



Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 08:46 AM EST

PDB ID : 6V0E
EMDB ID : EMD-20995
Title : Lipophilic Envelope-spanning Tunnel B (LetB), Model 3
Authors : Isom, G.L.; Coudray, N.; MacRae, M.R.; McManus, C.T.; Ekiert, D.C.; Bhabha, G.
Deposited on : 2019-11-18
Resolution : 3.06 Å(reported)
Based on initial model : 5UW2

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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

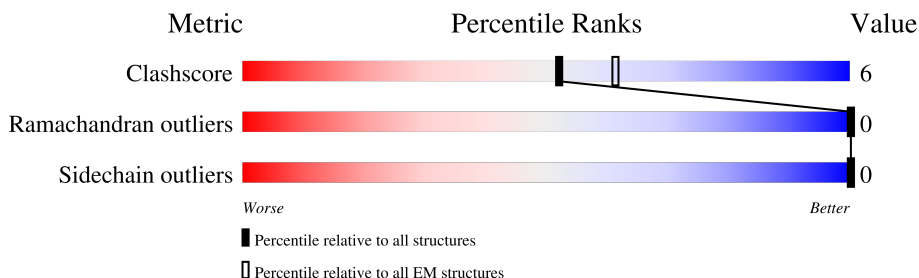
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY







The reported resolution of this entry is 3.06 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	832	
1	B	832	
1	C	832	
1	D	832	
1	E	832	
1	F	832	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16602 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.

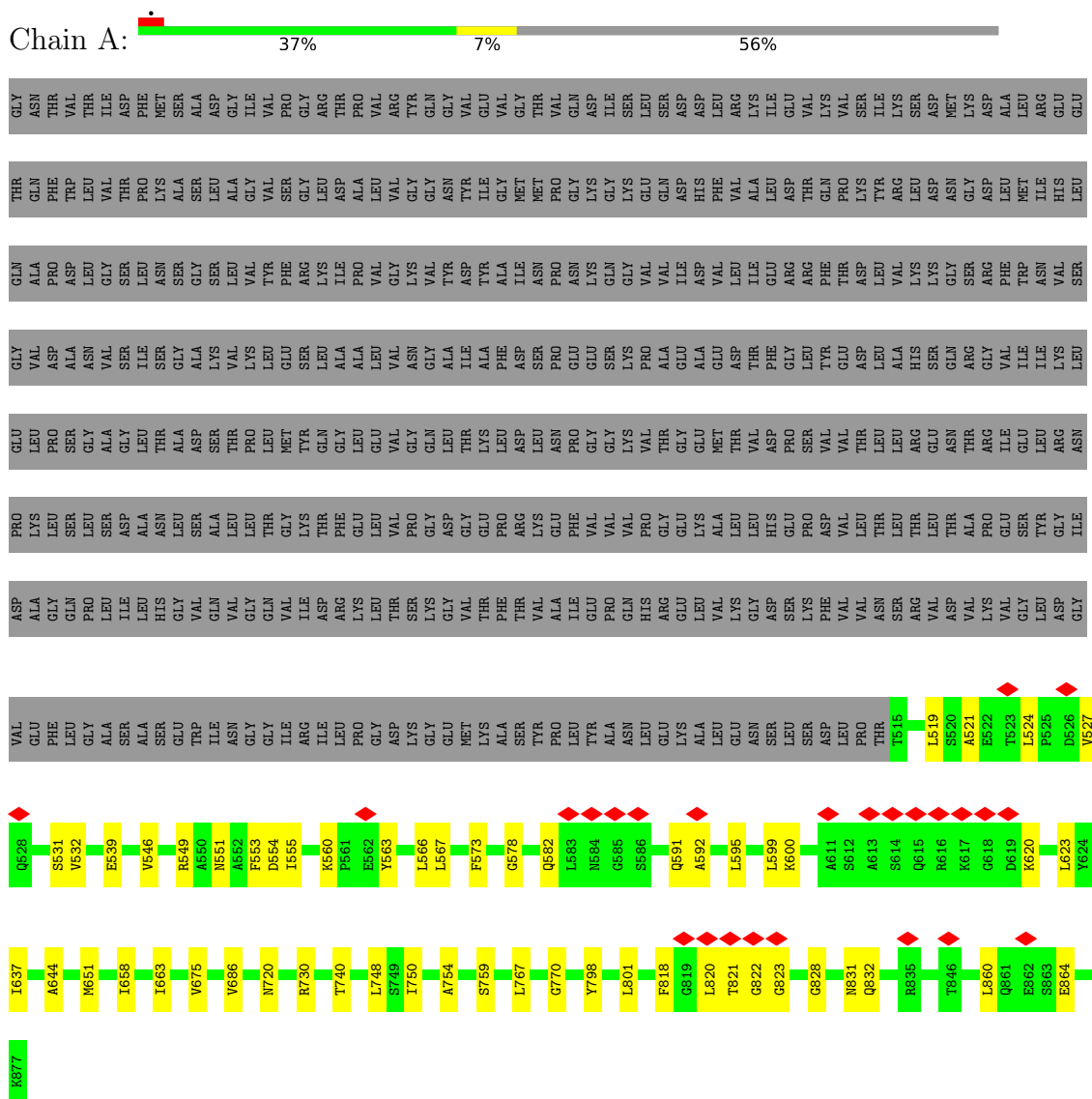
- Molecule 1 is a protein called Intermembrane transport protein YebT.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	363	Total	C	N	O	S	0	0
			2767	1757	487	519	4		
1	B	363	Total	C	N	O	S	0	0
			2767	1757	487	519	4		
1	C	363	Total	C	N	O	S	0	0
			2767	1757	487	519	4		
1	D	363	Total	C	N	O	S	0	0
			2767	1757	487	519	4		
1	E	363	Total	C	N	O	S	0	0
			2767	1757	487	519	4		
1	F	363	Total	C	N	O	S	0	0
			2767	1757	487	519	4		

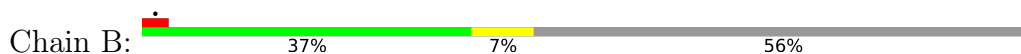
3 Residue-property plots

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: Intermembrane transport protein YebT



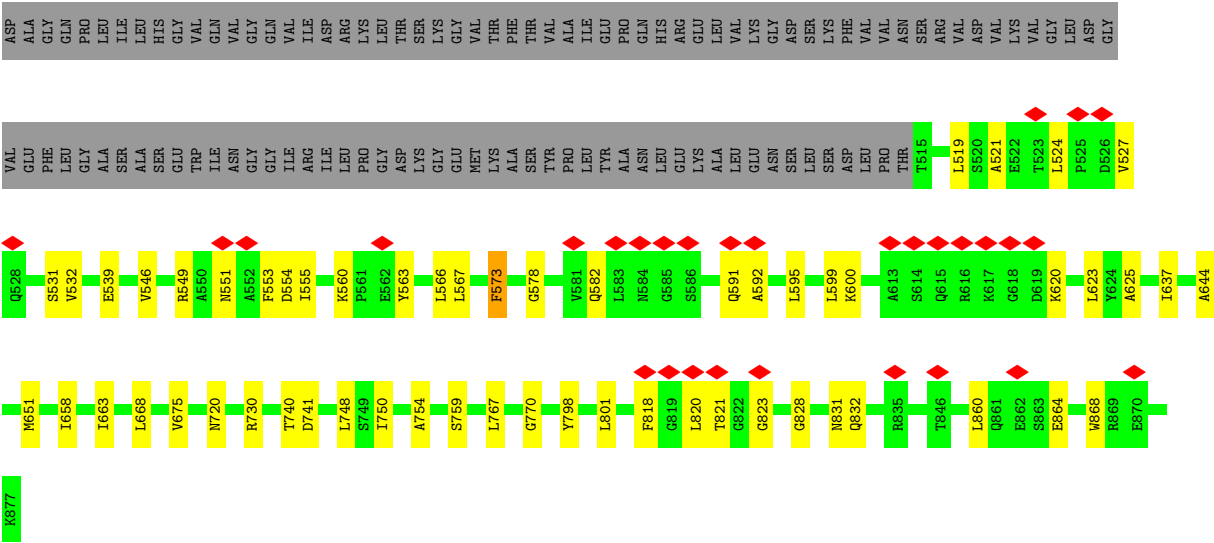
- Molecule 1: Intermembrane transport protein YebT



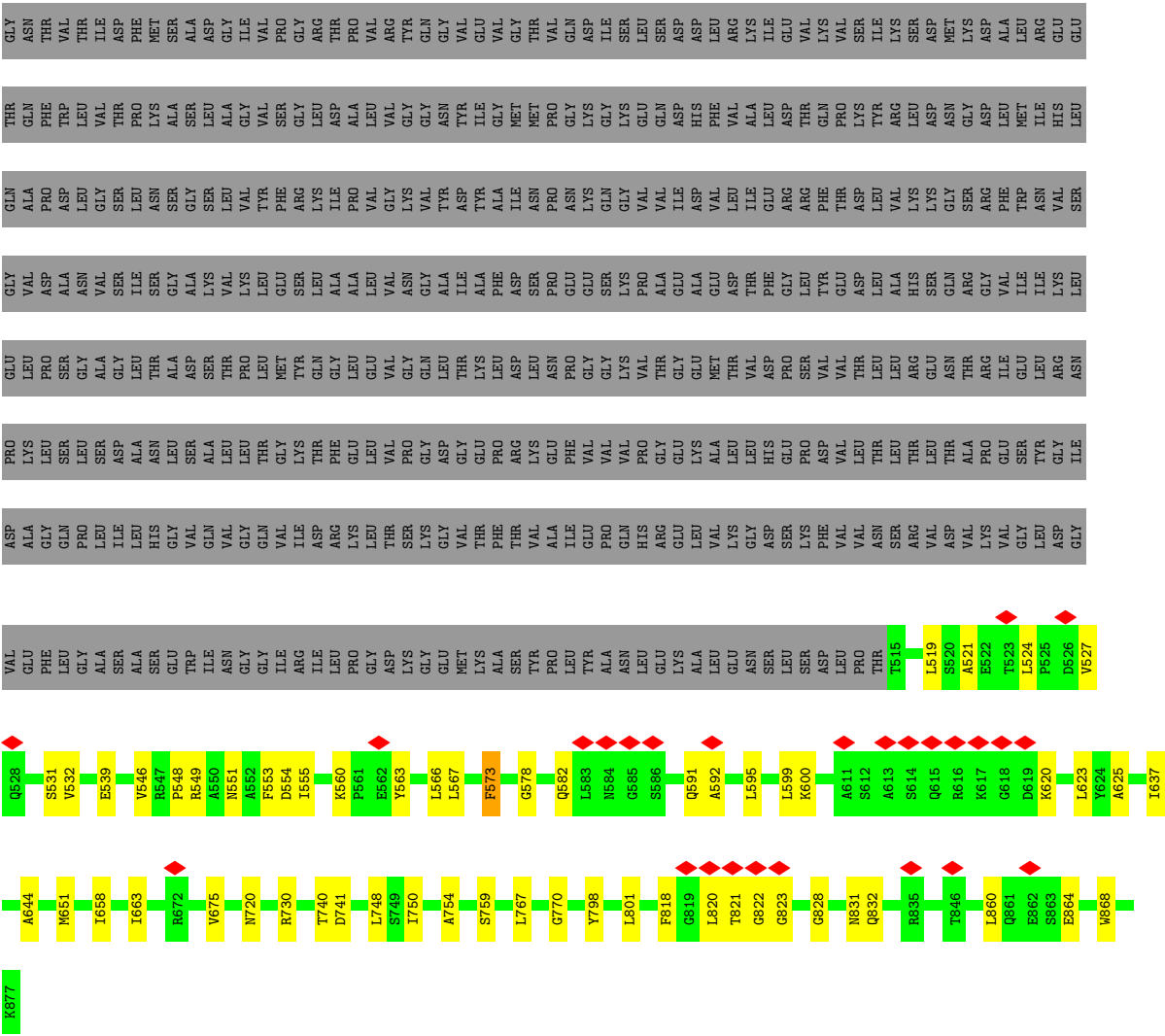
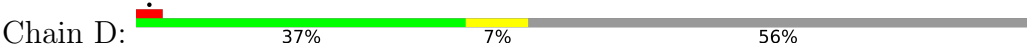


Frequency	Percentage
Daily	37%
Weekly	7%
Monthly	56%





● Molecule 1: Intermembrane transport protein YebT



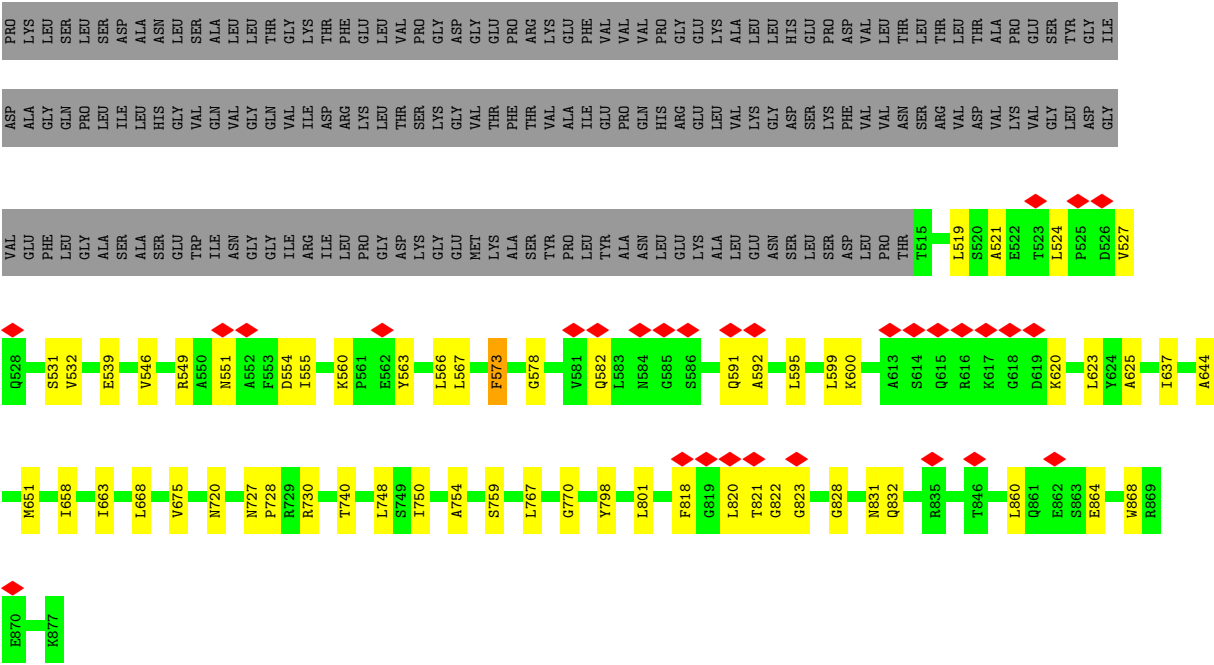
Chain E:



8377	A644	Q528	VAL	GLU	GLN	ASP	PRO	GLU	GLY	THR	GLN	GLY	GLN	THR	GLY
	M651	S531 V532	LEU	PHE	LEU	GLY	LYS	LEU	LEU	PRO	ASP	PRO	GLN	GLN	ASN
	I663	E539	ALA	SER	LEU	LEU	LEU	ALA	GLY	ALA	GLY	GLY	VAL	VAL	ILE
	I668	V546	ALA	SER	LEU	ASP	ASP	ALA	GLY	GLY	THR	THR	THR	THR	ASP
	R672	R549 A550	GLU	GLY	HIS	LEU	LEU	ALA	GLY	ALA	THR	LEU	PRO	PHE	MET
	V675	N551	ILE	ASN	GLN	VAL	SER	LEU	GLY	ASP	ASP	GLY	GLY	SER	ALA
	N720	A552	GLY	GLY	GLN	VAL	LEU	LEU	GLN	THR	THR	VAL	VAL	GLY	GLY
	R730	F553 D554 I555	ILE	ILE	VAL	GLY	THR	GLY	GLY	LEU	MET	GLY	TYR	PRO	ILE
	T740	K560	ILE	ILE	ASP	ASP	THR	THR	THR	GLN	GLY	LEU	LEU	ARG	GLY
	D741	P561	LEU	LEU	ARG	ARG	PHE	LEU	GLY	GLY	GLY	ALA	ALA	ASP	THR
	L748	E562	PRO	PRO	LYS	LYS	LEU	LEU	LEU	LEU	PRO	VAL	VAL	PRO	ALA
	S749	Y563	GLY	GLY	THR	THR	VAL	VAL	VAL	GLU	GLY	VAL	VAL	LEU	ARG
	I750	L566 L567	LYS	GLY	LYS	GLY	PRO	GLY	GLY	GLN	GLY	ASN	GLY	TYR	GLN
	A754	F573	GLY	GLY	VAL	GLY	ASP	GLY	GLY	LEU	ALA	TYR	ASN	ASN	GLY
	S759	G578	MET	MET	THR	THR	THR	GLY	THR	LEU	LYS	ILE	GLY	GLY	VAL
	L767	G578	ALA	ALA	PHE	PHE	ARG	ARG	THR	LEU	ASP	ILE	MET	GLY	VAL
	G770	V581 Q582	THR	THR	VAL	VAL	LYS	GLY	VAL	ASN	ASN	PRO	MET	THR	THR
	F818	L583	PRO	LEU	ALA	ALA	GLY	GLY	GLY	ASN	ASN	GLY	PRO	VAL	VAL
	G819	N584	ALA	ALA	GLY	GLY	PHE	GLY	VAL	PRO	GLY	GLY	LYS	ASP	ASP
	L820	G585	ASN	ASN	GLN	GLN	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ILE	ILE
	T821	S586	LEU	LEU	HIS	HIS	PRO	PRO	VAL	LYS	LYS	GLY	LYS	SER	LEU
	G822	Q591	LYS	LYS	ARG	ARG	GLY	GLY	THR	VAL	VAL	VAL	GLN	SER	LEU
	G823	A592	ALA	ALA	LEU	LEU	GLY	LEU	GLY	GLY	GLY	ILE	ILE	ASP	ASP
	V824	L595	LEU	LEU	VAL	VAL	ALA	ALA	MET	GLY	GLY	VAL	PHE	LEU	ARG
	V825	L595	GLY	ASN	LYS	GLY	LEU	LEU	THR	THR	THR	ILE	ALA	ARG	LYS
	G828	L599 K600	SER	SER	ASP	ASP	HIS	LEU	ASP	THR	ASP	GLY	ALA	ILE	ILE
	N831	Q832	LEU	LEU	LYS	LYS	GLY	GLY	THR	PRO	THR	ARG	GLY	GLY	VAL
	R835	A611 S612 A613	PRO	PRO	VAL	VAL	VAL	THR	VAL	THR	THR	LEU	THR	LYS	VAL
	T846	S614 Q615 R616	THR	THR	ASN	ASN	THR	THR	LEU	LEU	LEU	ALA	VAL	LEU	LYS
	E854	Q615 R616 K617	ARG	ARG	VAL	VAL	THR	THR	VAL	GLY	GLY	HIS	VAL	ARG	LYS
	L860	G618	ASP	ASP	VAL	VAL	ALA	LEU	THR	THR	THR	ARG	VAL	LEU	ASP
	E864	D619	LYS	LYS	GLY	GLY	THR	THR	GLY	GLY	GLY	ASN	GLY	TRP	ALA
	-	K620	GLY	GLY	LEU	LEU	GLY	GLY	THR	GLY	GLY	ASN	GLY	ILE	ARG
	-	D526	GLY	GLY	THR	THR	ILE	THR	ASN	THR	THR	LEU	VAL	THR	GLU

Chain F:

[illegible]



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	101464	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.385	Depositor
Minimum map value	-0.184	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	366.8, 366.8, 366.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/2822	0.62	1/3831 (0.0%)
1	B	0.41	0/2822	0.62	2/3831 (0.1%)
1	C	0.41	0/2822	0.62	2/3831 (0.1%)
1	D	0.41	0/2822	0.62	2/3831 (0.1%)
1	E	0.41	0/2822	0.62	1/3831 (0.0%)
1	F	0.41	0/2822	0.62	2/3831 (0.1%)
All	All	0.41	0/16932	0.62	10/22986 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	567	LEU	CA-CB-CG	5.89	128.86	115.30
1	B	567	LEU	CA-CB-CG	5.89	128.85	115.30
1	D	567	LEU	CA-CB-CG	5.89	128.84	115.30
1	C	567	LEU	CA-CB-CG	5.88	128.82	115.30
1	A	567	LEU	CA-CB-CG	5.88	128.81	115.30
1	F	567	LEU	CA-CB-CG	5.87	128.81	115.30
1	C	573	PHE	CB-CG-CD1	5.09	124.36	120.80
1	F	573	PHE	CB-CG-CD1	5.06	124.34	120.80
1	D	573	PHE	CB-CG-CD1	5.06	124.34	120.80
1	B	573	PHE	CB-CG-CD1	5.01	124.31	120.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2767	0	2795	37	0
1	B	2767	0	2795	36	0
1	C	2767	0	2795	37	0
1	D	2767	0	2795	38	0
1	E	2767	0	2795	36	0
1	F	2767	0	2795	38	0
All	All	16602	0	16770	190	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 6.

All (190) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:818:PHE:HB3	1:D:823:GLY:H	1.55	0.71
1:A:823:GLY:H	1:F:818:PHE:HB3	1.57	0.69
1:A:818:PHE:HB3	1:B:823:GLY:H	1.58	0.68
1:D:818:PHE:HB3	1:E:823:GLY:H	1.60	0.66
1:C:546:VAL:HG23	1:C:555:ILE:HG12	1.80	0.63
1:E:546:VAL:HG23	1:E:555:ILE:HG12	1.80	0.63
1:D:546:VAL:HG23	1:D:555:ILE:HG12	1.80	0.63
1:F:546:VAL:HG23	1:F:555:ILE:HG12	1.80	0.63
1:B:546:VAL:HG23	1:B:555:ILE:HG12	1.80	0.63
1:A:546:VAL:HG23	1:A:555:ILE:HG12	1.81	0.61
1:A:637:ILE:HG22	1:A:730:ARG:HG3	1.83	0.61
1:D:637:ILE:HG22	1:D:730:ARG:HG3	1.83	0.61
1:E:637:ILE:HG22	1:E:730:ARG:HG3	1.83	0.61
1:E:818:PHE:HB3	1:F:823:GLY:H	1.64	0.61
1:F:637:ILE:HG22	1:F:730:ARG:HG3	1.83	0.61
1:B:637:ILE:HG22	1:B:730:ARG:HG3	1.83	0.60
1:B:818:PHE:HB3	1:C:823:GLY:H	1.66	0.60
1:C:637:ILE:HG22	1:C:730:ARG:HG3	1.83	0.60
1:A:754:ALA:HB2	1:A:860:LEU:HD13	1.86	0.58
1:E:521:ALA:HB2	1:E:623:LEU:HB3	1.86	0.58
1:E:651:MET:HB3	1:E:663:ILE:HD12	1.86	0.58
1:F:651:MET:HB3	1:F:663:ILE:HD12	1.86	0.58
1:A:651:MET:HB3	1:A:663:ILE:HD12	1.86	0.58
1:C:754:ALA:HB2	1:C:860:LEU:HD13	1.85	0.58
1:D:521:ALA:HB2	1:D:623:LEU:HB3	1.86	0.58
1:D:759:SER:OG	1:E:828:GLY:O	2.22	0.58
1:F:754:ALA:HB2	1:F:860:LEU:HD13	1.86	0.58
1:D:651:MET:HB3	1:D:663:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:ALA:HB2	1:C:623:LEU:HB3	1.86	0.57
1:D:754:ALA:HB2	1:D:860:LEU:HD13	1.86	0.57
1:B:754:ALA:HB2	1:B:860:LEU:HD13	1.85	0.57
1:F:521:ALA:HB2	1:F:623:LEU:HB3	1.86	0.57
1:A:759:SER:OG	1:B:828:GLY:O	2.22	0.57
1:B:651:MET:HB3	1:B:663:ILE:HD12	1.86	0.57
1:C:651:MET:HB3	1:C:663:ILE:HD12	1.86	0.57
1:D:527:VAL:HG21	1:D:531:SER:H	1.70	0.56
1:B:521:ALA:HB2	1:B:623:LEU:HB3	1.86	0.56
1:B:527:VAL:HG21	1:B:531:SER:H	1.71	0.56
1:C:527:VAL:HG21	1:C:531:SER:H	1.70	0.56
1:A:527:VAL:HG21	1:A:531:SER:H	1.71	0.56
1:F:527:VAL:HG21	1:F:531:SER:H	1.70	0.56
1:E:527:VAL:HG21	1:E:531:SER:H	1.70	0.56
1:E:754:ALA:HB2	1:E:860:LEU:HD13	1.86	0.56
1:A:521:ALA:HB2	1:A:623:LEU:HB3	1.86	0.56
1:A:560:LYS:HB2	1:A:563:TYR:HD2	1.71	0.56
1:D:578:GLY:HA2	1:E:592:ALA:HB2	1.88	0.56
1:E:759:SER:OG	1:F:828:GLY:O	2.24	0.55
1:A:821:THR:HA	1:F:820:LEU:HB3	1.89	0.55
1:D:560:LYS:HB2	1:D:563:TYR:HD2	1.72	0.55
1:F:560:LYS:HB2	1:F:563:TYR:HD2	1.71	0.55
1:B:560:LYS:HB2	1:B:563:TYR:HD2	1.72	0.55
1:C:820:LEU:HB3	1:D:821:THR:HA	1.88	0.55
1:E:560:LYS:HB2	1:E:563:TYR:HD2	1.71	0.54
1:B:759:SER:OG	1:C:828:GLY:O	2.25	0.54
1:C:560:LYS:HB2	1:C:563:TYR:HD2	1.72	0.53
1:D:644:ALA:HB2	1:D:675:VAL:HG11	1.91	0.53
1:D:554:ASP:OD1	1:D:620:LYS:NZ	2.39	0.53
1:A:644:ALA:HB2	1:A:675:VAL:HG11	1.91	0.53
1:B:578:GLY:HA2	1:C:592:ALA:HB2	1.91	0.53
1:C:554:ASP:OD1	1:C:620:LYS:NZ	2.39	0.53
1:C:720:ASN:HD21	1:C:740:THR:HA	1.74	0.52
1:F:644:ALA:HB2	1:F:675:VAL:HG11	1.91	0.52
1:F:720:ASN:HD21	1:F:740:THR:HA	1.75	0.52
1:A:549:ARG:HH12	1:A:551:ASN:HD22	1.56	0.52
1:A:720:ASN:HD21	1:A:740:THR:HA	1.74	0.52
1:E:554:ASP:OD1	1:E:620:LYS:NZ	2.39	0.52
1:C:644:ALA:HB2	1:C:675:VAL:HG11	1.91	0.52
1:A:578:GLY:HA2	1:B:592:ALA:HB2	1.92	0.52
1:D:720:ASN:HD21	1:D:740:THR:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:LEU:HB3	1:B:821:THR:HA	1.92	0.52
1:B:720:ASN:HD21	1:B:740:THR:HA	1.74	0.52
1:E:644:ALA:HB2	1:E:675:VAL:HG11	1.91	0.52
1:E:720:ASN:HD21	1:E:740:THR:HA	1.74	0.52
1:E:549:ARG:HH12	1:E:551:ASN:HD22	1.56	0.52
1:D:820:LEU:HB3	1:E:821:THR:HA	1.92	0.52
1:B:549:ARG:HH12	1:B:551:ASN:HD22	1.56	0.52
1:B:644:ALA:HB2	1:B:675:VAL:HG11	1.91	0.51
1:A:831:ASN:OD1	1:A:832:GLN:NE2	2.43	0.51
1:B:831:ASN:OD1	1:B:832:GLN:NE2	2.43	0.51
1:C:549:ARG:HH12	1:C:551:ASN:HD22	1.56	0.51
1:D:549:ARG:HH12	1:D:551:ASN:HD22	1.56	0.51
1:E:831:ASN:OD1	1:E:832:GLN:NE2	2.43	0.51
1:F:549:ARG:HH12	1:F:551:ASN:HD22	1.56	0.51
1:C:831:ASN:OD1	1:C:832:GLN:NE2	2.43	0.51
1:D:831:ASN:OD1	1:D:832:GLN:NE2	2.43	0.51
1:F:831:ASN:OD1	1:F:832:GLN:NE2	2.43	0.50
1:A:828:GLY:O	1:F:759:SER:OG	2.28	0.50
1:C:759:SER:OG	1:D:828:GLY:O	2.29	0.50
1:E:578:GLY:HA2	1:F:592:ALA:HB2	1.93	0.50
1:A:554:ASP:OD1	1:A:620:LYS:NZ	2.39	0.49
1:B:554:ASP:OD1	1:B:620:LYS:NZ	2.39	0.49
1:B:521:ALA:HB1	1:B:524:LEU:HD12	1.95	0.49
1:C:818:PHE:HD2	1:D:822:GLY:HA2	1.78	0.49
1:B:748:LEU:HD13	1:B:750:ILE:HG23	1.95	0.48
1:C:521:ALA:HB1	1:C:524:LEU:HD12	1.95	0.48
1:A:748:LEU:HD13	1:A:750:ILE:HG23	1.95	0.48
1:E:748:LEU:HD13	1:E:750:ILE:HG23	1.95	0.48
1:F:521:ALA:HB1	1:F:524:LEU:HD12	1.95	0.48
1:C:578:GLY:HA2	1:D:592:ALA:HB2	1.96	0.48
1:E:521:ALA:HB1	1:E:524:LEU:HD12	1.95	0.47
1:F:554:ASP:OD1	1:F:620:LYS:NZ	2.39	0.47
1:A:822:GLY:HA2	1:F:818:PHE:HD2	1.79	0.47
1:A:592:ALA:HB2	1:F:578:GLY:HA2	1.96	0.47
1:B:563:TYR:HA	1:B:566:LEU:HD13	1.97	0.47
1:D:864:GLU:OE2	1:D:868:TRP:NE1	2.33	0.47
1:A:563:TYR:HA	1:A:566:LEU:HD13	1.97	0.47
1:A:521:ALA:HB1	1:A:524:LEU:HD12	1.95	0.47
1:C:748:LEU:HD13	1:C:750:ILE:HG23	1.95	0.47
1:D:521:ALA:HB1	1:D:524:LEU:HD12	1.95	0.47
1:D:748:LEU:HD13	1:D:750:ILE:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:532:VAL:HG21	1:E:539:GLU:HB3	1.97	0.47
1:C:563:TYR:HA	1:C:566:LEU:HD13	1.97	0.47
1:E:864:GLU:OE2	1:E:868:TRP:NE1	2.33	0.47
1:E:820:LEU:HB3	1:F:821:THR:HA	1.97	0.47
1:F:748:LEU:HD13	1:F:750:ILE:HG23	1.95	0.46
1:F:532:VAL:HG21	1:F:539:GLU:HB3	1.97	0.46
1:D:532:VAL:HG21	1:D:539:GLU:HB3	1.97	0.46
1:B:532:VAL:HG21	1:B:539:GLU:HB3	1.97	0.46
1:F:563:TYR:HA	1:F:566:LEU:HD13	1.97	0.46
1:A:532:VAL:HG21	1:A:539:GLU:HB3	1.97	0.45
1:B:820:LEU:HB3	1:C:821:THR:HA	1.98	0.45
1:D:563:TYR:HA	1:D:566:LEU:HD13	1.97	0.45
1:B:524:LEU:HD23	1:B:524:LEU:HA	1.85	0.45
1:D:519:LEU:HD11	1:D:573:PHE:HD2	1.81	0.45
1:E:563:TYR:HA	1:E:566:LEU:HD13	1.97	0.45
1:C:532:VAL:HG21	1:C:539:GLU:HB3	1.97	0.45
1:E:668:LEU:HB2	1:F:658:ILE:HG13	1.97	0.45
1:F:767:LEU:HD23	1:F:770:GLY:HA2	1.98	0.45
1:E:519:LEU:HD11	1:E:573:PHE:HD2	1.82	0.45
1:B:527:VAL:HG23	1:B:600:LYS:HD2	1.99	0.45
1:C:519:LEU:HD11	1:C:573:PHE:HD2	1.81	0.45
1:E:767:LEU:HD23	1:E:770:GLY:HA2	1.99	0.45
1:E:527:VAL:HG23	1:E:600:LYS:HD2	1.99	0.45
1:B:668:LEU:HB2	1:C:658:ILE:HG13	1.99	0.45
1:D:767:LEU:HD23	1:D:770:GLY:HA2	1.98	0.45
1:C:767:LEU:HD23	1:C:770:GLY:HA2	1.98	0.44
1:D:527:VAL:HG23	1:D:600:LYS:HD2	1.99	0.44
1:A:527:VAL:HG23	1:A:600:LYS:HD2	1.99	0.44
1:F:519:LEU:HD11	1:F:573:PHE:HD2	1.82	0.44
1:B:767:LEU:HD23	1:B:770:GLY:HA2	1.99	0.44
1:B:519:LEU:HD11	1:B:573:PHE:HD2	1.82	0.44
1:A:595:LEU:HG	1:A:599:LEU:HD13	2.00	0.44
1:C:527:VAL:HG23	1:C:600:LYS:HD2	1.99	0.44
1:D:595:LEU:HG	1:D:599:LEU:HD13	2.00	0.44
1:C:595:LEU:HG	1:C:599:LEU:HD13	2.00	0.43
1:F:527:VAL:HG23	1:F:600:LYS:HD2	1.99	0.43
1:F:595:LEU:HG	1:F:599:LEU:HD13	2.00	0.43
1:A:519:LEU:HD11	1:A:573:PHE:HD2	1.81	0.43
1:B:595:LEU:HG	1:B:599:LEU:HD13	2.00	0.43
1:E:595:LEU:HG	1:E:599:LEU:HD13	2.00	0.43
1:A:658:ILE:HG13	1:F:668:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:LEU:HD23	1:A:770:GLY:HA2	1.99	0.43
1:B:864:GLU:OE2	1:B:868:TRP:NE1	2.33	0.43
1:D:521:ALA:O	1:D:553:PHE:N	2.48	0.43
1:E:521:ALA:O	1:E:553:PHE:N	2.48	0.42
1:C:668:LEU:HB2	1:D:658:ILE:HG13	2.01	0.42
1:E:582:GLN:HE22	1:E:591:GLN:HE22	1.68	0.42
1:D:524:LEU:HD21	1:D:625:ALA:HA	2.01	0.42
1:D:582:GLN:HE22	1:D:591:GLN:HE22	1.68	0.42
1:F:524:LEU:HA	1:F:524:LEU:HD23	1.85	0.42
1:F:582:GLN:HE22	1:F:591:GLN:HE22	1.68	0.42
1:F:864:GLU:OE2	1:F:868:TRP:NE1	2.33	0.42
1:C:582:GLN:HE22	1:C:591:GLN:HE22	1.68	0.41
1:E:524:LEU:HD21	1:E:625:ALA:HA	2.01	0.41
1:C:864:GLU:OE2	1:C:868:TRP:NE1	2.33	0.41
1:C:524:LEU:HD21	1:C:625:ALA:HA	2.01	0.41
1:F:524:LEU:HD21	1:F:625:ALA:HA	2.01	0.41
1:A:582:GLN:HE22	1:A:591:GLN:HE22	1.68	0.41
1:B:521:ALA:O	1:B:553:PHE:N	2.47	0.41
1:B:727:ASN:HA	1:B:728:PRO:HD3	1.95	0.41
1:C:521:ALA:O	1:C:553:PHE:N	2.48	0.41
1:A:521:ALA:O	1:A:553:PHE:N	2.47	0.41
1:A:524:LEU:HA	1:A:524:LEU:HD23	1.85	0.41
1:B:582:GLN:HE22	1:B:591:GLN:HE22	1.68	0.41
1:E:818:PHE:HD2	1:F:822:GLY:HA2	1.86	0.41
1:D:548:PRO:HG2	1:E:563:TYR:HE1	1.85	0.41
1:F:727:ASN:HA	1:F:728:PRO:HD3	1.95	0.41
1:A:524:LEU:HD21	1:A:625:ALA:HA	2.02	0.41
1:A:798:TYR:HB3	1:A:801:LEU:HD12	2.03	0.41
1:A:864:GLU:OE2	1:A:868:TRP:NE1	2.33	0.41
1:B:524:LEU:HD21	1:B:625:ALA:HA	2.01	0.41
1:B:798:TYR:HB3	1:B:801:LEU:HD12	2.03	0.41
1:C:741:ASP:OD1	1:C:741:ASP:N	2.55	0.40
1:C:798:TYR:HB3	1:C:801:LEU:HD12	2.03	0.40
1:D:741:ASP:OD1	1:D:741:ASP:N	2.55	0.40
1:A:635:GLY:HA3	1:A:686:VAL:HG21	2.04	0.40
1:F:798:TYR:HB3	1:F:801:LEU:HD12	2.03	0.40
1:D:524:LEU:HD23	1:D:524:LEU:HA	1.85	0.40
1:D:798:TYR:HB3	1:D:801:LEU:HD12	2.03	0.40
1:E:741:ASP:OD1	1:E:741:ASP:N	2.55	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	A	361/832 (43%)	341 (94%)	20 (6%)	0	100	100
1	B	361/832 (43%)	342 (95%)	19 (5%)	0	100	100
1	C	361/832 (43%)	342 (95%)	19 (5%)	0	100	100
1	D	361/832 (43%)	342 (95%)	19 (5%)	0	100	100
1	E	361/832 (43%)	342 (95%)	19 (5%)	0	100	100
1	F	361/832 (43%)	342 (95%)	19 (5%)	0	100	100
All	All	2166/4992 (43%)	2051 (95%)	115 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	291/683 (43%)	291 (100%)	0	100	100
1	B	291/683 (43%)	291 (100%)	0	100	100
1	C	291/683 (43%)	291 (100%)	0	100	100
1	D	291/683 (43%)	291 (100%)	0	100	100
1	E	291/683 (43%)	291 (100%)	0	100	100
1	F	291/683 (43%)	291 (100%)	0	100	100
All	All	1746/4098 (43%)	1746 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	551	ASN
1	A	591	GLN
1	A	832	GLN
1	B	551	ASN
1	B	591	GLN
1	B	832	GLN
1	C	551	ASN
1	C	591	GLN
1	C	832	GLN
1	D	551	ASN
1	D	591	GLN
1	D	832	GLN
1	E	551	ASN
1	E	591	GLN
1	E	832	GLN
1	F	551	ASN
1	F	591	GLN
1	F	832	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 monosaccharides 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.

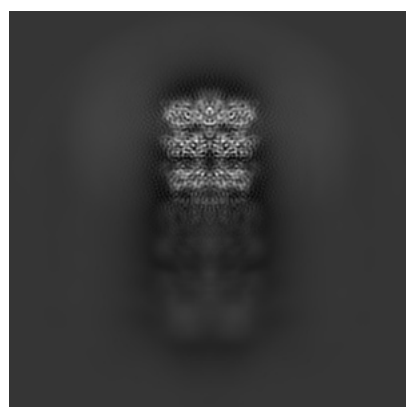
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20995. These allow visual inspection of the internal detail of the map and identification of artifacts.

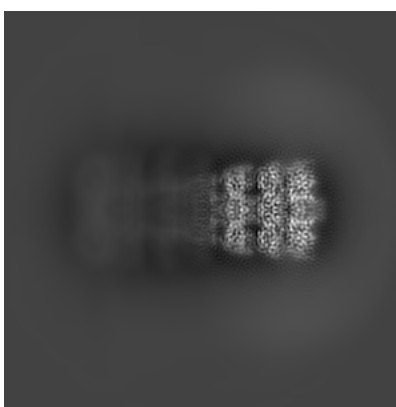
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

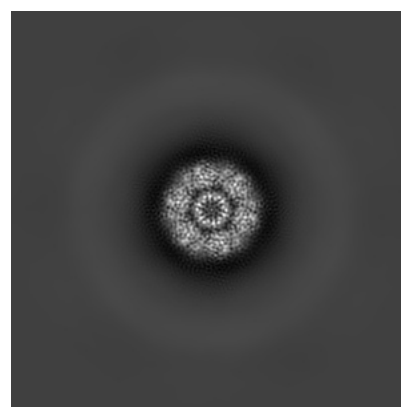
6.1.1 Primary map



X



Y



Z

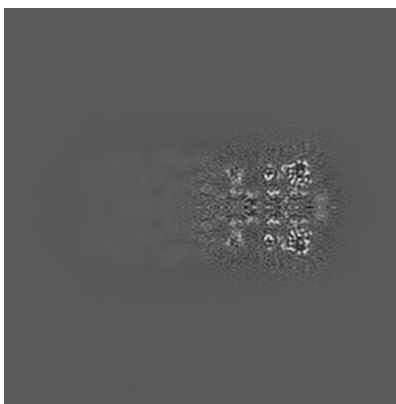
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

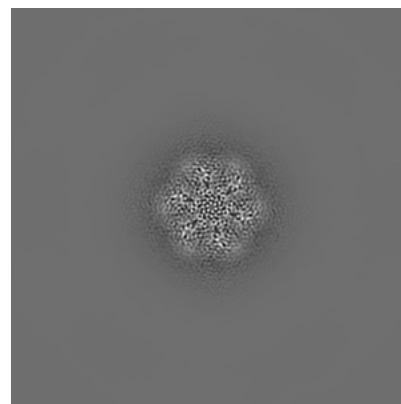
6.2.1 Primary map



X Index: 140



Y Index: 140

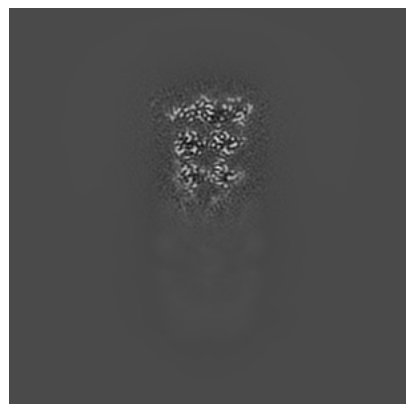


Z Index: 140

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

6.3 Largest variance slices [i](#)

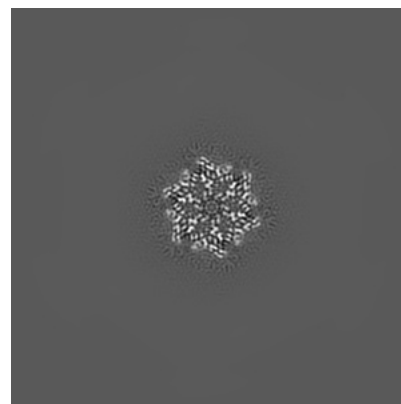
6.3.1 Primary map



X Index: 121



Y Index: 134

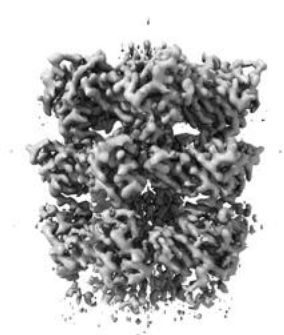


Z Index: 188

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

6.4 Orthogonal surface views [i](#)

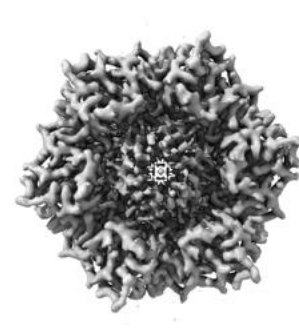
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

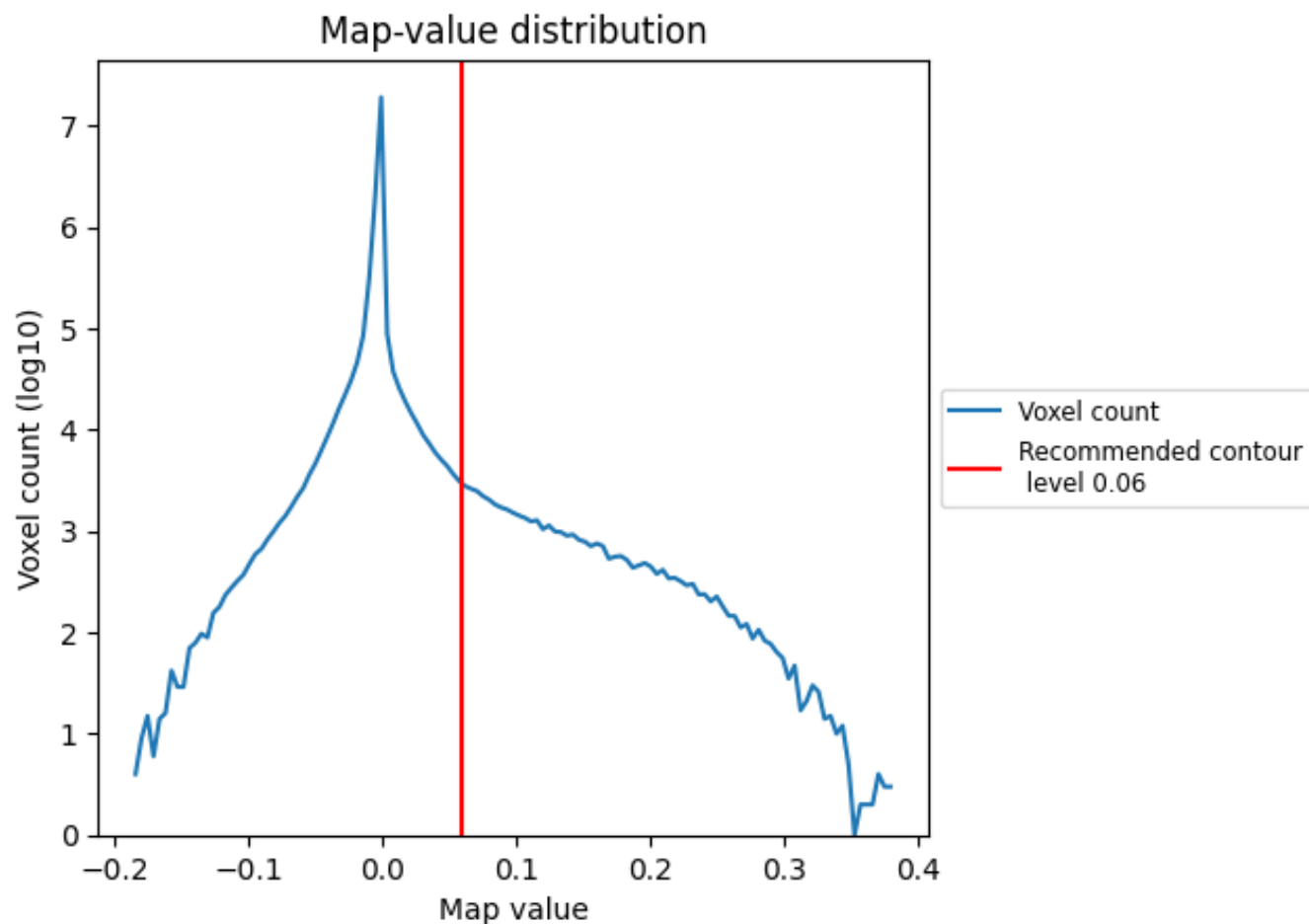
6.5 Mask visualisation

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

7 Map analysis [i](#)

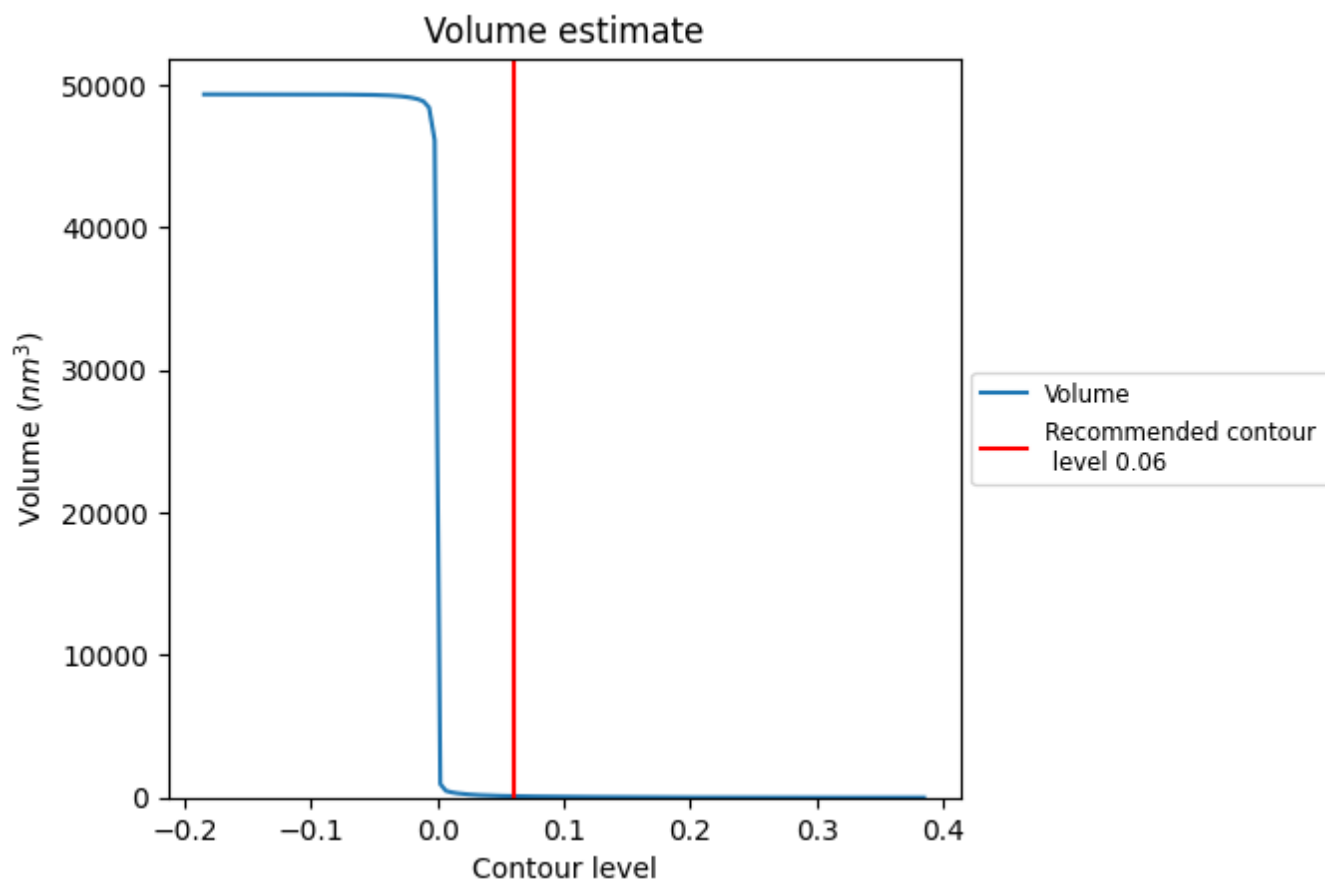
This section contains the results of statistical analysis of the map.

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.

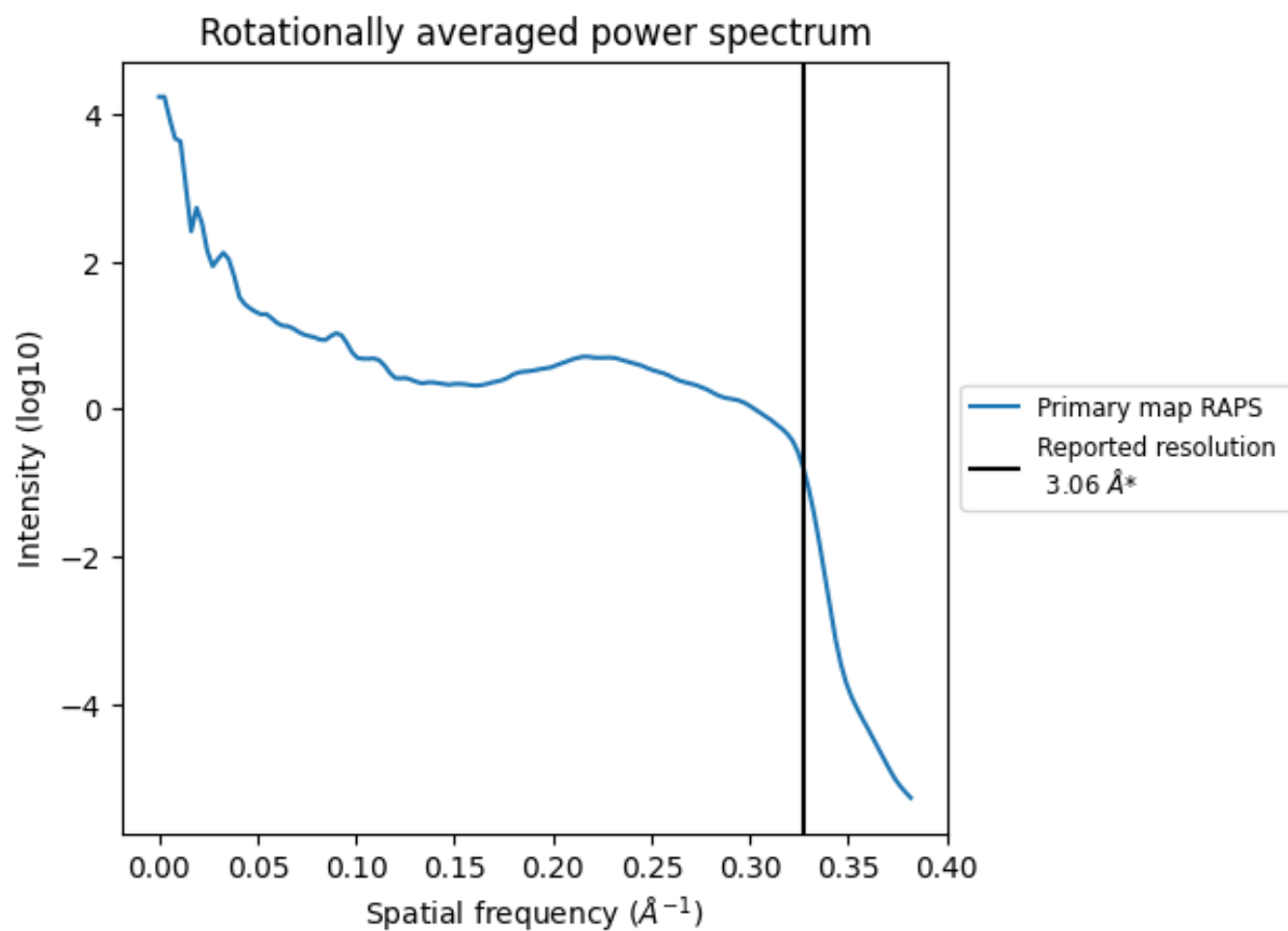
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 99 nm³; this corresponds to an approximate mass of 89 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 0.327 Å⁻¹

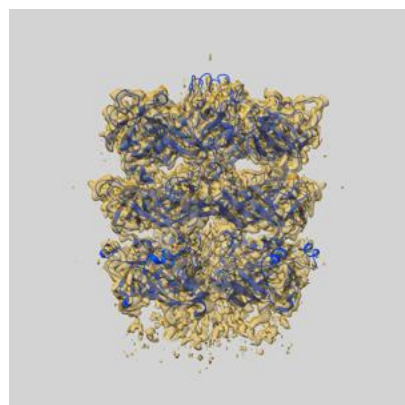
8 Fourier-Shell correlation ⓘ

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

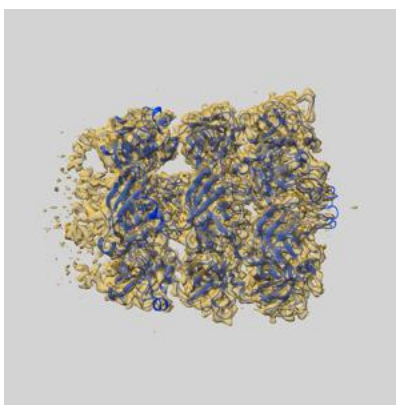
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20995 and PDB model 6V0E. Per-residue inclusion information can be found in section [3](#) on page [4](#).

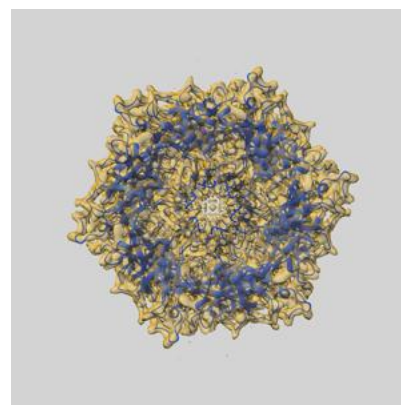
9.1 Map-model overlay [i](#)



X



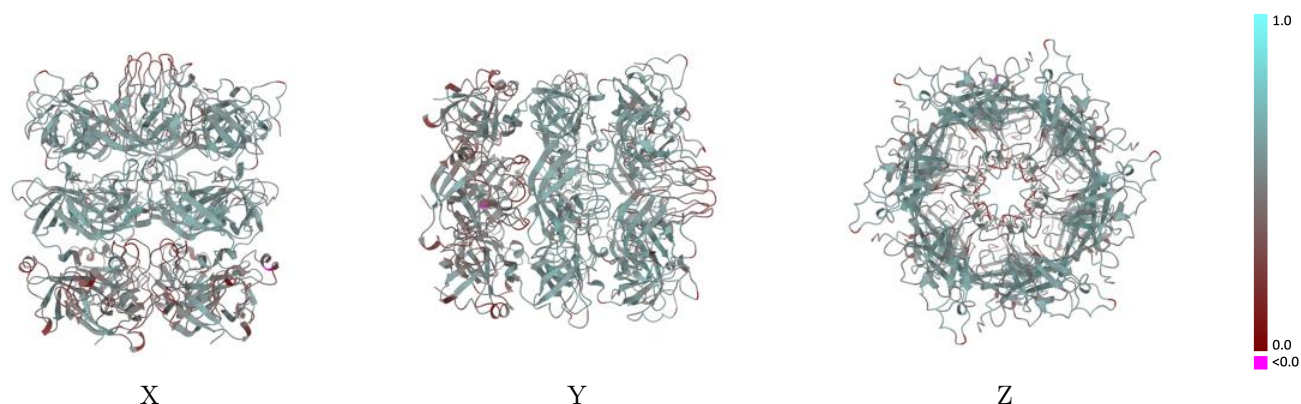
Y



Z

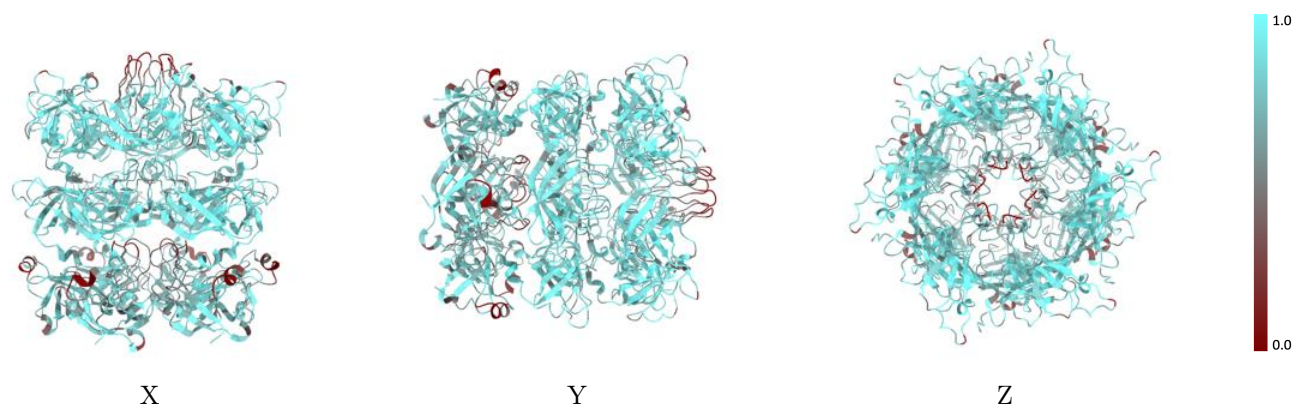
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



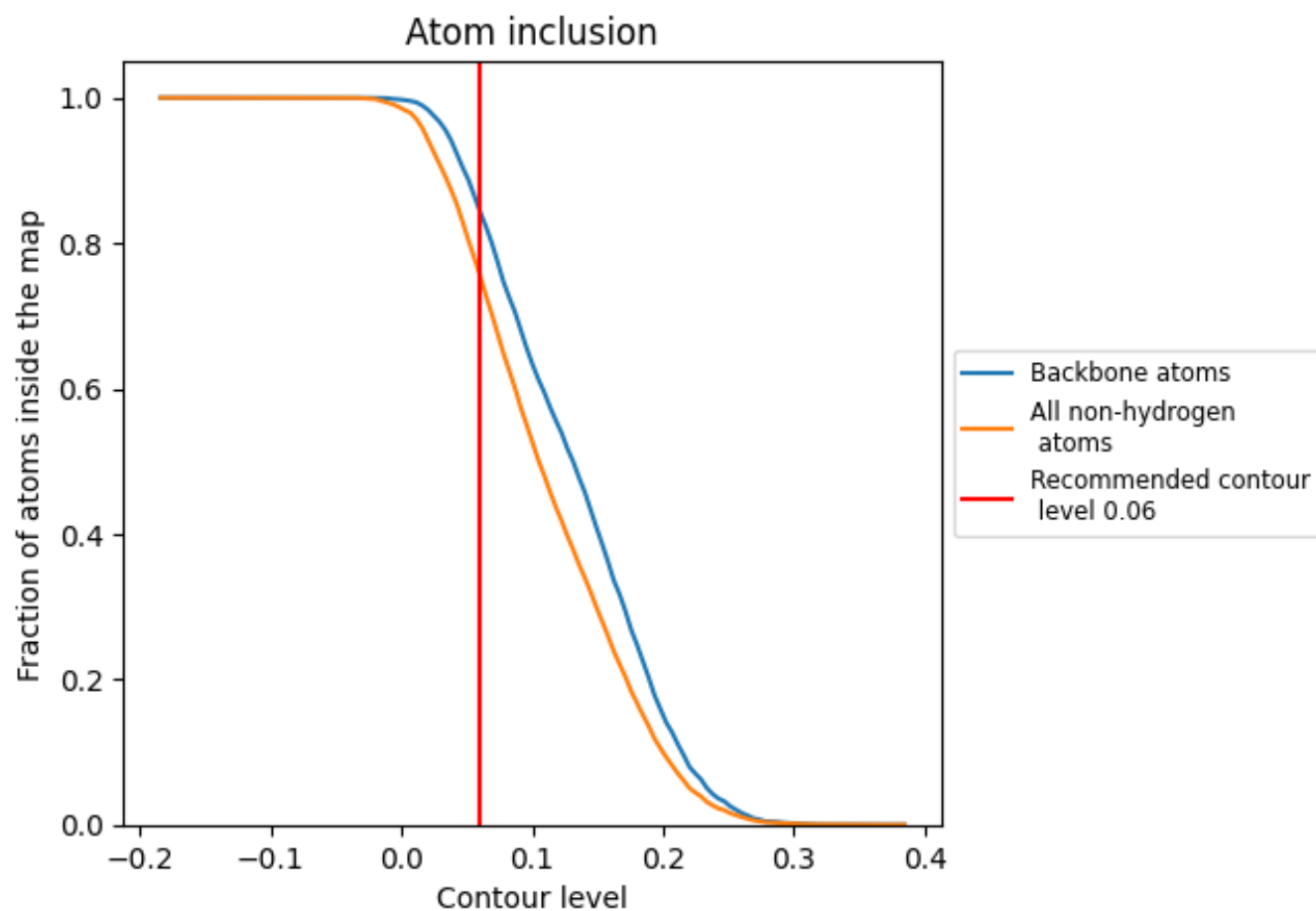
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 76% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7559	<div><div></div></div> 0.5010
A	<div><div></div></div> 0.7569	<div><div></div></div> 0.5040
B	<div><div></div></div> 0.7558	<div><div></div></div> 0.5010
C	<div><div></div></div> 0.7551	<div><div></div></div> 0.5000
D	<div><div></div></div> 0.7580	<div><div></div></div> 0.5040
E	<div><div></div></div> 0.7551	<div><div></div></div> 0.4990
F	<div><div></div></div> 0.7547	<div><div></div></div> 0.5000

1.0

0.0

<0.0