



Full wwPDB EM Validation Report ⓘ

Feb 10, 2025 – 11:35 PM EST

PDB ID : 9DZ2
EMDB ID : EMD-47323
Title : Cryo-EM structure of Sudan ebolavirus glycoprotein complexed with hNPC1-C
Authors : Bu, F.; Ye, G.; Liu, B.; Li, F.
Deposited on : 2024-10-15
Resolution : 3.31 Å(reported)
Based on initial model : 5f1b

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.dev113
MolProbity : 4.02b-467
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) : 2.40

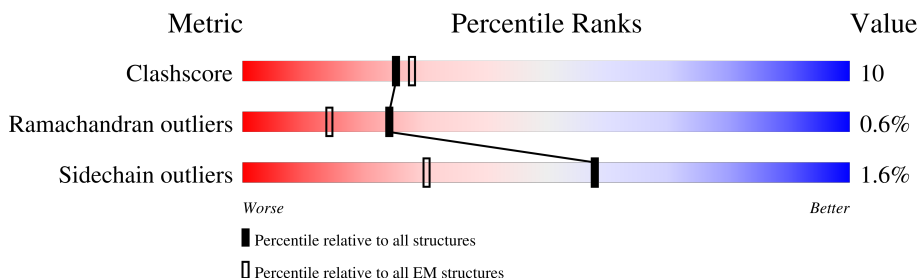
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.31 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	C	280	
1	D	280	
2	A	195	
2	E	195	
2	I	195	
3	B	165	
3	F	165	
3	J	165	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9523 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 NPC intracellular cholesterol transporter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	212	Total	C	N	O	S	0	0
			1723	1117	278	324	4		
1	D	209	Total	C	N	O	S	0	0
			1701	1101	275	321	4		

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	351	MET	-	initiating methionine	UNP O15118
C	352	ASP	-	expression tag	UNP O15118
C	353	ALA	-	expression tag	UNP O15118
C	354	MET	-	expression tag	UNP O15118
C	355	LYS	-	expression tag	UNP O15118
C	356	ARG	-	expression tag	UNP O15118
C	357	GLY	-	expression tag	UNP O15118
C	358	LEU	-	expression tag	UNP O15118
C	359	CYS	-	expression tag	UNP O15118
C	360	CYS	-	expression tag	UNP O15118
C	361	VAL	-	expression tag	UNP O15118
C	362	LEU	-	expression tag	UNP O15118
C	363	LEU	-	expression tag	UNP O15118
C	364	LEU	-	expression tag	UNP O15118
C	365	CYS	-	expression tag	UNP O15118
C	366	GLY	-	expression tag	UNP O15118
C	367	ALA	-	expression tag	UNP O15118
C	368	VAL	-	expression tag	UNP O15118
C	369	PHE	-	expression tag	UNP O15118
C	370	VAL	-	expression tag	UNP O15118
C	371	SER	-	expression tag	UNP O15118
C	372	ALA	-	expression tag	UNP O15118
C	373	SER	-	expression tag	UNP O15118
C	621	GLY	-	expression tag	UNP O15118
C	622	SER	-	expression tag	UNP O15118
C	623	TRP	-	expression tag	UNP O15118

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Chain	Residue	Modelled	Actual	Comment	Reference
C	624	SER	-	expression tag	UNP O15118
C	625	HIS	-	expression tag	UNP O15118
C	626	PRO	-	expression tag	UNP O15118
C	627	GLN	-	expression tag	UNP O15118
C	628	PHE	-	expression tag	UNP O15118
C	629	GLU	-	expression tag	UNP O15118
C	630	LYS	-	expression tag	UNP O15118
D	351	MET	-	initiating methionine	UNP O15118
D	352	ASP	-	expression tag	UNP O15118
D	353	ALA	-	expression tag	UNP O15118
D	354	MET	-	expression tag	UNP O15118
D	355	LYS	-	expression tag	UNP O15118
D	356	ARG	-	expression tag	UNP O15118
D	357	GLY	-	expression tag	UNP O15118
D	358	LEU	-	expression tag	UNP O15118
D	359	CYS	-	expression tag	UNP O15118
D	360	CYS	-	expression tag	UNP O15118
D	361	VAL	-	expression tag	UNP O15118
D	362	LEU	-	expression tag	UNP O15118
D	363	LEU	-	expression tag	UNP O15118
D	364	LEU	-	expression tag	UNP O15118
D	365	CYS	-	expression tag	UNP O15118
D	366	GLY	-	expression tag	UNP O15118
D	367	ALA	-	expression tag	UNP O15118
D	368	VAL	-	expression tag	UNP O15118
D	369	PHE	-	expression tag	UNP O15118
D	370	VAL	-	expression tag	UNP O15118
D	371	SER	-	expression tag	UNP O15118
D	372	ALA	-	expression tag	UNP O15118
D	373	SER	-	expression tag	UNP O15118
D	621	GLY	-	expression tag	UNP O15118
D	622	SER	-	expression tag	UNP O15118
D	623	TRP	-	expression tag	UNP O15118
D	624	SER	-	expression tag	UNP O15118
D	625	HIS	-	expression tag	UNP O15118
D	626	PRO	-	expression tag	UNP O15118
D	627	GLN	-	expression tag	UNP O15118
D	628	PHE	-	expression tag	UNP O15118
D	629	GLU	-	expression tag	UNP O15118
D	630	LYS	-	expression tag	UNP O15118

- Molecule 2 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	157	Total	C	N	O	S	0	0
			1198	763	203	226	6		
2	A	161	Total	C	N	O	S	0	0
			1230	783	208	233	6		
2	E	156	Total	C	N	O	S	0	0
			1189	757	201	225	6		

- Molecule 3 is a protein called Shed GP.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	105	Total	C	N	O	S	0	0
			835	528	152	149	6		
3	B	102	Total	C	N	O	S	0	0
			812	515	146	145	6		
3	F	105	Total	C	N	O	S	0	0
			835	528	152	149	6		

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	638	GLY	-	expression tag	UNP Q7T9D9
J	639	SER	-	expression tag	UNP Q7T9D9
J	640	GLY	-	expression tag	UNP Q7T9D9
J	641	TYR	-	expression tag	UNP Q7T9D9
J	642	ILE	-	expression tag	UNP Q7T9D9
J	643	PRO	-	expression tag	UNP Q7T9D9
J	644	GLU	-	expression tag	UNP Q7T9D9
J	645	ALA	-	expression tag	UNP Q7T9D9
J	646	PRO	-	expression tag	UNP Q7T9D9
J	647	ARG	-	expression tag	UNP Q7T9D9
J	648	ASP	-	expression tag	UNP Q7T9D9
J	649	GLY	-	expression tag	UNP Q7T9D9
J	650	GLN	-	expression tag	UNP Q7T9D9
J	651	ALA	-	expression tag	UNP Q7T9D9
J	652	TYR	-	expression tag	UNP Q7T9D9
J	653	VAL	-	expression tag	UNP Q7T9D9
J	654	ARG	-	expression tag	UNP Q7T9D9
J	655	LYS	-	expression tag	UNP Q7T9D9
J	656	ASP	-	expression tag	UNP Q7T9D9
J	657	GLY	-	expression tag	UNP Q7T9D9
J	658	GLU	-	expression tag	UNP Q7T9D9
J	659	TRP	-	expression tag	UNP Q7T9D9
J	660	VAL	-	expression tag	UNP Q7T9D9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	661	LEU	-	expression tag	UNP Q7T9D9
J	662	LEU	-	expression tag	UNP Q7T9D9
J	663	SER	-	expression tag	UNP Q7T9D9
J	664	THR	-	expression tag	UNP Q7T9D9
J	665	PHE	-	expression tag	UNP Q7T9D9
J	666	LEU	-	expression tag	UNP Q7T9D9
J	667	GLY	-	expression tag	UNP Q7T9D9
J	668	HIS	-	expression tag	UNP Q7T9D9
J	669	HIS	-	expression tag	UNP Q7T9D9
J	670	HIS	-	expression tag	UNP Q7T9D9
J	671	HIS	-	expression tag	UNP Q7T9D9
J	672	HIS	-	expression tag	UNP Q7T9D9
J	673	HIS	-	expression tag	UNP Q7T9D9
B	638	GLY	-	expression tag	UNP Q7T9D9
B	639	SER	-	expression tag	UNP Q7T9D9
B	640	GLY	-	expression tag	UNP Q7T9D9
B	641	TYR	-	expression tag	UNP Q7T9D9
B	642	ILE	-	expression tag	UNP Q7T9D9
B	643	PRO	-	expression tag	UNP Q7T9D9
B	644	GLU	-	expression tag	UNP Q7T9D9
B	645	ALA	-	expression tag	UNP Q7T9D9
B	646	PRO	-	expression tag	UNP Q7T9D9
B	647	ARG	-	expression tag	UNP Q7T9D9
B	648	ASP	-	expression tag	UNP Q7T9D9
B	649	GLY	-	expression tag	UNP Q7T9D9
B	650	GLN	-	expression tag	UNP Q7T9D9
B	651	ALA	-	expression tag	UNP Q7T9D9
B	652	TYR	-	expression tag	UNP Q7T9D9
B	653	VAL	-	expression tag	UNP Q7T9D9
B	654	ARG	-	expression tag	UNP Q7T9D9
B	655	LYS	-	expression tag	UNP Q7T9D9
B	656	ASP	-	expression tag	UNP Q7T9D9
B	657	GLY	-	expression tag	UNP Q7T9D9
B	658	GLU	-	expression tag	UNP Q7T9D9
B	659	TRP	-	expression tag	UNP Q7T9D9
B	660	VAL	-	expression tag	UNP Q7T9D9
B	661	LEU	-	expression tag	UNP Q7T9D9
B	662	LEU	-	expression tag	UNP Q7T9D9
B	663	SER	-	expression tag	UNP Q7T9D9
B	664	THR	-	expression tag	UNP Q7T9D9
B	665	PHE	-	expression tag	UNP Q7T9D9
B	666	LEU	-	expression tag	UNP Q7T9D9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	667	GLY	-	expression tag	UNP Q7T9D9
B	668	HIS	-	expression tag	UNP Q7T9D9
B	669	HIS	-	expression tag	UNP Q7T9D9
B	670	HIS	-	expression tag	UNP Q7T9D9
B	671	HIS	-	expression tag	UNP Q7T9D9
B	672	HIS	-	expression tag	UNP Q7T9D9
B	673	HIS	-	expression tag	UNP Q7T9D9
F	638	GLY	-	expression tag	UNP Q7T9D9
F	639	SER	-	expression tag	UNP Q7T9D9
F	640	GLY	-	expression tag	UNP Q7T9D9
F	641	TYR	-	expression tag	UNP Q7T9D9
F	642	ILE	-	expression tag	UNP Q7T9D9
F	643	PRO	-	expression tag	UNP Q7T9D9
F	644	GLU	-	expression tag	UNP Q7T9D9
F	645	ALA	-	expression tag	UNP Q7T9D9
F	646	PRO	-	expression tag	UNP Q7T9D9
F	647	ARG	-	expression tag	UNP Q7T9D9
F	648	ASP	-	expression tag	UNP Q7T9D9
F	649	GLY	-	expression tag	UNP Q7T9D9
F	650	GLN	-	expression tag	UNP Q7T9D9
F	651	ALA	-	expression tag	UNP Q7T9D9
F	652	TYR	-	expression tag	UNP Q7T9D9
F	653	VAL	-	expression tag	UNP Q7T9D9
F	654	ARG	-	expression tag	UNP Q7T9D9
F	655	LYS	-	expression tag	UNP Q7T9D9
F	656	ASP	-	expression tag	UNP Q7T9D9
F	657	GLY	-	expression tag	UNP Q7T9D9
F	658	GLU	-	expression tag	UNP Q7T9D9
F	659	TRP	-	expression tag	UNP Q7T9D9
F	660	VAL	-	expression tag	UNP Q7T9D9
F	661	LEU	-	expression tag	UNP Q7T9D9
F	662	LEU	-	expression tag	UNP Q7T9D9
F	663	SER	-	expression tag	UNP Q7T9D9
F	664	THR	-	expression tag	UNP Q7T9D9
F	665	PHE	-	expression tag	UNP Q7T9D9
F	666	LEU	-	expression tag	UNP Q7T9D9
F	667	GLY	-	expression tag	UNP Q7T9D9
F	668	HIS	-	expression tag	UNP Q7T9D9
F	669	HIS	-	expression tag	UNP Q7T9D9
F	670	HIS	-	expression tag	UNP Q7T9D9
F	671	HIS	-	expression tag	UNP Q7T9D9
F	672	HIS	-	expression tag	UNP Q7T9D9

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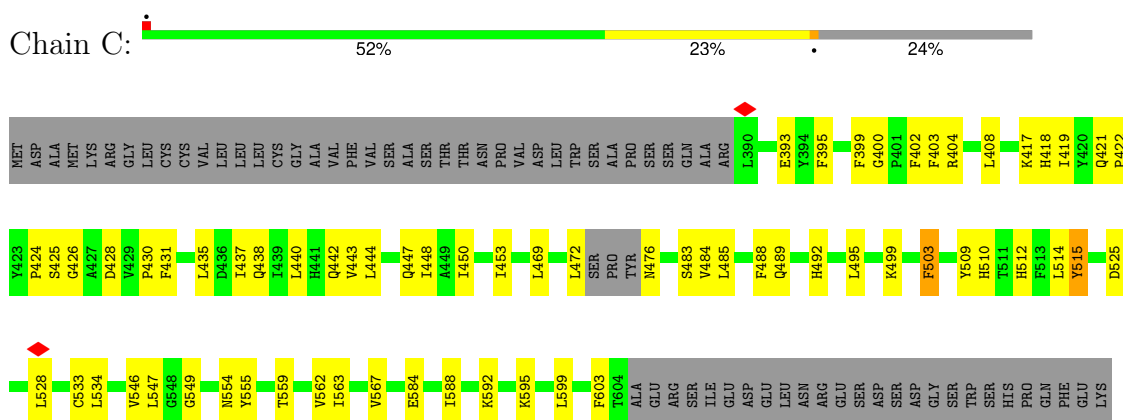
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Chain	Residue	Modelled	Actual	Comment	Reference
F	673	HIS	-	expression tag	UNP Q7T9D9

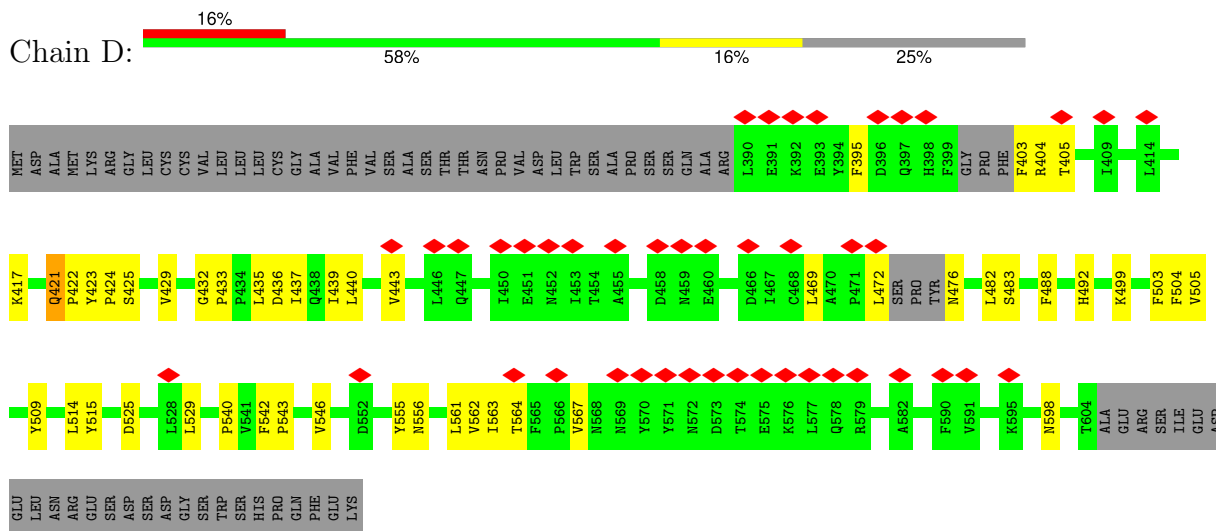
3 Residue-property plots

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: NPC intracellular cholesterol transporter 1



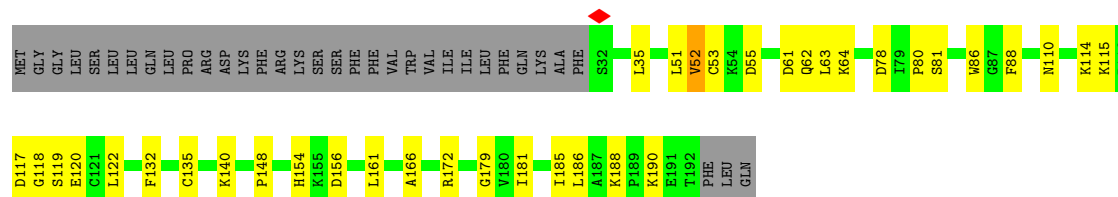
- Molecule 1: NPC intracellular cholesterol transporter 1



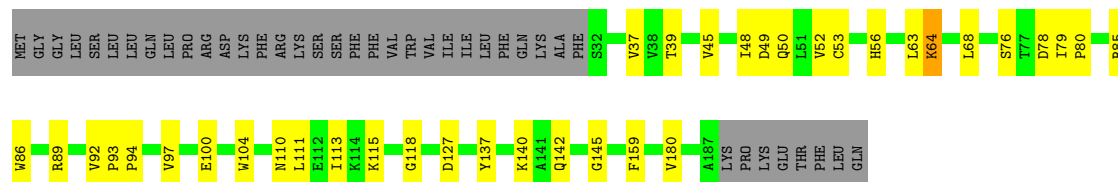
- Molecule 2: Envelope glycoprotein



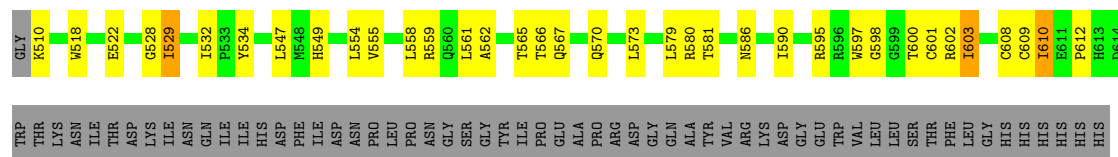
- Molecule 2: Envelope glycoprotein



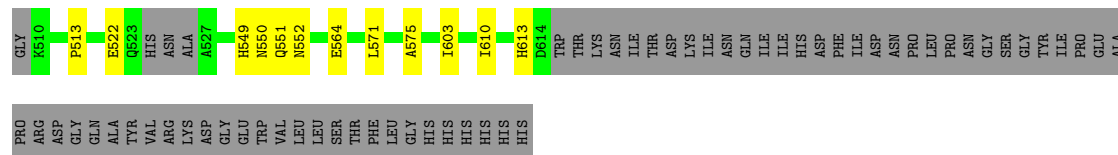
- Molecule 2: Envelope glycoprotein



- Molecule 3: Shed GP



- Molecule 3: Shed GP



- Molecule 3: Shed GP



ASN	GLN	ILE	HIS	ASP	PHE	ASP	ASN	ASN	PRO	LEU	PRO	ASN	GLY	SER	GLY	TYR	ILE	PRO	GLU	ALA	PRO	ARG	ASP	GLY	GLN	ALA	TYR	VAL	ARG	LYS	ASP	GLY	GLU	TRP	VAL	LEU	LEU	SER	THR	PHE	LEU	GLY	HIS	HIS	HIS	HIS	HIS	HIS	TRP	THR	LYS	ASN	ILE	THR	ASP	LYS	ILE																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
R510	Q523	H524	N525	A526	A527	W531	Y534	F535	E545	N550	Q551	L558	L561	A562	T566	Q570	L571	F572	L573	R580	L585	K588	R595	R596	W597	C601	R602	I603	C608	C609	I610	E611	D614																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				</

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	159976	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 ($e^-/\text{\AA}^2$)	53.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.548	Depositor
Minimum map value	-0.294	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.00825	Depositor
Map size (Å)	283.30664, 283.30664, 283.30664	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88533324, 0.88533324, 0.88533324	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	C	0.28	0/1775	0.50	0/2428
1	D	0.26	0/1750	0.47	0/2392
2	A	0.27	0/1262	0.54	0/1716
2	E	0.27	0/1220	0.54	0/1660
2	I	0.29	0/1229	0.59	2/1671 (0.1%)
3	B	0.25	0/831	0.54	0/1129
3	F	0.27	0/856	0.58	0/1165
3	J	0.26	0/856	0.55	0/1165
All	All	0.27	0/9779	0.53	2/13326 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	124	PRO	CA-N-CD	-8.37	99.79	111.50
2	I	124	PRO	N-CD-CG	-6.66	93.22	103.20

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	C	1723	0	1634	47	0
1	D	1701	0	1614	35	0
2	A	1230	0	1204	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1189	0	1158	31	0
2	I	1198	0	1171	34	0
3	B	812	0	789	8	0
3	F	835	0	808	26	0
3	J	835	0	808	31	0
All	All	9523	0	9186	191	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 10.

All (191) 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:444:LEU:HA	1:C:447:GLN:HE21	1.47	0.78
2:E:64:LYS:NZ	2:E:100:GLU:OE1	2.17	0.77
3:J:598:GLY:O	3:F:596:ARG:NH1	2.22	0.72
3:J:608:CYS:SG	3:J:609:CYS:N	2.63	0.71
2:I:43:LEU:HB2	3:J:554:LEU:HD12	1.72	0.70
2:I:50:GLN:HG2	2:I:51:LEU:H	1.57	0.69
1:C:499:LYS:HE3	1:C:528:LEU:HB3	1.75	0.68
3:B:522:GLU:HG3	3:F:571:LEU:HB3	1.74	0.68
2:E:180:VAL:HG13	3:F:562:ALA:HB1	1.74	0.68
1:D:482:LEU:HB2	1:D:564:THR:HB	1.78	0.66
1:D:499:LYS:HB2	1:D:529:LEU:HD21	1.77	0.66
1:D:472:LEU:O	1:D:476:ASN:N	2.28	0.66
1:C:438:GLN:N	1:C:438:GLN:OE1	2.30	0.65
2:A:115:LYS:HD2	2:A:119:SER:HB2	1.79	0.65
2:E:76:SER:O	2:E:85:ARG:NH2	2.30	0.65
2:E:78:ASP:OD1	2:E:79:ILE:N	2.29	0.65
1:C:472:LEU:O	1:C:476:ASN:N	2.30	0.64
2:E:52:VAL:HG23	2:E:53:CYS:H	1.61	0.64
1:C:431:PHE:HE2	1:C:510:HIS:HD2	1.45	0.64
1:C:422:PRO:HG2	1:C:426:GLY:HA3	1.79	0.63
1:C:431:PHE:CE2	1:C:510:HIS:HD2	2.16	0.63
1:C:418:HIS:HE1	1:C:431:PHE:HD2	1.46	0.62
2:A:61:ASP:O	2:A:64:LYS:NZ	2.32	0.62
1:C:448:ILE:HD12	1:C:492:HIS:CE1	2.35	0.61
2:I:180:VAL:HG23	3:J:562:ALA:HB1	1.82	0.61
1:C:425:SER:O	2:I:142:GLN:NE2	2.33	0.61
1:D:504:PHE:HE1	2:E:113:ILE:HG12	1.67	0.59
2:I:184:LEU:HD11	3:J:558:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:79:ILE:HG23	2:E:80:PRO:HD3	1.84	0.59
3:J:586:ASN:O	3:J:590:ILE:HG13	2.01	0.59
2:E:127:ASP:O	3:F:580:ARG:NH2	2.37	0.57
1:C:503:PHE:HE2	2:I:111:LEU:HD13	1.70	0.57
1:C:546:VAL:HA	1:C:562:VAL:HB	1.86	0.56
1:D:504:PHE:HZ	2:E:111:LEU:HD22	1.70	0.56
1:D:546:VAL:HA	1:D:562:VAL:HB	1.88	0.56
1:C:547:LEU:HD13	1:C:555:TYR:HB3	1.86	0.56
3:J:609:CYS:O	3:J:610:ILE:HB	2.06	0.56
1:D:492:HIS:O	1:D:492:HIS:ND1	2.38	0.56
1:C:447:GLN:HE22	1:C:485:LEU:HG	1.70	0.55
3:J:603:ILE:HG23	3:J:612:PRO:HG3	1.88	0.55
1:C:489:GLN:N	1:C:489:GLN:OE1	2.40	0.55
2:I:115:LYS:N	2:I:119:SER:O	2.31	0.55
2:A:117:ASP:OD1	2:A:118:GLY:N	2.34	0.55
2:I:52:VAL:HG13	2:I:53:CYS:H	1.71	0.55
3:J:547:LEU:HD13	3:J:549:HIS:CD2	2.42	0.55
1:C:431:PHE:CZ	1:C:514:LEU:HD21	2.42	0.55
3:J:600:THR:HG23	2:E:56:HIS:CE1	2.42	0.55
1:D:404:ARG:N	1:D:567:VAL:O	2.39	0.54
1:C:515:TYR:CZ	1:C:525:ASP:HA	2.42	0.54
2:I:117:ASP:OD1	2:I:118:GLY:N	2.35	0.54
3:F:611:GLU:N	3:F:611:GLU:OE1	2.41	0.53
2:E:68:LEU:HD11	3:F:558:LEU:HG	1.91	0.53
1:C:431:PHE:HE2	1:C:510:HIS:CD2	2.27	0.53
3:J:561:LEU:O	3:J:565:THR:HG23	2.08	0.53
1:D:429:VAL:HG21	1:D:514:LEU:HD11	1.91	0.53
1:C:595:LYS:HA	1:C:595:LYS:HE2	1.91	0.52
1:D:543:PRO:HB2	1:D:555:TYR:CD2	2.44	0.52
1:C:400:GLY:O	1:C:402:PHE:N	2.43	0.52
1:D:437:ILE:HD11	1:D:509:TYR:CE2	2.45	0.52
2:E:37:VAL:HG12	2:E:39:THR:HG23	1.91	0.51
3:J:612:PRO:HA	3:B:603:ILE:HD12	1.92	0.51
2:E:180:VAL:HG21	3:F:566:THR:OG1	2.10	0.51
2:I:122:LEU:O	2:I:172:ARG:NH1	2.42	0.51
2:A:114:LYS:HA	2:A:120:GLU:HA	1.92	0.51
1:C:588:ILE:HG22	1:C:603:PHE:CZ	2.46	0.50
2:I:97:VAL:HG11	3:J:573:LEU:HD11	1.94	0.50
2:I:50:GLN:O	3:J:595:ARG:NH2	2.40	0.50
2:A:35:LEU:HD21	2:A:185:ILE:HG13	1.93	0.50
1:C:549:GLY:HA3	1:C:559:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:GLY:H	1:D:435:LEU:HD12	1.77	0.49
1:D:436:ASP:O	1:D:440:LEU:N	2.42	0.49
2:E:159:PHE:CZ	3:F:570:GLN:NE2	2.81	0.49
2:I:52:VAL:HG13	2:I:53:CYS:N	2.27	0.49
2:E:97:VAL:HG13	3:F:573:LEU:HD21	1.95	0.49
2:E:48:ILE:HG21	3:F:588:LYS:HD3	1.95	0.49
2:E:53:CYS:CB	3:F:596:ARG:HH21	2.26	0.49
1:C:418:HIS:CE1	1:C:431:PHE:HD2	2.29	0.49
1:C:489:GLN:NE2	1:C:534:LEU:O	2.46	0.49
3:B:613:HIS:H	3:F:603:ILE:HD12	1.78	0.49
1:D:423:TYR:HB3	1:D:424:PRO:HD3	1.95	0.49
2:I:50:GLN:O	2:I:51:LEU:HB3	2.13	0.48
1:D:437:ILE:HD13	1:D:440:LEU:HD12	1.95	0.48
2:E:79:ILE:CG2	2:E:80:PRO:HD3	2.43	0.48
1:C:417:LYS:HB2	1:C:431:PHE:O	2.13	0.48
1:C:592:LYS:HE3	1:C:592:LYS:HA	1.95	0.48
1:C:404:ARG:N	1:C:567:VAL:O	2.37	0.48
1:C:488:PHE:HB2	1:C:495:LEU:HD11	1.95	0.48
3:J:601:CYS:SG	3:J:602:ARG:N	2.86	0.48
2:A:154:HIS:CE1	2:A:156:ASP:HB2	2.49	0.48
3:B:564:GLU:N	3:B:564:GLU:OE1	2.46	0.48
1:D:422:PRO:HB2	1:D:425:SER:O	2.14	0.47
2:I:164:ARG:HG3	3:J:518:TRP:HH2	1.78	0.47
1:D:432:GLY:N	1:D:556:ASN:O	2.46	0.47
1:C:442:GLN:HB3	1:C:599:LEU:HD11	1.96	0.47
3:J:528:GLY:O	3:J:529:ILE:HG22	2.14	0.47
2:A:62:GLN:HB3	2:A:190:LYS:HZ2	1.80	0.47
2:E:49:ASP:OD1	2:E:50:GLN:N	2.47	0.47
1:D:488:PHE:CZ	1:D:509:TYR:HA	2.50	0.47
2:I:39:THR:O	2:I:42:THR:HG22	2.15	0.46
2:I:122:LEU:HB2	2:I:172:ARG:HB3	1.97	0.46
1:D:543:PRO:HA	1:D:546:VAL:HG22	1.97	0.46
1:C:435:LEU:HA	1:C:440:LEU:HD12	1.96	0.46
2:E:89:ARG:HH11	2:E:92:VAL:HG23	1.80	0.46
1:C:499:LYS:HG2	1:C:528:LEU:HB2	1.97	0.46
1:C:437:ILE:HA	1:C:440:LEU:HB3	1.97	0.46
1:C:450:ILE:O	1:C:453:ILE:HG12	2.16	0.46
1:C:419:ILE:HA	1:C:430:PRO:HA	1.97	0.46
3:J:597:TRP:HB3	3:F:597:TRP:NE1	2.30	0.46
1:D:443:VAL:HG21	1:D:561:LEU:HD22	1.97	0.46
1:D:488:PHE:HZ	1:D:509:TYR:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:115:LYS:HD3	2:I:119:SER:HB2	1.97	0.46
1:D:421:GLN:NE2	2:E:142:GLN:O	2.49	0.46
2:E:53:CYS:HB2	3:F:596:ARG:HH21	1.80	0.46
3:F:523:GLN:NE2	3:F:525:ASN:HB2	2.31	0.46
2:I:49:ASP:O	3:J:595:ARG:NH1	2.49	0.45
1:D:542:PHE:CD1	1:D:542:PHE:N	2.83	0.45
1:C:419:ILE:HG22	1:C:430:PRO:HB3	1.98	0.45
2:E:63:LEU:HB3	3:F:585:LEU:HD22	1.97	0.45
3:J:566:THR:O	3:J:570:GLN:HG2	2.16	0.45
1:D:515:TYR:CE1	1:D:525:ASP:HA	2.52	0.44
2:I:105:ALA:O	2:I:136:ARG:HG3	2.17	0.44
2:I:96:VAL:HG12	3:J:579:LEU:HG	1.99	0.44
2:E:110:ASN:HB3	2:E:140:LYS:HD3	1.98	0.44
2:A:122:LEU:HB2	2:A:172:ARG:HB3	1.99	0.44
2:E:49:ASP:O	3:F:595:ARG:NE	2.50	0.44
2:A:51:LEU:O	2:A:52:VAL:HB	2.18	0.44
1:D:395:PHE:CD1	1:D:405:THR:HG21	2.52	0.44
1:D:439:ILE:HD12	1:D:598:ASN:HB3	1.99	0.44
3:F:601:CYS:HB3	3:F:608:CYS:HB3	1.74	0.44
3:F:610:ILE:HG12	3:F:610:ILE:O	2.16	0.44
2:A:132:PHE:HB3	2:A:135:CYS:SG	2.58	0.44
3:B:513:PRO:HB3	3:B:552:ASN:HB3	2.00	0.44
1:C:403:PHE:CE1	1:C:469:LEU:HD13	2.53	0.44
2:I:120:GLU:N	2:I:120:GLU:OE1	2.51	0.44
2:A:52:VAL:CG1	2:A:53:CYS:N	2.81	0.44
1:D:417:LYS:HB3	1:D:433:PRO:HD3	2.00	0.44
2:A:78:ASP:HB3	2:A:80:PRO:HD2	2.00	0.43
1:D:437:ILE:HD11	1:D:509:TYR:CZ	2.53	0.43
3:J:510:LYS:O	3:J:510:LYS:HD3	2.18	0.43
1:C:484:VAL:HG23	1:C:546:VAL:HG23	2.00	0.43
2:I:51:LEU:HD12	2:I:52:VAL:N	2.32	0.43
2:I:165:LEU:HD23	2:I:165:LEU:HA	1.92	0.43
1:C:431:PHE:HZ	1:C:514:LEU:HD21	1.80	0.43
1:D:483:SER:HB2	1:D:563:ILE:HG23	1.99	0.43
2:I:90:SER:OG	2:I:149:GLY:HA2	2.19	0.43
2:A:166:ALA:HB3	2:A:181:ILE:HD11	2.01	0.43
2:I:140:LYS:HB3	2:I:140:LYS:HE3	1.90	0.43
2:E:45:VAL:HG22	3:F:561:LEU:HD13	2.01	0.43
2:I:159:PHE:CZ	3:J:570:GLN:NE2	2.87	0.43
2:E:115:LYS:HB2	2:E:118:GLY:HA3	1.99	0.43
1:C:395:PHE:HA	1:C:399:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:52:VAL:CG1	2:A:53:CYS:H	2.32	0.42
2:A:161:LEU:HD11	2:A:179:GLY:HA3	2.01	0.42
2:A:63:LEU:HD23	2:A:185:ILE:HG12	2.01	0.42
1:D:403:PHE:CE1	1:D:469:LEU:HD13	2.54	0.42
3:F:550:ASN:OD1	3:F:551:GLN:N	2.52	0.42
3:J:522:GLU:HG3	3:B:571:LEU:HB3	2.02	0.42
2:E:104:TRP:HE1	3:F:545:GLU:CD	2.20	0.42
2:I:74:GLY:HA3	3:J:510:LYS:NZ	2.34	0.42
3:J:532:ILE:HG22	3:J:534:TYR:H	1.84	0.42
3:F:534:TYR:HD2	3:F:535:PHE:CE1	2.38	0.42
1:C:512:HIS:NE2	1:C:533:CYS:SG	2.93	0.42
2:I:63:LEU:HD23	2:I:185:ILE:HG12	2.01	0.42
3:J:555:VAL:O	3:J:559:ARG:HG3	2.19	0.42
2:A:186:LEU:HD13	2:A:190:LYS:HA	2.02	0.42
2:I:126:PRO:HG2	2:I:129:VAL:HG21	2.02	0.42
3:J:567:GLN:HG3	3:F:531:TRP:CG	2.54	0.41
2:A:78:ASP:HB2	2:A:81:SER:HB3	2.01	0.41
1:D:503:PHE:CZ	2:E:86:TRP:HD1	2.38	0.41
1:D:437:ILE:HD13	1:D:437:ILE:N	2.35	0.41
1:D:505:VAL:HG23	2:E:145:GLY:HA2	2.02	0.41
3:B:550:ASN:OD1	3:B:551:GLN:N	2.53	0.41
2:A:110:ASN:O	2:A:140:LYS:HA	2.20	0.41
1:C:418:HIS:CE1	1:C:431:PHE:HB2	2.55	0.41
1:C:421:GLN:HE21	2:I:143:GLY:C	2.23	0.41
2:I:97:VAL:HG12	3:J:581:THR:HB	2.02	0.41
2:A:110:ASN:HB3	2:A:140:LYS:HG2	2.02	0.41
1:C:393:GLU:OE1	1:C:393:GLU:N	2.52	0.41
1:C:440:LEU:O	1:C:443:VAL:HG12	2.21	0.41
2:I:164:ARG:NH1	3:B:575:ALA:O	2.54	0.41
1:D:561:LEU:HD23	1:D:561:LEU:O	2.20	0.41
2:E:93:PRO:HA	2:E:94:PRO:HD3	1.93	0.41
1:C:515:TYR:CE2	1:C:525:ASP:HA	2.56	0.41
2:A:88:PHE:HB2	2:A:148:PRO:O	2.21	0.41
1:C:483:SER:HB2	1:C:563:ILE:HG12	2.02	0.40
1:C:584:GLU:O	1:C:588:ILE:HG12	2.21	0.40
3:F:523:GLN:HE22	3:F:525:ASN:HB2	1.86	0.40
2:I:127:ASP:O	3:J:580:ARG:NH2	2.30	0.40
3:J:567:GLN:HG3	3:F:531:TRP:CD2	2.57	0.40
2:A:188:LYS:O	2:A:190:LYS:HG3	2.21	0.40
1:D:540:PRO:HG2	1:D:542:PHE:HE1	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	208/280 (74%)	194 (93%)	13 (6%)	1 (0%)	25	57
1	D	203/280 (72%)	190 (94%)	13 (6%)	0	100	100
2	A	159/195 (82%)	147 (92%)	11 (7%)	1 (1%)	22	53
2	E	154/195 (79%)	146 (95%)	8 (5%)	0	100	100
2	I	155/195 (80%)	142 (92%)	13 (8%)	0	100	100
3	B	98/165 (59%)	92 (94%)	5 (5%)	1 (1%)	13	42
3	F	103/165 (62%)	94 (91%)	7 (7%)	2 (2%)	6	30
3	J	103/165 (62%)	97 (94%)	4 (4%)	2 (2%)	6	30
All	All	1183/1640 (72%)	1102 (93%)	74 (6%)	7 (1%)	24	53

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	52	VAL
3	J	529	ILE
3	J	610	ILE
1	C	424	PRO
3	F	527	ALA
3	B	610	ILE
3	F	610	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	191/250 (76%)	185 (97%)	6 (3%)	35	62
1	D	189/250 (76%)	188 (100%)	1 (0%)	86	91
2	A	134/165 (81%)	132 (98%)	2 (2%)	60	77
2	E	129/165 (78%)	127 (98%)	2 (2%)	58	76
2	I	130/165 (79%)	127 (98%)	3 (2%)	45	69
3	B	84/138 (61%)	83 (99%)	1 (1%)	67	81
3	F	86/138 (62%)	86 (100%)	0	100	100
3	J	86/138 (62%)	85 (99%)	1 (1%)	67	81
All	All	1029/1409 (73%)	1013 (98%)	16 (2%)	58	76

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	408	LEU
1	C	428	ASP
1	C	503	PHE
1	C	509	TYR
1	C	515	TYR
1	C	554	ASN
2	I	55	ASP
2	I	56	HIS
2	I	77	THR
3	J	603	ILE
2	A	55	ASP
2	A	86	TRP
3	B	549	HIS
1	D	421	GLN
2	E	64	LYS
2	E	137	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	418	HIS
1	C	421	GLN
1	C	447	GLN
2	A	62	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.

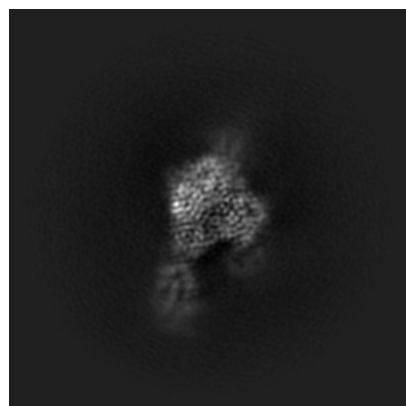
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47323. These allow visual inspection of the internal detail of the map and identification of artifacts.

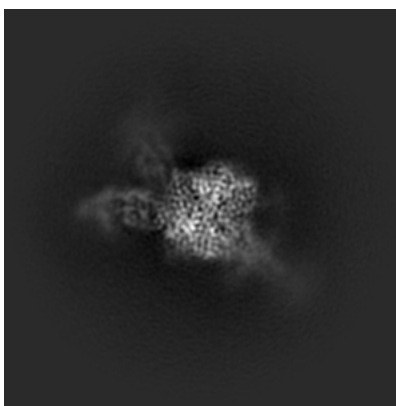
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

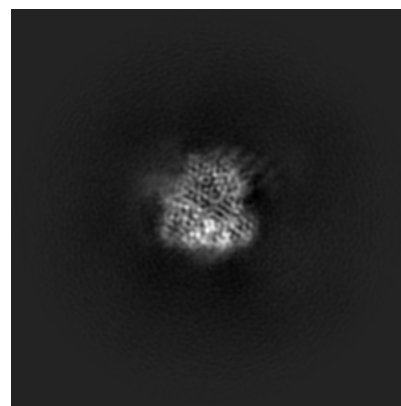
6.1.1 Primary map



X

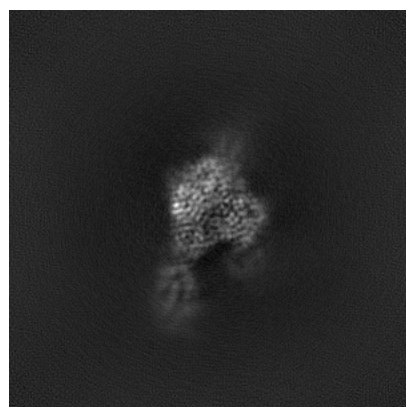


Y

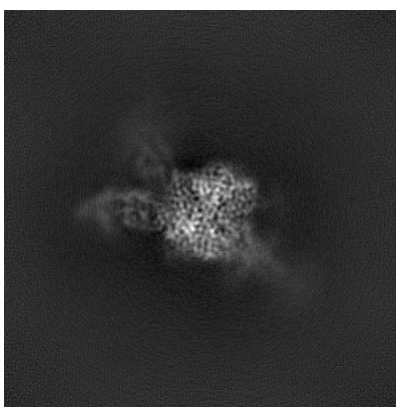


Z

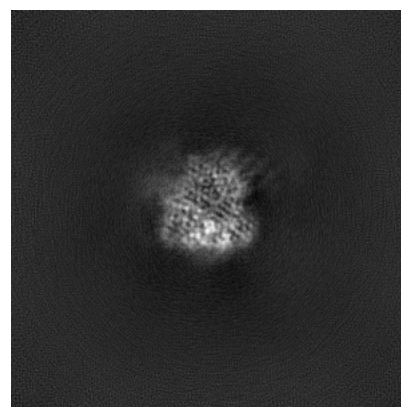
6.1.2 Raw map



X



Y

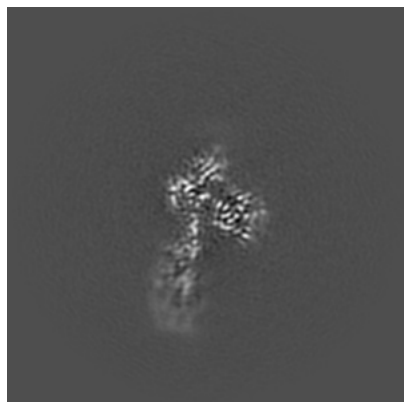


Z

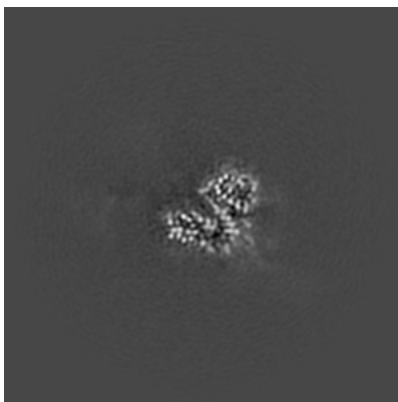
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

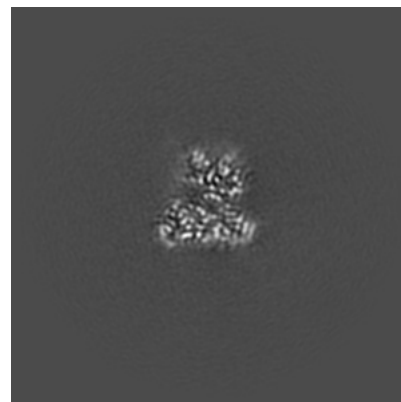
6.2.1 Primary map



X Index: 160

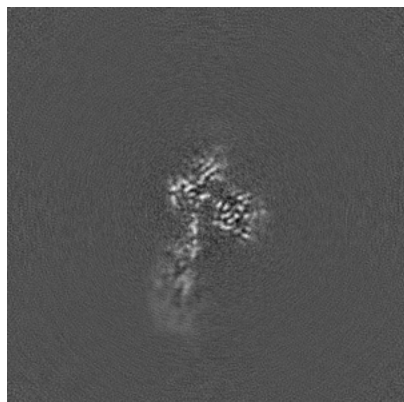


Y Index: 160

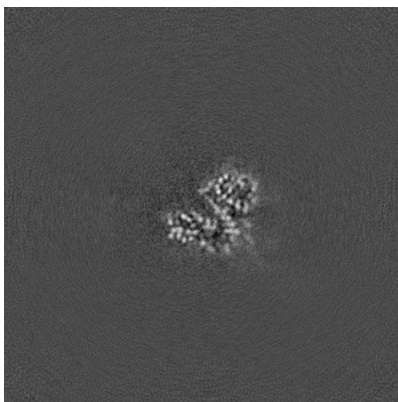


Z Index: 160

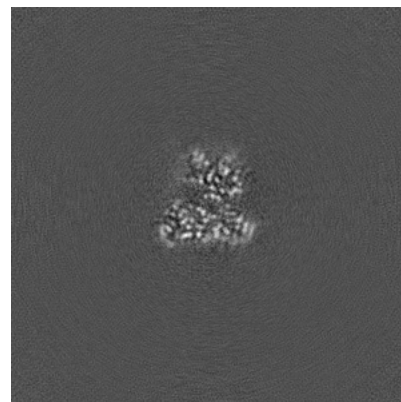
6.2.2 Raw map



X Index: 160



Y Index: 160

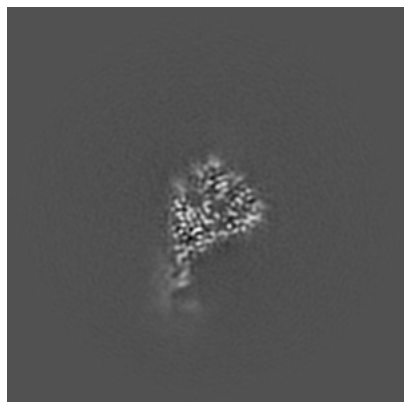


Z Index: 160

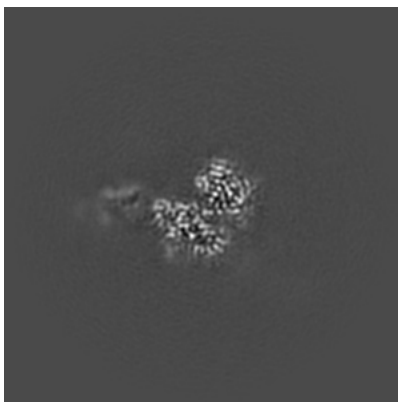
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

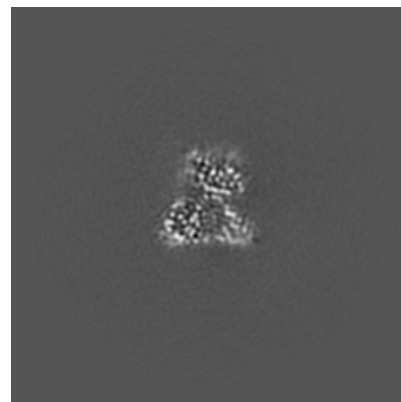
6.3.1 Primary map



X Index: 149

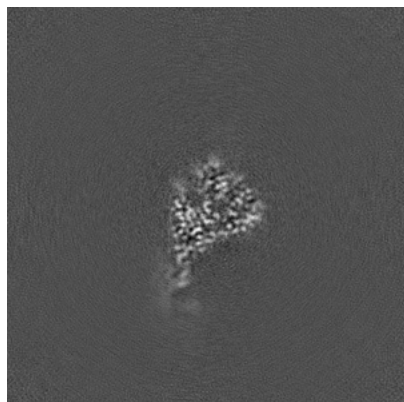


Y Index: 149

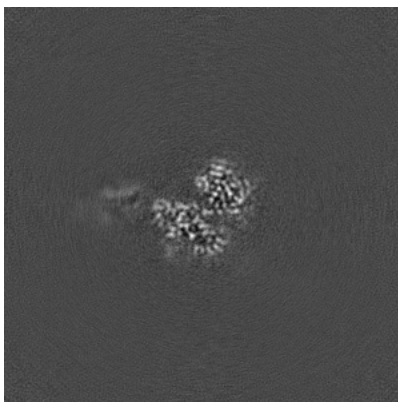


Z Index: 158

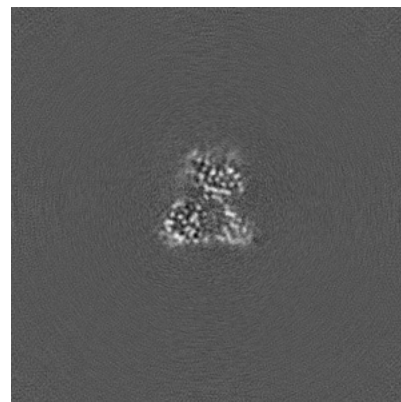
6.3.2 Raw map



X Index: 149



Y Index: 149

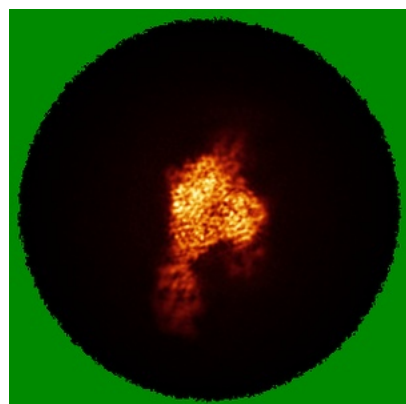


Z Index: 158

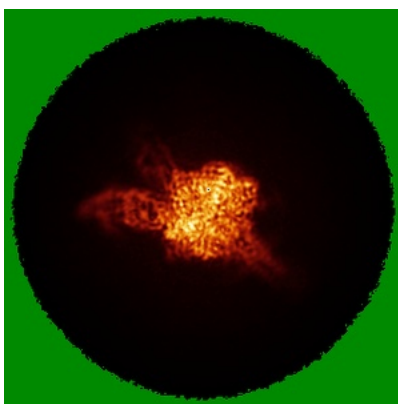
The images above show the largest variance slices of the map in three orthogonal directions.

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

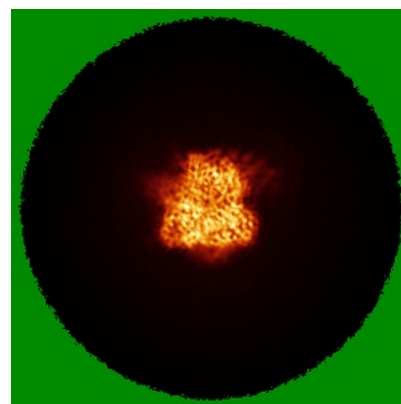
6.4.1 Primary map



X

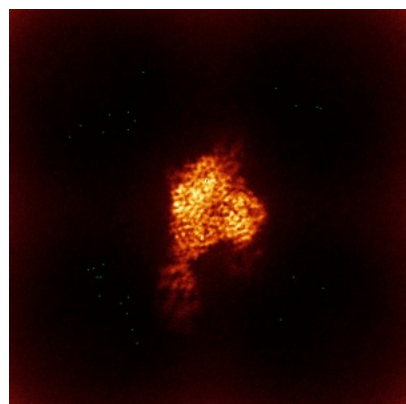


Y

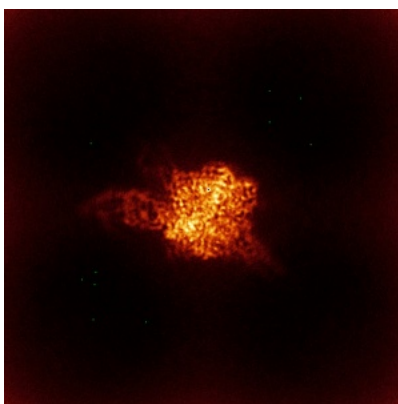


Z

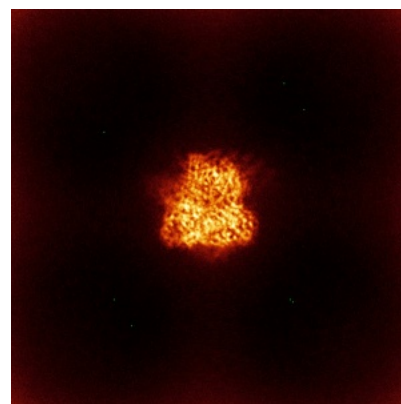
6.4.2 Raw map



X



Y

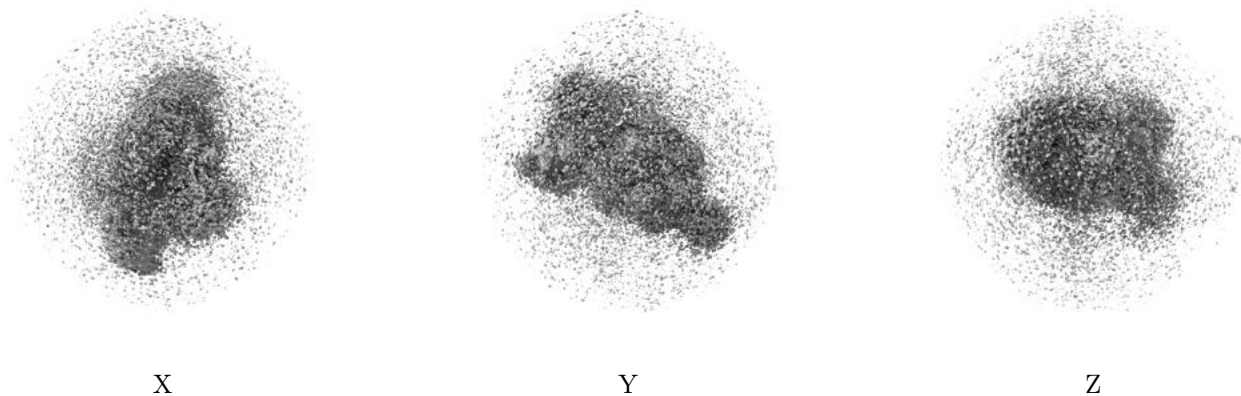


Z

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.

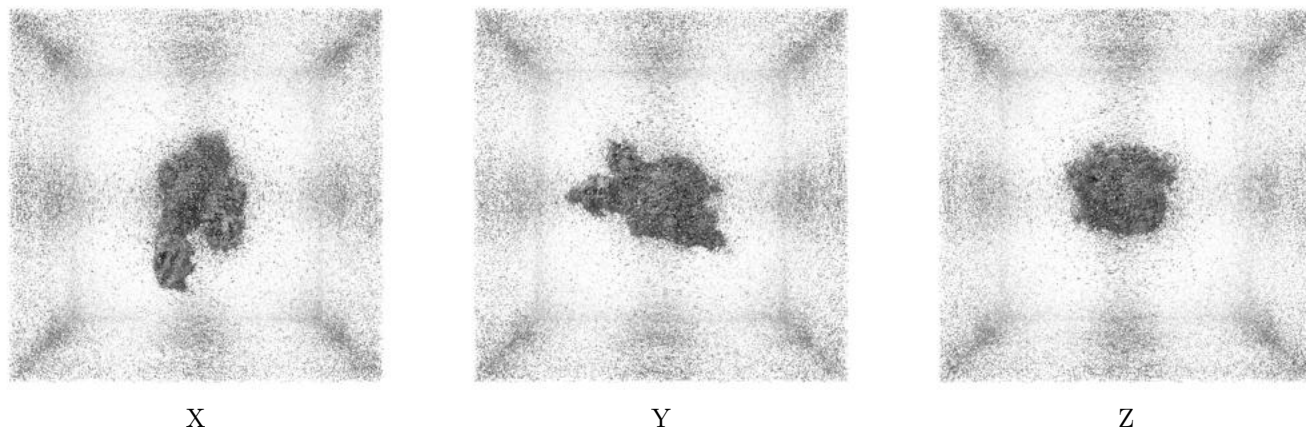
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00825. 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.

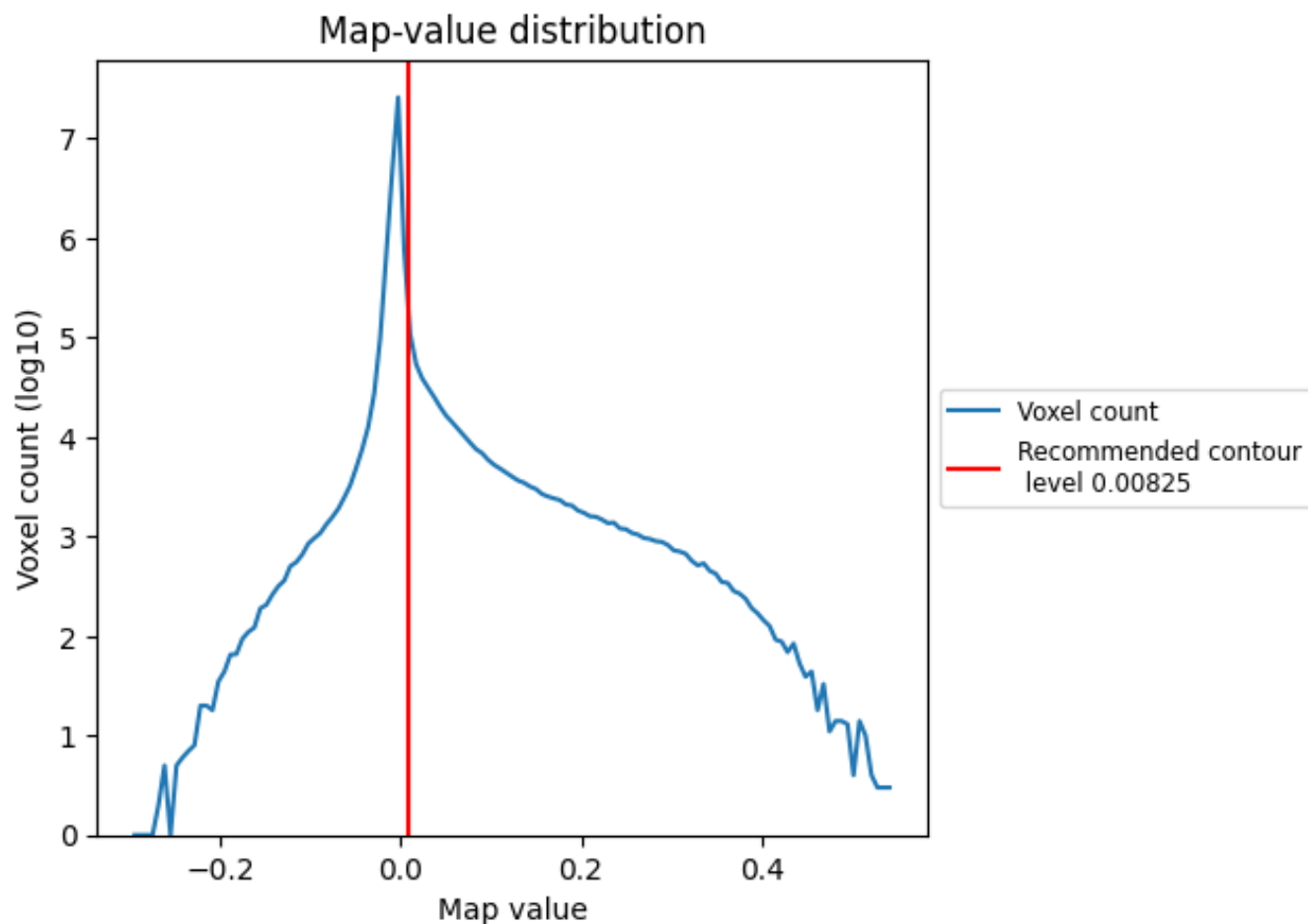
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

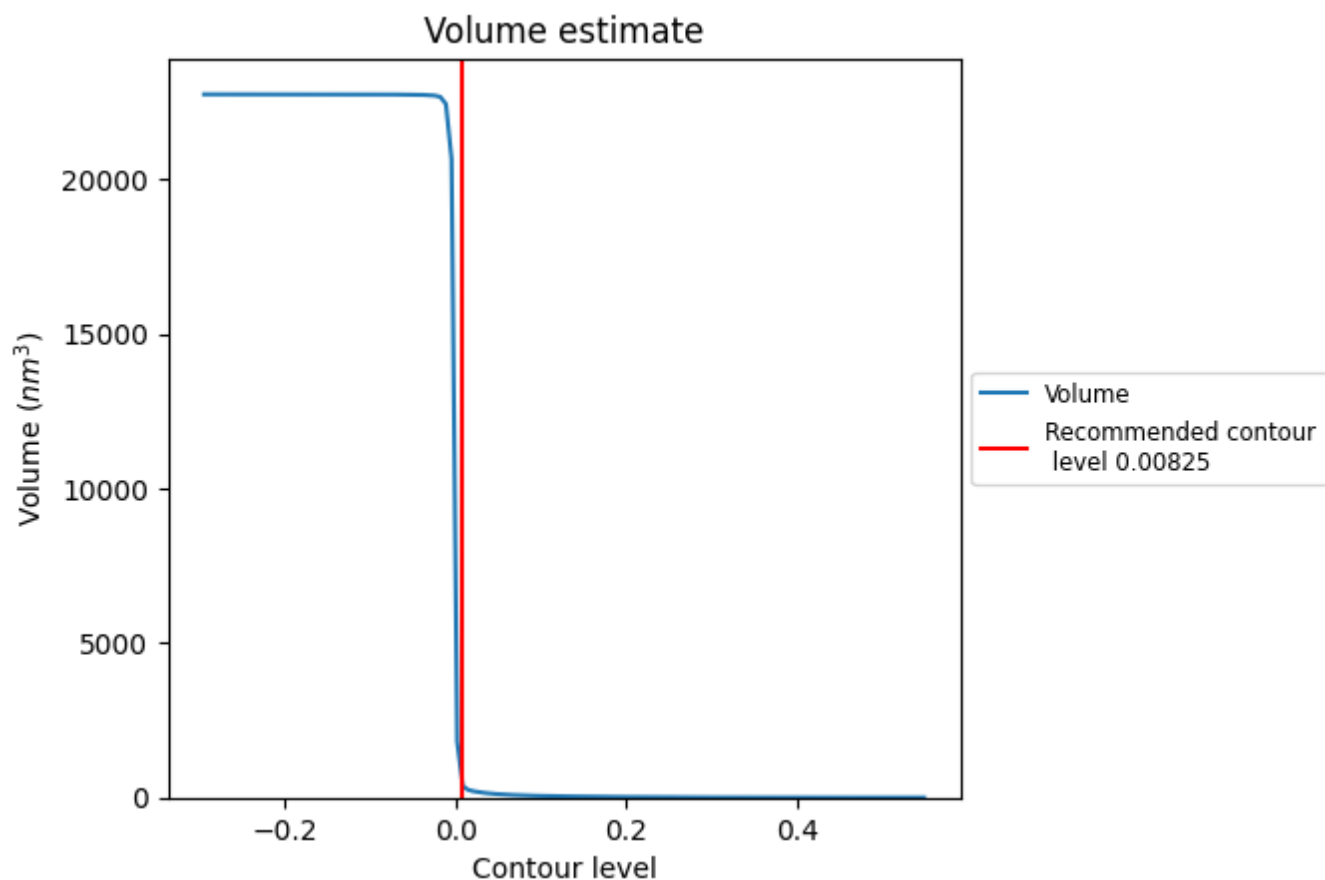
This section contains the results of statistical analysis of the map.

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.

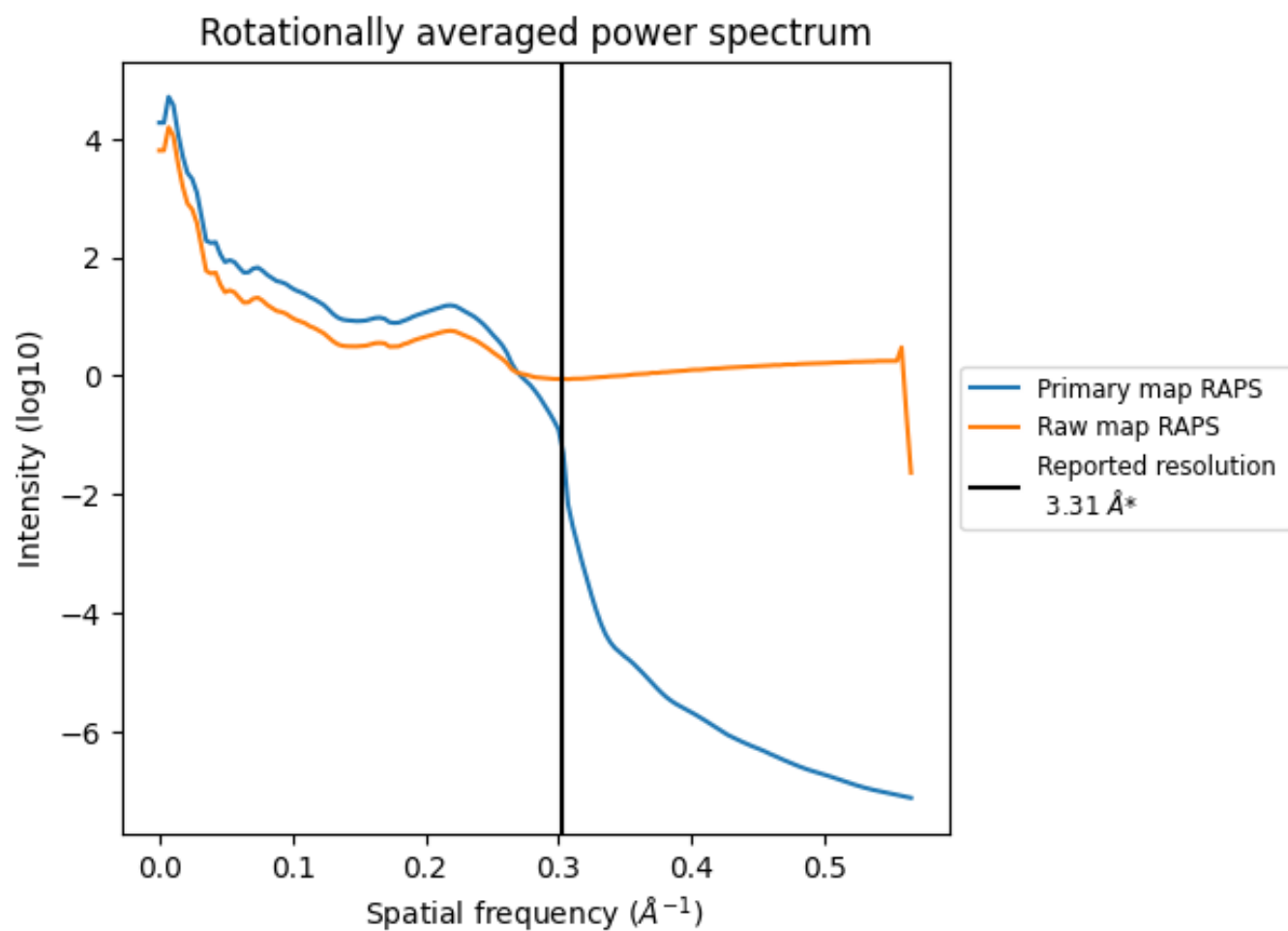
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 434 nm³; this corresponds to an approximate mass of 392 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 ⓘ

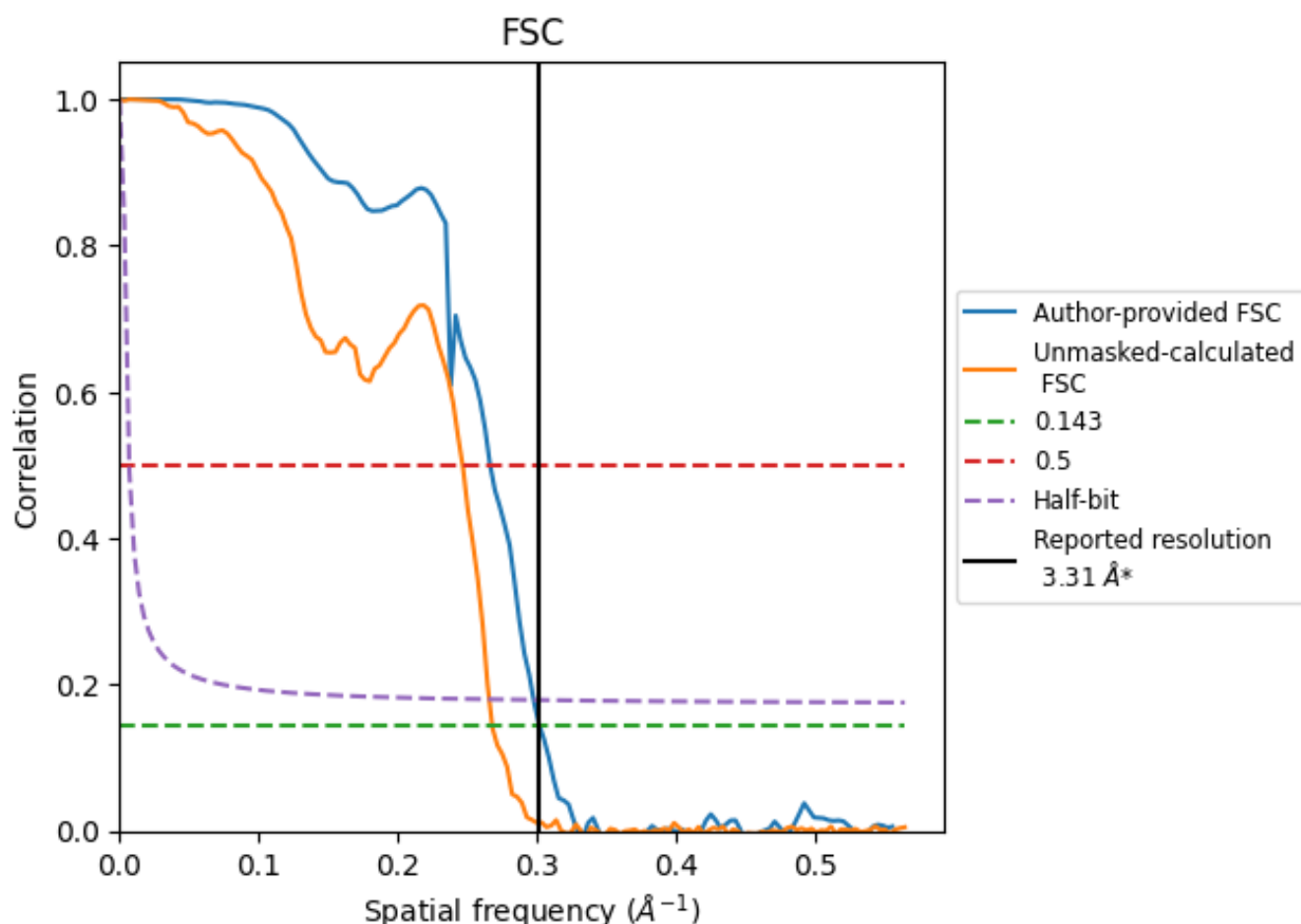


*Reported resolution corresponds to spatial frequency of 0.302 \AA^{-1}

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 0.302 Å⁻¹

8.2 Resolution estimates [i](#)

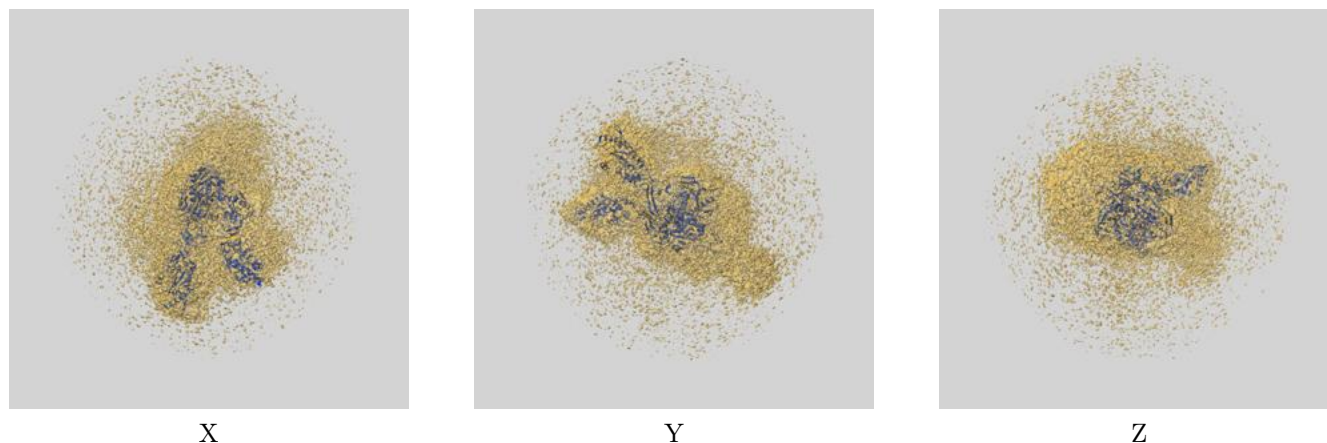
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.31	-	-
Author-provided FSC curve	3.31	3.75	3.36
Unmasked-calculated*	3.73	4.05	3.76

*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 3.73 differs from the reported value 3.31 by more than 10 %

9 Map-model fit [i](#)

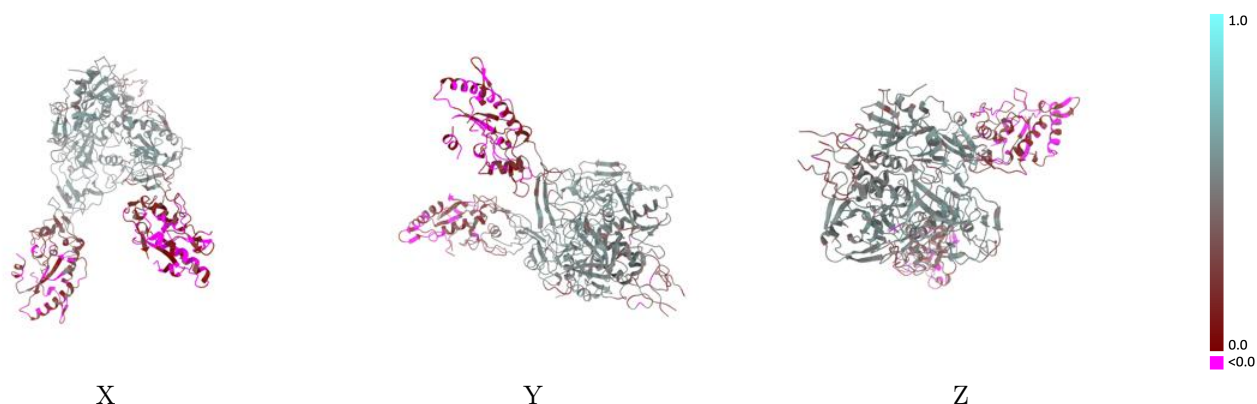
This section contains information regarding the fit between EMDB map EMD-47323 and PDB model 9DZ2. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



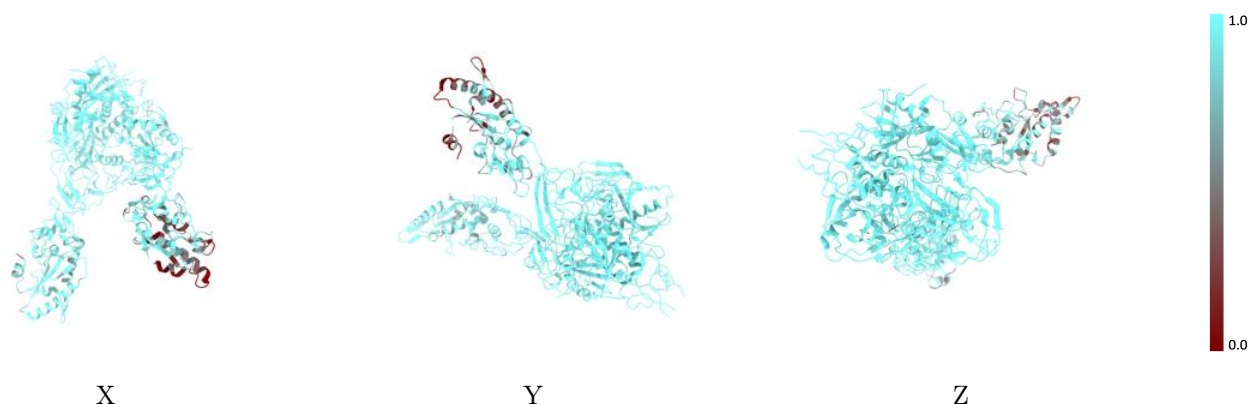
The images above show the 3D surface view of the map at the recommended contour level 0.00825 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



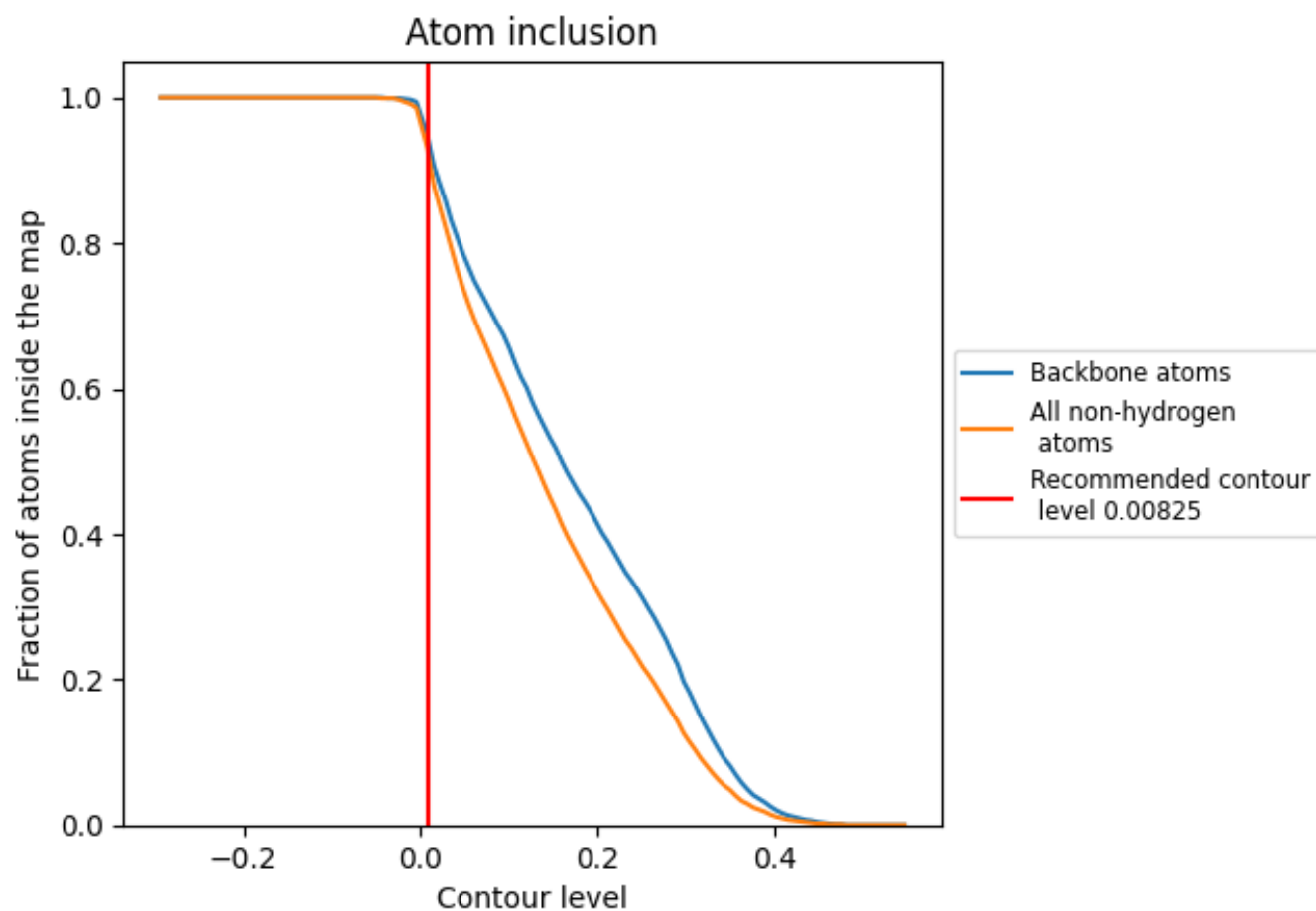
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00825).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.00825) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9290	<div></div> 0.3580
A	<div></div> 0.9940	<div></div> 0.5040
B	<div></div> 0.9960	<div></div> 0.4800
C	<div></div> 0.9260	<div></div> 0.1720
D	<div></div> 0.7000	<div></div> 0.0640
E	<div></div> 0.9870	<div></div> 0.5030
F	<div></div> 0.9960	<div></div> 0.4520
I	<div></div> 0.9960	<div></div> 0.5190
J	<div></div> 0.9940	<div></div> 0.4720

1.0

0.0

<0.0