show the largest variance slices of the map in three orthogonal directions.

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

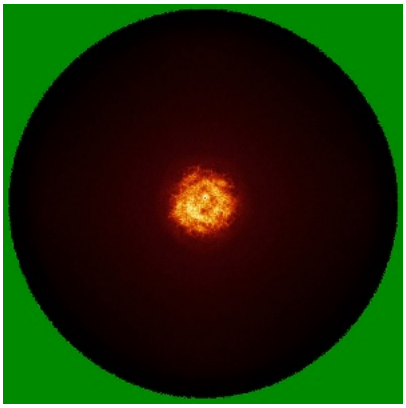
6.4.1 Primary map



X



Y

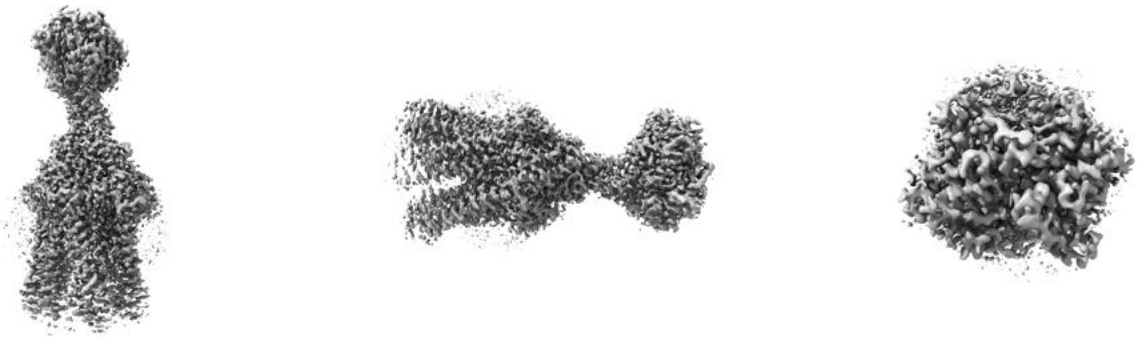


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 7.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

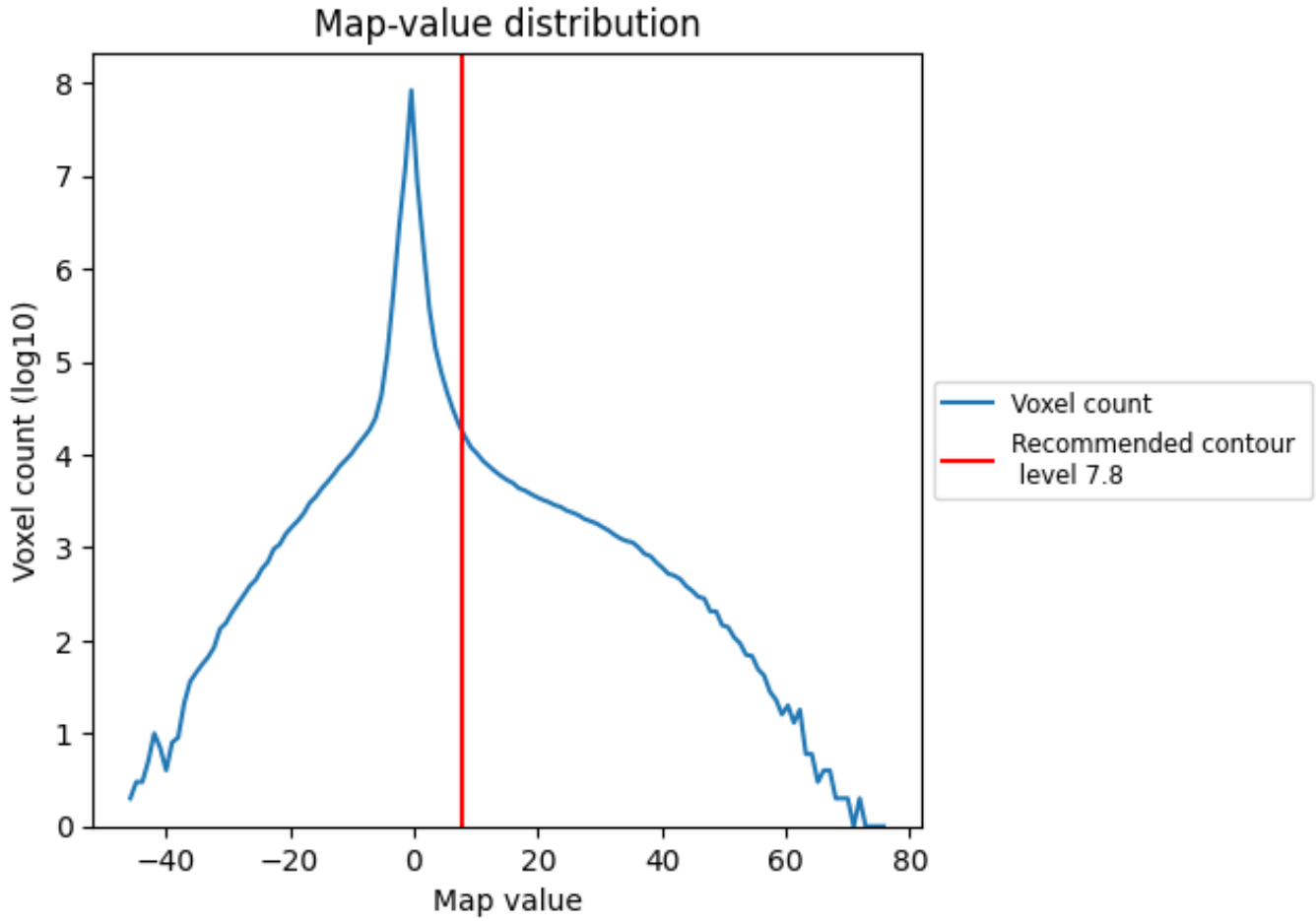
6.6 Mask visualisation (i)

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

7 Map analysis

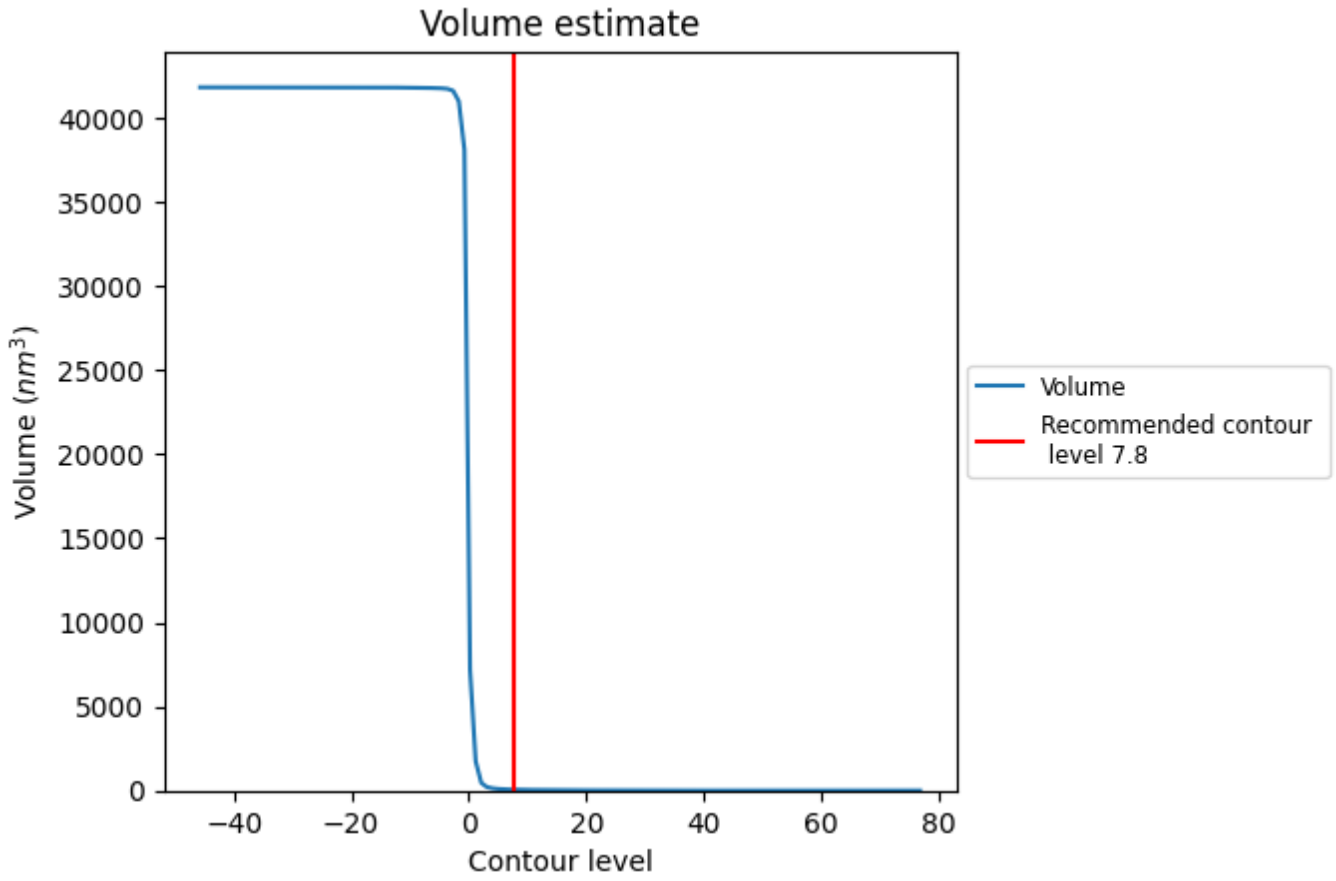
This section contains the results of statistical analysis of the map.

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.

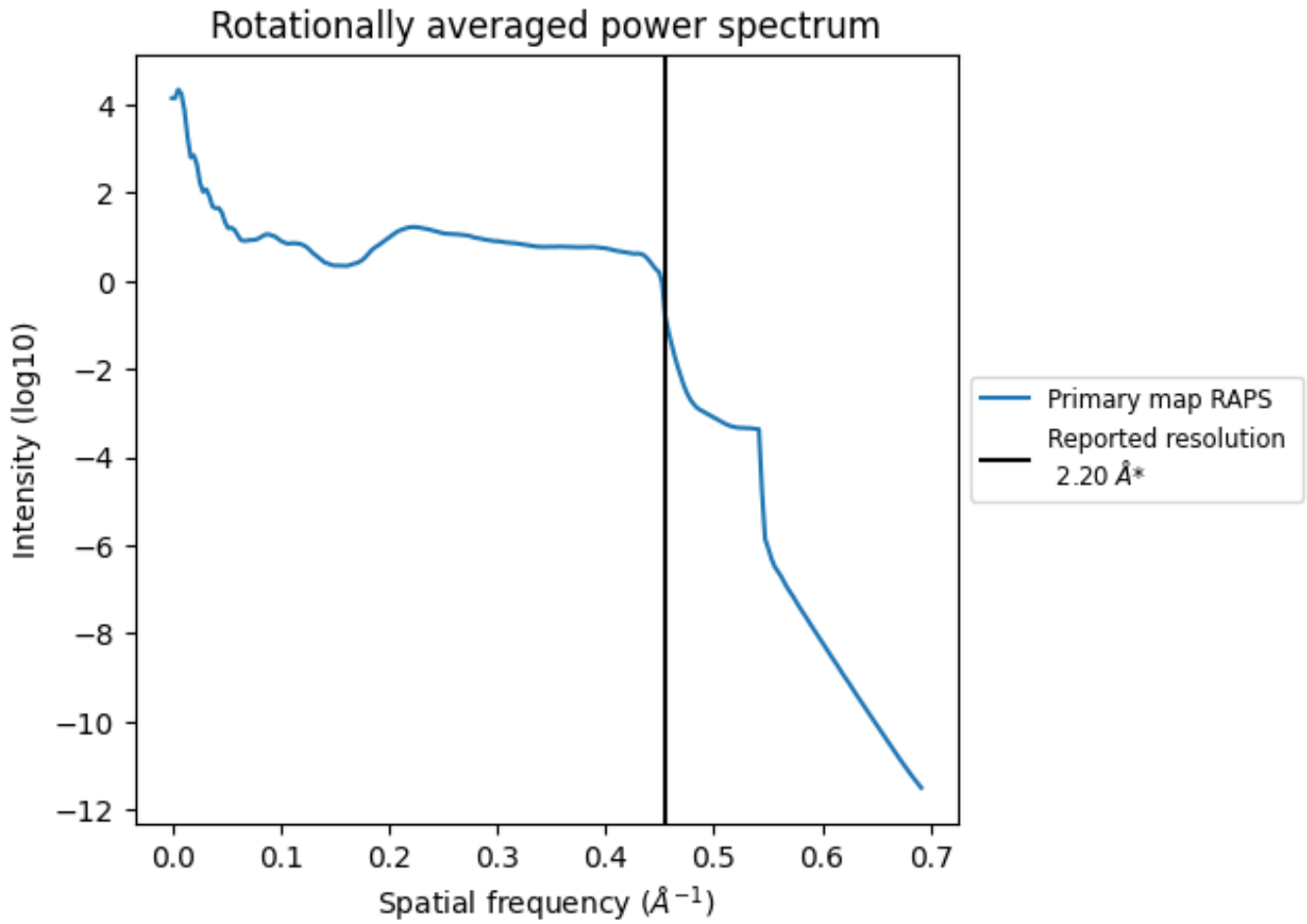
7.2 Volume estimate (i)



The volume at the recommended contour level is 54 nm^3; this corresponds to an approximate mass of 49 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 0.455 Å^{-1}

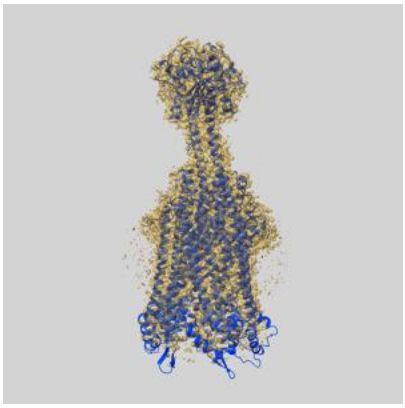
8 Fourier-Shell correlation (i)

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

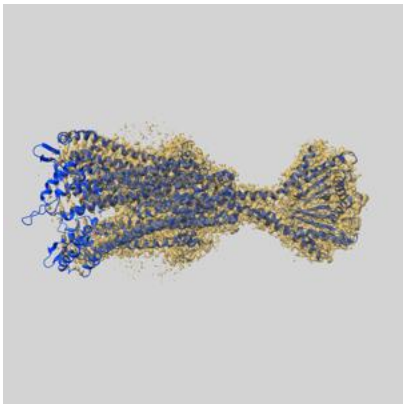
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43563 and PDB model 8VVN. Per-residue inclusion information can be found in section 3 on page 7.

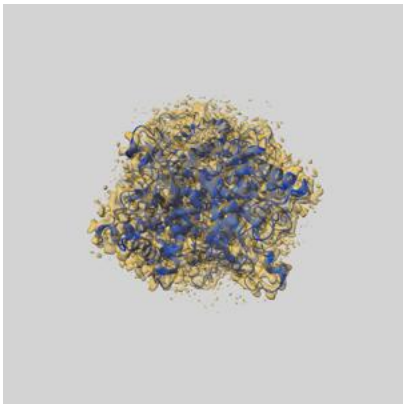
9.1 Map-model overlay



X



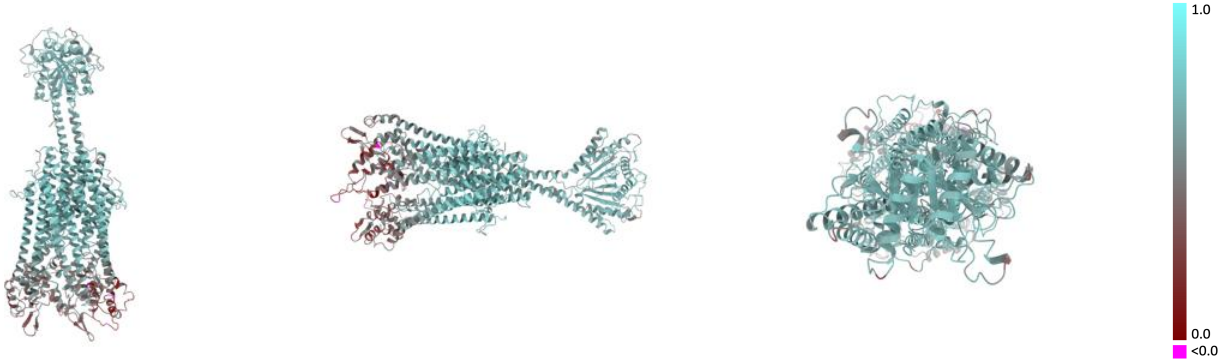
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.8 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.

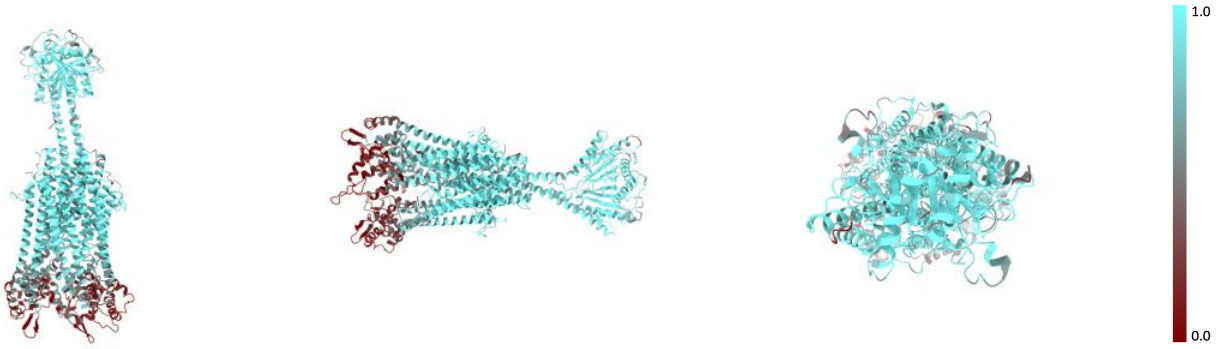
9.2 Q-score mapped to coordinate model (i)



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.

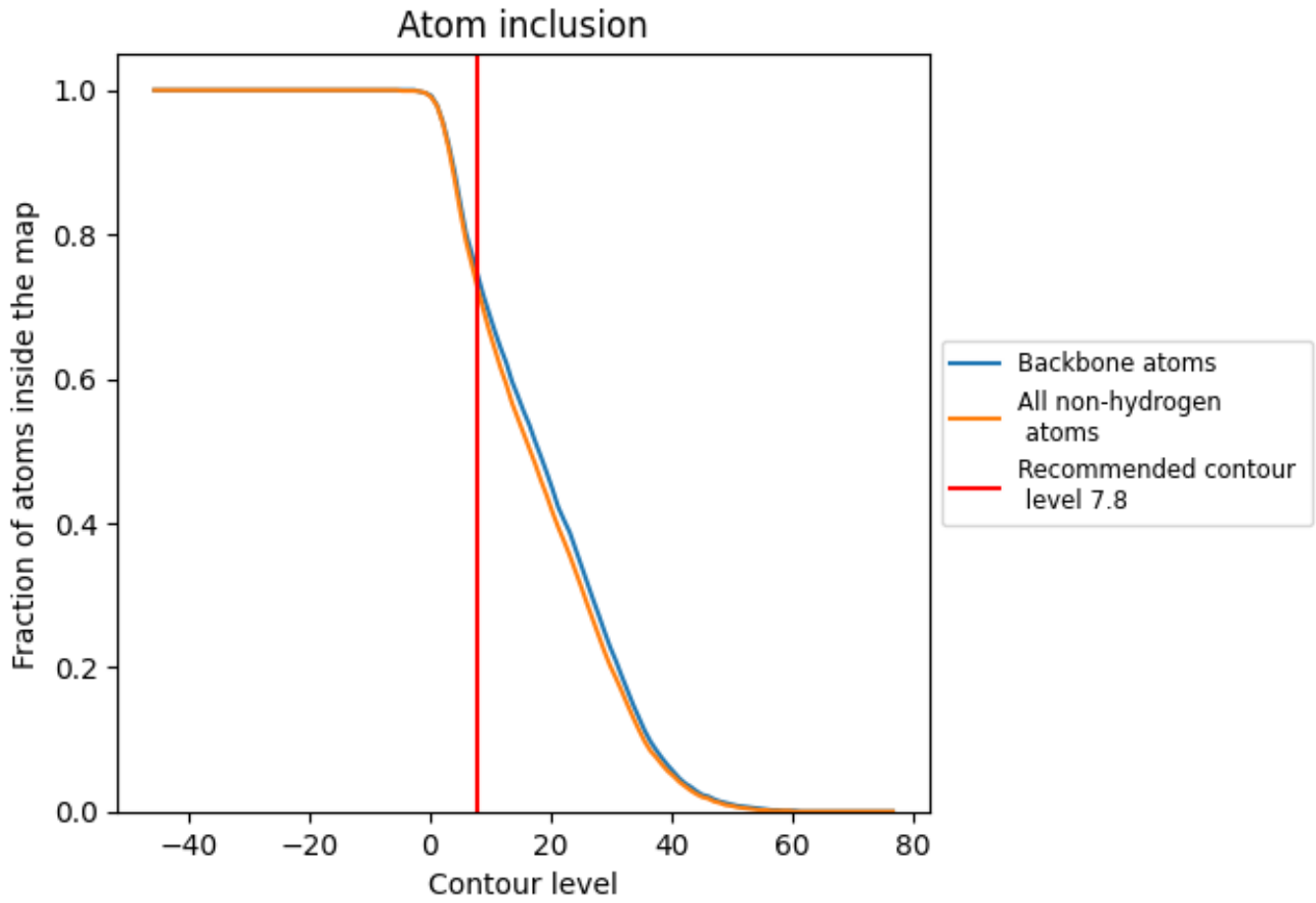
9.3 Atom inclusion mapped to coordinate model (i)



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 (7.8).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 73% 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 (7.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7290	0.5950
A	0.8770	0.6540
B	0.8920	0.6500
C	0.7300	0.6040
D	0.5980	0.5140
E	0.6240	0.5570
F	0.7230	0.6020
G	0.6780	0.5860