



## Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 06:33 pm BST

PDB ID : 7R11  
EMDB ID : EMD-14227  
Title : Dissociated S1 domain of Beta 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 : 3.50 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
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) : 2.39

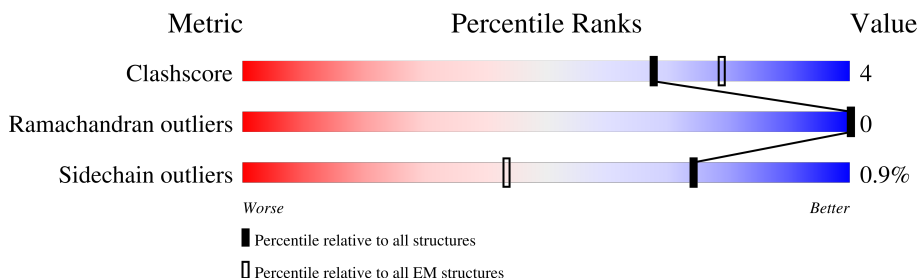
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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  $\geq 3$ , 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 6870 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	587	Total	C	N	O	S	1	0
			4802	3078	795	900	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	250	Total	C	N	O	S	0	0
			1969	1258	329	372	10		

There are 95 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	GLY	-	expression tag	UNP P0DTC2
A	-25	ILE	-	expression tag	UNP P0DTC2
A	-24	LEU	-	expression tag	UNP P0DTC2
A	-23	PRO	-	expression tag	UNP P0DTC2
A	-22	SER	-	expression tag	UNP P0DTC2
A	-21	PRO	-	expression tag	UNP P0DTC2
A	-20	GLY	-	expression tag	UNP P0DTC2
A	-19	MET	-	expression tag	UNP P0DTC2
A	-18	PRO	-	expression tag	UNP P0DTC2
A	-17	ALA	-	expression tag	UNP P0DTC2
A	-16	LEU	-	expression tag	UNP P0DTC2
A	-15	LEU	-	expression tag	UNP P0DTC2
A	-14	SER	-	expression tag	UNP P0DTC2
A	-13	LEU	-	expression tag	UNP P0DTC2
A	-12	VAL	-	expression tag	UNP P0DTC2
A	-11	SER	-	expression tag	UNP P0DTC2
A	-10	LEU	-	expression tag	UNP P0DTC2
A	-9	LEU	-	expression tag	UNP P0DTC2
A	-8	SER	-	expression tag	UNP P0DTC2
A	-7	VAL	-	expression tag	UNP P0DTC2
A	-6	LEU	-	expression tag	UNP P0DTC2
A	-5	LEU	-	expression tag	UNP P0DTC2
A	-4	MET	-	expression tag	UNP P0DTC2
A	-3	GLY	-	expression tag	UNP P0DTC2
A	-2	CYS	-	expression tag	UNP P0DTC2
A	-1	VAL	-	expression tag	UNP P0DTC2
A	0	ALA	-	expression tag	UNP P0DTC2
A	1	GLU	-	expression tag	UNP P0DTC2
A	2	THR	-	expression tag	UNP P0DTC2
A	3	GLY	-	expression tag	UNP P0DTC2
A	21	PHE	LEU	variant	UNP P0DTC2
A	83	ALA	ASP	variant	UNP P0DTC2
A	218	GLY	ASP	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	246	ILE	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	SER	ARG	variant	UNP P0DTC2

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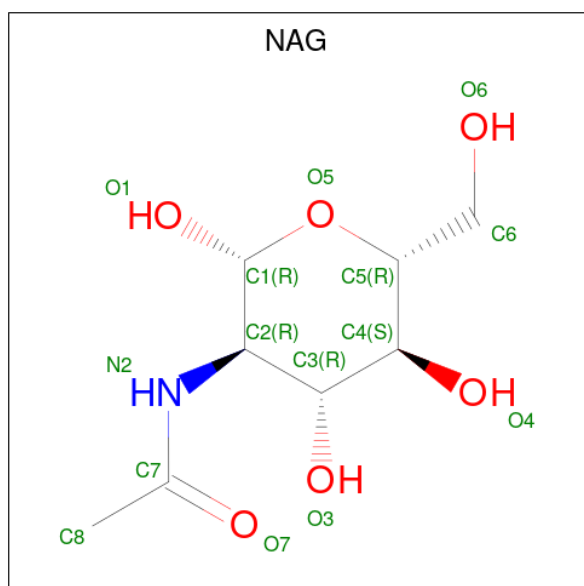
Chain	Residue	Modelled	Actual	Comment	Reference
A	685	SER	ARG	variant	UNP P0DTC2
A	701	VAL	ALA	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	SER	-	expression tag	UNP P0DTC2
A	1210	GLY	-	expression tag	UNP P0DTC2
A	1211	ARG	-	expression tag	UNP P0DTC2
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

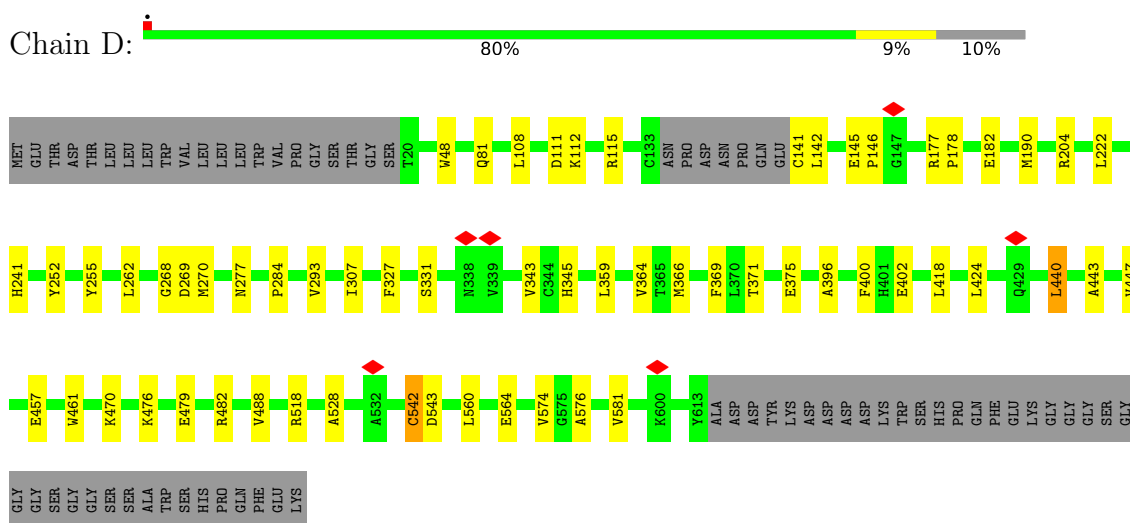
Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total	Zn	0
			1	1	



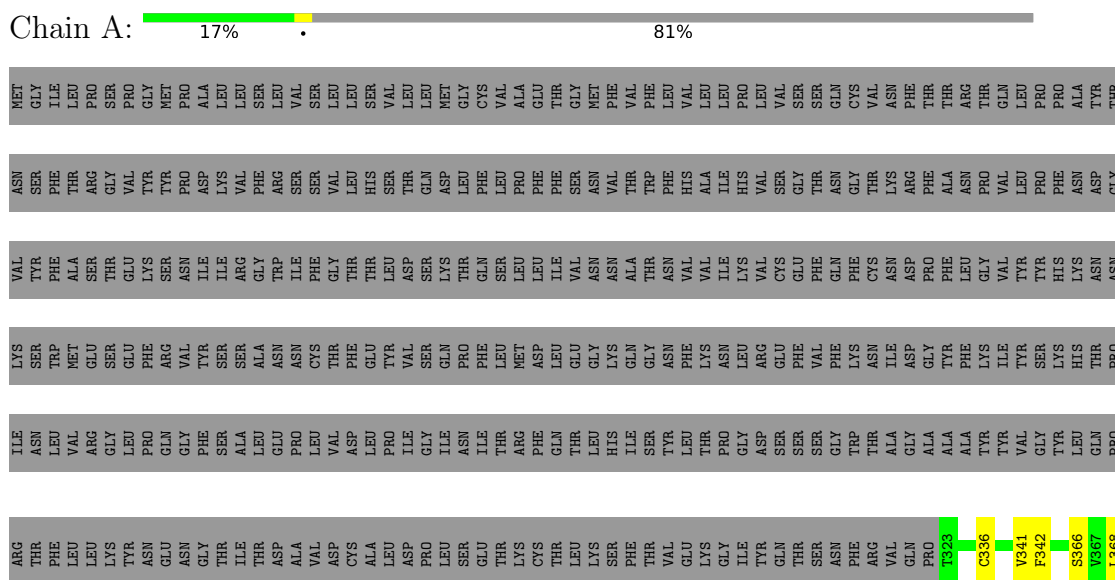
### 3 Residue-property plots

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



[illegible]

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	121000	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	8.079	Depositor
Minimum map value	-5.552	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.5	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	0.27	0/4940	0.43	0/6708
2	A	0.28	0/2019	0.49	0/2748
All	All	0.27	0/6959	0.45	0/9456

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	4802	0	4586	32	0
2	A	1969	0	1890	16	0
3	A	28	0	26	0	0
3	D	70	0	65	0	0
4	D	1	0	0	0	0
All	All	6870	0	6567	48	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.

All (48) 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:536:ASN:HA	2:A:551:VAL:HG13	1.83	0.61
1:D:177:ARG:HB3	1:D:178:PRO:HD3	1.86	0.58
1:D:252:TYR:HB3	1:D:255:TYR:HD2	1.72	0.55
1:D:574:VAL:HG23	1:D:576:ALA:H	1.73	0.52
2:A:396:TYR:HE2	2:A:516:GLU:OE1	1.93	0.52
1:D:560:LEU:HD11	1:D:564:GLU:HG3	1.90	0.52
2:A:431:GLY:HA3	2:A:513:LEU:O	2.10	0.51
1:D:293:VAL:HG22	1:D:366:MET:CE	2.41	0.51
1:D:482:ARG:HG2	1:D:488:VAL:HG22	1.93	0.51
1:D:268:GLY:O	1:D:277:ASN:ND2	2.43	0.50
2:A:439:ASN:O	2:A:443:SER:OG	2.30	0.50
2:A:341:VAL:HG13	2:A:342:PHE:HD1	1.76	0.50
1:D:115:ARG:NH2	1:D:182:GLU:OE2	2.44	0.50
1:D:364:VAL:O	1:D:364:VAL:HG23	2.12	0.49
2:A:382:VAL:HG11	2:A:387:LEU:HD21	1.94	0.49
1:D:402:GLU:HB2	1:D:518:ARG:HG3	1.95	0.49
1:D:528:ALA:HB2	1:D:574:VAL:HG12	1.96	0.47
1:D:141:CYS:SG	1:D:142:LEU:N	2.85	0.47
1:D:343:VAL:HG12	1:D:345:HIS:H	1.79	0.47
2:A:396:TYR:CE2	2:A:516:GLU:OE1	2.68	0.46
2:A:382:VAL:HG11	2:A:387:LEU:CD2	2.46	0.46
2:A:394:ASN:N	2:A:394:ASN:OD1	2.49	0.46
1:D:177:ARG:HH21	1:D:470:LYS:NZ	2.14	0.45
2:A:393:THR:O	2:A:523:THR:OG1	2.33	0.45
2:A:537:LYS:O	2:A:539:VAL:HG13	2.16	0.45
1:D:284:PRO:HB3	1:D:440:LEU:HD23	1.99	0.45
1:D:48:TRP:CZ3	1:D:359:LEU:HB2	2.52	0.45
1:D:269:ASP:OD1	1:D:270:MET:N	2.48	0.44
1:D:371:THR:O	1:D:375:GLU:HG2	2.16	0.44
2:A:401:VAL:HG22	2:A:509:ARG:HG2	1.98	0.44
1:D:108:LEU:HD11	1:D:190:MET:HB2	1.98	0.43
2:A:442:ASP:O	2:A:448:ASN:ND2	2.50	0.43
1:D:457:GLU:OE2	1:D:461:TRP:NE1	2.52	0.43
2:A:428:ASP:N	2:A:428:ASP:OD1	2.49	0.42
1:D:542:CYS:SG	1:D:543:ASP:N	2.92	0.42
2:A:342:PHE:CZ	2:A:368:LEU:HD11	2.55	0.42
1:D:327:PHE:O	1:D:331:SER:OG	2.26	0.42
1:D:418:LEU:HD23	1:D:424:LEU:HD22	2.02	0.42
1:D:241:HIS:NE2	1:D:262:LEU:HD13	2.34	0.42
1:D:145:GLU:HA	1:D:146:PRO:HA	1.75	0.42
1:D:307:ILE:HG23	1:D:369:PHE:HD1	1.85	0.42
1:D:443:ALA:O	1:D:447:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:476:LYS:O	1:D:479:GLU:HG3	2.20	0.41
1:D:111:ASP:OD1	1:D:112:LYS:N	2.53	0.41
1:D:396:ALA:HB3	1:D:400:PHE:CD2	2.55	0.41
1:D:204:ARG:HG2	1:D:222:LEU:HD23	2.03	0.40
2:A:366:SER:O	2:A:370:ASN:OD1	2.38	0.40
1:D:252:TYR:HB3	1:D:255:TYR:CD2	2.55	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	D	584/654 (89%)	564 (97%)	20 (3%)	0	100	100
2	A	246/1284 (19%)	238 (97%)	8 (3%)	0	100	100
All	All	830/1938 (43%)	802 (97%)	28 (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%)	515 (99%)	4 (1%)	79	88
2	A	219/1112 (20%)	216 (99%)	3 (1%)	62	79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	738/1685 (44%)	731 (99%)	7 (1%)	74	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	81	GLN
1	D	440	LEU
1	D	542	CYS
1	D	581	VAL
2	A	336	CYS
2	A	370	ASN
2	A	389	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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
3	NAG	D	706	1	14,14,15	0.38	0	17,19,21	0.58	0
3	NAG	D	701	1	14,14,15	0.29	0	17,19,21	0.42	0
3	NAG	D	705	1	14,14,15	0.21	0	17,19,21	0.37	0
3	NAG	A	1301	2	14,14,15	0.28	0	17,19,21	0.58	0
3	NAG	D	704	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	D	703	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	A	1302	2	14,14,15	0.22	0	17,19,21	0.40	0

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
3	NAG	D	706	1	-	1/6/23/26	0/1/1/1
3	NAG	D	701	1	-	0/6/23/26	0/1/1/1
3	NAG	D	705	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	2	-	1/6/23/26	0/1/1/1
3	NAG	D	704	1	-	2/6/23/26	0/1/1/1
3	NAG	D	703	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	703	NAG	C4-C5-C6-O6
3	D	705	NAG	O5-C5-C6-O6
3	D	704	NAG	O5-C5-C6-O6
3	D	705	NAG	C4-C5-C6-O6
3	D	703	NAG	O5-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	A	1302	NAG	C8-C7-N2-C2
3	A	1302	NAG	O7-C7-N2-C2
3	D	704	NAG	C4-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	D	706	NAG	C3-C2-N2-C7
3	A	1301	NAG	C3-C2-N2-C7



There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

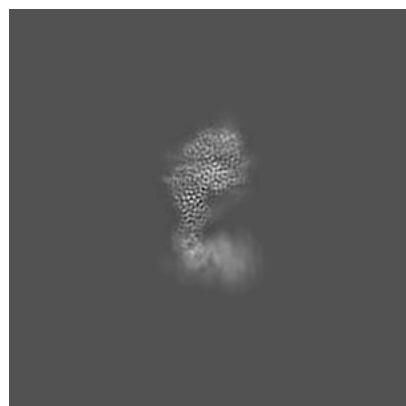
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14227. 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](#)

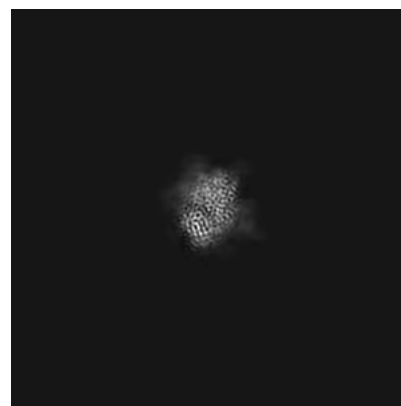
#### 6.1.1 Primary map



X



Y

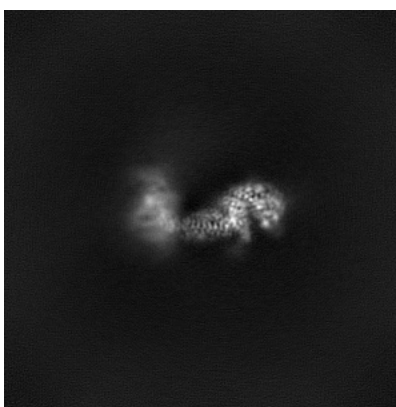


Z

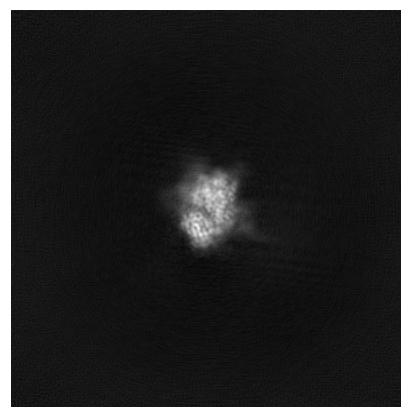
#### 6.1.2 Raw map



X



Y

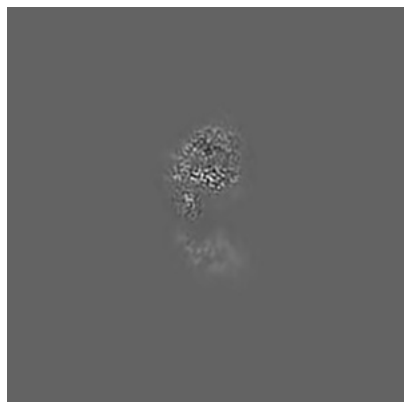


Z

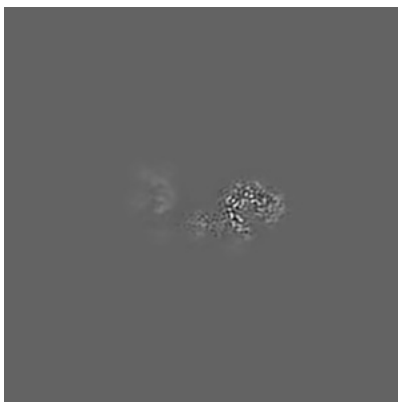
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

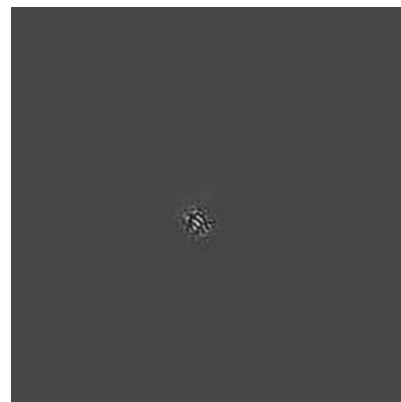
### 6.2.1 Primary map



X Index: 180

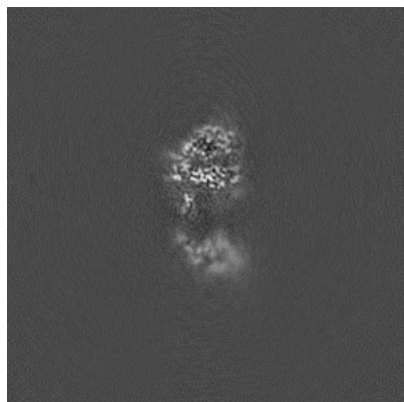


Y Index: 180

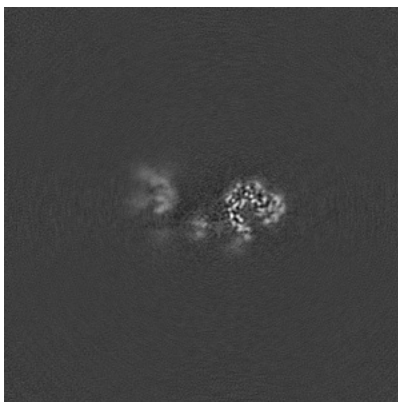


Z Index: 180

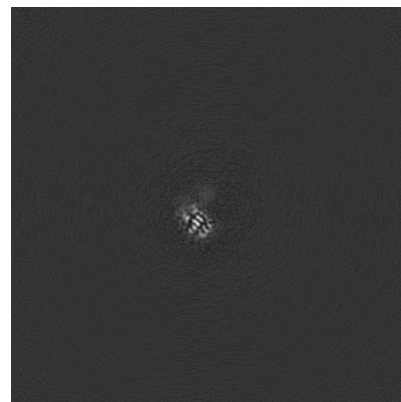
### 6.2.2 Raw map



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](#)

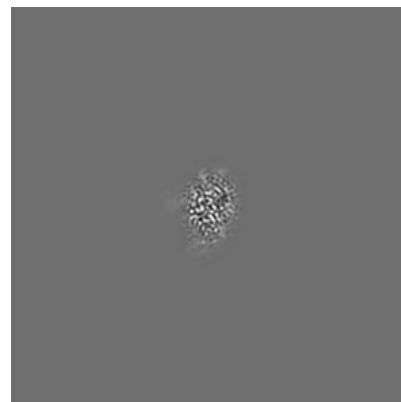
### 6.3.1 Primary map



X Index: 165



Y Index: 167



Z Index: 209

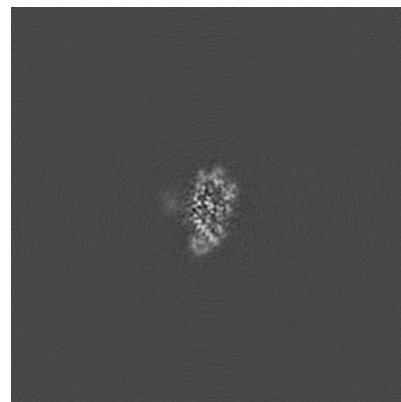
### 6.3.2 Raw map



X Index: 165



Y Index: 167

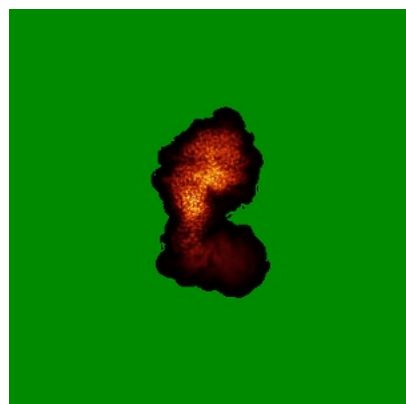


Z Index: 207

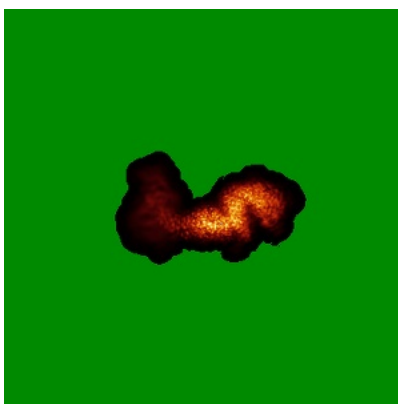
The images above show the largest variance slices of the map in three orthogonal directions.

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

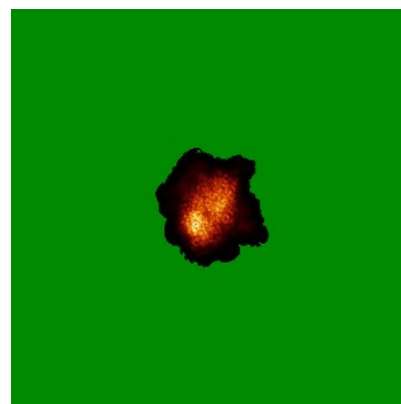
### 6.4.1 Primary map



X

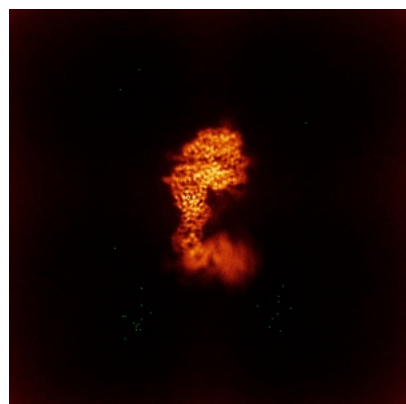


Y

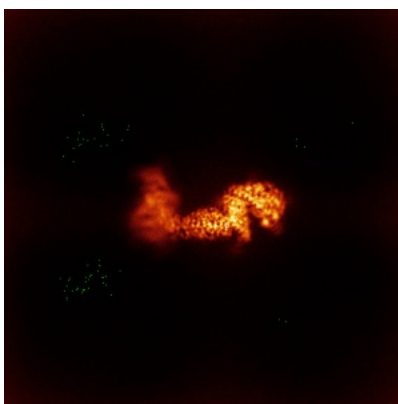


Z

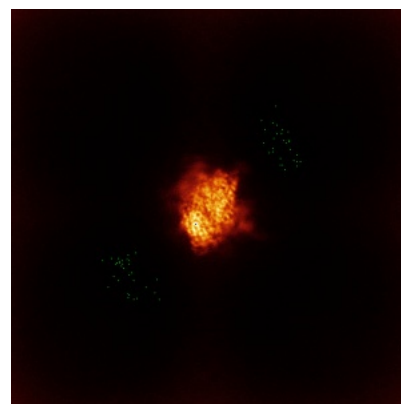
### 6.4.2 Raw map



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.

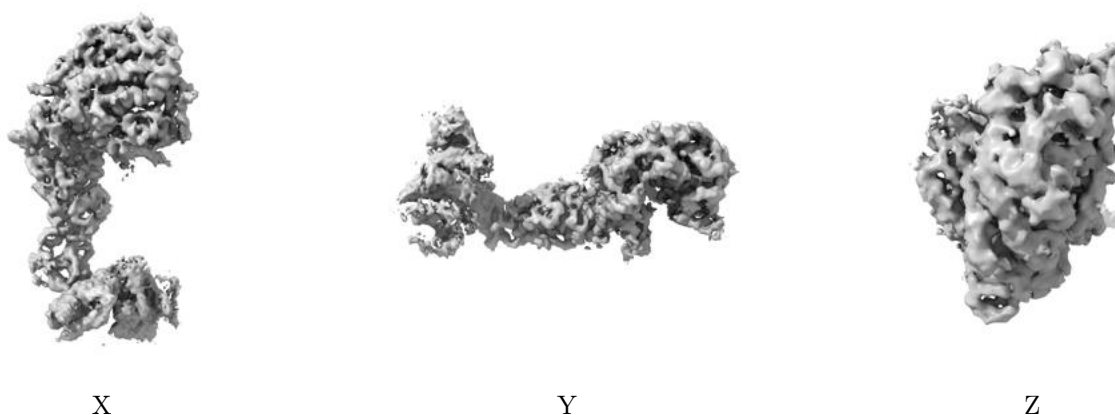
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

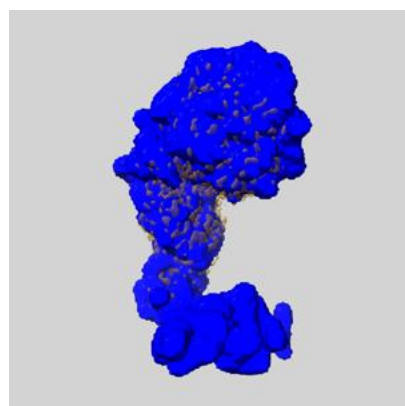
## 6.6 Mask visualisation [i](#)

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

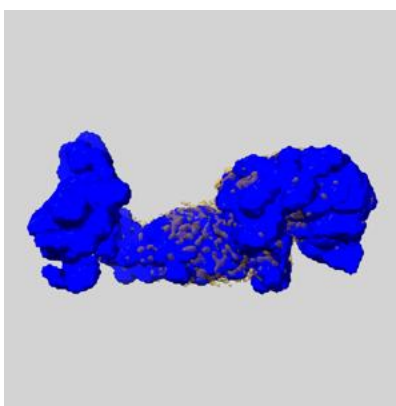
A mask typically either:

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

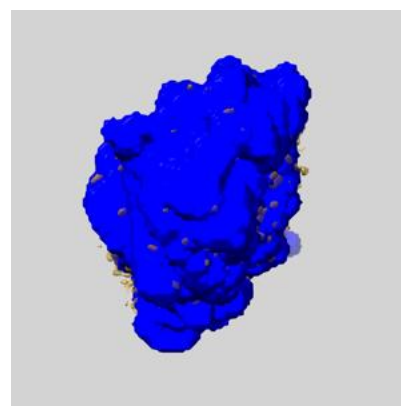
### 6.6.1 emd\_14227\_msk\_1.map [i](#)



X



Y

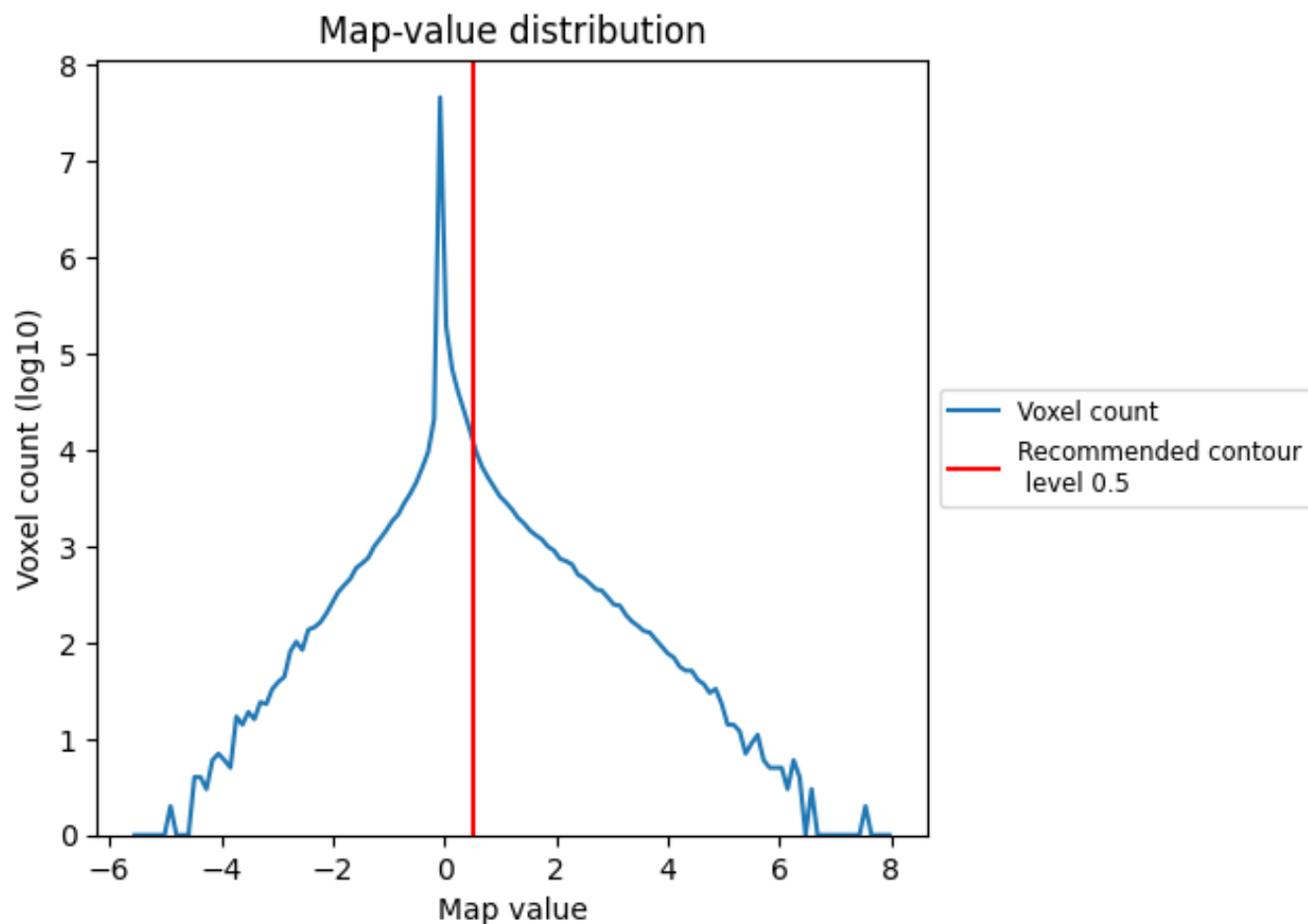


Z

## 7 Map analysis [i](#)

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

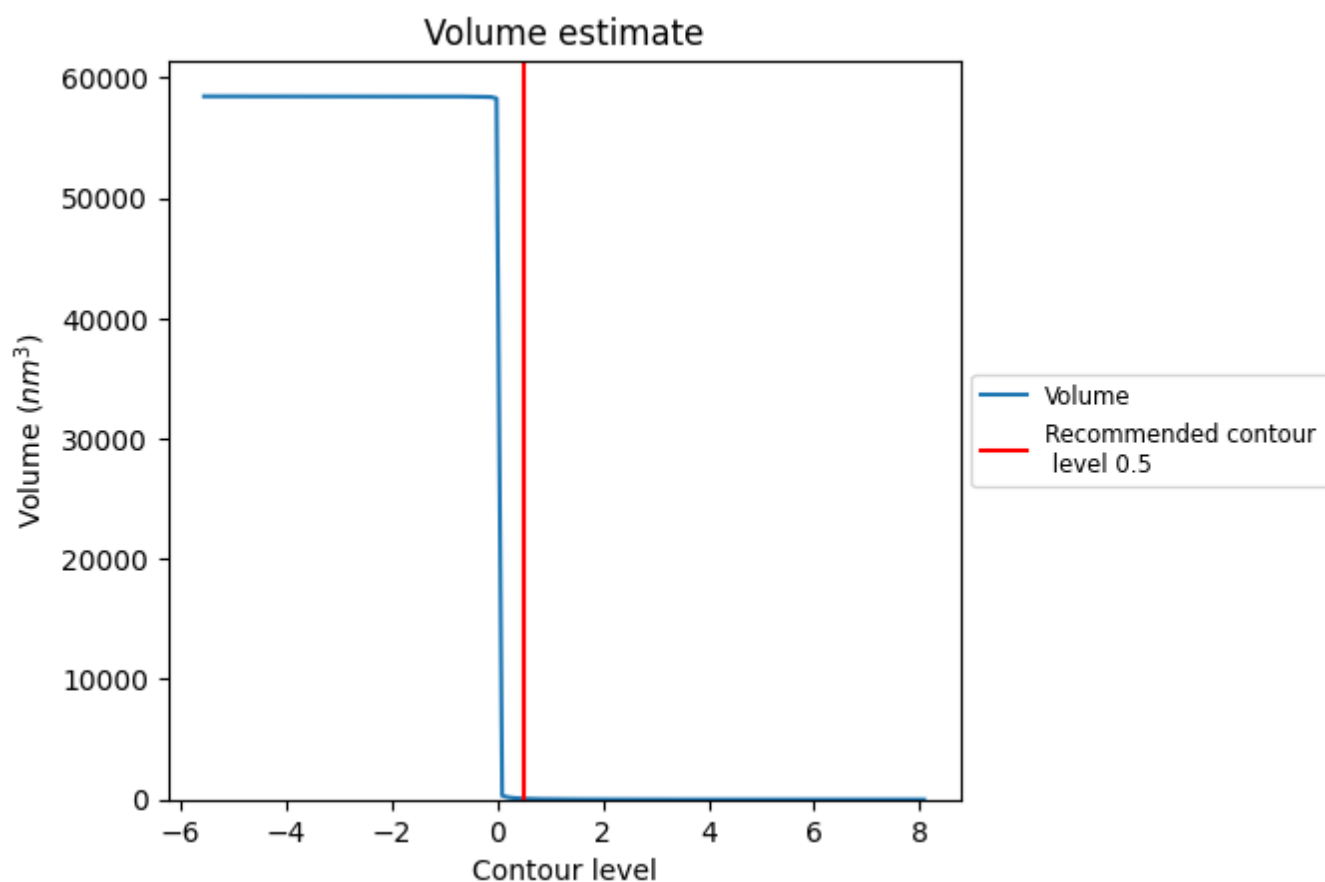
### 7.1 Map-value distribution [i](#)



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.



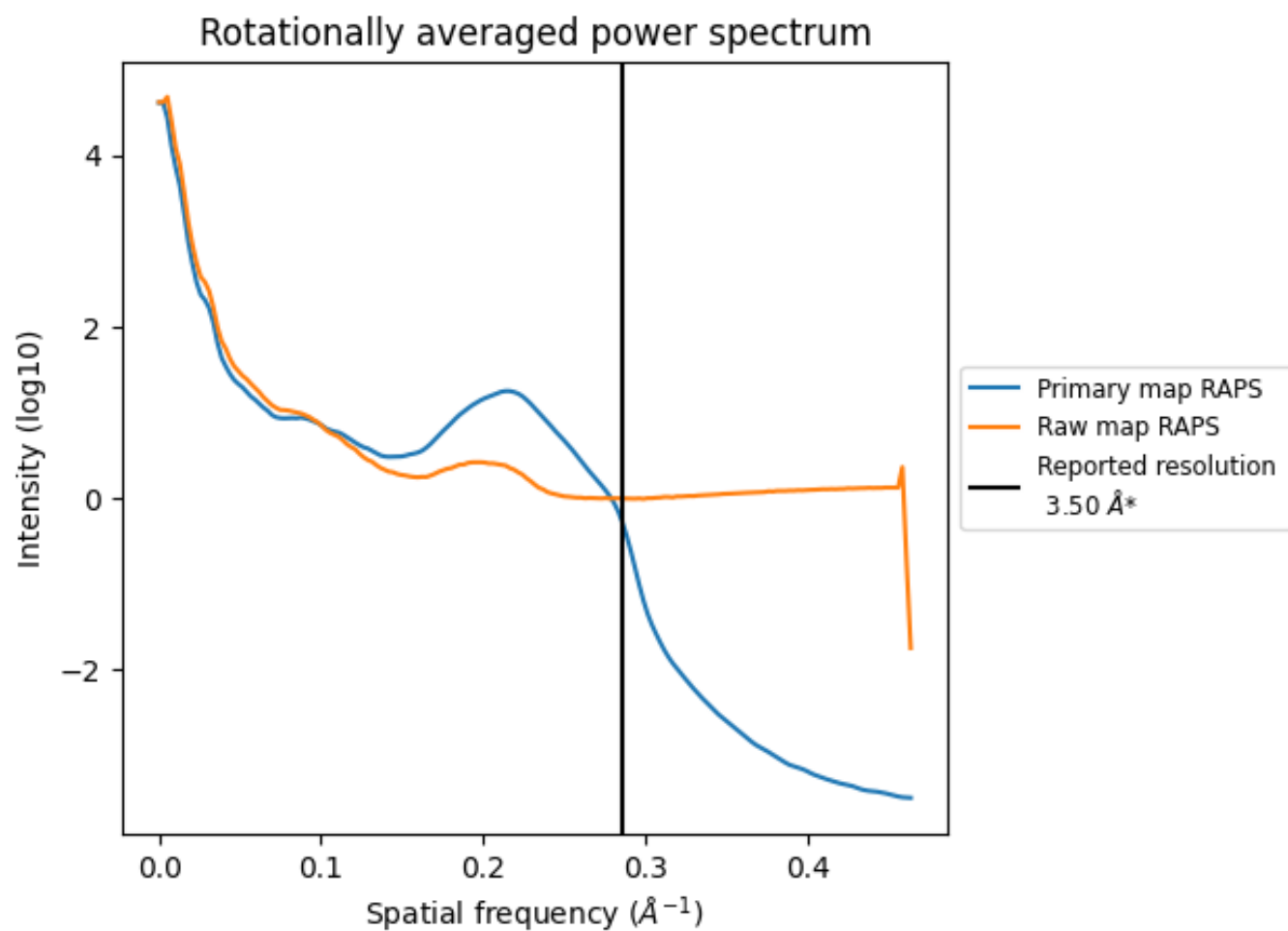
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 75 nm<sup>3</sup>; this corresponds to an approximate mass of 68 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 ⓘ

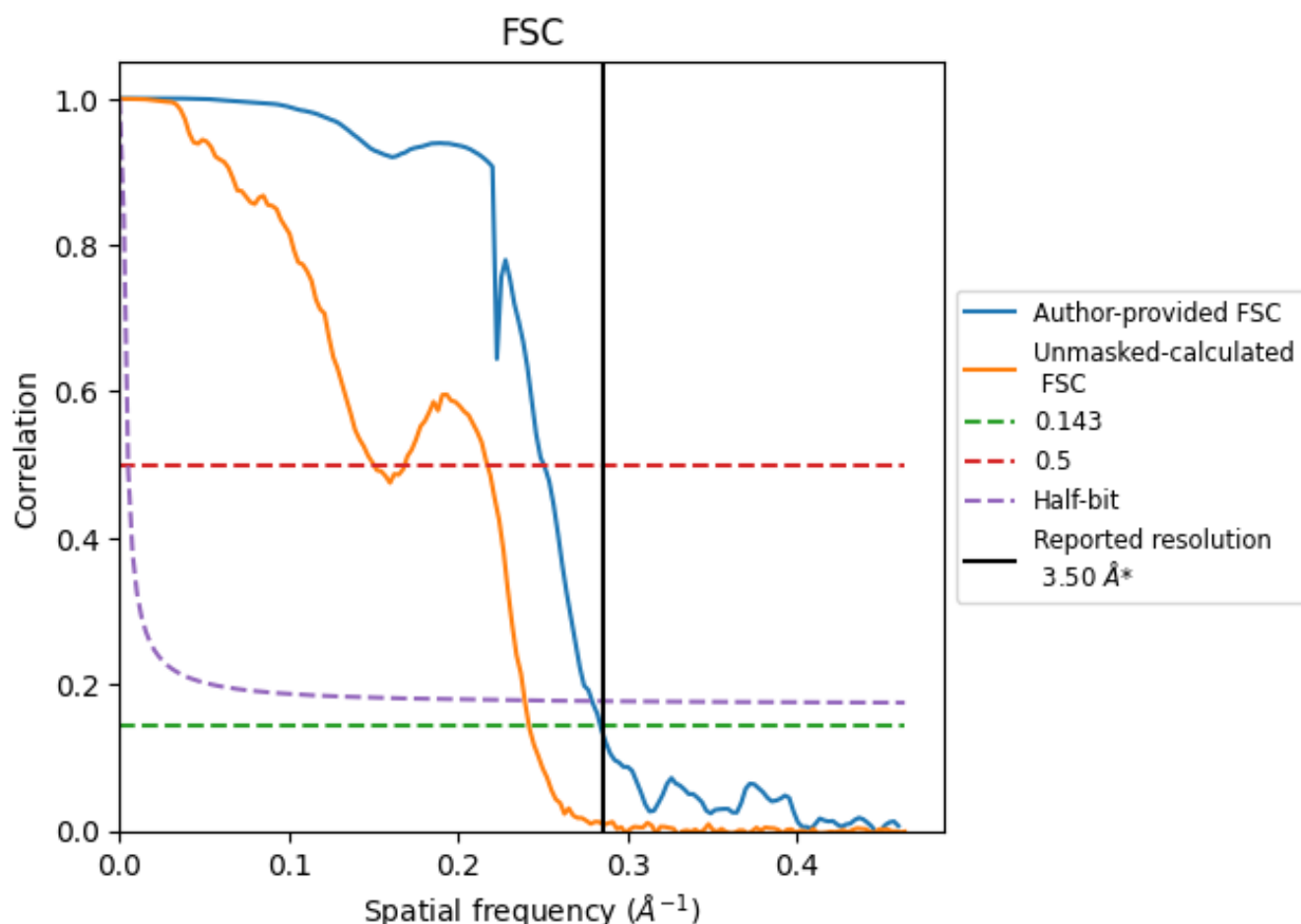


\*Reported resolution corresponds to spatial frequency of  $0.286 \text{ \AA}^{-1}$

## 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 0.286  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

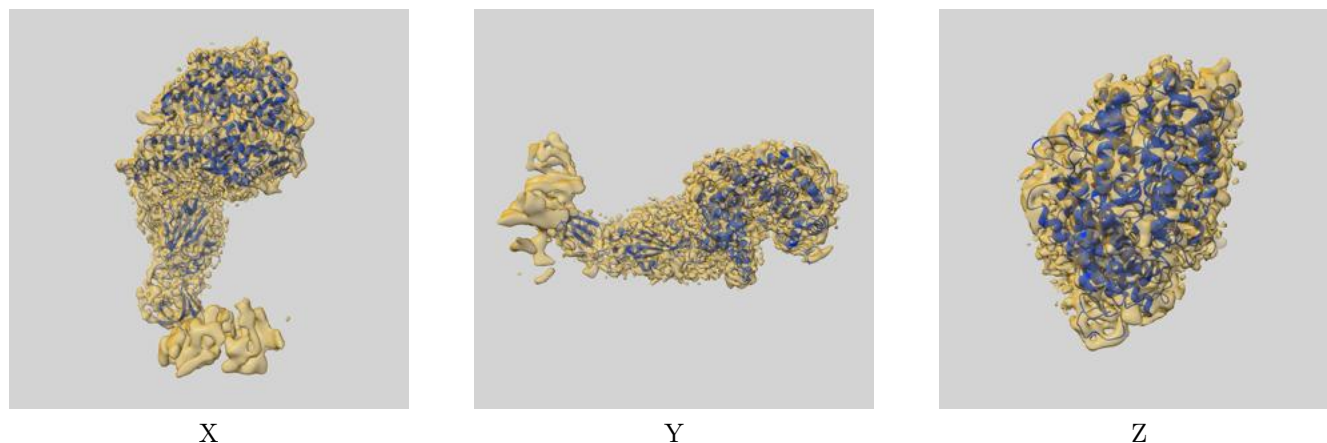
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.52	3.99	3.58
Unmasked-calculated*	4.13	6.66	4.18

\*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 4.13 differs from the reported value 3.5 by more than 10 %

## 9 Map-model fit [i](#)

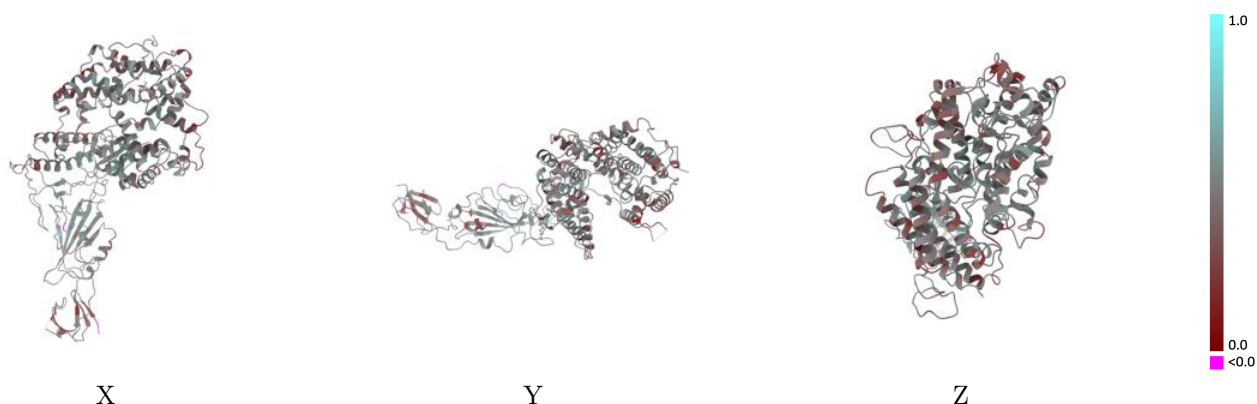
This section contains information regarding the fit between EMDB map EMD-14227 and PDB model 7R11. Per-residue inclusion information can be found in section [3](#) on page [9](#).

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.5 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](#)



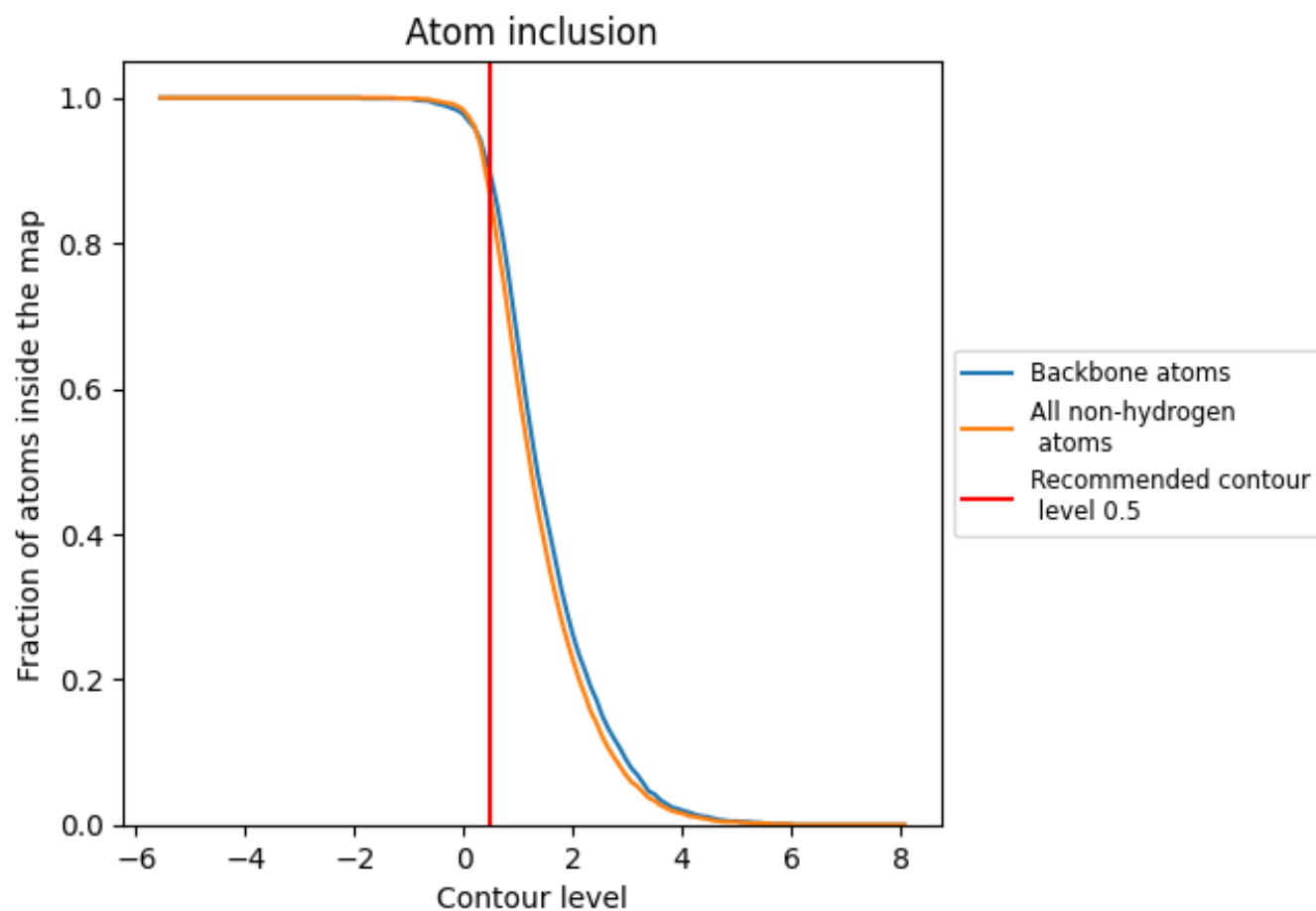
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 86% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8610	<div></div> 0.4550
A	<div></div> 0.8630	<div></div> 0.4600
D	<div></div> 0.8600	<div></div> 0.4530

