



wwPDB EM Validation Summary Report ⓘ

Mar 14, 2026 – 06:01 AM UTC

PDB ID : 7R12 / pdb_00007r12
EMDB ID : EMD-14228
Title : Dissociated S1 domain of Mink Variant SARS-CoV-2 Spike bound to ACE2
(Non-Uniform Refinement)
Authors : Benton, D.J.; Wrobel, A.G.; Gamblin, S.J.
Deposited on : 2022-02-02
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

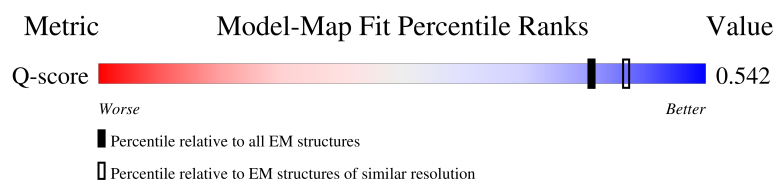
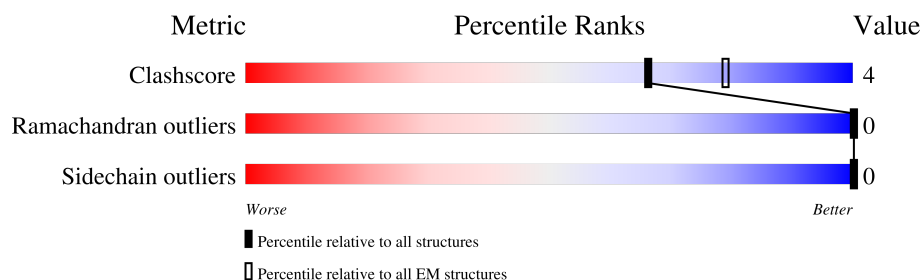
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	D	654	
2	A	1284	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6858 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	588	Total	C	N	O	S	0	0
			4801	3076	794	902	29		

There are 59 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	MET	-	initiating methionine	UNP Q9BYF1
D	0	GLU	-	expression tag	UNP Q9BYF1
D	1	THR	-	expression tag	UNP Q9BYF1
D	2	ASP	-	expression tag	UNP Q9BYF1
D	3	THR	-	expression tag	UNP Q9BYF1
D	4	LEU	-	expression tag	UNP Q9BYF1
D	5	LEU	-	expression tag	UNP Q9BYF1
D	6	LEU	-	expression tag	UNP Q9BYF1
D	7	TRP	-	expression tag	UNP Q9BYF1
D	8	VAL	-	expression tag	UNP Q9BYF1
D	9	LEU	-	expression tag	UNP Q9BYF1
D	10	LEU	-	expression tag	UNP Q9BYF1
D	11	LEU	-	expression tag	UNP Q9BYF1
D	12	TRP	-	expression tag	UNP Q9BYF1
D	13	VAL	-	expression tag	UNP Q9BYF1
D	14	PRO	-	expression tag	UNP Q9BYF1
D	15	GLY	-	expression tag	UNP Q9BYF1
D	16	SER	-	expression tag	UNP Q9BYF1
D	17	THR	-	expression tag	UNP Q9BYF1
D	18	GLY	-	expression tag	UNP Q9BYF1
D	614	ALA	-	expression tag	UNP Q9BYF1
D	615	ASP	-	expression tag	UNP Q9BYF1
D	616	ASP	-	expression tag	UNP Q9BYF1
D	617	TYR	-	expression tag	UNP Q9BYF1
D	618	LYS	-	expression tag	UNP Q9BYF1
D	619	ASP	-	expression tag	UNP Q9BYF1
D	620	ASP	-	expression tag	UNP Q9BYF1
D	621	ASP	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	622	ASP	-	expression tag	UNP Q9BYF1
D	623	LYS	-	expression tag	UNP Q9BYF1
D	624	TRP	-	expression tag	UNP Q9BYF1
D	625	SER	-	expression tag	UNP Q9BYF1
D	626	HIS	-	expression tag	UNP Q9BYF1
D	627	PRO	-	expression tag	UNP Q9BYF1
D	628	GLN	-	expression tag	UNP Q9BYF1
D	629	PHE	-	expression tag	UNP Q9BYF1
D	630	GLU	-	expression tag	UNP Q9BYF1
D	631	LYS	-	expression tag	UNP Q9BYF1
D	632	GLY	-	expression tag	UNP Q9BYF1
D	633	GLY	-	expression tag	UNP Q9BYF1
D	634	GLY	-	expression tag	UNP Q9BYF1
D	635	SER	-	expression tag	UNP Q9BYF1
D	636	GLY	-	expression tag	UNP Q9BYF1
D	637	GLY	-	expression tag	UNP Q9BYF1
D	638	GLY	-	expression tag	UNP Q9BYF1
D	639	SER	-	expression tag	UNP Q9BYF1
D	640	GLY	-	expression tag	UNP Q9BYF1
D	641	GLY	-	expression tag	UNP Q9BYF1
D	642	SER	-	expression tag	UNP Q9BYF1
D	643	SER	-	expression tag	UNP Q9BYF1
D	644	ALA	-	expression tag	UNP Q9BYF1
D	645	TRP	-	expression tag	UNP Q9BYF1
D	646	SER	-	expression tag	UNP Q9BYF1
D	647	HIS	-	expression tag	UNP Q9BYF1
D	648	PRO	-	expression tag	UNP Q9BYF1
D	649	GLN	-	expression tag	UNP Q9BYF1
D	650	PHE	-	expression tag	UNP Q9BYF1
D	651	GLU	-	expression tag	UNP Q9BYF1
D	652	LYS	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	251	Total	C	N	O	S	0	0
			1972	1259	330	373	10		

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	initiating methionine	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	GLY	-	expression tag	UNP P0DTC2
A	-26	ILE	-	expression tag	UNP P0DTC2
A	-25	LEU	-	expression tag	UNP P0DTC2
A	-24	PRO	-	expression tag	UNP P0DTC2
A	-23	SER	-	expression tag	UNP P0DTC2
A	-22	PRO	-	expression tag	UNP P0DTC2
A	-21	GLY	-	expression tag	UNP P0DTC2
A	-20	MET	-	expression tag	UNP P0DTC2
A	-19	PRO	-	expression tag	UNP P0DTC2
A	-18	ALA	-	expression tag	UNP P0DTC2
A	-17	LEU	-	expression tag	UNP P0DTC2
A	-16	LEU	-	expression tag	UNP P0DTC2
A	-15	SER	-	expression tag	UNP P0DTC2
A	-14	LEU	-	expression tag	UNP P0DTC2
A	-13	VAL	-	expression tag	UNP P0DTC2
A	-12	SER	-	expression tag	UNP P0DTC2
A	-11	LEU	-	expression tag	UNP P0DTC2
A	-10	LEU	-	expression tag	UNP P0DTC2
A	-9	SER	-	expression tag	UNP P0DTC2
A	-8	VAL	-	expression tag	UNP P0DTC2
A	-7	LEU	-	expression tag	UNP P0DTC2
A	-6	LEU	-	expression tag	UNP P0DTC2
A	-5	MET	-	expression tag	UNP P0DTC2
A	-4	GLY	-	expression tag	UNP P0DTC2
A	-3	CYS	-	expression tag	UNP P0DTC2
A	-2	VAL	-	expression tag	UNP P0DTC2
A	-1	ALA	-	expression tag	UNP P0DTC2
A	0	GLU	-	expression tag	UNP P0DTC2
A	1	THR	-	expression tag	UNP P0DTC2
A	2	GLY	-	expression tag	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	453	PHE	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	692	VAL	ILE	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	SER	-	expression tag	UNP P0DTC2
A	1210	GLY	-	expression tag	UNP P0DTC2
A	1211	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1212	GLU	-	expression tag	UNP P0DTC2
A	1213	ASN	-	expression tag	UNP P0DTC2
A	1214	LEU	-	expression tag	UNP P0DTC2
A	1215	TYR	-	expression tag	UNP P0DTC2
A	1216	PHE	-	expression tag	UNP P0DTC2
A	1217	GLN	-	expression tag	UNP P0DTC2
A	1218	GLY	-	expression tag	UNP P0DTC2
A	1219	GLY	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	TYR	-	expression tag	UNP P0DTC2
A	1225	ILE	-	expression tag	UNP P0DTC2
A	1226	PRO	-	expression tag	UNP P0DTC2
A	1227	GLU	-	expression tag	UNP P0DTC2
A	1228	ALA	-	expression tag	UNP P0DTC2
A	1229	PRO	-	expression tag	UNP P0DTC2
A	1230	ARG	-	expression tag	UNP P0DTC2
A	1231	ASP	-	expression tag	UNP P0DTC2
A	1232	GLY	-	expression tag	UNP P0DTC2
A	1233	GLN	-	expression tag	UNP P0DTC2
A	1234	ALA	-	expression tag	UNP P0DTC2
A	1235	TYR	-	expression tag	UNP P0DTC2
A	1236	VAL	-	expression tag	UNP P0DTC2
A	1237	ARG	-	expression tag	UNP P0DTC2
A	1238	LYS	-	expression tag	UNP P0DTC2
A	1239	ASP	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	TRP	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	LEU	-	expression tag	UNP P0DTC2
A	1246	SER	-	expression tag	UNP P0DTC2
A	1247	THR	-	expression tag	UNP P0DTC2
A	1248	PHE	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	GLY	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2

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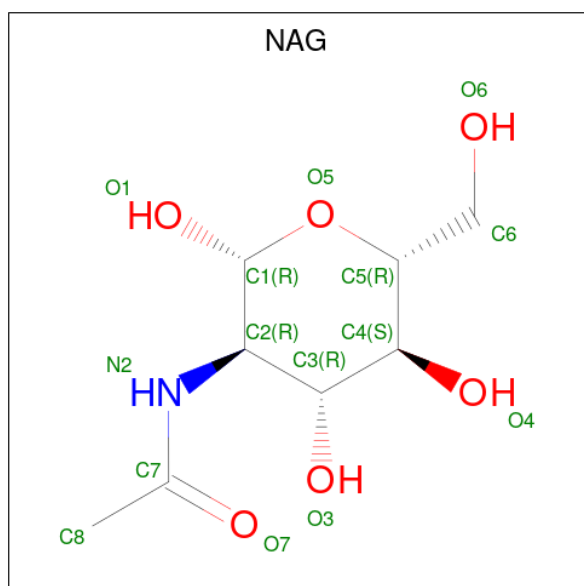
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Chain	Residue	Modelled	Actual	Comment	Reference
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
3	D	1	Total Zn 1 1	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

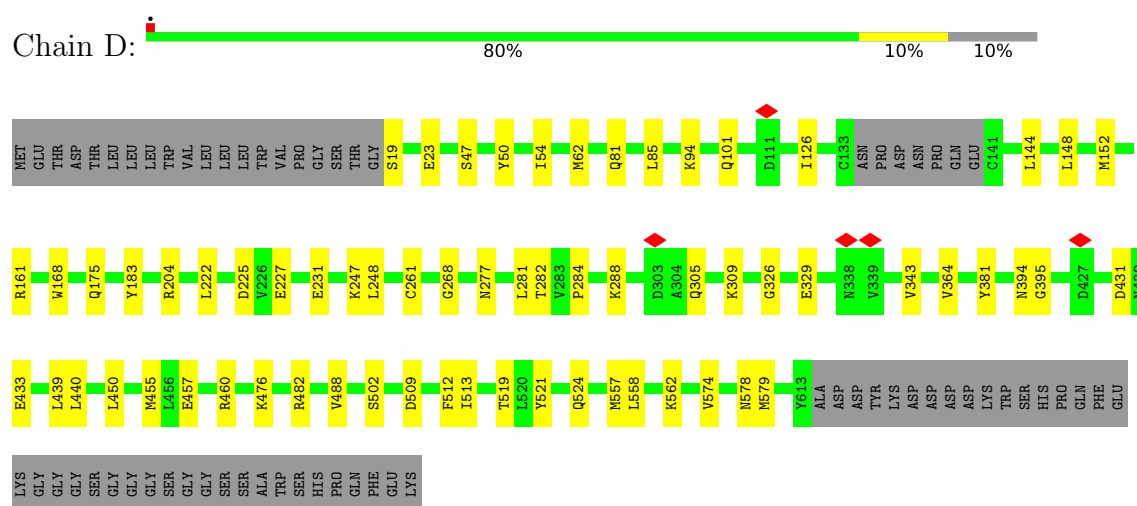


Mol	Chain	Residues	Atoms	AltConf
4	D	1	Total C N O 14 8 1 5	0
4	D	1	Total C N O 14 8 1 5	0
4	D	1	Total C N O 14 8 1 5	0
4	D	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0

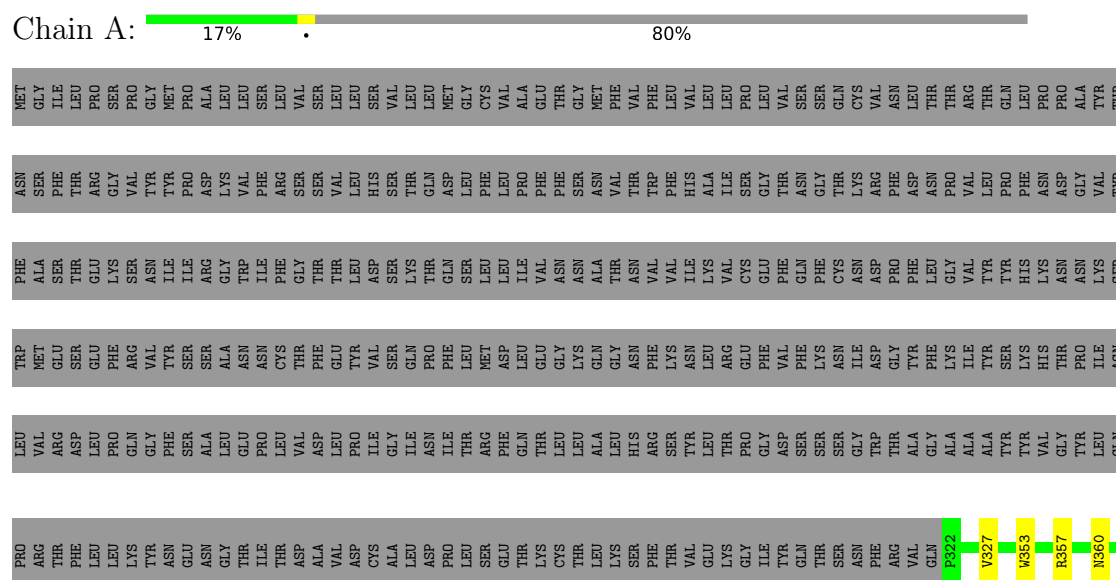
3 Residue-property plots

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: Angiotensin-converting enzyme 2



• Molecule 2: Spike glycoprotein



ARG	VAL	THR	PRO	ILE	SER	LEU	PHE	GLY	MET	SER	GLN	GLN	S366
LYS	ASN	ASP	HIS	THR	LEU	LEU	ILE	LEU	LEU	THR	GLN	GLN	S370
GLY	ILE	ASN	GLY	GLY	SER	ALA	ASP	GLY	LEU	GLY	PHE	PHE	N370
GLY	GLN	THR	VAL	ARG	THR	THR	ASP	CYS	GLY	SER	SER	GLY	S371
TRP	GLU	PHE	VAL	GLN	ALA	ILE	LEU	THR	ALA	VAL	ASP	ASP	A372
VAL	ILE	SER	PHE	GLN	SER	SER	PHE	LEU	ASN	PHE	ILE	ILE	S383
LEU	ASP	GLY	HIS	LEU	ALA	SER	ASN	ASN	SER	GLN	ALA	ALA	K386
LEU	ARG	ASN	VAL	GLN	GLY	TRP	VAL	VAL	VAL	THR	THR	THR	L387
SER	LEU	CYS	THR	THR	LEU	THR	THR	THR	TYR	ALA	THR	THR	
THR	ASN	ASP	VAL	VAL	LEU	PHE	LEU	THR	SER	GLY	THR	D574	
LEU	VAL	VAL	PRO	THR	GLN	GLY	ALA	ALA	ASN	CYS	GLY	GLY	L390
ALA	ALA	ILE	GLN	GLN	ASP	ALA	ASP	ILE	ASN	LEU	C890	C890	
HIS	LYS	GLY	ALA	GLN	VAL	GLY	ALA	ALA	SER	ILE	SER	SER	F392
HIS	ASN	ILE	GLU	LEU	VAL	ALA	PHE	VAL	ILE	GLY	PHE	PHE	
HIS	LEU	VAL	LYS	ILE	ASN	ALA	GLY	GLU	ALA	ALA	GLY	GLY	Y396
HIS	ASN	ASN	ASN	ARG	GLN	LEU	ILE	GLN	ILE	GLU	GLY	GLY	
HIS	GLU	ASN	PHE	ALA	ASN	GLN	LYS	ASP	PRO	HIS	VAL	VAL	E406
	SER	THR	THR	ALA	ALA	ILE	GLN	GLN	THR	VAL	SER	SER	V407
	LEU	VAL	THR	GLU	GLN	PRO	TYR	ARG	ASN	ASN	VAL	VAL	R408
	ILE	TYR	ALA	ILE	ALA	ALA	GLY	THR	PHE	ASN	ILE	ILE	
	ASP	ASP	PRO	ARG	LEU	ALA	ASP	GLY	THR	SER	THR	THR	Q414
	LEU	PRO	ALA	ALA	ASN	MET	CYS	GLU	ILE	TYR	PRO	GLY	Y421
	GLN	LEU	ILE	SER	THR	GLN	LEU	PHE	SER	GLU	THR	GLY	
	GLU	GLN	CYS	ALA	LEU	MET	GLY	ASP	VAL	CYS	THR	THR	D442
	LEU	PRO	HIS	ASN	VAL	ALA	ASP	ALA	THR	ASP	ASN	ASN	
	GLY	LEU	HIS	LEU	VAL	ALA	ILE	GLN	THR	ILE	THR	THR	N448
	LYS	GLU	GLY	ALA	GLN	ARG	ALA	VAL	GLU	PRO	SER	SER	
	TYR	ASP	LYS	ALA	LEU	PHE	ALA	LYS	ILE	ILE	GLY	GLY	R457
	GLU	SER	ALA	THR	SER	ASN	ARG	GLN	PRO	ALA	VAL	VAL	
	GLN	PHE	HIS	LYS	SER	GLY	ASP	ILE	VAL	GLY	ALA	ALA	R466
	SER	LYS	PHE	MET	ASN	ILE	LEU	TYR	VAL	ILE	VAL	VAL	
	GLY	GLU	PRO	GLU	PHE	GLY	ILE	LYS	SER	ILE	VAL	VAL	F490
	ARG	GLU	PRO	GLU	GLY	VAL	CYS	THR	MET	CYS	LEU	LEU	
	GLU	LEU	GLU	CYS	ALA	THR	ALA	PRO	THR	ALA	TYR	TYR	Q493
	ASN	ASP	VAL	VAL	ILE	GLN	GLN	PRO	LYS	SER	GLN	GLN	S494
	LEU	LYS	VAL	LEU	SER	ASN	LYS	ILE	THR	TYR	VAL	VAL	Y495
	TYR	TYR	PHE	GLY	SER	VAL	PHE	LYS	SER	GLN	ASN	ASN	
	PHE	PHE	VAL	GLN	VAL	LEU	ASN	ASP	VAL	THR	THR	THR	L517
	GLN	LYS	SER	SER	LEU	TYR	GLY	PHE	ASP	GLN	CYS	CYS	L519
	GLY	ASN	ASN	LYS	ASN	GLU	LEU	GLY	THR	THR	THR	THR	H519
	GLY	HIS	GLY	ARG	ASP	ASN	THR	GLY	THR	ASN	GLU	GLU	
	GLY	THR	THR	VAL	ILE	GLN	VAL	PHE	MET	SER	VAL	VAL	
	GLY	SER	HIS	ASP	LEU	LYS	LEU	ASN	TYR	PRO	PRO	PRO	T523
	SER	PRO	TRP	PHE	SER	LEU	PRO	PHE	ILE	SER	VAL	VAL	
	GLY	VAL	VAL	GLY	ARG	ILE	PRO	SER	CYS	ARG	ALA	ALA	L533
	TYR	VAL	VAL	GLY	LEU	ILE	LEU	GLN	GLY	ALA	ILE	ILE	
	ILE	ASP	THR	LYS	PRO	ASN	LEU	ILE	ASP	SER	HIS	HIS	N542
	PRO	GLN	GLN	GLY	ASP	GLN	THR	LEU	SER	SER	ALA	ALA	F543
	GLU	GLY	ARG	THR	PRO	PHE	ASP	PRO	THR	VAL	ASP	ASP	
	ALA	ASP	ASN	HIS	GLU	ASN	GLY	ASN	GLU	ALA	GLN	GLN	L546
	PRO	ILE	PHE	LEU	ALA	SER	MET	PRO	CYS	SER	LEU	LEU	
	ARG	SER	TYR	MET	VAL	ALA	ILE	SER	SER	GLN	THR	THR	S855
	ASP	GLY	GLU	SER	GLU	ILE	ALA	LYS	ASN	SER	PRO	PRO	
	GLY	ILE	PRO	PHE	GLN	GLY	GLN	THR	LEU	VAL	THR	THR	LYS
	GLN	ASN	PRO	PRO	ILE	ILE	THR	LYS	LEU	ILE	TRP	TRP	LYS
	ALA	ALA	ILE	GLN	ASP	ILE	SER	ARG	LEU	ALA	ARG	ARG	PHE
	TYR	VAL	THR	ALA	LEU	GLN	THR	ALA	THR	TYR	VAL	VAL	PHE
	VAL	VAL	THR	ALA	LEU	ASP	ALA	SER	GLN	THR	THR	THR	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	393000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	10.960	Depositor
Minimum map value	-7.763	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	388.08, 388.08, 388.08	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.078, 1.078, 1.078	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAG

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	D	0.14	0/4935	0.29	0/6701
2	A	0.14	0/2022	0.31	0/2751
All	All	0.14	0/6957	0.29	0/9452

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4801	0	4585	37	0
2	A	1972	0	1895	15	0
3	D	1	0	0	0	0
4	A	28	0	26	0	0
4	D	56	0	52	0	0
All	All	6858	0	6558	52	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 4.

The worst 5 of 52 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)
2:A:408:ARG:O	2:A:414:GLN:NE2	2.26	0.69
1:D:227:GLU:O	1:D:231:GLU:HG2	1.96	0.65
2:A:442:ASP:O	2:A:448:ASN:ND2	2.31	0.64
1:D:183:TYR:OH	1:D:509:ASP:OD1	2.16	0.64
1:D:557:MET:HE2	1:D:558:LEU:HD12	1.82	0.62

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	D	584/654 (89%)	571 (98%)	13 (2%)	0	100	100
2	A	247/1284 (19%)	237 (96%)	10 (4%)	0	100	100
All	All	831/1938 (43%)	808 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	D	519/573 (91%)	519 (100%)	0	100	100
2	A	220/1112 (20%)	220 (100%)	0	100	100
All	All	739/1685 (44%)	739 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	33	ASN
1	D	42	GLN
1	D	117	ASN
1	D	239	HIS
2	A	370	ASN

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](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	D	903	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	D	902	1	14,14,15	0.22	0	17,19,21	0.47	0
4	NAG	D	905	1	14,14,15	0.23	0	17,19,21	0.46	0
4	NAG	A	1302	2	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	D	904	1	14,14,15	0.26	0	17,19,21	0.41	0
4	NAG	A	1301	2	14,14,15	0.55	0	17,19,21	0.81	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	903	1	-	0/6/23/26	0/1/1/1
4	NAG	D	902	1	-	2/6/23/26	0/1/1/1
4	NAG	D	905	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1302	2	-	2/6/23/26	0/1/1/1
4	NAG	D	904	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1301	NAG	C1-O5-C5	2.54	115.59	112.19

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1302	NAG	C4-C5-C6-O6
4	D	902	NAG	O5-C5-C6-O6
4	D	904	NAG	O5-C5-C6-O6
4	D	904	NAG	C4-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

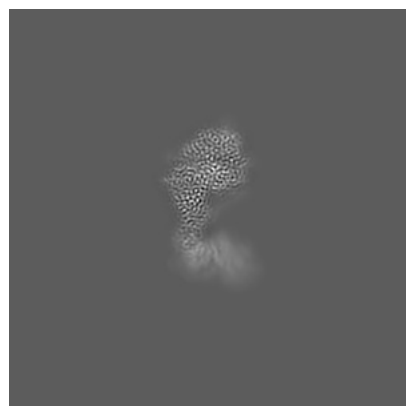
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14228. 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](#)

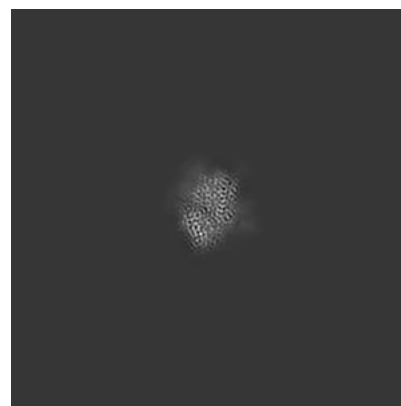
6.1.1 Primary map



X

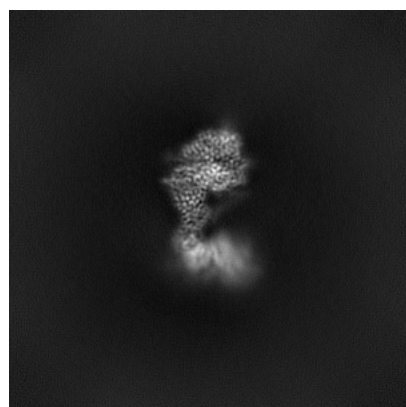


Y

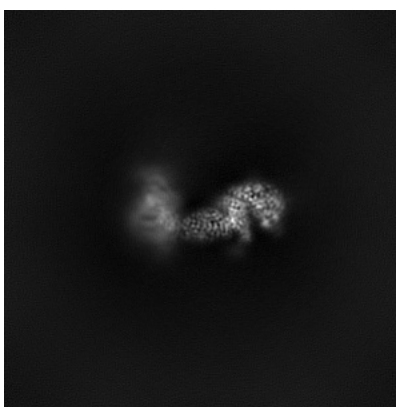


Z

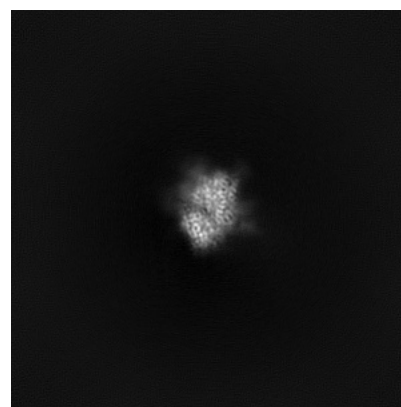
6.1.2 Raw map



X



Y

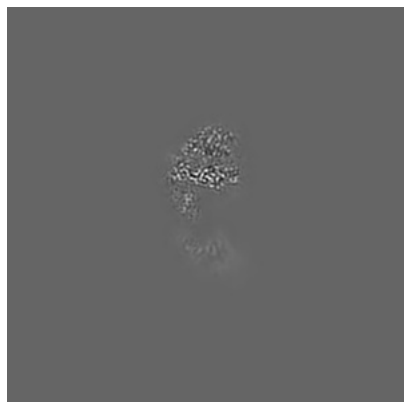


Z

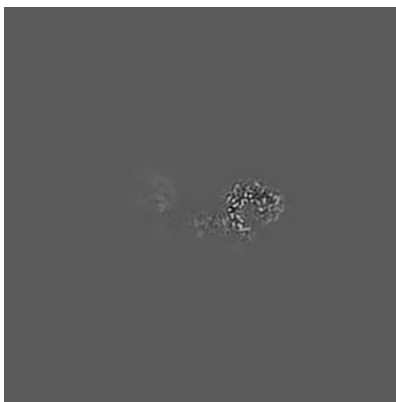
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

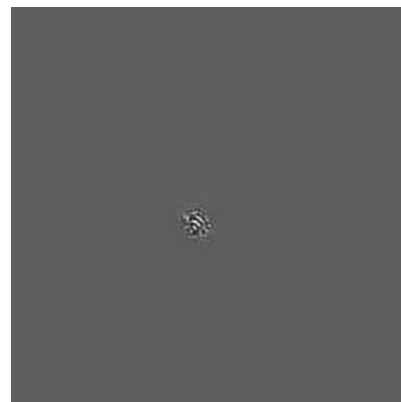
6.2.1 Primary map



X Index: 180

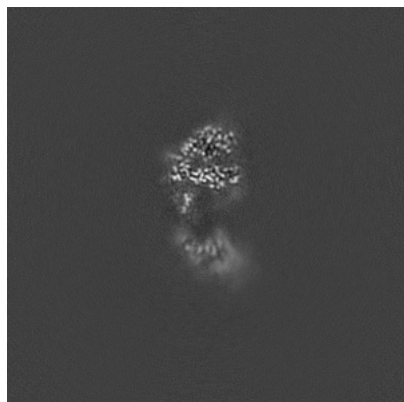


Y Index: 180

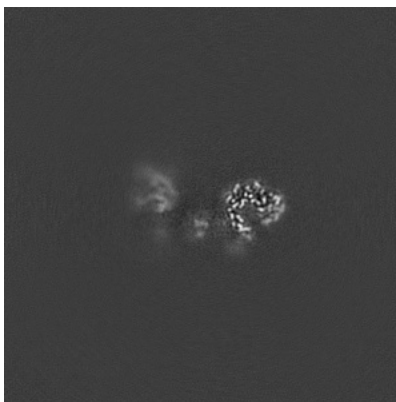


Z Index: 180

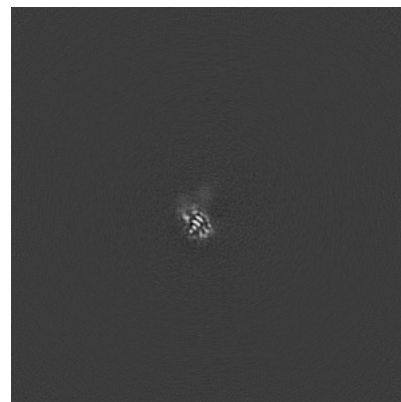
6.2.2 Raw map



X Index: 180



Y Index: 180

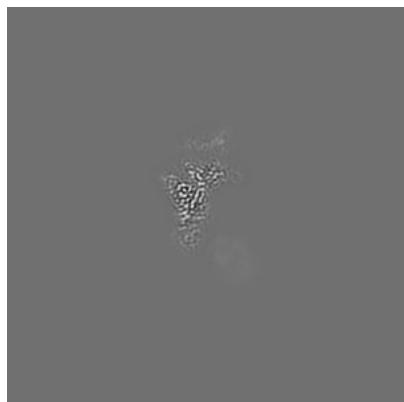


Z Index: 180

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

6.3 Largest variance slices [i](#)

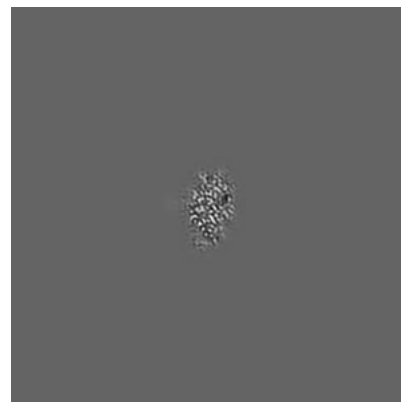
6.3.1 Primary map



X Index: 165

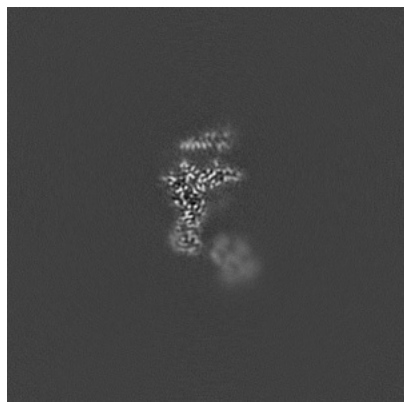


Y Index: 167



Z Index: 209

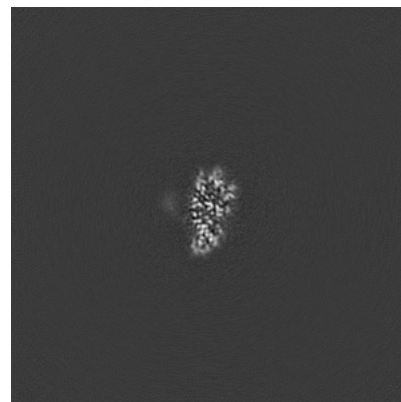
6.3.2 Raw map



X Index: 169



Y Index: 167

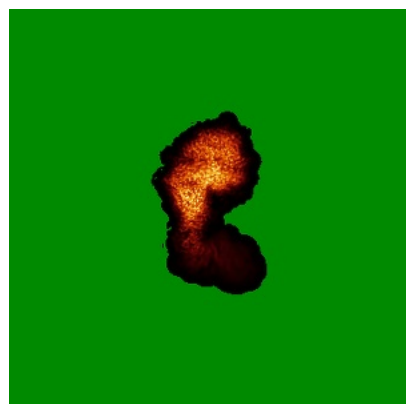


Z Index: 206

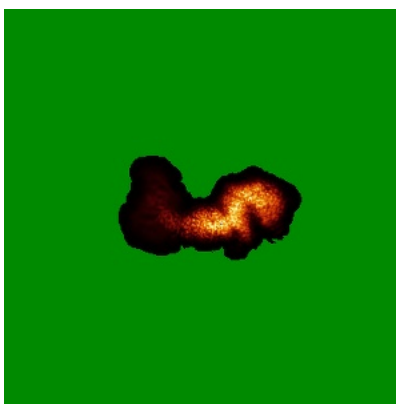
The images above show the largest variance slices of the map in three orthogonal directions.

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

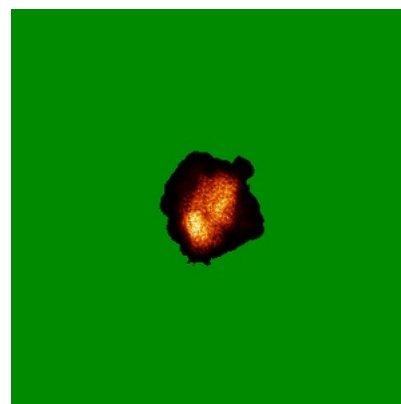
6.4.1 Primary map



X

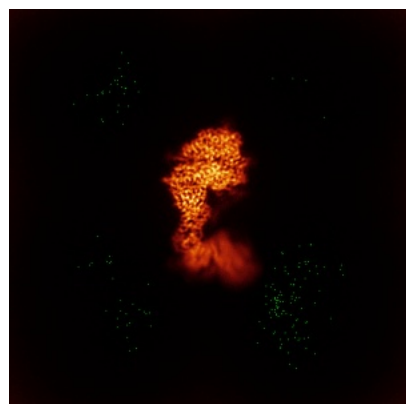


Y

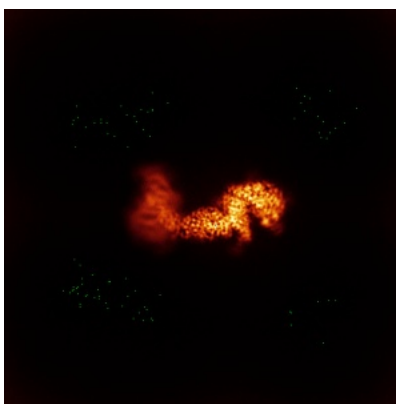


Z

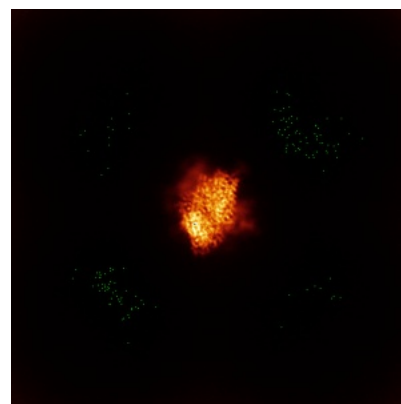
6.4.2 Raw map



X



Y

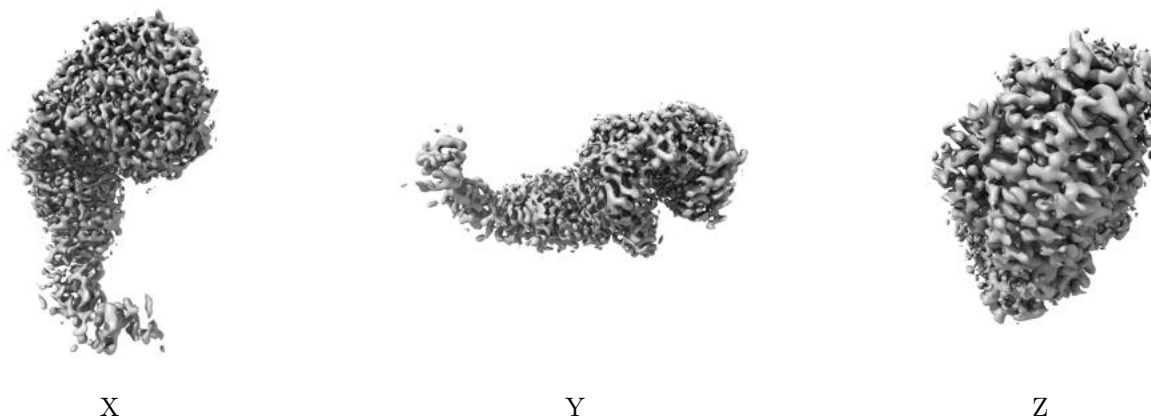


Z

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.

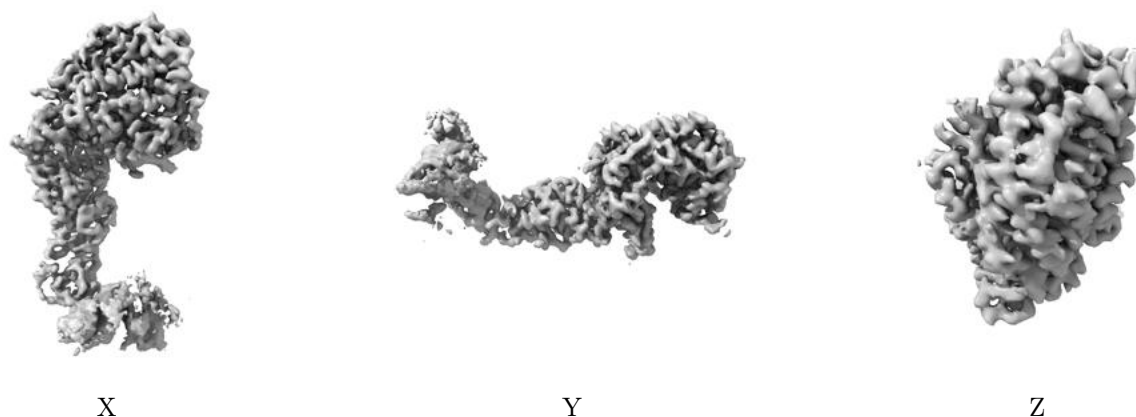
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. 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.

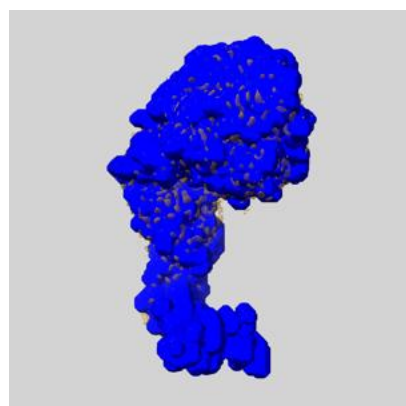
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

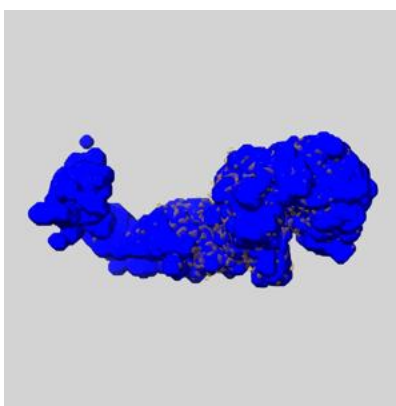
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

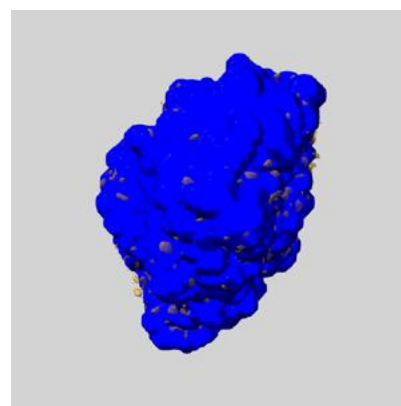
6.6.1 emd_14228_msk_1.map [i](#)



X



Y

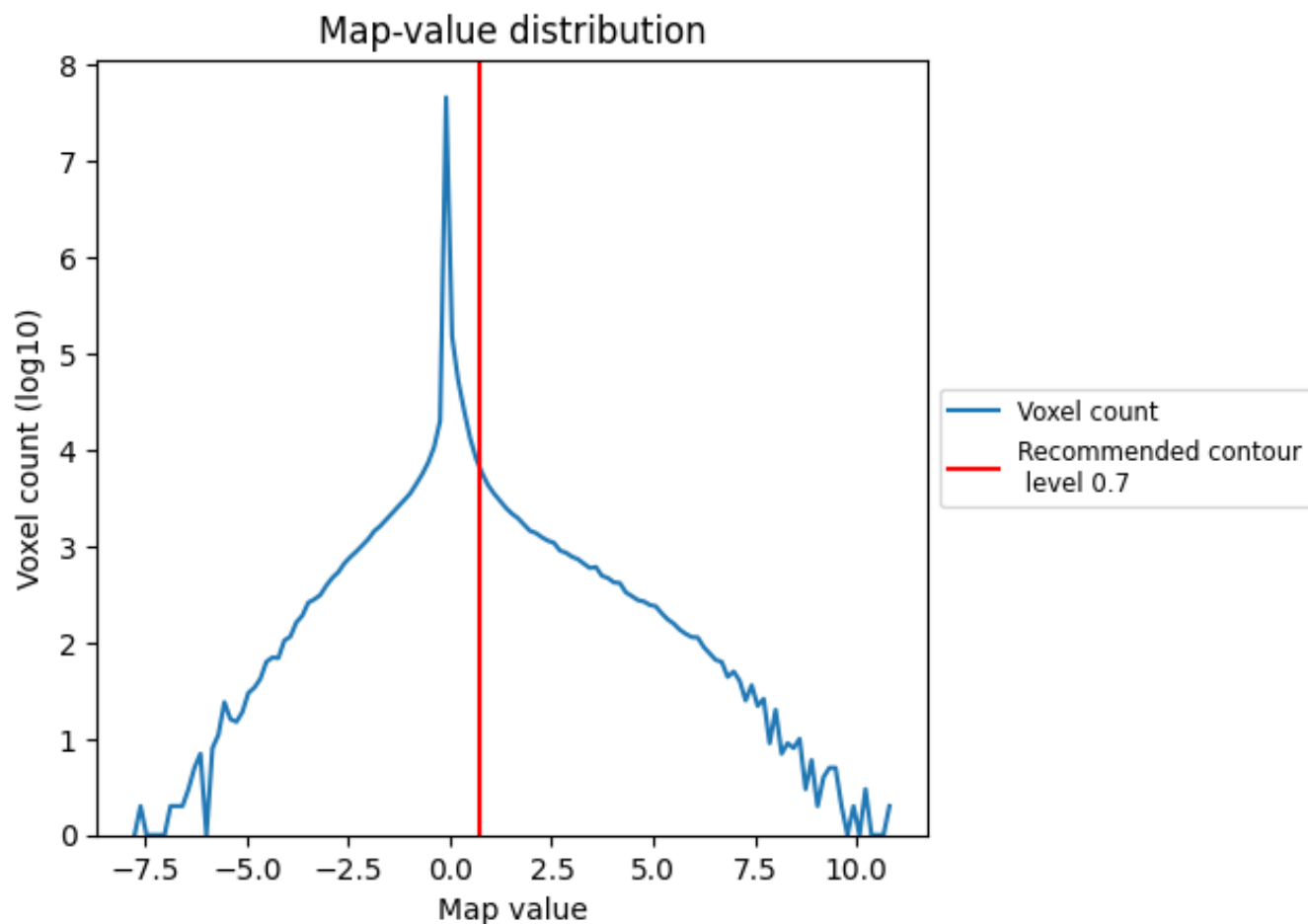


Z

7 Map analysis [i](#)

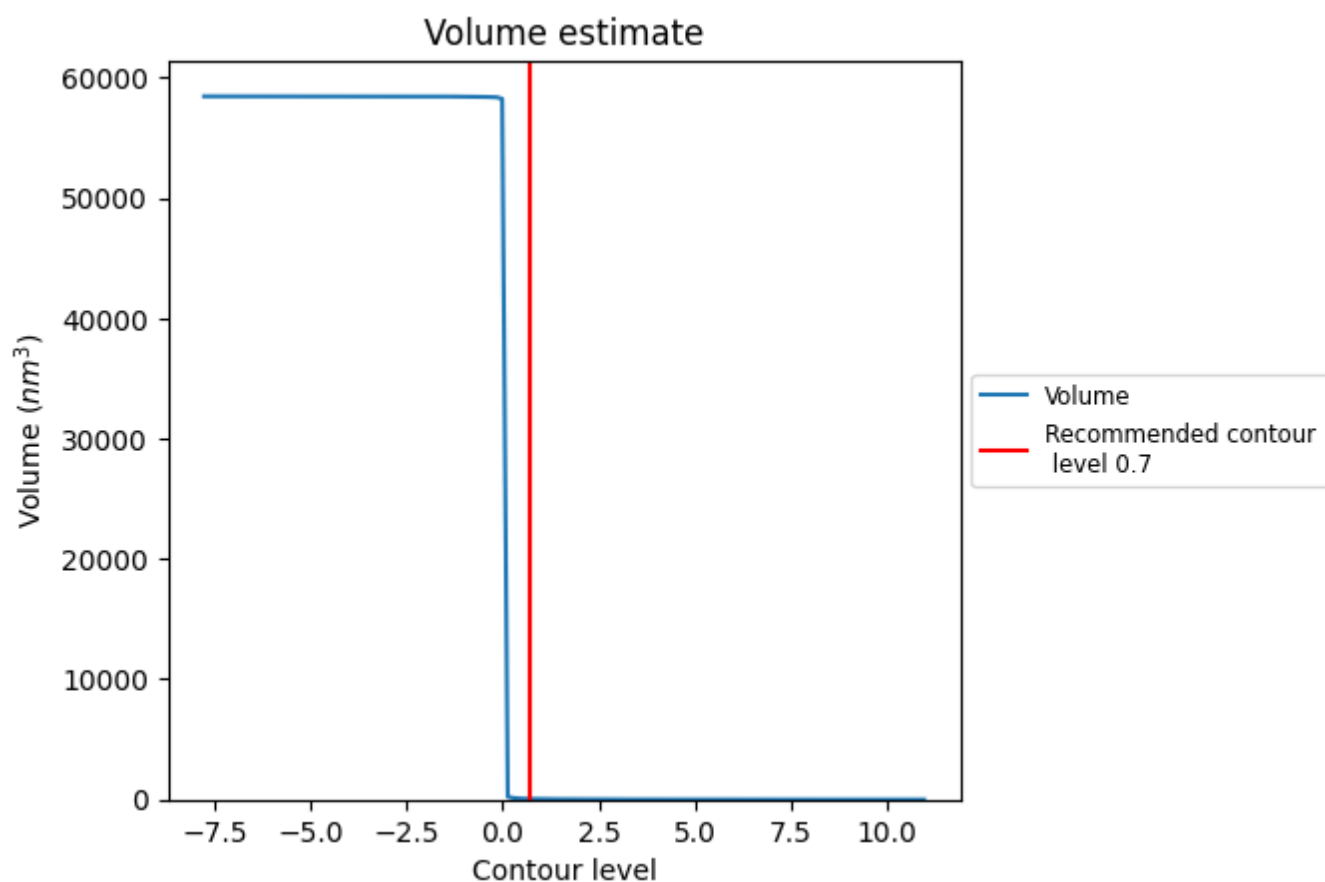
This section contains the results of statistical analysis of the map.

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.

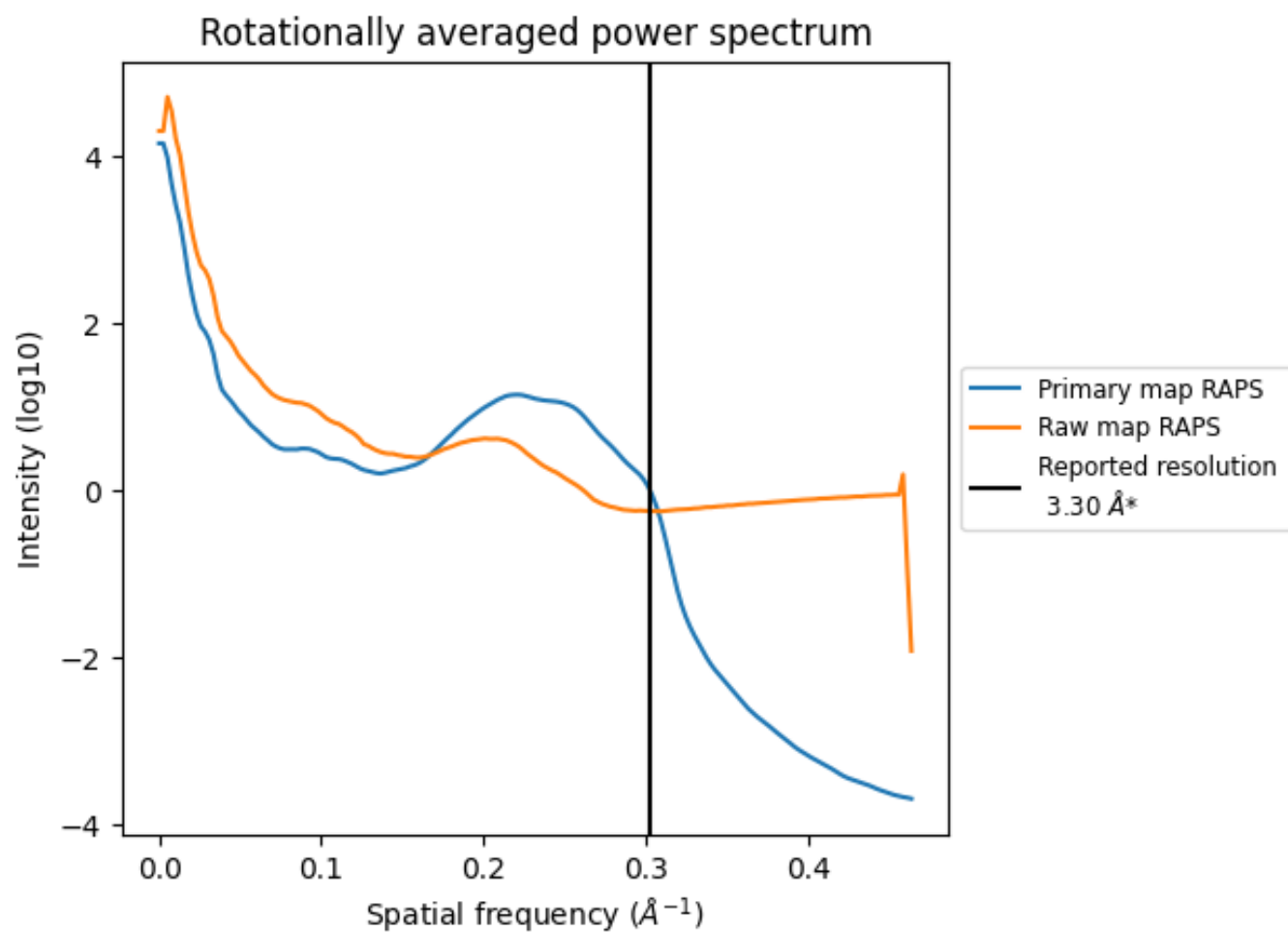
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 58 nm^3 ; this corresponds to an approximate mass of 52 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 ⓘ

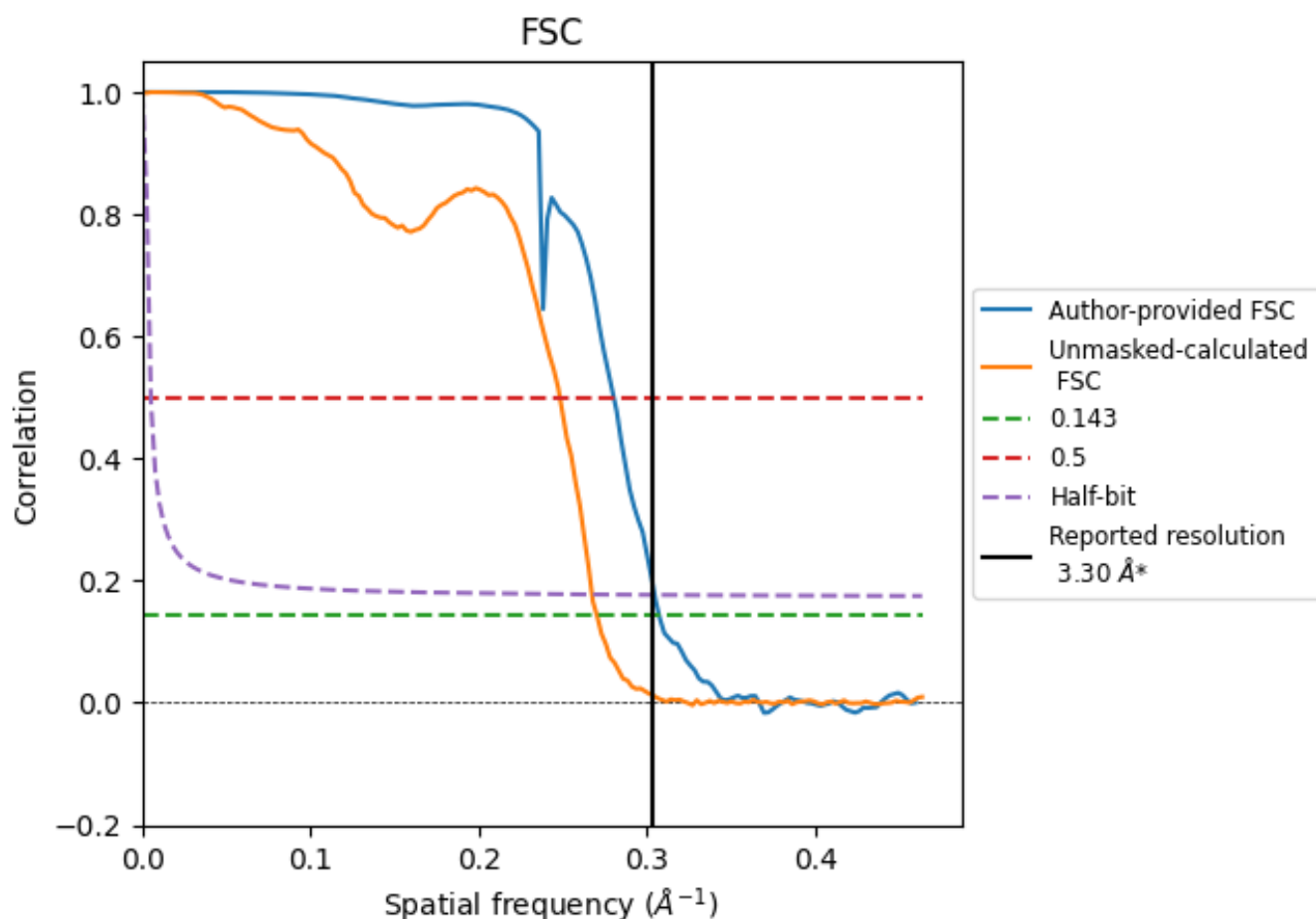


*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

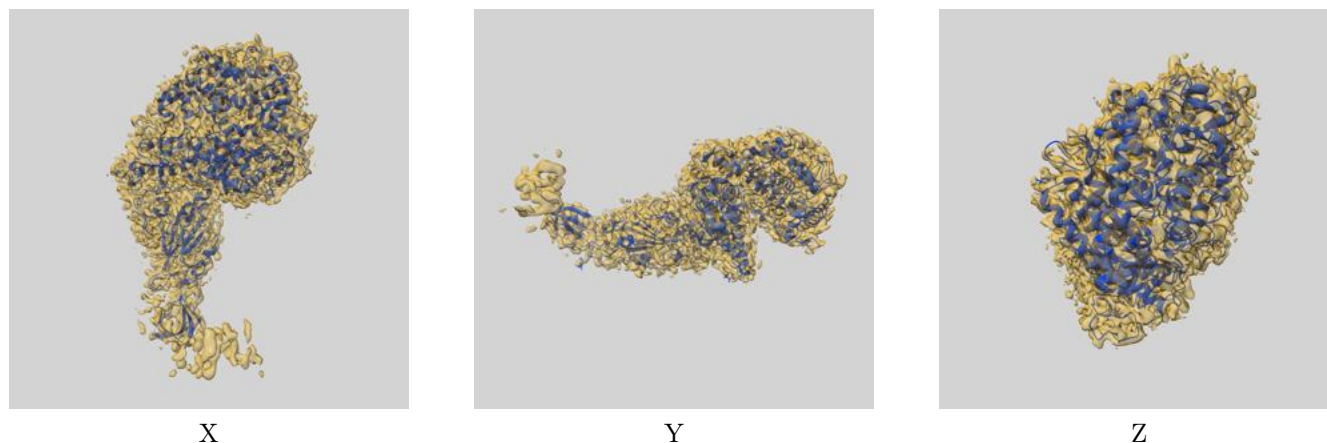
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.25	3.57	3.28
Unmasked-calculated*	3.70	4.03	3.74

*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 3.70 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14228 and PDB model 7R12. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.7 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](#)



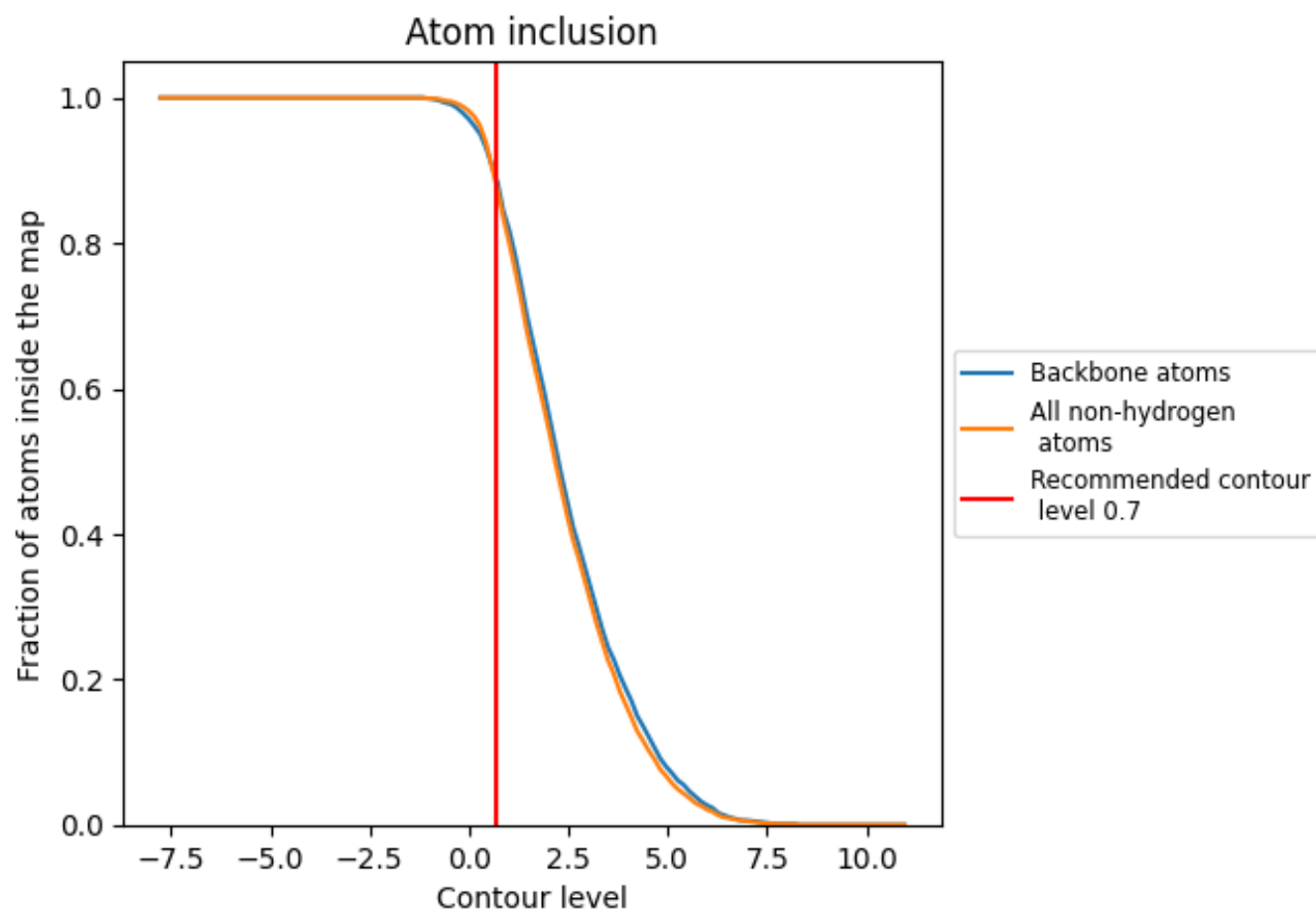
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8780	0.5420
A	0.8670	0.5320
D	0.8820	0.5460

