Full wwPDB EM Validation Report ⓘ

Apr 29, 2024 – 08:10 AM EDT

PDB ID	:	8SQA
EMDB ID	:	EMD-40700
Title	:	The cryo-EM structure of the EcBAM/EspP(beta8-12) complex
Authors	:	Wu, R.; Noinaj, N.
Deposited on	:	2023-05-04
Resolution	:	4.20 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:

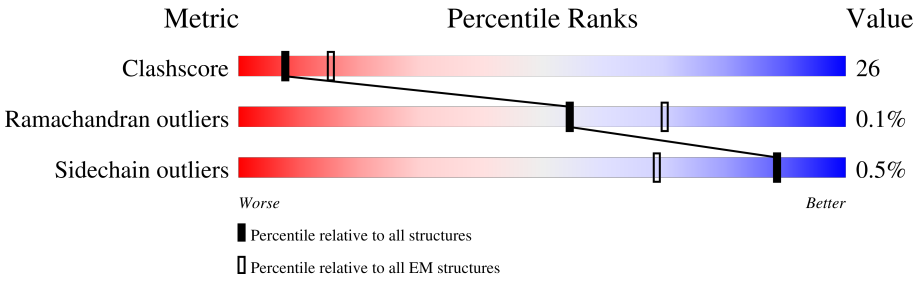
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	786	10% 51% 45%
2	B	372	47% 52%
3	C	319	11% 8% 81%
4	D	225	48% 47%
5	E	93	46% 45% 9%
6	F	551	5% 7% 88%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12156 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 Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	765	Total	C	N	O	S	0	0
			6052	3821	1023	1192	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	806	CYS	ILE	conflict	UNP C3TPJ2

- Molecule 2 is a protein called Outer membrane protein assembly factor BamB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	369	Total	C	N	O	S	0	0
			2776	1742	473	555	6		

- Molecule 3 is a protein called Outer membrane protein assembly factor BamC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	61	Total	C	N	O	S	0	0
			437	277	74	85	1		

- Molecule 4 is a protein called Outer membrane protein assembly factor BamD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	215	Total	C	N	O	S	0	0
			1740	1098	306	329	7		

- Molecule 5 is a protein called Outer membrane protein assembly factor BamE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	85	Total	C	N	O	S	0	0
			668	421	117	128	2		

- Molecule 6 is a protein called Maltose/maltodextrin-binding periplasmic protein,Autotrans

porter protein EspP translocator.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	68	Total	C	N	O	S	0	0
			483	303	86	92	2		

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	750	MET	-	expression tag	UNP P0AEY0
F	751	GLY	-	expression tag	UNP P0AEY0
F	1064	VAL	ALA	conflict	UNP P0AEY0
F	1119	GLY	-	linker	UNP P0AEY0
F	1120	SER	-	linker	UNP P0AEY0
F	1121	ILE	-	linker	UNP P0AEY0
F	1122	GLU	-	linker	UNP P0AEY0
F	1123	LEU	-	linker	UNP P0AEY0
F	1124	VAL	-	linker	UNP P0AEY0
F	1125	SER	-	linker	UNP P0AEY0
F	1126	ALA	-	linker	UNP P0AEY0
F	1127	PRO	-	linker	UNP P0AEY0
F	1128	LYS	-	linker	UNP P0AEY0
F	1129	ASP	-	linker	UNP P0AEY0
F	1130	THR	-	linker	UNP P0AEY0
F	1131	ASN	-	linker	UNP P0AEY0
F	1132	GLU	-	linker	UNP P0AEY0
F	1133	ASN	-	linker	UNP P0AEY0
F	1134	VAL	-	linker	UNP P0AEY0
F	1135	PHE	-	linker	UNP P0AEY0
F	1136	LYS	-	linker	UNP P0AEY0
F	1137	ALA	-	linker	UNP P0AEY0
F	1138	SER	-	linker	UNP P0AEY0
F	1139	LYS	-	linker	UNP P0AEY0
F	1140	GLN	-	linker	UNP P0AEY0
F	1141	THR	-	linker	UNP P0AEY0
F	1142	ILE	-	linker	UNP P0AEY0
F	1143	GLY	-	linker	UNP P0AEY0
F	1144	PHE	-	linker	UNP P0AEY0
F	1145	SER	-	linker	UNP P0AEY0
F	1146	ASP	-	linker	UNP P0AEY0
F	1147	VAL	-	linker	UNP P0AEY0
F	1148	THR	-	linker	UNP P0AEY0
F	1149	PRO	-	linker	UNP P0AEY0
F	1150	VAL	-	linker	UNP P0AEY0
F	1151	ILE	-	linker	UNP P0AEY0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1152	THR	-	linker	UNP P0AEY0
F	1153	THR	-	linker	UNP P0AEY0
F	1154	ARG	-	linker	UNP P0AEY0
F	1155	GLU	-	linker	UNP P0AEY0
F	1156	THR	-	linker	UNP P0AEY0
F	1157	ASP	-	linker	UNP P0AEY0
F	1158	ASP	-	linker	UNP P0AEY0
F	1159	LYS	-	linker	UNP P0AEY0
F	1160	ILE	-	linker	UNP P0AEY0
F	1161	THR	-	linker	UNP P0AEY0
F	1162	TRP	-	linker	UNP P0AEY0
F	1163	SER	-	linker	UNP P0AEY0
F	1164	LEU	-	linker	UNP P0AEY0
F	1165	THR	-	linker	UNP P0AEY0
F	1166	GLY	-	linker	UNP P0AEY0
F	1167	TYR	-	linker	UNP P0AEY0
F	1168	ASN	-	linker	UNP P0AEY0
F	1169	THR	-	linker	UNP P0AEY0
F	1170	VAL	-	linker	UNP P0AEY0
F	1171	ALA	-	linker	UNP P0AEY0
F	1172	ASN	-	linker	UNP P0AEY0
F	1173	LYS	-	linker	UNP P0AEY0
F	1174	GLU	-	linker	UNP P0AEY0
F	1175	ALA	-	linker	UNP P0AEY0
F	1176	THR	-	linker	UNP P0AEY0
F	1177	ARG	-	linker	UNP P0AEY0
F	1178	ASN	-	linker	UNP P0AEY0
F	1179	ALA	-	linker	UNP P0AEY0
F	1180	ALA	-	linker	UNP P0AEY0
F	1181	ALA	-	linker	UNP P0AEY0
F	1182	LEU	-	linker	UNP P0AEY0
F	1183	PHE	-	linker	UNP P0AEY0
F	1184	SER	-	linker	UNP P0AEY0
F	1185	VAL	-	linker	UNP P0AEY0
F	1186	ASP	-	linker	UNP P0AEY0
F	1187	TYR	-	linker	UNP P0AEY0
F	1188	LYS	-	linker	UNP P0AEY0
F	1189	ALA	-	linker	UNP P0AEY0
F	1190	PHE	-	linker	UNP P0AEY0
F	1191	LEU	-	linker	UNP P0AEY0
F	1192	ASN	-	linker	UNP P0AEY0
F	1193	GLU	-	linker	UNP P0AEY0

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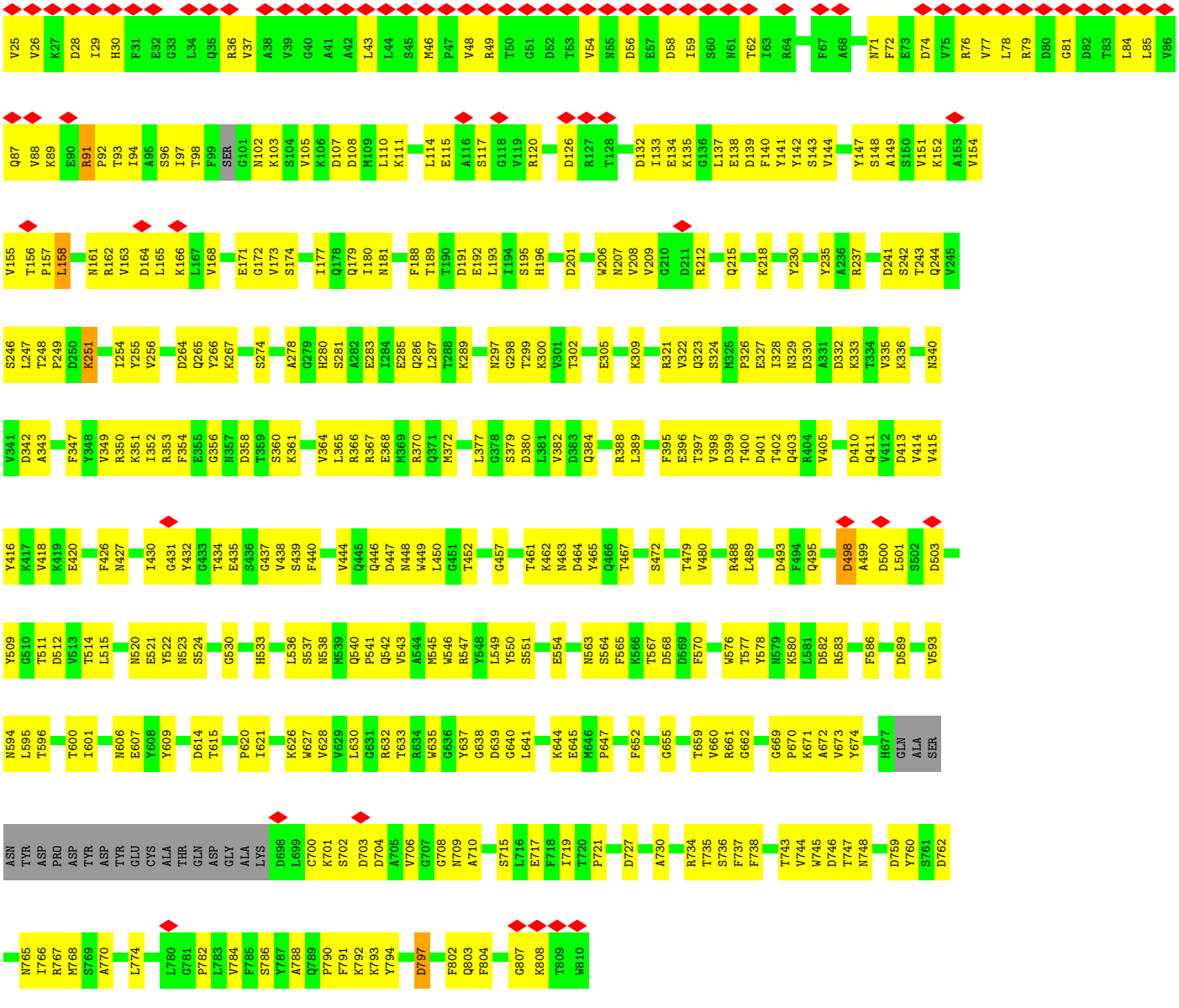
Chain	Residue	Modelled	Actual	Comment	Reference
F	1194	VAL	-	linker	UNP P0AEY0
F	1208	CYS	VAL	conflict	UNP Q7BSW5

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.

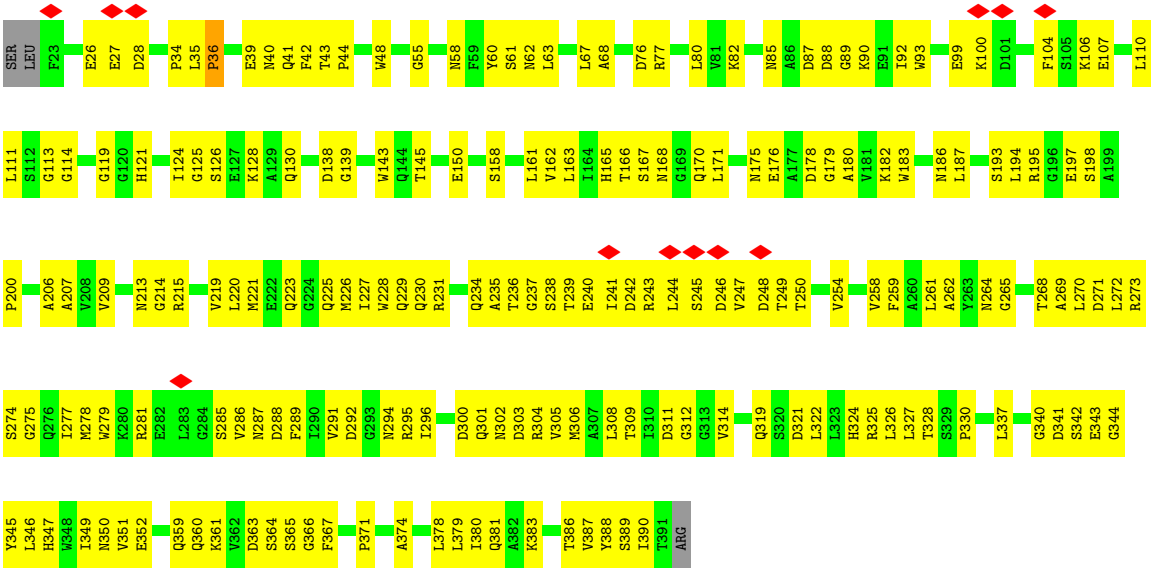
• Molecule 1: Outer membrane protein assembly factor BamA

Chain A:



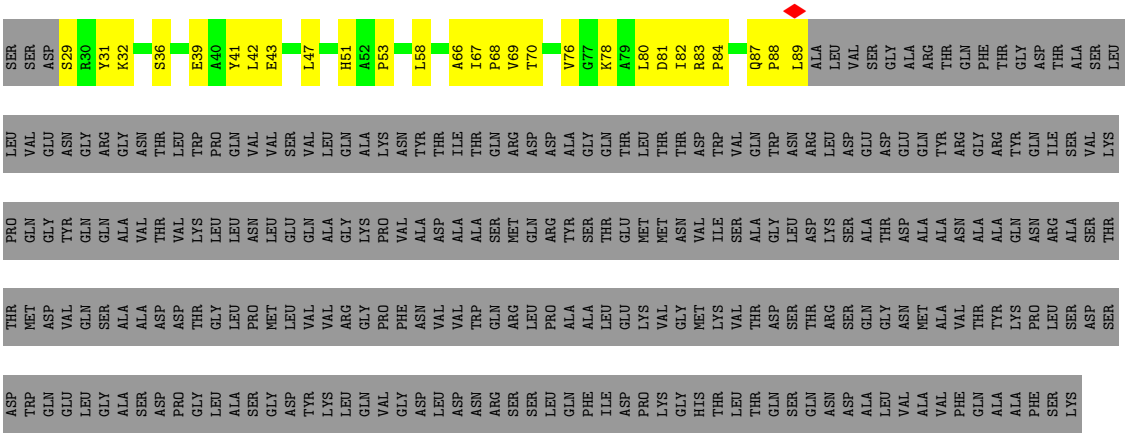
• Molecule 2: Outer membrane protein assembly factor BamB

Chain B:



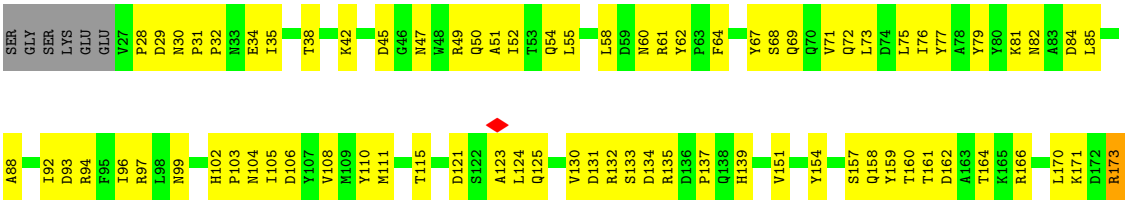
• Molecule 3: Outer membrane protein assembly factor BamC

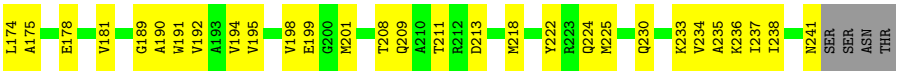
Chain C:



• Molecule 4: Outer membrane protein assembly factor BamD

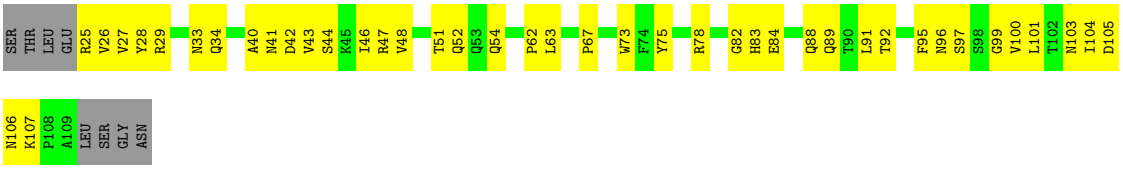
Chain D:





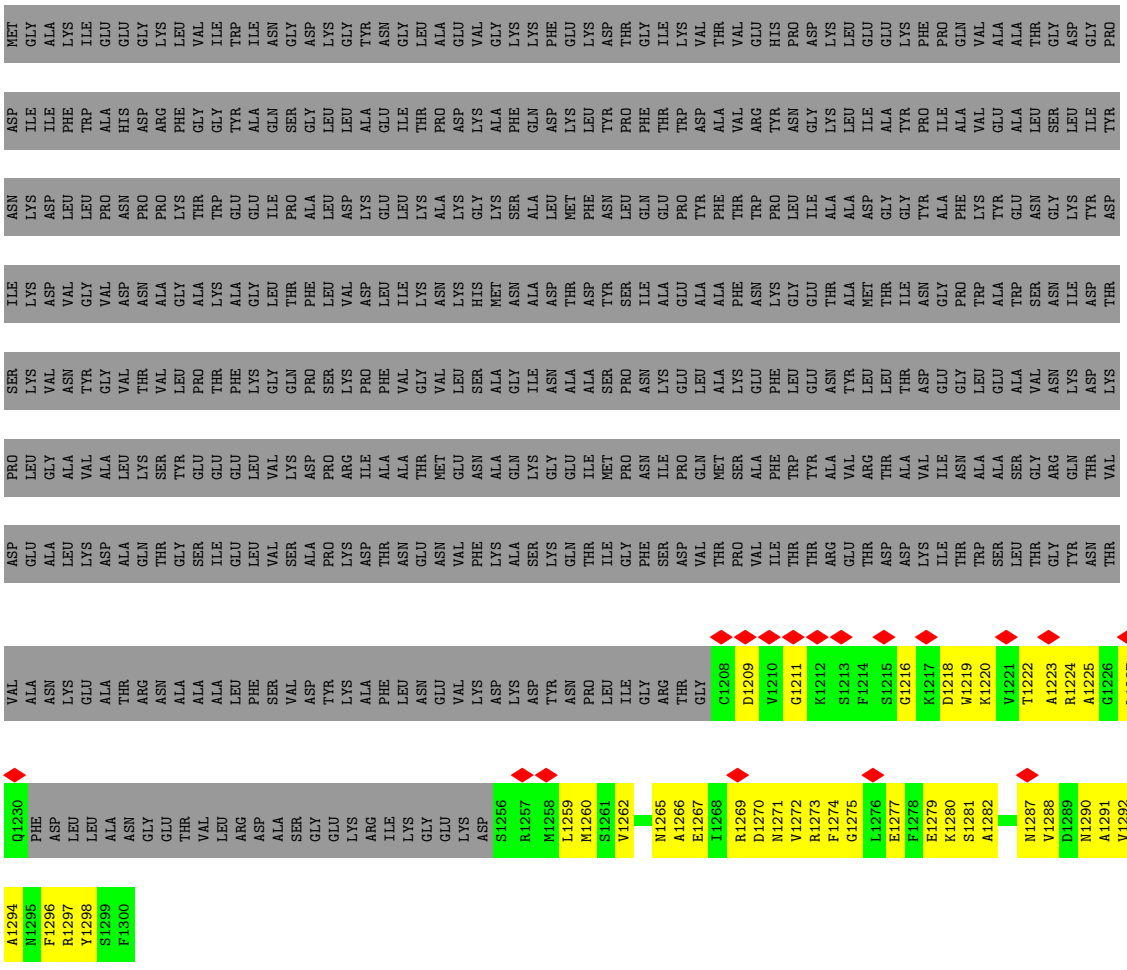
• Molecule 5: Outer membrane protein assembly factor BamE

Chain E:



• Molecule 6: Maltose/maltodextrin-binding periplasmic protein,Autotransporter protein EspP translocator

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92335	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	53.47	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.669	Depositor
Minimum map value	-0.876	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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	0.41	0/6188	0.51	1/8388 (0.0%)
2	B	0.39	0/2826	0.57	0/3853
3	C	0.37	0/447	0.53	0/612
4	D	0.48	0/1780	0.49	0/2419
5	E	0.43	0/683	0.53	0/932
6	F	0.32	0/489	0.50	0/659
All	All	0.41	0/12413	0.52	1/16863 (0.0%)

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	A	0	2
2	B	0	3
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	324	SER	C-N-CA	-6.33	105.88	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	LEU	Peptide
1	A	498	ASP	Peptide
2	B	227	ILE	Peptide
2	B	285	SER	Peptide

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Mol	Chain	Res	Type	Group
2	B	36	PRO	Peptide

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	6052	0	5789	287	0
2	B	2776	0	2713	166	0
3	C	437	0	434	26	0
4	D	1740	0	1683	95	0
5	E	668	0	649	36	0
6	F	483	0	419	33	0
All	All	12156	0	11687	608	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 26.

All (608) 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:A:195:SER:HG	1:A:196:HIS:N	1.63	0.96
4:D:38:THR:HB	4:D:54:GLN:HE22	1.35	0.89
4:D:85:LEU:HD12	4:D:115:THR:HG23	1.63	0.81
2:B:219:VAL:HG22	2:B:226:MET:HB3	1.64	0.79
1:A:195:SER:O	1:A:196:HIS:N	2.17	0.78
1:A:79:ARG:NH2	1:A:81:GLY:O	2.17	0.77
1:A:98:THR:HB	1:A:166:LYS:HA	1.67	0.77
2:B:243:ARG:HG3	2:B:244:LEU:HD12	1.67	0.76
1:A:500:ASP:HA	1:A:540:GLN:HE22	1.51	0.75
4:D:42:LYS:HG2	4:D:51:ALA:HB2	1.68	0.75
5:E:44:SER:O	5:E:47:ARG:NH2	2.20	0.75
4:D:106:ASP:HB3	4:D:154:TYR:HD2	1.51	0.74
1:A:499:ALA:O	1:A:540:GLN:NE2	2.20	0.74
2:B:119:GLY:O	2:B:121:HIS:N	2.21	0.74
2:B:326:LEU:HB2	2:B:342:SER:HB2	1.70	0.73
6:F:1279:GLU:HB2	6:F:1291:ALA:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:SER:OG	2:B:264:ASN:OD1	2.06	0.73
4:D:35:ILE:O	4:D:54:GLN:NE2	2.22	0.73
1:A:765:ASN:O	1:A:767:ARG:NH1	2.22	0.72
1:A:26:VAL:HG23	1:A:48:VAL:HG13	1.71	0.71
3:C:67:ILE:HG13	3:C:68:PRO:HD2	1.72	0.71
1:A:669:GLY:O	1:A:671:LYS:NZ	2.23	0.71
1:A:154:VAL:HB	1:A:166:LYS:HB3	1.71	0.71
1:A:201:ASP:O	1:A:212:ARG:NH1	2.21	0.71
2:B:235:ALA:HA	2:B:264:ASN:HD22	1.56	0.70
6:F:1282:ALA:HA	6:F:1287:ASN:HA	1.73	0.70
1:A:36:ARG:HG3	1:A:37:VAL:HG13	1.73	0.70
4:D:77:TYR:HE1	4:D:81:LYS:HZ2	1.39	0.70
5:E:26:VAL:HG11	5:E:83:HIS:HA	1.74	0.70
4:D:93:ASP:OD2	4:D:97:ARG:NH1	2.24	0.69
1:A:102:ASN:ND2	1:A:105:VAL:O	2.25	0.69
1:A:368:GLU:OE2	1:A:388:ARG:NE	2.23	0.69
1:A:645:GLU:OE1	1:A:748:ASN:ND2	2.26	0.69
1:A:762:ASP:OD2	1:A:765:ASN:ND2	2.25	0.69
2:B:272:LEU:HG	2:B:273:ARG:HG2	1.75	0.68
1:A:746:ASP:OD1	1:A:747:THR:N	2.26	0.68
3:C:53:PRO:HD2	4:D:237:ILE:HD13	1.75	0.68
2:B:76:ASP:OD2	2:B:80:LEU:N	2.25	0.68
2:B:219:VAL:HA	2:B:226:MET:HA	1.74	0.68
5:E:25:ARG:O	5:E:29:ARG:NH2	2.26	0.68
1:A:30:HIS:ND1	1:A:84:LEU:O	2.26	0.68
2:B:271:ASP:OD2	2:B:274:SER:N	2.27	0.68
1:A:93:THR:OG1	1:A:94:ILE:N	2.27	0.68
2:B:288:ASP:OD1	2:B:289:PHE:N	2.21	0.68
1:A:264:ASP:OD1	1:A:265:GLN:N	2.26	0.67
1:A:700:CYS:SG	1:A:701:LYS:N	2.62	0.67
2:B:341:ASP:OD1	2:B:345:TYR:N	2.28	0.67
2:B:261:LEU:HD13	2:B:286:VAL:HG21	1.77	0.67
4:D:131:ASP:OD1	4:D:132:ARG:N	2.26	0.67
6:F:1227:LEU:HG	6:F:1228:GLY:H	1.59	0.67
1:A:115:GLU:O	1:A:120:ARG:NH2	2.27	0.67
4:D:34:GLU:OE2	4:D:34:GLU:N	2.27	0.67
5:E:96:ASN:N	5:E:100:VAL:O	2.28	0.67
1:A:594:ASN:OD1	1:A:595:LEU:N	2.28	0.66
1:A:244:GLN:NE2	2:B:167:SER:O	2.28	0.66
2:B:143:TRP:NE1	2:B:176:GLU:O	2.29	0.66
1:A:614:ASP:OD1	1:A:615:THR:N	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:SER:HB2	1:A:803:GLN:HB2	1.75	0.66
2:B:300:ASP:HB3	2:B:304:ARG:HB3	1.78	0.66
1:A:719:ILE:HD12	1:A:734:ARG:HD3	1.77	0.65
6:F:1260:MET:O	6:F:1280:LYS:N	2.29	0.65
2:B:67:LEU:HD23	2:B:374:ALA:HB3	1.77	0.65
1:A:134:GLU:HG2	1:A:151:VAL:HG23	1.79	0.65
1:A:501:LEU:O	1:A:674:TYR:OH	2.14	0.65
1:A:577:THR:HG22	1:A:578:TYR:H	1.61	0.65
4:D:96:ILE:HD13	4:D:105:ILE:HD11	1.79	0.64
1:A:117:SER:OG	1:A:132:ASP:OD2	2.15	0.64
1:A:46:MET:O	1:A:49:ARG:NH1	2.31	0.64
2:B:63:LEU:HD23	2:B:114:GLY:HA2	1.79	0.64
1:A:26:VAL:HG22	1:A:54:VAL:HG21	1.79	0.64
1:A:115:GLU:HG2	1:A:120:ARG:HE	1.60	0.64
1:A:431:GLY:O	1:A:439:SER:N	2.24	0.64
3:C:41:TYR:OH	4:D:162:ASP:OD1	2.14	0.64
6:F:1218:ASP:HB3	6:F:1269:ARG:HD2	1.80	0.64
5:E:89:GLN:HE21	5:E:106:ASN:HD21	1.46	0.64
2:B:61:SER:OG	2:B:62:ASN:N	2.31	0.64
2:B:341:ASP:O	2:B:367:PHE:HB2	1.98	0.64
1:A:533:HIS:ND1	1:A:568:ASP:OD1	2.31	0.63
2:B:170:GLN:NE2	2:B:186:ASN:OD1	2.27	0.63
4:D:133:SER:O	4:D:173:ARG:NH1	2.32	0.63
1:A:158:LEU:N	1:A:162:ARG:O	2.25	0.63
1:A:162:ARG:HH22	4:D:61:ARG:HG2	1.63	0.63
1:A:278:ALA:O	1:A:280:HIS:ND1	2.32	0.63
2:B:175:ASN:ND2	2:B:178:ASP:OD2	2.31	0.63
2:B:206:ALA:HA	2:B:220:LEU:HA	1.80	0.63
2:B:363:ASP:OD1	2:B:364:SER:N	2.32	0.62
1:A:162:ARG:NH1	4:D:60:ASN:O	2.32	0.62
1:A:283:GLU:N	1:A:283:GLU:OE1	2.31	0.62
2:B:48:TRP:H	2:B:389:SER:HG	1.46	0.62
5:E:96:ASN:OD1	5:E:97:SER:N	2.33	0.62
2:B:200:PRO:HA	2:B:209:VAL:HG22	1.79	0.62
1:A:244:GLN:NE2	2:B:168:ASN:OD1	2.31	0.62
2:B:186:ASN:ND2	2:B:187:LEU:O	2.33	0.62
1:A:583:ARG:NH2	1:A:586:PHE:O	2.25	0.62
6:F:1265:ASN:HA	6:F:1275:GLY:HA3	1.82	0.62
2:B:241:ILE:HG22	2:B:242:ASP:H	1.65	0.62
2:B:48:TRP:N	2:B:389:SER:OG	2.32	0.61
6:F:1227:LEU:HA	6:F:1259:LEU:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLN:HG3	1:A:218:LYS:HE2	1.82	0.61
2:B:220:LEU:HB3	2:B:223:GLN:HE22	1.64	0.61
1:A:140:PHE:O	1:A:143:SER:OG	2.15	0.61
1:A:177:ILE:HA	1:A:254:ILE:HG13	1.82	0.61
2:B:55:GLY:O	2:B:77:ARG:N	2.33	0.61
1:A:449:TRP:CE2	1:A:450:LEU:HD13	2.36	0.61
2:B:319:GLN:NE2	2:B:321:ASP:OD1	2.33	0.61
1:A:536:LEU:N	1:A:565:PHE:O	2.33	0.61
2:B:178:ASP:OD1	2:B:180:ALA:N	2.34	0.61
2:B:319:GLN:HE21	2:B:321:ASP:N	1.98	0.61
2:B:166:THR:HG23	2:B:168:ASN:H	1.65	0.60
2:B:207:ALA:N	2:B:219:VAL:O	2.20	0.60
1:A:582:ASP:OD1	1:A:583:ARG:N	2.33	0.60
5:E:106:ASN:OD1	5:E:107:LYS:N	2.35	0.60
1:A:71:ASN:O	1:A:91:ARG:NH1	2.34	0.60
2:B:300:ASP:O	2:B:302:ASN:N	2.34	0.60
1:A:582:ASP:OD2	1:A:589:ASP:N	2.35	0.60
6:F:1209:ASP:O	6:F:1224:ARG:NH2	2.35	0.60
4:D:49:ARG:HA	4:D:52:ILE:HD12	1.83	0.59
2:B:381:GLN:HG3	2:B:386:THR:HB	1.83	0.59
1:A:462:LYS:HG3	1:A:467:THR:HG22	1.84	0.59
2:B:110:LEU:O	2:B:126:SER:OG	2.15	0.59
6:F:1222:THR:OG1	6:F:1265:ASN:O	2.17	0.59
1:A:401:ASP:OD1	1:A:403:GLN:N	2.36	0.59
1:A:509:TYR:CE1	1:A:533:HIS:HD2	2.20	0.59
2:B:163:LEU:HD12	2:B:171:LEU:HD21	1.83	0.59
2:B:223:GLN:HE21	2:B:225:GLN:HB3	1.68	0.58
1:A:244:GLN:NE2	2:B:167:SER:OG	2.32	0.58
1:A:247:LEU:HD13	1:A:254:ILE:HG22	1.85	0.58
2:B:166:THR:OG1	2:B:167:SER:N	2.34	0.58
5:E:41:ASN:O	5:E:44:SER:OG	2.15	0.58
2:B:281:ARG:NH1	2:B:314:VAL:O	2.27	0.58
1:A:237:ARG:HG3	1:A:266:TYR:HE2	1.69	0.58
6:F:1225:ALA:HA	6:F:1262:VAL:HG23	1.85	0.58
1:A:463:ASN:OD1	1:A:464:ASP:N	2.33	0.58
1:A:659:THR:HG23	1:A:660:VAL:HG23	1.84	0.58
2:B:239:THR:H	2:B:243:ARG:HH12	1.50	0.58
4:D:79:TYR:HB3	4:D:88:ALA:HB2	1.85	0.58
1:A:652:PHE:N	1:A:708:GLY:O	2.36	0.58
2:B:238:SER:H	2:B:243:ARG:HH22	1.52	0.58
4:D:32:PRO:O	4:D:35:ILE:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:HA	1:A:171:GLU:HA	1.85	0.58
1:A:743:THR:HB	1:A:766:ILE:HG12	1.84	0.58
1:A:768:MET:SD	1:A:768:MET:N	2.77	0.57
1:A:368:GLU:OE2	1:A:388:ARG:HB3	2.04	0.57
1:A:396:GLU:HG2	1:A:397:THR:HG23	1.85	0.57
2:B:300:ASP:C	2:B:302:ASN:H	2.07	0.57
5:E:27:VAL:HG23	5:E:28:TYR:H	1.68	0.57
1:A:498:ASP:OD1	1:A:503:ASP:HB3	2.04	0.57
2:B:363:ASP:OD2	2:B:388:TYR:OH	2.15	0.57
4:D:82:ASN:ND2	4:D:84:ASP:OD2	2.38	0.57
1:A:321:ARG:HB2	1:A:323:GLN:HE22	1.68	0.57
1:A:630:LEU:HB3	1:A:717:GLU:HB2	1.86	0.57
4:D:84:ASP:OD1	4:D:84:ASP:N	2.36	0.57
1:A:342:ASP:OD1	1:A:343:ALA:N	2.38	0.57
1:A:520:ASN:O	1:A:521:GLU:HG3	2.04	0.57
2:B:248:ASP:N	2:B:287:ASN:O	2.32	0.57
6:F:1216:GLY:HA3	6:F:1219:TRP:CE3	2.39	0.57
2:B:243:ARG:HA	2:B:264:ASN:ND2	2.19	0.57
1:A:768:MET:HB2	1:A:791:PHE:CZ	2.40	0.57
2:B:63:LEU:HA	2:B:114:GLY:HA2	1.86	0.57
1:A:192:GLU:N	1:A:192:GLU:OE1	2.35	0.57
2:B:309:THR:HG23	2:B:314:VAL:HG11	1.86	0.57
3:C:42:LEU:HD13	3:C:76:VAL:HG21	1.85	0.57
1:A:25:VAL:N	1:A:54:VAL:HG22	2.19	0.56
2:B:322:LEU:HD11	2:B:347:HIS:CE1	2.40	0.56
1:A:177:ILE:HG12	1:A:254:ILE:HD11	1.87	0.56
1:A:399:ASP:OD1	1:A:400:THR:N	2.38	0.56
1:A:302:THR:O	1:A:305:GLU:HG2	2.05	0.56
2:B:311:ASP:OD1	2:B:312:GLY:N	2.38	0.56
1:A:29:ILE:HD11	1:A:48:VAL:HG21	1.86	0.56
1:A:246:SER:OG	1:A:247:LEU:N	2.39	0.56
5:E:92:THR:OG1	5:E:105:ASP:OD1	2.22	0.56
6:F:1277:GLU:HB3	6:F:1293:ASN:HB2	1.86	0.56
2:B:138:ASP:OD1	2:B:139:GLY:N	2.39	0.56
1:A:28:ASP:OD2	1:A:30:HIS:NE2	2.40	0.55
1:A:717:GLU:HG2	1:A:738:PHE:HB3	1.88	0.55
1:A:72:PHE:HA	1:A:91:ARG:HH12	1.69	0.55
6:F:1220:LYS:HB3	6:F:1267:GLU:HB3	1.87	0.55
4:D:162:ASP:OD2	4:D:166:ARG:NH1	2.39	0.55
6:F:1266:ALA:N	6:F:1274:PHE:O	2.34	0.55
1:A:354:PHE:CZ	1:A:365:LEU:HB3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:LEU:H	2:B:80:LEU:HD23	1.72	0.55
2:B:363:ASP:OD1	2:B:365:SER:N	2.33	0.55
4:D:158:GLN:OE1	4:D:158:GLN:N	2.39	0.55
1:A:791:PHE:CE2	1:A:792:LYS:HB2	2.42	0.54
1:A:206:TRP:NE1	1:A:207:ASN:OD1	2.40	0.54
4:D:235:ALA:HA	4:D:238:ILE:HG22	1.88	0.54
3:C:29:SER:O	3:C:32:LYS:NZ	2.40	0.54
4:D:106:ASP:N	4:D:106:ASP:OD1	2.39	0.54
1:A:353:ARG:HB2	1:A:415:VAL:HG12	1.90	0.54
4:D:68:SER:O	4:D:72:GLN:NE2	2.31	0.54
1:A:364:VAL:HG22	1:A:367:ARG:HH22	1.73	0.54
5:E:52:GLN:HG2	5:E:95:PHE:CE2	2.42	0.54
1:A:541:PRO:HA	1:A:546:TRP:HE1	1.73	0.54
1:A:607:GLU:HB3	1:A:641:LEU:HD12	1.88	0.54
1:A:156:THR:O	1:A:163:VAL:HA	2.08	0.54
2:B:39:GLU:OE1	2:B:41:GLN:N	2.41	0.54
1:A:29:ILE:HG23	1:A:30:HIS:HA	1.89	0.53
5:E:103:ASN:OD1	5:E:104:ILE:N	2.41	0.53
3:C:66:ALA:H	4:D:171:LYS:HZ1	1.55	0.53
1:A:305:GLU:O	1:A:309:LYS:HG3	2.08	0.53
1:A:545:MET:O	1:A:549:LEU:HG	2.09	0.53
2:B:100:LYS:HE3	2:B:104:PHE:H	1.74	0.53
3:C:47:LEU:HD21	4:D:171:LYS:HD2	1.89	0.53
1:A:237:ARG:HG3	1:A:266:TYR:CE2	2.43	0.53
4:D:230:GLN:HA	4:D:233:LYS:HE2	1.91	0.53
1:A:103:LYS:NZ	2:B:28:ASP:OD2	2.33	0.53
2:B:330:PRO:HB2	2:B:337:LEU:HD12	1.90	0.53
4:D:42:LYS:HE2	4:D:47:ASN:HD21	1.74	0.53
1:A:330:ASP:N	1:A:330:ASP:OD1	2.42	0.53
2:B:85:ASN:OD1	2:B:89:GLY:N	2.42	0.53
1:A:255:TYR:OH	2:B:60:TYR:N	2.42	0.53
2:B:113:GLY:N	2:B:125:GLY:O	2.42	0.53
4:D:42:LYS:HD3	4:D:50:GLN:HB2	1.91	0.53
4:D:73:LEU:O	4:D:76:ILE:HG13	2.09	0.53
1:A:479:THR:HG22	1:A:480:VAL:H	1.75	0.52
2:B:223:GLN:N	2:B:223:GLN:OE1	2.40	0.52
1:A:171:GLU:OE1	1:A:171:GLU:N	2.42	0.52
1:A:43:LEU:HD22	1:A:49:ARG:HH22	1.73	0.52
1:A:405:VAL:HG12	1:A:411:GLN:O	2.10	0.52
2:B:178:ASP:OD1	2:B:179:GLY:N	2.43	0.52
5:E:62:PRO:HG3	5:E:73:TRP:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ASN:C	1:A:522:TYR:H	2.13	0.52
2:B:111:LEU:HD23	2:B:124:ILE:HG21	1.90	0.52
2:B:161:LEU:HD21	2:B:182:LYS:HD3	1.92	0.52
4:D:175:ALA:O	4:D:178:GLU:HG3	2.10	0.52
6:F:1271:ASN:HD22	6:F:1298:TYR:HE1	1.58	0.52
5:E:51:THR:H	5:E:54:GLN:NE2	2.08	0.52
1:A:704:ASP:OD1	1:A:704:ASP:N	2.40	0.52
6:F:1260:MET:HB3	6:F:1280:LYS:HB3	1.92	0.52
1:A:639:ASP:OD1	1:A:640:GLY:N	2.43	0.52
2:B:271:ASP:HB3	2:B:275:GLY:H	1.76	0.52
2:B:351:VAL:HG13	2:B:352:GLU:H	1.75	0.52
2:B:85:ASN:ND2	2:B:88:ASP:HB2	2.25	0.51
1:A:105:VAL:HG21	1:A:141:TYR:HE1	1.76	0.51
1:A:446:GLN:OE1	1:A:448:ASN:N	2.43	0.51
2:B:237:GLY:H	2:B:243:ARG:CZ	2.24	0.51
5:E:33:ASN:OD1	5:E:33:ASN:N	2.44	0.51
1:A:633:THR:HG1	1:A:635:TRP:HE1	1.58	0.51
2:B:247:VAL:HG12	2:B:249:THR:HA	1.92	0.51
4:D:110:TYR:CD2	4:D:159:TYR:HB3	2.45	0.51
1:A:538:ASN:N	1:A:563:ASN:O	2.37	0.51
2:B:231:ARG:HH12	2:B:234:GLN:HG3	1.76	0.51
1:A:148:SER:O	1:A:172:GLY:N	2.37	0.51
1:A:242:SER:OG	1:A:243:THR:N	2.44	0.51
2:B:39:GLU:OE1	2:B:40:ASN:N	2.44	0.51
3:C:67:ILE:CG1	3:C:68:PRO:HD2	2.40	0.51
3:C:87:GLN:HB2	3:C:89:LEU:N	2.26	0.51
1:A:286:GLN:HA	1:A:289:LYS:HD2	1.93	0.51
1:A:302:THR:HA	1:A:305:GLU:OE2	2.10	0.51
2:B:158:SER:OG	2:B:221:MET:SD	2.58	0.51
1:A:281:SER:OG	1:A:285:GLU:OE2	2.20	0.51
1:A:30:HIS:CE1	1:A:84:LEU:H	2.29	0.51
1:A:372:MET:SD	1:A:372:MET:N	2.84	0.51
1:A:401:ASP:OD1	1:A:402:THR:N	2.43	0.51
1:A:430:ILE:H	6:F:1294:ALA:HB3	1.75	0.51
1:A:626:LYS:HG2	1:A:721:PRO:HG3	1.92	0.51
2:B:234:GLN:HG2	2:B:241:ILE:HG13	1.92	0.51
6:F:1267:GLU:HG3	6:F:1273:ARG:HG2	1.93	0.51
1:A:457:GLY:N	1:A:472:SER:OG	2.44	0.50
2:B:213:ASN:HD21	2:B:215:ARG:NE	2.09	0.50
2:B:269:ALA:HB3	2:B:278:MET:HB2	1.92	0.50
2:B:309:THR:OG1	2:B:311:ASP:OD1	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASN:OD1	1:A:300:LYS:N	2.21	0.50
2:B:92:ILE:HG22	2:B:93:TRP:HD1	1.76	0.50
2:B:193:SER:OG	2:B:194:LEU:O	2.28	0.50
1:A:541:PRO:HA	1:A:546:TRP:NE1	2.27	0.50
2:B:44:PRO:HB2	2:B:360:GLN:OE1	2.12	0.50
3:C:42:LEU:O	3:C:43:GLU:HG3	2.10	0.50
2:B:258:VAL:N	2:B:270:LEU:O	2.45	0.50
1:A:465:TYR:HA	1:A:495:GLN:HB3	1.94	0.50
2:B:36:PRO:O	2:B:359:GLN:NE2	2.42	0.50
2:B:246:ASP:O	2:B:287:ASN:HA	2.12	0.50
1:A:702:SER:OG	1:A:703:ASP:N	2.44	0.50
1:A:736:SER:OG	1:A:737:PHE:N	2.45	0.50
2:B:207:ALA:O	2:B:219:VAL:N	2.39	0.50
4:D:75:LEU:HD11	4:D:79:TYR:CZ	2.47	0.50
6:F:1281:SER:HB3	6:F:1288:VAL:HB	1.93	0.50
1:A:364:VAL:HG22	1:A:367:ARG:NH2	2.26	0.50
1:A:512:ASP:HA	1:A:530:GLY:HA2	1.94	0.50
2:B:279:TRP:CE2	2:B:312:GLY:HA2	2.47	0.50
3:C:39:GLU:N	3:C:39:GLU:OE1	2.45	0.50
3:C:51:HIS:NE2	4:D:241:ASN:OD1	2.45	0.50
1:A:249:PRO:HG3	2:B:246:ASP:HB3	1.93	0.49
1:A:360:SER:OG	1:A:420:GLU:OE2	2.30	0.49
4:D:131:ASP:OD1	4:D:133:SER:N	2.45	0.49
5:E:48:VAL:HA	5:E:101:LEU:HD23	1.94	0.49
1:A:354:PHE:HE2	1:A:366:ARG:HD3	1.76	0.49
3:C:29:SER:OG	3:C:32:LYS:NZ	2.30	0.49
5:E:82:GLY:O	5:E:84:GLU:HG2	2.12	0.49
1:A:489:LEU:HG	1:A:511:THR:HB	1.93	0.49
1:A:735:THR:HB	1:A:774:LEU:HD23	1.94	0.49
1:A:94:ILE:HD12	1:A:163:VAL:HG23	1.94	0.49
1:A:189:THR:OG1	1:A:192:GLU:OE1	2.29	0.49
1:A:551:SER:OG	1:A:644:LYS:HA	2.11	0.49
3:C:84:PRO:HG3	4:D:77:TYR:CD2	2.48	0.49
2:B:213:ASN:OD1	2:B:214:GLY:N	2.45	0.49
2:B:215:ARG:NH1	2:B:229:GLN:OE1	2.46	0.49
2:B:228:TRP:CH2	2:B:275:GLY:HA3	2.48	0.49
2:B:291:VAL:HG13	2:B:296:ILE:HG13	1.95	0.49
3:C:31:TYR:HE2	4:D:85:LEU:HD23	1.78	0.49
2:B:254:VAL:HB	2:B:259:PHE:HE2	1.78	0.49
4:D:47:ASN:OD1	4:D:47:ASN:N	2.45	0.49
6:F:1281:SER:O	6:F:1288:VAL:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:178:GLU:CD	4:D:201:MET:HG3	2.33	0.49
1:A:134:GLU:O	1:A:138:GLU:HG2	2.13	0.49
2:B:167:SER:O	2:B:167:SER:OG	2.31	0.49
1:A:546:TRP:HB3	1:A:550:TYR:CZ	2.48	0.48
1:A:435:GLU:HB2	6:F:1288:VAL:HG13	1.94	0.48
5:E:42:ASP:N	5:E:42:ASP:OD1	2.43	0.48
1:A:431:GLY:HA3	6:F:1292:VAL:O	2.13	0.48
2:B:128:LYS:O	2:B:130:GLN:HG2	2.13	0.48
4:D:198:VAL:HG11	4:D:218:MET:HB2	1.94	0.48
1:A:30:HIS:N	1:A:84:LEU:O	2.47	0.48
1:A:87:GLN:HG2	1:A:88:VAL:H	1.78	0.48
1:A:133:ILE:O	1:A:137:LEU:HG	2.13	0.48
1:A:246:SER:HB3	1:A:255:TYR:HB2	1.95	0.48
4:D:50:GLN:N	4:D:50:GLN:OE1	2.46	0.48
1:A:351:LYS:O	1:A:413:ASP:HB2	2.14	0.48
2:B:165:HIS:CG	2:B:166:THR:N	2.81	0.48
3:C:87:GLN:HB2	3:C:88:PRO:C	2.33	0.48
1:A:347:PHE:HA	1:A:410:ASP:O	2.13	0.48
1:A:600:THR:HG21	1:A:606:ASN:O	2.14	0.48
1:A:280:HIS:HA	1:A:283:GLU:OE2	2.14	0.48
1:A:432:TYR:HB2	1:A:438:VAL:HA	1.96	0.48
1:A:578:TYR:HE1	1:A:580:LYS:HB2	1.78	0.48
1:A:91:ARG:N	1:A:92:PRO:HD2	2.29	0.48
1:A:782:PRO:O	1:A:807:GLY:N	2.45	0.48
2:B:292:ASP:O	2:B:294:ASN:N	2.44	0.48
4:D:137:PRO:O	4:D:139:HIS:N	2.46	0.48
5:E:42:ASP:OD1	5:E:43:VAL:N	2.45	0.48
5:E:27:VAL:HG23	5:E:28:TYR:N	2.28	0.47
1:A:488:ARG:HB3	1:A:512:ASP:OD1	2.14	0.47
1:A:670:PRO:HB3	1:A:760:TYR:CD2	2.49	0.47
1:A:793:LYS:NZ	1:A:794:TYR:O	2.35	0.47
1:A:797:ASP:N	1:A:797:ASP:OD1	2.48	0.47
5:E:40:ALA:O	5:E:43:VAL:HG22	2.14	0.47
5:E:91:LEU:HD12	5:E:105:ASP:O	2.13	0.47
1:A:542:GLN:NE2	1:A:545:MET:SD	2.88	0.47
4:D:189:GLY:O	4:D:191:TRP:N	2.47	0.47
1:A:577:THR:HG22	1:A:578:TYR:N	2.28	0.47
2:B:163:LEU:HD23	2:B:163:LEU:H	1.79	0.47
2:B:231:ARG:NH1	2:B:234:GLN:HG3	2.29	0.47
2:B:279:TRP:CD2	2:B:312:GLY:HA2	2.49	0.47
4:D:195:VAL:HG21	4:D:222:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:222:TYR:CE2	4:D:230:GLN:HB3	2.50	0.47
5:E:95:PHE:HB3	5:E:99:GLY:HA2	1.96	0.47
1:A:299:THR:O	1:A:302:THR:OG1	2.22	0.47
4:D:201:MET:SD	4:D:211:THR:HG22	2.54	0.47
1:A:207:ASN:O	1:A:209:VAL:HG23	2.15	0.47
1:A:578:TYR:CE1	1:A:580:LYS:HB2	2.49	0.47
4:D:208:THR:OG1	4:D:209:GLN:N	2.48	0.47
1:A:134:GLU:HB3	1:A:135:LYS:HE2	1.97	0.47
1:A:450:LEU:O	1:A:452:THR:OG1	2.30	0.47
3:C:67:ILE:HG21	4:D:151:VAL:HG21	1.96	0.47
5:E:78:ARG:NH1	5:E:88:GLN:OE1	2.38	0.47
1:A:662:GLY:HA3	1:A:790:PRO:HG3	1.96	0.47
1:A:710:ALA:O	1:A:744:VAL:HA	2.15	0.47
2:B:239:THR:H	2:B:243:ARG:NH1	2.13	0.47
1:A:413:ASP:OD1	1:A:413:ASP:N	2.48	0.47
4:D:123:ALA:HB3	4:D:125:GLN:HE22	1.80	0.47
1:A:94:ILE:HG13	1:A:163:VAL:O	2.15	0.46
1:A:215:GLN:O	1:A:218:LYS:N	2.47	0.46
1:A:326:PRO:HB2	1:A:328:ILE:HD11	1.97	0.46
1:A:426:PHE:HB3	6:F:1298:TYR:HB3	1.96	0.46
1:A:554:GLU:OE2	1:A:554:GLU:N	2.30	0.46
1:A:138:GLU:OE1	1:A:149:ALA:HB3	2.15	0.46
1:A:206:TRP:O	1:A:207:ASN:ND2	2.49	0.46
1:A:621:ILE:HG12	1:A:627:TRP:O	2.13	0.46
4:D:92:ILE:HG23	4:D:108:VAL:HG12	1.98	0.46
1:A:173:VAL:HG23	1:A:174:SER:H	1.81	0.46
4:D:157:SER:O	4:D:160:THR:HG23	2.15	0.46
1:A:43:LEU:HD22	1:A:49:ARG:NH2	2.31	0.46
2:B:328:THR:HG22	2:B:340:GLY:H	1.80	0.46
4:D:42:LYS:HA	4:D:45:ASP:OD2	2.15	0.46
2:B:303:ASP:OD2	2:B:324:HIS:N	2.49	0.46
1:A:165:LEU:HD12	1:A:165:LEU:HA	1.73	0.46
1:A:188:PHE:HD2	1:A:193:LEU:HD21	1.79	0.46
2:B:223:GLN:NE2	2:B:225:GLN:H	2.14	0.46
6:F:1281:SER:OG	6:F:1282:ALA:N	2.49	0.46
1:A:93:THR:HG1	1:A:94:ILE:H	1.61	0.46
2:B:228:TRP:CZ2	2:B:275:GLY:HA3	2.50	0.46
4:D:209:GLN:HG3	4:D:213:ASP:OD2	2.15	0.46
1:A:36:ARG:HB2	4:D:64:PHE:CZ	2.50	0.46
2:B:300:ASP:C	2:B:302:ASN:N	2.69	0.46
2:B:386:THR:OG1	2:B:387:VAL:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:1272:VAL:HA	6:F:1297:ARG:O	2.16	0.46
1:A:615:THR:HB	1:A:633:THR:HG23	1.98	0.46
1:A:719:ILE:HD12	1:A:734:ARG:HH21	1.81	0.46
5:E:62:PRO:HG3	5:E:73:TRP:CE3	2.50	0.46
5:E:96:ASN:HB3	5:E:100:VAL:H	1.81	0.46
1:A:431:GLY:HA2	6:F:1292:VAL:HG23	1.97	0.45
1:A:638:GLY:O	1:A:709:ASN:ND2	2.45	0.45
2:B:247:VAL:HG22	2:B:286:VAL:HB	1.98	0.45
4:D:178:GLU:HA	4:D:181:VAL:HG12	1.99	0.45
1:A:266:TYR:HE1	1:A:330:ASP:HA	1.81	0.45
4:D:102:HIS:CD2	4:D:104:ASN:H	2.34	0.45
1:A:247:LEU:HD12	1:A:248:THR:H	1.81	0.45
2:B:34:PRO:O	2:B:35:LEU:HD22	2.16	0.45
4:D:55:LEU:HD11	4:D:71:VAL:HG13	1.98	0.45
4:D:192:VAL:HB	5:E:34:GLN:HE21	1.82	0.45
1:A:364:VAL:HG12	1:A:365:LEU:HD12	1.97	0.45
1:A:370:ARG:HG3	1:A:384:GLN:NE2	2.31	0.45
2:B:213:ASN:OD1	2:B:215:ARG:N	2.49	0.45
1:A:479:THR:HG22	1:A:480:VAL:N	2.32	0.45
1:A:802:PHE:HE1	1:A:804:PHE:HB3	1.80	0.45
5:E:51:THR:HG22	5:E:100:VAL:HG22	1.98	0.45
1:A:570:PHE:O	1:A:601:ILE:HG22	2.17	0.45
1:A:606:ASN:OD1	1:A:647:PRO:HG3	2.16	0.45
1:A:632:ARG:HB2	1:A:715:SER:OG	2.17	0.45
2:B:236:THR:OG1	2:B:237:GLY:N	2.49	0.45
2:B:58:ASN:HA	2:B:383:LYS:NZ	2.31	0.45
4:D:236:LYS:HB2	4:D:236:LYS:HE3	1.71	0.45
1:A:48:VAL:HG12	1:A:48:VAL:O	2.16	0.45
1:A:58:ASP:O	1:A:62:THR:HG22	2.17	0.45
1:A:92:PRO:HA	1:A:93:THR:HA	1.75	0.45
1:A:440:PHE:O	1:A:461:THR:HA	2.17	0.45
2:B:262:ALA:HB1	2:B:265:GLY:H	1.82	0.45
3:C:36:SER:O	3:C:78:LYS:NZ	2.30	0.45
4:D:29:ASP:O	4:D:30:ASN:ND2	2.50	0.45
1:A:74:ASP:H	1:A:89:LYS:HG2	1.82	0.45
1:A:94:ILE:HD11	1:A:165:LEU:HB2	1.98	0.45
1:A:266:TYR:O	1:A:267:LYS:HD3	2.16	0.45
1:A:500:ASP:HA	1:A:540:GLN:NE2	2.24	0.45
2:B:85:ASN:HD21	2:B:90:LYS:HB2	1.82	0.45
1:A:365:LEU:HD11	1:A:395:PHE:CZ	2.51	0.44
1:A:430:ILE:N	6:F:1294:ALA:HB3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:GLU:HG3	2:B:243:ARG:NH1	2.32	0.44
2:B:271:ASP:OD2	2:B:273:ARG:N	2.50	0.44
4:D:31:PRO:HB2	4:D:34:GLU:CD	2.38	0.44
1:A:400:THR:OG1	1:A:401:ASP:N	2.50	0.44
1:A:576:TRP:CD1	1:A:577:THR:N	2.85	0.44
1:A:655:GLY:HA2	1:A:660:VAL:HB	1.99	0.44
1:A:661:ARG:HD2	1:A:738:PHE:CE1	2.52	0.44
2:B:268:THR:HG21	2:B:277:ILE:HG12	1.99	0.44
2:B:366:GLY:O	2:B:383:LYS:HG2	2.17	0.44
2:B:378:LEU:C	2:B:379:LEU:HD12	2.38	0.44
4:D:132:ARG:NH1	4:D:135:ARG:HG3	2.32	0.44
1:A:97:ILE:HD13	1:A:165:LEU:HD23	1.99	0.44
1:A:283:GLU:O	1:A:287:LEU:HB2	2.17	0.44
2:B:319:GLN:HE21	2:B:321:ASP:H	1.64	0.44
5:E:26:VAL:HG12	5:E:29:ARG:CZ	2.47	0.44
1:A:759:ASP:OD1	1:A:760:TYR:N	2.51	0.44
2:B:213:ASN:OD1	2:B:215:ARG:HG2	2.18	0.44
3:C:83:ARG:HA	4:D:77:TYR:HE2	1.83	0.44
1:A:111:LYS:HE3	1:A:111:LYS:HB2	1.74	0.44
1:A:248:THR:OG1	1:A:249:PRO:HD2	2.18	0.44
1:A:356:GLY:O	1:A:358:ASP:N	2.50	0.44
1:A:379:SER:OG	1:A:380:ASP:N	2.50	0.44
1:A:593:VAL:HG22	1:A:594:ASN:H	1.83	0.44
2:B:296:ILE:HD13	2:B:308:LEU:HD12	2.00	0.44
3:C:69:VAL:HG13	3:C:70:THR:N	2.32	0.44
1:A:235:TYR:HA	1:A:264:ASP:O	2.17	0.44
4:D:125:GLN:HB3	4:D:130:VAL:HG12	1.98	0.44
4:D:230:GLN:O	4:D:234:VAL:HG23	2.16	0.44
1:A:576:TRP:CD1	1:A:577:THR:O	2.71	0.44
1:A:620:PRO:HA	1:A:628:VAL:HG22	1.99	0.44
2:B:195:ARG:HG3	2:B:197:GLU:CD	2.39	0.44
4:D:67:TYR:O	4:D:71:VAL:HG23	2.18	0.44
1:A:352:ILE:HG13	1:A:414:VAL:HG23	2.00	0.44
1:A:607:GLU:HB3	1:A:641:LEU:HB2	1.98	0.44
2:B:80:LEU:HD11	2:B:82:LYS:HE3	2.00	0.44
4:D:32:PRO:HB3	4:D:62:TYR:CE2	2.53	0.44
2:B:42:PHE:CG	2:B:43:THR:N	2.86	0.43
2:B:165:HIS:NE2	2:B:166:THR:O	2.51	0.43
2:B:327:LEU:HA	2:B:327:LEU:HD23	1.72	0.43
2:B:378:LEU:HD22	2:B:390:ILE:HB	1.99	0.43
3:C:84:PRO:HB3	4:D:73:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:199:GLU:CG	5:E:67:PRO:HG3	2.48	0.43
1:A:157:PRO:HA	1:A:163:VAL:HG12	2.00	0.43
4:D:121:ASP:HA	4:D:132:ARG:HE	1.82	0.43
1:A:349:VAL:HG23	1:A:377:LEU:HB2	2.00	0.43
1:A:365:LEU:HD21	1:A:395:PHE:CE2	2.53	0.43
6:F:1227:LEU:HD12	6:F:1259:LEU:O	2.18	0.43
2:B:234:GLN:CG	2:B:241:ILE:HG13	2.49	0.43
4:D:35:ILE:HD11	4:D:58:LEU:HD13	2.00	0.43
5:E:43:VAL:O	5:E:46:ILE:HG12	2.17	0.43
5:E:52:GLN:HG2	5:E:95:PHE:CD2	2.53	0.43
1:A:77:VAL:O	1:A:78:LEU:HD23	2.18	0.43
1:A:139:ASP:HA	1:A:142:TYR:CD2	2.54	0.43
1:A:241:ASP:OD1	1:A:241:ASP:N	2.51	0.43
4:D:31:PRO:HB2	4:D:34:GLU:OE2	2.19	0.43
1:A:152:LYS:HB2	1:A:168:VAL:HG12	1.99	0.43
1:A:533:HIS:ND1	1:A:567:THR:O	2.48	0.43
2:B:76:ASP:OD2	2:B:80:LEU:HD23	2.19	0.43
4:D:105:ILE:HD12	4:D:108:VAL:HG21	2.00	0.43
5:E:75:TYR:HB2	5:E:91:LEU:HD23	2.01	0.43
2:B:182:LYS:HG2	2:B:183:TRP:CD1	2.54	0.43
4:D:174:LEU:HD23	4:D:174:LEU:HA	1.65	0.43
1:A:191:ASP:OD2	1:A:727:ASP:HB2	2.19	0.43
1:A:208:VAL:O	1:A:208:VAL:HG23	2.19	0.43
3:C:81:ASP:OD1	3:C:81:ASP:N	2.47	0.43
1:A:305:GLU:HB2	1:A:322:VAL:HG21	2.01	0.43
1:A:329:ASN:OD1	1:A:332:ASP:N	2.36	0.43
1:A:444:VAL:HG23	1:A:444:VAL:O	2.18	0.43
2:B:195:ARG:HG3	2:B:197:GLU:OE2	2.19	0.43
4:D:191:TRP:CE2	4:D:224:GLN:HG2	2.54	0.43
1:A:62:THR:HG23	1:A:77:VAL:HG21	2.01	0.43
1:A:147:TYR:O	1:A:251:LYS:HG2	2.19	0.43
1:A:743:THR:HG1	1:A:745:TRP:HZ3	1.65	0.43
2:B:345:TYR:CE2	2:B:361:LYS:HB2	2.53	0.43
2:B:371:PRO:HB3	2:B:380:ILE:HG13	2.00	0.43
4:D:137:PRO:C	4:D:139:HIS:H	2.21	0.43
6:F:1270:ASP:OD1	6:F:1270:ASP:N	2.44	0.43
1:A:523:ASN:O	1:A:524:SER:OG	2.34	0.42
4:D:82:ASN:HB3	4:D:84:ASP:OD1	2.19	0.42
1:A:91:ARG:HH21	1:A:126:ASP:HB3	1.83	0.42
2:B:100:LYS:HD3	2:B:106:LYS:HE2	2.01	0.42
2:B:303:ASP:OD2	2:B:325:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:54:GLN:OE1	5:E:54:GLN:N	2.35	0.42
2:B:87:ASP:OD1	2:B:87:ASP:N	2.40	0.42
4:D:99:ASN:OD1	4:D:99:ASN:N	2.52	0.42
1:A:595:LEU:HD23	1:A:596:THR:N	2.35	0.42
2:B:187:LEU:HD23	2:B:187:LEU:HA	1.92	0.42
2:B:243:ARG:HA	2:B:264:ASN:HD21	1.83	0.42
6:F:1227:LEU:HG	6:F:1228:GLY:N	2.31	0.42
1:A:389:LEU:HD12	1:A:389:LEU:HA	1.84	0.42
1:A:395:PHE:N	1:A:395:PHE:CD1	2.88	0.42
4:D:170:LEU:HA	4:D:170:LEU:HD23	1.70	0.42
1:A:195:SER:OG	1:A:196:HIS:N	2.40	0.42
1:A:274:SER:O	1:A:340:ASN:ND2	2.51	0.42
1:A:547:ARG:NH2	1:A:748:ASN:HB2	2.35	0.42
2:B:272:LEU:HG	2:B:273:ARG:N	2.34	0.42
1:A:432:TYR:HA	1:A:437:GLY:O	2.20	0.42
1:A:784:VAL:HG13	1:A:784:VAL:O	2.19	0.42
1:A:808:LYS:HD2	1:A:808:LYS:HA	1.92	0.42
4:D:133:SER:OG	4:D:134:ASP:N	2.52	0.42
6:F:1211:GLY:HA3	6:F:1223:ALA:O	2.19	0.42
1:A:446:GLN:OE1	1:A:447:ASP:N	2.52	0.42
2:B:67:LEU:HD12	2:B:68:ALA:N	2.35	0.42
2:B:341:ASP:CG	2:B:343:GLU:H	2.23	0.42
2:B:344:GLY:HA3	2:B:363:ASP:O	2.20	0.42
3:C:82:ILE:HD11	4:D:111:MET:SD	2.60	0.42
4:D:102:HIS:HD2	4:D:104:ASN:H	1.67	0.42
4:D:225:MET:HB3	5:E:88:GLN:HE22	1.85	0.42
1:A:74:ASP:HB2	1:A:89:LYS:HG2	2.01	0.42
1:A:350:ARG:HE	1:A:350:ARG:HB3	1.65	0.42
1:A:382:VAL:HG13	1:A:416:TYR:OH	2.20	0.42
1:A:672:ALA:HB2	1:A:706:VAL:HG11	2.00	0.42
2:B:128:LYS:HB3	2:B:128:LYS:HE2	1.74	0.42
1:A:56:ASP:HA	1:A:59:ILE:HD13	2.01	0.41
1:A:181:ASN:HD21	2:B:150:GLU:CD	2.22	0.41
1:A:735:THR:OG1	1:A:736:SER:N	2.53	0.41
4:D:28:PRO:HG2	4:D:30:ASN:OD1	2.20	0.41
4:D:161:THR:O	4:D:164:THR:OG1	2.21	0.41
1:A:72:PHE:HA	1:A:91:ARG:NH1	2.33	0.41
4:D:102:HIS:CG	4:D:103:PRO:HD2	2.55	0.41
5:E:63:LEU:HD12	5:E:63:LEU:HA	1.76	0.41
1:A:76:ARG:NH2	1:A:87:GLN:OE1	2.43	0.41
1:A:91:ARG:H	1:A:91:ARG:HD3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LYS:N	1:A:333:LYS:O	2.53	0.41
1:A:633:THR:OG1	1:A:635:TRP:NE1	2.52	0.41
2:B:345:TYR:CZ	2:B:361:LYS:HB2	2.55	0.41
2:B:380:ILE:HG12	2:B:381:GLN:N	2.35	0.41
4:D:94:ARG:NH1	4:D:94:ARG:HB2	2.34	0.41
1:A:323:GLN:N	1:A:323:GLN:OE1	2.54	0.41
1:A:637:TYR:HE1	1:A:639:ASP:HB2	1.84	0.41
2:B:346:LEU:HD21	2:B:390:ILE:HG13	2.02	0.41
1:A:327:GLU:OE1	1:A:336:LYS:HD2	2.20	0.41
1:A:364:VAL:HA	1:A:367:ARG:NH1	2.35	0.41
1:A:543:VAL:HG12	1:A:673:VAL:HB	2.02	0.41
2:B:271:ASP:H	2:B:275:GLY:HA2	1.85	0.41
2:B:303:ASP:O	2:B:305:VAL:N	2.49	0.41
3:C:80:LEU:HD23	3:C:81:ASP:N	2.35	0.41
1:A:180:ILE:HG12	1:A:256:VAL:CG1	2.51	0.41
1:A:727:ASP:HA	1:A:730:ALA:CB	2.50	0.41
2:B:99:GLU:O	2:B:107:GLU:HG2	2.19	0.41
2:B:145:THR:OG1	2:B:179:GLY:O	2.27	0.41
2:B:162:VAL:HG23	2:B:162:VAL:O	2.20	0.41
1:A:110:LEU:O	1:A:114:LEU:HD23	2.21	0.41
1:A:670:PRO:HB3	1:A:760:TYR:CG	2.56	0.41
2:B:223:GLN:NE2	2:B:225:GLN:O	2.53	0.41
2:B:309:THR:H	2:B:314:VAL:CG1	2.34	0.41
3:C:42:LEU:HD12	3:C:43:GLU:H	1.86	0.41
1:A:107:ASP:OD1	1:A:107:ASP:N	2.53	0.41
3:C:58:LEU:HD21	4:D:237:ILE:HD12	2.03	0.41
1:A:179:GLN:OE1	2:B:77:ARG:NH2	2.54	0.41
1:A:434:THR:H	6:F:1290:ASN:HB3	1.85	0.41
1:A:770:ALA:O	1:A:788:ALA:HB1	2.21	0.41
2:B:26:GLU:N	2:B:27:GLU:OE2	2.53	0.41
2:B:198:SER:HB2	2:B:249:THR:HB	2.02	0.41
2:B:240:GLU:HA	2:B:243:ARG:HD2	2.03	0.41
2:B:306:MET:HB2	2:B:306:MET:HE2	1.95	0.41
4:D:190:ALA:O	4:D:192:VAL:N	2.54	0.41
1:A:298:GLY:O	1:A:302:THR:HG23	2.21	0.41
4:D:102:HIS:CD2	4:D:104:ASN:HD22	2.39	0.41
1:A:30:HIS:HB2	1:A:85:LEU:HA	2.04	0.40
1:A:398:VAL:HG12	1:A:418:VAL:HG12	2.03	0.40
1:A:427:ASN:HA	6:F:1296:PHE:O	2.21	0.40
1:A:140:PHE:O	1:A:144:VAL:HG23	2.21	0.40
1:A:155:VAL:HB	1:A:163:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASN:OD1	1:A:162:ARG:HG3	2.21	0.40
1:A:326:PRO:HB3	1:A:335:VAL:HG21	2.03	0.40
1:A:361:LYS:HA	4:D:135:ARG:NH1	2.36	0.40
1:A:467:THR:OG1	1:A:493:ASP:HB3	2.21	0.40
1:A:514:THR:OG1	1:A:515:LEU:N	2.55	0.40
1:A:537:SER:HA	1:A:564:SER:HA	2.04	0.40
1:A:74:ASP:HB2	1:A:89:LYS:HB3	2.03	0.40
1:A:609:TYR:CD1	1:A:641:LEU:HD21	2.56	0.40
2:B:380:ILE:HG12	2:B:381:GLN:H	1.85	0.40
4:D:69:GLN:OE1	4:D:69:GLN:N	2.39	0.40
4:D:194:VAL:HG13	4:D:195:VAL:N	2.36	0.40
1:A:96:SER:OG	1:A:164:ASP:HA	2.21	0.40
1:A:108:ASP:OD1	1:A:108:ASP:N	2.52	0.40
1:A:354:PHE:CE1	1:A:365:LEU:HD23	2.56	0.40
2:B:229:GLN:HG2	2:B:230:GLN:N	2.36	0.40
2:B:248:ASP:C	2:B:250:THR:H	2.25	0.40
2:B:349:ILE:HG22	2:B:350:ASN:O	2.22	0.40
4:D:124:LEU:HD23	4:D:124:LEU:H	1.85	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	755/786 (96%)	630 (83%)	125 (17%)	0	100	100
2	B	365/372 (98%)	277 (76%)	87 (24%)	1 (0%)	41	76
3	C	59/319 (18%)	43 (73%)	16 (27%)	0	100	100
4	D	213/225 (95%)	179 (84%)	34 (16%)	0	100	100
5	E	83/93 (89%)	67 (81%)	16 (19%)	0	100	100
6	F	64/551 (12%)	53 (83%)	11 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1539/2346 (66%)	1249 (81%)	289 (19%)	1 (0%)	54 85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	301	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	653/670 (98%)	649 (99%)	4 (1%)	86 92
2	B	300/303 (99%)	299 (100%)	1 (0%)	92 95
3	C	44/257 (17%)	44 (100%)	0	100 100
4	D	180/189 (95%)	179 (99%)	1 (1%)	86 92
5	E	74/81 (91%)	74 (100%)	0	100 100
6	F	41/446 (9%)	41 (100%)	0	100 100
All	All	1292/1946 (66%)	1286 (100%)	6 (0%)	89 93

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ARG
1	A	230	TYR
1	A	251	LYS
1	A	797	ASP
2	B	295	ARG
4	D	173	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	540	GLN
2	B	319	GLN
4	D	54	GLN
4	D	104	ASN
5	E	89	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	29:ILE	C	30:HIS	N	5.03

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	195:SER	C	196:HIS	N	3.15
1	A	279:GLY	C	280:HIS	N	3.11
1	B	120:GLY	C	121:HIS	N	3.01

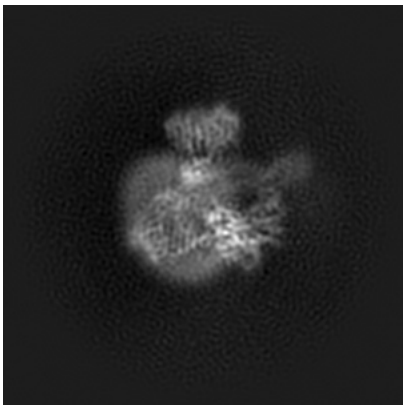
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40700. These allow visual inspection of the internal detail of the map and identification of artifacts.

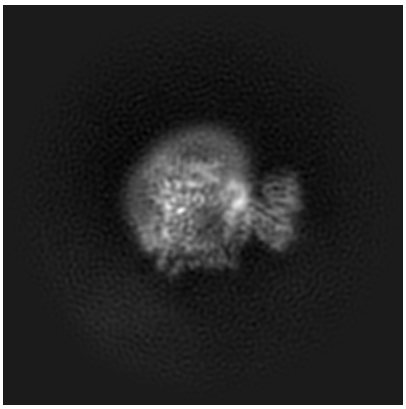
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

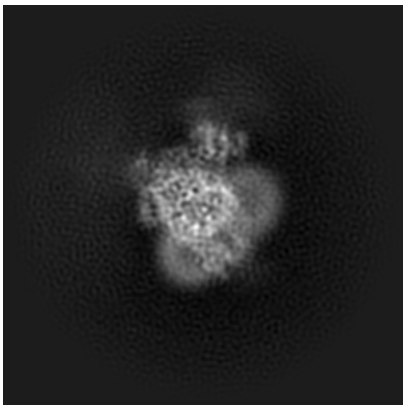
6.1.1 Primary map



X

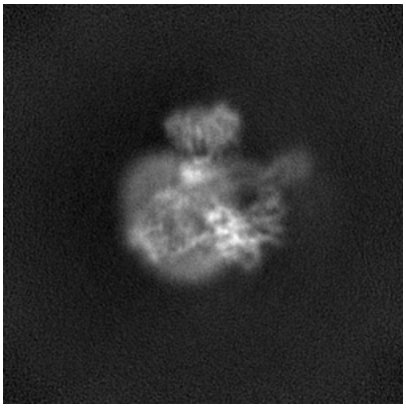


Y

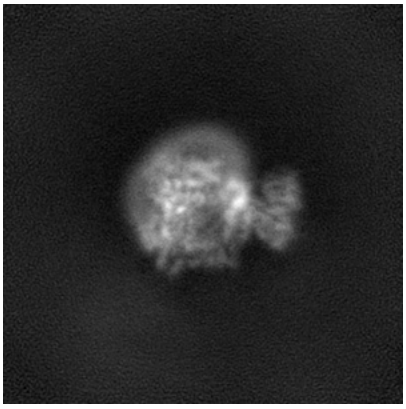


Z

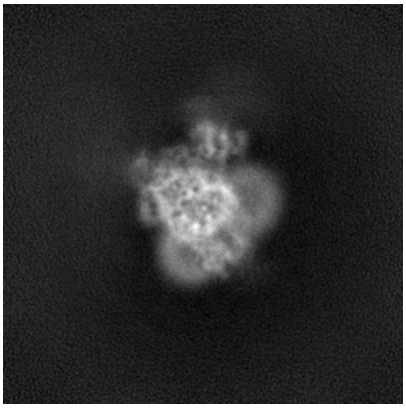
6.1.2 Raw map



X



Y

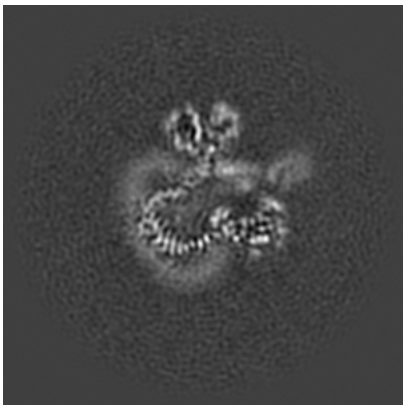


Z

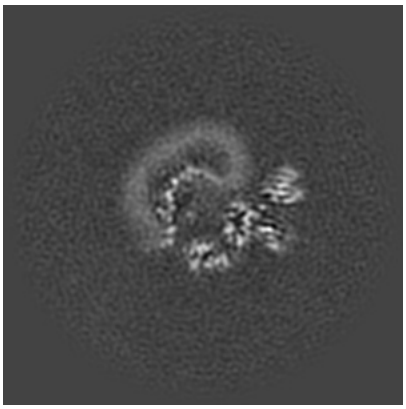
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

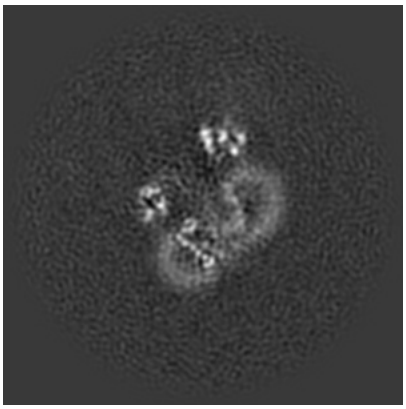
6.2.1 Primary map



X Index: 128

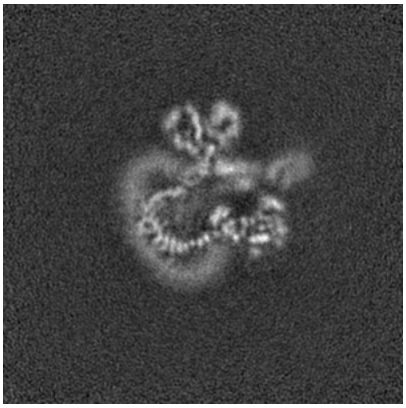


Y Index: 128

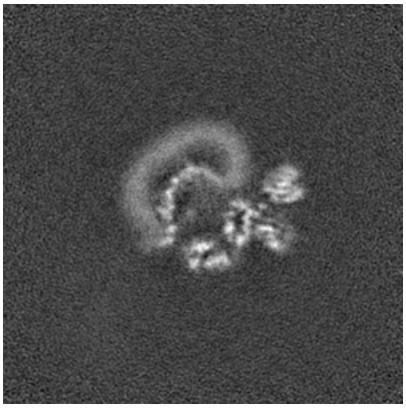


Z Index: 128

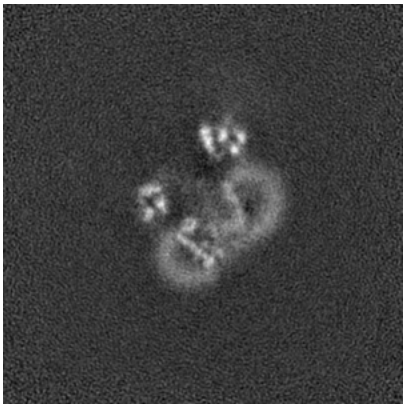
6.2.2 Raw map



X Index: 128



Y Index: 128

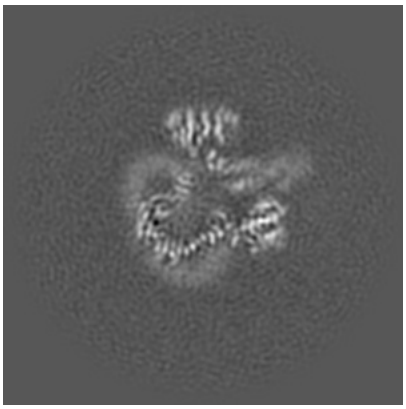


Z Index: 128

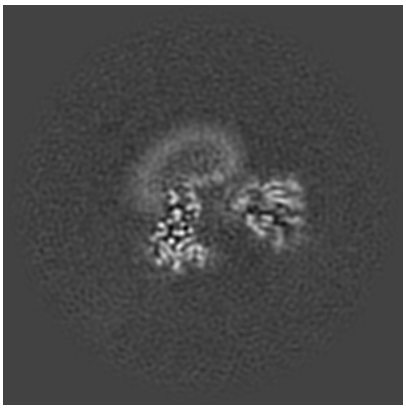
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

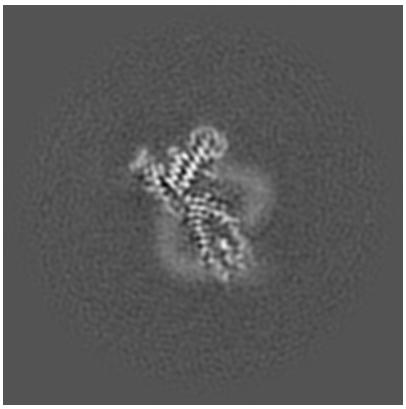
6.3.1 Primary map



X Index: 131

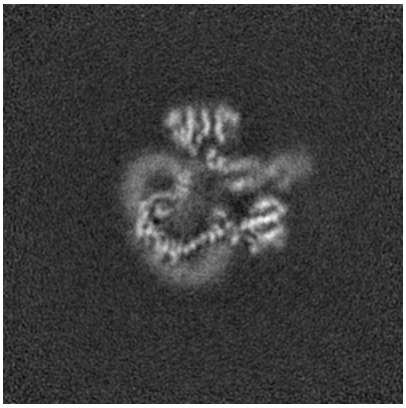


Y Index: 138

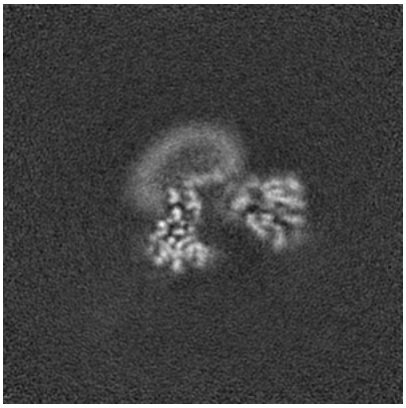


Z Index: 104

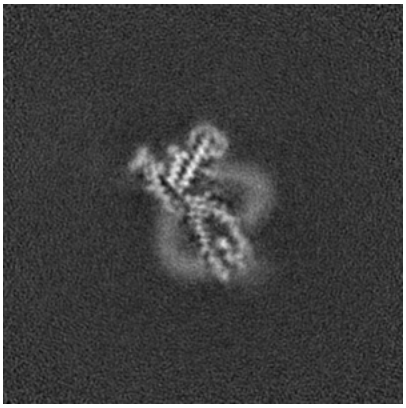
6.3.2 Raw map



X Index: 131



Y Index: 138

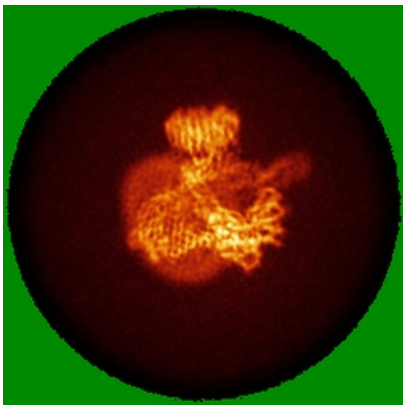


Z Index: 104

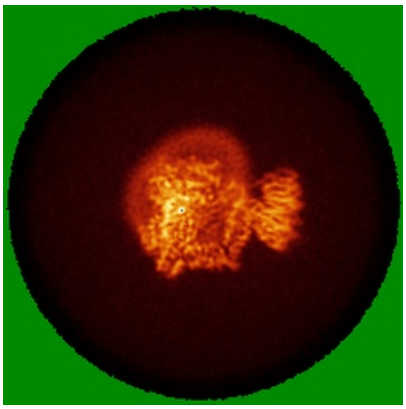
The images above show the largest variance slices of the map in three orthogonal directions.

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

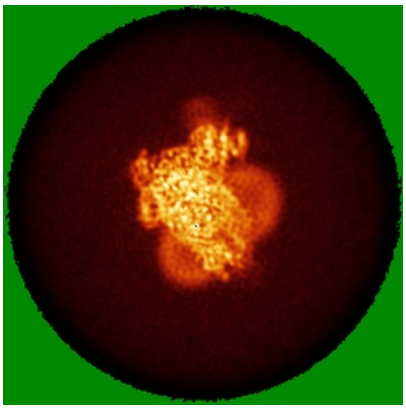
6.4.1 Primary map



X

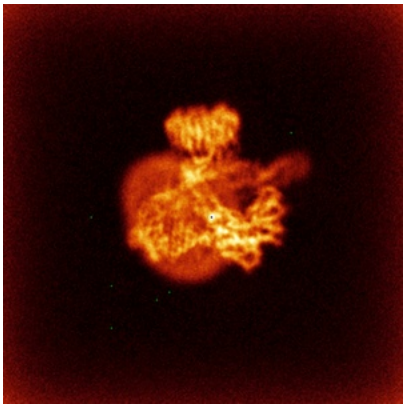


Y

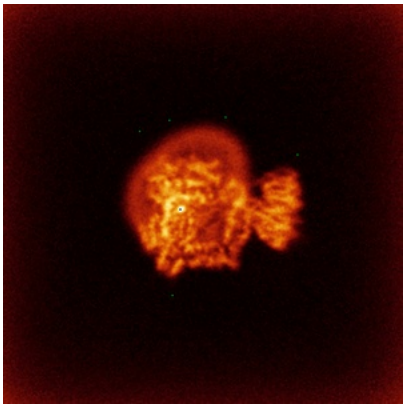


Z

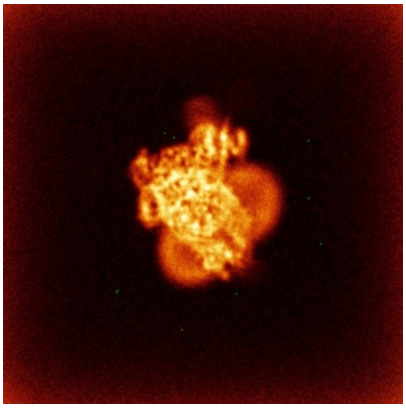
6.4.2 Raw map



X



Y

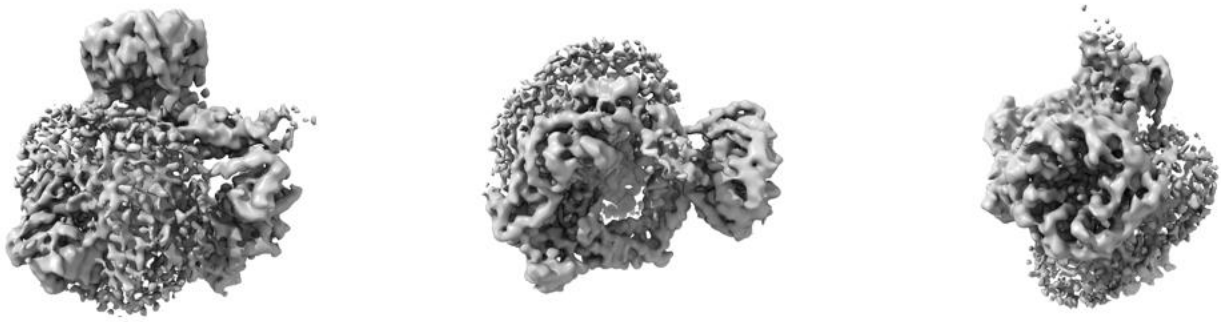


Z

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 0.35. 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.

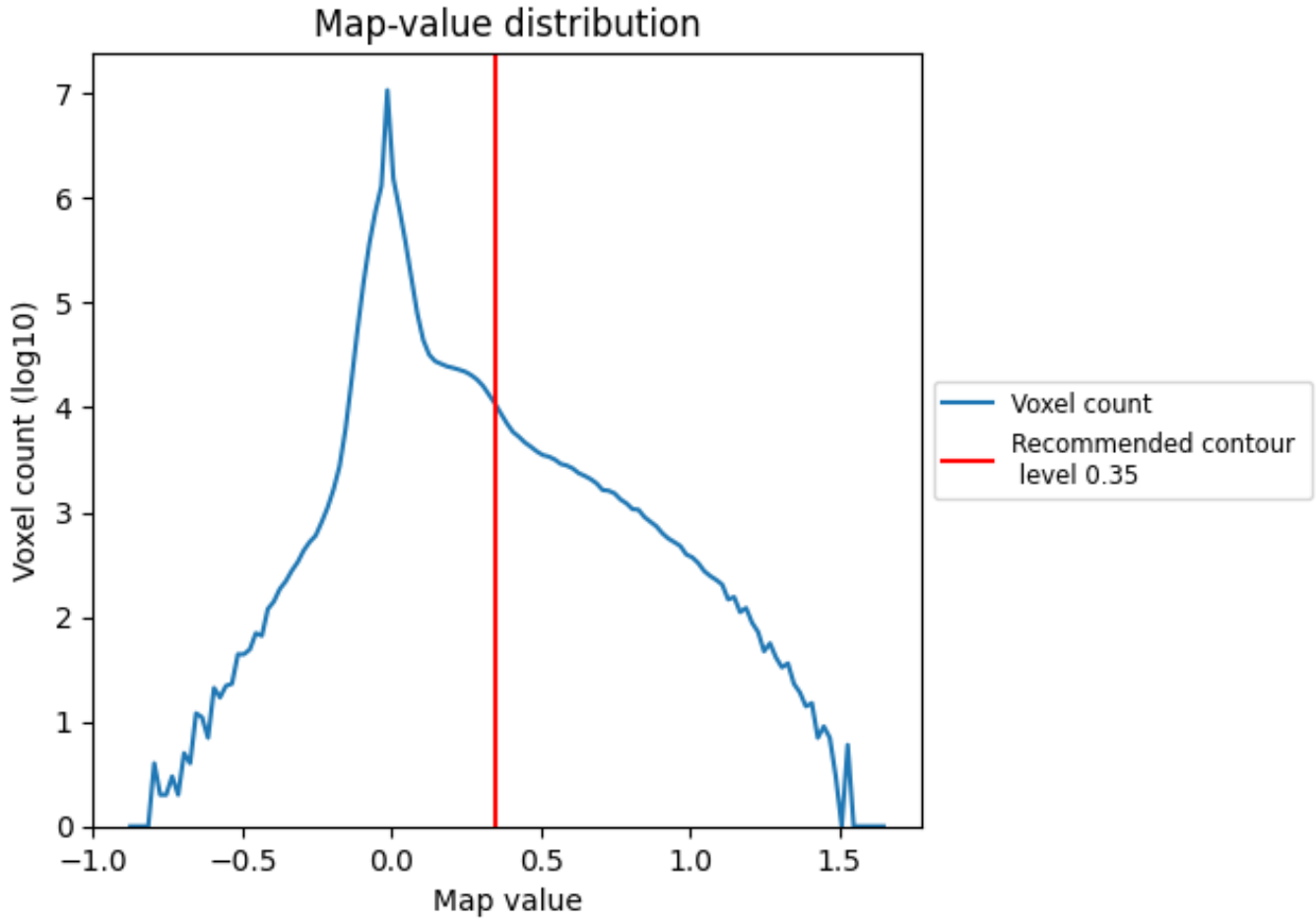
6.6 Mask visualisation (i)

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

7 Map analysis

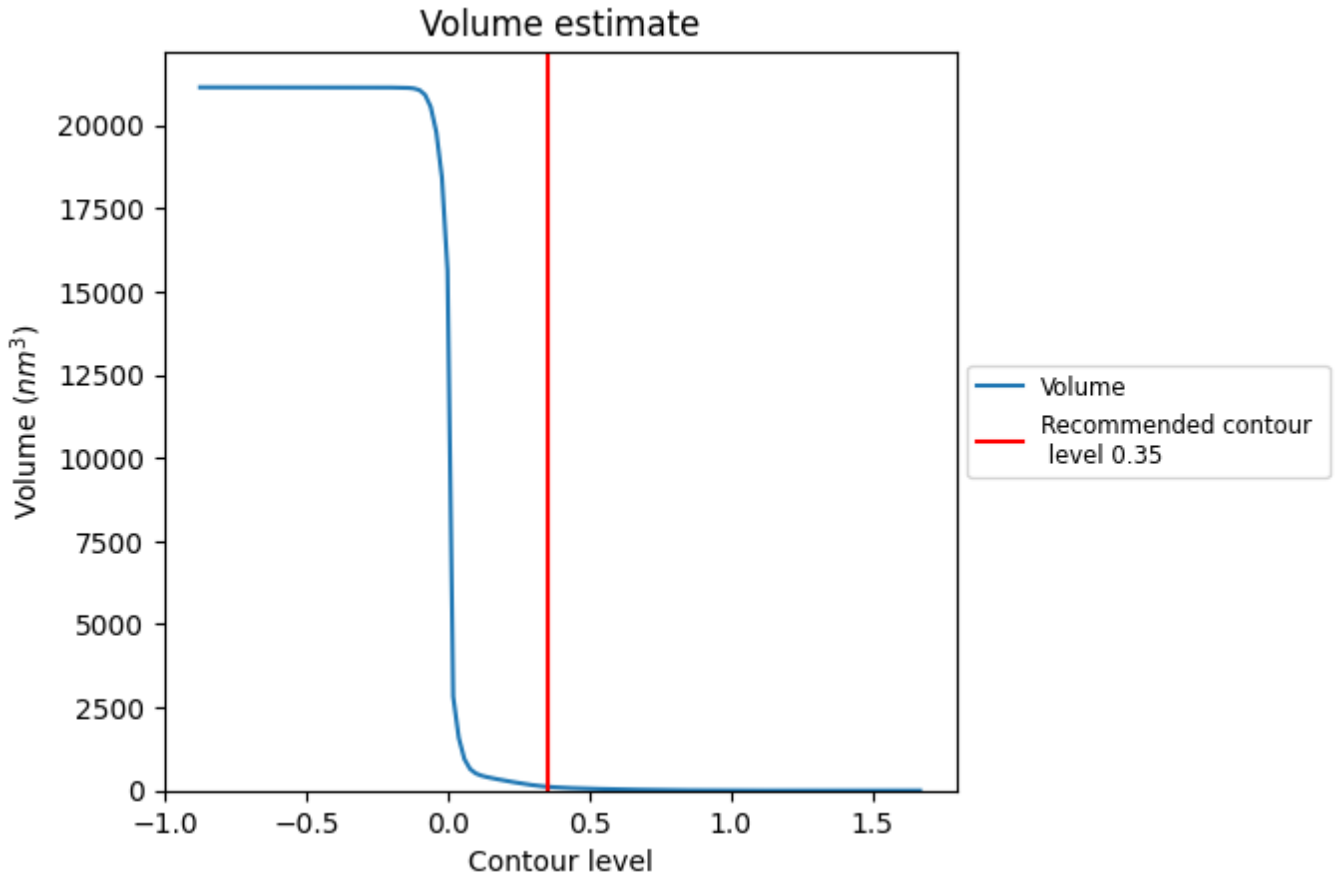
This section contains the results of statistical analysis of the map.

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.

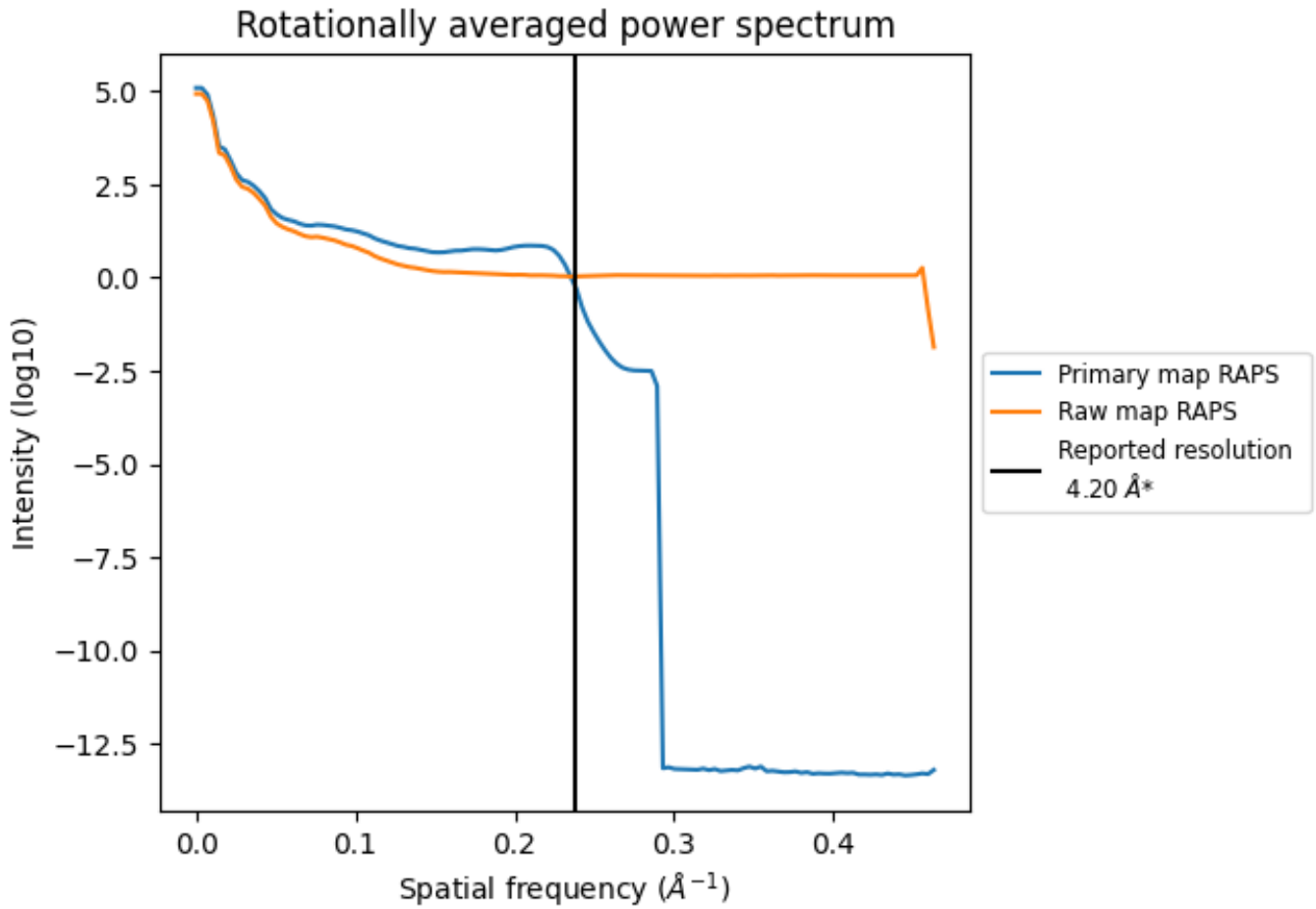
7.2 Volume estimate



The volume at the recommended contour level is 117 nm^3; this corresponds to an approximate mass of 106 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)

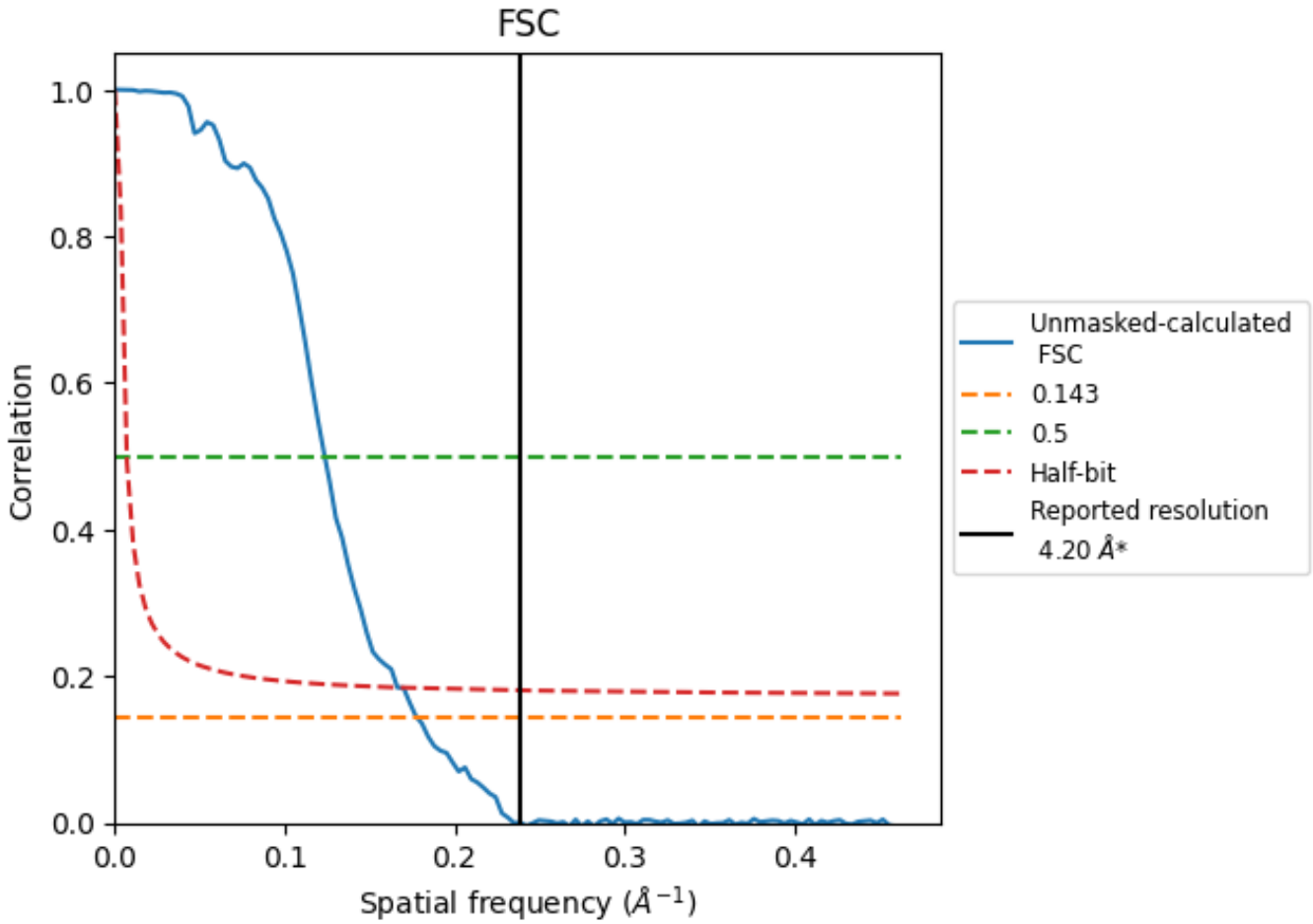


*Reported resolution corresponds to spatial frequency of 0.238 $Å^{-1}$

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 0.238 Å^{-1}

8.2 Resolution estimates (i)

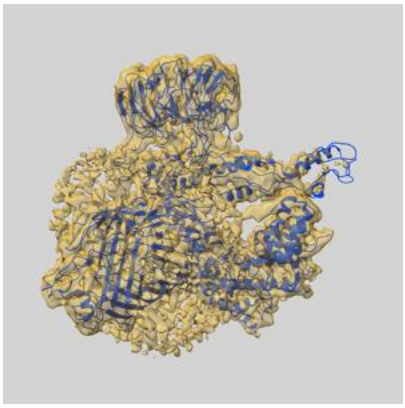
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.61	8.10	6.01

*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 5.61 differs from the reported value 4.2 by more than 10 %

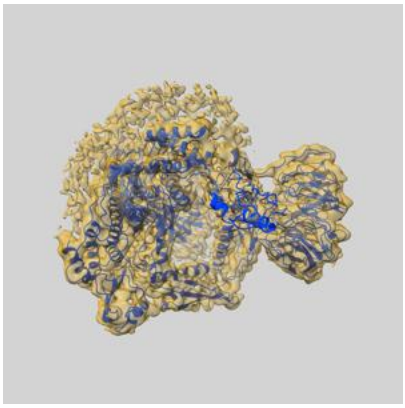
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40700 and PDB model 8SQA. Per-residue inclusion information can be found in section 3 on page 7.

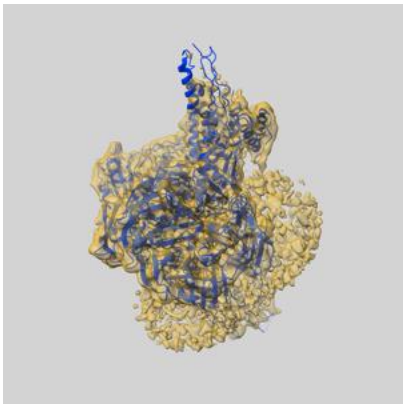
9.1 Map-model overlay



X



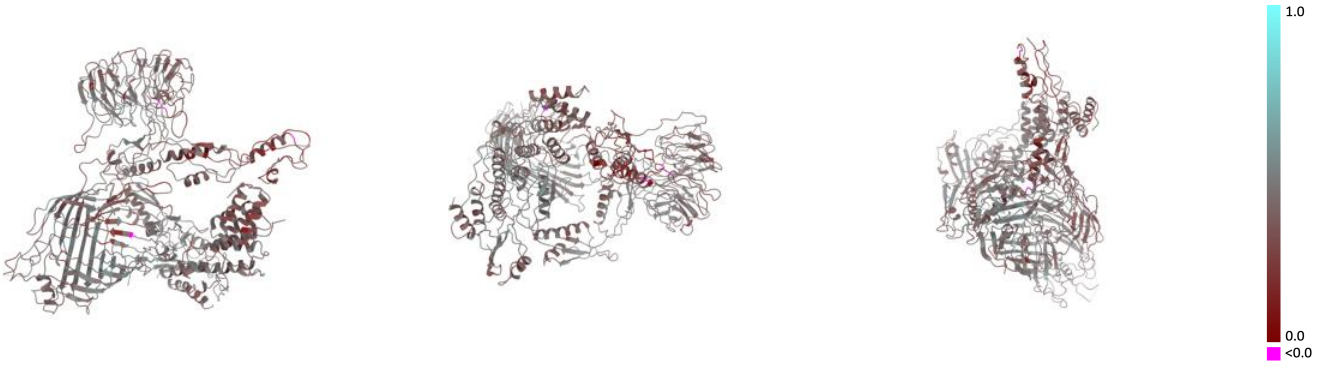
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

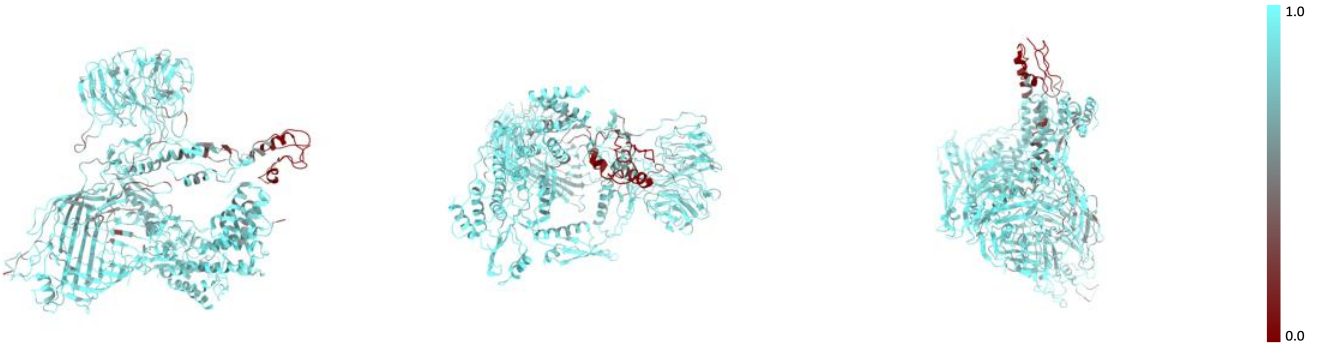
9.2 Q-score mapped to coordinate model (i)



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.

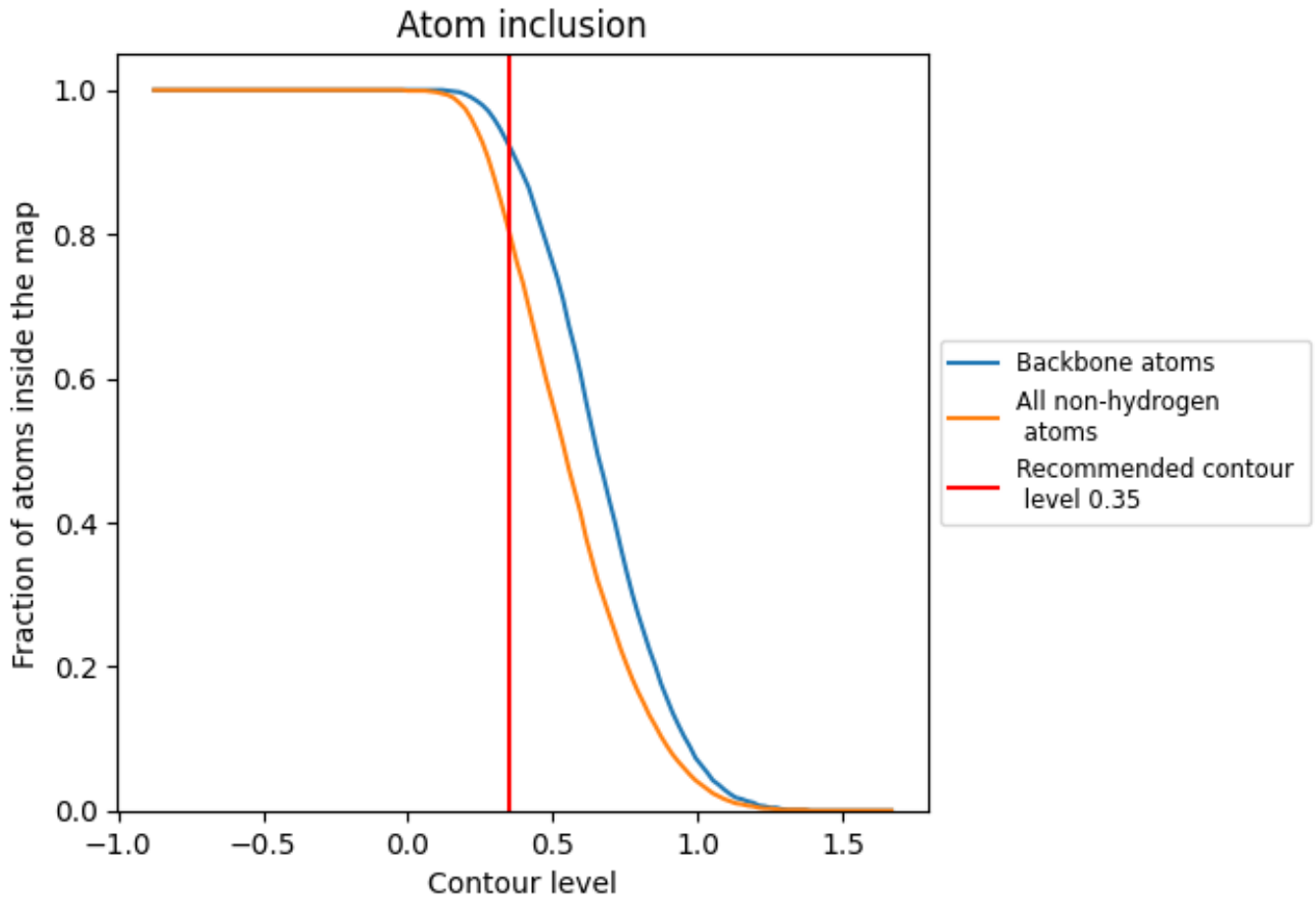
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 80% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8020	0.4080
A	0.7740	0.4140
B	0.8190	0.4020
C	0.8330	0.4200
D	0.8760	0.4000
E	0.9070	0.4320
F	0.6260	0.3470