



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:36 AM UTC

PDB ID : 8QPU / pdb_00008qpu
EMDB ID : EMD-18562
Title : Release Complex: BAM bound EspP and Extended SurA
Authors : Fenn, K.L.; Ranson, N.A.
Deposited on : 2023-10-03
Resolution : 5.20 Å (reported)
Based on initial models : 3SLT, 8PZ2, 7TTC

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

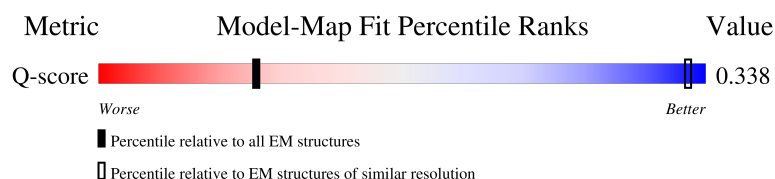
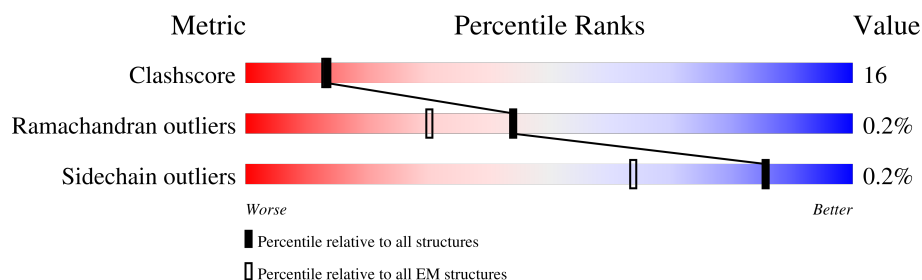
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	712 (4.70 - 5.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	790	29% 60% 36% .
2	B	373	46% 61% 37% .
3	D	226	11% 68% 28% .
4	E	104	14% 52% 30% 18%

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Mol	Chain	Length	Quality of chain
5	F	450	30%23%12%65%
6	C	320	33%42%11%46%
7	P	364	72%73%9%18%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15075 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	762	Total	C	N	O	S	0	0
			6027	3808	1018	1185	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	425	CYS	SER	engineered mutation	UNP P0A940

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	364	Total	C	N	O	S	0	0
			2737	1718	470	543	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	218	Total	C	N	O	S	0	0
			1760	1109	309	335	7		

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

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

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	114	GLY	-	expression tag	UNP P0A937
E	115	GLY	-	expression tag	UNP P0A937
E	116	HIS	-	expression tag	UNP P0A937

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Chain	Residue	Modelled	Actual	Comment	Reference
E	117	HIS	-	expression tag	UNP P0A937
E	118	HIS	-	expression tag	UNP P0A937
E	119	HIS	-	expression tag	UNP P0A937
E	120	HIS	-	expression tag	UNP P0A937
E	121	HIS	-	expression tag	UNP P0A937
E	122	HIS	-	expression tag	UNP P0A937
E	123	HIS	-	expression tag	UNP P0A937

- Molecule 5 is a protein called Chaperone SurA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	158	Total	C	N	O	S	0	0
			1264	778	235	241	10		

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-21	GLY	-	expression tag	UNP P0ABZ6
F	-20	SER	-	expression tag	UNP P0ABZ6
F	-19	SER	-	expression tag	UNP P0ABZ6
F	-18	ALA	-	expression tag	UNP P0ABZ6
F	-17	TRP	-	expression tag	UNP P0ABZ6
F	-16	SER	-	expression tag	UNP P0ABZ6
F	-15	HIS	-	expression tag	UNP P0ABZ6
F	-14	PRO	-	expression tag	UNP P0ABZ6
F	-13	GLN	-	expression tag	UNP P0ABZ6
F	-12	PHE	-	expression tag	UNP P0ABZ6
F	-11	GLU	-	expression tag	UNP P0ABZ6
F	-10	LYS	-	expression tag	UNP P0ABZ6
F	-9	GLY	-	expression tag	UNP P0ABZ6
F	-8	GLY	-	expression tag	UNP P0ABZ6
F	-7	GLY	-	expression tag	UNP P0ABZ6
F	-6	SER	-	expression tag	UNP P0ABZ6
F	-5	GLY	-	expression tag	UNP P0ABZ6
F	-4	GLY	-	expression tag	UNP P0ABZ6
F	-3	GLY	-	expression tag	UNP P0ABZ6
F	-2	SER	-	expression tag	UNP P0ABZ6
F	-1	GLY	-	expression tag	UNP P0ABZ6
F	0	GLY	-	expression tag	UNP P0ABZ6
F	1	SER	-	expression tag	UNP P0ABZ6
F	2	ALA	-	expression tag	UNP P0ABZ6
F	3	TRP	-	expression tag	UNP P0ABZ6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	4	SER	-	expression tag	UNP P0ABZ6
F	5	HIS	-	expression tag	UNP P0ABZ6
F	6	PRO	-	expression tag	UNP P0ABZ6
F	7	GLN	-	expression tag	UNP P0ABZ6
F	8	PHE	-	expression tag	UNP P0ABZ6
F	9	GLU	-	expression tag	UNP P0ABZ6
F	10	LYS	-	expression tag	UNP P0ABZ6
F	11	SER	-	expression tag	UNP P0ABZ6
F	12	SER	-	expression tag	UNP P0ABZ6
F	13	GLY	-	expression tag	UNP P0ABZ6
F	14	GLU	-	expression tag	UNP P0ABZ6
F	15	ASN	-	expression tag	UNP P0ABZ6
F	16	LEU	-	expression tag	UNP P0ABZ6
F	17	TYR	-	expression tag	UNP P0ABZ6
F	18	PHE	-	expression tag	UNP P0ABZ6
F	19	GLN	-	expression tag	UNP P0ABZ6
F	20	GLY	-	expression tag	UNP P0ABZ6
F	27	CYS	LYS	engineered mutation	UNP P0ABZ6

- Molecule 6 is a protein called Outer membrane protein assembly factor BamC.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	174	Total	C	N	O	S	0	0
			1096	677	198	217	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	125	ALA	GLN	conflict	UNP P0A903
C	126	GLN	ALA	conflict	UNP P0A903

- Molecule 7 is a protein called Serine protease EspP.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	299	Total	C	N	O	S	1	0
			1523	901	311	310	1		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	937	GLY	-	expression tag	UNP Q7BSW5
P	938	GLY	-	expression tag	UNP Q7BSW5

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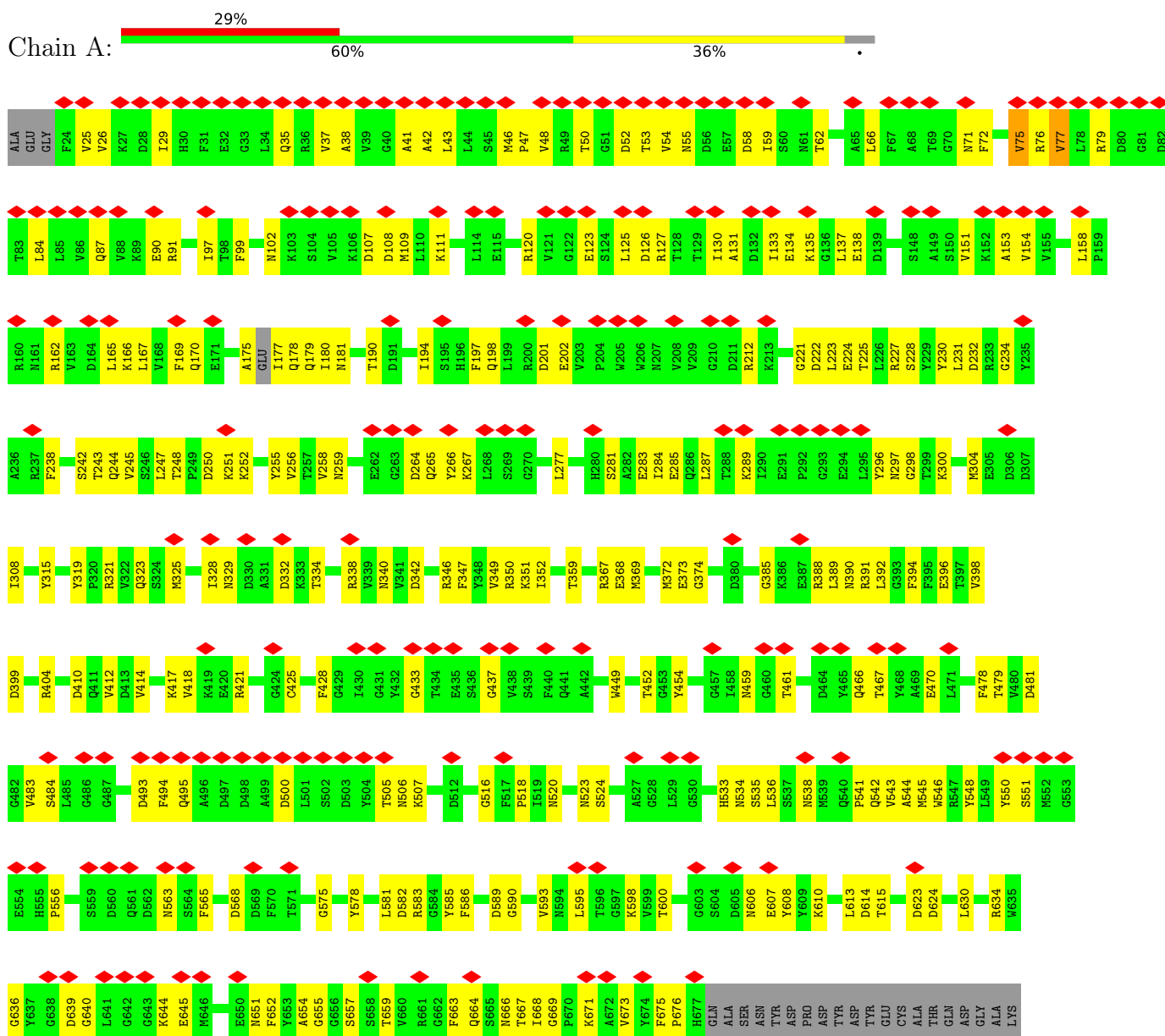
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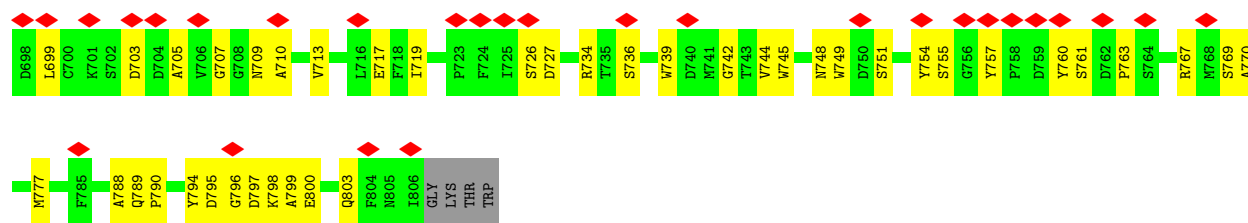
Chain	Residue	Modelled	Actual	Comment	Reference
P	976	GLY	-	insertion	UNP Q7BSW5
P	977	GLU	-	insertion	UNP Q7BSW5
P	978	ASN	-	insertion	UNP Q7BSW5
P	979	LEU	-	insertion	UNP Q7BSW5
P	980	TYR	-	insertion	UNP Q7BSW5
P	981	PHE	-	insertion	UNP Q7BSW5
P	982	GLN	-	insertion	UNP Q7BSW5
P	983	GLY	-	insertion	UNP Q7BSW5
P	984	GLY	-	insertion	UNP Q7BSW5
P	1299	CYS	SER	conflict	UNP Q7BSW5

3 Residue-property plots

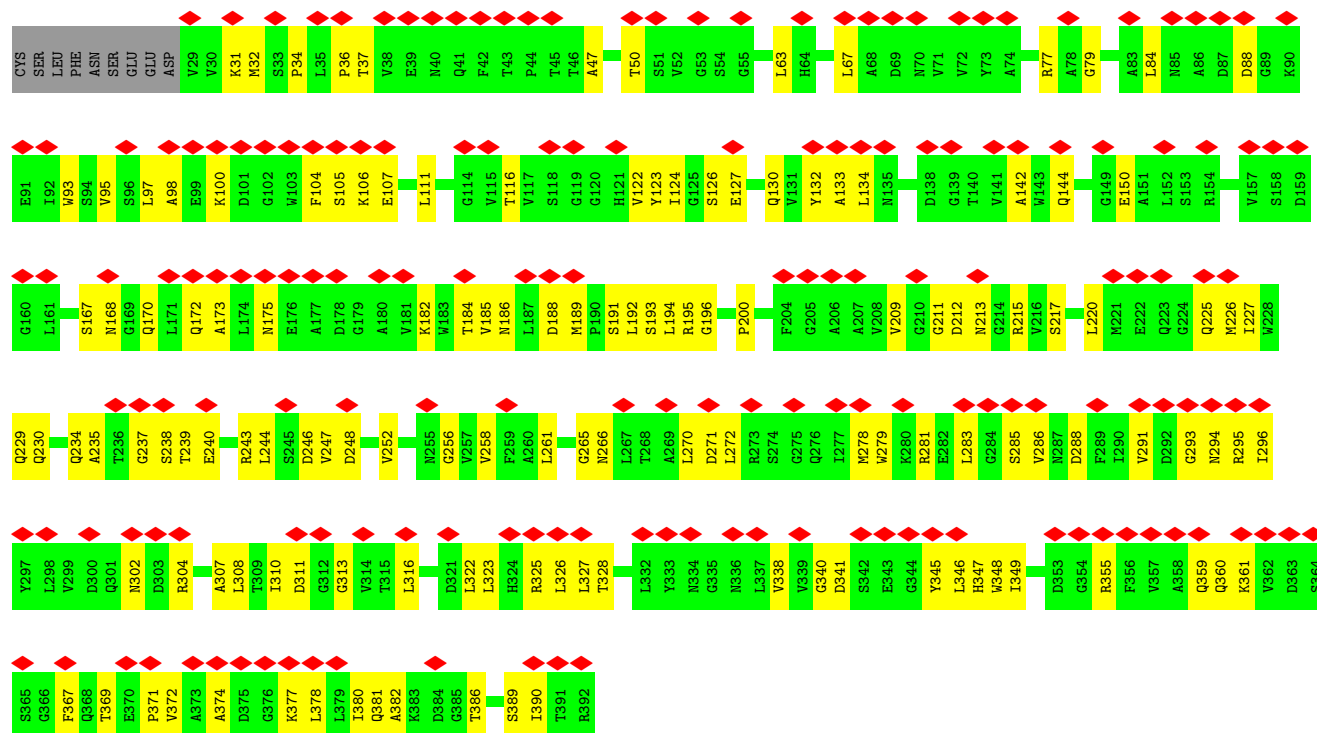
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

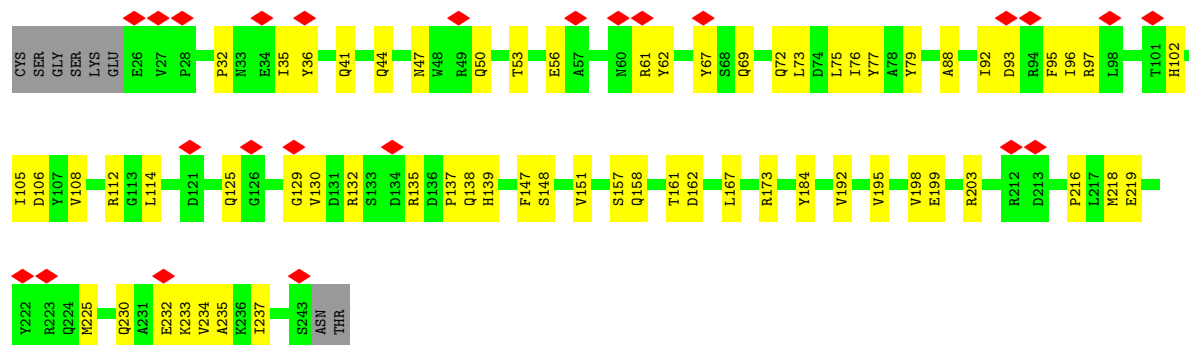




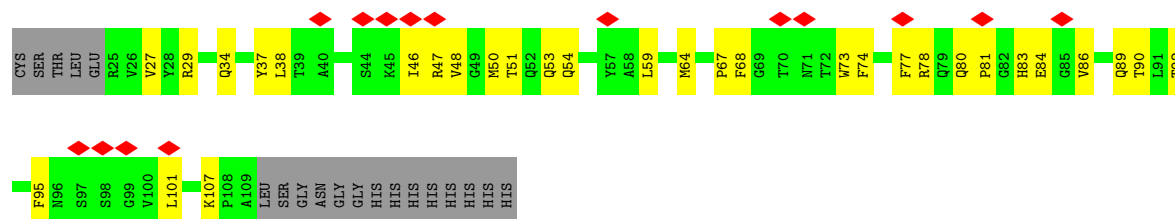
• Molecule 2: Outer membrane protein assembly factor BamB



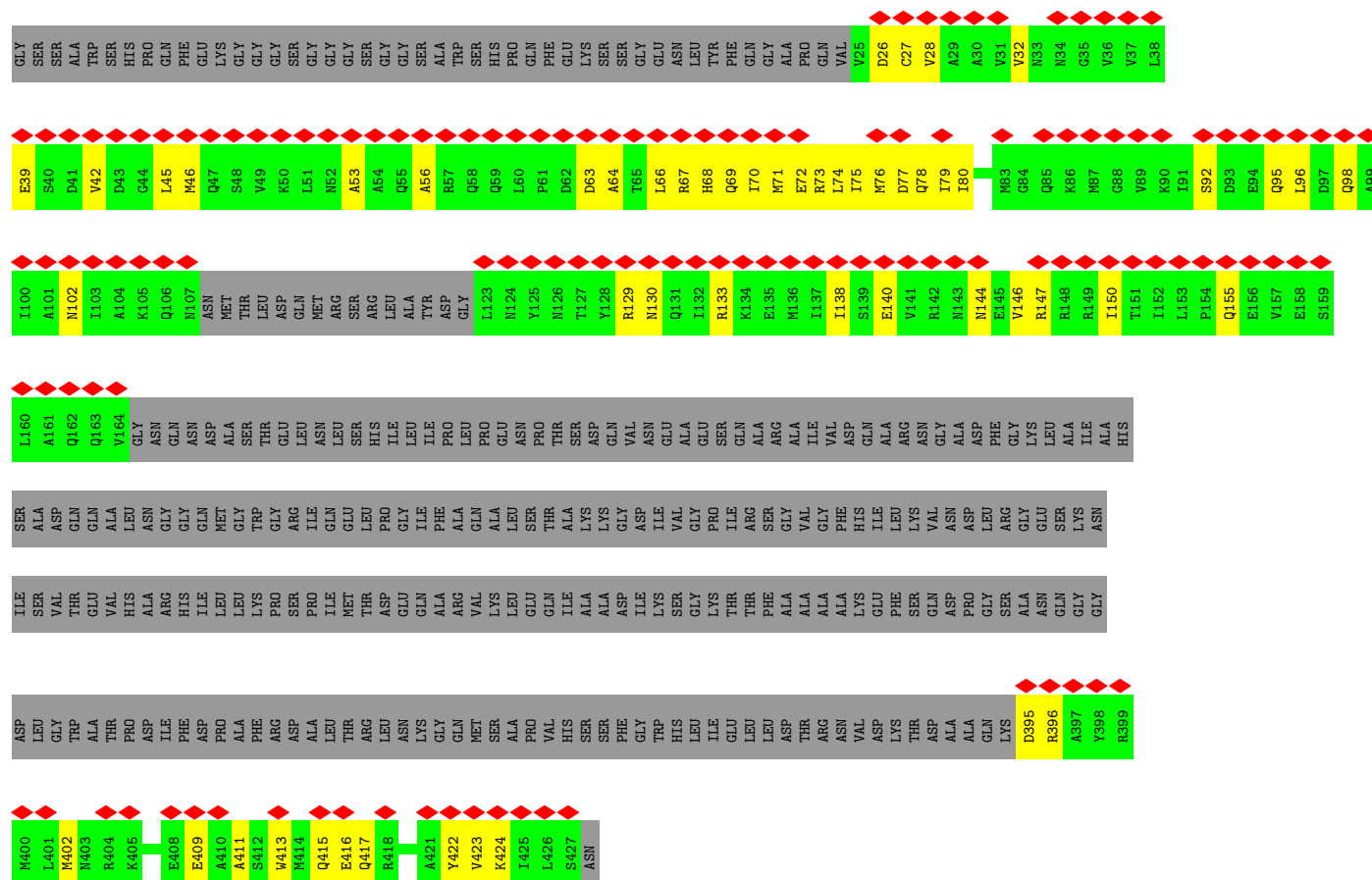
• Molecule 3: Outer membrane protein assembly factor BamD



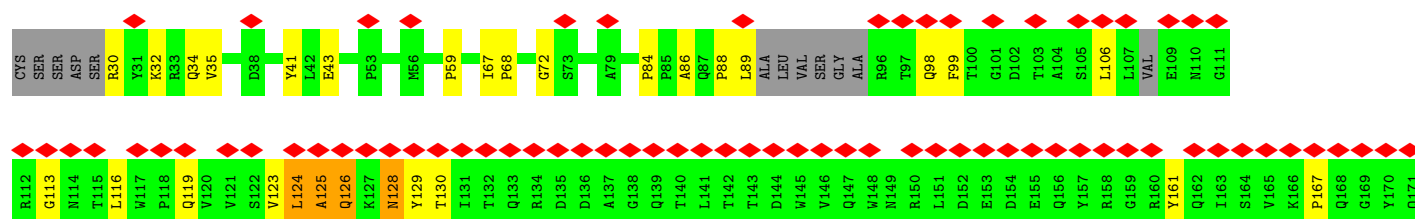
• Molecule 4: Outer membrane protein assembly factor BamE

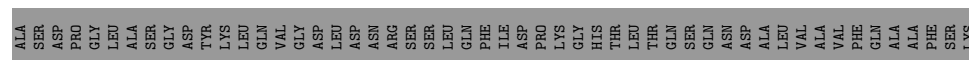
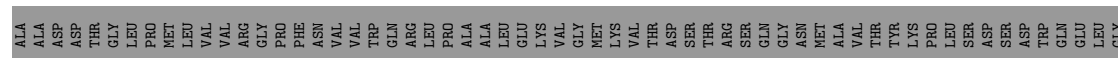
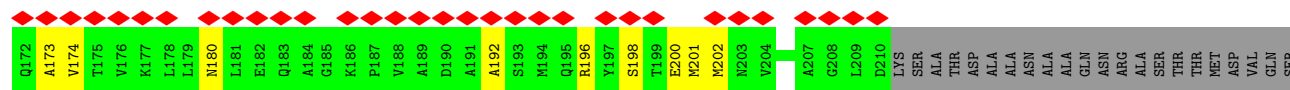


• Molecule 5: Chaperone SurA

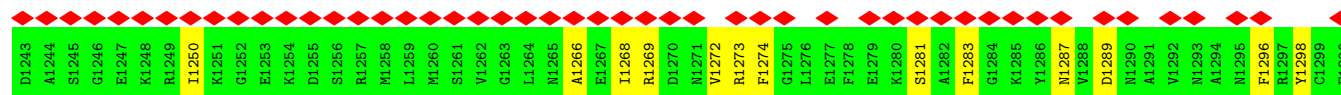
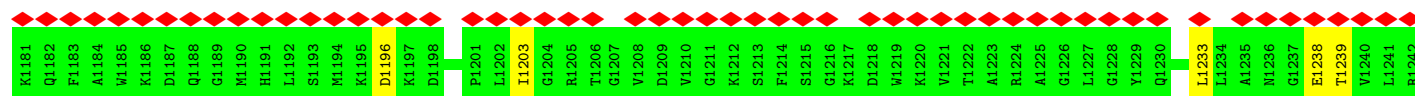
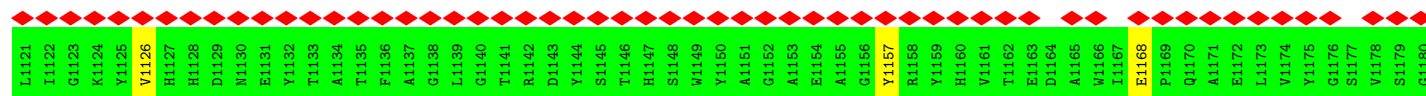
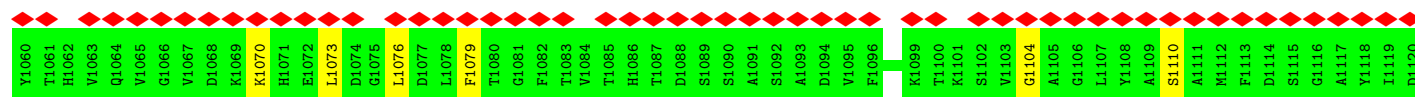
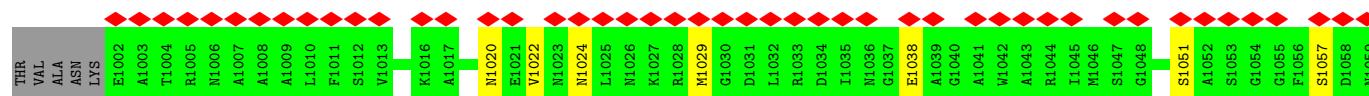
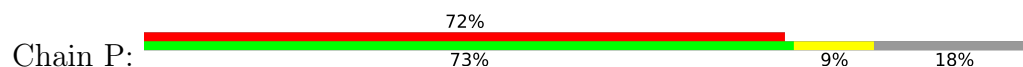


• Molecule 6: Outer membrane protein assembly factor BamC





● Molecule 7: Serine protease EspP



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24485	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 ($e^-/\text{\AA}^2$)	37.4	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.497	Depositor
Minimum map value	-0.373	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.137	Depositor
Map size (Å)	222.0, 222.0, 222.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.15	0/6164	0.40	0/8359
2	B	0.12	0/2787	0.35	0/3800
3	D	0.15	0/1800	0.39	0/2446
4	E	0.12	0/683	0.34	0/932
5	F	0.14	0/1271	0.39	0/1706
6	C	0.22	0/1108	0.43	1/1518 (0.1%)
7	P	0.17	0/1526	0.34	0/2104
All	All	0.15	0/15339	0.38	1/20865 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	124	LEU	O-C-N	-6.05	115.67	122.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6027	0	5773	211	0
2	B	2737	0	2691	103	0
3	D	1760	0	1699	49	0
4	E	668	0	649	28	0
5	F	1264	0	1288	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	1096	0	910	38	0
7	P	1523	0	805	21	0
All	All	15075	0	13815	464	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 16.

All (464) 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)
5:F:63:ASP:O	5:F:67:ARG:HB2	1.73	0.88
1:A:372:MET:HE3	1:A:373:GLU:H	1.41	0.85
3:D:192:VAL:HB	4:E:34:GLN:HG3	1.64	0.80
1:A:479:THR:HG22	1:A:483:VAL:HG12	1.67	0.76
1:A:76:ARG:HG3	5:F:27:CYS:HA	1.67	0.76
5:F:411:ALA:O	5:F:415:GLN:NE2	2.19	0.75
6:C:125:ALA:H	6:C:130:THR:H	1.31	0.75
7:P:1203:ILE:HA	7:P:1233:LEU:H	1.52	0.74
1:A:350:ARG:HG2	1:A:351:LYS:HG3	1.69	0.73
2:B:291:VAL:HG22	2:B:293:GLY:H	1.52	0.73
1:A:598:LYS:HG2	1:A:610:LYS:HB3	1.71	0.73
2:B:381:GLN:NE2	2:B:382:ALA:O	2.23	0.71
2:B:67:LEU:HD11	2:B:374:ALA:HB3	1.72	0.71
3:D:132:ARG:HE	3:D:135:ARG:HG3	1.56	0.70
5:F:66:LEU:HD12	5:F:69:GLN:HE21	1.56	0.70
2:B:286:VAL:HG12	2:B:288:ASP:H	1.57	0.70
2:B:32:MET:O	2:B:325:ARG:NH1	2.25	0.70
3:D:167:LEU:HG	6:C:67:ILE:HD13	1.74	0.69
6:C:125:ALA:N	6:C:130:THR:H	1.89	0.69
1:A:542:GLN:NE2	1:A:545:MET:SD	2.66	0.69
6:C:125:ALA:H	6:C:130:THR:N	1.89	0.69
1:A:739:TRP:HD1	1:A:770:ALA:HB2	1.59	0.68
1:A:479:THR:HG23	1:A:481:ASP:H	1.59	0.68
5:F:96:LEU:HD12	5:F:133:ARG:HB2	1.75	0.68
1:A:396:GLU:HB2	1:A:421:ARG:HB3	1.75	0.68
2:B:191:SER:OG	2:B:192:LEU:N	2.27	0.68
2:B:200:PRO:HB3	2:B:209:VAL:HB	1.76	0.67
5:F:63:ASP:HA	5:F:66:LEU:HB3	1.76	0.67
2:B:377:LYS:NZ	2:B:389:SER:OG	2.28	0.66
1:A:541:PRO:HA	1:A:546:TRP:HZ2	1.58	0.66
1:A:224:GLU:OE1	1:A:227:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:LEU:HD21	1:A:613:LEU:HD12	1.78	0.66
5:F:130:ASN:OD1	5:F:133:ARG:NH1	2.28	0.66
5:F:72:GLU:O	5:F:76:MET:HG2	1.95	0.66
1:A:194:ILE:HA	1:A:197:PHE:HD2	1.61	0.65
3:D:230:GLN:O	3:D:233:LYS:HB3	1.96	0.65
1:A:467:THR:H	1:A:494:PHE:HA	1.61	0.65
1:A:108:ASP:OD1	1:A:109:MET:N	2.28	0.65
2:B:235:ALA:O	2:B:243:ARG:NH1	2.30	0.65
6:C:86:ALA:O	6:C:196:ARG:NH1	2.30	0.65
2:B:279:TRP:HH2	2:B:308:LEU:HD21	1.61	0.65
6:C:125:ALA:N	6:C:130:THR:O	2.30	0.65
7:P:1238:GLU:HA	7:P:1250:ILE:O	1.97	0.65
1:A:153:ALA:HB1	1:A:165:LEU:HD11	1.80	0.64
1:A:349:VAL:HG23	1:A:374:GLY:H	1.62	0.64
1:A:26:VAL:HG21	1:A:84:LEU:HG	1.80	0.64
1:A:630:LEU:HB3	1:A:717:GLU:HB3	1.80	0.64
5:F:70:ILE:HG22	5:F:73:ARG:HH21	1.62	0.64
4:E:51:THR:O	4:E:54:GLN:NE2	2.30	0.64
2:B:230:GLN:HE21	2:B:270:LEU:HD22	1.63	0.64
1:A:234:GLY:HA2	1:A:296:TYR:HB3	1.79	0.63
7:P:1283:PHE:HA	7:P:1287:ASN:HA	1.80	0.63
1:A:398:VAL:HG23	1:A:418:VAL:HG12	1.79	0.63
1:A:478:PHE:HB3	1:A:483:VAL:HG13	1.79	0.63
6:C:113:GLY:HA3	6:C:173:ALA:HB3	1.81	0.63
1:A:523:ASN:HD21	1:A:578:TYR:HD2	1.46	0.63
5:F:98:GLN:NE2	5:F:102:ASN:OD1	2.32	0.63
6:C:119:GLN:O	6:C:123:VAL:HG23	1.99	0.63
6:C:30:ARG:HG3	6:C:32:LYS:HB2	1.80	0.62
1:A:321:ARG:N	1:A:342:ASP:OD1	2.32	0.62
6:C:98:GLN:H	6:C:106:LEU:HG	1.64	0.62
5:F:402:MET:HE3	5:F:402:MET:O	2.00	0.62
1:A:346:ARG:NH1	4:E:37:TYR:O	2.32	0.62
1:A:245:VAL:HG12	1:A:256:VAL:HG22	1.82	0.62
3:D:47:ASN:ND2	3:D:50:GLN:OE1	2.33	0.62
5:F:39:GLU:HA	5:F:42:VAL:HG12	1.82	0.62
1:A:29:ILE:HG22	1:A:84:LEU:HB2	1.82	0.62
1:A:651:ASN:ND2	1:A:707:GLY:O	2.33	0.62
3:D:158:GLN:HE22	6:C:192:ALA:HB3	1.64	0.62
1:A:754:TYR:HD2	1:A:757:TYR:HB2	1.65	0.61
2:B:237:GLY:H	2:B:243:ARG:HH11	1.48	0.61
2:B:111:LEU:HA	2:B:126:SER:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:GLU:OE1	1:A:388:ARG:HB3	2.01	0.61
2:B:31:LYS:NZ	2:B:32:MET:O	2.30	0.61
1:A:548:TYR:OH	1:A:606:ASN:OD1	2.18	0.60
2:B:235:ALA:HB1	2:B:243:ARG:HD2	1.83	0.60
4:E:50:MET:HG3	4:E:54:GLN:HG2	1.82	0.60
1:A:134:GLU:HG3	1:A:151:VAL:HG23	1.82	0.60
1:A:600:THR:HG21	1:A:607:GLU:HA	1.83	0.60
2:B:281:ARG:HD2	2:B:283:LEU:HG	1.83	0.60
1:A:654:ALA:HB3	1:A:668:ILE:HB	1.83	0.60
1:A:72:PHE:HD1	1:A:90:GLU:HG2	1.66	0.60
1:A:542:GLN:O	1:A:546:TRP:NE1	2.35	0.60
1:A:242:SER:OG	1:A:244:GLN:OE1	2.20	0.59
2:B:63:LEU:O	2:B:369:THR:OG1	2.12	0.59
2:B:167:SER:O	2:B:168:ASN:ND2	2.35	0.59
1:A:668:ILE:HG22	1:A:744:VAL:HG12	1.84	0.59
2:B:37:THR:O	2:B:359:GLN:NE2	2.35	0.59
2:B:323:LEU:O	2:B:325:ARG:NH1	2.36	0.59
3:D:77:TYR:CD2	6:C:84:PRO:HD3	2.36	0.59
3:D:158:GLN:NE2	6:C:192:ALA:HB3	2.18	0.59
1:A:769:SER:HB2	1:A:790:PRO:HA	1.85	0.58
1:A:287:LEU:HD23	1:A:308:ILE:HD13	1.86	0.58
3:D:233:LYS:HE2	4:E:68:PHE:HB2	1.84	0.58
1:A:135:LYS:HE2	2:B:238:SER:HB2	1.86	0.58
2:B:281:ARG:NH2	2:B:313:GLY:O	2.37	0.57
6:C:88:PRO:HD3	6:C:196:ARG:HH12	1.69	0.57
5:F:77:ASP:HB2	5:F:138:ILE:HD13	1.85	0.57
1:A:99:PHE:HE1	1:A:107:ASP:HB3	1.69	0.57
1:A:127:ARG:HD3	5:F:424:LYS:HE2	1.87	0.57
2:B:258:VAL:HG13	2:B:272:LEU:HD11	1.86	0.57
2:B:371:PRO:HB3	2:B:380:ILE:HD12	1.86	0.57
3:D:93:ASP:HA	3:D:96:ILE:HG12	1.86	0.57
1:A:190:THR:O	1:A:194:ILE:HG12	2.05	0.56
7:P:1266:ALA:HB3	7:P:1274:PHE:HB3	1.86	0.56
1:A:250:ASP:HB3	2:B:326:LEU:HD11	1.88	0.56
2:B:240:GLU:HA	2:B:243:ARG:HE	1.70	0.56
1:A:461:THR:HG22	1:A:466:GLN:HE22	1.69	0.56
2:B:378:LEU:HB3	2:B:390:ILE:HG22	1.88	0.56
3:D:88:ALA:O	3:D:92:ILE:HG12	2.06	0.56
4:E:46:ILE:HD11	4:E:59:LEU:HD21	1.88	0.56
1:A:247:LEU:HD11	1:A:251:LYS:HA	1.88	0.56
6:C:124:LEU:O	6:C:125:ALA:C	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:VAL:HG23	2:B:296:ILE:HG13	1.88	0.56
1:A:283:GLU:OE1	1:A:315:TYR:OH	2.25	0.55
1:A:719:ILE:HD12	1:A:734:ARG:HD3	1.87	0.55
5:F:96:LEU:HD21	5:F:129:ARG:HE	1.70	0.55
1:A:177:ILE:HD11	1:A:180:ILE:HD11	1.87	0.55
2:B:322:LEU:HD22	2:B:327:LEU:HD21	1.88	0.55
2:B:173:ALA:HB3	2:B:182:LYS:HB2	1.88	0.55
2:B:100:LYS:HD3	2:B:105:SER:HB3	1.88	0.55
6:C:125:ALA:O	6:C:126:GLN:C	2.49	0.55
1:A:663:PHE:O	1:A:799:ALA:HA	2.06	0.55
2:B:124:ILE:HG22	2:B:132:TYR:HB2	1.88	0.55
7:P:1038:GLU:O	7:P:1070:LYS:N	2.40	0.55
1:A:325:MET:SD	1:A:338:ARG:HB2	2.46	0.55
1:A:493:ASP:HB2	1:A:507:LYS:HG3	1.88	0.55
1:A:607:GLU:HB2	1:A:644:LYS:HD2	1.87	0.55
4:E:37:TYR:HA	4:E:77:PHE:CE1	2.42	0.55
2:B:77:ARG:NH2	2:B:127:GLU:OE1	2.40	0.55
1:A:459:ASN:OD1	1:A:470:GLU:HG2	2.06	0.54
5:F:92:SER:OG	5:F:95:GLN:OE1	2.19	0.54
2:B:116:THR:HG23	2:B:123:TYR:HD2	1.72	0.54
5:F:140:GLU:OE1	5:F:144:ASN:ND2	2.37	0.54
1:A:201:ASP:OD1	1:A:202:GLU:N	2.41	0.54
1:A:520:ASN:OD1	1:A:523:ASN:N	2.41	0.54
3:D:198:VAL:HB	3:D:218:MET:HE2	1.90	0.54
1:A:55:ASN:HD21	1:A:58:ASP:HB2	1.73	0.54
2:B:307:ALA:HB3	2:B:316:LEU:HB2	1.87	0.54
2:B:234:GLN:HB2	2:B:266:ASN:HD21	1.72	0.54
1:A:323:GLN:HE22	1:A:325:MET:HE1	1.73	0.54
1:A:461:THR:HG22	1:A:466:GLN:NE2	2.22	0.54
4:E:64:MET:HB3	4:E:74:PHE:HB2	1.88	0.54
1:A:533:HIS:ND1	1:A:568:ASP:OD1	2.23	0.54
3:D:32:PRO:HB3	3:D:62:TYR:CZ	2.43	0.54
5:F:395:ASP:HB2	5:F:396:ARG:HH21	1.73	0.54
2:B:225:GLN:NE2	2:B:226:MET:O	2.41	0.53
1:A:323:GLN:HE21	1:A:340:ASN:HB2	1.72	0.53
1:A:495:GLN:HA	1:A:505:THR:HG23	1.89	0.53
1:A:675:PHE:HD1	1:A:676:PRO:HD2	1.72	0.53
1:A:719:ILE:HD13	1:A:736:SER:HB2	1.89	0.53
7:P:1051:SER:HA	7:P:1057:SER:HA	1.90	0.53
2:B:338:VAL:HG11	2:B:378:LEU:HD21	1.91	0.53
1:A:175:ALA:O	1:A:178:GLN:NE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:90:THR:HG22	4:E:107:LYS:HB3	1.91	0.53
1:A:520:ASN:ND2	1:A:523:ASN:OD1	2.40	0.53
3:D:114:LEU:HD21	6:C:35:VAL:HG23	1.92	0.52
1:A:726:SER:OG	1:A:727:ASP:N	2.42	0.52
4:E:77:PHE:CD2	4:E:89:GLN:HB3	2.44	0.52
1:A:248:THR:OG1	1:A:250:ASP:OD1	2.21	0.52
2:B:234:GLN:N	2:B:266:ASN:OD1	2.39	0.52
1:A:175:ALA:O	1:A:177:ILE:N	2.43	0.52
1:A:494:PHE:HE1	1:A:506:ASN:HB2	1.73	0.52
1:A:589:ASP:OD1	1:A:590:GLY:N	2.43	0.52
1:A:352:ILE:HD11	1:A:369:MET:HE3	1.92	0.52
1:A:359:THR:O	3:D:135:ARG:NH1	2.42	0.52
1:A:548:TYR:O	1:A:551:SER:OG	2.27	0.52
5:F:53:ALA:HA	5:F:56:ALA:HB3	1.92	0.52
1:A:300:LYS:O	1:A:304:MET:HG2	2.10	0.52
2:B:34:PRO:HG3	2:B:323:LEU:HD23	1.92	0.52
1:A:367:ARG:HA	3:D:184:TYR:OH	2.10	0.52
1:A:452:THR:HG23	1:A:454:TYR:H	1.73	0.52
6:C:198:SER:O	6:C:201:MET:HG2	2.10	0.52
7:P:1269:ARG:O	7:P:1273:ARG:NH1	2.40	0.52
1:A:769:SER:OG	1:A:770:ALA:N	2.40	0.51
1:A:373:GLU:O	4:E:34:GLN:NE2	2.35	0.51
3:D:225:MET:HE1	4:E:78:ARG:HD3	1.93	0.51
1:A:154:VAL:HB	1:A:166:LYS:HB3	1.91	0.51
1:A:319:TYR:HE2	1:A:404:ARG:HD2	1.76	0.51
4:E:29:ARG:HD2	4:E:83:HIS:H	1.75	0.51
1:A:713:VAL:HA	1:A:742:GLY:HA2	1.93	0.51
2:B:79:GLY:HA2	2:B:111:LEU:HD13	1.93	0.51
4:E:89:GLN:HA	4:E:107:LYS:O	2.11	0.51
1:A:575:GLY:HA2	1:A:595:LEU:O	2.11	0.51
6:C:125:ALA:HA	6:C:129:TYR:HA	1.92	0.51
1:A:243:THR:HG22	1:A:258:VAL:HG23	1.91	0.51
1:A:800:GLU:N	1:A:800:GLU:OE1	2.43	0.51
2:B:226:MET:HE3	2:B:227:ILE:N	2.26	0.50
1:A:99:PHE:CE1	1:A:107:ASP:HB3	2.47	0.50
2:B:271:ASP:OD1	2:B:272:LEU:N	2.44	0.50
6:C:113:GLY:HA2	6:C:116:LEU:HD13	1.92	0.50
1:A:250:ASP:HB2	1:A:252:LYS:HD2	1.94	0.50
1:A:125:LEU:HD21	1:A:130:ILE:HD11	1.94	0.50
6:C:201:MET:HE3	6:C:202:MET:HE3	1.92	0.50
1:A:25:VAL:HG13	1:A:52:ASP:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:TYR:CZ	1:A:328:ILE:HD11	2.47	0.50
1:A:608:TYR:HA	1:A:640:GLY:HA2	1.94	0.50
2:B:196:GLY:O	2:B:248:ASP:HB3	2.11	0.50
2:B:213:ASN:O	2:B:215:ARG:NH2	2.44	0.50
5:F:75:ILE:O	5:F:79:ILE:HG12	2.11	0.50
5:F:146:VAL:HG13	5:F:409:GLU:HG2	1.94	0.50
1:A:29:ILE:HD13	1:A:50:THR:HG21	1.94	0.49
1:A:158:LEU:HB2	1:A:162:ARG:HB2	1.93	0.49
2:B:50:THR:HG21	2:B:84:LEU:HD13	1.94	0.49
2:B:220:LEU:HG	2:B:227:ILE:HD11	1.93	0.49
1:A:797:ASP:N	1:A:797:ASP:OD1	2.45	0.49
4:E:67:PRO:HB2	6:C:59:PRO:HB3	1.94	0.49
1:A:181:ASN:ND2	2:B:150:GLU:OE2	2.45	0.49
1:A:368:GLU:HG3	1:A:392:LEU:HD11	1.94	0.49
2:B:170:GLN:HG3	2:B:186:ASN:HB3	1.93	0.49
2:B:172:GLN:HG2	2:B:184:THR:HA	1.94	0.49
2:B:237:GLY:H	2:B:243:ARG:NH1	2.09	0.49
1:A:349:VAL:HA	1:A:412:VAL:O	2.13	0.49
1:A:404:ARG:HA	1:A:412:VAL:HA	1.95	0.49
1:A:518:PRO:HA	1:A:524:SER:HA	1.95	0.49
3:D:125:GLN:HB3	3:D:130:VAL:HB	1.95	0.49
6:C:43:GLU:OE1	6:C:43:GLU:N	2.45	0.49
1:A:399:ASP:OD1	1:A:417:LYS:HB3	2.13	0.49
2:B:367:PHE:CD2	2:B:380:ILE:HG12	2.47	0.49
3:D:32:PRO:O	3:D:36:TYR:HD1	1.96	0.49
1:A:48:VAL:HG13	1:A:50:THR:H	1.77	0.48
2:B:127:GLU:OE2	2:B:195:ARG:NH2	2.45	0.48
5:F:74:LEU:O	5:F:78:GLN:HG2	2.13	0.48
1:A:198:GLN:N	1:A:222:ASP:OD1	2.41	0.48
1:A:267:LYS:HB3	1:A:334:THR:HG22	1.95	0.48
1:A:304:MET:O	1:A:308:ILE:HG12	2.13	0.48
6:C:88:PRO:HG2	6:C:99:PHE:HA	1.96	0.48
1:A:76:ARG:HE	5:F:28:VAL:H	1.61	0.48
3:D:69:GLN:O	3:D:73:LEU:HD23	2.12	0.48
5:F:71:MET:O	5:F:75:ILE:HG12	2.13	0.48
1:A:788:ALA:O	1:A:789:GLN:NE2	2.46	0.48
3:D:125:GLN:O	3:D:129:GLY:N	2.47	0.48
4:E:34:GLN:H	4:E:78:ARG:HB2	1.76	0.48
7:P:1196:ASP:HA	7:P:1239:THR:HA	1.95	0.48
2:B:93:TRP:HZ3	2:B:95:VAL:HG22	1.78	0.48
5:F:42:VAL:O	5:F:46:MET:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:SER:HA	1:A:284:ILE:HD13	1.95	0.47
1:A:428:PHE:HB3	7:P:1296:PHE:HE1	1.78	0.47
1:A:663:PHE:CE2	1:A:767:ARG:HB3	2.48	0.47
1:A:703:ASP:N	1:A:703:ASP:OD1	2.45	0.47
2:B:215:ARG:HB3	2:B:229:GLN:HG3	1.96	0.47
5:F:147:ARG:HH21	5:F:150:ILE:HG12	1.79	0.47
7:P:1020:ASN:C	7:P:1022:VAL:N	2.71	0.47
3:D:106:ASP:OD2	3:D:157:SER:OG	2.28	0.47
1:A:391:ARG:NH1	1:A:581:LEU:H	2.12	0.47
6:C:125:ALA:H	6:C:130:THR:C	2.23	0.47
1:A:277:LEU:HD23	1:A:277:LEU:H	1.79	0.47
1:A:428:PHE:HB3	7:P:1296:PHE:CE1	2.50	0.47
2:B:130:GLN:OE1	2:B:144:GLN:NE2	2.47	0.47
3:D:195:VAL:HG13	3:D:218:MET:SD	2.54	0.47
1:A:533:HIS:NE2	1:A:535:SER:OG	2.48	0.47
3:D:93:ASP:O	3:D:97:ARG:HG2	2.14	0.47
3:D:225:MET:HE1	4:E:78:ARG:HH11	1.79	0.47
7:P:1281:SER:HA	7:P:1289:ASP:HA	1.97	0.47
1:A:639:ASP:OD1	1:A:639:ASP:N	2.46	0.47
1:A:655:GLY:O	1:A:666:ASN:N	2.34	0.47
1:A:664:GLN:HG3	1:A:798:LYS:HE2	1.97	0.47
1:A:75:VAL:C	1:A:76:ARG:HD2	2.39	0.47
1:A:232:ASP:HA	1:A:298:GLY:H	1.80	0.47
2:B:212:ASP:HA	2:B:246:ASP:HB2	1.97	0.47
2:B:256:GLY:HA2	2:B:272:LEU:HB2	1.95	0.47
4:E:80:GLN:HB3	4:E:86:VAL:HG12	1.96	0.47
5:F:64:ALA:O	5:F:68:HIS:ND1	2.33	0.47
1:A:673:VAL:CG1	1:A:699:LEU:HB3	2.45	0.47
2:B:237:GLY:HA3	2:B:243:ARG:HD3	1.96	0.47
6:C:124:LEU:O	6:C:126:GLN:N	2.48	0.47
1:A:120:ARG:O	1:A:123:GLU:HG3	2.15	0.47
5:F:75:ILE:HA	5:F:78:GLN:HG2	1.97	0.47
1:A:127:ARG:HA	1:A:130:ILE:HD12	1.97	0.47
1:A:329:ASN:ND2	1:A:332:ASP:OD2	2.48	0.47
1:A:657:SER:OG	1:A:803:GLN:OE1	2.29	0.47
2:B:345:TYR:CD1	2:B:361:LYS:HA	2.50	0.47
1:A:120:ARG:HD3	1:A:123:GLU:HG2	1.97	0.46
1:A:352:ILE:N	1:A:373:GLU:OE1	2.38	0.46
1:A:754:TYR:HB2	1:A:757:TYR:HD1	1.80	0.46
1:A:126:ASP:OD1	1:A:126:ASP:N	2.46	0.46
1:A:133:ILE:HG13	1:A:137:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:GLN:HA	2:B:185:VAL:O	2.15	0.46
1:A:285:GLU:O	1:A:289:LYS:HG3	2.15	0.46
1:A:390:ASN:HB3	1:A:582:ASP:O	2.16	0.46
2:B:31:LYS:NZ	2:B:325:ARG:HH12	2.12	0.46
3:D:199:GLU:OE1	3:D:203:ARG:NH2	2.49	0.46
1:A:228:SER:HA	1:A:231:LEU:HG	1.97	0.46
1:A:767:ARG:CZ	1:A:794:TYR:HB2	2.45	0.46
2:B:322:LEU:HB3	2:B:325:ARG:HG3	1.98	0.46
3:D:32:PRO:HA	3:D:35:ILE:HG12	1.97	0.46
5:F:422:TYR:CE2	5:F:424:LYS:HD3	2.51	0.46
6:C:30:ARG:HG2	6:C:34:GLN:HE22	1.81	0.46
7:P:1104:GLY:HA3	7:P:1126:VAL:HA	1.98	0.46
2:B:31:LYS:HA	2:B:31:LYS:HD2	1.72	0.46
5:F:72:GLU:HA	5:F:75:ILE:HG12	1.98	0.46
1:A:645:GLU:OE2	1:A:748:ASN:ND2	2.49	0.46
2:B:261:LEU:HD13	2:B:286:VAL:HB	1.97	0.46
2:B:381:GLN:HG2	2:B:386:THR:HA	1.98	0.46
3:D:147:PHE:HB3	3:D:167:LEU:CD2	2.46	0.46
4:E:77:PHE:O	4:E:78:ARG:HD2	2.16	0.46
6:C:128:ASN:O	6:C:129:TYR:C	2.59	0.46
1:A:77:VAL:HG13	5:F:26:ASP:HB3	1.99	0.45
2:B:133:ALA:O	2:B:142:ALA:N	2.48	0.45
3:D:67:TYR:HD2	6:C:89:LEU:HB2	1.81	0.45
3:D:147:PHE:HB3	3:D:167:LEU:HD22	1.98	0.45
1:A:479:THR:HG23	1:A:481:ASP:N	2.29	0.45
1:A:719:ILE:HA	1:A:736:SER:HB2	1.98	0.45
2:B:193:SER:OG	2:B:194:LEU:N	2.49	0.45
5:F:416:GLU:OE2	5:F:417:GLN:HG3	2.16	0.45
2:B:328:THR:HG22	2:B:340:GLY:H	1.81	0.45
2:B:378:LEU:HB3	2:B:390:ILE:CG2	2.46	0.45
7:P:1268:ILE:H	7:P:1272:VAL:HG23	1.82	0.45
1:A:614:ASP:OD1	1:A:615:THR:N	2.50	0.45
4:E:74:PHE:HD1	4:E:92:THR:HG23	1.82	0.45
1:A:493:ASP:HA	1:A:507:LYS:HA	1.99	0.45
2:B:36:PRO:HB2	2:B:359:GLN:NE2	2.31	0.45
7:P:1024:ASN:O	7:P:1029:MET:N	2.48	0.45
1:A:43:LEU:HA	1:A:46:MET:HE2	1.99	0.45
3:D:102:HIS:HB3	3:D:105:ILE:HG23	1.99	0.45
3:D:137:PRO:O	3:D:139:HIS:N	2.49	0.45
4:E:95:PHE:CD1	4:E:101:LEU:HA	2.52	0.45
5:F:76:MET:O	5:F:80:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:ASN:HD22	2:B:304:ARG:HD2	1.82	0.45
2:B:79:GLY:O	2:B:97:LEU:N	2.50	0.45
1:A:72:PHE:HA	1:A:90:GLU:HA	1.97	0.44
1:A:180:ILE:HD13	1:A:256:VAL:HB	1.99	0.44
1:A:264:ASP:OD1	1:A:265:GLN:N	2.48	0.44
1:A:484:SER:N	1:A:516:GLY:O	2.33	0.44
1:A:749:TRP:CZ3	1:A:760:TYR:HB2	2.52	0.44
2:B:348:TRP:HE1	2:B:360:GLN:CD	2.25	0.44
3:D:162:ASP:OD1	6:C:41:TYR:OH	2.24	0.44
4:E:53:GLN:OE1	4:E:53:GLN:N	2.44	0.44
6:C:167:PRO:O	6:C:174:VAL:N	2.33	0.44
7:P:1157:TYR:O	7:P:1168:GLU:HA	2.17	0.44
1:A:745:TRP:CD1	1:A:763:PRO:HG3	2.52	0.44
1:A:664:GLN:HB3	1:A:667:THR:HB	1.99	0.44
1:A:37:VAL:HG13	1:A:42:ALA:HB2	2.00	0.44
1:A:651:ASN:OD1	1:A:709:ASN:HA	2.17	0.44
3:D:79:TYR:HB3	3:D:88:ALA:HB2	2.00	0.44
5:F:69:GLN:O	5:F:72:GLU:HG3	2.18	0.44
1:A:433:GLY:O	1:A:437:GLY:N	2.50	0.44
3:D:137:PRO:HA	3:D:173:ARG:HH12	1.83	0.44
1:A:46:MET:HB3	1:A:66:LEU:HD21	1.99	0.44
2:B:296:ILE:HD11	2:B:310:ILE:HG22	1.98	0.44
3:D:72:GLN:O	3:D:76:ILE:HG12	2.16	0.44
1:A:259:ASN:HD21	2:B:168:ASN:HD21	1.65	0.44
6:C:89:LEU:C	6:C:106:LEU:HD21	2.42	0.44
1:A:751:SER:O	1:A:755:SER:OG	2.27	0.44
2:B:345:TYR:CZ	2:B:361:LYS:HD3	2.53	0.44
1:A:35:GLN:CD	1:A:35:GLN:H	2.25	0.44
1:A:550:TYR:HE1	1:A:556:PRO:HD2	1.82	0.44
2:B:97:LEU:HD12	2:B:132:TYR:CZ	2.52	0.44
2:B:168:ASN:HB2	2:B:170:GLN:OE1	2.18	0.44
3:D:41:GLN:O	3:D:44:GLN:HB3	2.17	0.44
1:A:62:THR:O	1:A:66:LEU:HD23	2.18	0.43
1:A:585:TYR:HD1	1:A:586:PHE:CE1	2.36	0.43
1:A:655:GLY:C	1:A:666:ASN:H	2.23	0.43
7:P:1020:ASN:C	7:P:1022:VAL:H	2.25	0.43
1:A:636:GLY:HA3	1:A:652:PHE:CZ	2.51	0.43
3:D:92:ILE:HG21	3:D:112:ARG:HB2	2.00	0.43
3:D:225:MET:HE2	3:D:225:MET:HA	2.00	0.43
1:A:38:ALA:HB3	1:A:41:ALA:HB3	2.01	0.43
1:A:202:GLU:HB3	1:A:212:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:CYS:HB2	7:P:1298:TYR:O	2.18	0.43
3:D:216:PRO:HA	3:D:219:GLU:HG3	2.00	0.43
7:P:1073:LEU:N	7:P:1076:LEU:O	2.52	0.43
1:A:108:ASP:HA	1:A:111:LYS:HE2	2.00	0.43
3:D:161:THR:HG22	6:C:72:GLY:HA2	2.01	0.43
4:E:81:PRO:HD2	4:E:84:GLU:HB2	2.00	0.43
2:B:372:VAL:O	2:B:378:LEU:HD12	2.18	0.43
7:P:1079:PHE:CB	7:P:1110:SER:O	2.65	0.43
2:B:252:VAL:HG21	2:B:291:VAL:HG11	2.01	0.43
1:A:47:PRO:HD2	1:A:62:THR:HG23	1.99	0.43
1:A:102:ASN:ND2	1:A:107:ASP:OD1	2.51	0.43
1:A:634:ARG:HH12	1:A:659:THR:HG22	1.83	0.43
5:F:32:VAL:HB	5:F:423:VAL:HG23	2.01	0.43
3:D:234:VAL:O	3:D:237:ILE:HB	2.18	0.43
2:B:98:ALA:HB1	2:B:106:LYS:HA	2.01	0.43
2:B:211:GLY:H	2:B:247:VAL:HG13	1.84	0.43
2:B:239:THR:O	2:B:243:ARG:NE	2.50	0.43
1:A:325:MET:SD	1:A:325:MET:N	2.92	0.42
2:B:104:PHE:N	2:B:107:GLU:OE2	2.50	0.42
2:B:341:ASP:OD2	2:B:347:HIS:NE2	2.42	0.42
6:C:67:ILE:HD12	6:C:68:PRO:HD2	2.01	0.42
1:A:197:PHE:HD1	1:A:222:ASP:HB3	1.84	0.42
2:B:32:MET:SD	2:B:32:MET:N	2.92	0.42
1:A:76:ARG:HB2	1:A:87:GLN:HG3	2.00	0.42
1:A:79:ARG:HD2	1:A:79:ARG:HA	1.81	0.42
3:D:219:GLU:OE2	3:D:235:ALA:HA	2.20	0.42
5:F:413:TRP:HE1	5:F:417:GLN:CD	2.27	0.42
1:A:179:GLN:HB3	1:A:255:TYR:CG	2.55	0.42
1:A:749:TRP:HB3	1:A:761:SER:HB2	2.02	0.42
1:A:669:GLY:O	1:A:671:LYS:NZ	2.32	0.42
2:B:122:VAL:CG1	2:B:134:LEU:HB2	2.50	0.42
2:B:278:MET:SD	2:B:278:MET:N	2.93	0.42
6:C:125:ALA:H	6:C:130:THR:CA	2.33	0.42
1:A:166:LYS:NZ	1:A:167:LEU:O	2.50	0.42
2:B:346:LEU:HB3	2:B:360:GLN:HB2	2.01	0.42
6:C:88:PRO:HA	6:C:200:GLU:OE2	2.20	0.42
2:B:265:GLY:HA2	2:B:285:SER:N	2.34	0.42
2:B:294:ASN:O	2:B:295:ARG:NE	2.53	0.42
7:P:1269:ARG:H	7:P:1272:VAL:CG2	2.32	0.42
1:A:385:GLY:O	1:A:389:LEU:HD23	2.20	0.42
1:A:795:ASP:OD1	1:A:796:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ALA:HB3	2:B:389:SER:HB3	2.02	0.42
6:C:161:TYR:O	6:C:180:ASN:N	2.53	0.42
1:A:170:GLN:N	1:A:170:GLN:OE1	2.53	0.42
1:A:536:LEU:HD11	1:A:565:PHE:HB3	2.02	0.42
1:A:593:VAL:HG12	1:A:615:THR:HG23	2.01	0.42
2:B:175:ASN:HB2	2:B:182:LYS:NZ	2.35	0.42
1:A:623:ASP:OD1	1:A:624:ASP:N	2.53	0.41
1:A:131:ALA:HB2	5:F:422:TYR:CE1	2.55	0.41
1:A:223:LEU:HD11	1:A:243:THR:HG21	2.02	0.41
1:A:671:LYS:HA	1:A:705:ALA:HA	2.01	0.41
1:A:777:MET:HE3	1:A:777:MET:HA	2.01	0.41
2:B:225:GLN:NE2	5:F:155:GLN:HG3	2.35	0.41
3:D:75:LEU:HD11	3:D:79:TYR:CZ	2.55	0.41
4:E:27:VAL:O	4:E:83:HIS:NE2	2.51	0.41
4:E:73:TRP:CG	4:E:95:PHE:HE2	2.38	0.41
1:A:54:VAL:HG21	1:A:59:ILE:HD11	2.02	0.41
1:A:578:TYR:HB3	1:A:593:VAL:CG2	2.50	0.41
1:A:38:ALA:O	1:A:42:ALA:N	2.33	0.41
1:A:578:TYR:HB3	1:A:593:VAL:HG22	2.02	0.41
1:A:410:ASP:OD1	1:A:410:ASP:N	2.54	0.41
1:A:449:TRP:O	1:A:452:THR:HG22	2.20	0.41
2:B:194:LEU:HD23	2:B:244:LEU:HD22	2.02	0.41
2:B:367:PHE:CZ	2:B:382:ALA:HB2	2.56	0.41
3:D:53:THR:O	3:D:56:GLU:HG2	2.20	0.41
4:E:74:PHE:CD1	4:E:92:THR:HG23	2.55	0.41
2:B:88:ASP:OD1	2:B:88:ASP:N	2.53	0.41
5:F:66:LEU:HA	5:F:69:GLN:NE2	2.35	0.41
5:F:147:ARG:NH2	5:F:402:MET:HE1	2.35	0.41
1:A:52:ASP:CG	1:A:53:THR:H	2.29	0.41
1:A:76:ARG:CB	1:A:87:GLN:HE21	2.34	0.41
1:A:134:GLU:HG2	1:A:138:GLU:OE2	2.21	0.41
3:D:148:SER:HA	3:D:151:VAL:HG12	2.02	0.41
4:E:47:ARG:NH1	4:E:48:VAL:O	2.54	0.41
1:A:392:LEU:HB3	1:A:394:PHE:CE1	2.56	0.41
1:A:582:ASP:OD1	1:A:583:ARG:N	2.53	0.41
1:A:673:VAL:HG11	1:A:699:LEU:HB3	2.03	0.41
1:A:745:TRP:CD2	1:A:763:PRO:HB3	2.56	0.41
2:B:188:ASP:OD1	2:B:189:MET:N	2.53	0.41
3:D:232:GLU:O	3:D:235:ALA:HB3	2.21	0.41
5:F:395:ASP:HB2	5:F:396:ARG:NH2	2.36	0.41
1:A:230:TYR:HD2	1:A:238:PHE:CE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:TYR:HB2	1:A:347:PHE:HE2	1.86	0.41
1:A:543:VAL:HG22	1:A:544:ALA:N	2.36	0.41
1:A:636:GLY:O	1:A:710:ALA:HA	2.20	0.41
2:B:349:ILE:HG13	2:B:355:ARG:O	2.21	0.41
1:A:221:GLY:O	1:A:225:THR:HG23	2.22	0.40
6:C:125:ALA:O	6:C:129:TYR:N	2.52	0.40
1:A:151:VAL:HG12	1:A:169:PHE:CD1	2.56	0.40
1:A:634:ARG:NH1	1:A:659:THR:HG22	2.37	0.40
2:B:217:SER:HB2	2:B:226:MET:SD	2.62	0.40
5:F:32:VAL:HA	5:F:423:VAL:HA	2.03	0.40
5:F:42:VAL:HA	5:F:45:LEU:HG	2.03	0.40
1:A:71:ASN:OD1	1:A:91:ARG:NH2	2.51	0.40
1:A:500:ASP:OD2	1:A:538:ASN:ND2	2.54	0.40
2:B:310:ILE:HG13	2:B:311:ASP:N	2.37	0.40
3:D:61:ARG:HG3	3:D:62:TYR:CD2	2.55	0.40
1:A:297:ASN:OD1	1:A:300:LYS:N	2.44	0.40
1:A:352:ILE:HG13	1:A:414:VAL:HG23	2.04	0.40
1:A:534:ASN:OD1	1:A:535:SER:N	2.55	0.40
4:E:38:LEU:HD23	4:E:77:PHE:CE1	2.56	0.40
5:F:413:TRP:HA	5:F:416:GLU:HG3	2.02	0.40
1:A:97:ILE:HD13	1:A:97:ILE:HA	1.92	0.40
2:B:367:PHE:HE2	2:B:380:ILE:HG23	1.87	0.40
3:D:95:PHE:CE2	3:D:108:VAL:HG21	2.56	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	756/790 (96%)	701 (93%)	54 (7%)	1 (0%)	48	83
2	B	362/373 (97%)	326 (90%)	36 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	216/226 (96%)	199 (92%)	16 (7%)	1 (0%)	24	63
4	E	83/104 (80%)	79 (95%)	4 (5%)	0	100	100
5	F	152/450 (34%)	146 (96%)	6 (4%)	0	100	100
6	C	168/320 (52%)	147 (88%)	19 (11%)	2 (1%)	10	42
7	P	298/364 (82%)	281 (94%)	17 (6%)	0	100	100
All	All	2035/2627 (78%)	1879 (92%)	152 (8%)	4 (0%)	44	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	563	ASN
3	D	138	GLN
6	C	126	GLN
6	C	125	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	651/672 (97%)	649 (100%)	2 (0%)	86	84
2	B	295/304 (97%)	295 (100%)	0	100	100
3	D	183/190 (96%)	183 (100%)	0	100	100
4	E	74/90 (82%)	74 (100%)	0	100	100
5	F	139/367 (38%)	139 (100%)	0	100	100
6	C	79/258 (31%)	78 (99%)	1 (1%)	61	73
7	P	16/289 (6%)	16 (100%)	0	100	100
All	All	1437/2170 (66%)	1434 (100%)	3 (0%)	85	85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	VAL
1	A	77	VAL
6	C	128	ASN

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

Mol	Chain	Res	Type
1	A	87	GLN
1	A	179	GLN
1	A	323	GLN
1	A	540	GLN
1	A	625	HIS
1	A	664	GLN
2	B	144	GLN
2	B	168	ASN
2	B	230	GLN
2	B	234	GLN
2	B	381	GLN
3	D	89	GLN
3	D	99	ASN
3	D	158	GLN
5	F	69	GLN
5	F	85	GLN
6	C	128	ASN
6	C	195	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

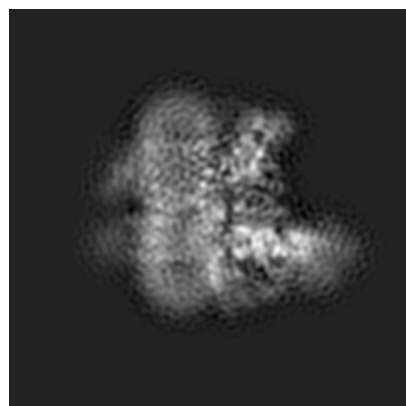
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18562. These allow visual inspection of the internal detail of the map and identification of artifacts.

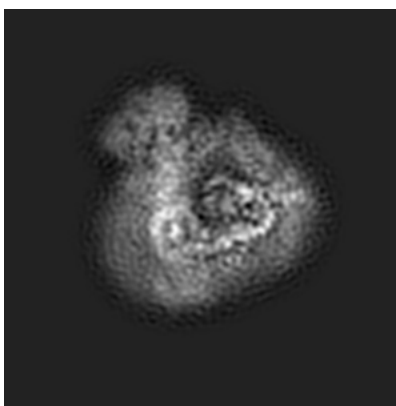
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

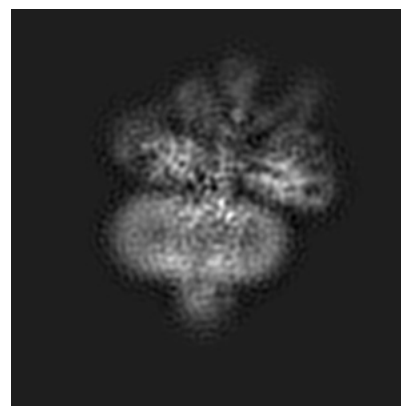
6.1.1 Primary map



X

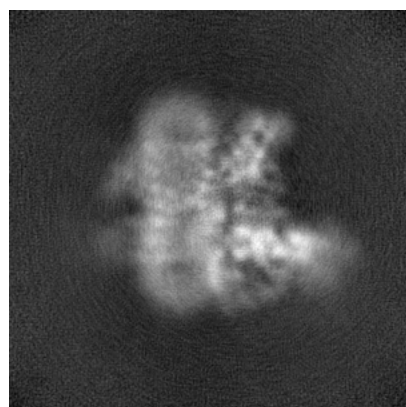


Y

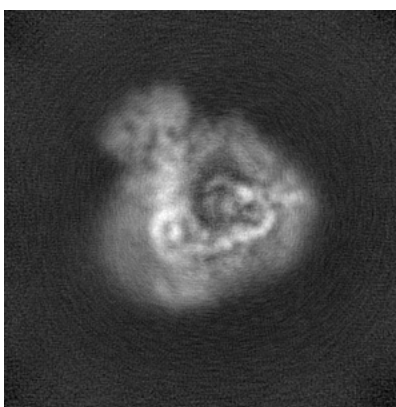


Z

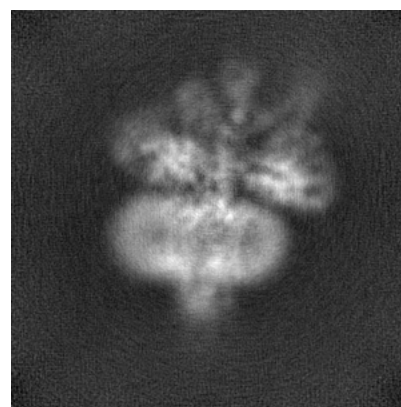
6.1.2 Raw map



X



Y

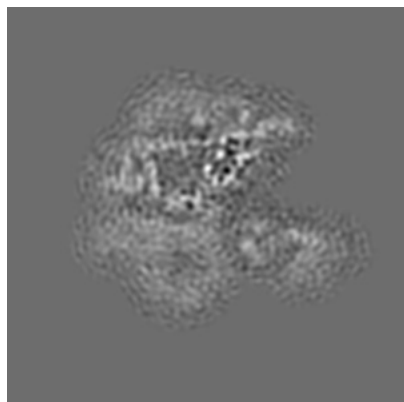


Z

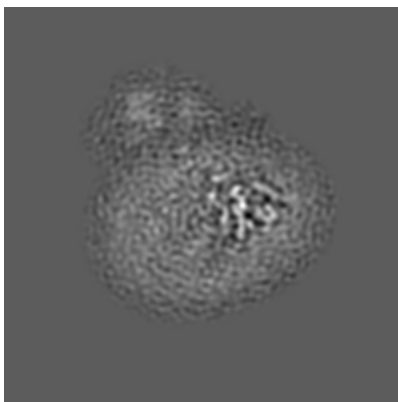
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

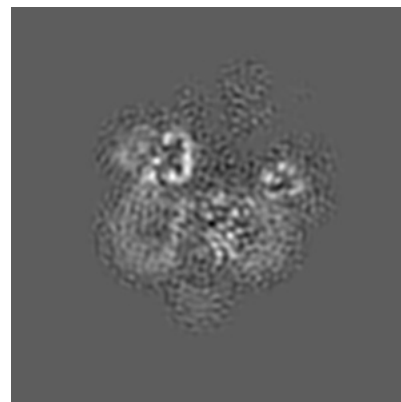
6.2.1 Primary map



X Index: 150

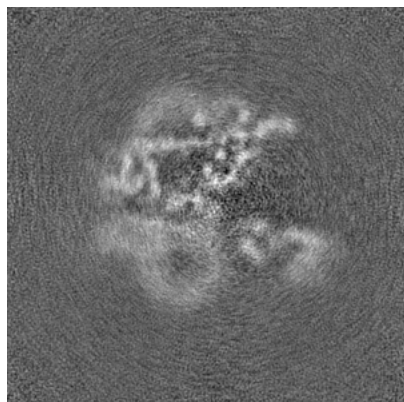


Y Index: 150

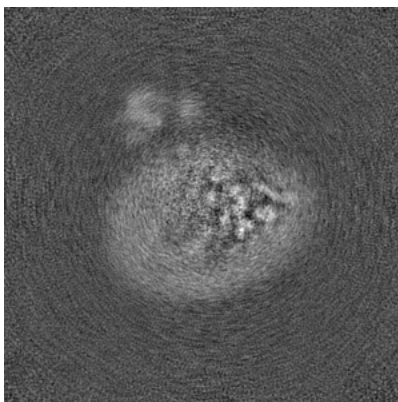


Z Index: 150

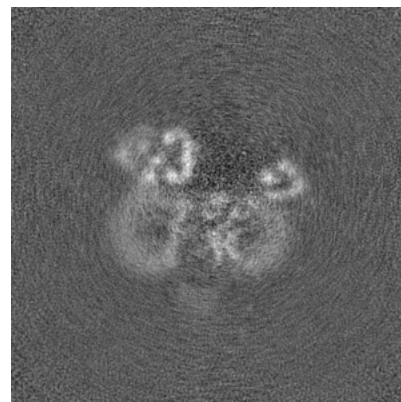
6.2.2 Raw map



X Index: 150



Y Index: 150

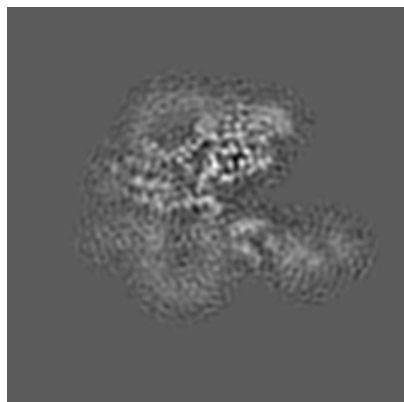


Z Index: 150

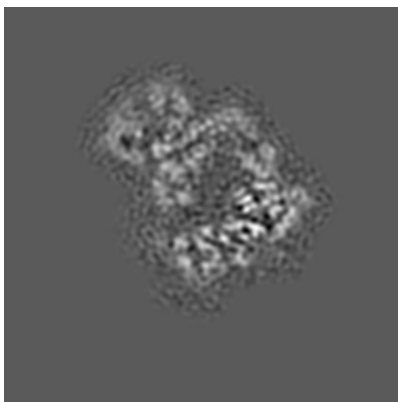
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

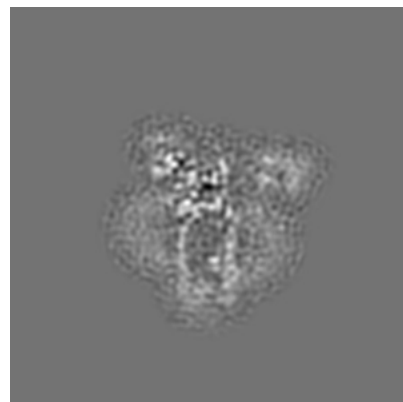
6.3.1 Primary map



X Index: 157

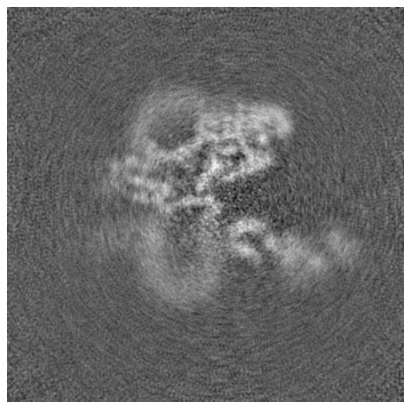


Y Index: 175

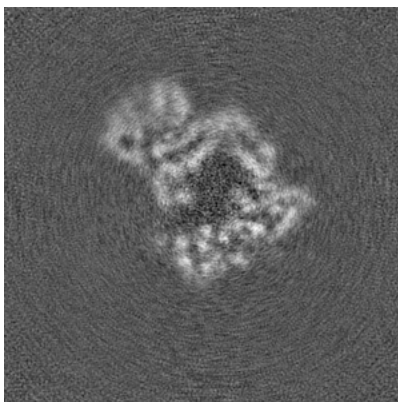


Z Index: 177

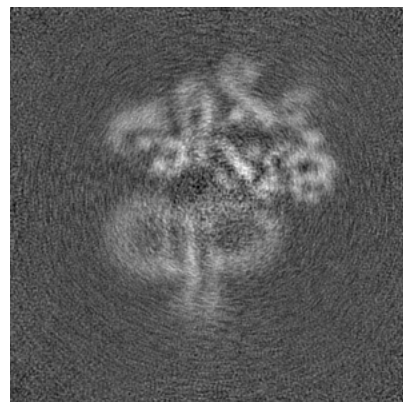
6.3.2 Raw map



X Index: 158



Y Index: 174

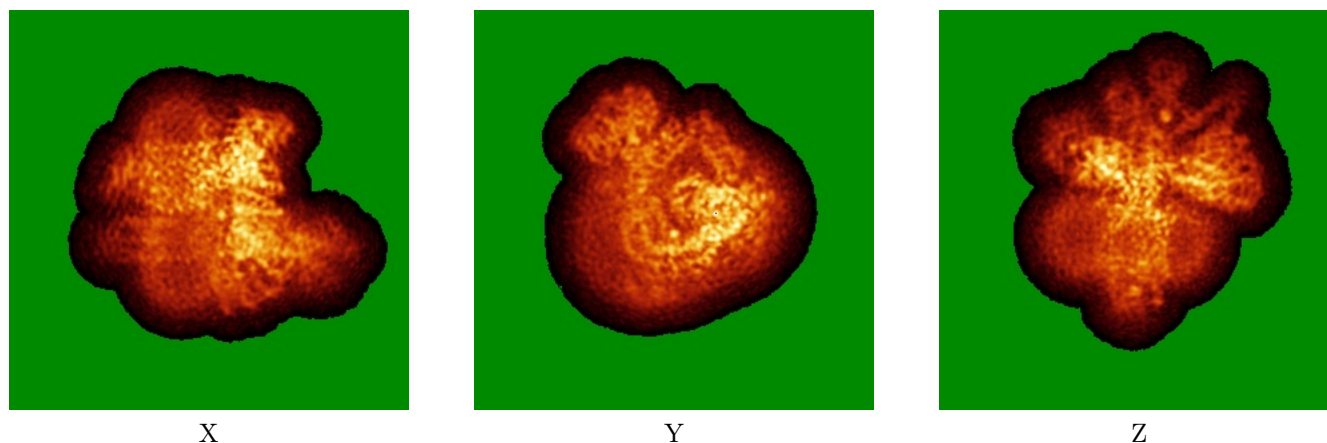


Z Index: 128

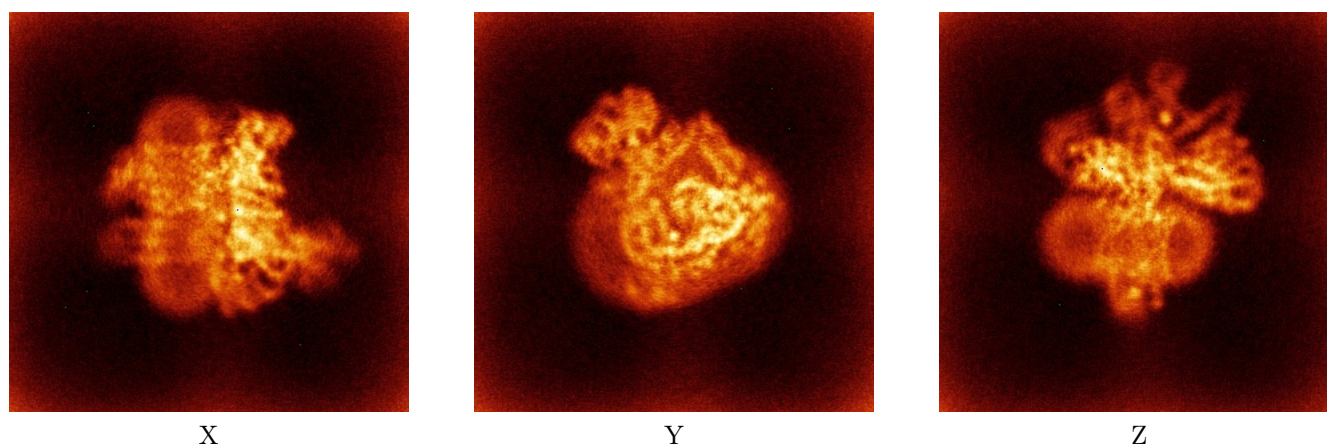
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

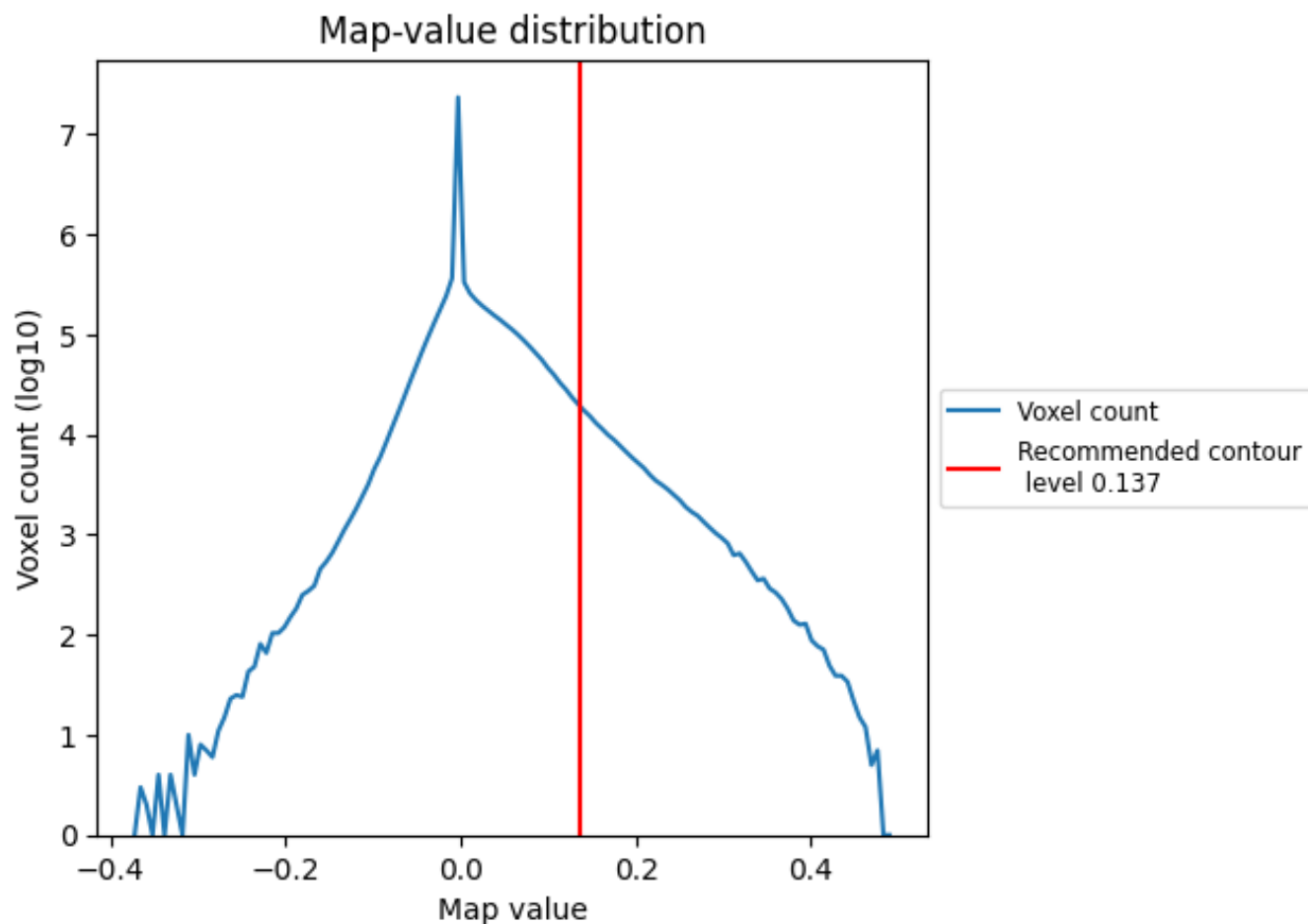
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

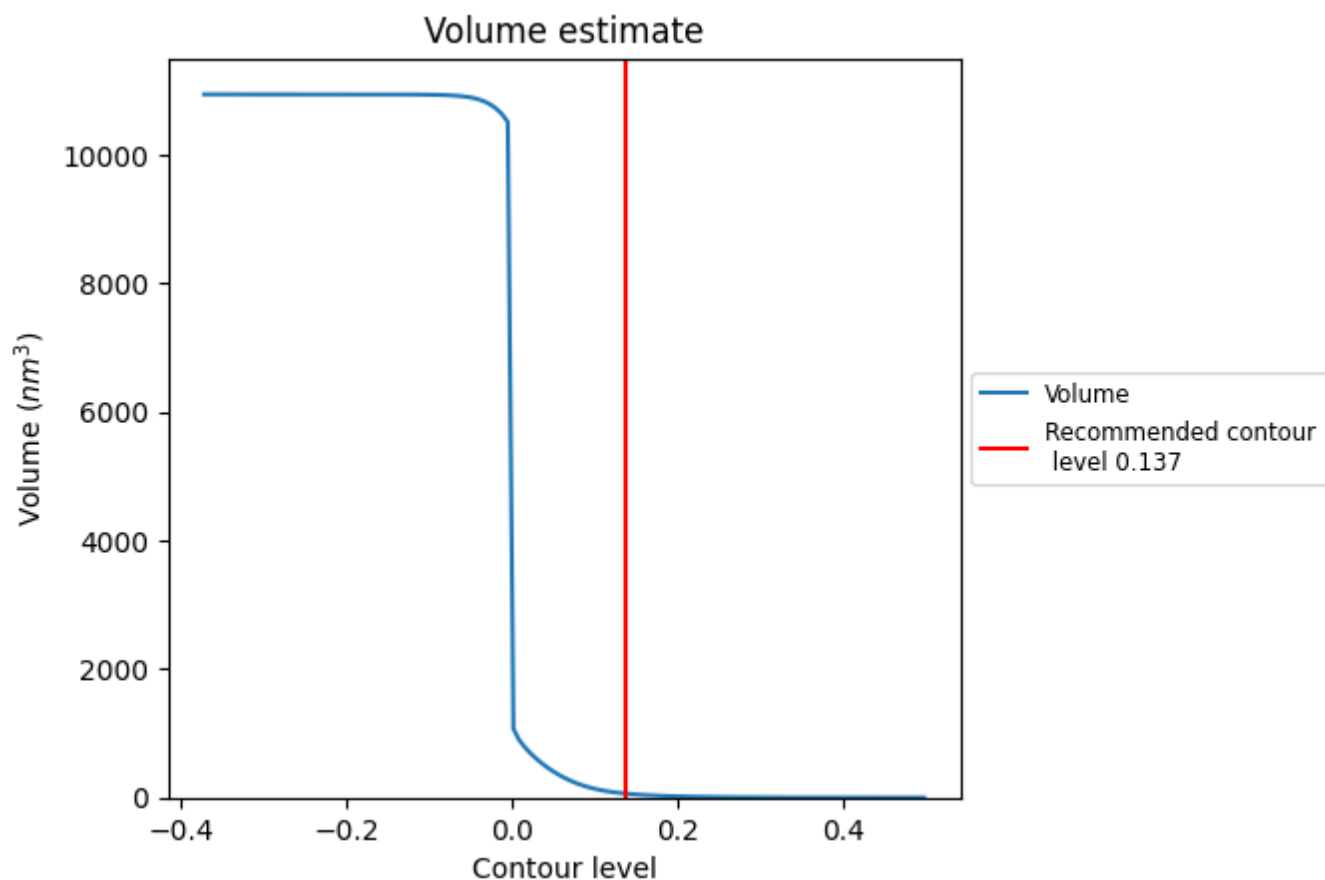
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

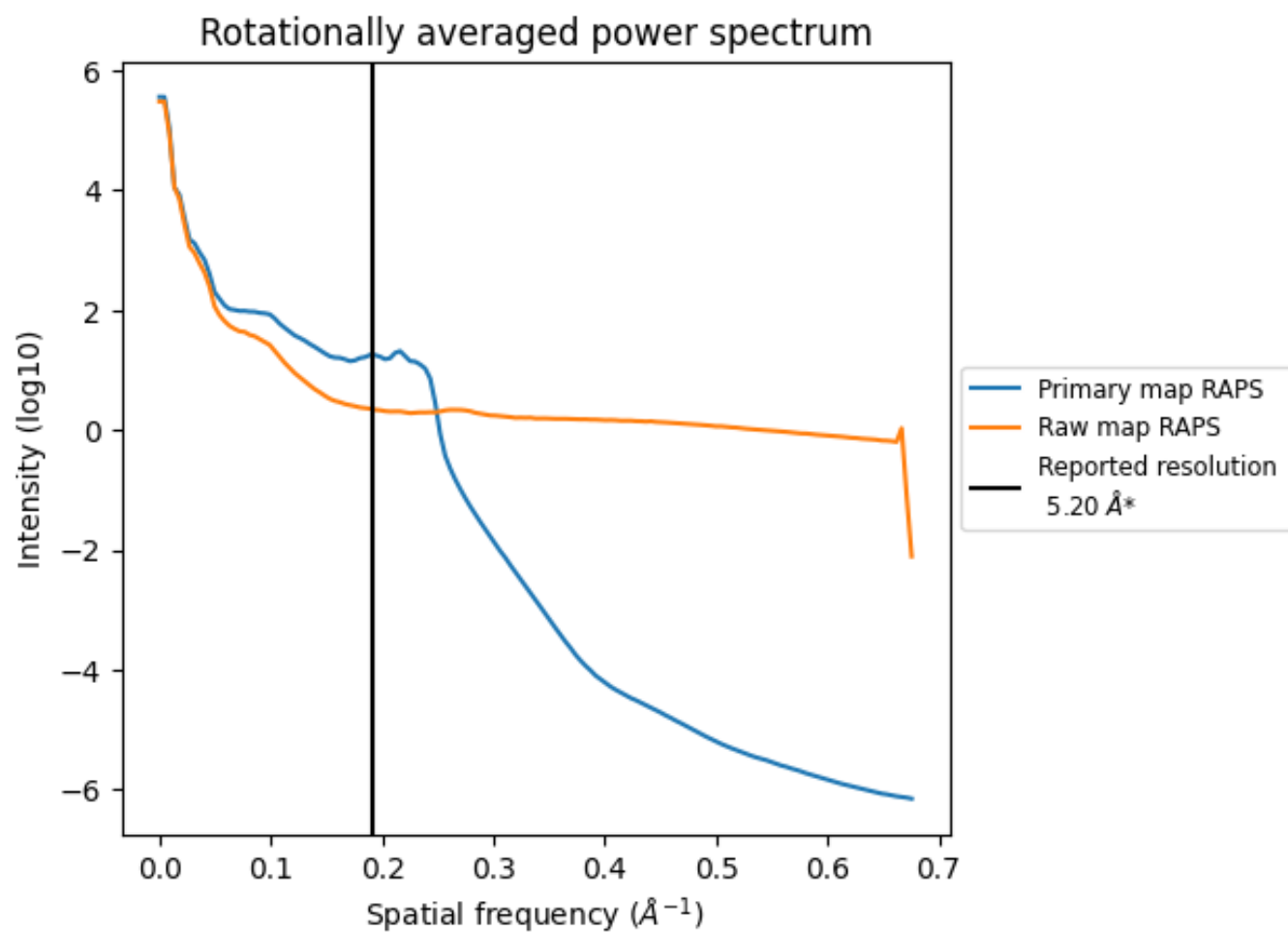
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 61 nm³; this corresponds to an approximate mass of 55 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

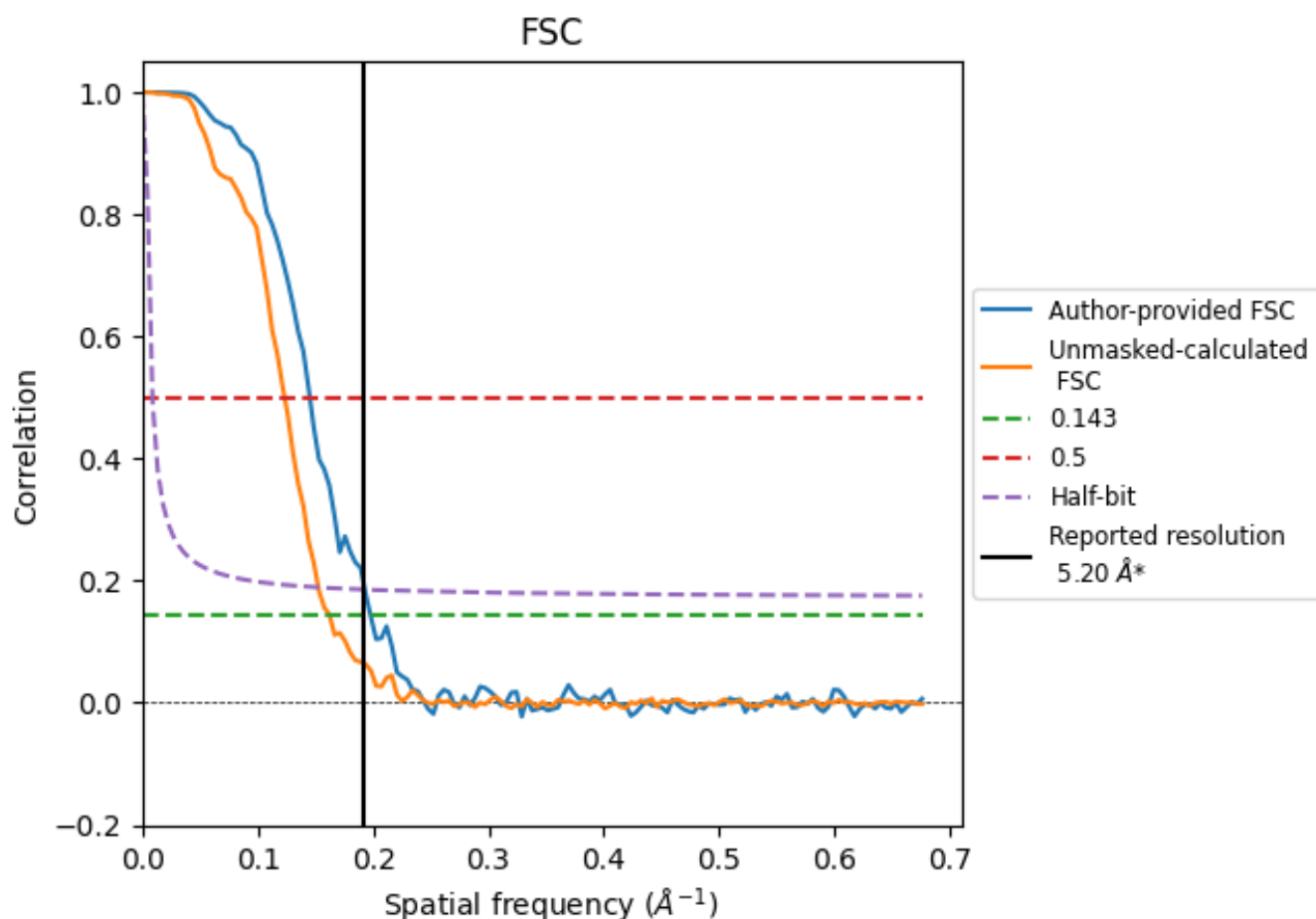


*Reported resolution corresponds to spatial frequency of 0.192 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.192 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

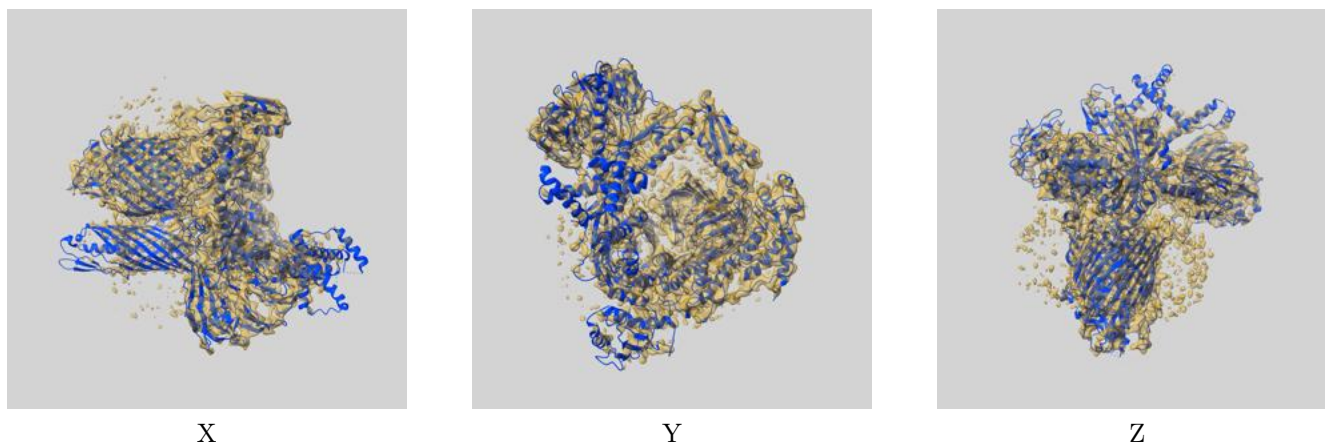
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.20	-	-
Author-provided FSC curve	5.06	6.88	5.18
Unmasked-calculated*	6.16	8.10	6.55

*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 6.16 differs from the reported value 5.2 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18562 and PDB model 8QPU. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



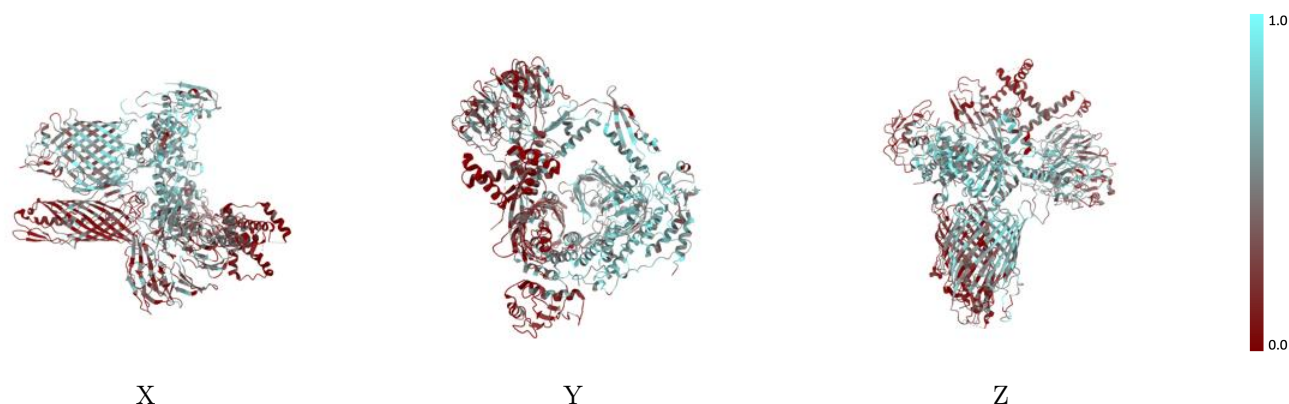
The images above show the 3D surface view of the map at the recommended contour level 0.137 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



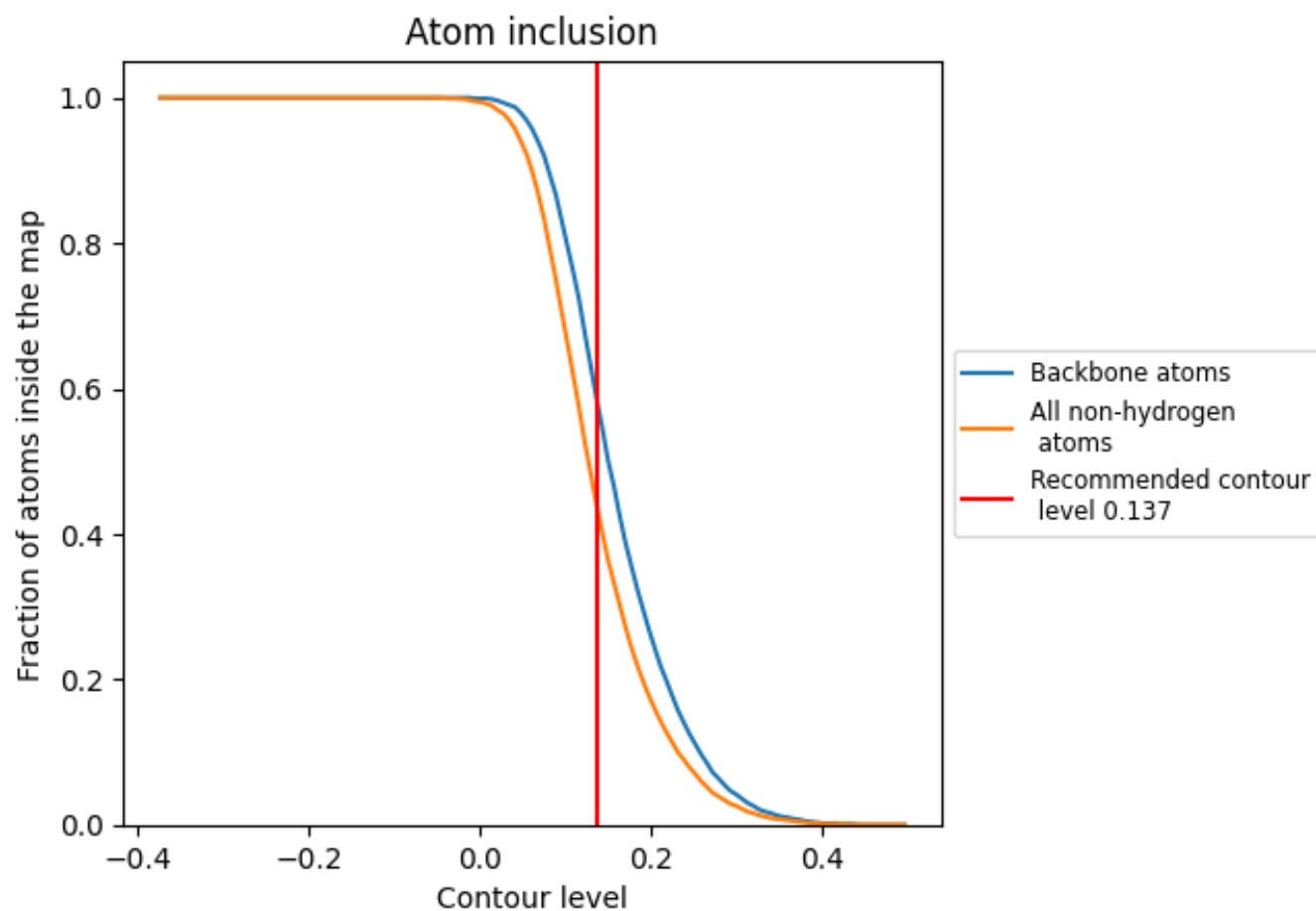
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.137).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 44% 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 (0.137) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4400	0.3380
A	0.5190	0.3670
B	0.4020	0.3310
C	0.3400	0.3140
D	0.6400	0.3730
E	0.6110	0.3860
F	0.1830	0.2690
P	0.1840	0.2460

1.0

0.0

<0.0