



## Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 03:30 AM UTC

PDB ID : 9K4A / pdb\_00009k4a  
EMDB ID : EMD-62051  
Title : Cryo-EM structure of depolymerase S2-4 from Klebsiella phage K64-1  
Authors : Zhao, R.; Du, T.; Ren, Z.; Gu, J.; Ru, H.  
Deposited on : 2024-10-21  
Resolution : 2.24 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.dev132  
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

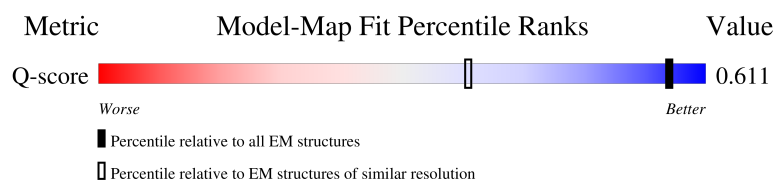
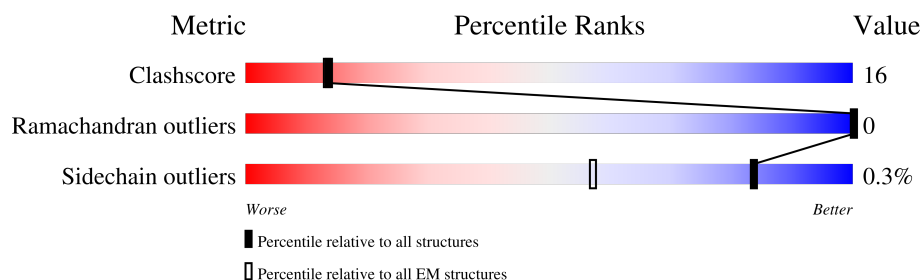
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*




The reported resolution of this entry is 2.24 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	3381 ( 1.75 - 2.74 )

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	A	922	
1	B	922	
1	C	922	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15447 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 Depolymerase, capsule K1-specific.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	668	Total	C	N	O	S	0	0
			5149	3220	858	1046	25		
1	B	668	Total	C	N	O	S	0	0
			5149	3220	858	1046	25		
1	C	668	Total	C	N	O	S	0	0
			5149	3220	858	1046	25		

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	initiating methionine	UNP A0A0A8J8T2
A	-32	GLY	-	expression tag	UNP A0A0A8J8T2
A	-31	SER	-	expression tag	UNP A0A0A8J8T2
A	-30	SER	-	expression tag	UNP A0A0A8J8T2
A	-29	HIS	-	expression tag	UNP A0A0A8J8T2
A	-28	HIS	-	expression tag	UNP A0A0A8J8T2
A	-27	HIS	-	expression tag	UNP A0A0A8J8T2
A	-26	HIS	-	expression tag	UNP A0A0A8J8T2
A	-25	HIS	-	expression tag	UNP A0A0A8J8T2
A	-24	HIS	-	expression tag	UNP A0A0A8J8T2
A	-23	SER	-	expression tag	UNP A0A0A8J8T2
A	-22	SER	-	expression tag	UNP A0A0A8J8T2
A	-21	GLY	-	expression tag	UNP A0A0A8J8T2
A	-20	LEU	-	expression tag	UNP A0A0A8J8T2
A	-19	VAL	-	expression tag	UNP A0A0A8J8T2
A	-18	PRO	-	expression tag	UNP A0A0A8J8T2
A	-17	ARG	-	expression tag	UNP A0A0A8J8T2
A	-16	GLY	-	expression tag	UNP A0A0A8J8T2
A	-15	SER	-	expression tag	UNP A0A0A8J8T2
A	-14	HIS	-	expression tag	UNP A0A0A8J8T2
A	-13	MET	-	expression tag	UNP A0A0A8J8T2
A	-12	ALA	-	expression tag	UNP A0A0A8J8T2
A	-11	SER	-	expression tag	UNP A0A0A8J8T2
A	-10	MET	-	expression tag	UNP A0A0A8J8T2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	THR	-	expression tag	UNP A0A0A8J8T2
A	-8	GLY	-	expression tag	UNP A0A0A8J8T2
A	-7	GLY	-	expression tag	UNP A0A0A8J8T2
A	-6	GLN	-	expression tag	UNP A0A0A8J8T2
A	-5	GLN	-	expression tag	UNP A0A0A8J8T2
A	-4	MET	-	expression tag	UNP A0A0A8J8T2
A	-3	GLY	-	expression tag	UNP A0A0A8J8T2
A	-2	ARG	-	expression tag	UNP A0A0A8J8T2
A	-1	GLY	-	expression tag	UNP A0A0A8J8T2
A	0	SER	-	expression tag	UNP A0A0A8J8T2
B	-33	MET	-	initiating methionine	UNP A0A0A8J8T2
B	-32	GLY	-	expression tag	UNP A0A0A8J8T2
B	-31	SER	-	expression tag	UNP A0A0A8J8T2
B	-30	SER	-	expression tag	UNP A0A0A8J8T2
B	-29	HIS	-	expression tag	UNP A0A0A8J8T2
B	-28	HIS	-	expression tag	UNP A0A0A8J8T2
B	-27	HIS	-	expression tag	UNP A0A0A8J8T2
B	-26	HIS	-	expression tag	UNP A0A0A8J8T2
B	-25	HIS	-	expression tag	UNP A0A0A8J8T2
B	-24	HIS	-	expression tag	UNP A0A0A8J8T2
B	-23	SER	-	expression tag	UNP A0A0A8J8T2
B	-22	SER	-	expression tag	UNP A0A0A8J8T2
B	-21	GLY	-	expression tag	UNP A0A0A8J8T2
B	-20	LEU	-	expression tag	UNP A0A0A8J8T2
B	-19	VAL	-	expression tag	UNP A0A0A8J8T2
B	-18	PRO	-	expression tag	UNP A0A0A8J8T2
B	-17	ARG	-	expression tag	UNP A0A0A8J8T2
B	-16	GLY	-	expression tag	UNP A0A0A8J8T2
B	-15	SER	-	expression tag	UNP A0A0A8J8T2
B	-14	HIS	-	expression tag	UNP A0A0A8J8T2
B	-13	MET	-	expression tag	UNP A0A0A8J8T2
B	-12	ALA	-	expression tag	UNP A0A0A8J8T2
B	-11	SER	-	expression tag	UNP A0A0A8J8T2
B	-10	MET	-	expression tag	UNP A0A0A8J8T2
B	-9	THR	-	expression tag	UNP A0A0A8J8T2
B	-8	GLY	-	expression tag	UNP A0A0A8J8T2
B	-7	GLY	-	expression tag	UNP A0A0A8J8T2
B	-6	GLN	-	expression tag	UNP A0A0A8J8T2
B	-5	GLN	-	expression tag	UNP A0A0A8J8T2
B	-4	MET	-	expression tag	UNP A0A0A8J8T2
B	-3	GLY	-	expression tag	UNP A0A0A8J8T2
B	-2	ARG	-	expression tag	UNP A0A0A8J8T2

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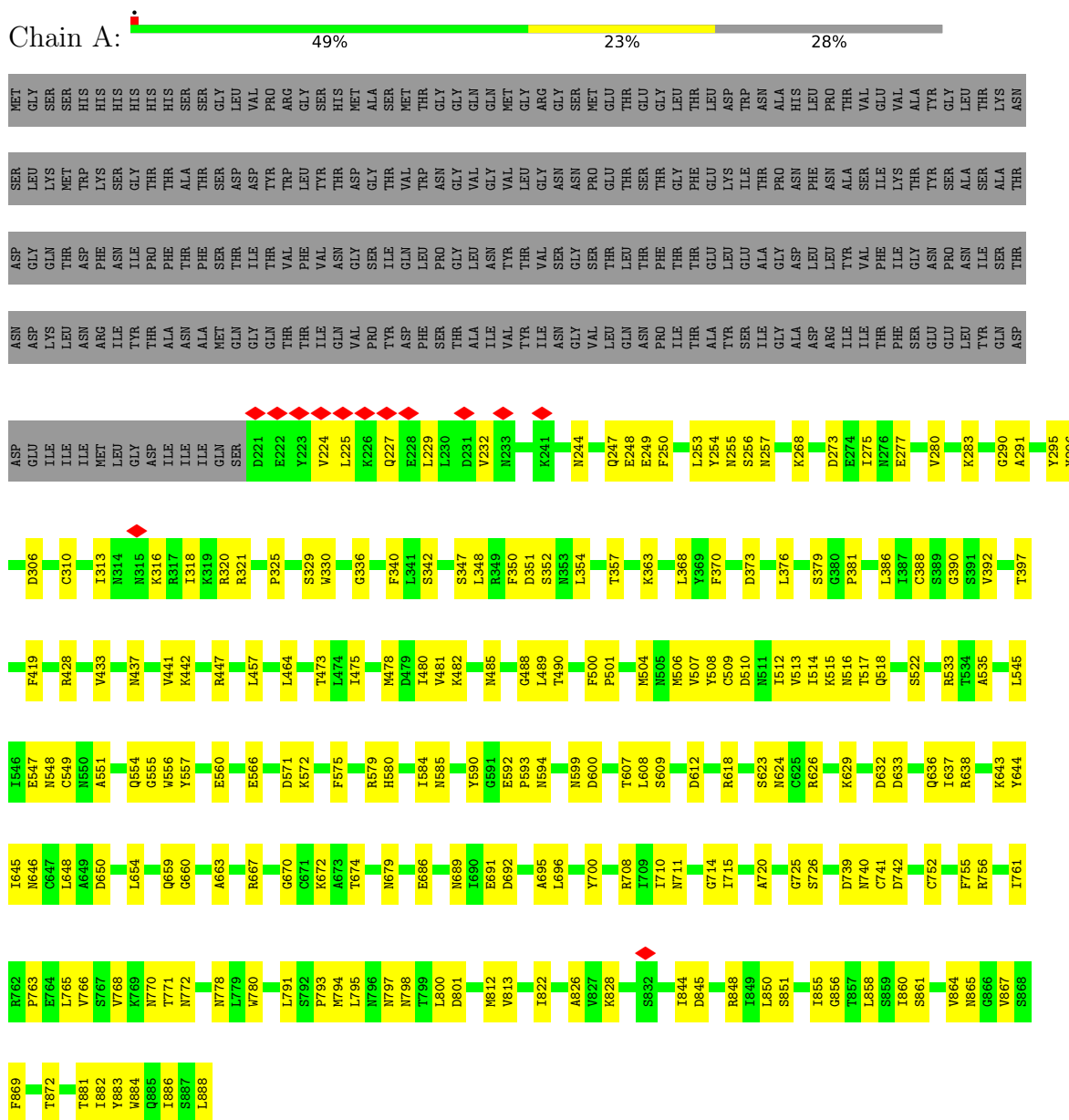
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP A0A0A8J8T2
B	0	SER	-	expression tag	UNP A0A0A8J8T2
C	-33	MET	-	initiating methionine	UNP A0A0A8J8T2
C	-32	GLY	-	expression tag	UNP A0A0A8J8T2
C	-31	SER	-	expression tag	UNP A0A0A8J8T2
C	-30	SER	-	expression tag	UNP A0A0A8J8T2
C	-29	HIS	-	expression tag	UNP A0A0A8J8T2
C	-28	HIS	-	expression tag	UNP A0A0A8J8T2
C	-27	HIS	-	expression tag	UNP A0A0A8J8T2
C	-26	HIS	-	expression tag	UNP A0A0A8J8T2
C	-25	HIS	-	expression tag	UNP A0A0A8J8T2
C	-24	HIS	-	expression tag	UNP A0A0A8J8T2
C	-23	SER	-	expression tag	UNP A0A0A8J8T2
C	-22	SER	-	expression tag	UNP A0A0A8J8T2
C	-21	GLY	-	expression tag	UNP A0A0A8J8T2
C	-20	LEU	-	expression tag	UNP A0A0A8J8T2
C	-19	VAL	-	expression tag	UNP A0A0A8J8T2
C	-18	PRO	-	expression tag	UNP A0A0A8J8T2
C	-17	ARG	-	expression tag	UNP A0A0A8J8T2
C	-16	GLY	-	expression tag	UNP A0A0A8J8T2
C	-15	SER	-	expression tag	UNP A0A0A8J8T2
C	-14	HIS	-	expression tag	UNP A0A0A8J8T2
C	-13	MET	-	expression tag	UNP A0A0A8J8T2
C	-12	ALA	-	expression tag	UNP A0A0A8J8T2
C	-11	SER	-	expression tag	UNP A0A0A8J8T2
C	-10	MET	-	expression tag	UNP A0A0A8J8T2
C	-9	THR	-	expression tag	UNP A0A0A8J8T2
C	-8	GLY	-	expression tag	UNP A0A0A8J8T2
C	-7	GLY	-	expression tag	UNP A0A0A8J8T2
C	-6	GLN	-	expression tag	UNP A0A0A8J8T2
C	-5	GLN	-	expression tag	UNP A0A0A8J8T2
C	-4	MET	-	expression tag	UNP A0A0A8J8T2
C	-3	GLY	-	expression tag	UNP A0A0A8J8T2
C	-2	ARG	-	expression tag	UNP A0A0A8J8T2
C	-1	GLY	-	expression tag	UNP A0A0A8J8T2
C	0	SER	-	expression tag	UNP A0A0A8J8T2

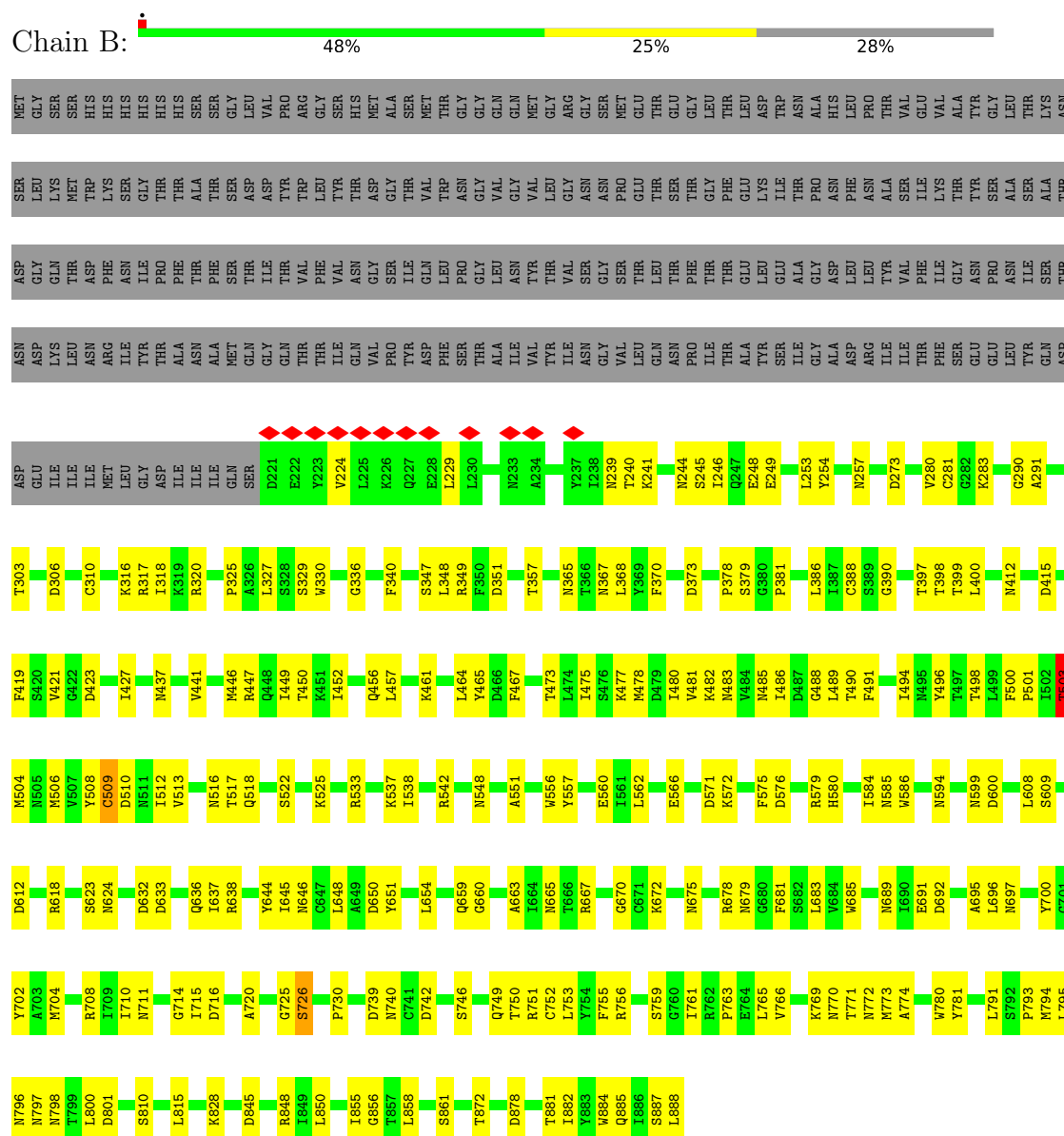
### 3 Residue-property plots

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.

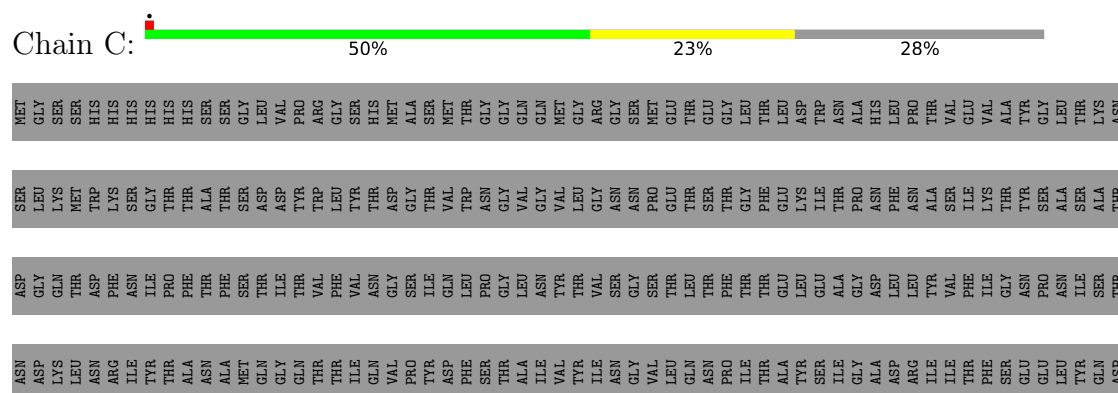
- Molecule 1: Depolymerase, capsule K1-specific



• Molecule 1: Depolymerase, capsule K1-specific



• Molecule 1: Depolymerase, capsule K1-specific



ASP	T303	Q554	G660	R762
GLU	V304	G556	A663	P763
ILE	E305	W556		V766
ILE	D306	Y557	R667	S767
ILE	F311	E566		V768
MET				R769
LEU				N770
GLY	K316	D571	G670	N771
ASP	R317	K572	C671	N772
ASP		C573	A673	
ILE	R320	F574	T674	W780
ILE	R321	F575	N675	Y781
ILE				
GLN	W330	R579	L683	L791
SER	D221	H580		S792
	E222	I584	N689	P793
	Y223	N585	I690	N794
	V224	Y590	E691	L795
	L225	G591	D692	N796
	K226	E592	A695	N797
	Q227	P593	L696	N798
	E228	N594	N697	N799
	L229			L800
	L230	N599	Y700	D801
	D231	D600	M704	S810
	V232	C601		G811
	N233	L608	R708	A826
		S609	I709	W827
	S236	D612	I710	K828
	Y237	T613	N711	L829
	L238	H614	G714	V841
	N239	D615	I715	R848
	T240	I616	D716	I849
	K241	G617	A720	L850
		R618		
	N244	S623	G725	I855
	S245	N624	P730	G856
	I246	D632		T857
	Q247	D633	D739	L858
	E248	Q636	N740	S861
	E249	I637	D742	N862
	F250	R638		I863
			Q749	T872
	L253	K643	T750	
	Y254	Y644	R751	S880
	N255	I645	C752	T881
	S256	N646	L753	I882
	N257	C647	Y754	
		L648	F755	Q885
	E277	A649		I886
		L545	S759	S887
		I546	G760	L888
	V280	E547	I761	
		N548		
	N286	C549		
		H550		
	G290	A551		
	A291	Y552		
		H553		
	Y296			



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	4015926	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.984	Depositor
Minimum map value	-1.935	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.27	Depositor
Map size (Å)	273.92, 273.92, 273.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.51	0/5235	0.78	0/7109
1	B	0.49	0/5235	0.79	2/7109 (0.0%)
1	C	0.50	0/5235	0.76	0/7109
All	All	0.50	0/15705	0.78	2/21327 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	585	ASN	N-CA-C	6.65	119.31	110.53
1	B	503	THR	N-CA-C	5.28	116.84	111.14

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5149	0	5016	171	0
1	B	5149	0	5016	180	0
1	C	5149	0	5016	161	0
All	All	15447	0	15048	484	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 16.

All (484) 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:A:556:TRP:O	1:A:579:ARG:HB3	1.65	0.96
1:C:556:TRP:O	1:C:579:ARG:HB3	1.69	0.93
1:B:556:TRP:O	1:B:579:ARG:HB3	1.70	0.91
1:A:851:SER:HB3	1:A:855:ILE:HD11	1.56	0.88
1:B:501:PRO:O	1:B:533:ARG:HA	1.74	0.86
1:B:750:THR:HG22	1:B:751:ARG:HE	1.40	0.86
1:A:501:PRO:O	1:A:533:ARG:HA	1.80	0.81
1:C:501:PRO:O	1:C:533:ARG:HA	1.79	0.81
1:A:386:LEU:HD22	1:A:506:MET:HE1	1.62	0.81
1:C:725:GLY:HA3	1:C:761:ILE:HD12	1.65	0.78
1:A:725:GLY:HA3	1:A:761:ILE:HD12	1.65	0.77
1:B:638:ARG:HG2	1:B:660:GLY:HA3	1.67	0.76
1:A:509:CYS:CB	1:A:512:ILE:HD11	2.16	0.75
1:A:509:CYS:HB3	1:A:512:ILE:HD11	1.68	0.75
1:A:691:GLU:HG3	1:A:710:ILE:HG23	1.68	0.74
1:B:691:GLU:HG3	1:B:710:ILE:HG23	1.69	0.74
1:A:612:ASP:HB2	1:A:636:GLN:HB3	1.69	0.74
1:C:638:ARG:HG2	1:C:660:GLY:HA3	1.68	0.74
1:B:239:ASN:HA	1:B:245:SER:HA	1.69	0.74
1:B:504:MET:HE2	1:B:506:MET:HE3	1.69	0.74
1:C:670:GLY:HA2	1:C:692:ASP:O	1.89	0.73
1:B:381:PRO:O	1:B:501:PRO:HB3	1.88	0.73
1:A:437:ASN:ND2	1:A:441:VAL:O	2.22	0.72
1:C:504:MET:HB3	1:C:506:MET:HE3	1.71	0.72
1:A:711:ASN:HD21	1:C:689:ASN:HD21	1.37	0.72
1:B:370:PHE:HB2	1:B:489:LEU:HD12	1.72	0.71
1:A:844:ILE:HB	1:A:860:ILE:HD11	1.70	0.71
1:C:239:ASN:HA	1:C:245:SER:HA	1.73	0.71
1:A:592:GLU:OE1	1:A:618:ARG:NE	2.24	0.71
1:B:398:THR:HG21	1:B:415:ASP:H	1.56	0.70
1:C:848:ARG:NH2	1:C:856:GLY:O	2.24	0.70
1:B:848:ARG:NH2	1:B:856:GLY:O	2.24	0.70
1:B:509:CYS:HB2	1:B:512:ILE:HD11	1.74	0.70
1:A:801:ASP:OD2	1:A:828:LYS:NZ	2.25	0.69
1:C:850:LEU:O	1:C:880:SER:HB3	1.92	0.69
1:B:708:ARG:NH1	1:B:739:ASP:OD2	2.26	0.68
1:C:290:GLY:HA2	1:C:330:TRP:CD1	2.28	0.68
1:B:390:GLY:O	1:B:508:TYR:HD2	1.77	0.68
1:C:386:LEU:HD22	1:C:506:MET:HE1	1.74	0.68
1:C:244:ASN:HB3	1:C:248:GLU:HG3	1.76	0.67
1:B:398:THR:HG22	1:B:399:THR:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:ASN:ND2	1:B:441:VAL:O	2.28	0.67
1:B:612:ASP:HB2	1:B:636:GLN:HB3	1.76	0.67
1:B:537:LYS:HE3	1:B:560:GLU:OE1	1.93	0.66
1:B:290:GLY:HA2	1:B:330:TRP:CD1	2.31	0.66
1:A:848:ARG:NH2	1:A:856:GLY:O	2.29	0.66
1:C:437:ASN:ND2	1:C:441:VAL:O	2.28	0.66
1:A:572:LYS:HD3	1:C:545:LEU:HD22	1.78	0.66
1:B:624:ASN:OD1	1:B:646:ASN:ND2	2.25	0.65
1:A:280:VAL:O	1:A:291:ALA:HA	1.95	0.65
1:A:273:ASP:OD1	1:A:316:LYS:NZ	2.26	0.65
1:C:691:GLU:HG3	1:C:710:ILE:HG23	1.78	0.65
1:B:801:ASP:OD2	1:B:828:LYS:NZ	2.29	0.64
1:C:580:HIS:HA	1:C:609:SER:O	1.97	0.64
1:A:504:MET:HB3	1:A:506:MET:HE3	1.79	0.64
1:A:708:ARG:NH1	1:A:739:ASP:OD2	2.29	0.64
1:A:257:ASN:HD22	1:C:253:LEU:HD23	1.62	0.64
1:C:303:THR:HG22	1:C:317:ARG:HG2	1.78	0.64
1:B:461:LYS:NZ	1:B:566:GLU:OE2	2.24	0.64
1:A:794:MET:HB3	1:B:885:GLN:NE2	2.13	0.63
1:A:812:MET:HE2	1:A:883:TYR:HB2	1.80	0.63
1:B:253:LEU:HD23	1:C:257:ASN:HD22	1.63	0.63
1:A:232:VAL:HG12	1:C:241:LYS:HA	1.78	0.63
1:C:584:ILE:HG23	1:C:593:PRO:HG2	1.81	0.63
1:C:692:ASP:HA	1:C:711:ASN:O	1.99	0.63
1:C:522:SER:OG	1:C:555:GLY:N	2.21	0.62
1:C:489:LEU:H	1:C:517:THR:HG22	1.64	0.62
1:C:386:LEU:CD2	1:C:506:MET:HE1	2.30	0.62
1:A:670:GLY:HA2	1:A:692:ASP:O	1.99	0.62
1:B:241:LYS:HA	1:C:232:VAL:HG12	1.80	0.61
1:B:449:ILE:HD13	1:B:457:LEU:HD22	1.81	0.61
1:B:299:ASN:ND2	1:C:286:ASN:O	2.33	0.61
1:B:368:LEU:HD12	1:B:486:ILE:HG12	1.82	0.61
1:B:386:LEU:HD22	1:B:506:MET:HE1	1.81	0.61
1:B:599:ASN:HD21	1:B:624:ASN:HD22	1.49	0.61
1:B:683:LEU:HD12	1:B:704:MET:HE1	1.83	0.61
1:B:850:LEU:HB2	1:B:881:THR:HB	1.82	0.61
1:B:365:ASN:HD22	1:B:483:ASN:HB2	1.65	0.61
1:A:370:PHE:HB2	1:A:489:LEU:HD12	1.83	0.61
1:A:545:LEU:HD13	1:B:572:LYS:HD2	1.83	0.61
1:B:378:PRO:HB3	1:B:500:PHE:CD1	2.36	0.61
1:A:433:VAL:HG22	1:A:437:ASN:ND2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:ASP:HA	1:A:624:ASN:O	2.01	0.61
1:A:689:ASN:HD21	1:B:711:ASN:HD21	1.49	0.60
1:B:273:ASP:OD1	1:B:316:LYS:NZ	2.29	0.60
1:A:659:GLN:NE2	1:A:686:GLU:H	1.99	0.60
1:B:599:ASN:ND2	1:B:624:ASN:HD22	2.00	0.60
1:C:320:ARG:HD2	1:C:330:TRP:CZ3	2.36	0.60
1:C:750:THR:HG23	1:C:751:ARG:HG2	1.83	0.60
1:C:484:VAL:HB	1:C:512:ILE:HD12	1.83	0.60
1:A:584:ILE:HG23	1:A:593:PRO:HG2	1.84	0.60
1:A:695:ALA:O	1:A:714:GLY:HA2	2.02	0.60
1:C:612:ASP:HB2	1:C:636:GLN:HB3	1.84	0.59
1:A:290:GLY:HA2	1:A:330:TRP:CD1	2.38	0.59
1:B:580:HIS:HA	1:B:609:SER:O	2.01	0.59
1:C:430:GLU:HA	1:C:442:LYS:HD2	1.84	0.59
1:C:600:ASP:HA	1:C:624:ASN:O	2.01	0.59
1:A:522:SER:HG	1:A:555:GLY:H	1.49	0.59
1:C:303:THR:O	1:C:317:ARG:NE	2.34	0.59
1:A:560:GLU:OE1	1:A:585:ASN:ND2	2.36	0.58
1:A:354:LEU:HB2	1:A:376:LEU:HD23	1.85	0.58
1:A:517:THR:OG1	1:A:549:CYS:SG	2.58	0.58
1:C:800:LEU:HD23	1:C:828:LYS:HG3	1.85	0.58
1:B:794:MET:SD	1:C:885:GLN:HG3	2.43	0.58
1:A:580:HIS:HA	1:A:609:SER:O	2.03	0.58
1:C:224:VAL:HG21	1:C:229:LEU:HD13	1.84	0.58
1:C:290:GLY:HA2	1:C:330:TRP:HD1	1.67	0.58
1:C:370:PHE:HB2	1:C:489:LEU:HD12	1.84	0.58
1:C:354:LEU:HB2	1:C:376:LEU:HD23	1.86	0.58
1:A:579:ARG:HA	1:A:607:THR:OG1	2.04	0.58
1:B:447:ARG:HH22	1:B:464:LEU:HD12	1.69	0.58
1:B:572:LYS:HA	1:B:600:ASP:O	2.03	0.58
1:B:600:ASP:HA	1:B:624:ASN:O	2.04	0.57
1:C:801:ASP:OD2	1:C:828:LYS:NZ	2.35	0.57
1:A:249:GLU:HG3	1:B:254:TYR:OH	2.02	0.57
1:B:551:ALA:HB3	1:B:575:PHE:HD2	1.69	0.57
1:C:708:ARG:NH1	1:C:739:ASP:OD2	2.38	0.57
1:A:679:ASN:ND2	1:A:700:TYR:HB2	2.20	0.57
1:C:280:VAL:O	1:C:291:ALA:HA	2.03	0.57
1:A:517:THR:HG1	1:A:549:CYS:HG	1.49	0.57
1:B:290:GLY:HA2	1:B:330:TRP:HD1	1.69	0.57
1:B:766:VAL:HB	1:B:793:PRO:HB3	1.86	0.57
1:C:296:TYR:CZ	1:C:316:LYS:HG2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ARG:HD2	1:A:330:TRP:CZ3	2.40	0.57
1:B:763:PRO:HB2	1:B:791:LEU:O	2.04	0.57
1:A:386:LEU:CD2	1:A:506:MET:HE1	2.34	0.56
1:A:813:VAL:HG11	1:A:822:ILE:HD11	1.88	0.56
1:B:244:ASN:HB3	1:B:248:GLU:HG3	1.87	0.56
1:A:566:GLU:HA	1:A:594:ASN:O	2.06	0.56
1:B:725:GLY:HA3	1:B:761:ILE:HD12	1.88	0.56
1:C:548:ASN:HA	1:C:572:LYS:O	2.06	0.56
1:C:572:LYS:HA	1:C:600:ASP:O	2.06	0.56
1:A:691:GLU:HG3	1:A:710:ILE:CG2	2.35	0.55
1:B:726:SER:HA	1:B:756:ARG:HD2	1.88	0.55
1:A:296:TYR:CZ	1:A:316:LYS:HG2	2.41	0.55
1:A:648:LEU:HD21	1:A:650:ASP:HB2	1.88	0.55
1:B:280:VAL:O	1:B:291:ALA:HA	2.06	0.55
1:C:696:LEU:HA	1:C:715:ILE:O	2.06	0.55
1:C:711:ASN:HA	1:C:740:ASN:O	2.05	0.55
1:B:446:MET:HE3	1:B:542:ARG:HG3	1.89	0.55
1:B:608:LEU:O	1:B:632:ASP:N	2.34	0.55
1:B:681:PHE:CD2	1:B:702:TYR:CE1	2.95	0.55
1:B:740:ASN:HA	1:B:770:ASN:O	2.06	0.55
1:A:357:THR:HA	1:A:379:SER:HB3	1.88	0.55
1:A:254:TYR:OH	1:C:249:GLU:HG3	2.06	0.55
1:A:623:SER:HA	1:A:645:ILE:O	2.07	0.55
1:B:327:LEU:HD23	1:B:349:ARG:HB3	1.88	0.55
1:A:572:LYS:HA	1:A:600:ASP:O	2.07	0.54
1:B:730:PRO:HB3	1:B:759:SER:HB3	1.88	0.54
1:A:244:ASN:HB3	1:A:248:GLU:HG3	1.90	0.54
1:B:249:GLU:HG3	1:C:254:TYR:OH	2.08	0.54
1:B:692:ASP:HA	1:B:711:ASN:O	2.06	0.54
1:A:850:LEU:HB2	1:A:881:THR:HB	1.90	0.54
1:B:485:ASN:ND2	1:B:513:VAL:HB	2.22	0.54
1:B:689:ASN:HD21	1:C:711:ASN:HD21	1.55	0.54
1:A:224:VAL:HG21	1:A:229:LEU:HD13	1.90	0.54
1:A:632:ASP:OD2	1:A:654:LEU:HD12	2.08	0.54
1:A:388:CYS:SG	1:A:481:VAL:HG11	2.47	0.54
1:C:487:ASP:OD1	1:C:516:ASN:ND2	2.39	0.54
1:B:489:LEU:H	1:B:517:THR:HG22	1.72	0.54
1:A:551:ALA:HB3	1:A:575:PHE:HD1	1.72	0.54
1:C:344:GLY:O	1:C:346:VAL:HG13	2.08	0.54
1:C:551:ALA:HB3	1:C:575:PHE:HD1	1.73	0.54
1:A:711:ASN:HA	1:A:740:ASN:O	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:VAL:HB	1:A:795:LEU:HD23	1.89	0.53
1:A:253:LEU:HD23	1:B:257:ASN:HD22	1.72	0.53
1:C:763:PRO:HB2	1:C:791:LEU:O	2.08	0.53
1:A:490:THR:HG23	1:A:518:GLN:HB2	1.91	0.53
1:A:740:ASN:HA	1:A:770:ASN:O	2.07	0.53
1:B:224:VAL:HG21	1:B:229:LEU:HD13	1.90	0.53
1:A:608:LEU:O	1:A:632:ASP:N	2.34	0.53
1:C:755:PHE:CZ	1:C:793:PRO:HG3	2.44	0.53
1:A:325:PRO:HA	1:A:347:SER:HB3	1.90	0.53
1:B:670:GLY:HA2	1:B:692:ASP:O	2.08	0.53
1:C:695:ALA:O	1:C:714:GLY:HA2	2.09	0.53
1:A:533:ARG:H	1:A:556:TRP:HB2	1.74	0.53
1:A:638:ARG:HG2	1:A:660:GLY:HA3	1.91	0.53
1:B:386:LEU:CD2	1:B:506:MET:HE1	2.39	0.53
1:B:400:LEU:HD23	1:B:475:ILE:HD11	1.92	0.53
1:A:755:PHE:CZ	1:A:793:PRO:HG3	2.44	0.52
1:B:488:GLY:HA2	1:B:516:ASN:O	2.09	0.52
1:B:584:ILE:HG22	1:B:584:ILE:O	2.09	0.52
1:A:674:THR:HG22	1:A:696:LEU:HB2	1.90	0.52
1:C:533:ARG:H	1:C:556:TRP:HB2	1.74	0.52
1:A:488:GLY:HA2	1:A:516:ASN:O	2.10	0.52
1:C:557:TYR:CE1	1:C:580:HIS:ND1	2.77	0.52
1:C:632:ASP:OD2	1:C:654:LEU:HD12	2.10	0.52
1:A:548:ASN:HA	1:A:572:LYS:O	2.09	0.52
1:A:557:TYR:CE1	1:A:580:HIS:ND1	2.78	0.52
1:C:770:ASN:HA	1:C:797:ASN:O	2.09	0.52
1:C:381:PRO:O	1:C:501:PRO:HB3	2.10	0.52
1:C:740:ASN:HA	1:C:770:ASN:O	2.10	0.52
1:A:253:LEU:O	1:A:256:SER:OG	2.26	0.52
1:B:566:GLU:HA	1:B:594:ASN:O	2.08	0.52
1:B:711:ASN:HA	1:B:740:ASN:O	2.09	0.52
1:A:296:TYR:CE1	1:A:316:LYS:HG2	2.45	0.52
1:B:306:ASP:HB2	1:B:336:GLY:O	2.10	0.52
1:A:599:ASN:HD21	1:A:624:ASN:HD22	1.57	0.52
1:A:480:ILE:HD12	1:A:510:ASP:HB2	1.92	0.52
1:A:428:ARG:O	1:A:473:THR:HA	2.10	0.51
1:A:533:ARG:O	1:A:556:TRP:N	2.41	0.51
1:A:710:ILE:HA	1:A:739:ASP:O	2.10	0.51
1:B:320:ARG:HD2	1:B:330:TRP:CZ3	2.45	0.51
1:C:488:GLY:HA2	1:C:516:ASN:O	2.10	0.51
1:C:253:LEU:O	1:C:256:SER:OG	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:ASP:HB2	1:C:336:GLY:O	2.11	0.51
1:C:710:ILE:HA	1:C:739:ASP:O	2.10	0.51
1:A:277:GLU:HG3	1:A:295:TYR:HB3	1.93	0.51
1:A:844:ILE:HD12	1:A:860:ILE:HD13	1.92	0.51
1:B:557:TYR:CD2	1:B:560:GLU:OE2	2.64	0.51
1:A:390:GLY:O	1:A:508:TYR:HD2	1.94	0.51
1:A:659:GLN:HE22	1:A:686:GLU:H	1.58	0.51
1:B:548:ASN:HA	1:B:572:LYS:O	2.10	0.51
1:A:696:LEU:HA	1:A:715:ILE:O	2.10	0.51
1:B:482:LYS:HA	1:B:510:ASP:O	2.10	0.51
1:B:452:ILE:HG12	1:B:457:LEU:HD23	1.91	0.51
1:C:801:ASP:OD2	1:C:826:ALA:HA	2.11	0.51
1:A:626:ARG:HG2	1:A:648:LEU:HB3	1.92	0.51
1:A:419:PHE:HD2	1:A:457:LEU:HD11	1.76	0.51
1:C:696:LEU:HG	1:C:715:ILE:HB	1.92	0.51
1:A:381:PRO:O	1:A:501:PRO:HB3	2.11	0.50
1:B:710:ILE:HA	1:B:739:ASP:O	2.11	0.50
1:C:623:SER:HA	1:C:645:ILE:O	2.11	0.50
1:A:485:ASN:OD1	1:A:513:VAL:HB	2.10	0.50
1:B:296:TYR:CZ	1:B:316:LYS:HG2	2.46	0.50
1:B:665:ASN:HD21	1:B:667:ARG:HH11	1.59	0.50
1:A:480:ILE:CD1	1:A:510:ASP:HB2	2.42	0.50
1:A:329:SER:HB3	1:A:352:SER:HB3	1.94	0.50
1:B:646:ASN:HA	1:B:670:GLY:O	2.11	0.50
1:A:392:VAL:HG22	1:A:478:MET:HG2	1.92	0.50
1:B:306:ASP:OD2	1:B:340:PHE:HB2	2.11	0.50
1:C:507:VAL:HG12	1:C:508:TYR:CD2	2.46	0.50
1:A:858:LEU:HD11	1:A:882:ILE:HD12	1.94	0.50
1:B:638:ARG:HA	1:B:663:ALA:HB2	1.93	0.50
1:C:277:GLU:CD	1:C:321:ARG:HH21	2.20	0.49
1:C:533:ARG:O	1:C:556:TRP:CB	2.59	0.49
1:A:667:ARG:NH2	1:B:692:ASP:OD1	2.44	0.49
1:C:515:LYS:HA	1:C:547:GLU:O	2.13	0.49
1:A:447:ARG:HH22	1:A:464:LEU:HD12	1.75	0.49
1:B:791:LEU:HD11	1:C:811:GLY:HA2	1.94	0.49
1:C:716:ASP:HA	1:C:749:GLN:HB2	1.94	0.49
1:C:798:ASN:N	1:C:887:SER:OG	2.46	0.49
1:A:255:ASN:ND2	1:A:275:ILE:HD13	2.26	0.49
1:A:794:MET:SD	1:B:810:SER:HB3	2.52	0.49
1:A:800:LEU:HD23	1:A:828:LYS:HG3	1.94	0.49
1:B:861:SER:HB3	1:B:872:THR:OG1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ARG:CD	1:C:330:TRP:CZ3	2.95	0.49
1:C:646:ASN:HA	1:C:670:GLY:O	2.11	0.49
1:B:478:MET:HE2	1:B:480:ILE:HG22	1.95	0.49
1:B:695:ALA:O	1:B:714:GLY:HA2	2.13	0.49
1:A:306:ASP:OD2	1:A:340:PHE:HB2	2.13	0.49
1:A:646:ASN:HA	1:A:670:GLY:O	2.13	0.49
1:A:763:PRO:HB2	1:A:791:LEU:O	2.12	0.49
1:B:696:LEU:HA	1:B:715:ILE:O	2.13	0.49
1:A:861:SER:HB3	1:A:872:THR:OG1	2.13	0.49
1:B:586:TRP:CD1	1:B:586:TRP:C	2.91	0.49
1:C:766:VAL:HB	1:C:793:PRO:HB3	1.94	0.48
1:A:533:ARG:N	1:A:556:TRP:HB2	2.28	0.48
1:A:692:ASP:HA	1:A:711:ASN:O	2.12	0.48
1:C:599:ASN:HA	1:C:623:SER:O	2.13	0.48
1:A:310:CYS:HA	1:A:318:ILE:O	2.12	0.48
1:B:490:THR:HG23	1:B:518:GLN:HB2	1.95	0.48
1:B:623:SER:HA	1:B:645:ILE:O	2.14	0.48
1:B:770:ASN:HA	1:B:797:ASN:O	2.13	0.48
1:C:566:GLU:HA	1:C:594:ASN:O	2.14	0.48
1:C:637:ILE:HG12	1:C:644:TYR:OH	2.13	0.48
1:B:373:ASP:OD1	1:B:373:ASP:N	2.47	0.48
1:B:491:PHE:CG	1:B:503:THR:CG2	2.97	0.48
1:B:659:GLN:O	1:B:685:TRP:HD1	1.96	0.48
1:C:624:ASN:OD1	1:C:646:ASN:ND2	2.31	0.48
1:C:862:ASN:OD1	1:C:863:ILE:N	2.46	0.48
1:B:504:MET:HE2	1:B:506:MET:CE	2.40	0.48
1:A:247:GLN:OE1	1:C:240:THR:HB	2.14	0.48
1:A:489:LEU:H	1:A:517:THR:HG22	1.78	0.48
1:A:794:MET:SD	1:B:885:GLN:HG3	2.53	0.48
1:A:482:LYS:HA	1:A:510:ASP:O	2.14	0.47
1:B:637:ILE:HG13	1:B:644:TYR:OH	2.13	0.47
1:C:850:LEU:HB2	1:C:881:THR:HB	1.96	0.47
1:A:509:CYS:SG	1:A:512:ILE:HD11	2.54	0.47
1:A:373:ASP:OD1	1:A:373:ASP:N	2.48	0.47
1:A:692:ASP:OD2	1:C:667:ARG:NH2	2.46	0.47
1:A:798:ASN:O	1:A:888:LEU:N	2.38	0.47
1:C:370:PHE:CZ	1:C:374:VAL:HG12	2.50	0.47
1:A:742:ASP:HA	1:A:772:ASN:HB3	1.96	0.47
1:C:515:LYS:HG2	1:C:547:GLU:HB3	1.95	0.47
1:A:500:PHE:H	1:A:522:SER:HA	1.79	0.47
1:C:390:GLY:O	1:C:508:TYR:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:VAL:HB	1:A:793:PRO:HB3	1.97	0.47
1:C:350:PHE:HB2	1:C:370:PHE:CD2	2.50	0.47
1:C:592:GLU:HB2	1:C:617:GLY:H	1.79	0.47
1:C:768:VAL:HB	1:C:795:LEU:HD23	1.97	0.47
1:C:349:ARG:HH11	1:C:371:ASN:HD21	1.63	0.47
1:A:812:MET:HE3	1:A:812:MET:HB2	1.76	0.47
1:B:557:TYR:CE1	1:B:580:HIS:ND1	2.83	0.47
1:C:321:ARG:HG3	1:C:321:ARG:HH11	1.80	0.47
1:C:533:ARG:N	1:C:556:TRP:HB2	2.29	0.47
1:C:730:PRO:HG3	1:C:759:SER:HB3	1.97	0.47
1:B:325:PRO:HA	1:B:347:SER:HB3	1.97	0.47
1:B:447:ARG:NH2	1:B:464:LEU:HD12	2.30	0.47
1:C:650:ASP:HA	1:C:674:THR:O	2.15	0.46
1:A:225:LEU:HD23	1:A:227:GLN:H	1.80	0.46
1:A:726:SER:HA	1:A:756:ARG:HD2	1.96	0.46
1:B:465:TYR:HE1	1:B:618:ARG:HH11	1.62	0.46
1:B:800:LEU:HD23	1:B:828:LYS:HG3	1.95	0.46
1:A:679:ASN:HD22	1:A:700:TYR:HB2	1.80	0.46
1:B:794:MET:SD	1:C:810:SER:HB3	2.55	0.46
1:B:858:LEU:HD11	1:B:882:ILE:HD12	1.96	0.46
1:C:492:ASN:HB3	1:C:493:ASN:H	1.66	0.46
1:C:858:LEU:HD11	1:C:882:ILE:HD12	1.96	0.46
1:A:504:MET:HE1	1:A:514:ILE:HD13	1.97	0.46
1:B:378:PRO:HB3	1:B:500:PHE:CE1	2.50	0.46
1:B:494:ILE:O	1:B:525:LYS:NZ	2.33	0.46
1:B:512:ILE:HD13	1:B:512:ILE:HG21	1.67	0.46
1:C:780:TRP:H	1:C:780:TRP:CD1	2.33	0.46
1:A:638:ARG:HA	1:A:663:ALA:HB2	1.97	0.46
1:A:770:ASN:HA	1:A:797:ASN:O	2.16	0.46
1:B:533:ARG:N	1:B:556:TRP:HB2	2.31	0.46
1:A:571:ASP:HA	1:A:599:ASN:O	2.16	0.46
1:A:741:CYS:HB2	1:A:771:THR:HG23	1.98	0.46
1:B:421:VAL:HG13	1:B:450:THR:O	2.15	0.46
1:C:442:LYS:O	1:C:590:TYR:HA	2.15	0.46
1:C:505:ASN:C	1:C:506:MET:HE2	2.40	0.46
1:C:580:HIS:HD2	1:C:609:SER:H	1.63	0.46
1:B:329:SER:OG	1:B:351:ASP:OD2	2.29	0.46
1:B:755:PHE:CZ	1:B:793:PRO:HG3	2.51	0.46
1:C:648:LEU:HD12	1:C:672:LYS:HD3	1.98	0.46
1:A:626:ARG:HA	1:A:648:LEU:O	2.16	0.46
1:A:643:LYS:HB3	1:A:643:LYS:HE3	1.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:LEU:HD13	1:A:888:LEU:HG	1.98	0.46
1:C:798:ASN:HB2	1:C:888:LEU:HB3	1.98	0.46
1:A:306:ASP:HB2	1:A:336:GLY:O	2.16	0.45
1:B:648:LEU:HD21	1:B:650:ASP:HB2	1.98	0.45
1:B:691:GLU:HG3	1:B:710:ILE:CG2	2.42	0.45
1:C:489:LEU:N	1:C:517:THR:HG22	2.29	0.45
1:C:700:TYR:HA	1:C:720:ALA:O	2.16	0.45
1:A:250:PHE:HE2	1:C:246:ILE:HG23	1.81	0.45
1:A:268:LYS:HG3	1:A:313:ILE:HG12	1.98	0.45
1:B:562:LEU:HD23	1:B:562:LEU:N	2.32	0.45
1:B:303:THR:HG22	1:B:317:ARG:HG2	1.98	0.45
1:B:465:TYR:HE1	1:B:618:ARG:NH1	2.15	0.45
1:C:404:VAL:HB	1:C:467:PHE:HB2	1.99	0.45
1:C:533:ARG:O	1:C:556:TRP:N	2.45	0.45
1:A:290:GLY:HA2	1:A:330:TRP:HD1	1.80	0.45
1:A:522:SER:OG	1:A:555:GLY:N	2.28	0.45
1:A:844:ILE:HB	1:A:860:ILE:CD1	2.45	0.45
1:B:716:ASP:OD2	1:B:746:SER:OG	2.27	0.45
1:B:750:THR:HG22	1:B:751:ARG:NE	2.18	0.45
1:A:869:PHE:CE1	1:A:886:ILE:HD11	2.52	0.45
1:B:765:LEU:HD23	1:B:765:LEU:HA	1.85	0.45
1:C:432:LEU:HD23	1:C:442:LYS:HG2	1.98	0.45
1:C:674:THR:HG22	1:C:696:LEU:HB2	1.98	0.45
1:B:771:THR:HB	1:B:798:ASN:OD1	2.17	0.45
1:C:608:LEU:O	1:C:632:ASP:N	2.33	0.45
1:B:310:CYS:HA	1:B:318:ILE:O	2.17	0.44
1:C:643:LYS:HE3	1:C:643:LYS:HB3	1.72	0.44
1:B:241:LYS:NZ	1:C:233:ASN:OD1	2.49	0.44
1:B:378:PRO:HB3	1:B:500:PHE:CG	2.52	0.44
1:C:753:LEU:O	1:C:781:TYR:HA	2.17	0.44
1:C:861:SER:HB3	1:C:872:THR:OG1	2.16	0.44
1:B:397:THR:HA	1:B:475:ILE:O	2.18	0.44
1:B:504:MET:HB3	1:B:506:MET:HE3	2.00	0.44
1:B:599:ASN:HA	1:B:623:SER:O	2.17	0.44
1:C:517:THR:HG1	1:C:549:CYS:HG	1.65	0.44
1:B:798:ASN:N	1:B:887:SER:OG	2.51	0.44
1:C:356:LEU:HD13	1:C:385:GLY:HA2	2.00	0.44
1:A:700:TYR:HA	1:A:720:ALA:O	2.17	0.44
1:A:321:ARG:HG3	1:A:321:ARG:HH11	1.83	0.44
1:B:580:HIS:HD2	1:B:609:SER:H	1.66	0.44
1:B:496:TYR:O	1:B:496:TYR:CD2	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:THR:HG23	1:C:518:GLN:HB2	2.00	0.44
1:C:798:ASN:O	1:C:887:SER:OG	2.23	0.43
1:C:516:ASN:HA	1:C:548:ASN:O	2.18	0.43
1:B:398:THR:HG22	1:B:399:THR:N	2.30	0.43
1:C:445:ILE:HD12	1:C:447:ARG:CG	2.48	0.43
1:A:342:SER:O	1:A:363:LYS:HG3	2.19	0.43
1:A:370:PHE:CG	1:A:489:LEU:HA	2.53	0.43
1:B:795:LEU:HD13	1:B:888:LEU:HG	2.01	0.43
1:C:367:ASN:OD1	1:C:485:ASN:HB3	2.18	0.43
1:C:742:ASP:HA	1:C:772:ASN:HB3	2.01	0.43
1:B:283:LYS:NZ	1:B:329:SER:O	2.40	0.43
1:A:515:LYS:HE2	1:A:547:GLU:OE2	2.19	0.43
1:A:765:LEU:HD23	1:A:765:LEU:HA	1.88	0.43
1:C:349:ARG:HH11	1:C:371:ASN:ND2	2.17	0.43
1:C:535:ALA:HB2	1:C:554:GLN:CD	2.44	0.43
1:A:768:VAL:HG12	1:A:798:ASN:CG	2.44	0.43
1:B:500:PHE:O	1:B:522:SER:HB2	2.18	0.43
1:B:691:GLU:HA	1:B:710:ILE:O	2.18	0.43
1:C:320:ARG:CD	1:C:330:TRP:CE3	3.02	0.43
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.89	0.43
1:B:240:THR:HB	1:C:247:GLN:OE1	2.18	0.43
1:B:467:PHE:HB3	1:B:473:THR:HG21	2.00	0.43
1:B:489:LEU:N	1:B:517:THR:HG22	2.34	0.43
1:A:637:ILE:HG12	1:A:644:TYR:OH	2.19	0.43
1:B:855:ILE:HD13	1:B:855:ILE:HA	1.83	0.43
1:B:480:ILE:HB	1:B:508:TYR:O	2.19	0.42
1:B:742:ASP:HA	1:B:772:ASN:HB3	2.01	0.42
1:C:829:LEU:HD13	1:C:841:VAL:HG23	2.01	0.42
1:B:659:GLN:HB2	1:B:683:LEU:HA	2.00	0.42
1:C:573:CYS:HB2	1:C:601:CYS:SG	2.59	0.42
1:C:683:LEU:HD12	1:C:704:MET:HE1	2.01	0.42
1:A:650:ASP:HA	1:A:674:THR:O	2.19	0.42
1:B:609:SER:HA	1:B:633:ASP:O	2.20	0.42
1:A:801:ASP:OD2	1:A:826:ALA:HA	2.19	0.42
1:B:576:ASP:C	1:B:576:ASP:OD2	2.63	0.42
1:B:752:CYS:N	1:B:780:TRP:O	2.43	0.42
1:B:753:LEU:O	1:B:781:TYR:HA	2.19	0.42
1:B:533:ARG:H	1:B:556:TRP:HB2	1.83	0.42
1:B:730:PRO:HB2	1:B:759:SER:O	2.20	0.42
1:B:769:LYS:HA	1:B:796:ASN:O	2.19	0.42
1:A:648:LEU:HA	1:A:672:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:ASN:OD1	1:A:865:ASN:ND2	2.41	0.42
1:C:675:ASN:HA	1:C:697:ASN:O	2.20	0.42
1:A:507:VAL:HG12	1:A:508:TYR:CD2	2.55	0.42
1:A:535:ALA:HB2	1:A:554:GLN:CD	2.44	0.42
1:A:768:VAL:HG12	1:A:798:ASN:ND2	2.35	0.42
1:A:864:VAL:HG12	1:A:867:VAL:HB	2.01	0.42
1:B:357:THR:HA	1:B:379:SER:HB3	2.01	0.42
1:B:678:ARG:HG2	1:B:679:ASN:OD1	2.20	0.42
1:C:585:ASN:HA	1:C:614:HIS:CD2	2.55	0.42
1:A:348:LEU:O	1:A:368:LEU:HA	2.20	0.42
1:B:281:CYS:O	1:B:291:ALA:HB2	2.20	0.42
1:B:716:ASP:HA	1:B:749:GLN:HB2	2.02	0.42
1:C:341:LEU:HD13	1:C:362:ILE:HD13	2.02	0.42
1:C:342:SER:O	1:C:363:LYS:HG3	2.20	0.42
1:B:557:TYR:HD2	1:B:560:GLU:OE2	2.03	0.42
1:C:609:SER:HA	1:C:633:ASP:O	2.19	0.42
1:A:547:GLU:HA	1:A:571:ASP:O	2.20	0.42
1:A:845:ASP:O	1:A:884:TRP:HA	2.20	0.42
1:B:571:ASP:HA	1:B:599:ASN:O	2.20	0.42
1:C:612:ASP:CB	1:C:636:GLN:HB3	2.48	0.42
1:B:557:TYR:CE2	1:B:560:GLU:OE2	2.72	0.41
1:B:700:TYR:HA	1:B:720:ALA:O	2.20	0.41
1:A:629:LYS:HB2	1:C:462:ILE:HG21	2.01	0.41
1:B:773:MET:HE1	1:B:780:TRP:CE3	2.55	0.41
1:C:433:VAL:HG21	1:C:616:ILE:HG22	2.02	0.41
1:B:348:LEU:O	1:B:368:LEU:HA	2.21	0.41
1:C:354:LEU:HB2	1:C:376:LEU:CD2	2.50	0.41
1:A:225:LEU:HD22	1:A:227:GLN:HB2	2.02	0.41
1:A:350:PHE:HB2	1:A:370:PHE:CD2	2.55	0.41
1:A:612:ASP:CB	1:A:636:GLN:HB3	2.44	0.41
1:A:844:ILE:HG12	1:A:886:ILE:HG12	2.02	0.41
1:A:609:SER:HA	1:A:633:ASP:O	2.21	0.41
1:A:691:GLU:HA	1:A:710:ILE:O	2.20	0.41
1:B:506:MET:HG3	1:B:538:ILE:HD13	2.02	0.41
1:C:571:ASP:HA	1:C:599:ASN:O	2.20	0.41
1:C:691:GLU:HA	1:C:710:ILE:O	2.21	0.41
1:B:347:SER:HA	1:B:367:ASN:O	2.21	0.41
1:C:370:PHE:HB3	1:C:488:GLY:O	2.21	0.41
1:A:752:CYS:N	1:A:780:TRP:O	2.45	0.41
1:B:427:ILE:HG23	1:B:475:ILE:HG13	2.03	0.41
1:B:506:MET:HG3	1:B:538:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:845:ASP:O	1:B:884:TRP:HA	2.21	0.41
1:A:329:SER:OG	1:A:351:ASP:OD2	2.39	0.41
1:A:428:ARG:HD2	1:A:590:TYR:CE2	2.56	0.41
1:A:780:TRP:CD1	1:A:780:TRP:H	2.38	0.41
1:B:632:ASP:OD2	1:B:654:LEU:HD12	2.20	0.41
1:B:651:TYR:HA	1:B:675:ASN:O	2.20	0.41
1:C:491:PHE:HD1	1:C:519:LEU:HD23	1.85	0.41
1:C:519:LEU:HD13	1:C:535:ALA:HB1	2.03	0.41
1:C:648:LEU:HD21	1:C:650:ASP:HB2	2.02	0.41
1:A:397:THR:HA	1:A:475:ILE:O	2.21	0.41
1:B:246:ILE:HG23	1:C:250:PHE:HE2	1.85	0.41
1:B:675:ASN:HA	1:B:697:ASN:O	2.21	0.41
1:B:648:LEU:HA	1:B:672:LYS:O	2.21	0.40
1:C:848:ARG:HD3	1:C:855:ILE:HD12	2.03	0.40
1:A:442:LYS:HB2	1:A:590:TYR:CD1	2.56	0.40
1:B:398:THR:OG1	1:B:419:PHE:HE2	2.05	0.40
1:B:423:ASP:CG	1:B:477:LYS:HE2	2.46	0.40
1:C:321:ARG:HG3	1:C:321:ARG:NH1	2.36	0.40
1:C:397:THR:HB	1:C:474:LEU:HD11	2.04	0.40
1:C:593:PRO:O	1:C:618:ARG:N	2.44	0.40
1:C:638:ARG:HA	1:C:663:ALA:HB2	2.03	0.40
1:C:305:GLU:HG3	1:C:311:PHE:HA	2.04	0.40
1:A:442:LYS:O	1:A:590:TYR:HA	2.22	0.40
1:B:412:ASN:OD1	1:B:456:GLN:HG2	2.20	0.40
1:C:674:THR:HA	1:C:696:LEU:O	2.21	0.40
1:A:283:LYS:HE3	1:A:329:SER:O	2.21	0.40
1:B:388:CYS:SG	1:B:481:VAL:HG11	2.61	0.40
1:B:648:LEU:HD12	1:B:672:LYS:HD3	2.04	0.40
1:B:774:ALA:HA	1:B:800:LEU:O	2.21	0.40
1:B:780:TRP:CD1	1:B:780:TRP:H	2.39	0.40
1:B:815:LEU:HD12	1:B:878:ASP:OD1	2.21	0.40
1:C:240:THR:OG1	1:C:249:GLU:OE1	2.32	0.40
1:C:388:CYS:SG	1:C:481:VAL:HG11	2.62	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	666/922 (72%)	641 (96%)	25 (4%)	0	100	100
1	B	666/922 (72%)	638 (96%)	28 (4%)	0	100	100
1	C	666/922 (72%)	643 (96%)	23 (4%)	0	100	100
All	All	1998/2766 (72%)	1922 (96%)	76 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	588/804 (73%)	588 (100%)	0	100	100
1	B	588/804 (73%)	584 (99%)	4 (1%)	76	81
1	C	588/804 (73%)	587 (100%)	1 (0%)	87	92
All	All	1764/2412 (73%)	1759 (100%)	5 (0%)	84	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	498	THR
1	B	503	THR
1	B	509	CYS
1	B	726	SER
1	C	552	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	ASN
1	A	483	ASN
1	A	495	ASN
1	A	511	ASN
1	A	518	GLN
1	A	599	ASN
1	A	641	ASN
1	A	659	GLN
1	A	679	ASN
1	A	689	ASN
1	A	697	ASN
1	A	699	GLN
1	A	732	ASN
1	A	796	ASN
1	A	885	GLN
1	B	299	ASN
1	B	365	ASN
1	B	371	ASN
1	B	483	ASN
1	B	485	ASN
1	B	493	ASN
1	B	495	ASN
1	B	511	ASN
1	B	599	ASN
1	B	641	ASN
1	B	665	ASN
1	B	689	ASN
1	B	697	ASN
1	B	699	GLN
1	C	371	ASN
1	C	483	ASN
1	C	511	ASN
1	C	619	ASN
1	C	665	ASN
1	C	675	ASN
1	C	689	ASN
1	C	697	ASN
1	C	823	ASN
1	C	885	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.

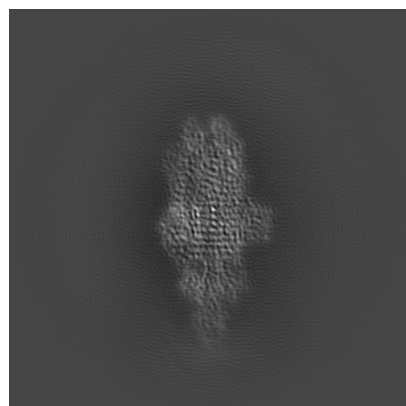
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62051. These allow visual inspection of the internal detail of the map and identification of artifacts.

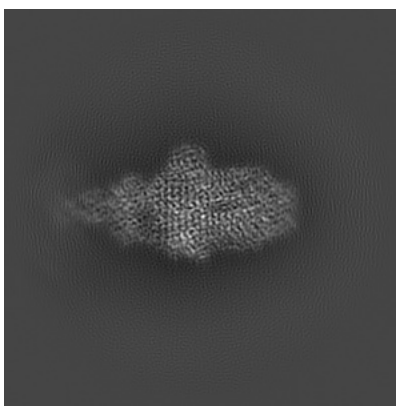
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

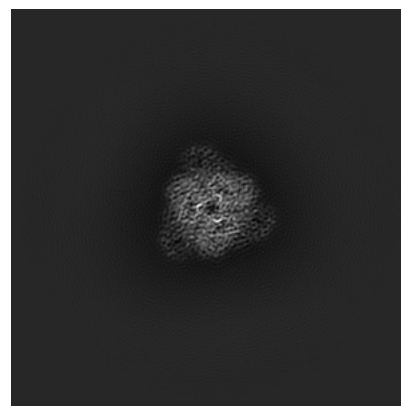
#### 6.1.1 Primary map



X

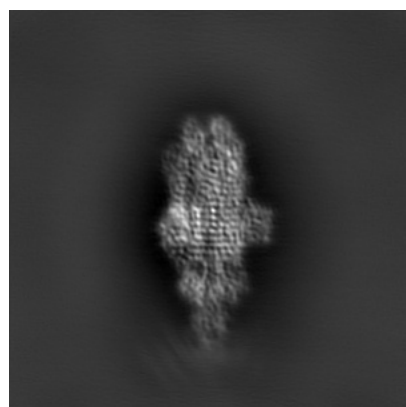


Y

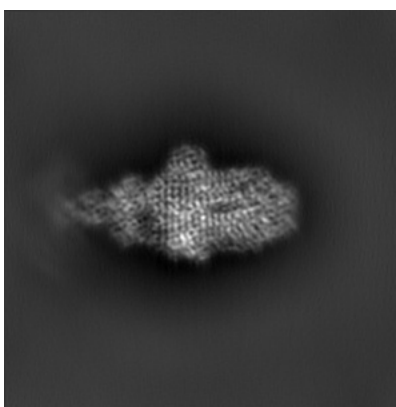


Z

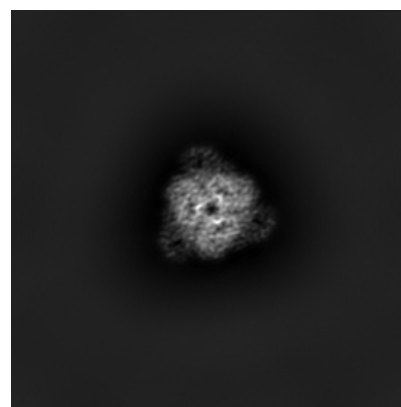
#### 6.1.2 Raw map



X



Y

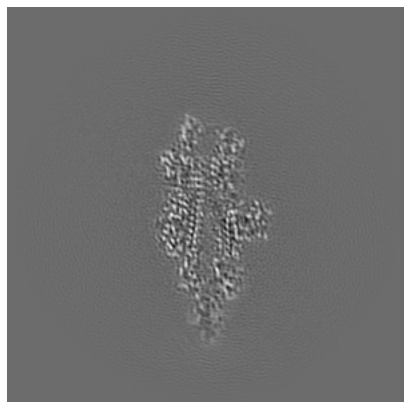


Z

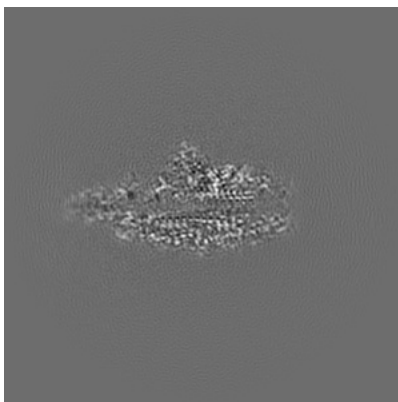
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

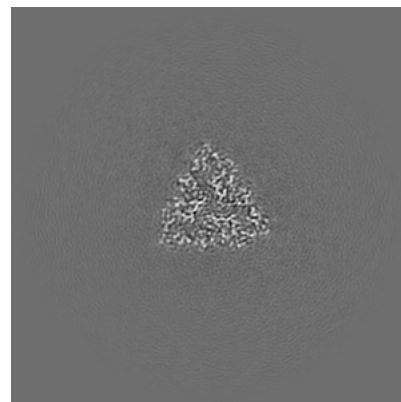
### 6.2.1 Primary map



X Index: 128

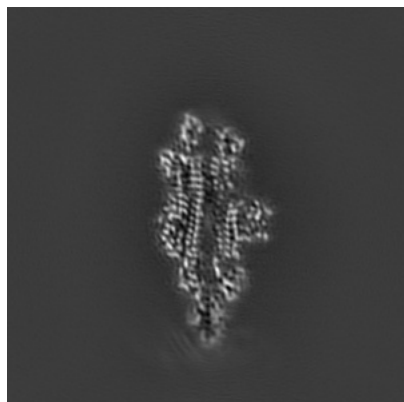


Y Index: 128

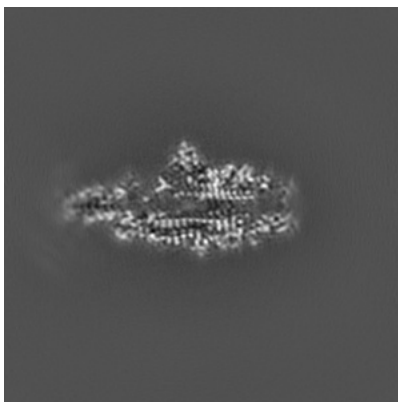


Z Index: 128

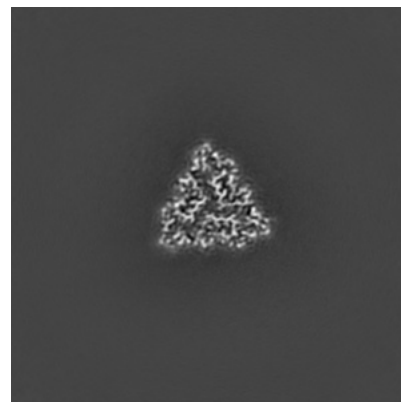
### 6.2.2 Raw map



X Index: 128



Y Index: 128

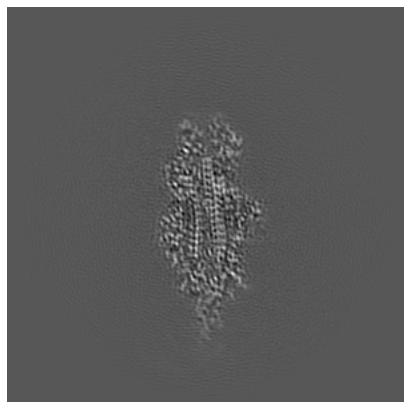


Z Index: 128

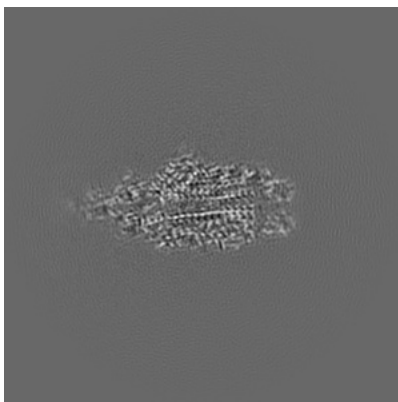
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

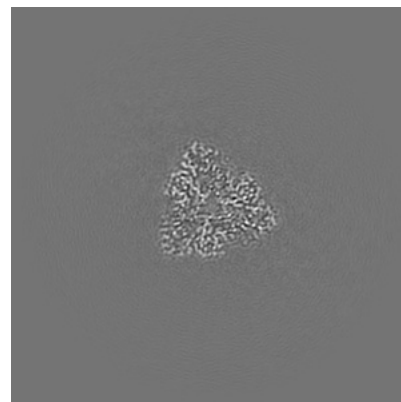
### 6.3.1 Primary map



X Index: 134



Y Index: 132

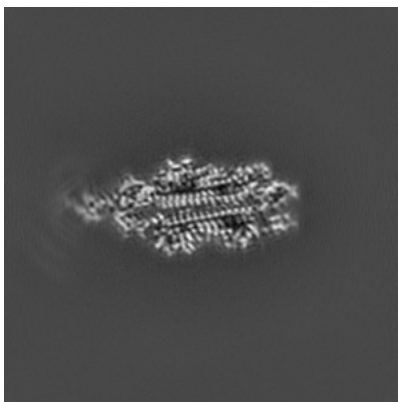


Z Index: 118

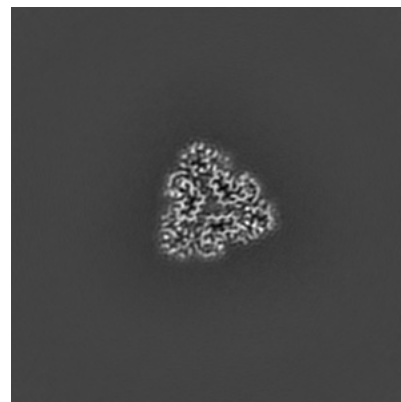
### 6.3.2 Raw map



X Index: 133



Y Index: 136

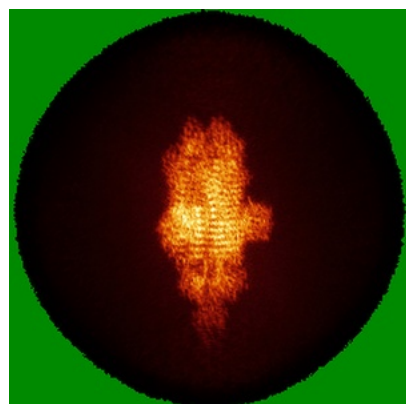


Z Index: 119

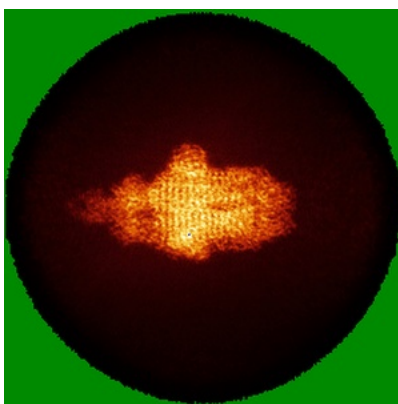
The images above show the largest variance slices of the map in three orthogonal directions.

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

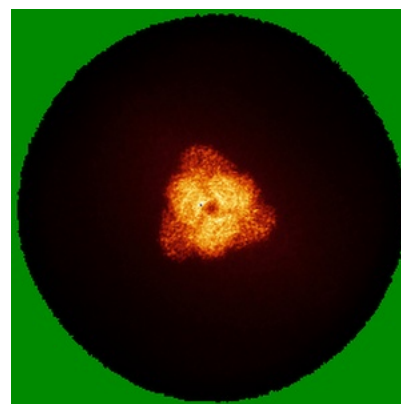
### 6.4.1 Primary map



X

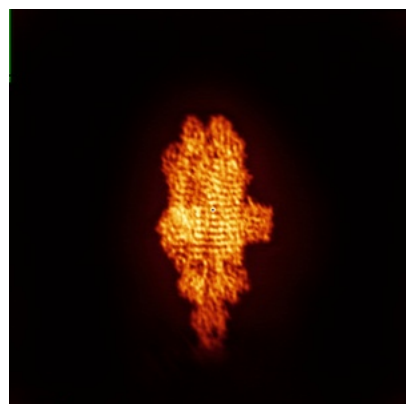


Y

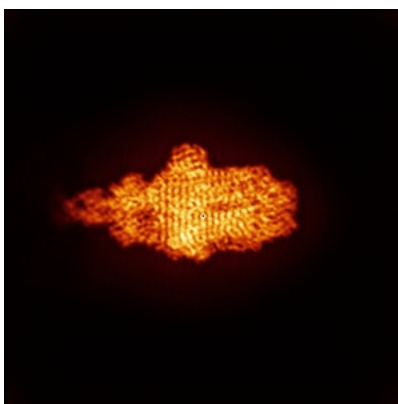


Z

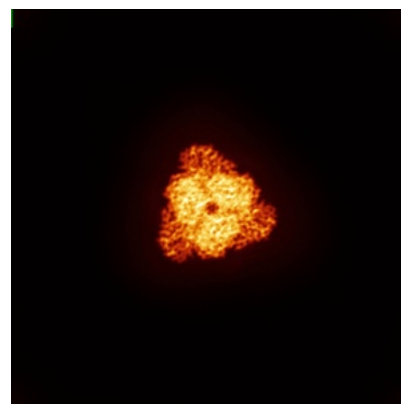
### 6.4.2 Raw map



X



Y

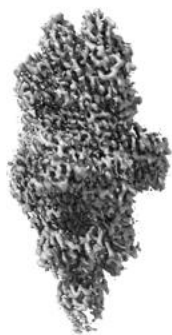


Z

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



X



Y



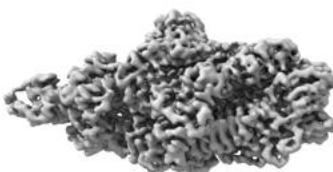
Z

The images above show the 3D surface view of the map at the recommended contour level 0.27. 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



X



Y



Z

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.

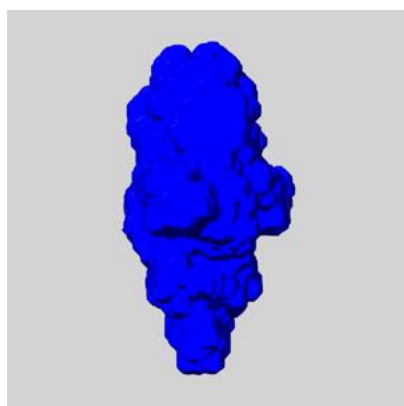
## 6.6 Mask visualisation [i](#)

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

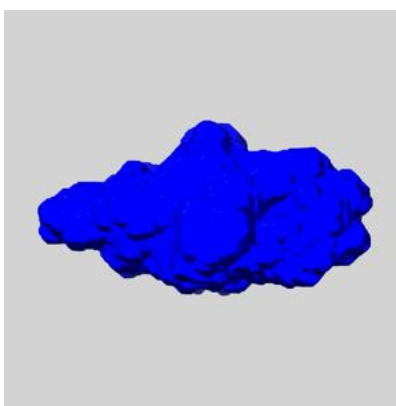
A mask typically either:

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

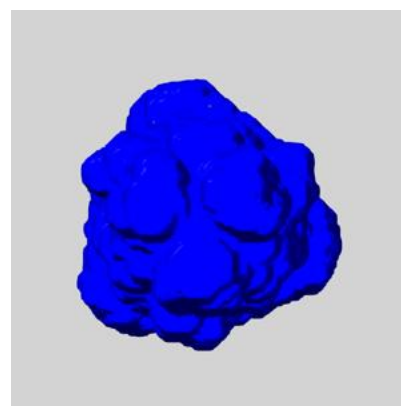
### 6.6.1 emd\_62051\_msk\_1.map [i](#)



X



Y

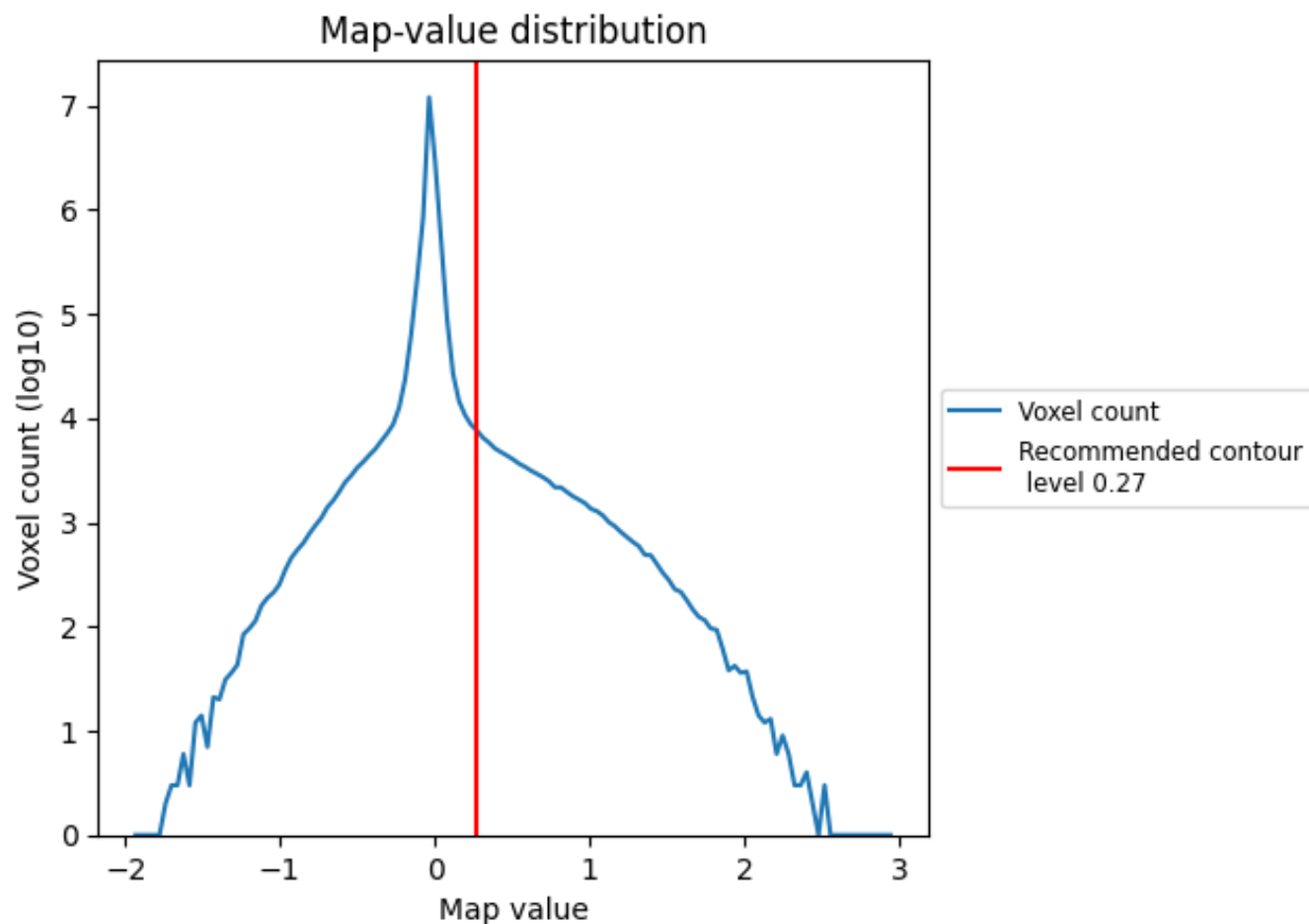


Z

## 7 Map analysis [i](#)

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

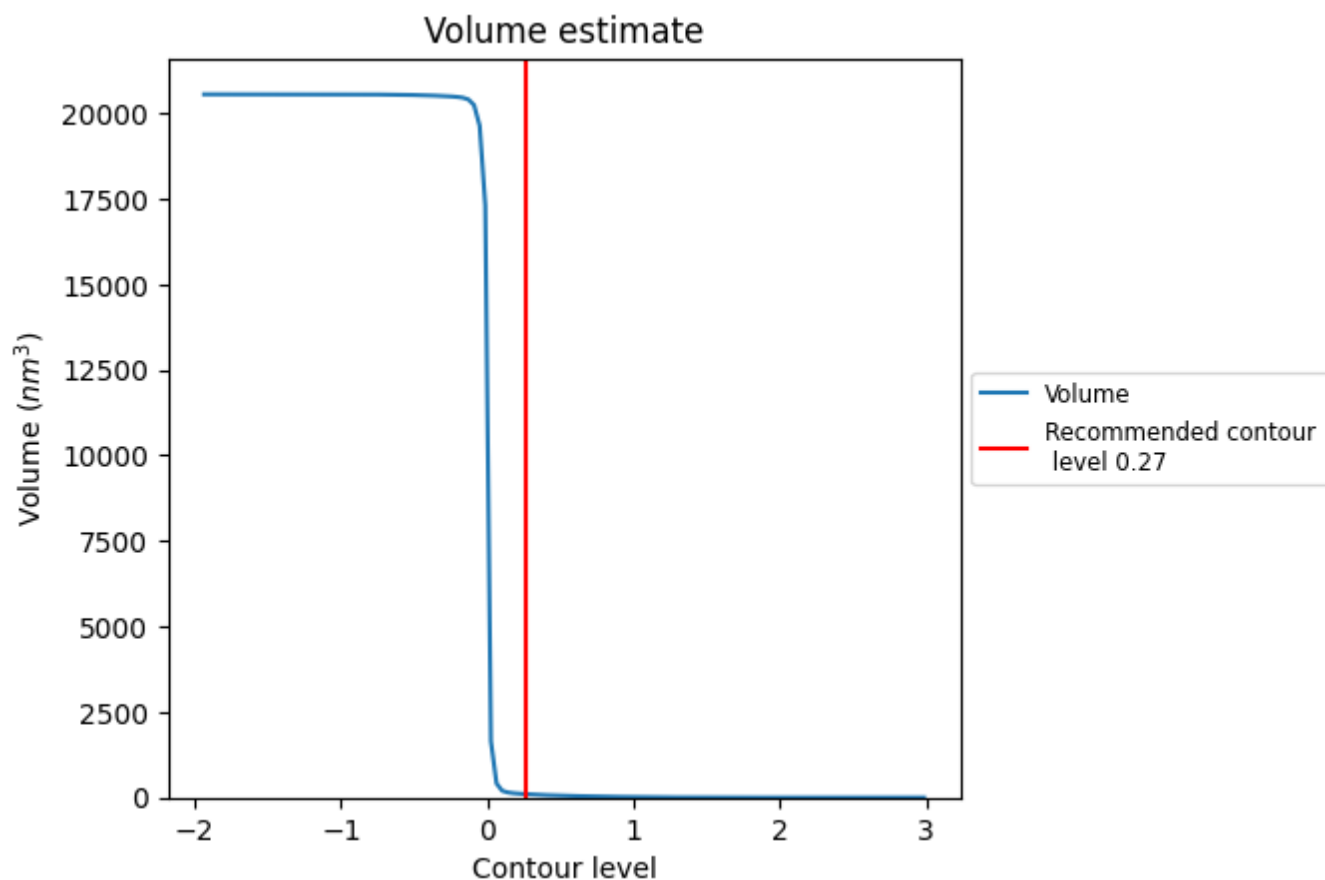
### 7.1 Map-value distribution [i](#)



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.



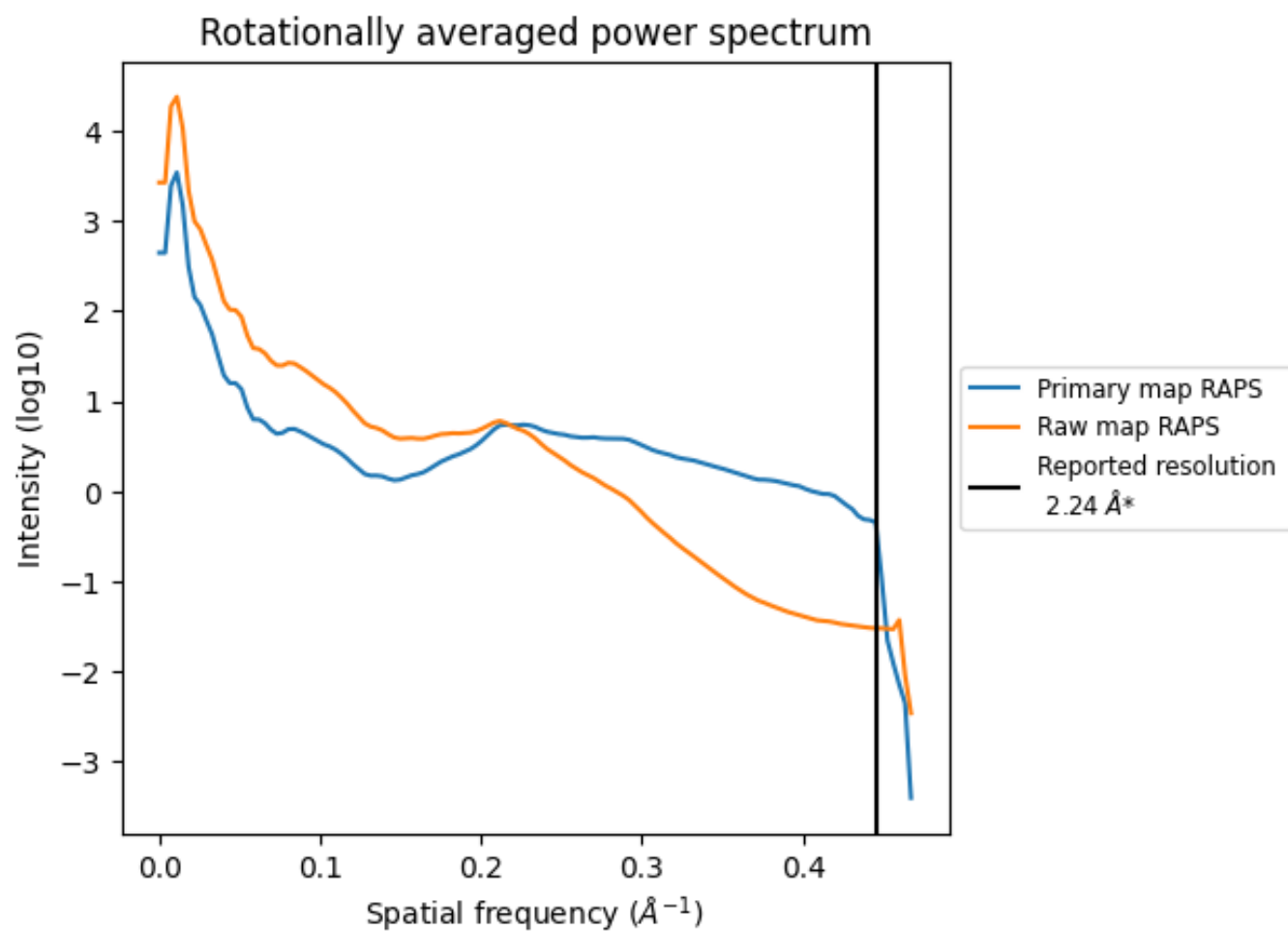
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 98  $\text{nm}^3$ ; this corresponds to an approximate mass of 89 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

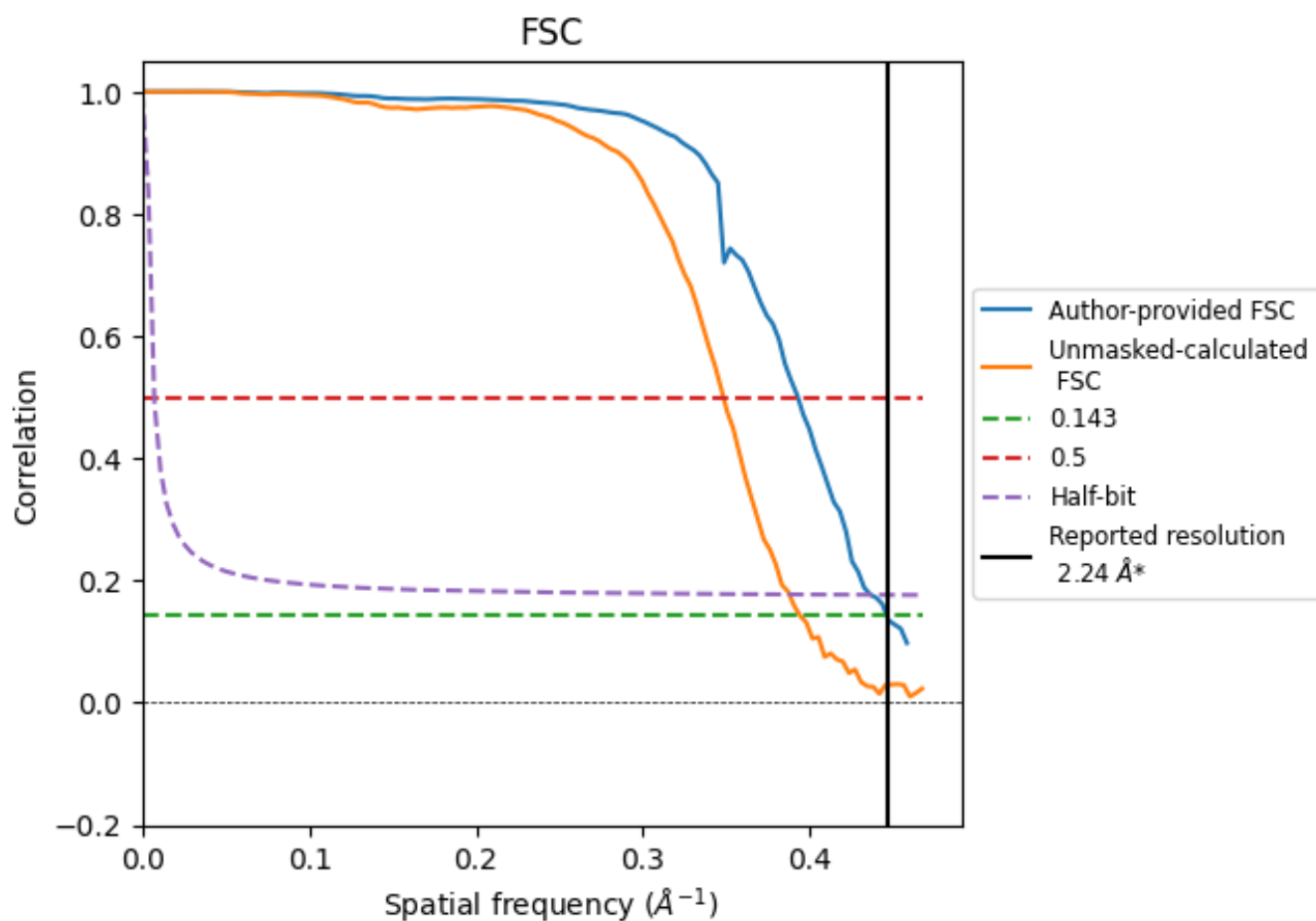


\*Reported resolution corresponds to spatial frequency of 0.446 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

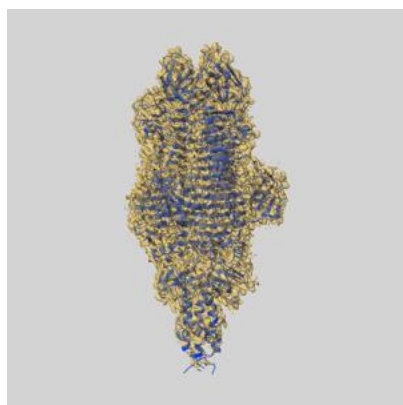
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.24	-	-
Author-provided FSC curve	2.24	2.55	2.29
Unmasked-calculated*	2.54	2.87	2.58

\*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 2.54 differs from the reported value 2.24 by more than 10 %

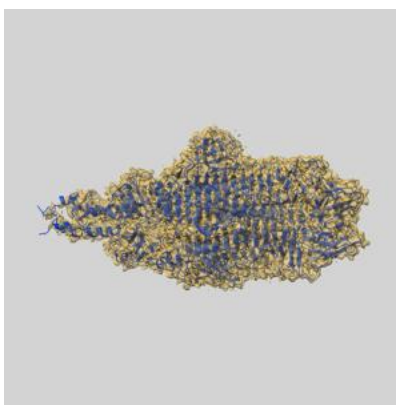
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62051 and PDB model 9K4A. Per-residue inclusion information can be found in section [3](#) on page [6](#).

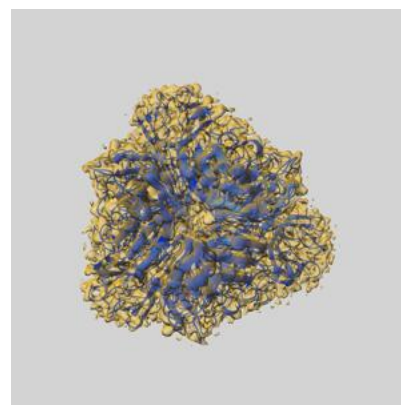
### 9.1 Map-model overlay [i](#)



X



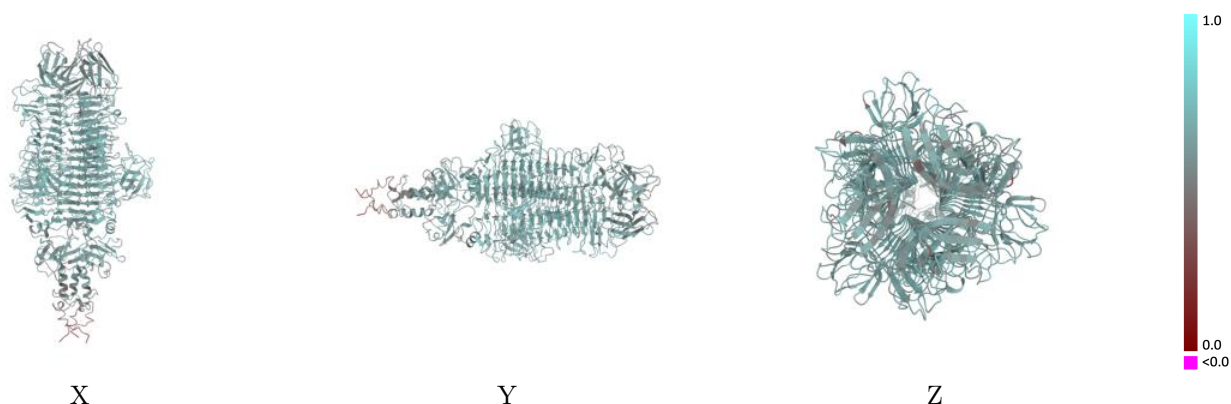
Y



Z

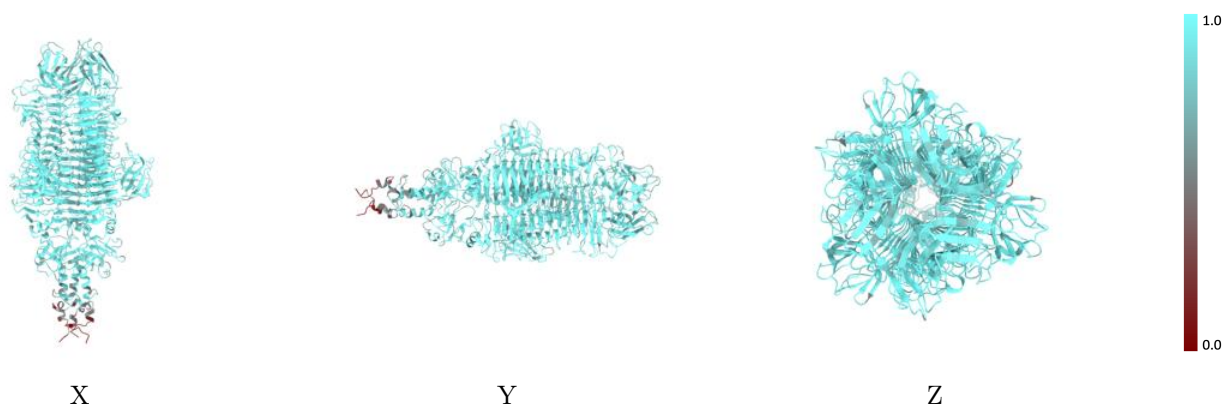
The images above show the 3D surface view of the map at the recommended contour level 0.27 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



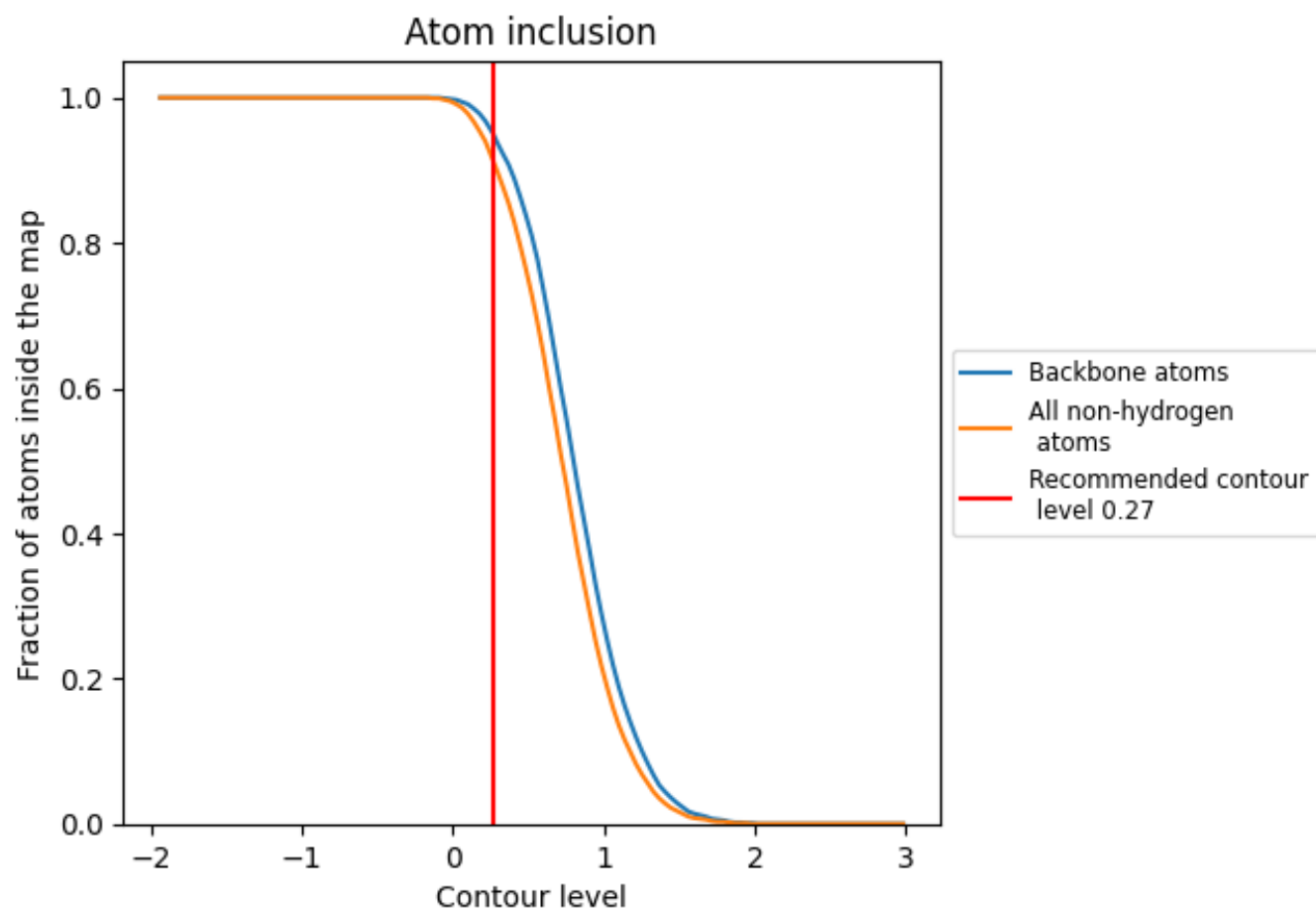
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.27).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9130	<div><div></div></div> 0.6110
A	<div><div></div></div> 0.9140	<div><div></div></div> 0.6080
B	<div><div></div></div> 0.9080	<div><div></div></div> 0.6080
C	<div><div></div></div> 0.9160	<div><div></div></div> 0.6190

