



Full wwPDB EM Validation Report ⓘ

May 25, 2025 – 06:06 PM EDT

PDB ID : 9DUM / pdb_00009dum
EMDB ID : EMD-47170
Title : Human PELP1-WDR18-TEX10 complex
Authors : Huang, J.; Tong, L.
Deposited on : 2024-10-03
Resolution : 3.56 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

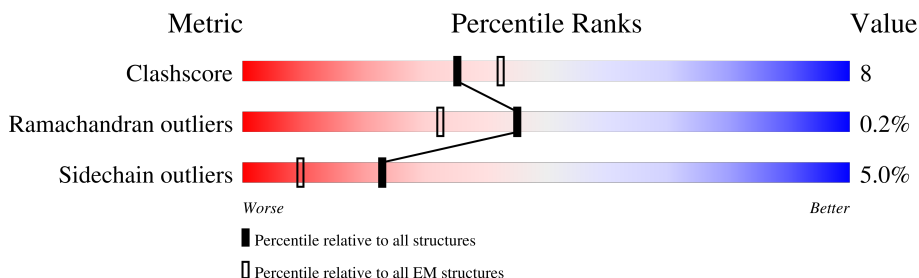
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.56 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	434	
1	B	434	
2	C	644	
2	D	644	
3	G	931	
3	H	931	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22662 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 WD repeat-containing protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	358	Total	C	N	O	S	0	0
			2718	1725	468	505	20		
1	B	376	Total	C	N	O	S	0	0
			2872	1819	500	533	20		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q9BV38
A	0	ASN	-	expression tag	UNP Q9BV38
B	-1	SER	-	expression tag	UNP Q9BV38
B	0	ASN	-	expression tag	UNP Q9BV38

- Molecule 2 is a protein called Proline-, glutamic acid- and leucine-rich protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	481	Total	C	N	O	S	0	0
			3655	2320	646	660	29		
2	D	485	Total	C	N	O	S	0	0
			3683	2337	653	664	29		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP Q8IZL8
C	0	ASN	-	expression tag	UNP Q8IZL8
D	-1	SER	-	expression tag	UNP Q8IZL8
D	0	ASN	-	expression tag	UNP Q8IZL8

- Molecule 3 is a protein called Testis-expressed protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	710	Total	C	N	O	S	0	0
			5690	3691	971	1004	24		
3	G	505	Total	C	N	O	S	0	0
			4044	2605	699	722	18		

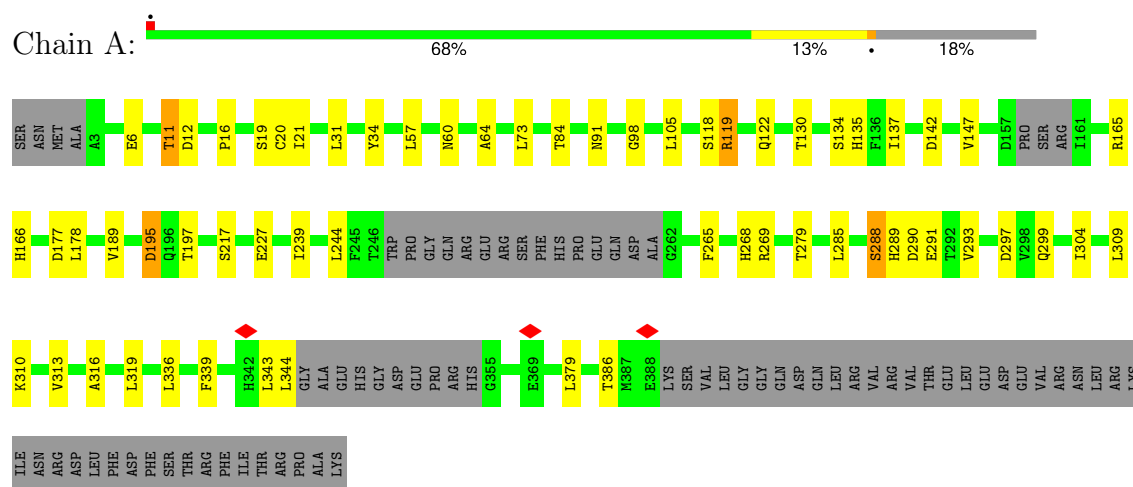
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	SER	-	expression tag	UNP Q9NXF1
H	0	ASN	-	expression tag	UNP Q9NXF1
G	-1	SER	-	expression tag	UNP Q9NXF1
G	0	ASN	-	expression tag	UNP Q9NXF1

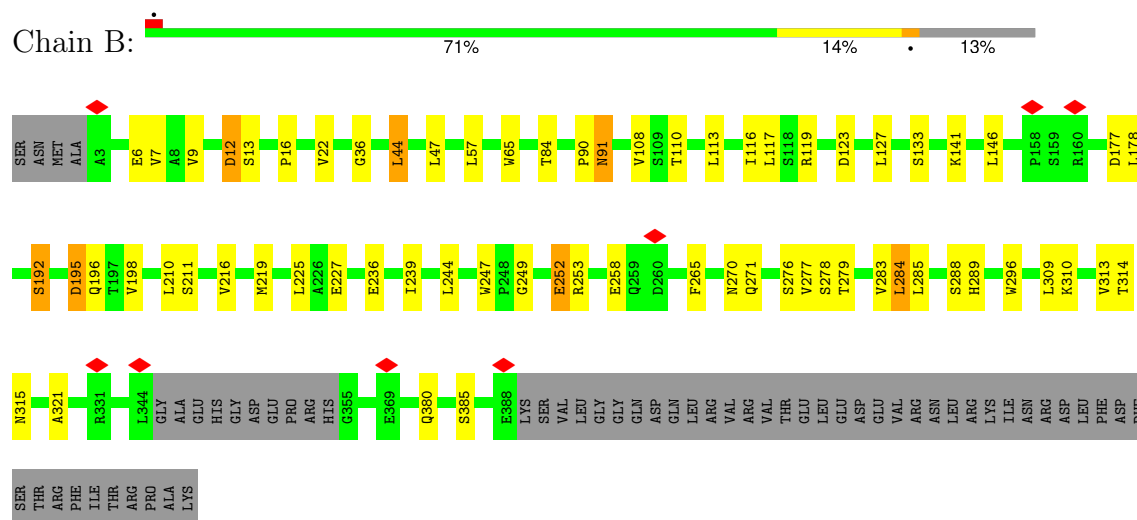
3 Residue-property plots

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: WD repeat-containing protein 18

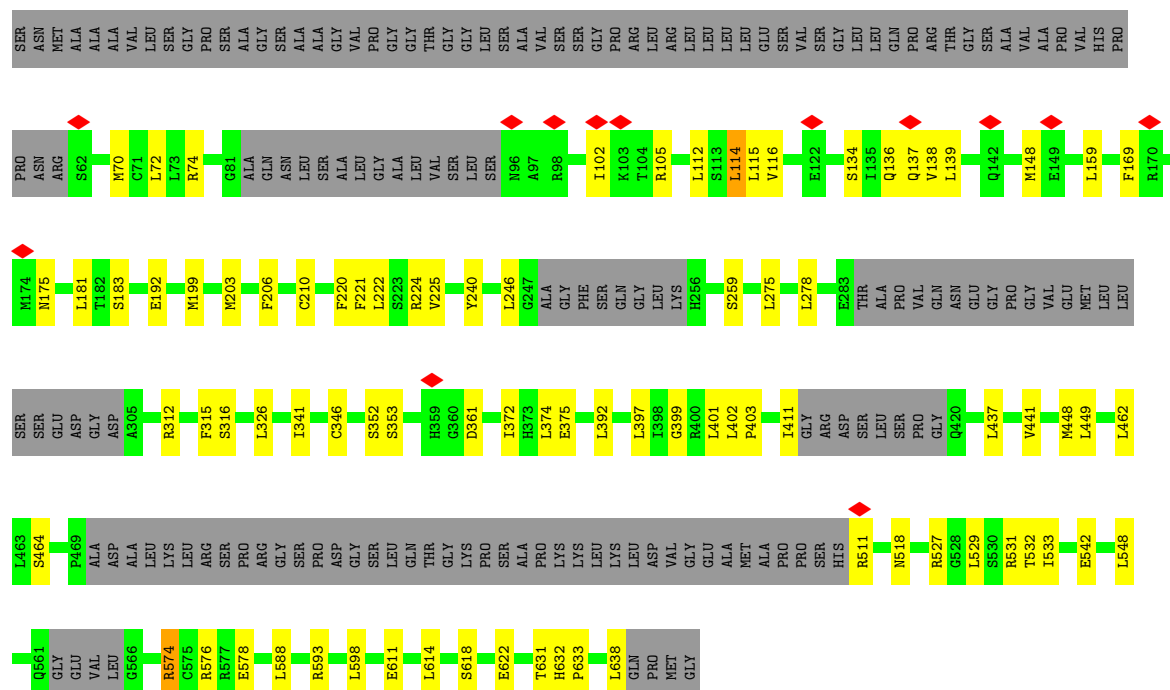


• Molecule 1: WD repeat-containing protein 18

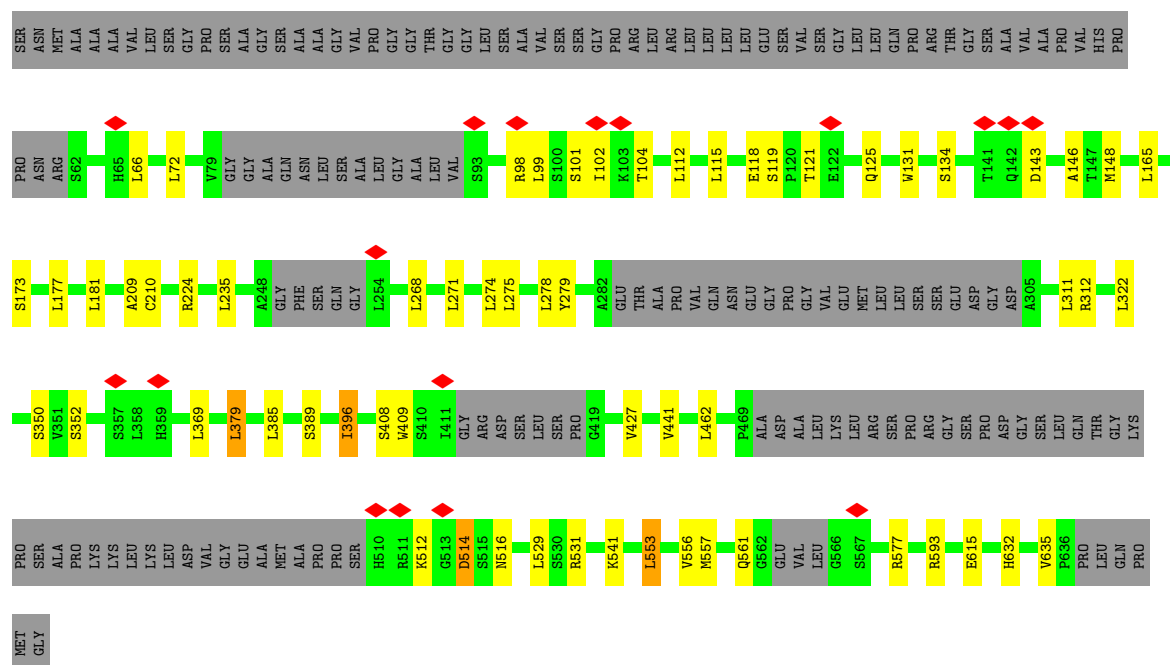


• Molecule 2: Proline-, glutamic acid- and leucine-rich protein 1

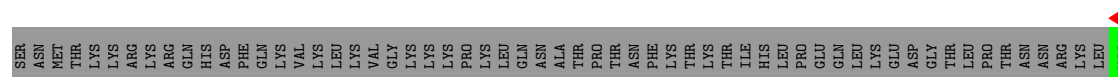
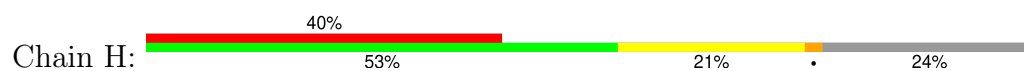




• Molecule 2: Proline-, glutamic acid- and leucine-rich protein 1



• Molecule 3: Testis-expressed protein 10





N890	H818	L713	T595	L502	V442	TRP	GLU	ALA	SER	VAL	ILE	LYS	ASP	GLY	ASP	ILE	SER	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	268599	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 ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.296	Depositor
Minimum map value	-1.700	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.284	Depositor
Map size (\AA)	324.9, 324.9, 324.9	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.083, 1.083, 1.083	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	0.21	0/2777	0.39	2/3777 (0.1%)
1	B	0.21	0/2940	0.42	1/4002 (0.0%)
2	C	0.12	0/3720	0.26	0/5043
2	D	0.12	0/3748	0.27	0/5079
3	G	0.14	0/4124	0.33	0/5597
3	H	0.18	0/5799	0.41	1/7860 (0.0%)
All	All	0.17	0/23108	0.35	4/31358 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	530	ILE	N-CA-C	-8.70	104.68	113.47
1	A	195	ASP	CA-CB-CG	6.67	119.27	112.60
1	B	195	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	290	ASP	CA-CB-CG	5.62	118.22	112.60

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	2718	0	2708	26	0
1	B	2872	0	2846	40	0
2	C	3655	0	3772	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3683	0	3805	39	0
3	G	4044	0	4169	71	0
3	H	5690	0	5920	150	0
All	All	22662	0	23220	352	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 8.

All (352) 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)
3:H:503:ILE:HD11	3:H:530:ILE:HD11	1.29	1.13
3:H:527:PHE:HA	3:H:530:ILE:HG22	1.34	1.07
3:H:503:ILE:HD11	3:H:530:ILE:CD1	1.95	0.97
1:B:270:ASN:ND2	3:H:742:VAL:HG13	1.81	0.94
3:H:527:PHE:CA	3:H:530:ILE:HG22	1.97	0.94
3:H:527:PHE:HA	3:H:530:ILE:CG2	1.98	0.92
3:H:527:PHE:O	3:H:530:ILE:HG22	1.74	0.86
1:B:270:ASN:HD21	3:H:742:VAL:HG13	1.41	0.84
3:H:527:PHE:C	3:H:530:ILE:HG22	2.03	0.84
1:B:270:ASN:HD21	3:H:742:VAL:CG1	1.94	0.81
3:G:705:VAL:HG23	3:G:707:HIS:H	1.50	0.76
3:H:503:ILE:CD1	3:H:530:ILE:CD1	2.66	0.73
3:H:700:GLN:NE2	3:H:766:VAL:O	2.24	0.70
1:B:44:LEU:HB2	1:B:315:ASN:HD22	1.56	0.70
3:G:474:LEU:HB3	3:G:478:GLN:HB3	1.74	0.68
2:C:533:ILE:HD11	2:C:548:LEU:HD13	1.76	0.68
3:H:636:LEU:HD21	3:H:653:LEU:HD11	1.77	0.67
3:H:527:PHE:O	3:H:530:ILE:CG2	2.41	0.66
3:H:710:GLN:HG2	3:H:717:LEU:HD21	1.76	0.66
3:G:512:GLN:NE2	3:G:513:ARG:O	2.27	0.66
2:C:210:CYS:HB2	2:C:246:LEU:HD23	1.77	0.66
3:G:593:GLN:NE2	3:G:626:PRO:O	2.29	0.66
3:G:769:ASP:OD2	3:G:821:LYS:NZ	2.29	0.66
2:D:177:LEU:HD23	2:D:209:ALA:HB3	1.80	0.63
3:H:474:LEU:HB3	3:H:478:GLN:HE22	1.63	0.63
1:A:119:ARG:HH12	3:G:535:GLU:HG2	1.64	0.63
3:G:276:GLN:N	3:G:276:GLN:OE1	2.31	0.63
1:B:9:VAL:HG22	1:B:22:VAL:HG22	1.81	0.63
1:A:122:GLN:HB2	1:A:142:ASP:HB3	1.80	0.62
2:C:70:MET:HE3	2:C:114:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:384:ARG:HE	3:H:388:LEU:HD22	1.65	0.62
3:G:510:TYR:O	3:G:513:ARG:NH2	2.34	0.61
1:B:211:SER:HB3	1:B:252:GLU:HG3	1.82	0.61
1:B:12:ASP:OD1	1:B:12:ASP:N	2.32	0.60
3:H:675:MET:HE2	3:H:675:MET:HA	1.81	0.60
3:G:754:GLN:HE22	3:G:789:VAL:HA	1.65	0.60
3:H:804:LEU:O	3:H:808:LEU:HG	2.01	0.60
1:B:309:LEU:HD12	1:B:313:VAL:HG22	1.84	0.60
3:H:66:MET:HE1	3:H:78:LEU:HG	1.84	0.60
1:A:239:ILE:HB	1:A:265:PHE:HB2	1.85	0.59
3:H:722:ASP:N	3:H:722:ASP:OD1	2.34	0.59
3:G:517:LEU:HD11	3:G:566:ASN:HD21	1.67	0.59
2:D:224:ARG:HG3	2:D:224:ARG:HH11	1.68	0.59
1:B:239:ILE:HB	1:B:265:PHE:HB2	1.83	0.58
3:H:129:ILE:HG13	3:H:171:TYR:OH	2.03	0.58
3:G:823:ASP:OD1	3:G:823:ASP:N	2.36	0.58
3:H:438:SER:HA	3:H:460:ILE:HD11	1.86	0.58
3:H:823:ASP:N	3:H:823:ASP:OD1	2.34	0.58
1:B:16:PRO:HG3	1:B:310:LYS:HD2	1.86	0.57
3:H:769:ASP:OD2	3:H:821:LYS:NZ	2.36	0.57
3:G:470:ASP:OD1	3:G:470:ASP:N	2.37	0.57
3:G:482:LEU:O	3:G:486:SER:OG	2.22	0.57
2:C:511:ARG:NH1	2:D:121:THR:OG1	2.37	0.57
1:A:244:LEU:HD23	3:G:279:ILE:HG21	1.87	0.57
2:C:462:LEU:HD13	2:C:529:LEU:HD13	1.87	0.56
2:D:278:LEU:HD11	2:D:311:LEU:HB3	1.87	0.56
2:C:169:PHE:HD1	2:C:206:PHE:HE1	1.53	0.56
3:H:535:GLU:HB3	3:H:583:ARG:HH21	1.70	0.56
3:G:700:GLN:HA	3:G:766:VAL:HG21	1.87	0.56
2:D:514:ASP:N	2:D:514:ASP:OD1	2.38	0.56
3:H:391:PHE:HA	3:H:395:PHE:HB2	1.85	0.56
3:H:366:LEU:HA	3:H:369:LEU:HB2	1.87	0.56
3:H:717:LEU:HB2	3:H:766:VAL:HG22	1.87	0.56
1:B:177:ASP:OD1	1:B:178:LEU:N	2.38	0.56
3:H:535:GLU:HG2	3:H:536:LEU:HD22	1.88	0.56
3:G:483:LEU:HD21	3:G:523:LEU:HD23	1.86	0.56
3:H:637:SER:HB2	3:H:683:PHE:CD1	2.41	0.56
1:B:196:GLN:HE22	3:H:652:MET:HG3	1.70	0.56
3:H:880:ASN:HD21	3:H:883:LEU:HD13	1.71	0.56
3:G:684:LEU:HD22	3:G:736:VAL:HG13	1.87	0.56
2:C:192:GLU:OE2	2:C:224:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ILE:HD13	1:A:189:VAL:HG21	1.89	0.55
1:A:309:LEU:HD12	1:A:313:VAL:HG22	1.88	0.55
3:H:60:LYS:HA	3:H:63:LEU:HD12	1.88	0.55
3:G:575:ASP:OD1	3:G:617:ARG:NH1	2.39	0.55
3:G:631:ASP:N	3:G:631:ASP:OD1	2.39	0.55
3:G:627:SER:O	3:G:629:PRO:HD3	2.07	0.55
2:C:199:MET:HE1	2:C:220:PHE:HD2	1.71	0.55
3:H:397:SER:OG	3:H:398:ARG:N	2.39	0.55
2:C:622:GLU:OE2	2:D:531:ARG:NH1	2.40	0.54
3:G:531:TYR:C	3:G:533:THR:H	2.16	0.54
1:A:386:THR:HG23	2:D:146:ALA:HB1	1.89	0.54
3:H:107:PHE:HE2	3:H:141:VAL:HG23	1.73	0.54
3:H:68:HIS:O	3:H:74:LYS:NZ	2.41	0.53
2:C:72:LEU:HD11	2:D:312:ARG:HH12	1.74	0.53
1:A:6:GLU:OE2	1:A:279:THR:OG1	2.20	0.53
3:H:503:ILE:CD1	3:H:530:ILE:HD13	2.39	0.53
1:A:297:ASP:HB2	1:A:304:ILE:HD11	1.88	0.53
2:C:542:GLU:OE2	2:C:593:ARG:NE	2.34	0.53
3:H:109:ASP:O	3:H:115:ARG:NH1	2.41	0.53
3:H:62:LEU:HD13	3:H:81:LEU:HD13	1.90	0.53
3:H:692:SER:HB2	3:H:695:GLU:HG2	1.90	0.53
2:C:102:ILE:HD13	2:C:105:ARG:HH21	1.74	0.53
3:G:761:LEU:HA	3:G:764:LEU:HD12	1.90	0.53
3:H:676:SER:O	3:H:678:VAL:N	2.42	0.53
1:B:288:SER:OG	1:B:289:HIS:N	2.41	0.52
3:G:556:PRO:HB2	3:G:595:THR:HG21	1.91	0.52
2:C:112:LEU:O	2:C:116:VAL:HG23	2.08	0.52
3:H:516:ILE:HG23	3:H:518:PRO:HD2	1.92	0.52
2:C:203:MET:HG2	2:C:246:LEU:HD21	1.92	0.52
3:H:684:LEU:HD23	3:H:740:LEU:HD13	1.92	0.52
1:B:90:PRO:HD2	1:B:133:SER:HB3	1.91	0.52
2:C:134:SER:O	2:C:138:VAL:HG23	2.10	0.52
2:C:136:GLN:HA	2:C:139:LEU:HD12	1.92	0.52
3:H:456:TRP:HA	3:H:459:MET:HG2	1.92	0.52
3:G:716:VAL:HG11	3:G:800:CYS:HA	1.92	0.52
3:H:362:ILE:HD12	3:H:363:ILE:N	2.23	0.52
1:A:11:THR:OG1	1:A:12:ASP:N	2.42	0.52
3:H:833:LEU:HD11	3:H:840:LEU:HD13	1.91	0.51
3:H:496:ARG:O	3:H:500:GLU:HG2	2.11	0.51
2:C:159:LEU:HD22	2:C:206:PHE:HE2	1.75	0.51
1:B:380:GLN:OE1	2:C:74:ARG:NH2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:555:LEU:HG	3:H:573:LEU:HD22	1.91	0.50
3:H:819:LEU:HB3	3:H:822:ARG:HH21	1.75	0.50
3:G:500:GLU:HA	3:G:503:ILE:HD12	1.93	0.50
3:H:320:PHE:O	3:H:324:ILE:HG12	2.12	0.50
3:G:806:TYR:O	3:G:810:THR:HG22	2.12	0.50
2:D:115:LEU:O	2:D:119:SER:HB2	2.11	0.50
1:A:268:HIS:CE1	1:A:288:SER:HB3	2.47	0.50
1:B:196:GLN:HE22	3:H:652:MET:CG	2.25	0.50
3:H:475:ASN:O	3:H:478:GLN:NE2	2.45	0.50
3:H:503:ILE:CD1	3:H:530:ILE:HD11	2.17	0.50
3:H:870:HIS:ND1	3:H:872:PRO:HD2	2.27	0.50
3:G:646:SER:HB3	3:G:649:LEU:HD12	1.92	0.50
2:C:527:ARG:NH1	2:C:578:GLU:OE2	2.44	0.50
1:B:244:LEU:HD22	2:C:638:LEU:HD21	1.94	0.49
1:B:47:LEU:HD11	1:B:108:VAL:HG21	1.93	0.49
3:G:705:VAL:HG22	3:G:708:VAL:HG23	1.93	0.49
1:A:177:ASP:OD1	1:A:178:LEU:N	2.45	0.49
3:H:107:PHE:CE2	3:H:141:VAL:HG23	2.46	0.49
3:H:599:ILE:HG23	3:H:600:TYR:CD1	2.47	0.49
1:B:278:SER:OG	1:B:279:THR:N	2.46	0.49
2:C:246:LEU:HD12	2:C:246:LEU:H	1.77	0.49
2:C:326:LEU:HD11	2:C:341:ILE:HD13	1.94	0.49
3:G:476:SER:HB2	3:G:516:ILE:HD11	1.94	0.48
2:D:593:ARG:HG2	2:D:593:ARG:HH11	1.78	0.48
3:H:737:PHE:HE1	3:H:778:VAL:HG23	1.78	0.48
3:G:748:GLN:O	3:G:752:ILE:HG13	2.13	0.48
2:D:98:ARG:HG2	2:D:104:THR:HB	1.94	0.48
3:H:238:LEU:O	3:H:242:SER:OG	2.29	0.48
3:G:788:VAL:HG12	3:G:788:VAL:O	2.13	0.48
1:A:84:THR:OG1	1:A:98:GLY:O	2.31	0.48
1:B:284:LEU:HD23	1:B:296:TRP:HD1	1.78	0.48
2:D:125:GLN:HG2	2:D:165:LEU:HD13	1.95	0.48
3:H:552:LEU:HD12	3:H:555:LEU:HD22	1.95	0.48
3:H:601:ASP:OD1	3:H:635:ARG:NH1	2.47	0.48
1:B:270:ASN:ND2	3:H:742:VAL:CG1	2.58	0.48
3:H:100:LEU:O	3:H:104:THR:OG1	2.28	0.48
3:H:720:LEU:HD23	3:H:818:HIS:ND1	2.28	0.48
3:H:91:ILE:HD13	3:G:913:VAL:HG13	1.96	0.48
3:H:888:ILE:HG12	3:H:907:LEU:HD21	1.95	0.48
2:D:173:SER:OG	2:D:209:ALA:HB2	2.14	0.47
3:H:495:ASN:ND2	3:H:498:ASP:OD2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:708:VAL:HG12	3:G:710:GLN:H	1.79	0.47
2:D:409:TRP:CD1	2:D:427:VAL:HG11	2.49	0.47
3:H:179:SER:O	3:H:181:ILE:N	2.47	0.47
3:H:599:ILE:HG13	3:H:606:ALA:HB3	1.96	0.47
3:G:816:ALA:HA	3:G:819:LEU:HD12	1.96	0.47
2:C:221:PHE:HB3	2:C:240:TYR:HB2	1.95	0.47
3:H:88:TYR:HB2	3:H:91:ILE:HG12	1.97	0.47
3:H:179:SER:O	3:H:182:LEU:HG	2.15	0.47
3:H:183:LEU:H	3:H:183:LEU:HD12	1.79	0.47
3:H:874:ARG:O	3:H:878:LEU:HG	2.15	0.47
3:H:509:LEU:HD22	3:H:523:LEU:HD11	1.96	0.47
3:H:561:HIS:O	3:H:565:ARG:NH2	2.48	0.47
2:C:399:GLY:HA2	2:C:448:MET:HE1	1.96	0.47
3:H:145:LEU:O	3:H:149:MET:HG3	2.15	0.47
3:G:505:ALA:O	3:G:508:THR:OG1	2.31	0.47
2:D:322:LEU:HD23	2:D:379:LEU:HD11	1.97	0.46
3:H:456:TRP:HA	3:H:459:MET:HE2	1.97	0.46
3:H:531:TYR:C	3:H:533:THR:H	2.23	0.46
3:G:507:TYR:O	3:G:511:GLN:N	2.43	0.46
3:G:441:MET:HA	3:G:441:MET:HE2	1.96	0.46
2:D:556:VAL:HG23	2:D:557:MET:HG3	1.98	0.46
1:A:130:THR:HG21	1:A:135:HIS:HB2	1.97	0.46
1:B:91:ASN:ND2	1:B:133:SER:OG	2.48	0.46
3:H:354:GLN:O	3:H:357:GLN:N	2.49	0.46
3:H:463:PHE:O	3:H:467:THR:HG22	2.15	0.46
3:H:95:HIS:O	3:H:99:ILE:HG13	2.15	0.46
2:C:312:ARG:HH12	2:D:72:LEU:HD11	1.80	0.46
1:A:137:ILE:HG12	1:A:147:VAL:HG22	1.97	0.46
3:H:234:PHE:CD1	3:H:234:PHE:C	2.94	0.46
3:G:691:PHE:O	3:G:696:LEU:HD13	2.15	0.46
3:H:631:ASP:O	3:H:635:ARG:HG2	2.15	0.46
3:H:746:ARG:HA	3:H:749:ASN:ND2	2.31	0.46
3:H:562:LEU:HD21	3:H:566:ASN:HB3	1.97	0.45
3:G:531:TYR:CE2	3:G:580:ALA:HB2	2.52	0.45
1:B:216:VAL:HG21	1:B:236:GLU:HG2	1.96	0.45
1:B:227:GLU:OE1	2:D:632:HIS:NE2	2.34	0.45
3:H:379:LEU:O	3:H:383:LEU:HG	2.16	0.45
3:H:746:ARG:HA	3:H:749:ASN:HD21	1.81	0.45
1:B:277:VAL:HG22	1:B:284:LEU:HD12	1.97	0.45
3:G:531:TYR:O	3:G:533:THR:N	2.50	0.45
3:G:804:LEU:HD11	3:G:825:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:352:SER:OG	2:C:353:SER:N	2.50	0.45
3:G:874:ARG:NH2	3:G:915:ILE:HD13	2.31	0.45
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.85	0.45
1:B:113:LEU:HD21	1:B:116:ILE:HG13	1.98	0.45
1:B:123:ASP:OD1	1:B:123:ASP:N	2.49	0.45
3:H:572:GLN:O	3:H:576:ILE:HG22	2.17	0.45
3:H:738:HIS:O	3:H:742:VAL:HG23	2.17	0.45
3:H:96:LEU:HD13	3:H:133:GLN:HG2	1.98	0.45
3:G:713:LEU:HB3	3:G:802:TYR:HE2	1.80	0.45
1:B:6:GLU:OE2	1:B:279:THR:OG1	2.33	0.45
1:B:7:VAL:HG13	1:B:321:ALA:HB2	1.98	0.45
2:C:574:ARG:O	2:C:578:GLU:HG2	2.16	0.45
3:H:397:SER:HB3	3:H:437:LEU:HD22	1.98	0.45
3:H:432:LEU:HD23	3:H:432:LEU:H	1.82	0.45
2:D:369:LEU:HD12	2:D:369:LEU:HA	1.83	0.45
3:H:362:ILE:HD12	3:H:363:ILE:HG13	2.00	0.45
3:H:637:SER:HB2	3:H:683:PHE:HD1	1.80	0.45
3:H:657:LEU:HD23	3:H:657:LEU:HA	1.81	0.44
3:G:717:LEU:HB2	3:G:765:THR:O	2.17	0.44
3:H:806:TYR:HD1	3:H:806:TYR:O	2.00	0.44
1:A:16:PRO:HG2	1:A:310:LYS:HD2	1.99	0.44
1:B:141:LYS:HE2	3:H:668:TYR:OH	2.17	0.44
2:D:99:LEU:HD23	2:D:134:SER:HB3	2.00	0.44
3:H:325:ILE:O	3:H:329:ILE:HG13	2.17	0.44
1:A:336:LEU:HD22	1:A:339:PHE:HE2	1.82	0.44
1:B:219:MET:HE3	1:B:219:MET:HB3	1.91	0.44
3:H:453:ASP:HB3	3:H:456:TRP:CE2	2.52	0.44
3:H:623:TYR:O	3:H:660:ARG:NH1	2.48	0.44
3:H:699:LEU:HD11	3:H:719:TYR:CG	2.52	0.44
3:G:618:LEU:HD23	3:G:618:LEU:HA	1.78	0.44
3:H:66:MET:O	3:H:74:LYS:NZ	2.38	0.44
3:H:367:TRP:CE2	3:H:443:SER:HB3	2.53	0.44
3:H:352:PRO:HB2	3:H:353:LEU:H	1.68	0.44
3:H:153:THR:HG22	3:H:156:ILE:H	1.82	0.44
3:H:234:PHE:C	3:H:234:PHE:HD1	2.26	0.43
3:H:707:HIS:O	3:H:720:LEU:HB2	2.17	0.43
3:H:830:VAL:HG23	3:H:873:LEU:HD11	1.99	0.43
3:H:461:ARG:HA	3:H:464:VAL:HG22	2.00	0.43
3:G:899:VAL:O	3:G:901:GLU:HG3	2.17	0.43
3:H:685:PHE:O	3:H:689:THR:HG22	2.17	0.43
3:H:711:THR:HG22	3:H:713:LEU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LEU:HD23	1:B:127:LEU:HA	1.89	0.43
3:H:329:ILE:O	3:H:333:VAL:HG23	2.18	0.43
3:H:546:LYS:H	3:H:546:LYS:HG3	1.65	0.43
3:G:718:LEU:HD23	3:G:803:SER:HB3	1.99	0.43
2:C:449:LEU:HD22	2:C:532:THR:HG21	2.00	0.43
2:D:396:ILE:H	2:D:396:ILE:HG12	1.53	0.43
1:B:195:ASP:O	1:B:196:GLN:HB2	2.18	0.43
2:C:614:LEU:HD11	2:D:441:VAL:HG12	2.00	0.43
3:H:371:LYS:HE3	3:H:371:LYS:HB3	1.66	0.43
2:C:181:LEU:HD11	2:C:210:CYS:HB3	2.01	0.43
3:H:596:ALA:HA	3:H:599:ILE:HG22	2.00	0.43
3:G:599:ILE:HG23	3:G:606:ALA:HB3	2.01	0.43
3:G:871:ALA:O	3:G:874:ARG:HG2	2.19	0.43
2:D:462:LEU:HD13	2:D:529:LEU:HD13	2.01	0.43
2:D:553:LEU:HD13	2:D:553:LEU:HA	1.82	0.43
2:D:181:LEU:HD11	2:D:210:CYS:SG	2.59	0.43
3:H:401:TYR:OH	3:H:430:HIS:O	2.32	0.43
2:D:389:SER:O	2:D:389:SER:OG	2.37	0.42
3:H:525:LYS:HE2	3:H:529:LYS:HD2	2.00	0.42
3:G:893:THR:O	3:G:896:SER:OG	2.36	0.42
3:H:461:ARG:NH1	3:H:493:GLN:OE1	2.52	0.42
3:H:737:PHE:CE1	3:H:778:VAL:HG23	2.53	0.42
3:G:801:CYS:HB3	3:G:843:MET:HE2	2.02	0.42
3:H:189:LEU:HD11	3:H:227:VAL:HG21	2.00	0.42
2:C:631:THR:O	2:C:633:PRO:HD3	2.19	0.42
2:C:633:PRO:HG2	2:D:635:VAL:O	2.19	0.42
3:G:527:PHE:HB3	3:G:551:TRP:CH2	2.53	0.42
2:C:275:LEU:HD12	2:C:275:LEU:HA	1.89	0.42
3:H:457:ILE:O	3:H:460:ILE:HG22	2.19	0.42
1:B:13:SER:HB2	1:B:314:THR:HG23	2.00	0.42
1:B:247:TRP:CE2	1:B:249:GLY:HA2	2.54	0.42
2:C:70:MET:CE	2:C:114:LEU:HD12	2.48	0.42
2:C:576:ARG:NH1	2:C:611:GLU:OE2	2.53	0.42
3:H:638:ARG:HA	3:H:641:ILE:HG22	2.02	0.42
3:H:127:PRO:HA	3:H:170:GLN:NE2	2.34	0.42
3:H:328:LEU:O	3:H:332:TRP:N	2.51	0.42
3:H:740:LEU:HD12	3:H:740:LEU:HA	1.87	0.42
3:G:633:LEU:HD12	3:G:633:LEU:HA	1.87	0.42
1:A:285:LEU:HD21	1:A:316:ALA:HB1	2.02	0.42
2:C:598:LEU:HD12	2:C:598:LEU:HA	1.94	0.42
2:D:275:LEU:HD11	2:D:279:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:625:LEU:O	3:G:660:ARG:NH2	2.53	0.42
1:A:227:GLU:OE1	2:C:632:HIS:NE2	2.45	0.42
3:H:433:LEU:HD12	3:H:433:LEU:H	1.85	0.42
3:G:868:LEU:HD23	3:G:868:LEU:HA	1.80	0.42
2:D:118:GLU:OE2	2:D:118:GLU:N	2.53	0.41
2:D:268:LEU:HD12	2:D:268:LEU:HA	1.81	0.41
3:H:235:LEU:HD13	3:H:235:LEU:HA	1.93	0.41
3:H:527:PHE:HA	3:H:530:ILE:HG21	1.92	0.41
1:A:64:ALA:O	1:A:73:LEU:HB2	2.20	0.41
2:C:402:LEU:HB2	2:C:403:PRO:HD3	2.00	0.41
3:H:713:LEU:HB3	3:H:802:TYR:HE2	1.85	0.41
3:G:478:GLN:HG2	3:G:481:ARG:HH21	1.85	0.41
3:G:517:LEU:N	3:G:518:PRO:HD2	2.35	0.41
3:G:849:VAL:HG12	3:G:850:ASN:H	1.84	0.41
1:A:165:ARG:O	1:A:166:HIS:ND1	2.53	0.41
3:H:326:PRO:HA	3:H:329:ILE:HD12	2.03	0.41
3:G:479:LEU:HA	3:G:479:LEU:HD12	1.82	0.41
2:D:112:LEU:HD11	2:D:131:TRP:CD1	2.56	0.41
2:D:271:LEU:HD23	2:D:271:LEU:HA	1.84	0.41
3:H:238:LEU:HD22	3:H:238:LEU:H	1.85	0.41
3:H:618:LEU:HA	3:H:618:LEU:HD23	1.80	0.41
3:G:440:ILE:H	3:G:440:ILE:HG12	1.65	0.41
3:G:531:TYR:C	3:G:533:THR:N	2.79	0.41
2:C:437:LEU:O	2:C:441:VAL:HG22	2.21	0.41
3:H:486:SER:O	3:H:490:MET:HG2	2.21	0.41
3:H:641:ILE:HG12	3:H:690:GLY:HA3	2.02	0.41
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.87	0.41
1:B:210:LEU:HD11	1:B:253:ARG:NE	2.36	0.41
2:C:315:PHE:CE1	2:C:372:ILE:HG23	2.56	0.41
2:D:101:SER:OG	2:D:102:ILE:N	2.54	0.41
3:G:522:LEU:HD23	3:G:522:LEU:HA	1.94	0.41
2:D:274:LEU:HD23	2:D:274:LEU:HA	1.92	0.41
2:D:512:LYS:HB3	2:D:512:LYS:HE3	1.87	0.41
2:D:516:ASN:O	2:D:516:ASN:ND2	2.52	0.41
2:D:143:ASP:HB2	2:D:148:MET:HE2	2.02	0.41
3:H:367:TRP:CZ2	3:H:443:SER:HB3	2.55	0.41
3:H:527:PHE:HB3	3:H:551:TRP:CH2	2.56	0.41
2:C:112:LEU:HA	2:C:115:LEU:HD12	2.03	0.41
2:C:588:LEU:HD23	2:C:588:LEU:HA	1.90	0.41
3:H:125:LEU:O	3:H:125:LEU:HD12	2.21	0.41
3:H:440:ILE:O	3:H:444:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:866:LEU:HD13	3:H:866:LEU:HA	1.95	0.41
3:G:602:PRO:HB2	3:G:642:MET:HE1	2.01	0.41
3:G:791:GLU:H	3:G:791:GLU:CD	2.28	0.41
3:G:864:LEU:HD12	3:G:864:LEU:HA	1.81	0.41
2:C:531:ARG:HE	2:C:531:ARG:HB2	1.66	0.41
3:H:184:LYS:HD2	3:H:184:LYS:O	2.20	0.41
3:H:399:PHE:HB2	3:H:400:PRO:HD3	2.03	0.41
3:G:768:PRO:HD2	3:G:771:THR:HB	2.02	0.41
3:G:811:ILE:O	3:G:812:GLU:HG2	2.21	0.41
3:G:889:LYS:H	3:G:889:LYS:HG2	1.66	0.41
2:C:392:LEU:HD23	2:C:392:LEU:HA	1.88	0.40
2:D:577:ARG:HD2	2:D:615:GLU:OE2	2.22	0.40
3:H:573:LEU:HD23	3:H:573:LEU:HA	1.91	0.40
1:A:379:LEU:HD12	1:A:379:LEU:HA	1.93	0.40
2:C:148:MET:H	2:C:148:MET:HG2	1.67	0.40
3:H:324:ILE:O	3:H:327:LEU:N	2.49	0.40
3:H:325:ILE:HA	3:H:328:LEU:HD23	2.03	0.40
3:H:354:GLN:O	3:H:355:VAL:C	2.63	0.40
3:H:857:LEU:HD23	3:H:857:LEU:HA	1.87	0.40
1:A:20:CYS:HB3	1:A:34:TYR:HD2	1.85	0.40
2:C:401:LEU:HD23	2:C:401:LEU:HA	1.87	0.40
2:C:574:ARG:HE	2:C:574:ARG:HB3	1.56	0.40
2:D:181:LEU:HD23	2:D:181:LEU:HA	1.94	0.40
3:H:151:HIS:HD2	3:H:156:ILE:HB	1.86	0.40
3:G:737:PHE:HE1	3:G:778:VAL:HG23	1.86	0.40
1:A:91:ASN:OD1	1:A:91:ASN:N	2.50	0.40
3:H:815:GLU:OE1	3:H:815:GLU:N	2.55	0.40
3:G:700:GLN:HE22	3:G:765:THR:HG1	1.65	0.40
1:B:36:GLY:HA3	1:B:65:TRP:HZ2	1.87	0.40
1:B:44:LEU:HB2	1:B:315:ASN:ND2	2.29	0.40
1:B:192:SER:HB2	1:B:198:VAL:HG22	2.02	0.40
1:B:271:GLN:H	1:B:271:GLN:HG3	1.71	0.40
3:H:115:ARG:HE	3:H:115:ARG:HB2	1.73	0.40
3:H:764:LEU:HD23	3:H:764:LEU:HA	1.95	0.40
3:G:435:LEU:HD23	3:G:435:LEU:HA	1.97	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	350/434 (81%)	325 (93%)	25 (7%)	0	100	100
1	B	372/434 (86%)	342 (92%)	30 (8%)	0	100	100
2	C	467/644 (72%)	457 (98%)	10 (2%)	0	100	100
2	D	471/644 (73%)	457 (97%)	14 (3%)	0	100	100
3	G	497/931 (53%)	447 (90%)	49 (10%)	1 (0%)	44	74
3	H	688/931 (74%)	652 (95%)	32 (5%)	4 (1%)	22	56
All	All	2845/4018 (71%)	2680 (94%)	160 (6%)	5 (0%)	45	74

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	180	SER
3	H	355	VAL
3	H	132	GLU
3	G	532	GLN
3	H	532	GLN

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	303/370 (82%)	283 (93%)	20 (7%)	14	42
1	B	319/370 (86%)	301 (94%)	18 (6%)	17	46
2	C	408/528 (77%)	389 (95%)	19 (5%)	22	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	411/528 (78%)	399 (97%)	12 (3%)	37	64
3	G	458/845 (54%)	436 (95%)	22 (5%)	21	51
3	H	646/845 (76%)	611 (95%)	35 (5%)	18	47
All	All	2545/3486 (73%)	2419 (95%)	126 (5%)	23	49

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	19	SER
1	A	21	ILE
1	A	57	LEU
1	A	60	ASN
1	A	105	LEU
1	A	118	SER
1	A	119	ARG
1	A	134	SER
1	A	195	ASP
1	A	197	THR
1	A	217	SER
1	A	269	ARG
1	A	288	SER
1	A	289	HIS
1	A	291	GLU
1	A	293	VAL
1	A	299	GLN
1	A	319	LEU
1	A	343	LEU
1	B	12	ASP
1	B	44	LEU
1	B	57	LEU
1	B	84	THR
1	B	91	ASN
1	B	110	THR
1	B	117	LEU
1	B	119	ARG
1	B	146	LEU
1	B	192	SER
1	B	225	LEU
1	B	252	GLU
1	B	258	GLU

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Mol	Chain	Res	Type
1	B	276	SER
1	B	283	VAL
1	B	284	LEU
1	B	285	LEU
1	B	385	SER
2	C	114	LEU
2	C	137	GLN
2	C	175	ASN
2	C	183	SER
2	C	222	LEU
2	C	225	VAL
2	C	259	SER
2	C	278	LEU
2	C	316	SER
2	C	346	CYS
2	C	361	ASP
2	C	374	LEU
2	C	375	GLU
2	C	397	LEU
2	C	411	ILE
2	C	464	SER
2	C	518	ASN
2	C	574	ARG
2	C	618	SER
2	D	66	LEU
2	D	235	LEU
2	D	350	SER
2	D	352	SER
2	D	379	LEU
2	D	385	LEU
2	D	396	ILE
2	D	408	SER
2	D	514	ASP
2	D	541	LYS
2	D	553	LEU
2	D	561	GLN
3	H	68	HIS
3	H	108	THR
3	H	122	LEU
3	H	235	LEU
3	H	293	SER
3	H	314	THR

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Mol	Chain	Res	Type
3	H	354	GLN
3	H	356	MET
3	H	365	LEU
3	H	366	LEU
3	H	371	LYS
3	H	401	TYR
3	H	433	LEU
3	H	449	THR
3	H	450	LEU
3	H	517	LEU
3	H	534	GLU
3	H	536	LEU
3	H	555	LEU
3	H	587	GLU
3	H	604	GLU
3	H	631	ASP
3	H	672	ASP
3	H	684	LEU
3	H	707	HIS
3	H	722	ASP
3	H	727	LEU
3	H	755	SER
3	H	778	VAL
3	H	785	HIS
3	H	786	THR
3	H	811	ILE
3	H	833	LEU
3	H	842	LEU
3	H	866	LEU
3	G	437	LEU
3	G	502	LEU
3	G	517	LEU
3	G	532	GLN
3	G	544	ARG
3	G	549	SER
3	G	555	LEU
3	G	585	ASN
3	G	642	MET
3	G	693	LYS
3	G	711	THR
3	G	727	LEU
3	G	732	VAL

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Mol	Chain	Res	Type
3	G	753	LEU
3	G	805	LEU
3	G	830	VAL
3	G	849	VAL
3	G	857	LEU
3	G	859	VAL
3	G	863	LEU
3	G	878	LEU
3	G	909	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	315	ASN
1	A	340	ASN
1	B	60	ASN
1	B	75	GLN
1	B	91	ASN
1	B	155	GLN
1	B	170	HIS
1	B	196	GLN
1	B	315	ASN
1	B	364	HIS
1	B	378	GLN
2	C	164	GLN
2	C	175	ASN
2	C	176	HIS
2	C	450	GLN
2	D	256	HIS
2	D	272	HIS
2	D	359	HIS
2	D	450	GLN
2	D	603	GLN
3	H	144	HIS
3	H	157	GLN
3	H	585	ASN
3	H	620	GLN
3	H	880	ASN
3	H	885	GLN
3	G	272	HIS
3	G	566	ASN

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Mol	Chain	Res	Type
3	G	585	ASN
3	G	615	GLN
3	G	700	GLN
3	G	725	GLN
3	G	850	ASN
3	G	880	ASN
3	G	886	GLN
3	G	900	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.

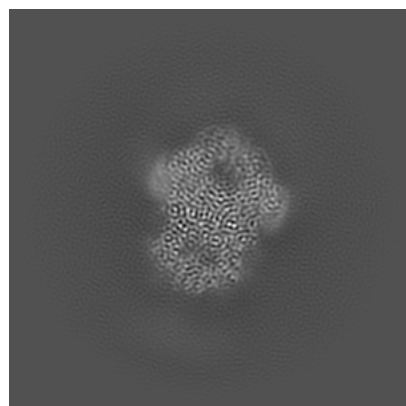
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47170. These allow visual inspection of the internal detail of the map and identification of artifacts.

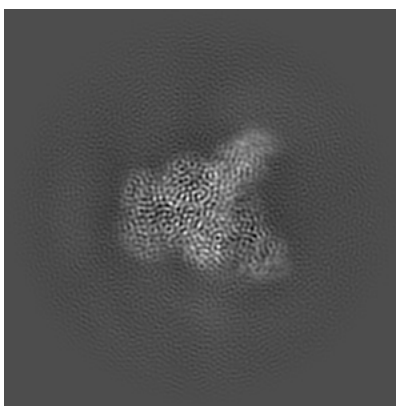
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

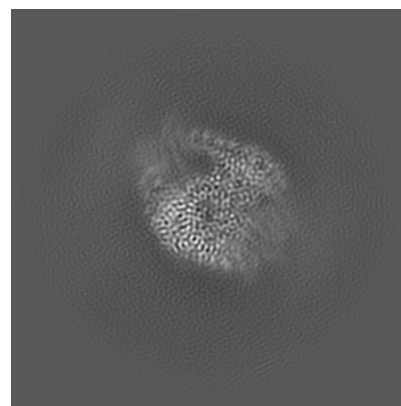
6.1.1 Primary map



X

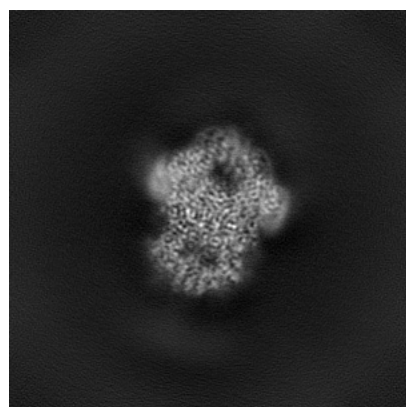


Y

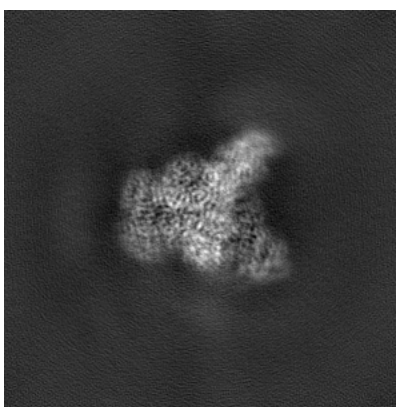


Z

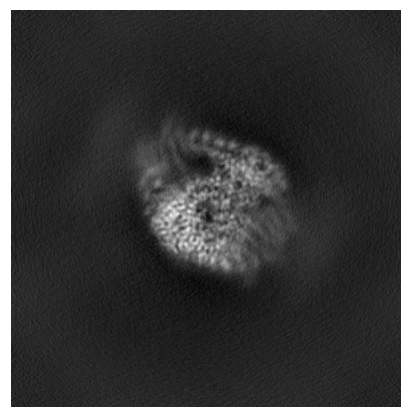
6.1.2 Raw map



X



Y

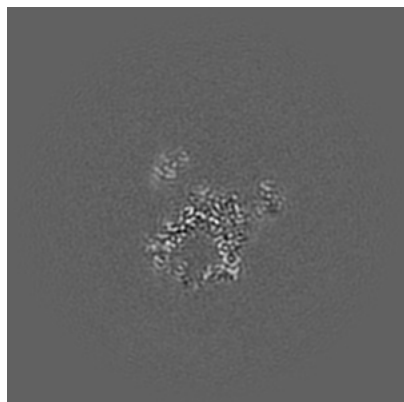


Z

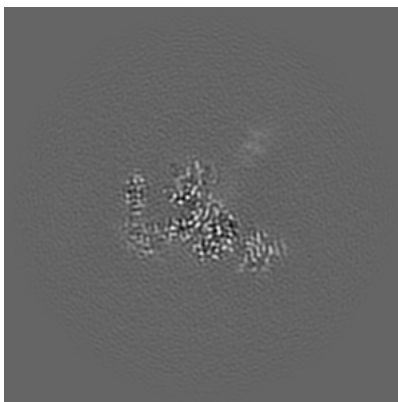
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

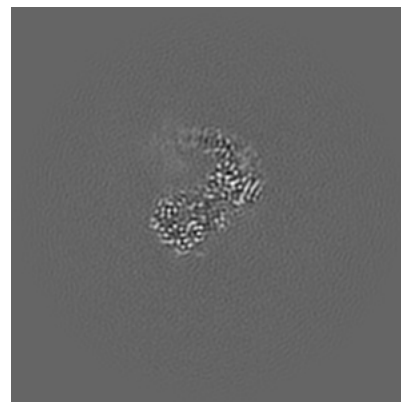
6.2.1 Primary map



X Index: 150

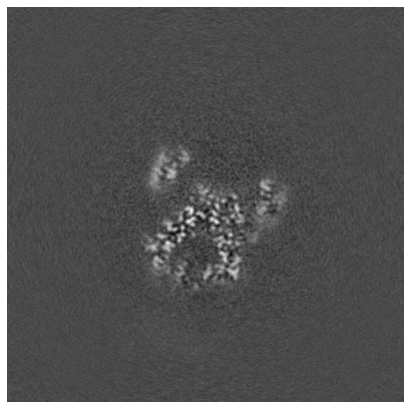


Y Index: 150

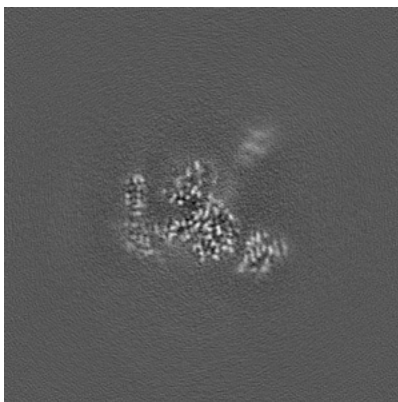


Z Index: 150

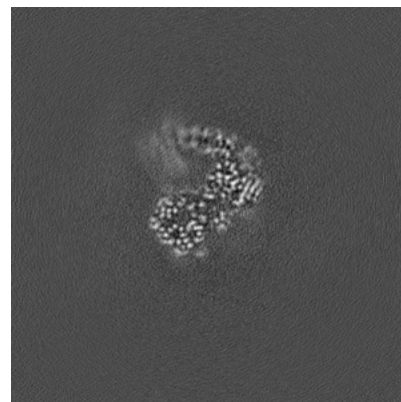
6.2.2 Raw map



X Index: 150



Y Index: 150

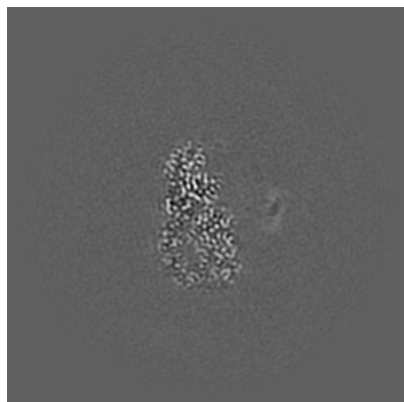


Z Index: 150

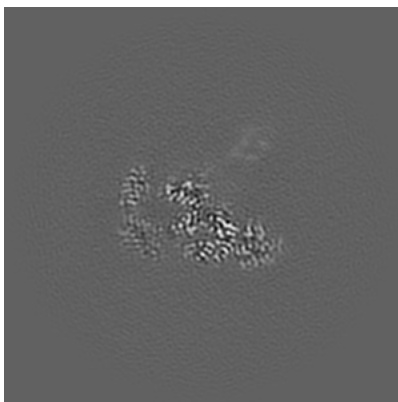
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

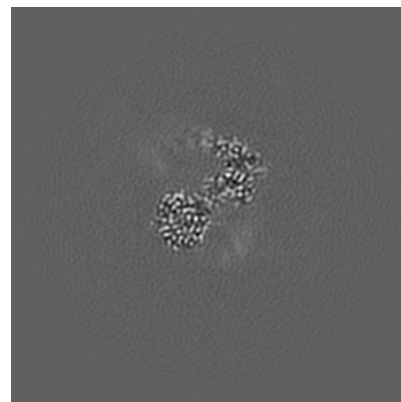
6.3.1 Primary map



X Index: 133

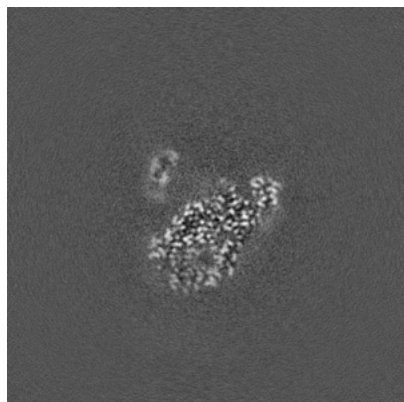


Y Index: 144

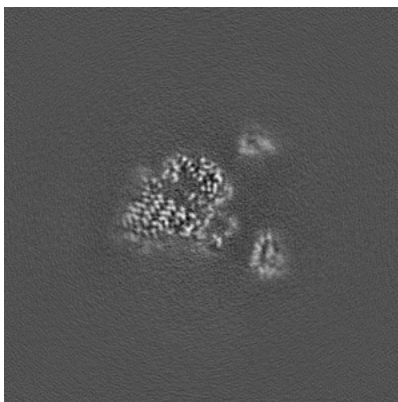


Z Index: 157

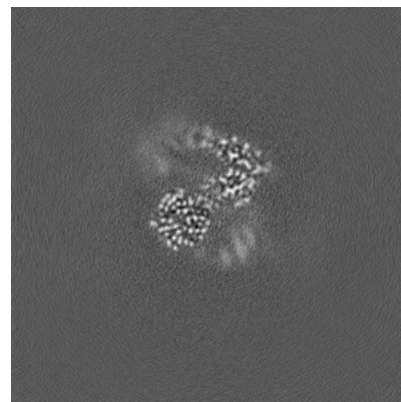
6.3.2 Raw map



X Index: 158



Y Index: 161

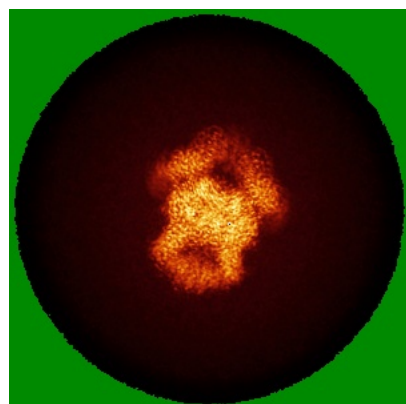


Z Index: 158

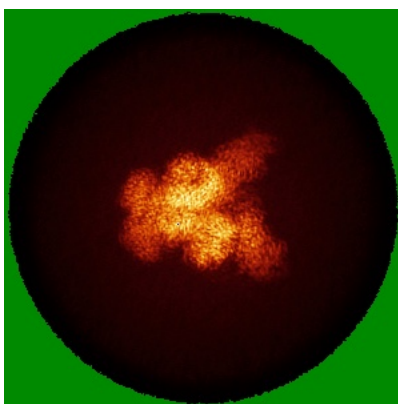
The images above show the largest variance slices of the map in three orthogonal directions.

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

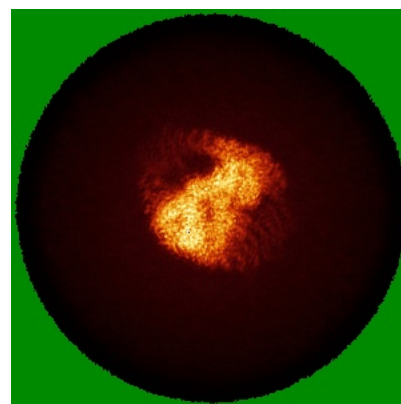
6.4.1 Primary map



X

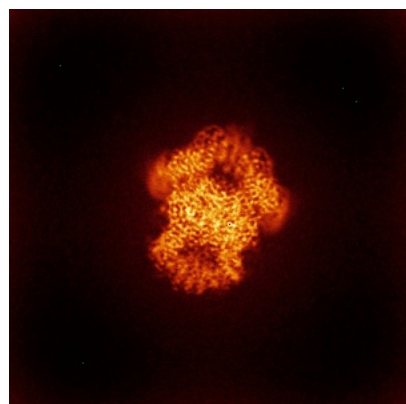


Y

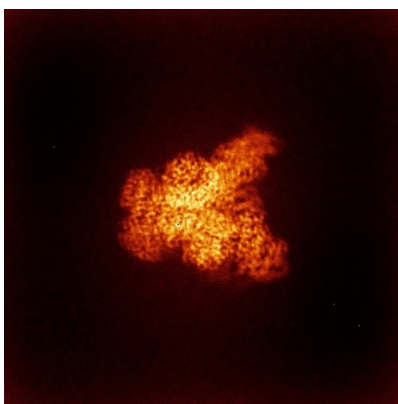


Z

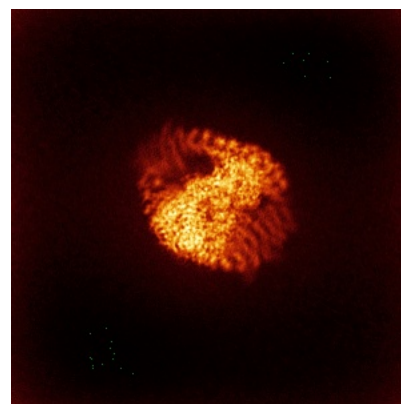
6.4.2 Raw map



X



Y

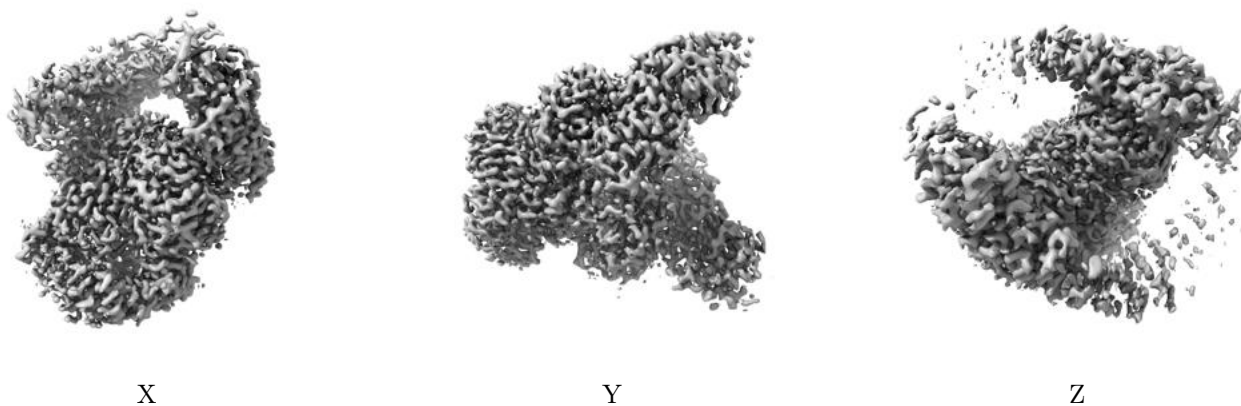


Z

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.

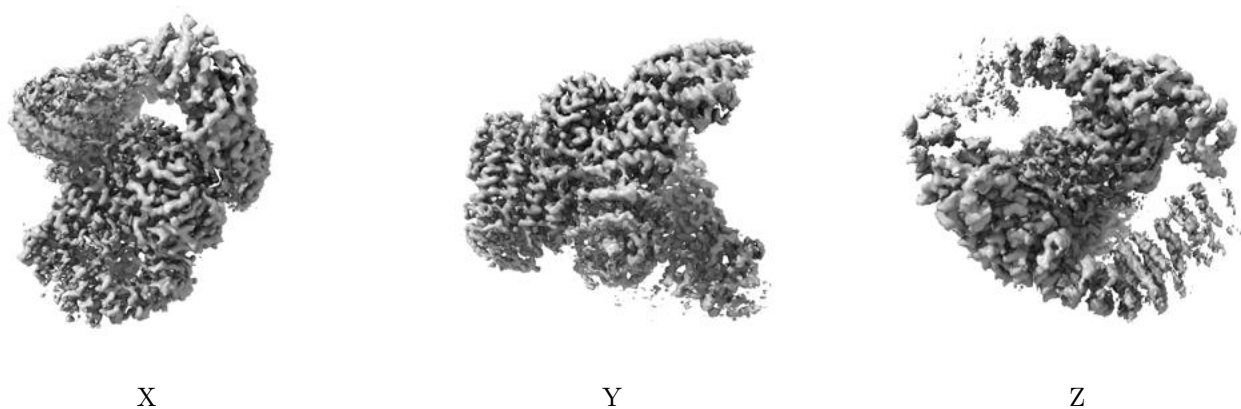
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.284. 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.

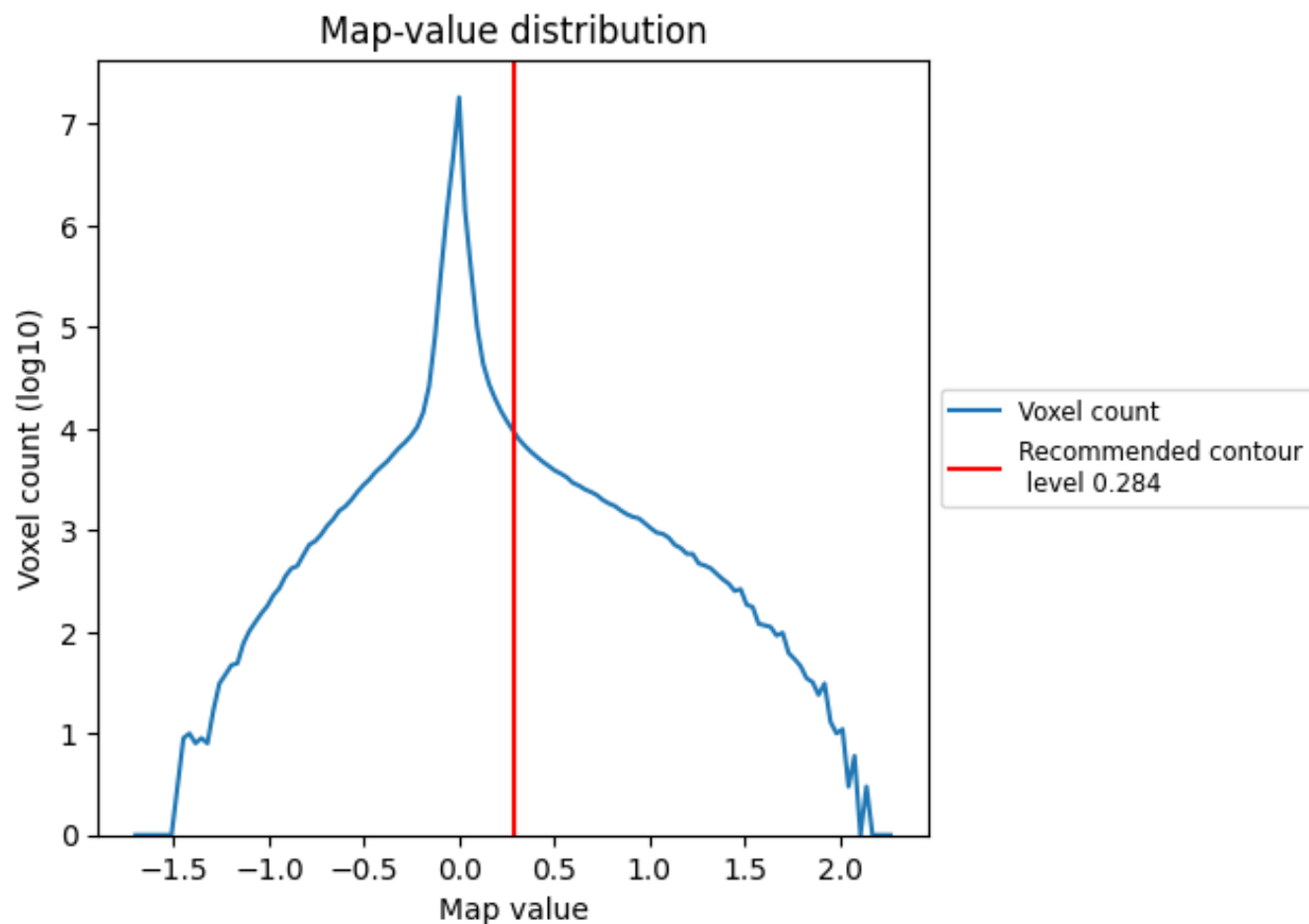
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

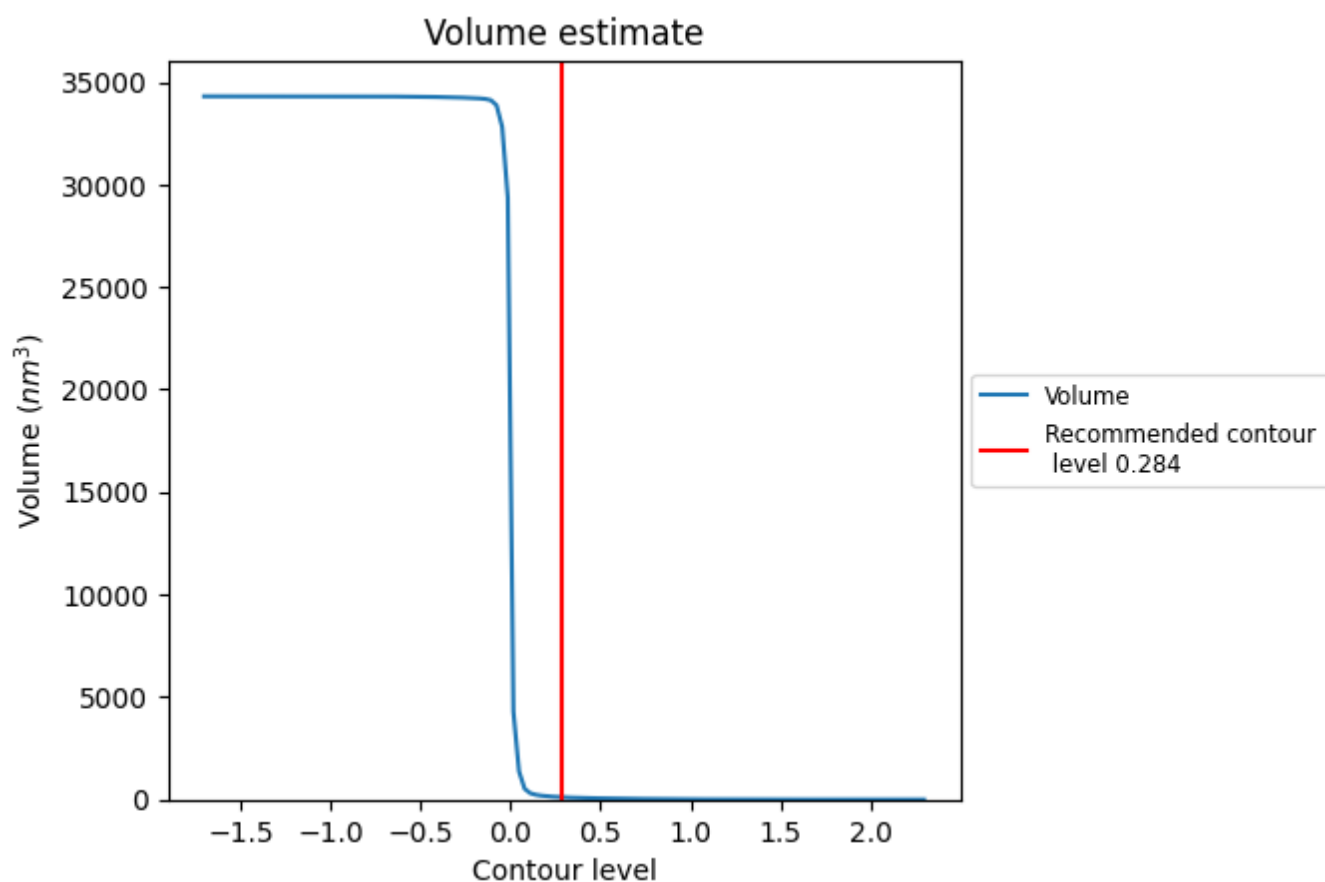
This section contains the results of statistical analysis of the map.

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.

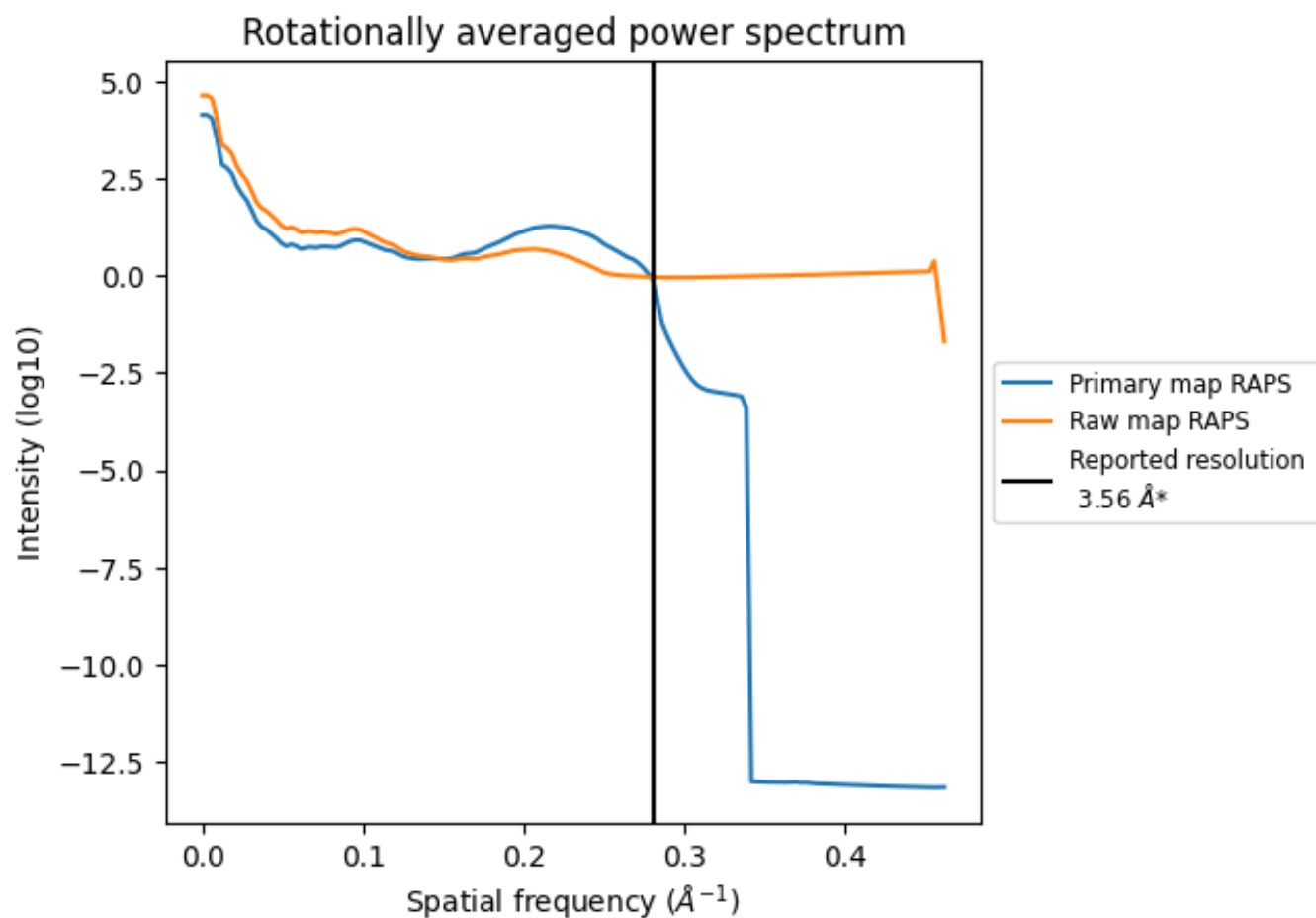
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm³; this corresponds to an approximate mass of 104 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 ⓘ

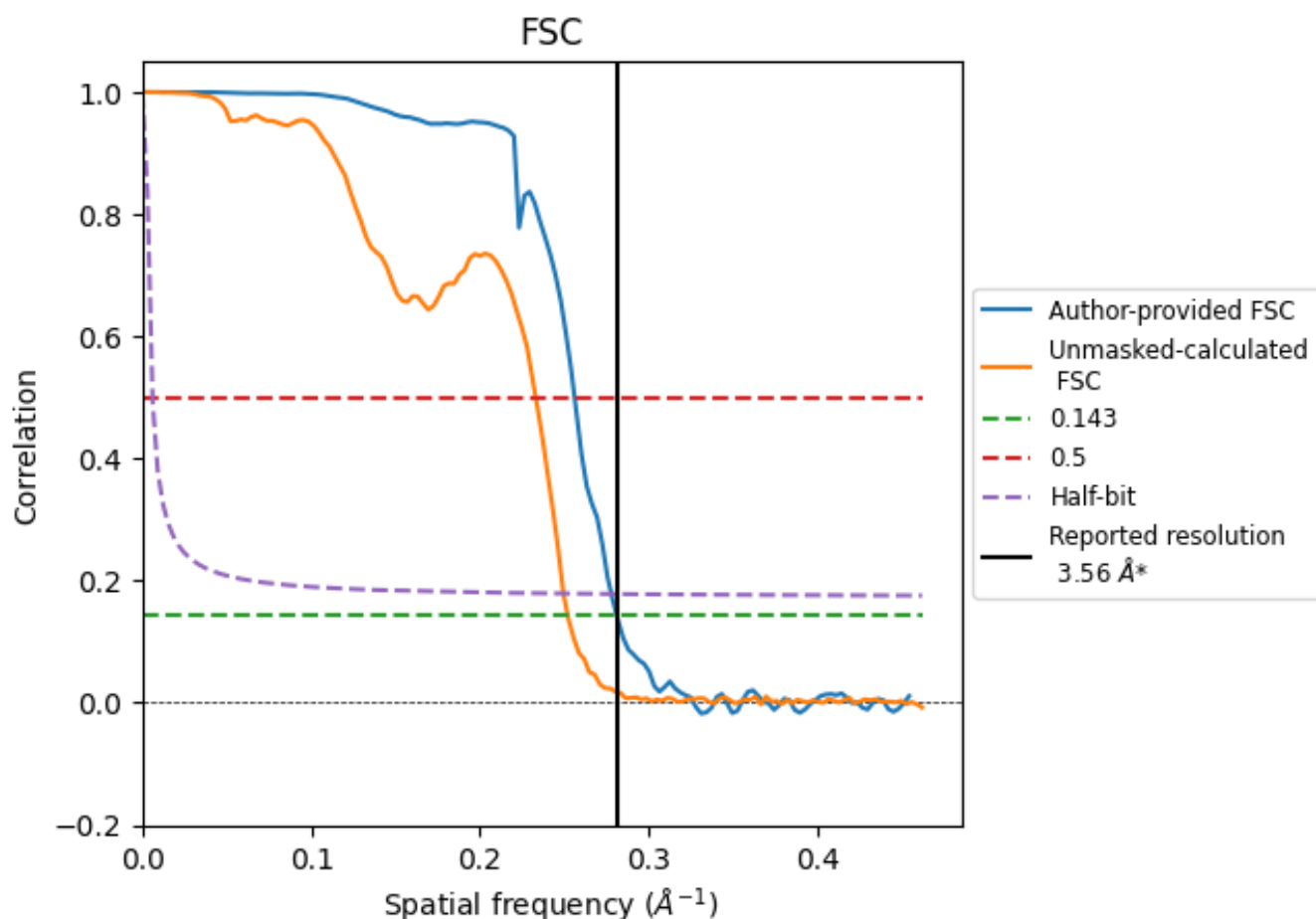


*Reported resolution corresponds to spatial frequency of 0.281 Å⁻¹

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 0.281 \AA^{-1}

8.2 Resolution estimates [i](#)

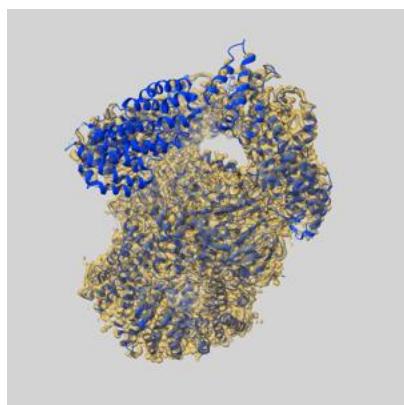
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.56	-	-
Author-provided FSC curve	3.56	3.91	3.60
Unmasked-calculated*	3.97	4.29	4.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.97 differs from the reported value 3.56 by more than 10 %

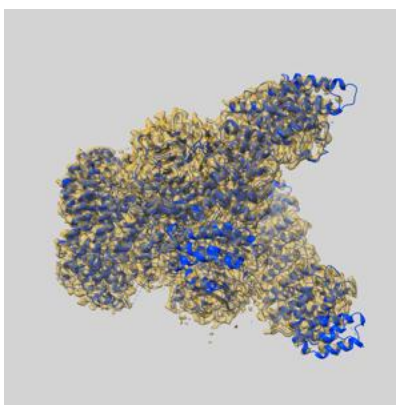
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47170 and PDB model 9DUM. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

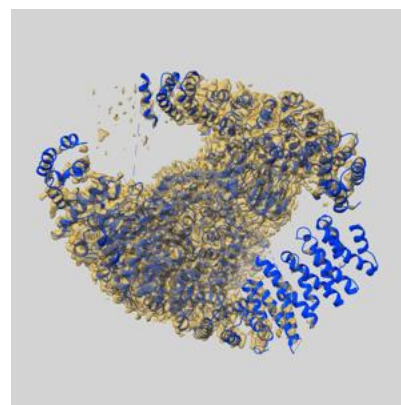
9.1 Map-model overlay [i](#)



X



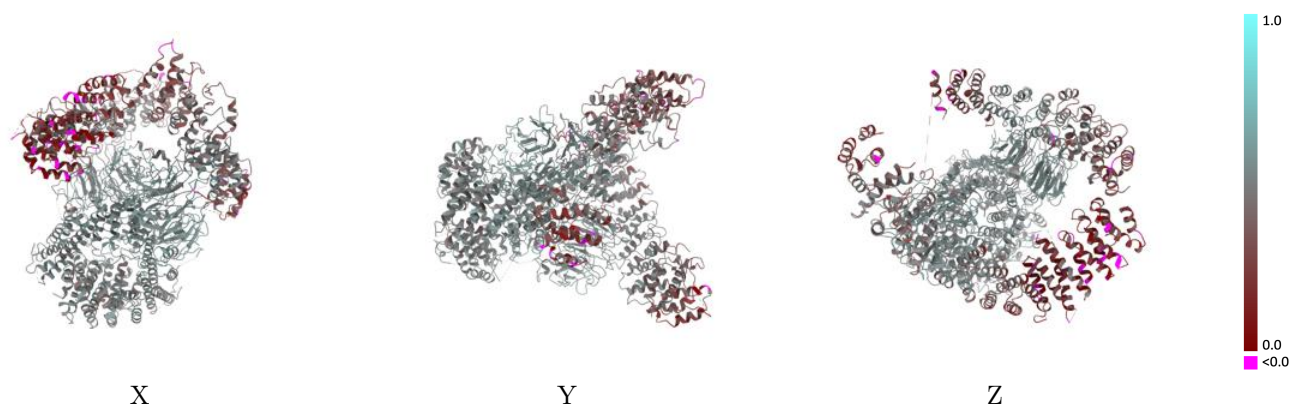
Y



Z

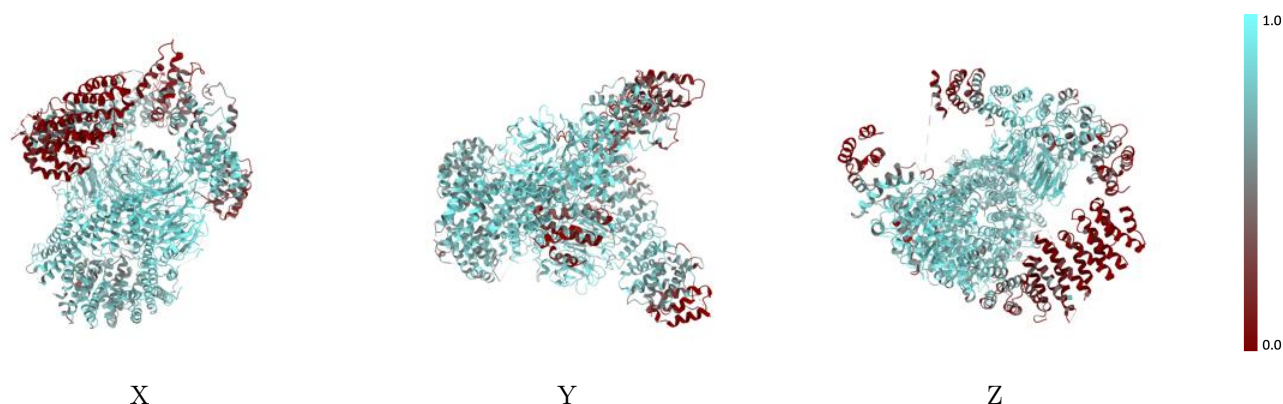
The images above show the 3D surface view of the map at the recommended contour level 0.284 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



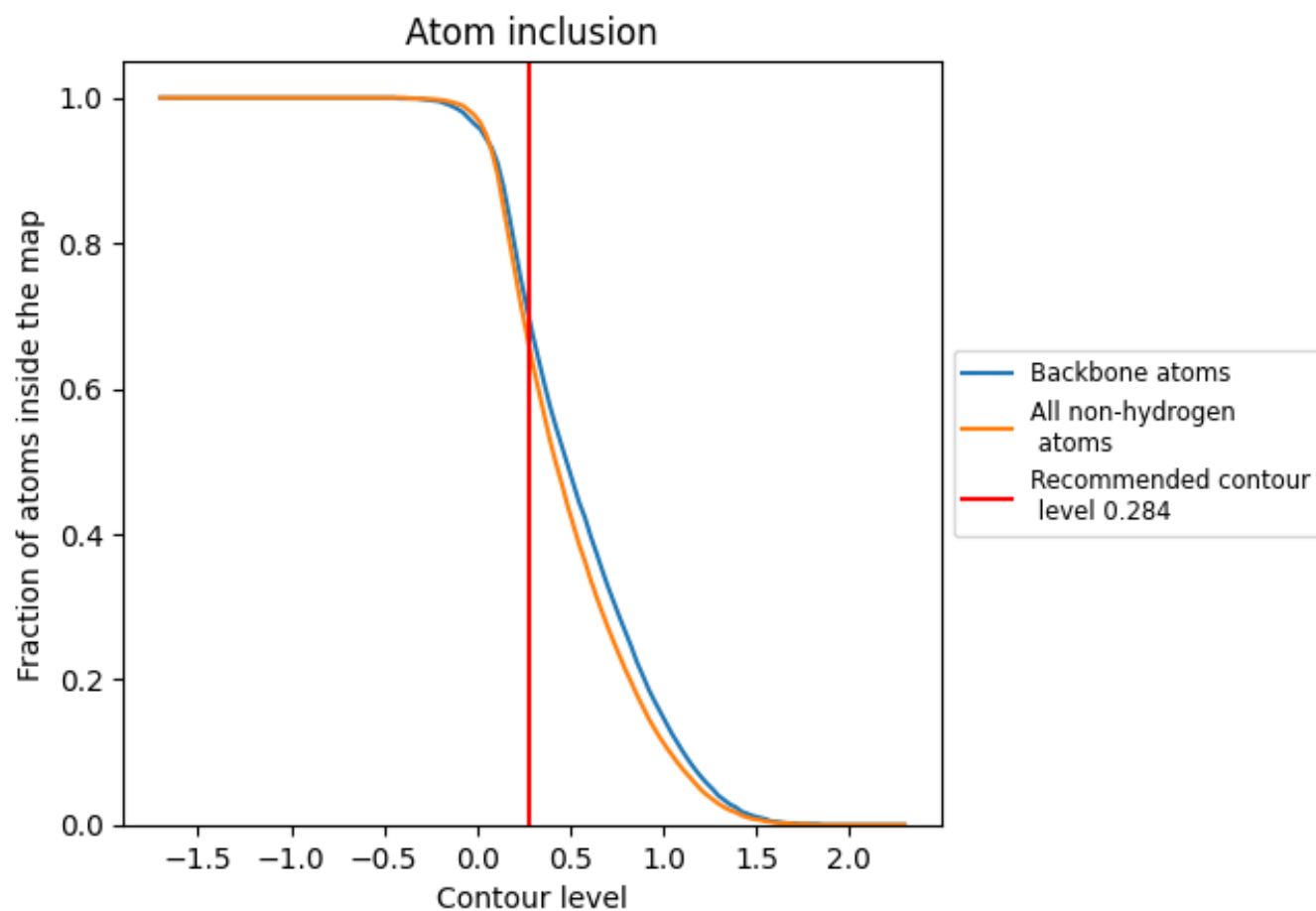
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.284).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 65% 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 (0.284) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6520	<div></div> 0.4530
A	<div></div> 0.8470	<div></div> 0.5450
B	<div></div> 0.8260	<div></div> 0.5390
C	<div></div> 0.7830	<div></div> 0.5190
D	<div></div> 0.7780	<div></div> 0.5160
G	<div></div> 0.5410	<div></div> 0.3940
H	<div></div> 0.3840	<div></div> 0.3240

1.0

0.0

<0.0