



Full wwPDB EM Validation Report ⓘ

Aug 18, 2026 – 07:23 am BST

PDB ID : 28JU / pdb_000028ju
EMDB ID : EMD-56559
Title : Poised Complex: BAM bound BepA
Authors : Fenn, K.L.; Ranson, N.A.
Deposited on : 2026-02-04
Resolution : 5.30 Å (reported)
Based on initial models : 28JQ, .

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:

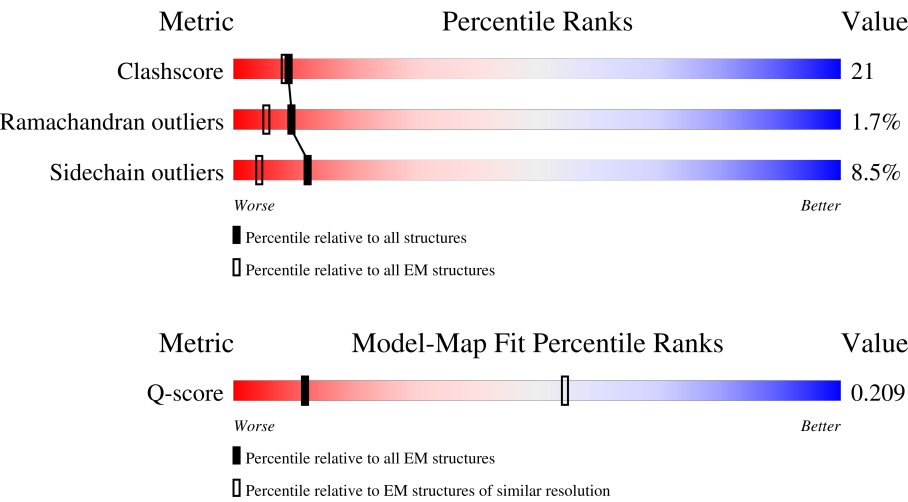
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 5.30 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	625 (4.80 - 5.80)

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	C	320	91% 30% 39% 25% 5%
2	D	226	32% 63% 30% . .
3	E	104	30% 67% 22% 11%
4	B	373	60% 77% 23%

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Mol	Chain	Length	Quality of chain
5	A	790	42% 68% 27% . .
6	F	492	59% 72% 13% 16%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16808 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 BamC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	317	Total	C	N	O	S	0	0
			2234	1382	405	442	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	218	Total	C	N	O	S	0	0
			1764	1111	309	337	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	93	Total	C	N	O	S	0	0
			724	454	126	142	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
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 4 is a protein called Outer membrane protein assembly factor BamB.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	372	Total	C	N	O	S	0	0
			2802	1757	479	560	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	770	Total	C	N	O	S	0	0
			6014	3791	1022	1185	16		

- Molecule 6 is a protein called Beta-barrel assembly-enhancing protease.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	415	Total	C	N	O	S	0	0
			3270	2023	602	633	12		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	488	GLY	-	expression tag	UNP P66948
F	489	SER	-	expression tag	UNP P66948
F	490	SER	-	expression tag	UNP P66948
F	491	ALA	-	expression tag	UNP P66948
F	492	TRP	-	expression tag	UNP P66948
F	493	SER	-	expression tag	UNP P66948
F	494	HIS	-	expression tag	UNP P66948
F	495	PRO	-	expression tag	UNP P66948
F	496	GLN	-	expression tag	UNP P66948
F	497	PHE	-	expression tag	UNP P66948
F	498	GLU	-	expression tag	UNP P66948
F	499	LYS	-	expression tag	UNP P66948
F	500	GLY	-	expression tag	UNP P66948
F	501	GLY	-	expression tag	UNP P66948
F	502	GLY	-	expression tag	UNP P66948
F	503	SER	-	expression tag	UNP P66948
F	504	GLY	-	expression tag	UNP P66948
F	505	GLY	-	expression tag	UNP P66948
F	506	GLY	-	expression tag	UNP P66948
F	507	SER	-	expression tag	UNP P66948
F	508	GLY	-	expression tag	UNP P66948
F	509	GLY	-	expression tag	UNP P66948
F	510	SER	-	expression tag	UNP P66948
F	511	ALA	-	expression tag	UNP P66948
F	512	TRP	-	expression tag	UNP P66948

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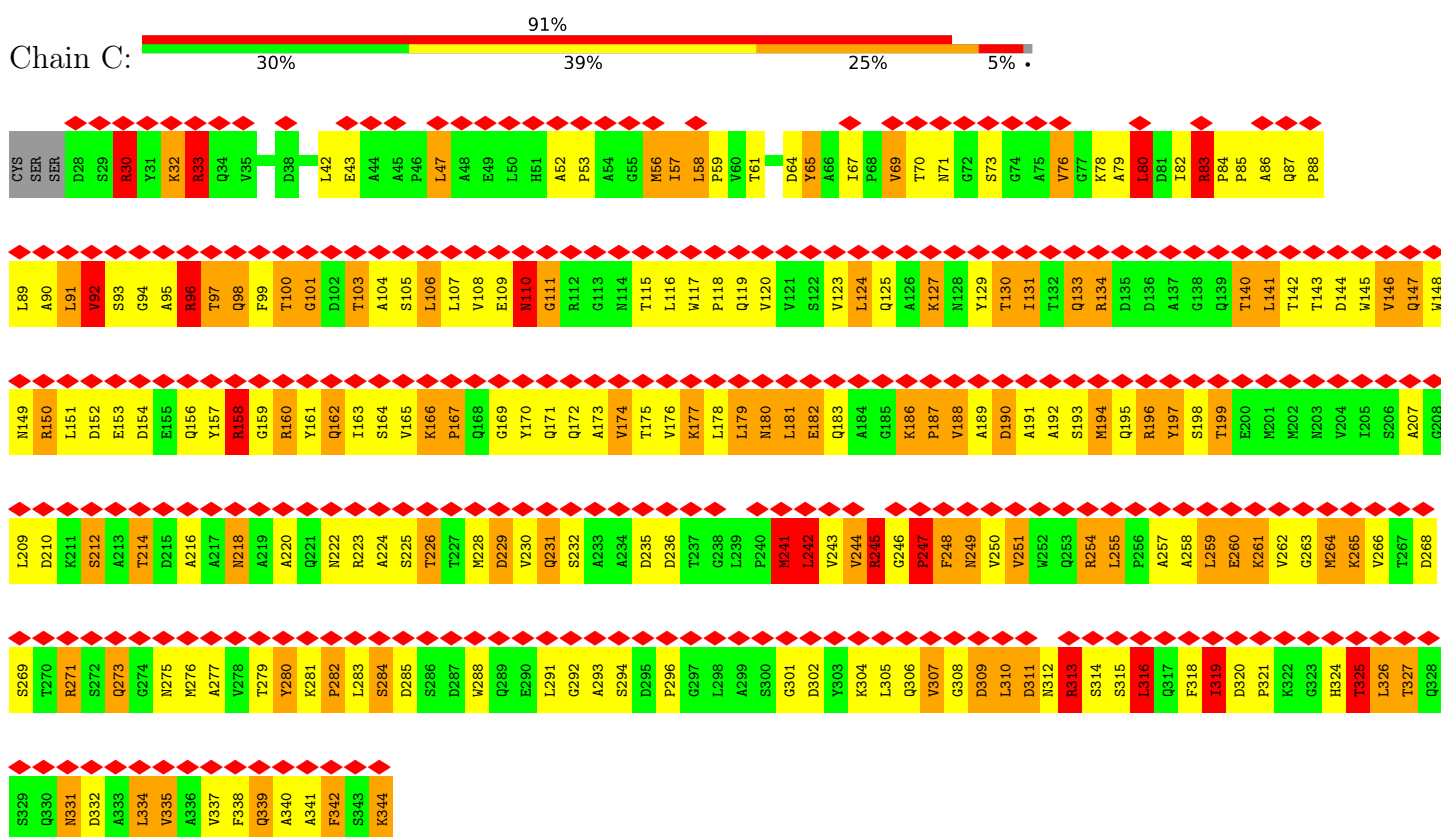
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Chain	Residue	Modelled	Actual	Comment	Reference
F	513	SER	-	expression tag	UNP P66948
F	514	HIS	-	expression tag	UNP P66948
F	515	PRO	-	expression tag	UNP P66948
F	516	GLN	-	expression tag	UNP P66948
F	517	PHE	-	expression tag	UNP P66948
F	518	GLU	-	expression tag	UNP P66948
F	519	LYS	-	expression tag	UNP P66948

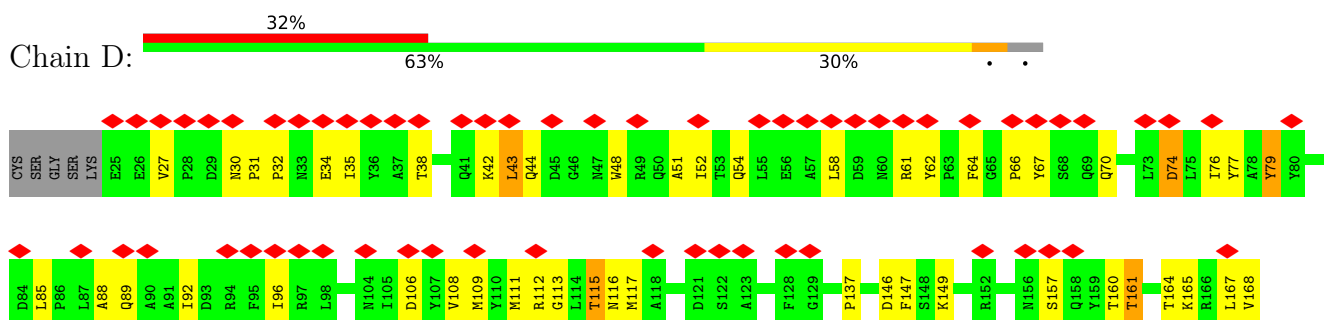
3 Residue-property plots

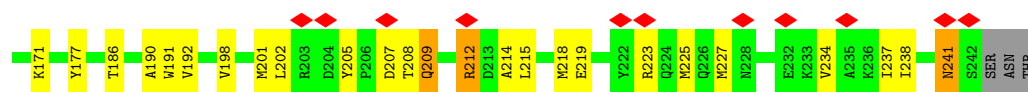
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

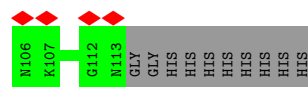
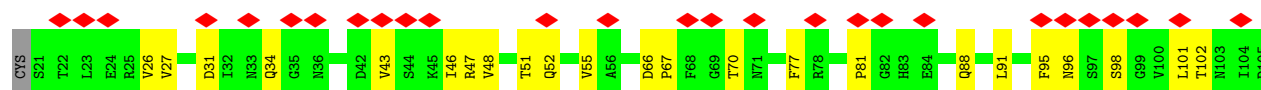


• Molecule 2: Outer membrane protein assembly factor BamD

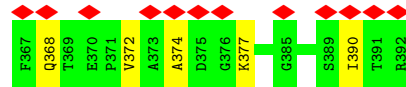
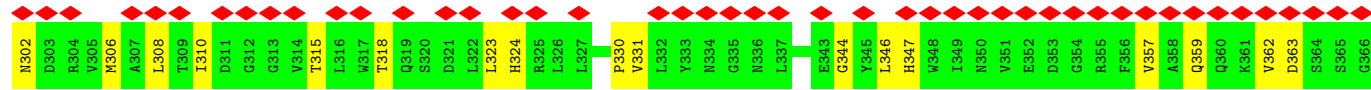
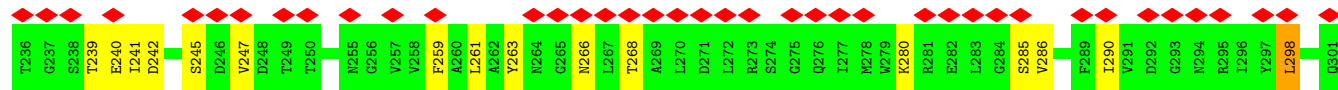
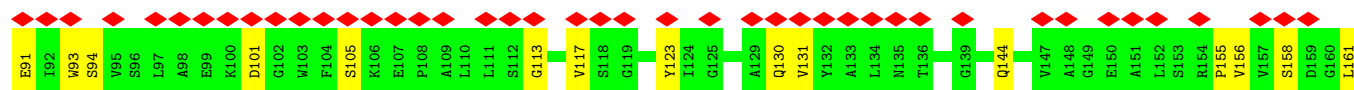
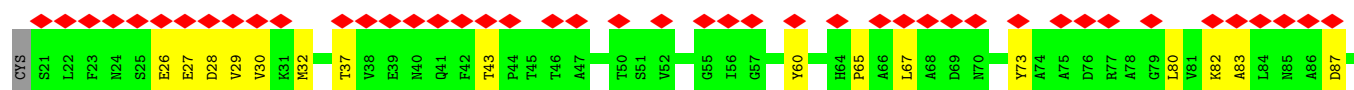
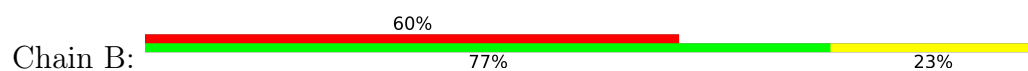




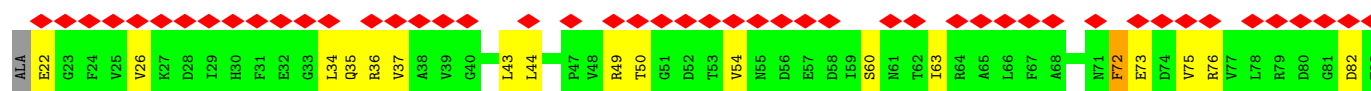
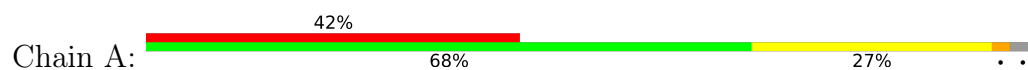
• Molecule 3: Outer membrane protein assembly factor BamE

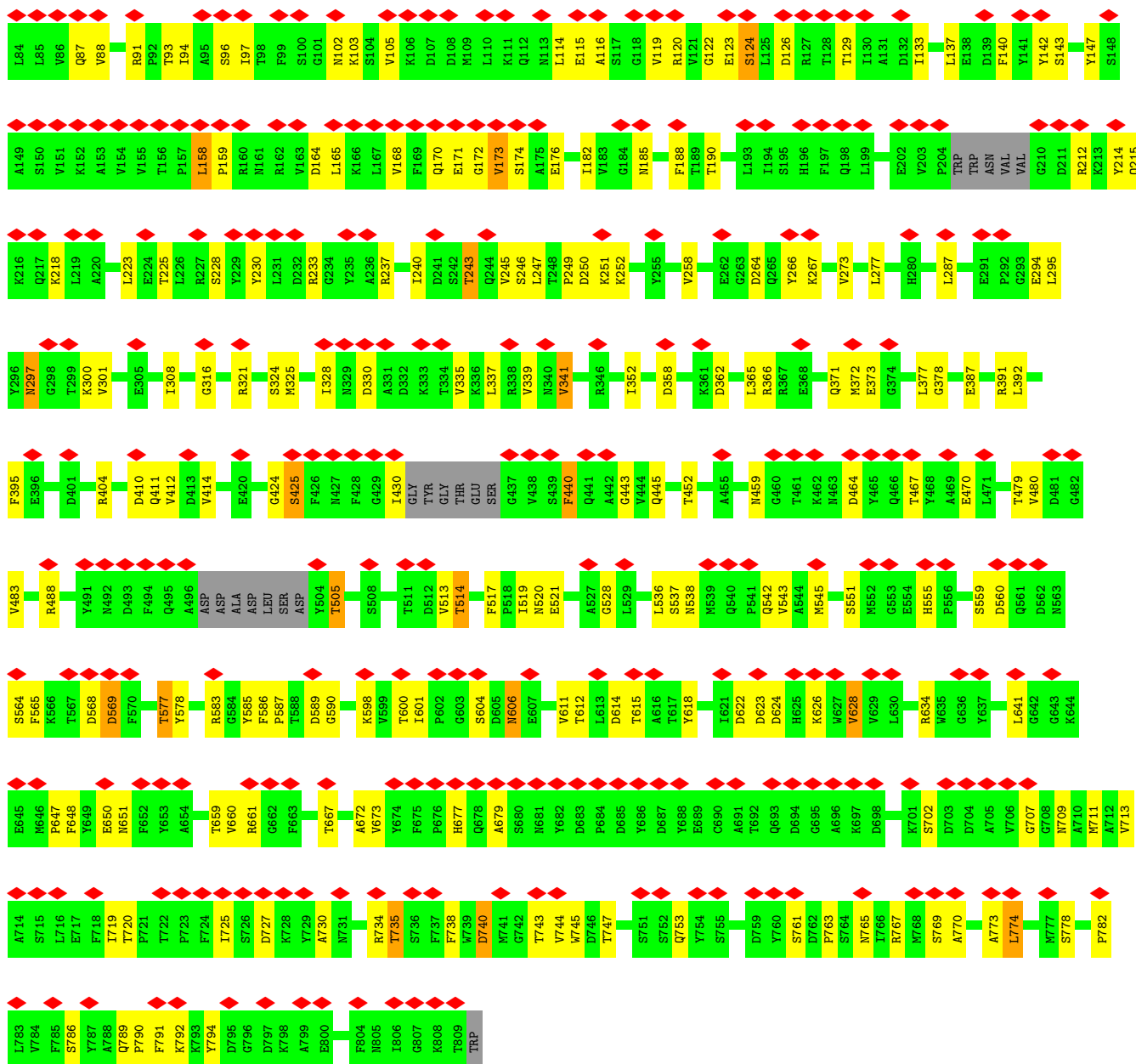


• Molecule 4: Outer membrane protein assembly factor BamB

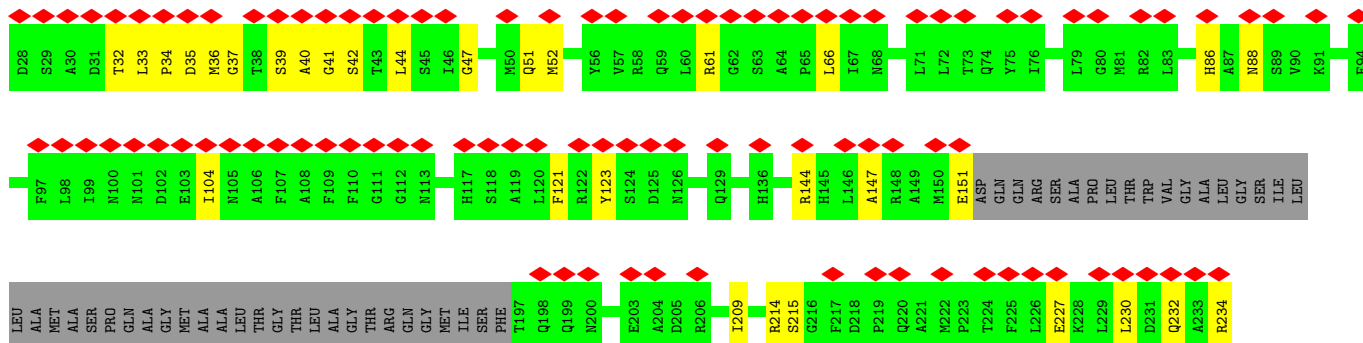


• Molecule 5: Outer membrane protein assembly factor BamA





● Molecule 6: Beta-barrel assembly-enhancing protease





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47000	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.035	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0115	Depositor
Map size (Å)	260.48, 260.48, 260.48	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	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	C	1.04	0/2271	1.25	7/3106 (0.2%)
2	D	0.29	0/1804	0.48	0/2451
3	E	0.27	0/739	0.38	0/1008
4	B	0.70	0/2853	1.03	0/3889
5	A	0.28	0/6145	0.46	0/8333
6	F	0.72	0/3324	1.17	0/4496
All	All	0.60	0/17136	0.87	7/23283 (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	C	0	12

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	342	PHE	CA-CB-CG	7.01	120.81	113.80
1	C	242	LEU	N-CA-CB	6.56	121.12	110.43
1	C	241	MET	CA-C-O	-5.48	114.85	121.32
1	C	197	TYR	CB-CA-C	5.26	119.79	110.85
1	C	316	LEU	N-CA-CB	5.25	119.36	110.49
1	C	242	LEU	CB-CG-CD1	5.14	126.13	110.70
1	C	342	PHE	N-CA-CB	5.02	118.26	109.72

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	150	ARG	Sidechain
1	C	158	ARG	Sidechain
1	C	160	ARG	Sidechain
1	C	196	ARG	Sidechain
1	C	245	ARG	Sidechain
1	C	254	ARG	Sidechain
1	C	271	ARG	Sidechain
1	C	30	ARG	Sidechain
1	C	313	ARG	Sidechain
1	C	33	ARG	Sidechain
1	C	83	ARG	Sidechain
1	C	96	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2234	0	2049	311	0
2	D	1764	0	1700	72	0
3	E	724	0	703	16	0
4	B	2802	0	2743	95	0
5	A	6014	0	5727	217	0
6	F	3270	0	3197	113	0
All	All	16808	0	16119	678	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 21.

All (678) 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:A:143:SER:CB	6:F:42:SER:CB	1.78	1.60
5:A:143:SER:CB	6:F:42:SER:HB3	1.02	1.48
4:B:29:VAL:HG11	5:A:170:GLN:C	1.45	1.40
1:C:150:ARG:NH1	1:C:196:ARG:NH1	1.70	1.39
1:C:57:ILE:HD13	1:C:58:LEU:N	1.32	1.39
1:C:337:VAL:O	1:C:341:ALA:CB	1.71	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:LEU:CG	1:C:174:VAL:HG23	1.53	1.34
1:C:150:ARG:HH12	1:C:196:ARG:NH1	1.21	1.34
5:A:140:PHE:HE1	6:F:42:SER:O	1.02	1.30
5:A:321:ARG:HD2	6:F:234:ARG:CZ	1.59	1.29
1:C:119:GLN:HE21	1:C:209:LEU:CB	1.45	1.28
1:C:106:LEU:CD2	1:C:174:VAL:HG21	1.64	1.26
5:A:140:PHE:CE1	6:F:42:SER:O	1.87	1.26
5:A:43:LEU:CD1	6:F:462:LEU:HD21	1.49	1.25
1:C:141:LEU:CD1	1:C:141:LEU:O	1.85	1.25
5:A:143:SER:OG	6:F:42:SER:CB	1.83	1.24
1:C:141:LEU:O	1:C:141:LEU:HD12	1.36	1.23
1:C:117:TRP:CH2	1:C:141:LEU:HG	1.75	1.20
1:C:96:ARG:O	1:C:98:GLN:OE1	1.60	1.19
5:A:49:ARG:HH12	6:F:428:GLN:NE2	1.40	1.19
1:C:64:ASP:O	1:C:65:TYR:CD2	1.96	1.18
1:C:106:LEU:HD23	1:C:174:VAL:CG2	1.73	1.18
1:C:117:TRP:HH2	1:C:141:LEU:HG	1.05	1.16
1:C:57:ILE:CD1	1:C:58:LEU:N	2.08	1.15
1:C:106:LEU:CD2	1:C:174:VAL:CG2	2.24	1.15
1:C:91:LEU:O	1:C:92:VAL:O	1.61	1.14
1:C:182:GLU:HA	1:C:187:PRO:HA	1.21	1.14
1:C:106:LEU:HG	1:C:174:VAL:CG2	1.79	1.13
1:C:106:LEU:CG	1:C:174:VAL:CG2	2.26	1.13
4:B:29:VAL:CG1	5:A:170:GLN:C	2.21	1.12
5:A:404:ARG:HD3	6:F:237:SER:HA	1.30	1.12
5:A:214:TYR:HE2	6:F:36:MET:HB3	1.15	1.11
5:A:404:ARG:HB3	6:F:237:SER:HB2	1.28	1.11
1:C:106:LEU:HD23	1:C:174:VAL:HG21	1.15	1.10
5:A:43:LEU:HD11	6:F:462:LEU:HD21	1.16	1.10
1:C:90:ALA:HB1	1:C:95:ALA:HB1	1.18	1.10
4:B:29:VAL:H	5:A:172:GLY:HA2	1.09	1.10
4:B:29:VAL:CG1	5:A:170:GLN:HB3	1.81	1.09
1:C:106:LEU:HG	1:C:174:VAL:HG23	1.10	1.09
1:C:264:MET:HA	1:C:280:TYR:HA	1.09	1.09
5:A:215:GLN:OE1	6:F:37:GLY:O	1.70	1.09
1:C:131:ILE:HD12	1:C:141:LEU:HD22	1.28	1.08
4:B:191:SER:HB2	6:F:33:LEU:CD2	1.83	1.08
4:B:27:GLU:OE1	5:A:103:LYS:NZ	1.86	1.08
1:C:337:VAL:O	1:C:341:ALA:HB3	1.43	1.07
5:A:49:ARG:NH1	6:F:428:GLN:NE2	2.00	1.07
1:C:283:LEU:O	1:C:284:SER:O	1.73	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ARG:HB2	1:C:141:LEU:HB2	1.27	1.06
5:A:214:TYR:CE2	6:F:36:MET:HB3	1.91	1.05
1:C:57:ILE:HD13	1:C:57:ILE:C	1.80	1.03
5:A:321:ARG:CD	6:F:234:ARG:CZ	2.33	1.03
4:B:29:VAL:HG11	5:A:170:GLN:O	1.58	1.02
4:B:191:SER:CB	6:F:33:LEU:HD23	1.88	1.02
6:F:484:TYR:HA	6:F:487:MET:HE3	1.39	1.02
1:C:131:ILE:HD12	1:C:141:LEU:CD2	1.89	1.02
6:F:51:GLN:HE21	6:F:480:ARG:HB3	1.25	1.02
1:C:90:ALA:CB	1:C:95:ALA:HB1	1.90	1.01
1:C:134:ARG:HA	1:C:141:LEU:HA	1.43	1.01
4:B:191:SER:HB2	6:F:33:LEU:HD23	1.02	1.01
1:C:337:VAL:O	1:C:341:ALA:N	1.94	1.01
5:A:143:SER:OG	6:F:42:SER:HB2	1.61	1.00
5:A:143:SER:HB3	6:F:42:SER:HB3	1.02	0.99
4:B:29:VAL:CG2	5:A:171:GLU:N	2.27	0.98
1:C:69:VAL:HB	2:D:164:THR:HG21	1.43	0.98
5:A:321:ARG:CD	6:F:234:ARG:NH2	2.27	0.97
5:A:215:GLN:CD	6:F:37:GLY:O	2.09	0.95
5:A:43:LEU:HD11	6:F:462:LEU:CD2	1.97	0.94
4:B:130:GLN:OE1	4:B:144:GLN:NE2	2.01	0.94
5:A:49:ARG:HH12	6:F:428:GLN:HE22	1.05	0.94
1:C:119:GLN:NE2	1:C:209:LEU:CB	2.31	0.94
1:C:337:VAL:O	1:C:341:ALA:HB2	1.66	0.94
1:C:141:LEU:CD1	1:C:141:LEU:C	2.40	0.93
1:C:218:ASN:HA	1:C:222:ASN:HA	1.46	0.93
1:C:106:LEU:CB	1:C:174:VAL:HG23	1.97	0.93
1:C:141:LEU:O	1:C:141:LEU:HD13	1.67	0.92
1:C:117:TRP:HH2	1:C:141:LEU:CG	1.81	0.92
1:C:134:ARG:CB	1:C:141:LEU:HB2	2.00	0.91
1:C:150:ARG:NH1	1:C:196:ARG:HH11	1.48	0.91
5:A:404:ARG:HB3	6:F:237:SER:CB	2.00	0.91
5:A:321:ARG:HD2	6:F:234:ARG:NH2	1.85	0.91
1:C:131:ILE:CD1	1:C:141:LEU:HD22	2.01	0.91
5:A:143:SER:HB2	6:F:42:SER:HB3	0.94	0.90
1:C:150:ARG:HH12	1:C:196:ARG:HH12	1.09	0.90
4:B:113:GLY:O	4:B:155:PRO:HD3	1.72	0.90
1:C:64:ASP:O	1:C:65:TYR:CG	2.24	0.90
4:B:28:ASP:OD2	5:A:252:LYS:NZ	2.05	0.90
5:A:49:ARG:HH12	6:F:428:GLN:CD	1.80	0.90
1:C:106:LEU:HD11	1:C:108:VAL:CG1	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:LEU:CD1	1:C:108:VAL:HG13	2.03	0.89
4:B:29:VAL:HG12	5:A:170:GLN:HB3	1.53	0.89
5:A:321:ARG:CD	6:F:234:ARG:NH1	2.33	0.89
1:C:337:VAL:O	1:C:341:ALA:CA	2.21	0.88
1:C:147:GLN:OE1	1:C:157:TYR:O	1.91	0.88
4:B:29:VAL:CG1	5:A:170:GLN:CB	2.50	0.88
1:C:242:LEU:HA	1:C:331:ASN:ND2	1.88	0.88
6:F:51:GLN:NE2	6:F:480:ARG:HB3	1.89	0.88
5:A:143:SER:HB2	6:F:42:SER:CB	1.67	0.87
1:C:186:LYS:O	1:C:188:VAL:HG23	1.74	0.87
6:F:40:ALA:N	6:F:151:GLU:OE1	2.08	0.86
1:C:167:PRO:HA	1:C:172:GLN:HA	1.58	0.86
4:B:29:VAL:N	5:A:172:GLY:HA2	1.89	0.86
1:C:145:TRP:HE1	1:C:180:ASN:HB2	1.41	0.86
1:C:141:LEU:C	1:C:141:LEU:HD13	2.01	0.85
1:C:264:MET:HA	1:C:280:TYR:CA	2.00	0.85
1:C:182:GLU:HA	1:C:187:PRO:CA	2.06	0.85
4:B:29:VAL:CG1	5:A:170:GLN:CA	2.54	0.84
5:A:49:ARG:NH1	6:F:428:GLN:CD	2.34	0.84
5:A:143:SER:CB	6:F:42:SER:HB2	2.03	0.83
1:C:106:LEU:HG	1:C:106:LEU:O	1.76	0.83
4:B:192:LEU:HD13	6:F:36:MET:SD	2.19	0.82
1:C:57:ILE:CD1	1:C:58:LEU:H	1.90	0.82
1:C:69:VAL:HB	2:D:164:THR:CG2	2.10	0.82
4:B:346:LEU:HD12	4:B:362:VAL:HG21	1.60	0.82
1:C:293:ALA:O	1:C:296:PRO:HD3	1.80	0.81
5:A:321:ARG:HD2	6:F:234:ARG:NH1	1.93	0.81
5:A:43:LEU:HD13	6:F:462:LEU:HD21	1.61	0.81
5:A:140:PHE:HE1	6:F:42:SER:C	1.88	0.81
2:D:64:PHE:CD2	6:F:445:GLN:CG	2.62	0.81
1:C:149:ASN:HA	1:C:156:GLN:HB3	1.64	0.80
4:B:29:VAL:HG13	5:A:170:GLN:CA	2.12	0.80
1:C:131:ILE:HG21	1:C:134:ARG:HB2	1.64	0.79
4:B:195:ARG:N	5:A:247:LEU:O	2.14	0.79
1:C:147:GLN:HA	1:C:158:ARG:HA	1.65	0.79
5:A:143:SER:HB3	6:F:42:SER:CB	1.77	0.79
1:C:96:ARG:O	1:C:98:GLN:CD	2.26	0.79
1:C:264:MET:CA	1:C:280:TYR:HA	2.03	0.78
1:C:116:LEU:HD21	1:C:174:VAL:HG22	1.64	0.78
1:C:131:ILE:CD1	1:C:141:LEU:CD2	2.58	0.78
1:C:105:SER:HA	1:C:175:THR:HA	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:404:ARG:CB	6:F:237:SER:HB2	2.11	0.77
1:C:159:GLY:HA2	1:C:181:LEU:HA	1.65	0.76
4:B:240:GLU:OE2	6:F:32:THR:O	2.03	0.76
5:A:43:LEU:CD1	6:F:462:LEU:CD2	2.44	0.76
1:C:157:TYR:HA	1:C:183:GLN:HA	1.67	0.75
4:B:60:TYR:CZ	5:A:249:PRO:HG2	2.21	0.75
1:C:57:ILE:HD13	1:C:58:LEU:CA	2.16	0.75
4:B:131:VAL:HG21	4:B:164:ILE:HD12	1.70	0.74
1:C:106:LEU:CD1	1:C:108:VAL:CG1	2.65	0.74
2:D:64:PHE:CD2	6:F:445:GLN:HG2	2.23	0.73
4:B:29:VAL:HG21	5:A:171:GLU:N	1.65	0.73
1:C:86:ALA:H	1:C:196:ARG:HG2	1.54	0.73
1:C:242:LEU:HB2	1:C:316:LEU:HB3	1.71	0.73
1:C:103:THR:HA	1:C:177:LYS:HA	1.71	0.73
5:A:404:ARG:CD	6:F:237:SER:HA	2.15	0.72
4:B:29:VAL:H	5:A:172:GLY:CA	1.96	0.72
1:C:106:LEU:HD12	1:C:108:VAL:HG13	1.71	0.72
5:A:36:ARG:NH2	5:A:122:GLY:O	2.22	0.72
1:C:106:LEU:CG	1:C:106:LEU:O	2.36	0.72
1:C:110:ASN:HB2	1:C:170:TYR:HA	1.72	0.72
4:B:26:GLU:OE1	5:A:174:SER:HB3	1.90	0.71
1:C:69:VAL:CB	2:D:164:THR:HG21	2.19	0.71
1:C:91:LEU:C	1:C:92:VAL:O	2.33	0.71
1:C:262:VAL:HG23	1:C:292:GLY:HA3	1.71	0.71
5:A:622:ASP:OD1	5:A:624:ASP:N	2.18	0.71
1:C:106:LEU:HD11	1:C:108:VAL:HG13	1.67	0.71
1:C:116:LEU:HD22	1:C:172:GLN:HB3	1.72	0.71
1:C:140:THR:HA	1:C:164:SER:HA	1.72	0.71
5:A:143:SER:CB	6:F:42:SER:OG	2.38	0.71
1:C:307:VAL:HA	1:C:316:LEU:HA	1.72	0.71
1:C:242:LEU:HD13	1:C:316:LEU:HD13	1.73	0.71
4:B:161:LEU:HD21	4:B:182:LYS:HD2	1.71	0.70
1:C:150:ARG:NH1	1:C:196:ARG:HH12	1.70	0.70
1:C:242:LEU:HD23	1:C:335:VAL:HG23	1.72	0.70
4:B:60:TYR:OH	5:A:249:PRO:HG2	1.92	0.70
5:A:321:ARG:NE	6:F:234:ARG:NH1	1.97	0.70
6:F:123:TYR:CE2	6:F:232:GLN:OE1	2.44	0.70
5:A:214:TYR:HE2	6:F:36:MET:CB	2.00	0.70
2:D:92:ILE:HD12	2:D:108:VAL:HG13	1.74	0.69
5:A:470:GLU:OE2	5:A:488:ARG:NH2	2.25	0.69
5:A:569:ASP:HA	5:A:604:SER:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:41:GLY:HA2	6:F:144:ARG:HH22	1.57	0.69
4:B:344:GLY:HA3	4:B:363:ASP:O	1.92	0.69
1:C:106:LEU:HD11	1:C:108:VAL:HG11	1.75	0.68
4:B:347:HIS:CE1	4:B:359:GLN:HE21	2.11	0.68
1:C:88:PRO:HB2	1:C:97:THR:HB	1.75	0.68
1:C:57:ILE:HD12	1:C:57:ILE:H	1.58	0.68
5:A:789:GLN:HE22	5:A:791:PHE:HB2	1.57	0.68
2:D:43:LEU:HD12	2:D:51:ALA:HB1	1.74	0.68
4:B:29:VAL:HG13	5:A:170:GLN:HB3	1.76	0.68
1:C:106:LEU:HB3	1:C:174:VAL:HG23	1.76	0.67
1:C:57:ILE:HD13	1:C:58:LEU:C	2.19	0.67
5:A:569:ASP:OD1	5:A:569:ASP:N	2.26	0.67
5:A:43:LEU:O	6:F:466:ARG:NH1	2.27	0.67
5:A:44:LEU:HG	6:F:466:ARG:HG2	1.76	0.67
1:C:186:LYS:O	1:C:188:VAL:CG2	2.43	0.67
1:C:307:VAL:HG22	1:C:316:LEU:HG	1.77	0.67
2:D:76:ILE:HD12	2:D:92:ILE:HG12	1.77	0.67
1:C:134:ARG:HB2	1:C:141:LEU:CB	2.18	0.66
1:C:220:ALA:HB3	1:C:226:THR:HA	1.77	0.66
5:A:215:GLN:HG3	5:A:218:LYS:HE3	1.76	0.66
5:A:49:ARG:NH1	6:F:428:GLN:HE22	1.76	0.66
6:F:329:ARG:NH2	6:F:353:ASP:OD1	2.24	0.66
2:D:27:VAL:HB	2:D:61:ARG:HH22	1.61	0.66
4:B:192:LEU:HD12	5:A:245:VAL:O	1.95	0.66
1:C:134:ARG:HA	1:C:141:LEU:CA	2.24	0.65
2:D:219:GLU:OE2	2:D:223:ARG:NE	2.27	0.65
4:B:286:VAL:HG21	5:A:249:PRO:HB3	1.77	0.65
1:C:161:TYR:HE1	1:C:178:LEU:HD12	1.61	0.65
1:C:209:LEU:O	1:C:212:SER:C	2.40	0.65
1:C:134:ARG:CB	1:C:141:LEU:CB	2.75	0.65
5:A:622:ASP:OD1	5:A:623:ASP:N	2.30	0.65
4:B:131:VAL:HG21	4:B:164:ILE:CD1	2.26	0.65
1:C:218:ASN:HA	1:C:222:ASN:CA	2.23	0.65
2:D:191:TRP:HB2	2:D:225:MET:HE2	1.79	0.65
1:C:57:ILE:HD12	1:C:58:LEU:H	1.62	0.65
1:C:57:ILE:O	1:C:58:LEU:HB2	1.96	0.64
4:B:29:VAL:HG13	5:A:170:GLN:CB	2.28	0.64
1:C:150:ARG:HH11	1:C:196:ARG:NH1	1.90	0.64
1:C:99:PHE:HA	1:C:104:ALA:HA	1.79	0.64
5:A:143:SER:HG	6:F:42:SER:CB	1.88	0.64
1:C:73:SER:O	2:D:161:THR:HG21	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:VAL:HG21	2:D:165:LYS:HG3	1.80	0.63
4:B:60:TYR:CZ	5:A:249:PRO:CG	2.81	0.63
1:C:117:TRP:CH2	1:C:141:LEU:CG	2.62	0.63
1:C:209:LEU:O	1:C:212:SER:O	2.16	0.63
1:C:89:LEU:HD21	2:D:70:GLN:HB2	1.81	0.63
5:A:377:LEU:HD12	5:A:412:VAL:HG21	1.81	0.63
1:C:106:LEU:HD21	1:C:174:VAL:HG21	1.76	0.63
5:A:479:THR:HG22	5:A:483:VAL:HB	1.81	0.63
1:C:32:LYS:HD2	1:C:152:ASP:HA	1.80	0.62
5:A:606:ASN:OD1	5:A:606:ASN:N	2.31	0.62
1:C:88:PRO:HA	1:C:199:THR:HG23	1.81	0.62
5:A:740:ASP:OD1	5:A:740:ASP:N	2.31	0.62
1:C:159:GLY:CA	1:C:181:LEU:HA	2.30	0.62
6:F:44:LEU:HD11	6:F:52:MET:CE	2.30	0.62
1:C:53:PRO:HD2	2:D:237:ILE:HD13	1.81	0.62
1:C:151:LEU:HG	2:D:44:GLN:HE21	1.65	0.62
2:D:27:VAL:O	2:D:61:ARG:NH1	2.33	0.62
5:A:243:THR:HB	5:A:258:VAL:HG12	1.80	0.62
1:C:181:LEU:HD11	1:C:197:TYR:HD2	1.65	0.61
4:B:261:LEU:HD21	4:B:285:SER:HB3	1.82	0.61
5:A:223:LEU:HD12	5:A:240:ILE:HD13	1.82	0.61
5:A:301:VAL:HG22	5:A:337:LEU:HD21	1.83	0.61
1:C:134:ARG:HG3	1:C:141:LEU:HB3	1.82	0.61
1:C:228:MET:HE2	1:C:246:GLY:HA3	1.83	0.61
5:A:250:ASP:OD1	5:A:252:LYS:HG3	2.01	0.61
2:D:79:TYR:HB3	2:D:88:ALA:HB2	1.83	0.60
4:B:239:THR:HG21	5:A:142:TYR:HD2	1.66	0.60
4:B:263:TYR:OH	5:A:251:LYS:NZ	2.28	0.60
4:B:32:MET:HG2	4:B:324:HIS:O	2.02	0.60
5:A:143:SER:HB2	6:F:42:SER:OG	2.01	0.60
1:C:117:TRP:HB3	1:C:118:PRO:HD3	1.84	0.60
1:C:262:VAL:HG23	1:C:292:GLY:CA	2.31	0.60
5:A:96:SER:OG	5:A:164:ASP:OD1	2.19	0.60
5:A:659:THR:OG1	5:A:660:VAL:N	2.33	0.60
1:C:229:ASP:CB	1:C:244:VAL:HG12	2.31	0.59
1:C:242:LEU:HB3	1:C:244:VAL:HG13	1.83	0.59
4:B:29:VAL:HG11	5:A:170:GLN:CA	2.19	0.59
5:A:75:VAL:HG22	5:A:88:VAL:HG22	1.83	0.59
5:A:185:ASN:ND2	5:A:188:PHE:O	2.35	0.59
1:C:131:ILE:CG2	1:C:141:LEU:HD22	2.32	0.59
5:A:176:GLU:OE1	5:A:212:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:ALA:CA	6:F:151:GLU:OE1	2.50	0.59
1:C:133:GLN:HG2	1:C:142:THR:HB	1.85	0.59
2:D:192:VAL:HG22	2:D:225:MET:HE1	1.84	0.59
4:B:27:GLU:CD	5:A:103:LYS:NZ	2.59	0.59
5:A:404:ARG:HB3	6:F:237:SER:CA	2.33	0.59
1:C:131:ILE:CG1	1:C:141:LEU:HD22	2.33	0.58
6:F:44:LEU:HD11	6:F:52:MET:HE1	1.84	0.58
1:C:246:GLY:O	1:C:247:PRO:C	2.46	0.58
2:D:202:LEU:HD12	2:D:218:MET:HE1	1.83	0.58
4:B:60:TYR:HA	4:B:368:GLN:HE22	1.67	0.58
5:A:365:LEU:HD21	5:A:395:PHE:CZ	2.38	0.58
5:A:568:ASP:OD1	5:A:568:ASP:N	2.35	0.58
1:C:142:THR:HA	1:C:162:GLN:HA	1.86	0.58
1:C:242:LEU:HA	1:C:331:ASN:HD21	1.63	0.58
4:B:91:GLU:OE2	4:B:94:SER:HB2	2.03	0.58
5:A:387:GLU:OE2	5:A:391:ARG:NH2	2.37	0.58
3:E:52:GLN:HG2	3:E:95:PHE:CE2	2.39	0.57
1:C:117:TRP:HZ2	1:C:134:ARG:HG3	1.69	0.57
3:E:51:THR:OG1	3:E:52:GLN:N	2.36	0.57
1:C:67:ILE:HG12	2:D:167:LEU:HB3	1.86	0.57
1:C:247:PRO:O	1:C:248:PHE:C	2.47	0.57
2:D:35:ILE:HG22	2:D:58:LEU:HD12	1.86	0.57
1:C:178:LEU:HD11	1:C:181:LEU:HB2	1.85	0.57
1:C:275:ASN:HA	1:C:306:GLN:HA	1.87	0.57
5:A:114:LEU:HD21	5:A:137:LEU:HD21	1.86	0.57
5:A:410:ASP:O	5:A:411:GLN:NE2	2.20	0.57
1:C:131:ILE:CG2	1:C:134:ARG:HB2	2.34	0.57
1:C:156:GLN:HB2	1:C:158:ARG:HH11	1.70	0.57
1:C:264:MET:O	1:C:265:LYS:C	2.47	0.57
2:D:241:ASN:O	2:D:241:ASN:ND2	2.37	0.57
3:E:52:GLN:HG2	3:E:95:PHE:HE2	1.69	0.57
5:A:214:TYR:O	6:F:37:GLY:HA3	2.04	0.57
1:C:255:LEU:O	1:C:259:LEU:HG	2.04	0.57
1:C:262:VAL:CG2	1:C:292:GLY:HA3	2.35	0.57
2:D:64:PHE:HD2	6:F:445:GLN:HG2	1.68	0.57
1:C:157:TYR:CD2	1:C:197:TYR:CE2	2.93	0.56
5:A:587:PRO:HG2	5:A:618:TYR:CZ	2.40	0.56
1:C:229:ASP:HA	1:C:244:VAL:HA	1.88	0.56
1:C:91:LEU:HG	1:C:207:ALA:HA	1.88	0.56
5:A:22:GLU:N	5:A:54:VAL:O	2.39	0.56
6:F:272:GLU:OE1	6:F:309:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:96:ASN:ND2	3:E:98:SER:OG	2.37	0.56
4:B:113:GLY:O	4:B:155:PRO:CD	2.50	0.56
6:F:61:ARG:HA	6:F:66:LEU:HD12	1.87	0.56
1:C:190:ASP:O	1:C:191:ALA:C	2.49	0.56
1:C:311:ASP:O	6:F:475:ARG:NH1	2.39	0.56
5:A:709:ASN:ND2	5:A:747:THR:OG1	2.35	0.56
2:D:89:GLN:NE2	2:D:116:ASN:OD1	2.40	0.55
1:C:152:ASP:HB2	2:D:44:GLN:HA	1.88	0.55
1:C:117:TRP:HH2	1:C:141:LEU:CB	2.19	0.55
1:C:242:LEU:CD2	1:C:335:VAL:HG23	2.36	0.55
1:C:98:GLN:HG2	1:C:105:SER:HB3	1.88	0.55
4:B:29:VAL:CG1	5:A:171:GLU:N	2.69	0.55
5:A:129:THR:O	5:A:133:ILE:HG13	2.07	0.55
1:C:150:ARG:HH11	1:C:196:ARG:HH11	1.48	0.55
1:C:269:SER:HA	1:C:276:MET:HA	1.88	0.55
1:C:57:ILE:HD12	1:C:57:ILE:N	2.22	0.55
1:C:325:THR:O	1:C:326:LEU:C	2.49	0.55
1:C:131:ILE:CD1	1:C:141:LEU:HD21	2.34	0.55
1:C:313:ARG:HH12	6:F:471:ILE:HG21	1.71	0.55
4:B:60:TYR:CD1	4:B:368:GLN:NE2	2.74	0.55
1:C:115:THR:HG23	1:C:214:THR:HG22	1.88	0.54
1:C:163:ILE:HG13	1:C:176:VAL:HG22	1.89	0.54
2:D:64:PHE:CD2	6:F:445:GLN:HG3	2.42	0.54
5:A:245:VAL:HB	6:F:36:MET:HE1	1.88	0.54
6:F:230:LEU:HD12	6:F:253:LEU:HD22	1.89	0.54
5:A:76:ARG:HB2	5:A:87:GLN:HB2	1.89	0.54
5:A:769:SER:OG	5:A:770:ALA:N	2.41	0.54
5:A:215:GLN:HA	6:F:37:GLY:HA3	1.88	0.54
1:C:59:PRO:HG3	3:E:67:PRO:HB2	1.90	0.54
1:C:131:ILE:HD12	1:C:141:LEU:HD21	1.86	0.54
4:B:29:VAL:HG13	5:A:170:GLN:HA	1.85	0.54
1:C:98:GLN:NE2	1:C:105:SER:O	2.40	0.54
4:B:161:LEU:CD2	4:B:182:LYS:HD2	2.38	0.54
6:F:284:MET:HB2	6:F:317:LEU:HD21	1.89	0.54
1:C:106:LEU:HD23	1:C:174:VAL:CB	2.34	0.54
1:C:100:THR:O	1:C:101:GLY:C	2.51	0.54
5:A:214:TYR:OH	6:F:36:MET:HE3	2.07	0.54
1:C:69:VAL:CG2	2:D:164:THR:HG21	2.38	0.53
1:C:107:LEU:HA	1:C:173:ALA:HA	1.90	0.53
1:C:157:TYR:CD1	1:C:183:GLN:HB2	2.43	0.53
5:A:365:LEU:HD21	5:A:395:PHE:HZ	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:TYR:CE1	1:C:178:LEU:HD12	2.42	0.53
1:C:326:LEU:O	1:C:327:THR:C	2.50	0.53
4:B:87:ASP:OD1	4:B:377:LYS:NZ	2.40	0.53
5:A:352:ILE:O	5:A:366:ARG:NH1	2.41	0.53
2:D:190:ALA:HB2	5:A:372:MET:HE2	1.89	0.53
1:C:131:ILE:HA	1:C:143:THR:HA	1.90	0.53
5:A:425:SER:HB3	5:A:782:PRO:HD2	1.89	0.53
1:C:89:LEU:HD21	2:D:70:GLN:CB	2.39	0.53
2:D:38:THR:O	2:D:42:LYS:HG2	2.08	0.53
6:F:442:ARG:HD3	6:F:445:GLN:OE1	2.09	0.53
1:C:258:ALA:HB2	1:C:342:PHE:HA	1.91	0.53
1:C:283:LEU:O	1:C:284:SER:C	2.49	0.53
5:A:246:SER:OG	5:A:247:LEU:N	2.41	0.53
5:A:464:ASP:N	5:A:464:ASP:OD1	2.41	0.53
1:C:127:LYS:HD2	1:C:146:VAL:HG13	1.91	0.52
5:A:589:ASP:OD1	5:A:590:GLY:N	2.42	0.52
5:A:297:ASN:HB2	5:A:300:LYS:HB3	1.91	0.52
5:A:49:ARG:NH1	6:F:428:GLN:OE1	2.42	0.52
1:C:131:ILE:HG21	1:C:134:ARG:CB	2.37	0.52
4:B:60:TYR:CE1	5:A:249:PRO:HG2	2.44	0.52
6:F:227:GLU:CD	6:F:257:ARG:HH11	2.17	0.52
1:C:84:PRO:HG3	2:D:74:ASP:OD1	2.10	0.52
5:A:36:ARG:HH22	5:A:123:GLU:HA	1.75	0.52
1:C:47:LEU:HD21	2:D:171:LYS:HD3	1.92	0.52
1:C:110:ASN:O	1:C:111:GLY:C	2.53	0.52
5:A:583:ARG:HD2	5:A:585:TYR:HE1	1.74	0.52
2:D:106:ASP:OD2	2:D:157:SER:OG	2.28	0.51
5:A:514:THR:HA	5:A:528:GLY:HA3	1.91	0.51
1:C:248:PHE:O	1:C:249:ASN:C	2.53	0.51
4:B:73:TYR:CD2	4:B:117:VAL:HG21	2.46	0.51
1:C:229:ASP:CA	1:C:244:VAL:HA	2.41	0.51
1:C:332:ASP:HA	1:C:335:VAL:HB	1.91	0.51
4:B:29:VAL:HG22	5:A:171:GLU:N	2.22	0.51
5:A:36:ARG:HH12	5:A:124:SER:N	2.08	0.51
5:A:614:ASP:O	5:A:615:THR:OG1	2.24	0.51
5:A:727:ASP:HA	5:A:730:ALA:HB2	1.91	0.51
4:B:290:ILE:HD11	4:B:330:PRO:O	2.11	0.51
5:A:158:LEU:HD13	5:A:159:PRO:HD2	1.91	0.51
1:C:260:GLU:HA	1:C:265:LYS:HA	1.93	0.51
1:C:334:LEU:O	1:C:338:PHE:N	2.43	0.51
1:C:140:THR:O	1:C:141:LEU:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:MET:HG3	1:C:280:TYR:HB2	1.92	0.51
5:A:661:ARG:HG3	5:A:738:PHE:CE2	2.45	0.51
1:C:98:GLN:O	1:C:105:SER:HB3	2.11	0.51
5:A:215:GLN:CG	6:F:37:GLY:O	2.59	0.51
5:A:672:ALA:O	5:A:702:SER:OG	2.27	0.51
5:A:102:ASN:ND2	5:A:105:VAL:O	2.40	0.50
6:F:484:TYR:HD1	6:F:487:MET:HE1	1.76	0.50
1:C:181:LEU:HD11	1:C:197:TYR:CD2	2.46	0.50
4:B:259:PHE:HZ	4:B:310:ILE:HG23	1.76	0.50
5:A:60:SER:HA	5:A:63:ILE:HG12	1.94	0.50
6:F:387:LEU:HD21	6:F:419:ALA:HA	1.93	0.50
1:C:91:LEU:O	1:C:92:VAL:C	2.50	0.50
1:C:242:LEU:HD12	1:C:316:LEU:HD22	1.94	0.50
1:C:119:GLN:HG3	1:C:209:LEU:CB	2.42	0.50
1:C:319:ILE:HA	1:C:325:THR:HA	1.94	0.50
1:C:97:THR:HA	1:C:106:LEU:HA	1.94	0.49
1:C:107:LEU:HD23	1:C:171:GLN:HB3	1.93	0.49
5:A:628:VAL:HB	5:A:719:ILE:HD12	1.94	0.49
1:C:241:MET:HE3	1:C:315:SER:HA	1.94	0.49
4:B:60:TYR:CE2	4:B:195:ARG:O	2.66	0.49
4:B:290:ILE:HD11	4:B:331:VAL:HA	1.95	0.49
5:A:237:ARG:NH2	5:A:330:ASP:OD2	2.46	0.49
5:A:601:ILE:HD12	5:A:601:ILE:H	1.76	0.49
1:C:337:VAL:C	1:C:341:ALA:HB3	2.30	0.49
3:E:47:ARG:HA	3:E:47:ARG:NH2	2.28	0.49
1:C:161:TYR:OH	1:C:197:TYR:HB3	2.12	0.49
4:B:191:SER:CB	6:F:33:LEU:CD2	2.69	0.49
4:B:194:LEU:HD11	4:B:263:TYR:CD2	2.48	0.49
1:C:57:ILE:HD12	1:C:58:LEU:N	2.15	0.49
1:C:209:LEU:HA	1:C:212:SER:O	2.12	0.49
1:C:291:LEU:HA	1:C:344:LYS:HG3	1.94	0.49
4:B:158:SER:HB3	4:B:221:MET:HE1	1.93	0.49
5:A:126:ASP:O	5:A:129:THR:OG1	2.31	0.49
1:C:99:PHE:CE2	1:C:195:GLN:HG2	2.47	0.49
1:C:117:TRP:CH2	1:C:141:LEU:HB3	2.48	0.49
1:C:242:LEU:CD1	1:C:316:LEU:HB3	2.43	0.49
4:B:302:ASN:O	4:B:323:LEU:HD23	2.13	0.49
4:B:123:TYR:OH	4:B:176:GLU:HG3	2.13	0.48
4:B:266:ASN:OD1	4:B:280:LYS:HE3	2.12	0.48
5:A:328:ILE:HG12	5:A:335:VAL:HG12	1.93	0.48
5:A:536:LEU:O	5:A:565:PHE:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:PRO:HB3	2:D:62:TYR:CE2	2.48	0.48
2:D:198:VAL:HG12	2:D:218:MET:HE3	1.96	0.48
1:C:178:LEU:HD22	1:C:194:MET:HG3	1.95	0.48
2:D:234:VAL:O	2:D:238:ILE:HG23	2.14	0.48
1:C:157:TYR:CG	1:C:183:GLN:HG3	2.49	0.48
1:C:285:ASP:HA	1:C:288:TRP:CB	2.44	0.48
4:B:101:ASP:O	4:B:105:SER:OG	2.24	0.48
2:D:137:PRO:HG3	2:D:177:TYR:CG	2.49	0.48
1:C:79:ALA:O	1:C:80:LEU:C	2.56	0.48
1:C:225:SER:O	1:C:226:THR:C	2.56	0.48
3:E:46:ILE:O	3:E:47:ARG:HD2	2.14	0.48
6:F:209:ILE:HG23	6:F:263:MET:HE1	1.95	0.48
1:C:148:TRP:NE1	1:C:161:TYR:OH	2.46	0.47
2:D:31:PRO:HG2	2:D:34:GLU:HG3	1.95	0.47
6:F:484:TYR:CA	6:F:487:MET:HE3	2.26	0.47
1:C:242:LEU:CB	1:C:244:VAL:HG13	2.44	0.47
5:A:719:ILE:HD13	5:A:734:ARG:NH2	2.29	0.47
5:A:765:ASN:O	5:A:767:ARG:NH2	2.43	0.47
1:C:158:ARG:HG3	1:C:182:GLU:HB2	1.95	0.47
1:C:313:ARG:NH1	6:F:471:ILE:HG21	2.29	0.47
4:B:60:TYR:CE1	5:A:249:PRO:CD	2.98	0.47
2:D:208:THR:OG1	2:D:209:GLN:N	2.48	0.47
4:B:60:TYR:CE1	5:A:249:PRO:HD2	2.49	0.47
1:C:89:LEU:HD22	2:D:67:TYR:CD1	2.49	0.47
1:C:159:GLY:HA3	1:C:181:LEU:HD23	1.97	0.47
1:C:165:VAL:HG22	1:C:174:VAL:HG13	1.95	0.47
1:C:251:VAL:HG22	1:C:342:PHE:CE2	2.49	0.47
5:A:264:ASP:OD1	5:A:264:ASP:N	2.48	0.47
1:C:157:TYR:CD1	1:C:183:GLN:HG3	2.49	0.47
3:E:31:ASP:OD1	3:E:81:PRO:HA	2.14	0.47
1:C:82:ILE:HB	2:D:111:MET:HE1	1.97	0.47
1:C:91:LEU:HD21	2:D:67:TYR:OH	2.14	0.47
1:C:310:LEU:O	1:C:311:ASP:C	2.58	0.47
5:A:266:TYR:OH	5:A:330:ASP:OD1	2.28	0.47
5:A:424:GLY:HA2	5:A:445:GLN:O	2.14	0.47
5:A:94:ILE:HD12	5:A:119:VAL:HG13	1.96	0.47
1:C:177:LYS:HB3	1:C:177:LYS:HE3	1.62	0.47
1:C:338:PHE:C	1:C:340:ALA:N	2.72	0.47
1:C:86:ALA:HB3	1:C:196:ARG:HA	1.95	0.46
1:C:129:TYR:O	1:C:130:THR:C	2.59	0.46
4:B:242:ASP:OD1	5:A:142:TYR:OH	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:PRO:HG3	1:C:99:PHE:N	2.31	0.46
1:C:93:SER:O	1:C:94:GLY:C	2.58	0.46
1:C:131:ILE:HG23	1:C:141:LEU:HD22	1.97	0.46
1:C:161:TYR:HD1	1:C:178:LEU:HA	1.80	0.46
1:C:324:HIS:O	1:C:325:THR:C	2.58	0.46
4:B:165:HIS:CE1	4:B:197:GLU:OE1	2.68	0.46
1:C:96:ARG:C	1:C:98:GLN:OE1	2.50	0.46
1:C:152:ASP:H	2:D:44:GLN:HB2	1.80	0.46
6:F:88:ASN:ND2	6:F:214:ARG:HH22	2.13	0.46
4:B:26:GLU:OE1	5:A:174:SER:CB	2.62	0.46
1:C:47:LEU:HD22	2:D:168:VAL:HG22	1.96	0.46
1:C:305:LEU:HA	1:C:318:PHE:HA	1.96	0.46
1:C:313:ARG:HH22	6:F:471:ILE:HB	1.81	0.46
2:D:92:ILE:HG21	2:D:112:ARG:HG3	1.97	0.46
5:A:324:SER:HB3	5:A:339:VAL:HG13	1.97	0.46
1:C:186:LYS:HA	1:C:186:LYS:HD3	1.38	0.46
4:B:239:THR:HG21	5:A:142:TYR:CD2	2.49	0.46
5:A:114:LEU:HD12	5:A:119:VAL:HB	1.97	0.46
5:A:560:ASP:HA	5:A:679:ALA:HB3	1.98	0.46
5:A:598:LYS:NZ	5:A:650:GLU:OE2	2.44	0.46
6:F:88:ASN:HD21	6:F:214:ARG:HH22	1.64	0.46
6:F:104:ILE:HD12	6:F:123:TYR:CG	2.51	0.46
1:C:288:TRP:CB	1:C:294:SER:HA	2.45	0.46
4:B:233:SER:OG	4:B:245:SER:HB2	2.16	0.46
1:C:251:VAL:HG22	1:C:342:PHE:CZ	2.50	0.46
3:E:34:GLN:NE2	5:A:373:GLU:O	2.48	0.46
5:A:294:GLU:HG2	5:A:295:LEU:N	2.31	0.46
5:A:443:GLY:HA2	5:A:459:ASN:HA	1.98	0.46
5:A:537:SER:HA	5:A:564:SER:HA	1.98	0.46
6:F:51:GLN:NE2	6:F:480:ARG:CB	2.72	0.46
1:C:106:LEU:HB3	1:C:174:VAL:CG2	2.45	0.45
1:C:157:TYR:CE1	1:C:183:GLN:HB2	2.50	0.45
5:A:43:LEU:C	6:F:466:ARG:HE	2.24	0.45
5:A:91:ARG:HD3	5:A:126:ASP:HA	1.98	0.45
1:C:107:LEU:HG	1:C:173:ALA:HB2	1.99	0.45
1:C:120:VAL:HG11	1:C:174:VAL:HG11	1.98	0.45
1:C:182:GLU:CA	1:C:187:PRO:HA	2.16	0.45
2:D:109:MET:HE1	2:D:112:ARG:HE	1.82	0.45
4:B:198:SER:HB2	4:B:247:VAL:O	2.17	0.45
5:A:277:LEU:HD23	5:A:341:VAL:HG21	1.97	0.45
5:A:316:GLY:HA2	5:A:377:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ASP:O	1:C:321:PRO:C	2.60	0.45
1:C:218:ASN:CA	1:C:222:ASN:HA	2.33	0.45
5:A:559:SER:HA	5:A:677:HIS:HA	1.98	0.45
5:A:773:ALA:HA	5:A:786:SER:HA	1.98	0.45
5:A:789:GLN:HA	5:A:790:PRO:HD3	1.84	0.45
1:C:261:LYS:HB2	1:C:261:LYS:HE3	1.51	0.45
2:D:225:MET:HB2	2:D:227:MET:HG2	1.97	0.45
1:C:153:GLU:O	1:C:154:ASP:C	2.59	0.45
5:A:250:ASP:OD1	5:A:250:ASP:C	2.60	0.45
5:A:404:ARG:HD3	6:F:237:SER:CA	2.22	0.45
3:E:27:VAL:HG12	5:A:517:PHE:HB2	1.99	0.45
5:A:404:ARG:CB	6:F:237:SER:CB	2.82	0.45
5:A:761:SER:O	5:A:761:SER:OG	2.32	0.45
6:F:44:LEU:HD11	6:F:52:MET:HE2	1.98	0.45
1:C:161:TYR:HA	1:C:179:LEU:H	1.83	0.44
1:C:181:LEU:HD12	1:C:189:ALA:HA	1.99	0.44
5:A:49:ARG:HG3	5:A:50:THR:N	2.32	0.44
4:B:83:ALA:HB2	4:B:93:TRP:CE2	2.52	0.44
1:C:70:THR:HB	2:D:160:THR:HG21	1.99	0.44
1:C:166:LYS:HB2	1:C:166:LYS:HE2	1.37	0.44
5:A:711:MET:HB2	5:A:744:VAL:HG22	1.99	0.44
1:C:134:ARG:CG	1:C:141:LEU:HB3	2.46	0.44
5:A:371:GLN:NE2	5:A:372:MET:O	2.47	0.44
1:C:309:ASP:HA	1:C:314:SER:HA	2.00	0.44
2:D:212:ARG:HD2	2:D:212:ARG:HA	1.90	0.44
3:E:47:ARG:HA	3:E:47:ARG:CZ	2.47	0.44
5:A:72:PHE:HB3	5:A:88:VAL:HG13	1.99	0.44
5:A:115:GLU:HG2	5:A:120:ARG:HD3	1.98	0.44
5:A:143:SER:OG	6:F:42:SER:OG	1.98	0.44
5:A:430:ILE:HG13	5:A:440:PHE:HA	2.00	0.44
1:C:78:LYS:O	1:C:79:ALA:C	2.60	0.44
1:C:103:THR:CA	1:C:177:LYS:HA	2.46	0.44
1:C:231:GLN:HB2	1:C:243:VAL:HB	2.00	0.44
2:D:48:TRP:O	2:D:52:ILE:HG13	2.18	0.44
4:B:60:TYR:CZ	5:A:249:PRO:CD	3.00	0.44
5:A:634:ARG:CZ	5:A:711:MET:HE1	2.48	0.44
5:A:392:LEU:HD23	5:A:392:LEU:HA	1.81	0.44
6:F:39:SER:C	6:F:151:GLU:OE2	2.61	0.44
6:F:144:ARG:HB3	6:F:147:ALA:HB3	2.00	0.44
4:B:261:LEU:CD2	4:B:285:SER:HB3	2.47	0.44
4:B:306:MET:HG2	4:B:318:THR:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:308:LEU:HD23	4:B:315:THR:HA	1.99	0.44
1:C:33:ARG:HB3	1:C:83:ARG:CZ	2.47	0.43
1:C:58:LEU:HD23	1:C:58:LEU:HA	1.75	0.43
2:D:192:VAL:CG2	2:D:225:MET:HE1	2.48	0.43
4:B:80:LEU:HD21	4:B:82:LYS:HE3	1.99	0.43
5:A:116:ALA:HB1	6:F:47:GLY:HA3	2.00	0.43
5:A:626:LYS:HD3	5:A:626:LYS:HA	1.82	0.43
6:F:464:GLN:NE2	6:F:468:ASP:OD2	2.51	0.43
1:C:337:VAL:C	1:C:341:ALA:H	2.14	0.43
2:D:31:PRO:O	2:D:35:ILE:HD12	2.18	0.43
2:D:89:GLN:HG2	2:D:115:THR:HG21	2.00	0.43
1:C:32:LYS:HB3	2:D:48:TRP:HH2	1.84	0.43
1:C:91:LEU:HD13	1:C:91:LEU:HA	1.86	0.43
1:C:257:ALA:O	1:C:258:ALA:C	2.62	0.43
5:A:44:LEU:HA	6:F:466:ARG:HE	1.83	0.43
5:A:542:GLN:HG2	5:A:545:MET:HE3	2.00	0.43
5:A:735:THR:HG22	5:A:774:LEU:HD12	1.99	0.43
5:A:745:TRP:CE2	5:A:763:PRO:HB3	2.54	0.43
5:A:792:LYS:HE3	5:A:794:TYR:HE1	1.84	0.43
1:C:223:ARG:O	1:C:224:ALA:C	2.61	0.43
1:C:281:LYS:O	1:C:282:PRO:C	2.62	0.43
2:D:212:ARG:HH22	2:D:238:ILE:HB	1.83	0.43
5:A:677:HIS:H	5:A:677:HIS:CD2	2.37	0.43
1:C:99:PHE:CZ	1:C:195:GLN:HA	2.53	0.43
4:B:266:ASN:CG	4:B:280:LYS:HE3	2.44	0.43
5:A:26:VAL:HG23	5:A:82:ASP:O	2.19	0.43
6:F:61:ARG:HD2	6:F:439:LEU:O	2.19	0.43
3:E:46:ILE:CD1	3:E:55:VAL:HG22	2.48	0.43
5:A:297:ASN:N	5:A:297:ASN:OD1	2.52	0.43
1:C:339:GLN:HE21	1:C:339:GLN:HB2	1.71	0.43
2:D:27:VAL:HG21	2:D:54:GLN:HG3	2.00	0.43
2:D:30:ASN:HB3	2:D:31:PRO:HD2	2.00	0.43
2:D:92:ILE:HD13	2:D:92:ILE:HA	1.89	0.43
5:A:73:GLU:HA	5:A:91:ARG:NH2	2.34	0.43
5:A:250:ASP:CG	5:A:252:LYS:HG3	2.43	0.43
5:A:520:ASN:OD1	5:A:521:GLU:N	2.38	0.43
1:C:228:MET:SD	1:C:342:PHE:CD2	3.12	0.43
4:B:60:TYR:HE2	4:B:195:ARG:O	2.01	0.43
1:C:115:THR:HG21	1:C:216:ALA:HB3	2.00	0.43
1:C:241:MET:C	1:C:241:MET:HE2	2.43	0.43
4:B:156:VAL:HG21	4:B:200:PRO:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:LEU:HA	1:C:344:LYS:HE3	2.01	0.42
4:B:195:ARG:HB2	5:A:246:SER:HG	1.84	0.42
5:A:287:LEU:HA	5:A:287:LEU:HD23	1.81	0.42
5:A:545:MET:HG3	5:A:648:PHE:CE1	2.54	0.42
1:C:84:PRO:HD3	2:D:77:TYR:CD2	2.54	0.42
1:C:151:LEU:HB2	2:D:44:GLN:O	2.19	0.42
1:C:228:MET:HE2	1:C:251:VAL:HG23	2.00	0.42
3:E:66:ASP:C	3:E:66:ASP:OD1	2.62	0.42
1:C:147:GLN:HA	1:C:158:ARG:CA	2.45	0.42
1:C:293:ALA:HB3	1:C:296:PRO:HB3	2.01	0.42
3:E:43:VAL:HG22	3:E:91:LEU:HD22	2.00	0.42
1:C:99:PHE:CD2	1:C:195:GLN:HG2	2.54	0.42
1:C:228:MET:O	1:C:229:ASP:CB	2.66	0.42
1:C:279:THR:HA	1:C:301:GLY:H	1.83	0.42
5:A:233:ARG:HA	5:A:233:ARG:HD3	1.84	0.42
6:F:34:PRO:HG2	6:F:36:MET:HG3	2.01	0.42
6:F:40:ALA:N	6:F:151:GLU:CD	2.77	0.42
2:D:112:ARG:HD2	2:D:146:ASP:OD2	2.19	0.42
3:E:77:PHE:O	3:E:88:GLN:HA	2.20	0.42
1:C:52:ALA:HB2	1:C:58:LEU:HG	2.02	0.42
2:D:117:MET:HE3	2:D:117:MET:HB2	1.89	0.42
2:D:149:LYS:HB3	2:D:149:LYS:HE2	1.75	0.42
4:B:65:PRO:O	4:B:372:VAL:HG21	2.19	0.42
5:A:34:LEU:HD23	5:A:37:VAL:O	2.20	0.42
5:A:505:THR:HG22	5:A:538:ASN:OD1	2.19	0.42
5:A:577:THR:OG1	5:A:578:TYR:N	2.52	0.42
1:C:30:ARG:HE	1:C:30:ARG:HB3	1.50	0.42
1:C:91:LEU:HB3	1:C:210:ASP:CB	2.49	0.42
1:C:134:ARG:HG3	1:C:141:LEU:CB	2.47	0.42
1:C:244:VAL:O	1:C:251:VAL:HG21	2.20	0.42
2:D:113:GLY:HA3	2:D:147:PHE:CE1	2.54	0.42
5:A:182:ILE:HG12	5:A:258:VAL:HG23	2.02	0.42
6:F:86:HIS:CD2	6:F:215:SER:HA	2.54	0.42
1:C:192:ALA:O	1:C:196:ARG:HG3	2.19	0.42
2:D:76:ILE:HG21	2:D:92:ILE:HD11	2.01	0.42
2:D:85:LEU:HD12	2:D:115:THR:HG23	2.01	0.42
2:D:201:MET:HE1	2:D:214:ALA:HB3	2.02	0.42
4:B:261:LEU:HD22	4:B:298:LEU:HD13	2.01	0.42
1:C:159:GLY:CA	1:C:181:LEU:HD23	2.49	0.42
2:D:113:GLY:N	2:D:146:ASP:OD2	2.53	0.42
5:A:273:VAL:HG23	5:A:339:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:MET:H	1:C:56:MET:HG2	1.45	0.41
2:D:207:ASP:OD1	2:D:207:ASP:C	2.63	0.41
4:B:175:ASN:HB3	4:B:178:ASP:OD1	2.20	0.41
5:A:634:ARG:NH2	5:A:711:MET:HE1	2.34	0.41
1:C:311:ASP:HB2	6:F:475:ARG:HH12	1.84	0.41
4:B:259:PHE:CZ	4:B:310:ILE:HG23	2.54	0.41
6:F:457:VAL:HG23	6:F:464:GLN:HB2	2.02	0.41
1:C:106:LEU:CD1	1:C:106:LEU:O	2.68	0.41
4:B:346:LEU:CD1	4:B:390:ILE:CD1	2.98	0.41
1:C:70:THR:O	1:C:71:ASN:C	2.63	0.41
1:C:89:LEU:HD22	2:D:67:TYR:HD1	1.85	0.41
1:C:90:ALA:O	1:C:91:LEU:HD22	2.20	0.41
1:C:134:ARG:HA	1:C:141:LEU:CB	2.50	0.41
1:C:236:ASP:OD1	5:A:122:GLY:O	2.39	0.41
1:C:268:ASP:H	1:C:277:ALA:HB3	1.84	0.41
5:A:173:VAL:HG11	5:A:252:LYS:HG2	2.03	0.41
6:F:278:LYS:HD3	6:F:300:TRP:HZ2	1.84	0.41
1:C:320:ASP:CB	1:C:324:HIS:HB2	2.50	0.41
4:B:241:ILE:HD13	5:A:147:TYR:CD1	2.55	0.41
5:A:115:GLU:HB3	5:A:120:ARG:HE	1.86	0.41
5:A:543:VAL:HG12	5:A:673:VAL:O	2.20	0.41
1:C:90:ALA:O	2:D:66:PRO:HB2	2.20	0.41
1:C:311:ASP:HB2	6:F:475:ARG:NH1	2.36	0.41
6:F:121:PHE:O	6:F:278:LYS:HE3	2.20	0.41
1:C:30:ARG:HA	1:C:33:ARG:HG3	2.02	0.41
4:B:67:LEU:HD23	4:B:374:ALA:HB3	2.03	0.41
5:A:97:ILE:HG22	5:A:165:LEU:HB2	2.03	0.41
6:F:437:TYR:HD1	6:F:442:ARG:HD2	1.86	0.41
1:C:117:TRP:CH2	1:C:141:LEU:CB	3.00	0.41
1:C:119:GLN:O	1:C:123:VAL:HG23	2.21	0.41
1:C:263:GLY:O	1:C:281:LYS:N	2.54	0.41
1:C:273:GLN:H	1:C:273:GLN:HG3	1.71	0.41
1:C:306:GLN:O	1:C:307:VAL:C	2.63	0.41
1:C:308:GLY:O	1:C:309:ASP:C	2.64	0.41
4:B:60:TYR:HA	4:B:368:GLN:NE2	2.34	0.41
5:A:225:THR:O	5:A:228:SER:OG	2.36	0.41
6:F:270:SER:O	6:F:306:ARG:NH2	2.48	0.41
1:C:124:LEU:HD12	1:C:124:LEU:HA	1.89	0.41
1:C:242:LEU:O	1:C:316:LEU:N	2.51	0.41
3:E:101:LEU:HD12	3:E:102:THR:N	2.35	0.41
1:C:108:VAL:O	1:C:109:GLU:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:30:VAL:HG12	4:B:324:HIS:HB3	2.03	0.40
5:A:377:LEU:HD23	5:A:378:GLY:N	2.36	0.40
5:A:606:ASN:HD22	5:A:647:PRO:CG	2.34	0.40
1:C:57:ILE:CD1	1:C:57:ILE:N	2.84	0.40
1:C:241:MET:SD	1:C:241:MET:N	2.94	0.40
1:C:292:GLY:CA	1:C:337:VAL:HA	2.50	0.40
1:C:325:THR:O	1:C:327:THR:N	2.54	0.40
4:B:29:VAL:HG22	5:A:171:GLU:H	1.86	0.40
5:A:519:ILE:HD13	5:A:519:ILE:HA	1.90	0.40
6:F:52:MET:HG2	6:F:484:TYR:CE1	2.56	0.40
1:C:145:TRP:CD1	1:C:160:ARG:HB2	2.56	0.40
4:B:192:LEU:HD13	6:F:36:MET:CE	2.51	0.40
1:C:33:ARG:HB3	1:C:83:ARG:HD2	2.04	0.40
1:C:292:GLY:C	1:C:337:VAL:HA	2.46	0.40
4:B:261:LEU:CD2	4:B:298:LEU:HD13	2.51	0.40
5:A:651:ASN:ND2	5:A:707:GLY:O	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	315/320 (98%)	192 (61%)	89 (28%)	34 (11%)	0	6
2	D	216/226 (96%)	209 (97%)	7 (3%)	0	100	100
3	E	91/104 (88%)	86 (94%)	5 (6%)	0	100	100
4	B	370/373 (99%)	355 (96%)	14 (4%)	1 (0%)	36	71
5	A	762/790 (96%)	692 (91%)	69 (9%)	1 (0%)	48	82
6	F	411/492 (84%)	406 (99%)	4 (1%)	1 (0%)	43	77
All	All	2165/2305 (94%)	1940 (90%)	188 (9%)	37 (2%)	9	34

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	65	TYR
1	C	92	VAL
1	C	229	ASP
1	C	247	PRO
1	C	248	PHE
1	C	284	SER
1	C	312	ASN
1	C	326	LEU
1	C	101	GLY
1	C	110	ASN
1	C	146	VAL
1	C	245	ARG
1	C	302	ASP
1	C	307	VAL
1	C	309	ASP
4	B	188	ASP
1	C	80	LEU
1	C	130	THR
1	C	265	LYS
1	C	304	LYS
1	C	325	THR
6	F	35	ASP
1	C	58	LEU
1	C	169	GLY
1	C	187	PRO
1	C	226	THR
1	C	280	TYR
1	C	282	PRO
1	C	319	ILE
1	C	85	PRO
1	C	316	LEU
1	C	167	PRO
1	C	259	LEU
5	A	267	LYS
1	C	244	VAL
1	C	111	GLY
1	C	131	ILE

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	C	205/258 (80%)	123 (60%)	82 (40%)	0	1
2	D	183/190 (96%)	171 (93%)	12 (7%)	15	36
3	E	81/90 (90%)	78 (96%)	3 (4%)	30	51
4	B	303/304 (100%)	297 (98%)	6 (2%)	48	65
5	A	640/672 (95%)	594 (93%)	46 (7%)	13	34
6	F	343/395 (87%)	342 (100%)	1 (0%)	86	84
All	All	1755/1909 (92%)	1605 (92%)	150 (8%)	12	29

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	30	ARG
1	C	32	LYS
1	C	33	ARG
1	C	42	LEU
1	C	43	GLU
1	C	47	LEU
1	C	56	MET
1	C	57	ILE
1	C	61	THR
1	C	69	VAL
1	C	76	VAL
1	C	80	LEU
1	C	83	ARG
1	C	87	GLN
1	C	91	LEU
1	C	92	VAL
1	C	96	ARG
1	C	97	THR
1	C	98	GLN
1	C	100	THR
1	C	103	THR
1	C	106	LEU

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Mol	Chain	Res	Type
1	C	110	ASN
1	C	124	LEU
1	C	125	GLN
1	C	127	LYS
1	C	133	GLN
1	C	134	ARG
1	C	140	THR
1	C	141	LEU
1	C	144	ASP
1	C	147	GLN
1	C	158	ARG
1	C	162	GLN
1	C	166	LYS
1	C	174	VAL
1	C	177	LYS
1	C	179	LEU
1	C	180	ASN
1	C	181	LEU
1	C	182	GLU
1	C	186	LYS
1	C	188	VAL
1	C	190	ASP
1	C	193	SER
1	C	194	MET
1	C	198	SER
1	C	199	THR
1	C	212	SER
1	C	214	THR
1	C	218	ASN
1	C	230	VAL
1	C	231	GLN
1	C	232	SER
1	C	235	ASP
1	C	241	MET
1	C	242	LEU
1	C	245	ARG
1	C	247	PRO
1	C	249	ASN
1	C	250	VAL
1	C	251	VAL
1	C	254	ARG
1	C	255	LEU

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Mol	Chain	Res	Type
1	C	260	GLU
1	C	261	LYS
1	C	264	MET
1	C	266	VAL
1	C	271	ARG
1	C	273	GLN
1	C	310	LEU
1	C	311	ASP
1	C	313	ARG
1	C	316	LEU
1	C	319	ILE
1	C	325	THR
1	C	327	THR
1	C	331	ASN
1	C	334	LEU
1	C	335	VAL
1	C	339	GLN
1	C	344	LYS
2	D	43	LEU
2	D	74	ASP
2	D	79	TYR
2	D	96	ILE
2	D	115	THR
2	D	161	THR
2	D	186	THR
2	D	205	TYR
2	D	209	GLN
2	D	212	ARG
2	D	215	LEU
2	D	241	ASN
3	E	26	VAL
3	E	48	VAL
3	E	70	THR
4	B	37	THR
4	B	43	THR
4	B	220	LEU
4	B	268	THR
4	B	298	LEU
4	B	357	VAL
5	A	35	GLN
5	A	72	PHE
5	A	93	THR

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Mol	Chain	Res	Type
5	A	124	SER
5	A	158	LEU
5	A	168	VAL
5	A	173	VAL
5	A	190	THR
5	A	230	TYR
5	A	243	THR
5	A	297	ASN
5	A	308	ILE
5	A	325	MET
5	A	341	VAL
5	A	358	ASP
5	A	362	ASP
5	A	414	VAL
5	A	425	SER
5	A	440	PHE
5	A	452	THR
5	A	467	THR
5	A	480	VAL
5	A	505	THR
5	A	513	VAL
5	A	514	THR
5	A	551	SER
5	A	555	HIS
5	A	569	ASP
5	A	577	THR
5	A	586	PHE
5	A	600	THR
5	A	606	ASN
5	A	611	VAL
5	A	612	THR
5	A	628	VAL
5	A	641	LEU
5	A	667	THR
5	A	713	VAL
5	A	720	THR
5	A	725	ILE
5	A	735	THR
5	A	740	ASP
5	A	743	THR
5	A	753	GLN
5	A	774	LEU

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Mol	Chain	Res	Type
5	A	778	SER
6	F	459	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	51	HIS
1	C	87	GLN
1	C	98	GLN
1	C	119	GLN
1	C	128	ASN
1	C	172	GLN
1	C	253	GLN
1	C	273	GLN
1	C	312	ASN
1	C	317	GLN
1	C	324	HIS
1	C	328	GLN
1	C	339	GLN
2	D	44	GLN
2	D	104	ASN
2	D	125	GLN
3	E	79	GLN
4	B	324	HIS
4	B	347	HIS
4	B	359	GLN
5	A	244	GLN
5	A	561	GLN
5	A	803	GLN
6	F	51	GLN
6	F	86	HIS
6	F	88	ASN
6	F	143	GLN
6	F	269	GLN
6	F	318	GLN
6	F	323	ASN
6	F	391	GLN
6	F	428	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

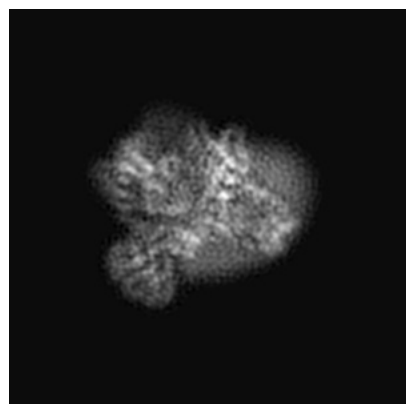
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56559. These allow visual inspection of the internal detail of the map and identification of artifacts.

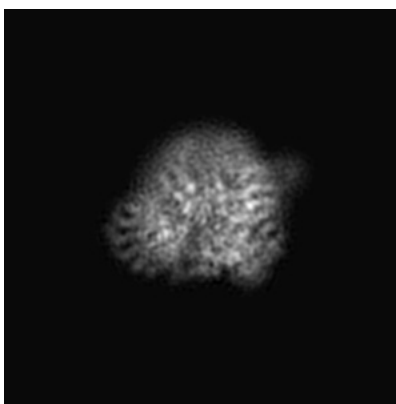
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

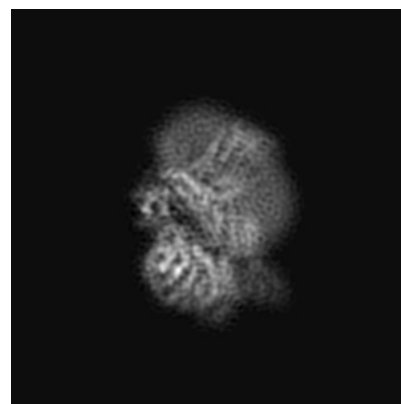
6.1.1 Primary map



X

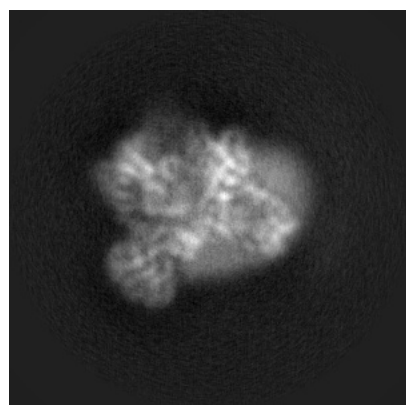


Y

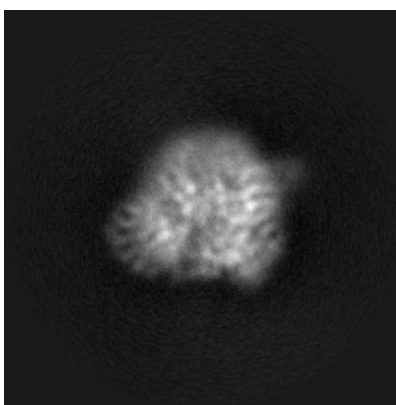


Z

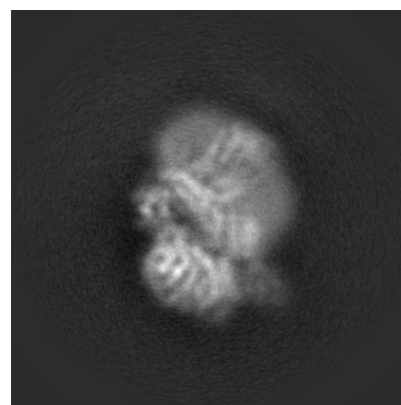
6.1.2 Raw map



X



Y

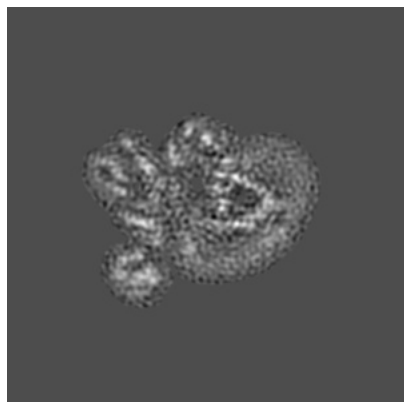


Z

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

6.2 Central slices [i](#)

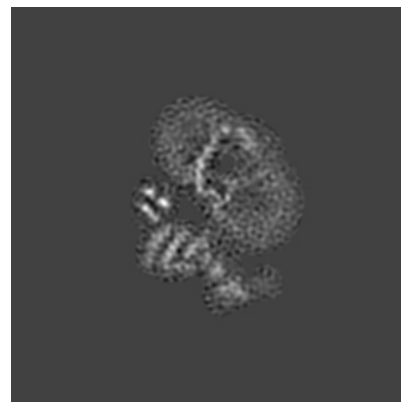
6.2.1 Primary map



X Index: 176

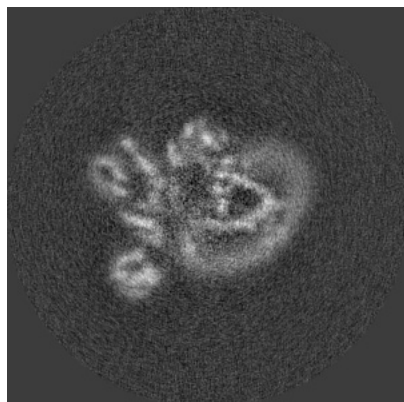


Y Index: 176

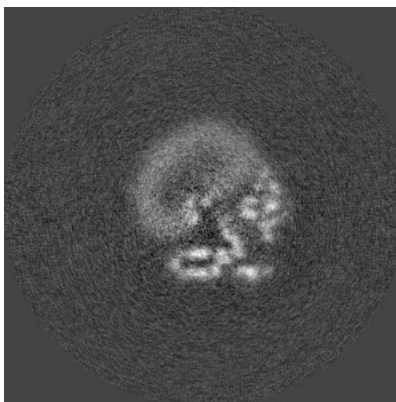


Z Index: 176

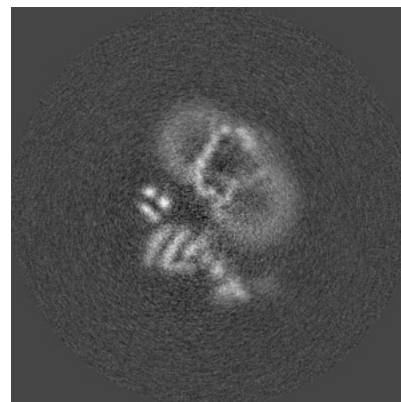
6.2.2 Raw map



X Index: 176



Y Index: 176

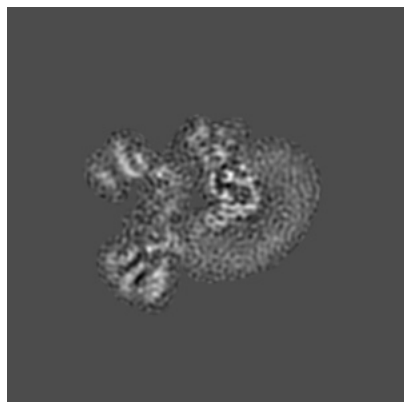


Z Index: 176

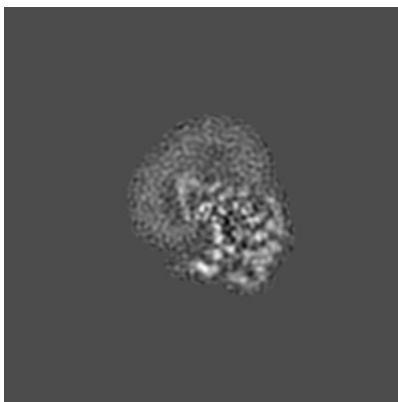
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

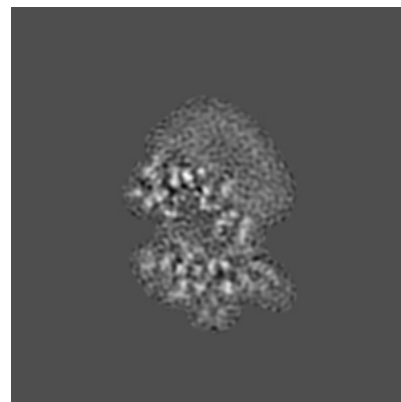
6.3.1 Primary map



X Index: 166

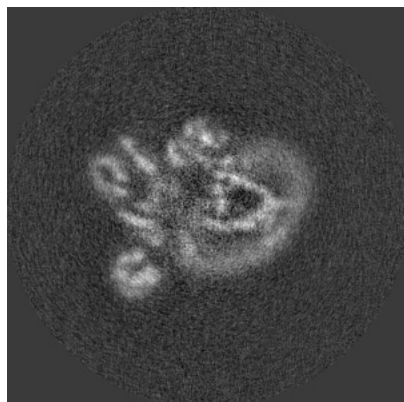


Y Index: 189

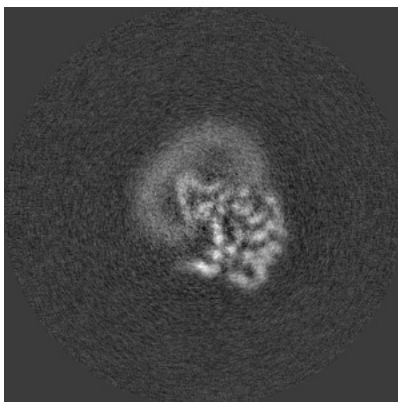


Z Index: 211

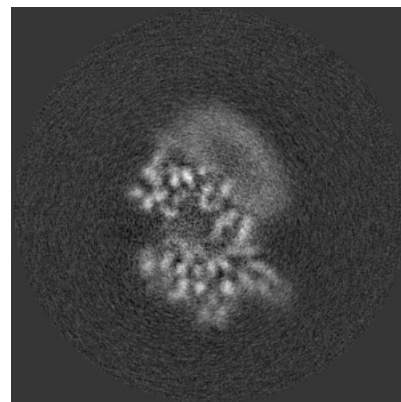
6.3.2 Raw map



X Index: 177



Y Index: 189

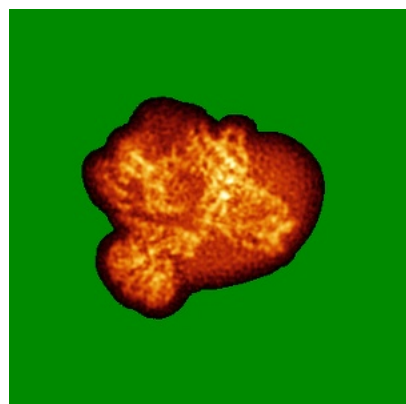


Z Index: 211

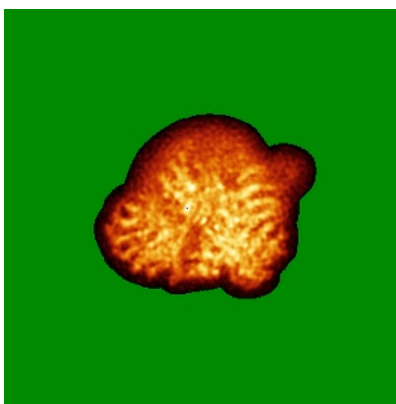
The images above show the largest variance slices of the map in three orthogonal directions.

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

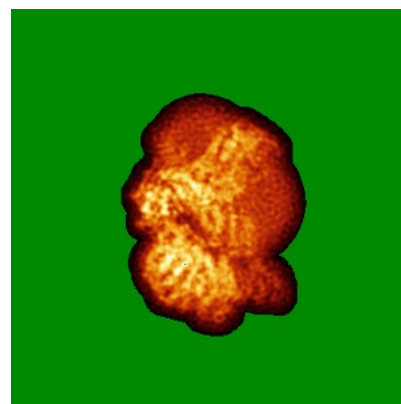
6.4.1 Primary map



X

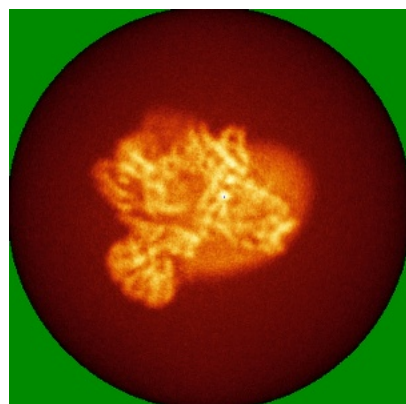


Y

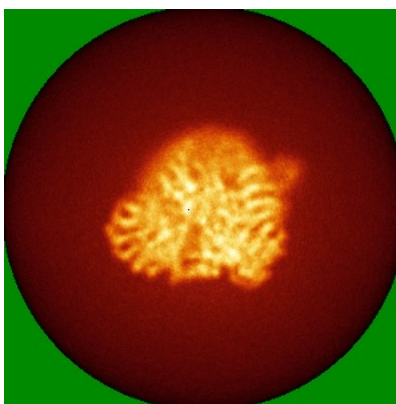


Z

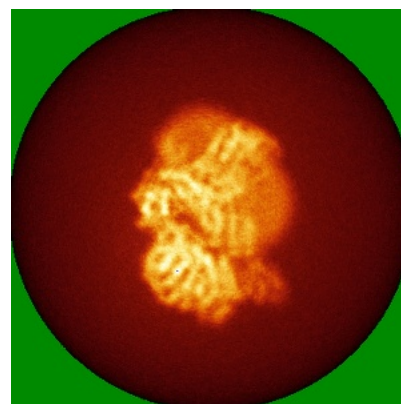
6.4.2 Raw map



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.

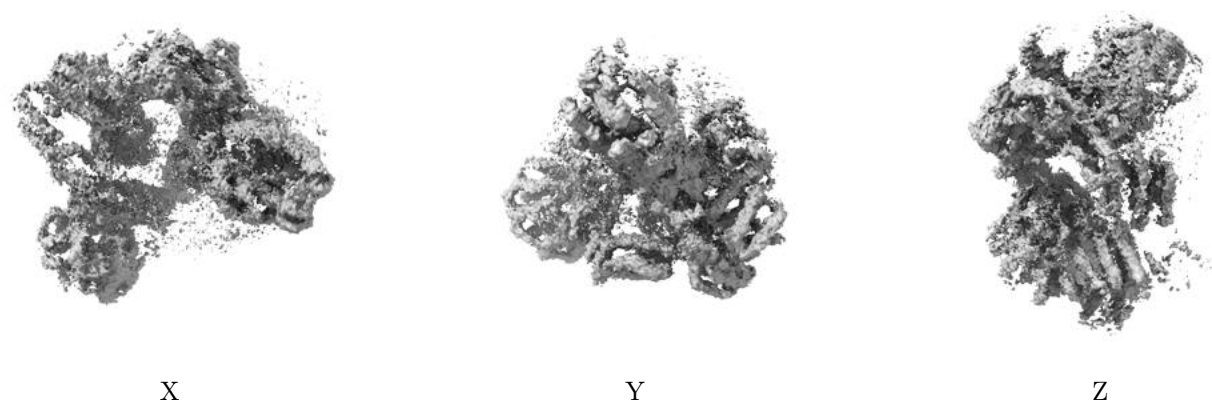
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0115. 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



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.

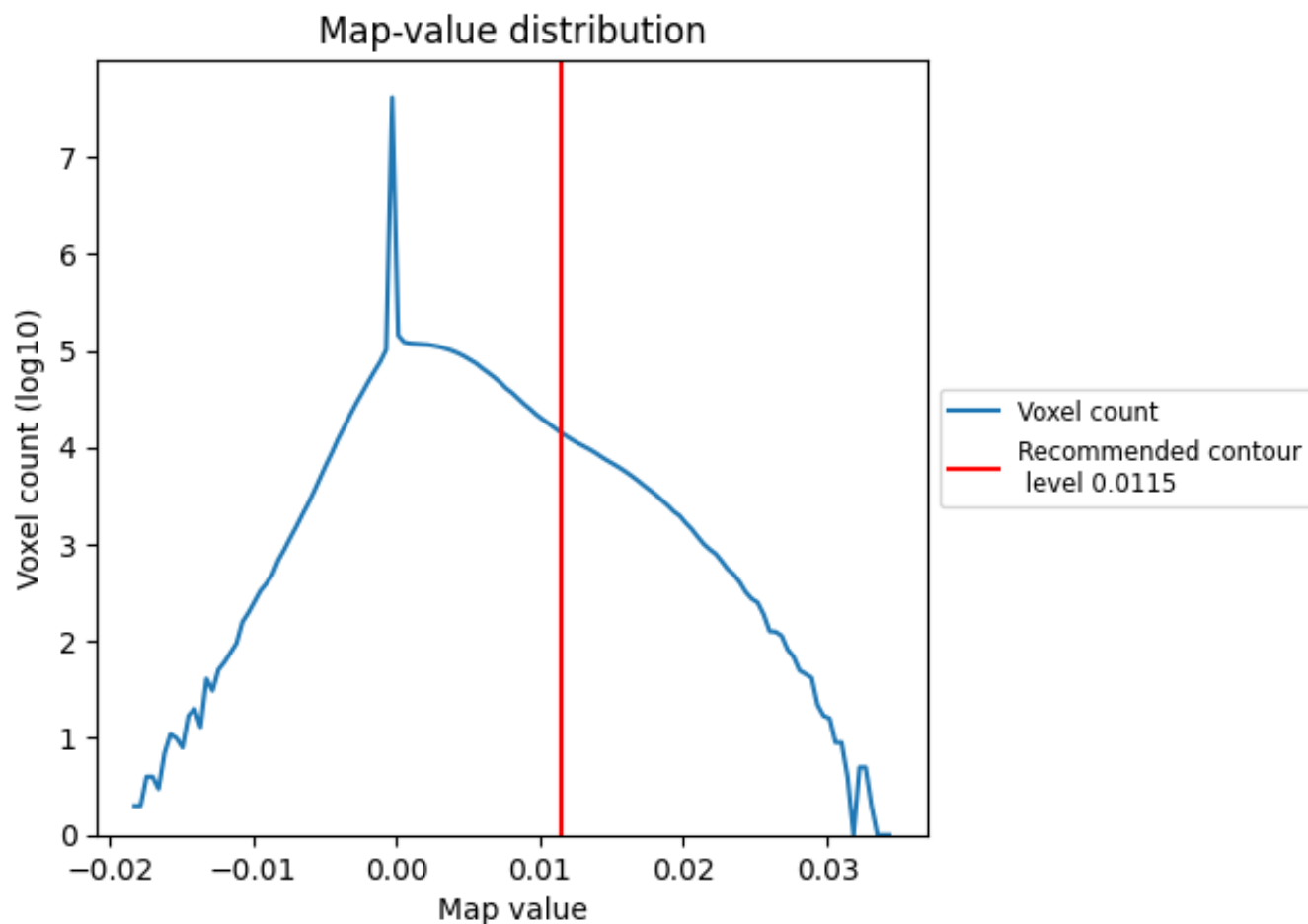
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

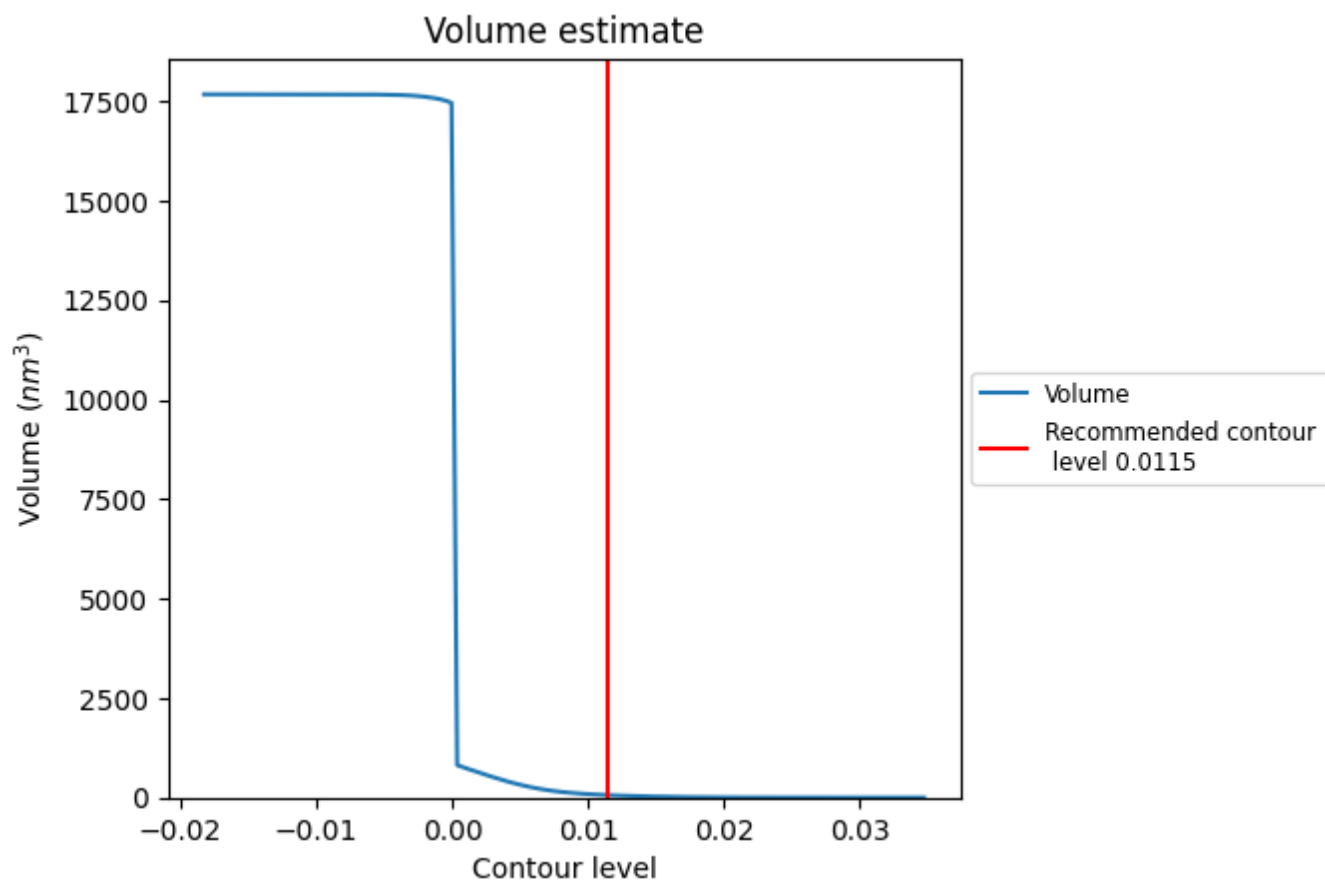
This section contains the results of statistical analysis of the map.

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.

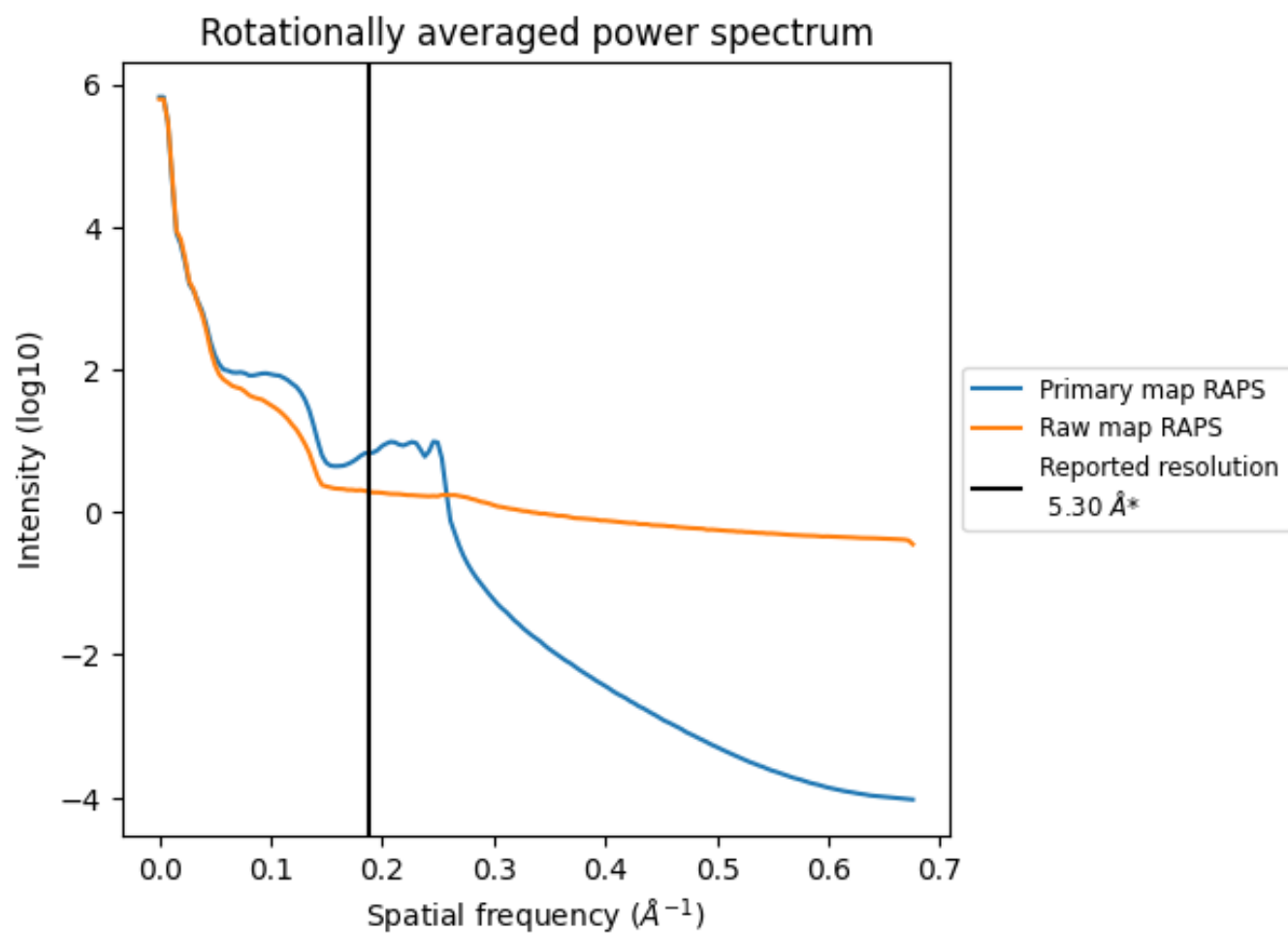
7.2 Volume estimate [i](#)



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 ⓘ

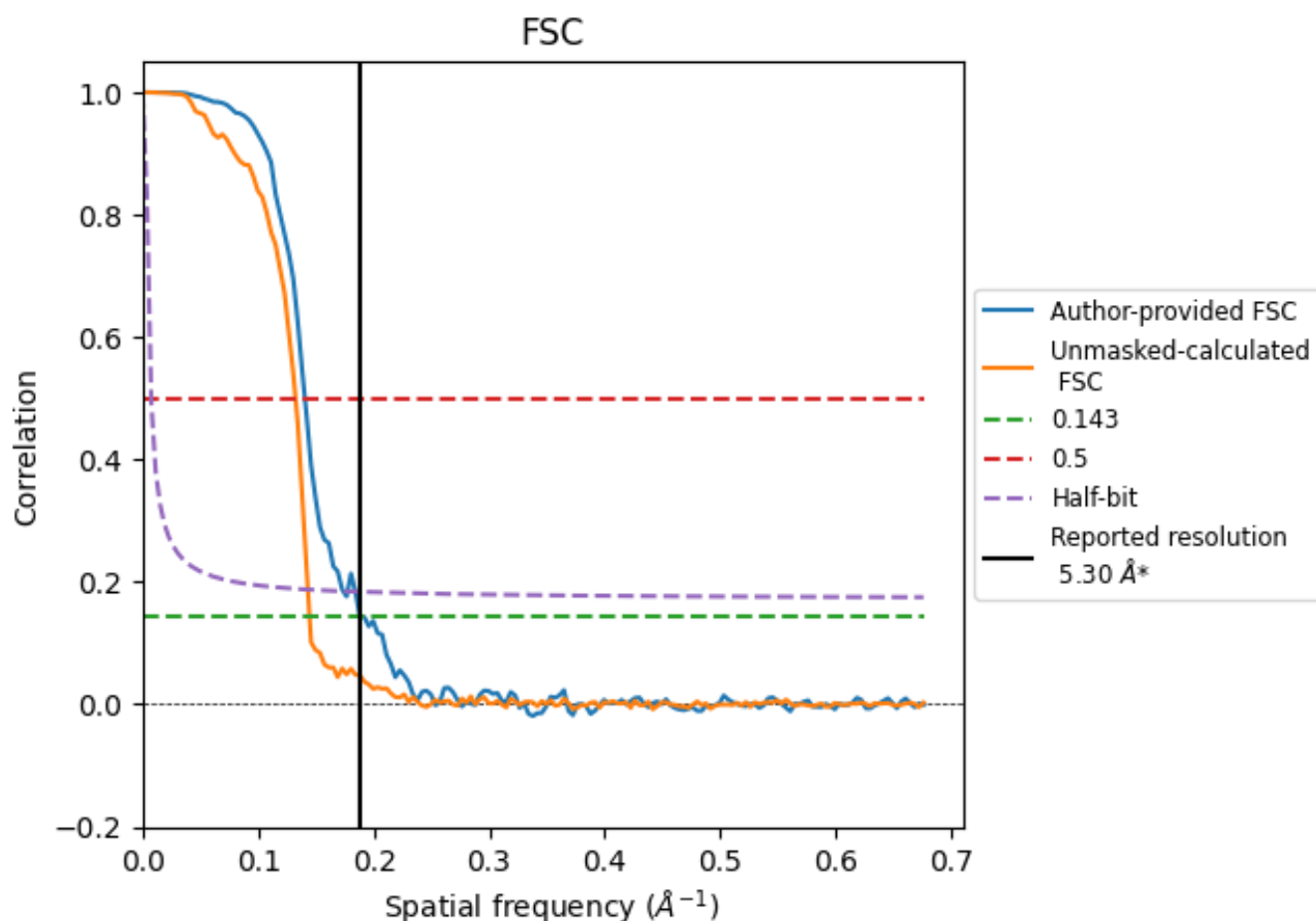


*Reported resolution corresponds to spatial frequency of 0.189 $\text{\AA}^{-1}$

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 0.189 Å⁻¹

8.2 Resolution estimates [i](#)

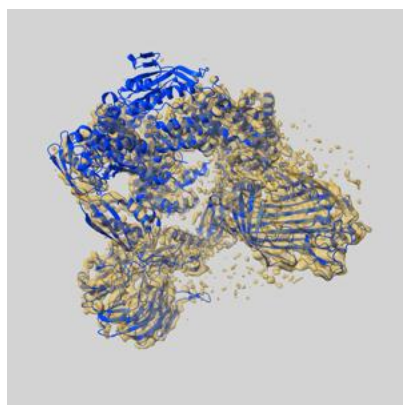
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.30	-	-
Author-provided FSC curve	5.30	7.11	5.75
Unmasked-calculated*	6.92	7.55	7.00

*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 6.92 differs from the reported value 5.3 by more than 10 %

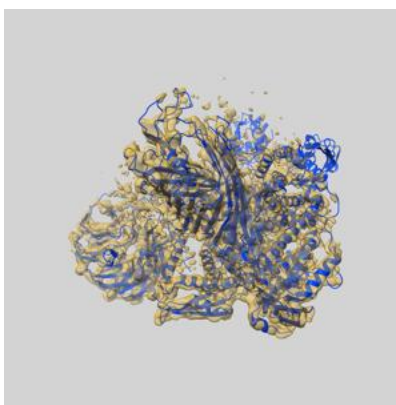
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56559 and PDB model 28JU. Per-residue inclusion information can be found in section [3](#) on page [7](#).

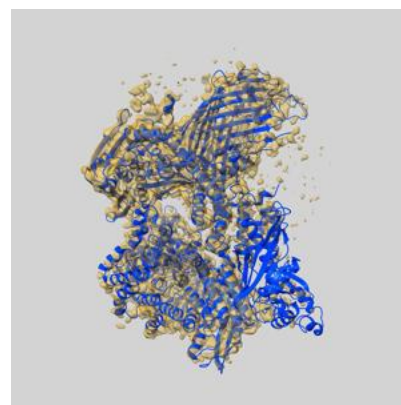
9.1 Map-model overlay [i](#)



X



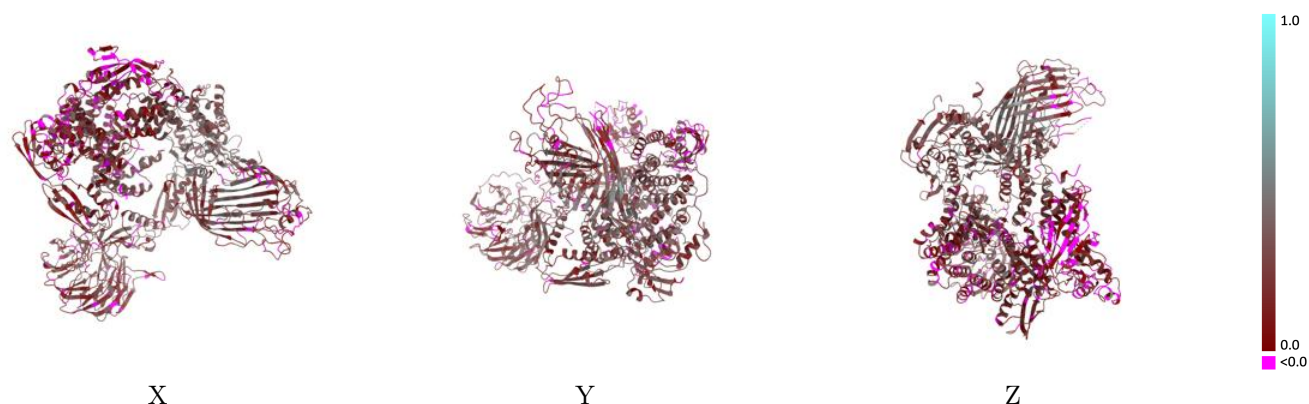
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0115 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](#)



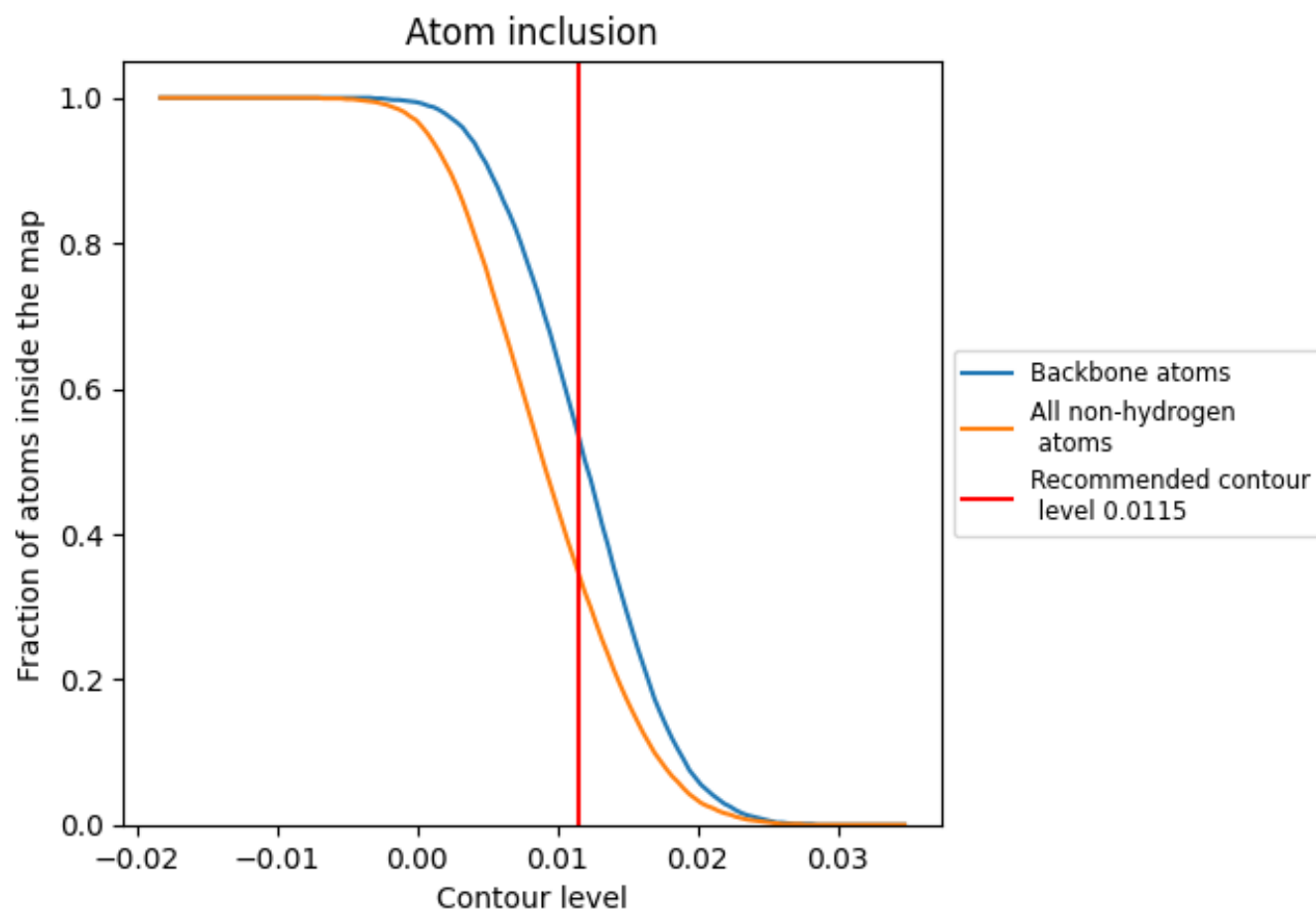
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0115).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 35% 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 (0.0115) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3470	0.2090
A	0.4290	0.2590
B	0.3440	0.1980
C	0.0910	0.0900
D	0.4600	0.2670
E	0.5080	0.2960
F	0.2790	0.1570

1.0

0.0

<0.0