



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:44 PM UTC

PDB ID : 8R65 / pdb_00008r65
EMDB ID : EMD-18947
Title : 1918 H1N1 Viral polymerase heterotrimer in complex with 4 repeat serine-5 phosphorylated PolII peptide with ordered PB2 C-terminal domains
Authors : Keown, J.R.; Carrique, L.; Fodor, E.; Grimes, J.M.
Deposited on : 2023-11-20
Resolution : 4.23 Å(reported)
Based on initial model : 7NHX

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

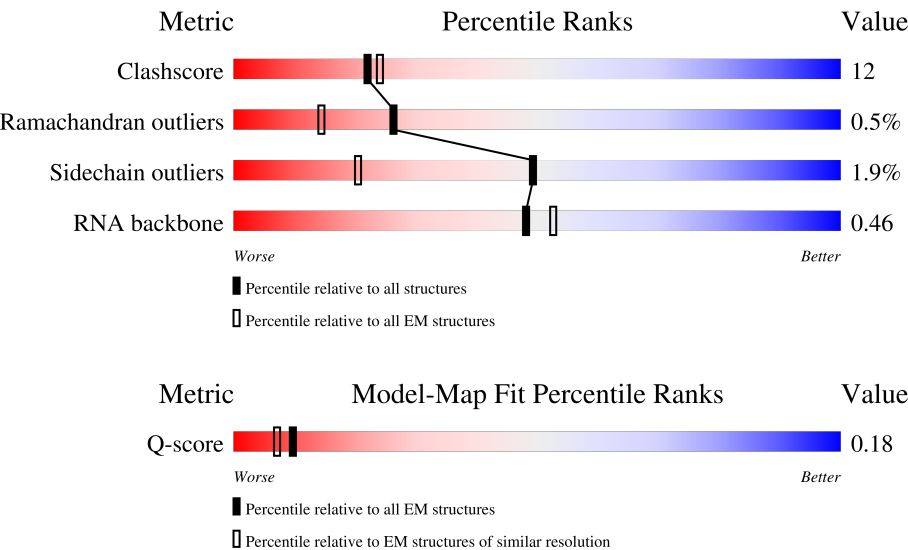
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

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

The reported resolution of this entry is 4.23 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	4685 (3.74 - 4.73)

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

Mol	Chain	Length	Quality of chain
1	A	716	
2	C	905	
3	D	15	

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Mol	Chain	Length	Quality of chain
4	E	17	6% 29% 18% 53%
5	X	28	32% 43% 14% 11%
6	B	757	78% 16% 5%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 35541 atoms, of which 17462 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	716	Total	C	H	N	O	S	0	0
			11519	3670	5724	985	1100	40		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	ALA	ASP	conflict	UNP Q3HM39

- Molecule 2 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	737	Total	C	H	N	O	S	0	0
			11651	3670	5805	1052	1084	40		

There are 146 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	760	GLU	-	expression tag	UNP Q3HM41
C	761	ASN	-	expression tag	UNP Q3HM41
C	762	LEU	-	expression tag	UNP Q3HM41
C	763	TYR	-	expression tag	UNP Q3HM41
C	764	PHE	-	expression tag	UNP Q3HM41
C	765	GLN	-	expression tag	UNP Q3HM41
C	766	GLY	-	expression tag	UNP Q3HM41
C	767	GLU	-	expression tag	UNP Q3HM41
C	768	LEU	-	expression tag	UNP Q3HM41
C	769	LYS	-	expression tag	UNP Q3HM41
C	770	THR	-	expression tag	UNP Q3HM41
C	771	ALA	-	expression tag	UNP Q3HM41
C	772	ALA	-	expression tag	UNP Q3HM41
C	773	LEU	-	expression tag	UNP Q3HM41
C	774	ALA	-	expression tag	UNP Q3HM41
C	775	GLN	-	expression tag	UNP Q3HM41

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Chain	Residue	Modelled	Actual	Comment	Reference
C	776	HIS	-	expression tag	UNP Q3HM41
C	777	ASP	-	expression tag	UNP Q3HM41
C	778	GLU	-	expression tag	UNP Q3HM41
C	779	ALA	-	expression tag	UNP Q3HM41
C	780	VAL	-	expression tag	UNP Q3HM41
C	781	ASP	-	expression tag	UNP Q3HM41
C	782	ASN	-	expression tag	UNP Q3HM41
C	783	LYS	-	expression tag	UNP Q3HM41
C	784	PHE	-	expression tag	UNP Q3HM41
C	785	ASN	-	expression tag	UNP Q3HM41
C	786	LYS	-	expression tag	UNP Q3HM41
C	787	GLU	-	expression tag	UNP Q3HM41
C	788	GLN	-	expression tag	UNP Q3HM41
C	789	GLN	-	expression tag	UNP Q3HM41
C	790	ASN	-	expression tag	UNP Q3HM41
C	791	ALA	-	expression tag	UNP Q3HM41
C	792	PHE	-	expression tag	UNP Q3HM41
C	793	TYR	-	expression tag	UNP Q3HM41
C	794	GLU	-	expression tag	UNP Q3HM41
C	795	ILE	-	expression tag	UNP Q3HM41
C	796	LEU	-	expression tag	UNP Q3HM41
C	797	HIS	-	expression tag	UNP Q3HM41
C	798	LEU	-	expression tag	UNP Q3HM41
C	799	PRO	-	expression tag	UNP Q3HM41
C	800	ASN	-	expression tag	UNP Q3HM41
C	801	LEU	-	expression tag	UNP Q3HM41
C	802	ASN	-	expression tag	UNP Q3HM41
C	803	GLU	-	expression tag	UNP Q3HM41
C	804	GLU	-	expression tag	UNP Q3HM41
C	805	GLN	-	expression tag	UNP Q3HM41
C	806	ARG	-	expression tag	UNP Q3HM41
C	807	ASN	-	expression tag	UNP Q3HM41
C	808	ALA	-	expression tag	UNP Q3HM41
C	809	PHE	-	expression tag	UNP Q3HM41
C	810	ILE	-	expression tag	UNP Q3HM41
C	811	GLN	-	expression tag	UNP Q3HM41
C	812	SER	-	expression tag	UNP Q3HM41
C	813	LEU	-	expression tag	UNP Q3HM41
C	814	LYS	-	expression tag	UNP Q3HM41
C	815	ASP	-	expression tag	UNP Q3HM41
C	816	ASP	-	expression tag	UNP Q3HM41
C	817	PRO	-	expression tag	UNP Q3HM41

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Chain	Residue	Modelled	Actual	Comment	Reference
C	818	SER	-	expression tag	UNP Q3HM41
C	819	GLN	-	expression tag	UNP Q3HM41
C	820	SER	-	expression tag	UNP Q3HM41
C	821	ALA	-	expression tag	UNP Q3HM41
C	822	ASN	-	expression tag	UNP Q3HM41
C	823	LEU	-	expression tag	UNP Q3HM41
C	824	LEU	-	expression tag	UNP Q3HM41
C	825	ALA	-	expression tag	UNP Q3HM41
C	826	GLU	-	expression tag	UNP Q3HM41
C	827	ALA	-	expression tag	UNP Q3HM41
C	828	LYS	-	expression tag	UNP Q3HM41
C	829	LYS	-	expression tag	UNP Q3HM41
C	830	LEU	-	expression tag	UNP Q3HM41
C	831	ASN	-	expression tag	UNP Q3HM41
C	832	ASP	-	expression tag	UNP Q3HM41
C	833	ALA	-	expression tag	UNP Q3HM41
C	834	GLN	-	expression tag	UNP Q3HM41
C	835	ALA	-	expression tag	UNP Q3HM41
C	836	PRO	-	expression tag	UNP Q3HM41
C	837	LYS	-	expression tag	UNP Q3HM41
C	838	VAL	-	expression tag	UNP Q3HM41
C	839	ASP	-	expression tag	UNP Q3HM41
C	840	ASN	-	expression tag	UNP Q3HM41
C	841	LYS	-	expression tag	UNP Q3HM41
C	842	PHE	-	expression tag	UNP Q3HM41
C	843	ASN	-	expression tag	UNP Q3HM41
C	844	LYS	-	expression tag	UNP Q3HM41
C	845	GLU	-	expression tag	UNP Q3HM41
C	846	GLN	-	expression tag	UNP Q3HM41
C	847	GLN	-	expression tag	UNP Q3HM41
C	848	ASN	-	expression tag	UNP Q3HM41
C	849	ALA	-	expression tag	UNP Q3HM41
C	850	PHE	-	expression tag	UNP Q3HM41
C	851	TYR	-	expression tag	UNP Q3HM41
C	852	GLU	-	expression tag	UNP Q3HM41
C	853	ILE	-	expression tag	UNP Q3HM41
C	854	LEU	-	expression tag	UNP Q3HM41
C	855	HIS	-	expression tag	UNP Q3HM41
C	856	LEU	-	expression tag	UNP Q3HM41
C	857	PRO	-	expression tag	UNP Q3HM41
C	858	ASN	-	expression tag	UNP Q3HM41
C	859	LEU	-	expression tag	UNP Q3HM41

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Chain	Residue	Modelled	Actual	Comment	Reference
C	860	ASN	-	expression tag	UNP Q3HM41
C	861	GLU	-	expression tag	UNP Q3HM41
C	862	GLU	-	expression tag	UNP Q3HM41
C	863	GLN	-	expression tag	UNP Q3HM41
C	864	ARG	-	expression tag	UNP Q3HM41
C	865	ASN	-	expression tag	UNP Q3HM41
C	866	ALA	-	expression tag	UNP Q3HM41
C	867	PHE	-	expression tag	UNP Q3HM41
C	868	ILE	-	expression tag	UNP Q3HM41
C	869	GLN	-	expression tag	UNP Q3HM41
C	870	SER	-	expression tag	UNP Q3HM41
C	871	LEU	-	expression tag	UNP Q3HM41
C	872	LYS	-	expression tag	UNP Q3HM41
C	873	ALA	-	expression tag	UNP Q3HM41
C	874	ASP	-	expression tag	UNP Q3HM41
C	875	PRO	-	expression tag	UNP Q3HM41
C	876	SER	-	expression tag	UNP Q3HM41
C	877	GLN	-	expression tag	UNP Q3HM41
C	878	SER	-	expression tag	UNP Q3HM41
C	879	ALA	-	expression tag	UNP Q3HM41
C	880	ASN	-	expression tag	UNP Q3HM41
C	881	LEU	-	expression tag	UNP Q3HM41
C	882	LEU	-	expression tag	UNP Q3HM41
C	883	ALA	-	expression tag	UNP Q3HM41
C	884	GLU	-	expression tag	UNP Q3HM41
C	885	ALA	-	expression tag	UNP Q3HM41
C	886	LYS	-	expression tag	UNP Q3HM41
C	887	LYS	-	expression tag	UNP Q3HM41
C	888	LEU	-	expression tag	UNP Q3HM41
C	889	ASN	-	expression tag	UNP Q3HM41
C	890	GLY	-	expression tag	UNP Q3HM41
C	891	ALA	-	expression tag	UNP Q3HM41
C	892	GLN	-	expression tag	UNP Q3HM41
C	893	ALA	-	expression tag	UNP Q3HM41
C	894	PRO	-	expression tag	UNP Q3HM41
C	895	LYS	-	expression tag	UNP Q3HM41
C	896	VAL	-	expression tag	UNP Q3HM41
C	897	ASP	-	expression tag	UNP Q3HM41
C	898	ALA	-	expression tag	UNP Q3HM41
C	899	ASN	-	expression tag	UNP Q3HM41
C	900	SER	-	expression tag	UNP Q3HM41
C	901	ALA	-	expression tag	UNP Q3HM41

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Chain	Residue	Modelled	Actual	Comment	Reference
C	902	GLY	-	expression tag	UNP Q3HM41
C	903	LYS	-	expression tag	UNP Q3HM41
C	904	SER	-	expression tag	UNP Q3HM41
C	905	THR	-	expression tag	UNP Q3HM41

- Molecule 3 is a RNA chain called RNA (5'-R(P*AP*GP*UP*AP*GP*AP*AP*AP*CP*AP*AP*GP*GP*CP*C)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	15	Total	C	H	N	O	P	0	0
			491	146	165	66	99	15		

- Molecule 4 is a RNA chain called RNA (5'-R(P*GP*GP*CP*CP*UP*GP*CP*U)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	8	Total	C	H	N	O	P	0	0
			255	75	86	28	58	8		

- Molecule 5 is a protein called RNA polymerase II 4 repeat peptide with serine5 phosphorylation.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	25	Total	C	N	O	P	0	0
			197	117	25	52	3		

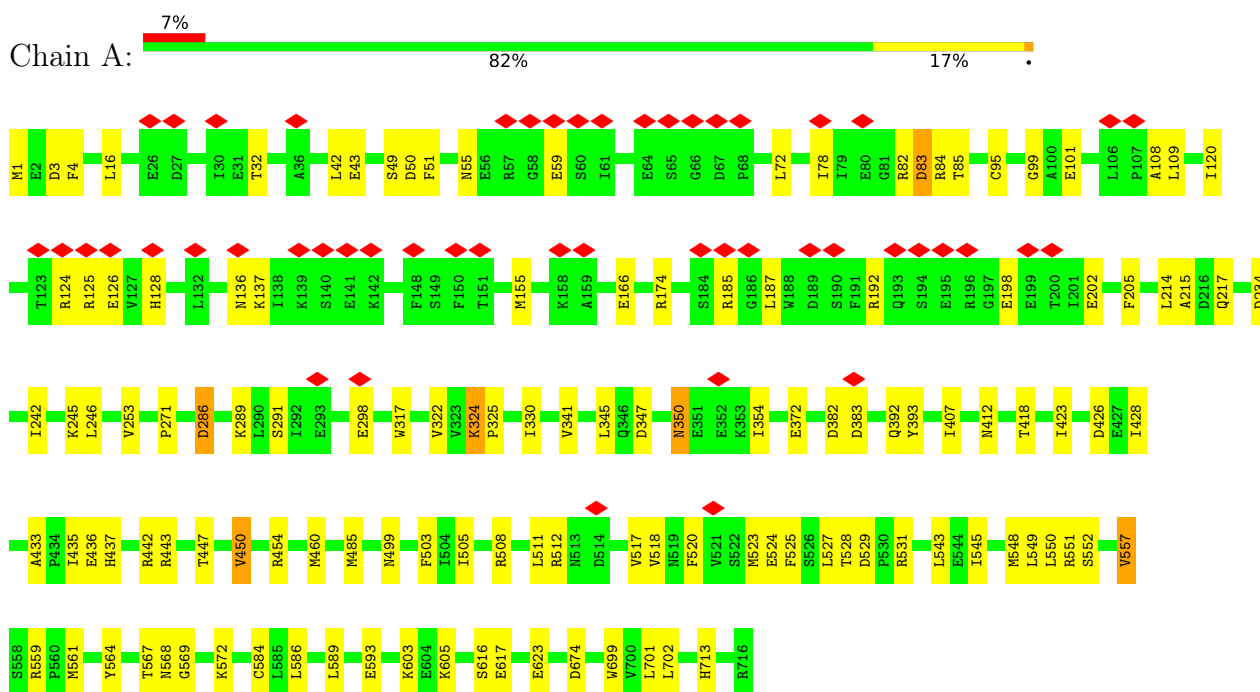
- Molecule 6 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	B	718	Total	C	H	N	O	S	0	0
			11428	3614	5682	1005	1083	44		

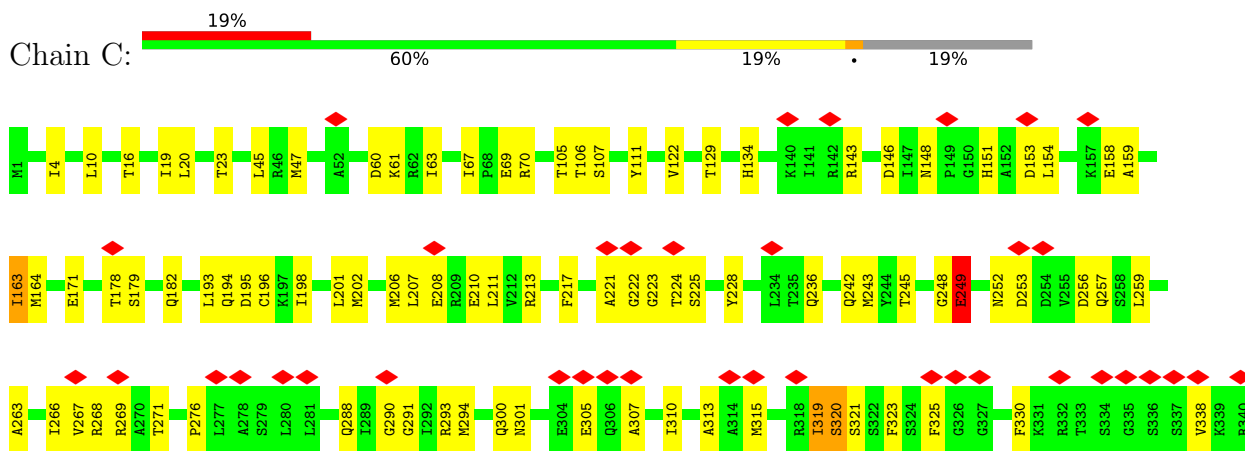
3 Residue-property plots

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: Polymerase acidic protein



• Molecule 2: Polymerase basic protein 2

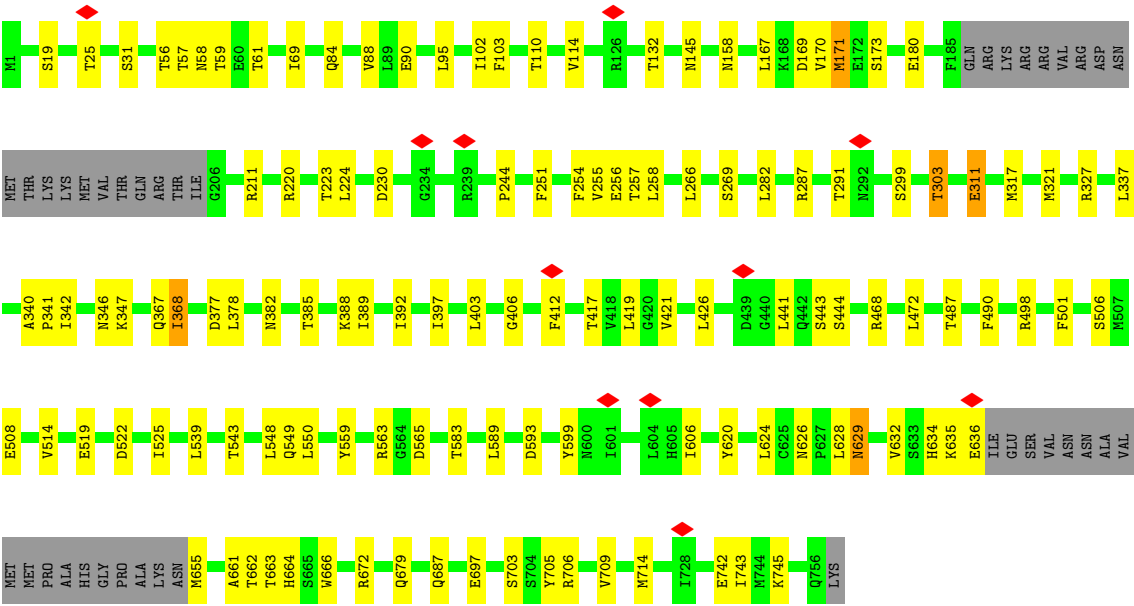


Chain B:

78%

16%

• 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16121	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.735	Depositor
Minimum map value	-0.245	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.144	Depositor
Map size (Å)	268.8, 268.8, 268.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.19	0/5918	0.29	0/7975
2	C	0.31	1/5944 (0.0%)	0.49	5/8017 (0.1%)
3	D	0.22	0/366	0.26	0/569
4	E	0.15	0/187	0.26	0/289
5	X	0.20	0/174	0.49	0/237
6	B	0.20	0/5858	0.28	0/7897
All	All	0.23	1/18447 (0.0%)	0.37	5/24984 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	319	ILE	C-O	-6.83	1.16	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	536	MET	N-CA-C	9.91	121.75	108.07
2	C	542	PRO	N-CA-C	-7.66	102.89	113.53
2	C	543	GLU	N-CA-C	-6.47	103.92	112.34
2	C	319	ILE	CA-C-O	-5.88	113.56	121.32
2	C	534	SER	N-CA-C	-5.10	105.16	111.33

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	422	ASN	Sidechain
2	C	493	ARG	Sidechain

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	A	5795	5724	5733	103	0
2	C	5846	5805	5964	229	0
3	D	326	165	165	5	0
4	E	169	86	87	3	0
5	X	197	0	161	15	0
6	B	5746	5682	5721	105	0
All	All	18079	17462	17831	414	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 12.

All (414) 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:437:HIS:CE1	2:C:646:ARG:HH12	1.39	1.40
2:C:223:GLY:N	2:C:525:GLU:OE2	1.64	1.29
2:C:243:MET:SD	2:C:530:THR:HG23	1.81	1.21
2:C:276:PRO:HB3	2:C:502:LEU:HD11	1.31	1.12
2:C:228:TYR:CE2	2:C:527:LEU:HA	1.87	1.09
1:A:437:HIS:CE1	2:C:646:ARG:NH1	2.21	1.08
2:C:271:THR:HG22	2:C:515:PRO:HB3	1.14	1.07
2:C:143:ARG:HH22	2:C:524:THR:CG2	1.72	1.03
2:C:266:ILE:HD12	2:C:269:ARG:HH12	1.23	1.00
2:C:225:SER:CB	2:C:526:LYS:HE2	1.93	0.99
2:C:225:SER:HB2	2:C:526:LYS:HE2	1.41	0.98
5:X:9:SER:HB3	5:X:12:SEP:HB2	1.42	0.98
2:C:143:ARG:NH2	2:C:524:THR:HG21	1.80	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4:ILE:HD13	6:B:743:ILE:HD11	1.48	0.95
2:C:271:THR:CG2	2:C:515:PRO:HB3	1.97	0.94
1:A:437:HIS:HE1	2:C:646:ARG:HH12	1.09	0.94
2:C:276:PRO:CB	2:C:502:LEU:HD11	1.99	0.93
2:C:143:ARG:NH1	2:C:524:THR:OG1	2.01	0.93
2:C:505:ARG:NH2	2:C:509:GLY:O	2.02	0.92
2:C:223:GLY:O	2:C:525:GLU:O	1.85	0.92
2:C:143:ARG:NH2	2:C:524:THR:CG2	2.35	0.90
2:C:243:MET:SD	2:C:530:THR:CG2	2.60	0.89
4:E:5:U:OP1	6:B:672:ARG:NH1	2.06	0.88
3:D:7:A:O2'	3:D:8:A:OP2	1.92	0.87
2:C:143:ARG:HH22	2:C:524:THR:HG23	1.41	0.85
2:C:158:GLU:OE2	2:C:182:GLN:NE2	2.10	0.84
6:B:180:GLU:OE1	6:B:211:ARG:NH1	2.11	0.83
1:A:372:GLU:OE2	1:A:508:ARG:NH1	2.14	0.81
2:C:143:ARG:HH12	2:C:524:THR:CB	1.92	0.80
4:E:6:G:OP2	4:E:6:G:N2	2.15	0.80
5:X:21:SER:O	5:X:23:SER:N	2.15	0.80
2:C:546:LEU:HD21	2:C:583:LEU:HD12	1.63	0.80
1:A:674:ASP:OD2	6:B:498:ARG:NH2	2.16	0.78
6:B:522:ASP:OD2	6:B:559:TYR:OH	1.99	0.78
6:B:636:GLU:N	6:B:636:GLU:OE1	2.17	0.77
1:A:435:ILE:HD11	2:C:242:GLN:HB2	1.68	0.75
6:B:299:SER:OG	6:B:487:THR:OG1	2.01	0.74
6:B:563:ARG:NH1	6:B:565:ASP:OD2	2.21	0.74
2:C:321:SER:HB3	2:C:494:VAL:HG13	1.70	0.74
2:C:360:TYR:OH	2:C:362:GLU:OE2	2.05	0.74
2:C:171:GLU:OE1	2:C:171:GLU:N	2.21	0.73
2:C:547:VAL:HG22	2:C:667:VAL:HB	1.69	0.73
6:B:58:ASN:ND2	6:B:61:THR:OG1	2.22	0.72
2:C:47:MET:HE1	6:B:666:TRP:HH2	1.55	0.71
2:C:266:ILE:HD12	2:C:269:ARG:NH1	2.04	0.71
2:C:208:GLU:OE1	6:B:705:TYR:OH	2.05	0.71
2:C:146:ASP:OD2	2:C:213:ARG:NH2	2.23	0.70
6:B:311:GLU:N	6:B:311:GLU:OE1	2.24	0.70
2:C:546:LEU:HD21	2:C:583:LEU:CD1	2.22	0.70
2:C:63:ILE:CD1	2:C:67:ILE:HD12	2.21	0.70
6:B:321:MET:HE2	6:B:419:LEU:HD13	1.73	0.70
1:A:545:ILE:HD11	1:A:561:MET:HE2	1.75	0.69
2:C:222:GLY:C	2:C:525:GLU:OE2	2.35	0.69
6:B:628:LEU:HD23	6:B:628:LEU:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLN:NE2	6:B:382:ASN:OD1	2.26	0.69
2:C:20:LEU:HD13	6:B:714:MET:HE3	1.74	0.69
2:C:223:GLY:O	2:C:224:THR:OG1	2.09	0.69
6:B:170:VAL:O	6:B:173:SER:OG	2.09	0.69
6:B:377:ASP:OD1	6:B:378:LEU:N	2.26	0.69
5:X:8:TYR:HB3	5:X:10:PRO:HD3	1.75	0.68
2:C:540:ASN:HD22	2:C:545:VAL:HG23	1.57	0.68
2:C:342:GLU:OE1	2:C:344:VAL:HG23	1.92	0.68
6:B:626:ASN:O	6:B:629:ASN:ND2	2.27	0.68
6:B:347:LYS:NZ	6:B:406:GLY:O	2.27	0.67
1:A:298:GLU:N	1:A:298:GLU:OE1	2.26	0.67
2:C:288:GLN:N	2:C:288:GLN:OE1	2.27	0.67
2:C:143:ARG:CZ	2:C:524:THR:HG21	2.24	0.67
1:A:442:ARG:NH1	1:A:593:GLU:OE2	2.28	0.67
2:C:194:GLN:OE1	2:C:194:GLN:N	2.28	0.66
2:C:111:TYR:OH	6:B:661:ALA:O	2.14	0.66
6:B:110:THR:O	6:B:114:VAL:HG12	1.96	0.66
1:A:166:GLU:N	1:A:166:GLU:OE1	2.27	0.66
1:A:437:HIS:HE1	2:C:646:ARG:NH1	1.72	0.65
2:C:518:VAL:O	2:C:519:SER:C	2.39	0.65
1:A:1:MET:SD	1:A:32:THR:OG1	2.51	0.65
2:C:537:TRP:CD1	2:C:543:GLU:HB3	2.31	0.65
6:B:508:GLU:N	6:B:508:GLU:OE1	2.30	0.65
2:C:4:ILE:CD1	6:B:743:ILE:HD11	2.23	0.65
6:B:287:ARG:O	6:B:291:THR:OG1	2.13	0.65
2:C:344:VAL:HG12	2:C:345:LEU:N	2.13	0.64
2:C:537:TRP:CD1	2:C:537:TRP:N	2.65	0.64
2:C:222:GLY:HA2	2:C:525:GLU:OE2	1.97	0.64
2:C:542:PRO:HB3	2:C:546:LEU:HD12	1.80	0.64
2:C:537:TRP:CD1	2:C:543:GLU:CB	2.81	0.63
5:X:9:SER:HB3	5:X:12:SEP:CB	2.25	0.63
2:C:271:THR:HG22	2:C:515:PRO:CB	2.09	0.63
2:C:537:TRP:CG	2:C:543:GLU:HB2	2.34	0.63
5:X:5:SEP:O	5:X:8:TYR:N	2.32	0.63
1:A:341:VAL:CG2	1:A:505:ILE:HD11	2.30	0.62
2:C:276:PRO:CB	2:C:502:LEU:CD1	2.75	0.62
6:B:258:LEU:HD22	6:B:337:LEU:HD21	1.80	0.62
1:A:291:SER:OG	1:A:499:ASN:OD1	2.10	0.62
2:C:315:MET:SD	2:C:315:MET:N	2.73	0.62
1:A:437:HIS:CE1	2:C:646:ARG:HH22	2.18	0.62
2:C:60:ASP:OD1	2:C:61:LYS:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:5:G:OP2	3:D:5:G:N2	2.32	0.61
1:A:126:GLU:OE1	1:A:128:HIS:N	2.32	0.61
6:B:224:LEU:HD23	6:B:244:PRO:HA	1.82	0.61
5:X:5:SEP:O	5:X:8:TYR:HB2	2.01	0.61
2:C:194:GLN:NE2	2:C:195:ASP:OD1	2.33	0.61
2:C:305:GLU:OE1	2:C:307:ALA:N	2.33	0.61
2:C:722:ALA:O	2:C:733:LEU:HD12	2.01	0.61
6:B:340:ALA:HB3	6:B:341:PRO:HD3	1.82	0.61
6:B:110:THR:HG21	6:B:258:LEU:HA	1.83	0.60
1:A:128:HIS:HA	1:A:155:MET:HE1	1.83	0.60
2:C:225:SER:HA	2:C:526:LYS:HE3	1.83	0.60
2:C:313:ALA:HB2	2:C:319:ILE:CG2	2.31	0.60
2:C:320:SER:HA	2:C:493:ARG:HA	1.82	0.60
6:B:679:GLN:OE1	6:B:679:GLN:N	2.34	0.60
1:A:568:ASN:OD1	1:A:569:GLY:N	2.35	0.60
2:C:19:ILE:O	2:C:23:THR:HG22	2.02	0.59
2:C:267:VAL:O	2:C:271:THR:HG23	2.01	0.59
1:A:217:GLN:NE2	6:B:59:THR:OG1	2.32	0.59
2:C:344:VAL:HG12	2:C:345:LEU:H	1.67	0.59
2:C:463:ILE:HD11	2:C:478:VAL:O	2.03	0.59
1:A:125:ARG:NH1	1:A:192:ARG:O	2.36	0.59
6:B:266:LEU:HD13	6:B:421:VAL:HG11	1.84	0.59
2:C:268:ARG:O	2:C:271:THR:OG1	2.20	0.59
2:C:225:SER:HA	2:C:526:LYS:CE	2.31	0.59
6:B:347:LYS:NZ	6:B:403:LEU:O	2.26	0.59
2:C:498:ILE:HG22	2:C:499:ASP:O	2.02	0.59
2:C:540:ASN:HA	2:C:544:SER:CB	2.33	0.59
2:C:456:ASN:ND2	2:C:471:THR:O	2.36	0.58
2:C:488:TYR:CE2	2:C:489:SER:O	2.57	0.58
2:C:538:GLU:CG	2:C:539:VAL:H	2.14	0.58
2:C:463:ILE:HD13	2:C:478:VAL:HB	1.85	0.58
1:A:50:ASP:OD1	1:A:51:PHE:N	2.37	0.58
2:C:4:ILE:HD12	2:C:4:ILE:H	1.68	0.58
1:A:16:LEU:HD12	1:A:42:LEU:HD13	1.86	0.58
2:C:276:PRO:HB2	2:C:502:LEU:CG	2.33	0.58
2:C:538:GLU:HG3	2:C:539:VAL:H	1.69	0.58
1:A:43:GLU:OE2	1:A:174:ARG:NE	2.37	0.57
2:C:225:SER:CA	2:C:526:LYS:HE2	2.32	0.57
1:A:16:LEU:CD1	1:A:42:LEU:HD13	2.33	0.57
2:C:463:ILE:CD1	2:C:478:VAL:HB	2.34	0.57
2:C:293:ARG:HE	2:C:664:ARG:HG3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ASP:O	1:A:350:ASN:ND2	2.38	0.57
2:C:269:ARG:NE	2:C:531:TYR:OH	2.37	0.57
2:C:540:ASN:ND2	2:C:545:VAL:HG23	2.19	0.57
1:A:205:PHE:CZ	6:B:171:MET:HE1	2.40	0.57
1:A:525:PHE:HB3	1:A:561:MET:HE3	1.86	0.57
6:B:88:VAL:HG21	6:B:317:MET:SD	2.45	0.57
5:X:24:PRO:O	5:X:25:THR:HG22	2.05	0.56
1:A:428:ILE:HD11	6:B:548:LEU:HD23	1.87	0.56
2:C:222:GLY:CA	2:C:525:GLU:OE2	2.54	0.56
6:B:367:GLN:OE1	6:B:368:ILE:N	2.38	0.56
2:C:323:PHE:CD1	2:C:512:LEU:HA	2.40	0.56
2:C:221:ALA:O	2:C:236:GLN:NE2	2.39	0.56
1:A:234:ASP:OD1	6:B:327:ARG:HG2	2.06	0.56
2:C:443:LYS:O	2:C:447:GLN:OE1	2.23	0.56
2:C:463:ILE:HD12	2:C:474:SER:OG	2.06	0.56
1:A:341:VAL:HG21	1:A:505:ILE:HD11	1.87	0.56
2:C:544:SER:O	2:C:545:VAL:C	2.49	0.55
1:A:435:ILE:HD13	2:C:242:GLN:OE1	2.06	0.55
1:A:437:HIS:CE1	2:C:646:ARG:CZ	2.88	0.55
5:X:12:SEP:CB	5:X:13:PRO:HD3	2.36	0.55
2:C:581:GLN:OE1	2:C:624:ALA:HB2	2.07	0.55
2:C:537:TRP:CG	2:C:543:GLU:CB	2.89	0.55
2:C:164:MET:HE1	6:B:706:ARG:HH21	1.72	0.55
1:A:124:ARG:NH2	1:A:198:GLU:OE1	2.39	0.55
2:C:269:ARG:NH1	2:C:269:ARG:HB3	2.22	0.55
2:C:163:ILE:HD11	2:C:211:LEU:HD12	1.89	0.55
6:B:632:VAL:HG12	6:B:634:HIS:H	1.70	0.55
2:C:105:THR:O	2:C:106:THR:OG1	2.21	0.55
2:C:344:VAL:CG1	2:C:345:LEU:H	2.20	0.55
1:A:433:ALA:N	1:A:436:GLU:OE1	2.36	0.54
2:C:537:TRP:O	2:C:541:GLY:N	2.38	0.54
2:C:243:MET:CE	2:C:530:THR:HG23	2.37	0.54
2:C:547:VAL:HG22	2:C:667:VAL:CB	2.37	0.54
6:B:697:GLU:OE1	6:B:703:SER:OG	2.25	0.54
2:C:325:PHE:HB3	2:C:330:PHE:CE1	2.42	0.54
6:B:171:MET:HE2	6:B:251:PHE:HZ	1.72	0.54
6:B:321:MET:CE	6:B:419:LEU:HD13	2.38	0.54
1:A:382:ASP:OD1	1:A:383:ASP:N	2.41	0.54
1:A:214:LEU:HD22	6:B:346:ASN:ND2	2.23	0.54
6:B:655:MET:SD	6:B:655:MET:N	2.81	0.54
2:C:535:MET:SD	2:C:535:MET:N	2.81	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:148:ASN:OD1	2:C:151:HIS:N	2.42	0.53
2:C:163:ILE:HD12	2:C:207:LEU:HB3	1.90	0.53
2:C:268:ARG:NH1	2:C:520:GLU:HA	2.23	0.53
2:C:537:TRP:CD1	2:C:543:GLU:HB2	2.43	0.53
2:C:202:MET:HE1	6:B:635:LYS:HE2	1.91	0.53
2:C:313:ALA:HB2	2:C:319:ILE:HG23	1.89	0.53
2:C:323:PHE:HD1	2:C:512:LEU:HA	1.74	0.53
2:C:338:VAL:HB	2:C:358:GLU:OE1	2.09	0.53
2:C:543:GLU:HG3	2:C:668:LEU:HD23	1.90	0.53
1:A:246:LEU:HD12	6:B:472:LEU:HD11	1.91	0.53
2:C:542:PRO:C	2:C:544:SER:N	2.63	0.53
1:A:101:GLU:N	1:A:101:GLU:OE1	2.42	0.52
1:A:437:HIS:HE1	2:C:646:ARG:CZ	2.22	0.52
2:C:47:MET:HE2	6:B:559:TYR:CE2	2.45	0.52
1:A:108:ALA:C	1:A:109:LEU:HD12	2.35	0.52
1:A:450:VAL:HG21	1:A:589:LEU:HD11	1.91	0.52
2:C:547:VAL:HG23	2:C:667:VAL:HG12	1.90	0.52
6:B:132:THR:HG21	6:B:145:ASN:HB3	1.89	0.52
6:B:519:GLU:OE1	6:B:664:HIS:ND1	2.41	0.52
1:A:205:PHE:CE2	6:B:171:MET:HE1	2.45	0.52
6:B:583:THR:HG21	6:B:589:LEU:HD11	1.90	0.52
2:C:534:SER:O	2:C:536:MET:N	2.43	0.52
1:A:437:HIS:CE1	2:C:646:ARG:NH2	2.78	0.52
6:B:258:LEU:HD22	6:B:337:LEU:CD2	2.40	0.52
2:C:543:GLU:C	2:C:547:VAL:HB	2.36	0.51
1:A:324:LYS:NZ	1:A:325:PRO:O	2.41	0.51
1:A:528:THR:O	1:A:564:TYR:OH	2.28	0.51
2:C:153:ASP:O	2:C:154:LEU:HD23	2.11	0.51
2:C:276:PRO:HB2	2:C:502:LEU:HG	1.92	0.51
6:B:269:SER:HB2	6:B:421:VAL:HG21	1.91	0.51
1:A:322:VAL:HG22	1:A:543:LEU:CD2	2.41	0.51
2:C:547:VAL:CG2	2:C:667:VAL:HG12	2.41	0.51
2:C:538:GLU:OE2	2:C:539:VAL:HG23	2.10	0.51
2:C:143:ARG:NH1	2:C:524:THR:CB	2.71	0.51
2:C:344:VAL:CG1	2:C:345:LEU:N	2.73	0.51
6:B:282:LEU:HD23	6:B:501:PHE:HZ	1.73	0.51
2:C:310:ILE:HG13	2:C:513:LEU:HD13	1.92	0.51
6:B:303:THR:O	6:B:303:THR:OG1	2.26	0.50
6:B:95:LEU:HD11	6:B:266:LEU:HD21	1.93	0.50
1:A:517:VAL:HG11	3:D:2:G:H21	1.77	0.50
1:A:242:ILE:HD13	6:B:426:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:317:MET:HE2	6:B:317:MET:HA	1.94	0.50
2:C:129:THR:OG1	2:C:245:THR:OG1	2.29	0.50
2:C:228:TYR:HE2	2:C:527:LEU:HG	1.77	0.50
2:C:343:GLU:O	2:C:344:VAL:HG23	2.12	0.50
2:C:537:TRP:O	2:C:538:GLU:C	2.54	0.50
2:C:10:LEU:O	2:C:16:THR:OG1	2.28	0.50
2:C:537:TRP:CB	2:C:543:GLU:HB2	2.42	0.50
1:A:109:LEU:HD13	1:A:120:ILE:HD13	1.93	0.50
1:A:286:ASP:N	1:A:286:ASP:OD1	2.45	0.50
2:C:248:GLY:O	2:C:249:GLU:C	2.53	0.50
2:C:193:LEU:HD12	2:C:193:LEU:O	2.12	0.50
2:C:343:GLU:C	2:C:344:VAL:HG23	2.37	0.49
2:C:542:PRO:HG2	2:C:668:LEU:HD21	1.95	0.49
6:B:110:THR:HG22	6:B:257:THR:HG22	1.93	0.49
1:A:485:MET:HE1	1:A:524:GLU:OE2	2.12	0.49
1:A:512:ARG:NH2	4:E:5:U:O2	2.46	0.49
2:C:276:PRO:HD2	2:C:500:ARG:O	2.13	0.49
2:C:313:ALA:HA	2:C:319:ILE:CG1	2.43	0.49
6:B:397:ILE:HG23	6:B:397:ILE:O	2.13	0.49
6:B:624:LEU:O	6:B:663:THR:HG23	2.13	0.49
6:B:662:THR:HG22	6:B:663:THR:N	2.28	0.49
1:A:82:ARG:O	1:A:83:ASP:CB	2.60	0.49
2:C:617:LYS:NZ	2:C:649:VAL:O	2.46	0.49
2:C:196:CYS:SG	2:C:198:ILE:HG22	2.53	0.48
2:C:463:ILE:HD11	2:C:478:VAL:C	2.38	0.48
2:C:517:GLU:O	2:C:519:SER:N	2.46	0.48
2:C:468:THR:HG23	2:C:468:THR:O	2.13	0.48
2:C:538:GLU:CG	2:C:539:VAL:N	2.77	0.48
1:A:518:VAL:HG13	1:A:518:VAL:O	2.11	0.48
3:D:7:A:HO2'	3:D:8:A:P	2.29	0.48
2:C:506:ASP:HB3	2:C:510:ASN:OD1	2.13	0.48
6:B:171:MET:HE2	6:B:251:PHE:CZ	2.49	0.48
6:B:255:VAL:HG11	6:B:412:PHE:CE2	2.48	0.48
6:B:19:SER:OG	6:B:506:SER:OG	2.08	0.47
1:A:330:ILE:O	1:A:330:ILE:HG22	2.14	0.47
2:C:4:ILE:HD12	2:C:4:ILE:N	2.29	0.47
1:A:246:LEU:HD12	6:B:472:LEU:CD1	2.44	0.47
1:A:345:LEU:HD11	1:A:503:PHE:CZ	2.50	0.47
2:C:365:MET:SD	2:C:365:MET:N	2.88	0.47
2:C:463:ILE:HG22	2:C:464:LEU:N	2.28	0.47
6:B:388:LYS:O	6:B:392:ILE:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:547:VAL:CG2	2:C:667:VAL:CG1	2.93	0.47
6:B:167:LEU:O	6:B:171:MET:HE3	2.13	0.47
1:A:49:SER:OG	1:A:78:ILE:HD11	2.15	0.47
2:C:491:THR:C	2:C:492:GLU:CD	2.83	0.47
2:C:542:PRO:CB	2:C:546:LEU:HD12	2.42	0.47
2:C:343:GLU:O	2:C:344:VAL:CG2	2.63	0.47
2:C:505:ARG:HH12	2:C:511:VAL:HG22	1.80	0.47
2:C:547:VAL:HG22	2:C:667:VAL:CG1	2.45	0.47
3:D:14:C:H2'	3:D:15:C:O4'	2.15	0.47
1:A:527:LEU:HD11	1:A:548:MET:HE2	1.97	0.46
2:C:313:ALA:HA	2:C:319:ILE:HG12	1.97	0.46
2:C:370:ALA:O	2:C:371:THR:OG1	2.29	0.46
2:C:163:ILE:N	2:C:163:ILE:HD13	2.29	0.46
2:C:325:PHE:CZ	2:C:431:MET:HG3	2.50	0.46
2:C:394:ILE:HG22	2:C:398:ILE:HD12	1.96	0.46
2:C:540:ASN:C	2:C:544:SER:HB3	2.40	0.46
2:C:543:GLU:HA	2:C:547:VAL:CG2	2.44	0.46
6:B:282:LEU:HD21	6:B:490:PHE:CE1	2.50	0.46
2:C:122:VAL:HG22	6:B:606:ILE:HD13	1.97	0.46
2:C:342:GLU:OE1	2:C:343:GLU:N	2.49	0.46
2:C:545:VAL:HG12	2:C:546:LEU:N	2.30	0.46
2:C:464:LEU:O	2:C:464:LEU:HD12	2.16	0.46
2:C:499:ASP:OD1	2:C:500:ARG:N	2.46	0.46
6:B:624:LEU:HG	6:B:662:THR:HG23	1.98	0.46
6:B:282:LEU:HD23	6:B:501:PHE:CZ	2.51	0.46
1:A:253:VAL:O	6:B:468:ARG:NH1	2.47	0.45
1:A:552:SER:HB2	5:X:14:SER:HB2	1.99	0.45
2:C:512:LEU:HD23	2:C:513:LEU:HG	1.98	0.45
2:C:531:TYR:O	2:C:535:MET:HE3	2.15	0.45
2:C:541:GLY:C	2:C:544:SER:H	2.24	0.45
2:C:45:LEU:HD23	2:C:45:LEU:O	2.16	0.45
1:A:428:ILE:HD11	6:B:548:LEU:CD2	2.47	0.45
2:C:63:ILE:HD13	2:C:67:ILE:HD12	1.95	0.45
2:C:225:SER:CA	2:C:526:LYS:CE	2.94	0.45
1:A:289:LYS:NZ	5:X:19:SEP:HB2	2.31	0.45
2:C:458:MET:O	2:C:458:MET:HG2	2.16	0.45
1:A:95:CYS:O	1:A:99:GLY:N	2.45	0.45
2:C:201:LEU:HD23	2:C:201:LEU:O	2.15	0.45
2:C:504:VAL:HB	2:C:513:LEU:HB2	1.98	0.45
2:C:106:THR:HG22	2:C:107:SER:N	2.32	0.45
2:C:365:MET:CE	2:C:374:LEU:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LYS:NZ	6:B:84:GLN:OE1	2.44	0.45
2:C:134:HIS:CE1	2:C:535:MET:CG	3.00	0.45
2:C:256:ASP:OD1	2:C:257:GLN:N	2.50	0.45
6:B:389:ILE:HA	6:B:392:ILE:HG22	1.98	0.45
1:A:511:LEU:HD23	1:A:572:LYS:HB2	1.98	0.44
2:C:129:THR:HG1	2:C:245:THR:HG1	1.57	0.44
1:A:586:LEU:HD21	6:B:550:LEU:HD12	1.99	0.44
2:C:547:VAL:HG12	2:C:548:ASN:HD22	1.82	0.44
6:B:56:THR:OG1	6:B:57:THR:N	2.50	0.44
6:B:417:THR:O	6:B:421:VAL:HG23	2.16	0.44
1:A:550:LEU:HG	1:A:557:VAL:HG22	1.99	0.44
2:C:313:ALA:CB	2:C:319:ILE:HG12	2.48	0.44
2:C:537:TRP:N	2:C:537:TRP:HD1	2.15	0.44
5:X:8:TYR:CB	5:X:10:PRO:HD3	2.45	0.44
6:B:443:SER:O	6:B:444:SER:C	2.60	0.44
1:A:55:ASN:ND2	1:A:59:GLU:OE2	2.51	0.44
1:A:623:GLU:OE2	1:A:713:HIS:NE2	2.51	0.44
6:B:90:GLU:OE1	6:B:90:GLU:HA	2.18	0.44
2:C:259:LEU:HD12	2:C:294:MET:SD	2.58	0.44
2:C:368:ARG:NH1	2:C:519:SER:CB	2.80	0.44
2:C:506:ASP:CG	2:C:507:GLN:H	2.25	0.44
6:B:102:ILE:HG23	6:B:103:PHE:N	2.32	0.44
6:B:593:ASP:OD2	6:B:620:TYR:OH	2.34	0.44
1:A:616:SER:O	1:A:617:GLU:C	2.60	0.44
6:B:114:VAL:HG23	6:B:254:PHE:CZ	2.53	0.44
1:A:418:THR:HG22	1:A:454:ARG:NH2	2.33	0.44
6:B:539:LEU:HD11	6:B:543:THR:CG2	2.47	0.44
1:A:108:ALA:CB	1:A:109:LEU:HD12	2.48	0.43
1:A:423:ILE:HG13	1:A:460:MET:HE3	1.99	0.43
1:A:567:THR:HG22	1:A:568:ASN:N	2.33	0.43
2:C:542:PRO:O	2:C:547:VAL:N	2.50	0.43
1:A:185:ARG:HG3	1:A:187:LEU:HD23	2.00	0.43
1:A:699:TRP:CZ3	1:A:702:LEU:HD23	2.53	0.43
2:C:541:GLY:O	2:C:545:VAL:N	2.51	0.43
1:A:407:ILE:HG13	1:A:702:LEU:HD22	2.00	0.43
2:C:159:ALA:O	2:C:163:ILE:HG12	2.19	0.43
2:C:517:GLU:O	2:C:518:VAL:C	2.61	0.43
6:B:539:LEU:HD11	6:B:543:THR:HG22	1.99	0.43
1:A:548:MET:HE1	5:X:20:PRO:HG3	2.01	0.43
2:C:245:THR:HG21	2:C:291:GLY:N	2.33	0.43
2:C:595:PHE:O	2:C:599:LEU:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASP:OD1	1:A:84:ARG:N	2.52	0.43
2:C:276:PRO:HB2	2:C:502:LEU:HD21	2.01	0.43
2:C:399:ILE:O	2:C:403:VAL:HG23	2.17	0.43
2:C:525:GLU:OE1	2:C:525:GLU:N	2.48	0.43
6:B:220:ARG:O	6:B:223:THR:HG22	2.19	0.43
2:C:178:THR:HG23	2:C:179:SER:N	2.33	0.43
2:C:320:SER:O	2:C:494:VAL:HG22	2.18	0.43
2:C:519:SER:O	2:C:520:GLU:CB	2.66	0.43
6:B:303:THR:HG22	6:B:490:PHE:HB2	2.00	0.43
5:X:18:THR:O	5:X:20:PRO:HD3	2.18	0.43
6:B:255:VAL:HG21	6:B:340:ALA:HB3	2.00	0.43
1:A:443:ARG:O	1:A:447:THR:HG22	2.18	0.43
2:C:63:ILE:HD12	2:C:67:ILE:HD12	1.99	0.43
2:C:245:THR:CG2	2:C:290:GLY:C	2.92	0.43
2:C:338:VAL:HB	2:C:358:GLU:CD	2.44	0.43
2:C:452:GLU:HB3	2:C:453:PRO:CD	2.48	0.43
2:C:313:ALA:HB2	2:C:319:ILE:HG21	2.01	0.43
2:C:481:SER:OG	2:C:483:MET:HE3	2.18	0.43
5:X:4:THR:HG23	5:X:4:THR:O	2.19	0.43
1:A:527:LEU:HD22	1:A:559:ARG:HH11	1.84	0.42
1:A:603:LYS:O	1:A:605:LYS:N	2.46	0.42
6:B:282:LEU:HD21	6:B:490:PHE:HE1	1.83	0.42
1:A:584:CYS:SG	6:B:25:THR:HG21	2.58	0.42
6:B:69:ILE:HD12	6:B:317:MET:HE3	2.01	0.42
1:A:136:ASN:OD1	1:A:137:LYS:N	2.53	0.42
2:C:228:TYR:CZ	2:C:527:LEU:HA	2.46	0.42
6:B:514:VAL:O	6:B:514:VAL:HG23	2.20	0.42
1:A:437:HIS:HE1	2:C:646:ARG:NH2	2.17	0.42
1:A:72:LEU:H	1:A:72:LEU:HD12	1.85	0.42
1:A:354:ILE:N	1:A:354:ILE:HD12	2.34	0.42
2:C:263:ALA:HA	2:C:266:ILE:HG22	2.02	0.42
2:C:105:THR:OG1	2:C:106:THR:N	2.52	0.42
1:A:85:THR:CG2	6:B:709:VAL:HG23	2.50	0.42
1:A:505:ILE:HD12	1:A:523:MET:HE3	2.01	0.42
2:C:319:ILE:O	2:C:493:ARG:HB3	2.19	0.42
2:C:543:GLU:HA	2:C:547:VAL:HB	2.01	0.42
1:A:426:ASP:O	6:B:549:GLN:NE2	2.52	0.42
2:C:463:ILE:CG2	2:C:464:LEU:N	2.83	0.42
1:A:271:PRO:HD2	1:A:701:LEU:HD11	2.02	0.42
1:A:215:ALA:HB2	6:B:342:ILE:HD13	2.02	0.41
2:C:548:ASN:HD22	2:C:548:ASN:N	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:724:VAL:HG12	2:C:726:ILE:HG23	2.02	0.41
1:A:82:ARG:O	1:A:83:ASP:HB3	2.21	0.41
2:C:252:ASN:OD1	2:C:253:ASP:N	2.54	0.41
1:A:3:ASP:OD1	1:A:4:PHE:N	2.53	0.41
2:C:486:ASP:C	2:C:486:ASP:OD1	2.61	0.41
1:A:529:ASP:OD1	1:A:531:ARG:NE	2.40	0.41
2:C:365:MET:HE1	2:C:374:LEU:HB2	2.03	0.41
1:A:109:LEU:HD12	1:A:109:LEU:N	2.35	0.41
1:A:286:ASP:OD2	1:A:528:THR:HG21	2.20	0.41
2:C:495:VAL:C	2:C:496:VAL:HG13	2.45	0.41
2:C:531:TYR:O	2:C:535:MET:CE	2.68	0.41
2:C:717:ALA:N	2:C:720:GLU:OE2	2.54	0.41
6:B:110:THR:HG21	6:B:258:LEU:CA	2.50	0.41
1:A:16:LEU:HD11	1:A:42:LEU:HD13	2.02	0.41
1:A:317:TRP:HZ3	1:A:545:ILE:HD12	1.85	0.41
2:C:300:GLN:OE1	2:C:301:ASN:N	2.53	0.41
2:C:537:TRP:HB3	2:C:544:SER:N	2.36	0.41
2:C:547:VAL:HA	2:C:667:VAL:HG11	2.03	0.41
6:B:548:LEU:HD21	6:B:599:TYR:HB3	2.03	0.41
2:C:463:ILE:HD13	2:C:475:MET:HB2	2.03	0.40
6:B:25:THR:O	6:B:25:THR:HG22	2.20	0.40
6:B:31:SER:OG	6:B:230:ASP:OD1	2.29	0.40
6:B:171:MET:HE3	6:B:171:MET:HB2	1.96	0.40
1:A:520:PHE:CD1	1:A:520:PHE:O	2.75	0.40
2:C:543:GLU:CA	2:C:547:VAL:HB	2.51	0.40
1:A:202:GLU:N	1:A:202:GLU:OE1	2.54	0.40
2:C:330:PHE:CZ	2:C:365:MET:HG3	2.57	0.40
6:B:158:ASN:ND2	6:B:169:ASP:OD2	2.52	0.40
6:B:368:ILE:O	6:B:368:ILE:CG1	2.70	0.40
2:C:134:HIS:CE1	2:C:243:MET:HE3	2.57	0.40
5:X:22:TYR:CG	5:X:23:SER:N	2.89	0.40
6:B:742:GLU:O	6:B:745:LYS:HG2	2.21	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	714/716 (100%)	669 (94%)	44 (6%)	1 (0%)	48 82
2	C	735/905 (81%)	668 (91%)	58 (8%)	9 (1%)	10 42
5	X	20/28 (71%)	17 (85%)	2 (10%)	1 (5%)	1 16
6	B	712/757 (94%)	669 (94%)	43 (6%)	0	100 100
All	All	2181/2406 (91%)	2023 (93%)	147 (7%)	11 (0%)	26 62

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	249	GLU
2	C	519	SER
2	C	545	VAL
5	X	22	TYR
2	C	518	VAL
2	C	520	GLU
2	C	535	MET
2	C	492	GLU
2	C	533	SER
2	C	641	ARG
1	A	83	ASP

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	639/639 (100%)	630 (99%)	9 (1%)	59 71
2	C	646/788 (82%)	629 (97%)	17 (3%)	40 60
5	X	22/24 (92%)	22 (100%)	0	100 100
6	B	634/669 (95%)	624 (98%)	10 (2%)	55 69
All	All	1941/2120 (92%)	1905 (98%)	36 (2%)	49 66

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286	ASP
1	A	324	LYS
1	A	350	ASN
1	A	393	TYR
1	A	412	ASN
1	A	450	VAL
1	A	549	LEU
1	A	551	ARG
1	A	557	VAL
2	C	69	GLU
2	C	70	ARG
2	C	163	ILE
2	C	206	MET
2	C	210	GLU
2	C	217	PHE
2	C	249	GLU
2	C	320	SER
2	C	490	SER
2	C	492	GLU
2	C	493	ARG
2	C	518	VAL
2	C	537	TRP
2	C	538	GLU
2	C	540	ASN
2	C	547	VAL
2	C	640	VAL
6	B	171	MET
6	B	256	GLU
6	B	303	THR
6	B	311	GLU
6	B	368	ILE
6	B	385	THR
6	B	441	LEU
6	B	525	ILE
6	B	629	ASN
6	B	687	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN

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Mol	Chain	Res	Type
1	A	217	GLN
1	A	392	GLN
1	A	412	ASN
1	A	437	HIS
2	C	73	GLN
2	C	75	GLN
2	C	127	HIS
2	C	134	HIS
2	C	151	HIS
2	C	233	HIS
2	C	540	ASN
2	C	548	ASN
6	B	65	GLN
6	B	77	ASN
6	B	136	ASN
6	B	314	ASN
6	B	346	ASN
6	B	567	GLN
6	B	600	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	14/15 (93%)	3 (21%)	0
4	E	7/17 (41%)	1 (14%)	0
All	All	21/32 (65%)	4 (19%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	D	6	A
3	D	11	A
3	D	15	C
4	E	7	C

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
5	SEP	X	12	5	8,9,10	1.63	1 (12%)	7,12,14	1.45	1 (14%)
5	SEP	X	5	5	8,9,10	1.57	1 (12%)	7,12,14	1.45	1 (14%)
5	SEP	X	19	5	8,9,10	1.55	1 (12%)	7,12,14	1.38	1 (14%)

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
5	SEP	X	12	5	-	6/6/8/10	-
5	SEP	X	5	5	-	6/6/8/10	-
5	SEP	X	19	5	-	0/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	X	12	SEP	P-O1P	3.56	1.61	1.50
5	X	5	SEP	P-O1P	3.46	1.61	1.50
5	X	19	SEP	P-O1P	3.40	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	12	SEP	OG-CB-CA	3.34	111.39	108.14
5	X	5	SEP	OG-CB-CA	3.26	111.32	108.14
5	X	19	SEP	OG-CB-CA	3.00	111.06	108.14

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	X	5	SEP	N-CA-CB-OG
5	X	5	SEP	C-CA-CB-OG
5	X	5	SEP	CB-OG-P-O1P
5	X	5	SEP	CB-OG-P-O2P
5	X	5	SEP	CB-OG-P-O3P
5	X	12	SEP	N-CA-CB-OG
5	X	12	SEP	C-CA-CB-OG
5	X	12	SEP	CA-CB-OG-P
5	X	12	SEP	CB-OG-P-O1P
5	X	12	SEP	CB-OG-P-O2P
5	X	12	SEP	CB-OG-P-O3P
5	X	5	SEP	CA-CB-OG-P

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	X	12	SEP	3	0
5	X	5	SEP	2	0
5	X	19	SEP	1	0

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.

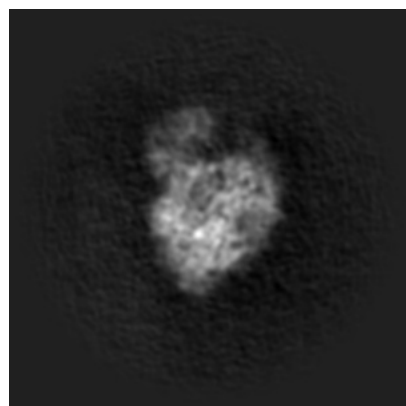
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18947. These allow visual inspection of the internal detail of the map and identification of artifacts.

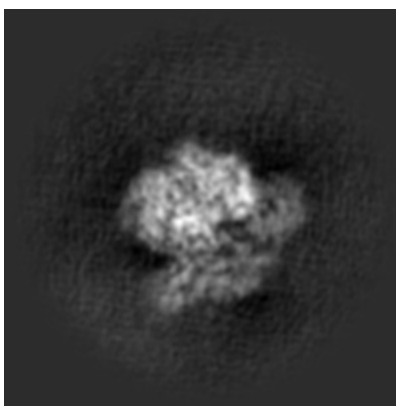
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

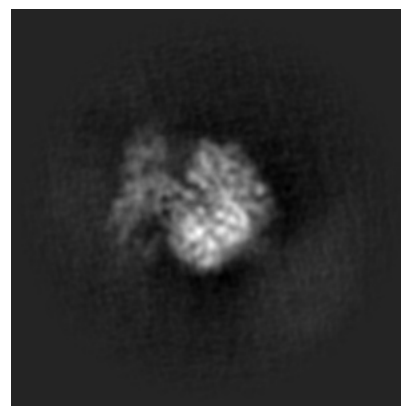
6.1.1 Primary map



X

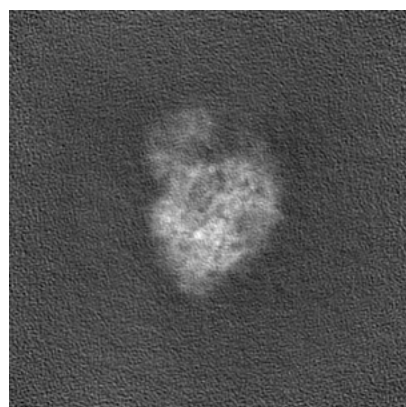


Y

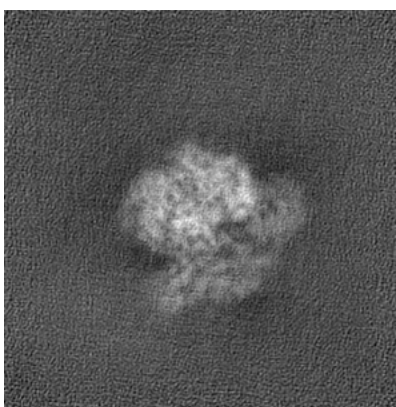


Z

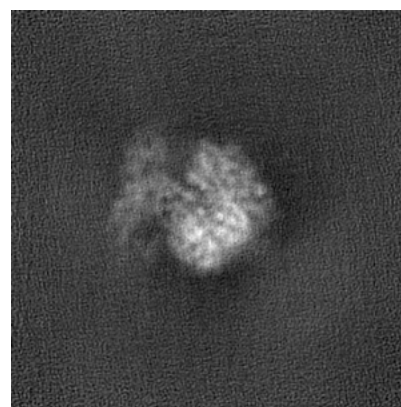
6.1.2 Raw map



X



Y

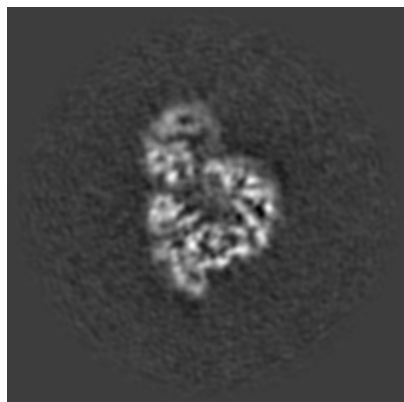


Z

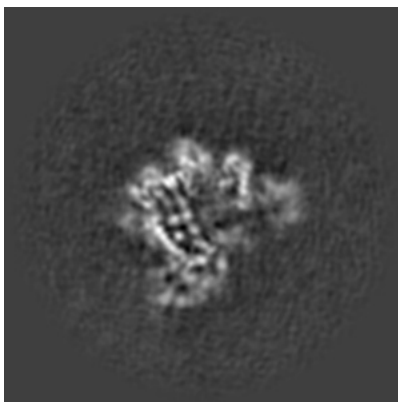
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

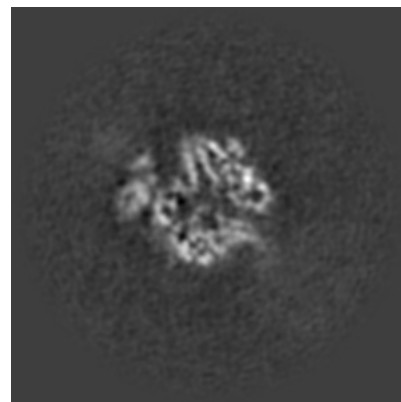
6.2.1 Primary map



X Index: 128

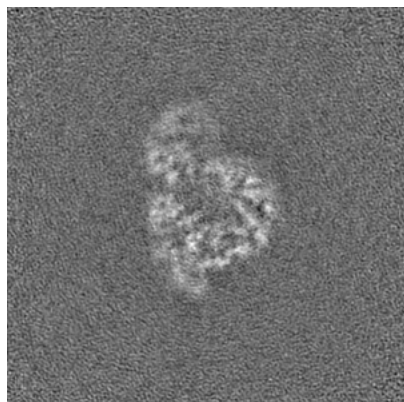


Y Index: 128

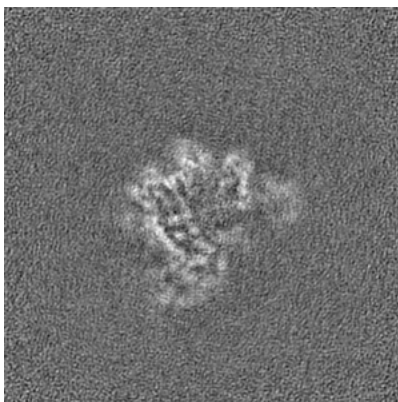


Z Index: 128

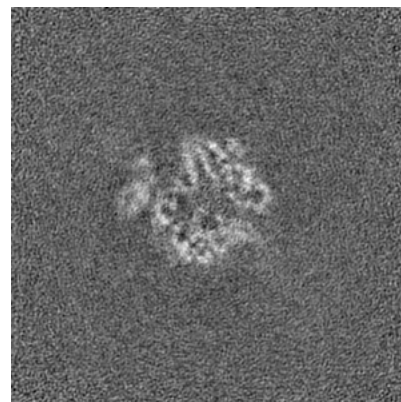
6.2.2 Raw map



X Index: 128



Y Index: 128

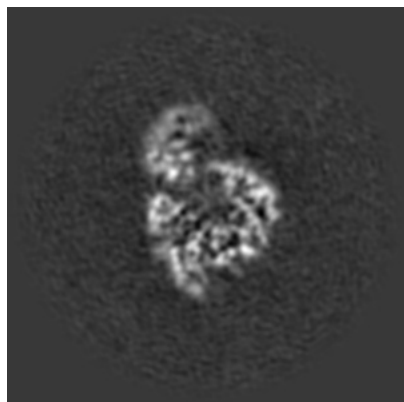


Z Index: 128

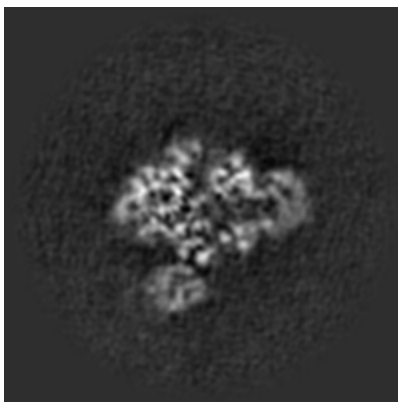
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

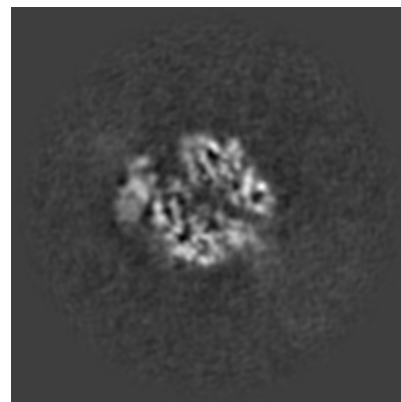
6.3.1 Primary map



X Index: 126

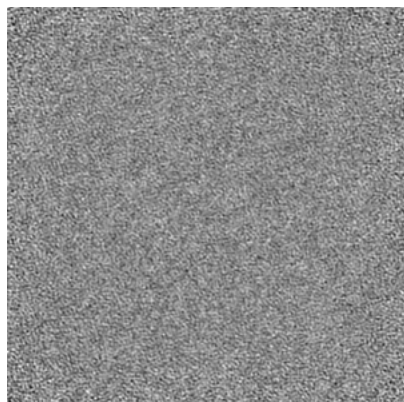


Y Index: 121

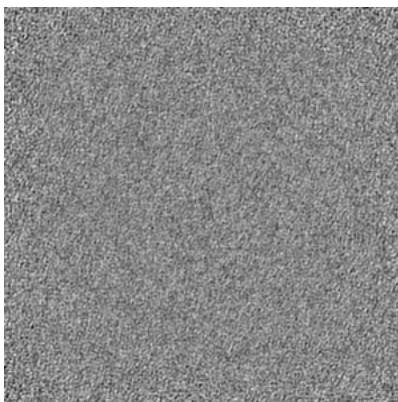


Z Index: 126

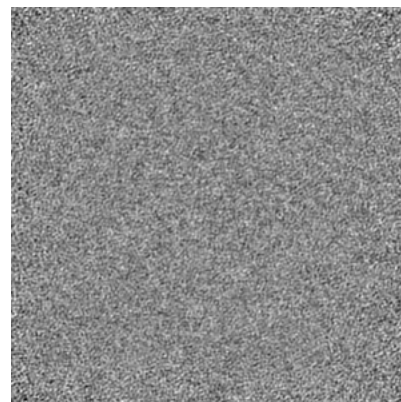
6.3.2 Raw map



X Index: 0



Y Index: 0

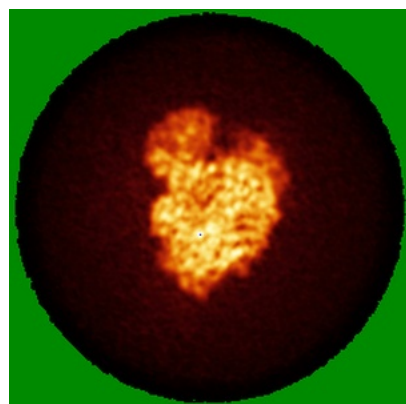


Z Index: 0

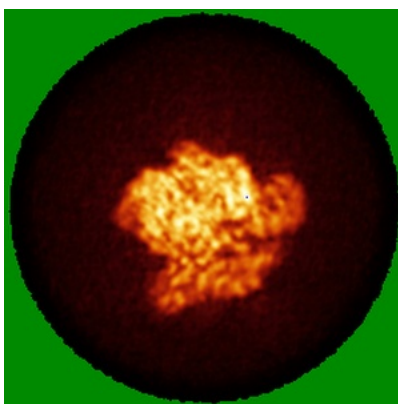
The images above show the largest variance slices of the map in three orthogonal directions.

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

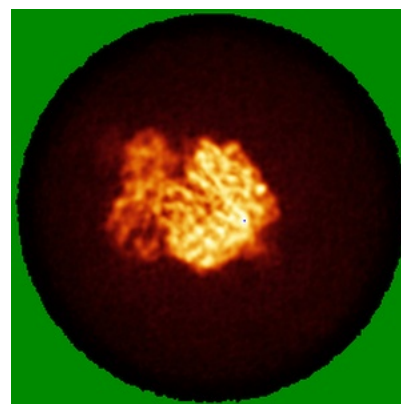
6.4.1 Primary map



X

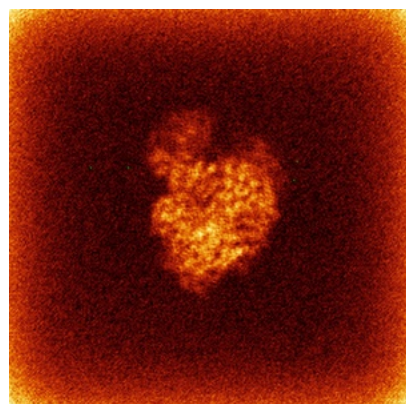


Y

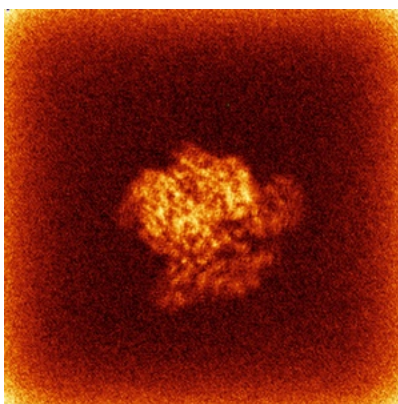


Z

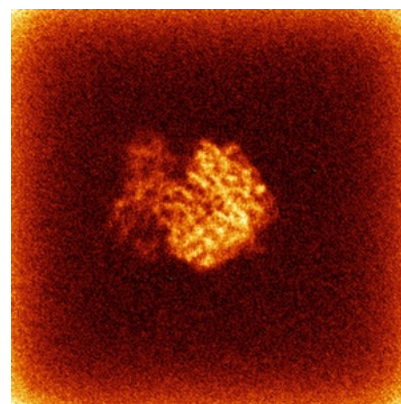
6.4.2 Raw map



X



Y

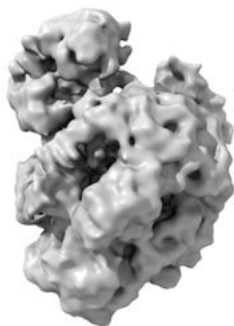


Z

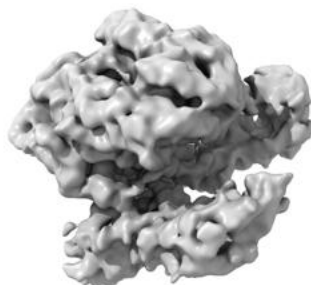
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

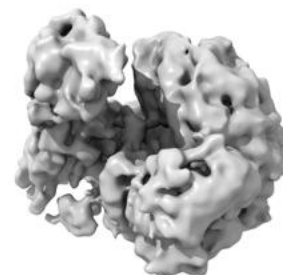
6.5.1 Primary map



X



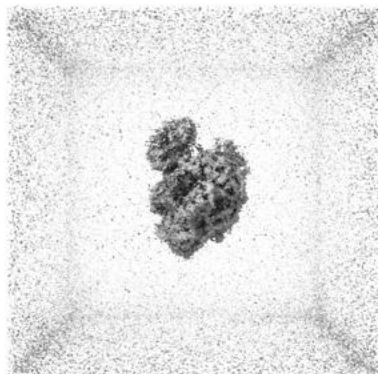
Y



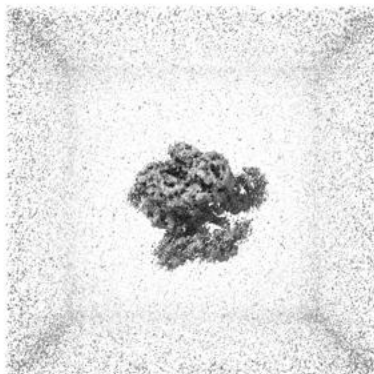
Z

The images above show the 3D surface view of the map at the recommended contour level 0.144. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

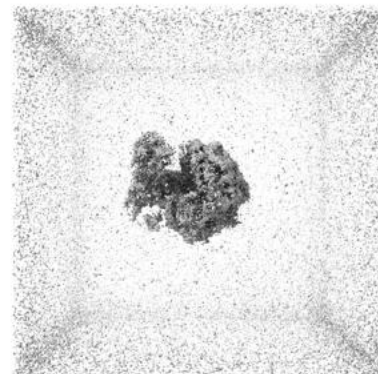
6.5.2 Raw map



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.

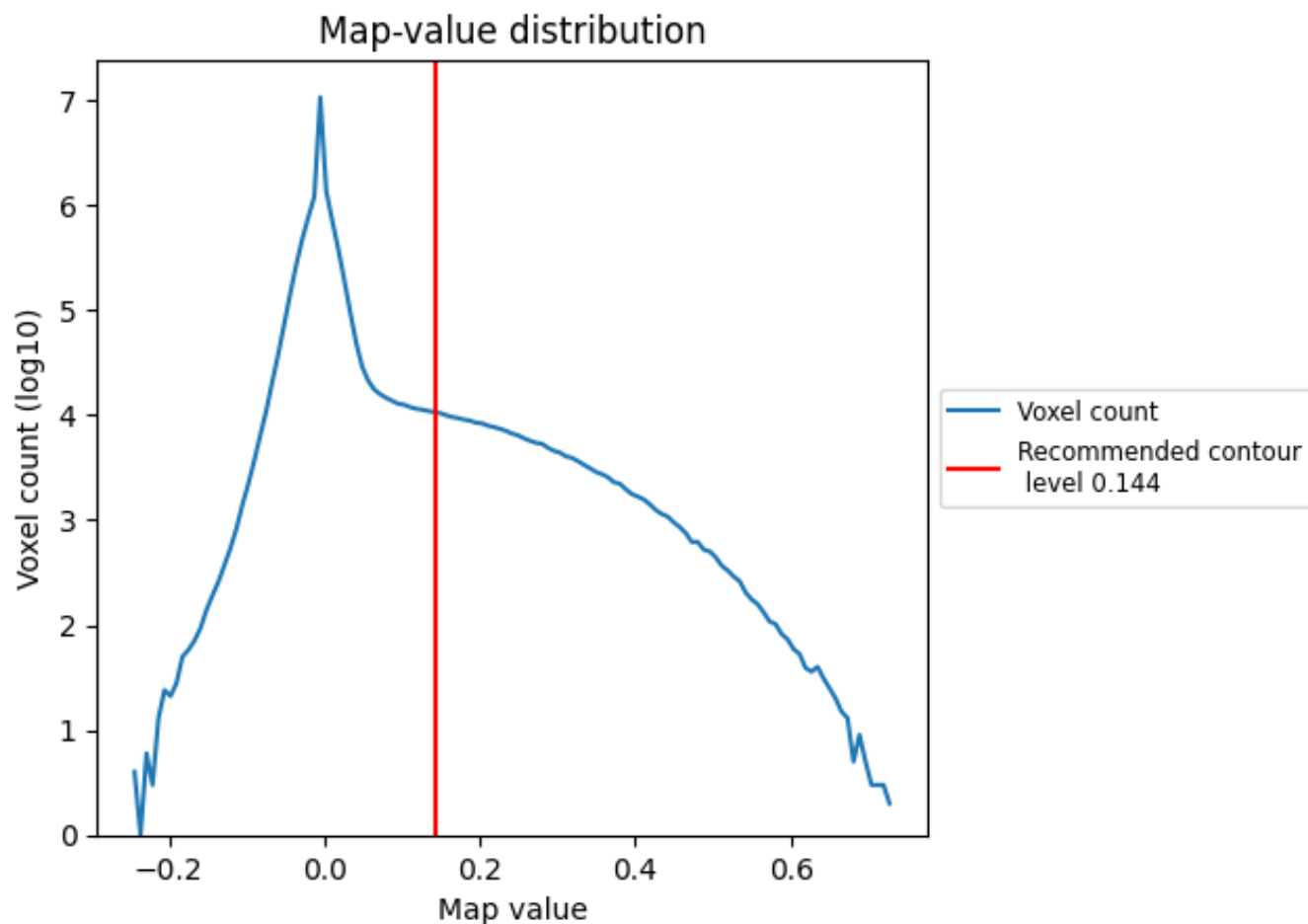
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

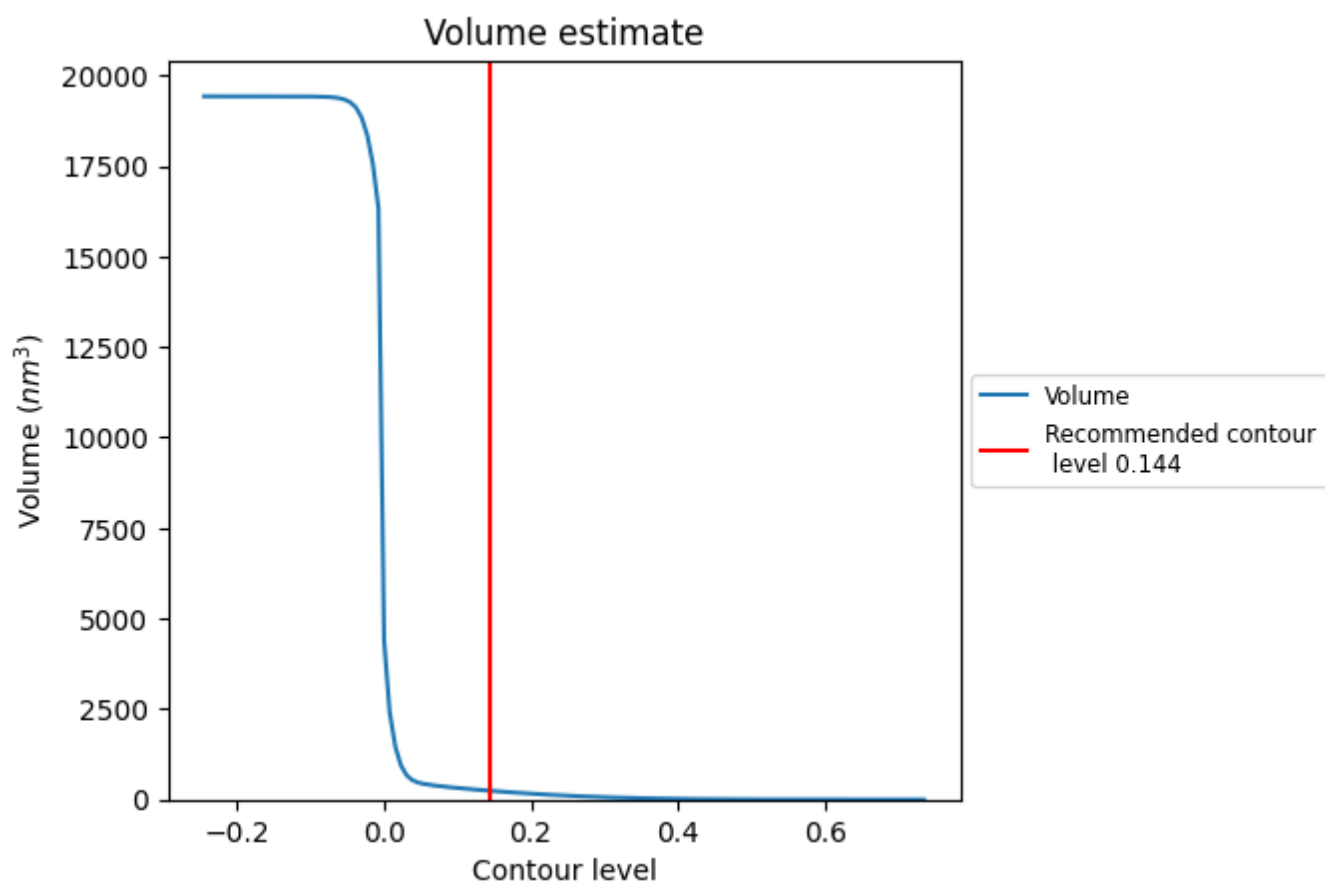
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

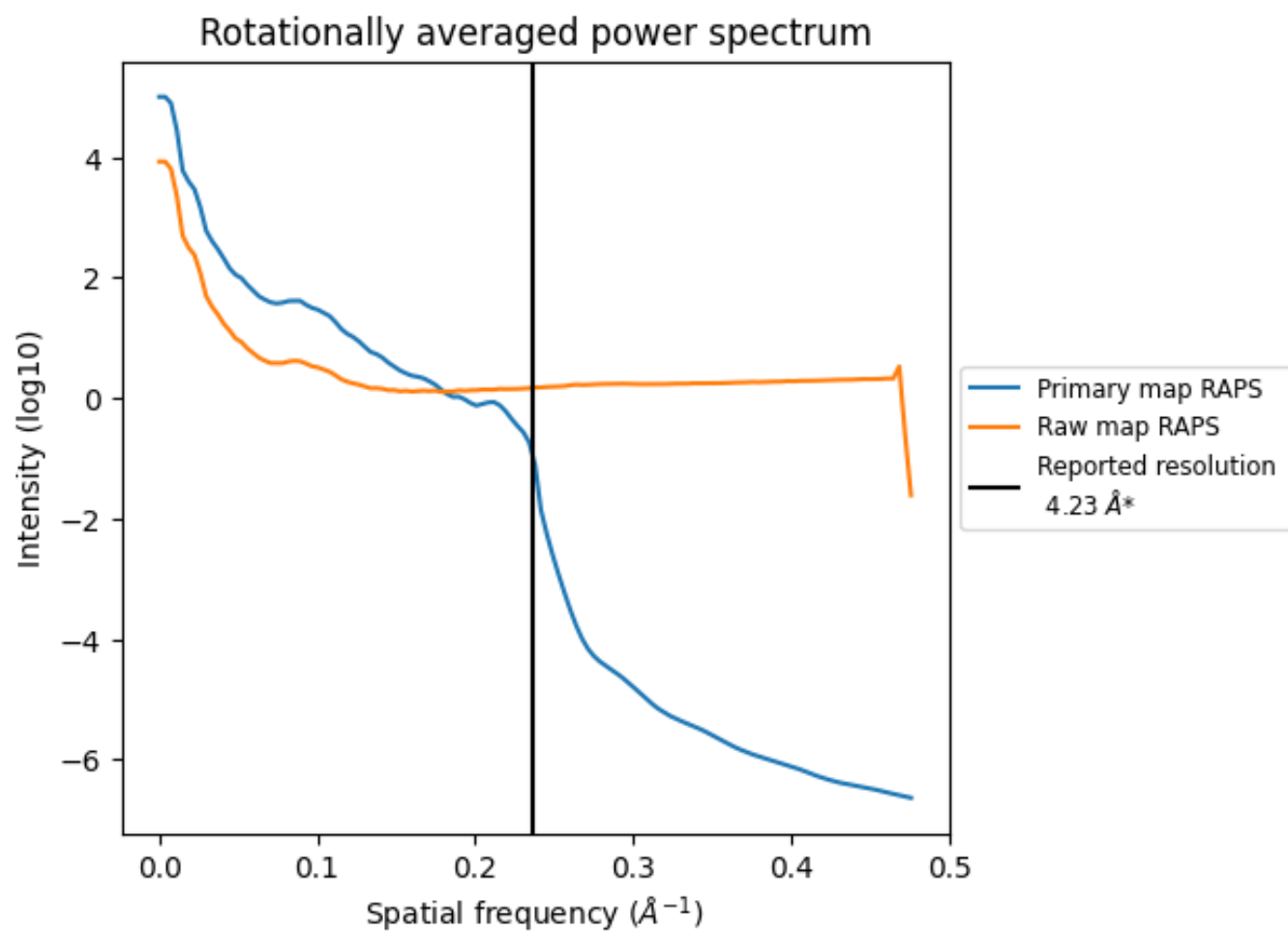
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 243 nm³; this corresponds to an approximate mass of 220 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 ⓘ

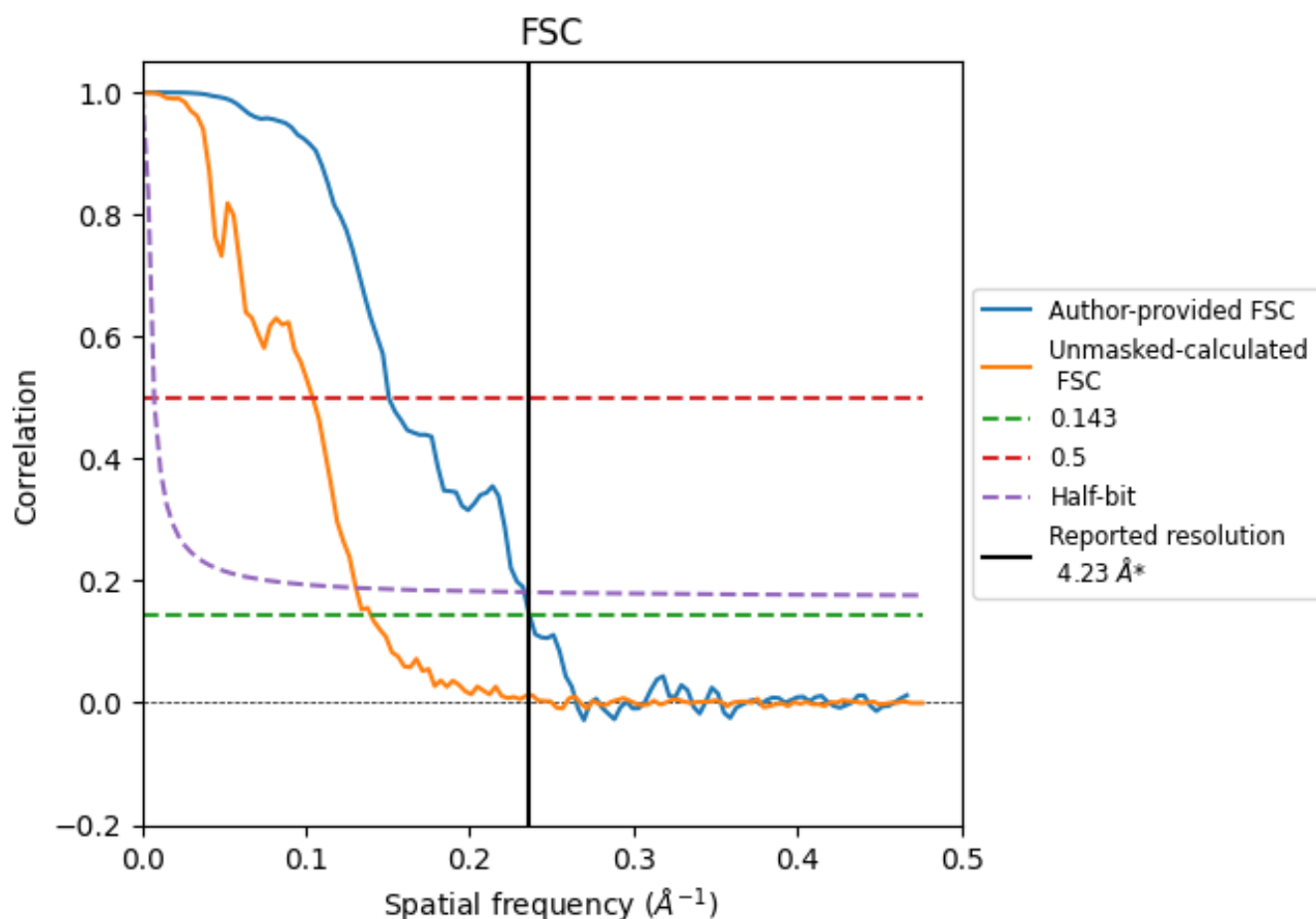


*Reported resolution corresponds to spatial frequency of 0.236 $\text{\AA}^{-1}$

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 0.236 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

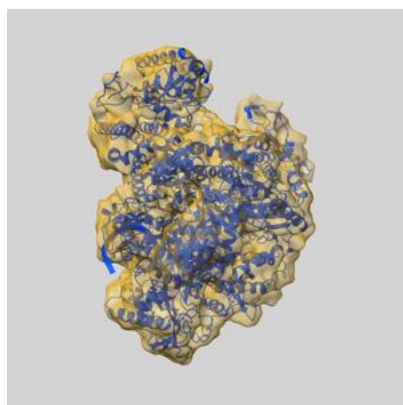
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.23	-	-
Author-provided FSC curve	4.23	6.64	4.29
Unmasked-calculated*	7.15	9.62	7.66

*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 7.15 differs from the reported value 4.23 by more than 10 %

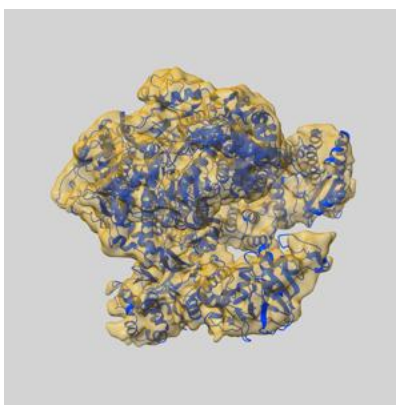
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18947 and PDB model 8R65. Per-residue inclusion information can be found in section [3](#) on page [9](#).

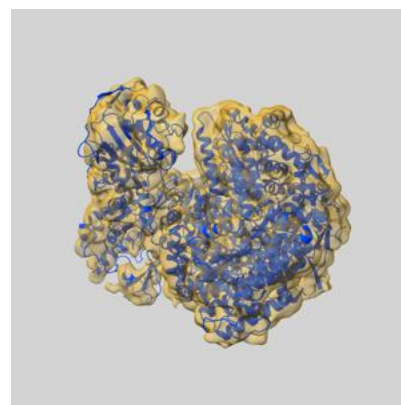
9.1 Map-model overlay [i](#)



X



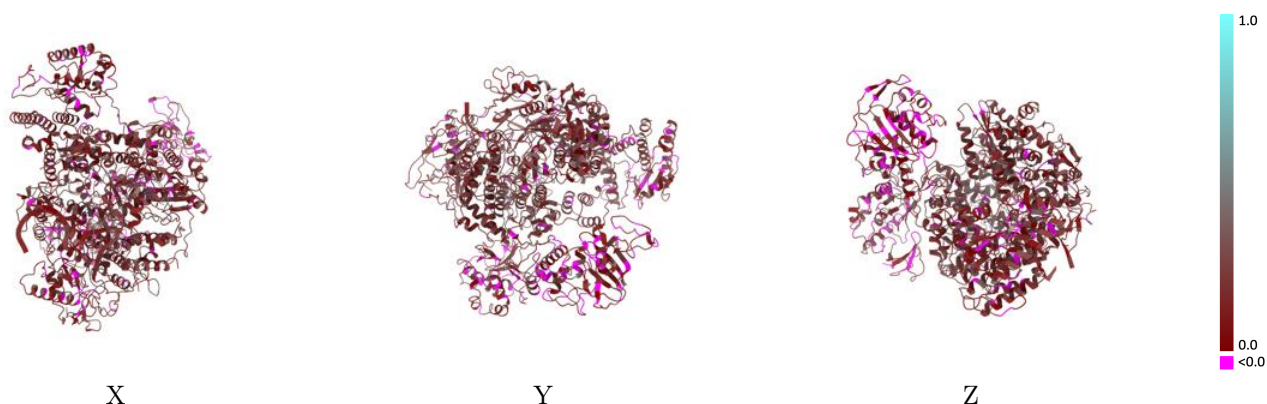
Y



Z

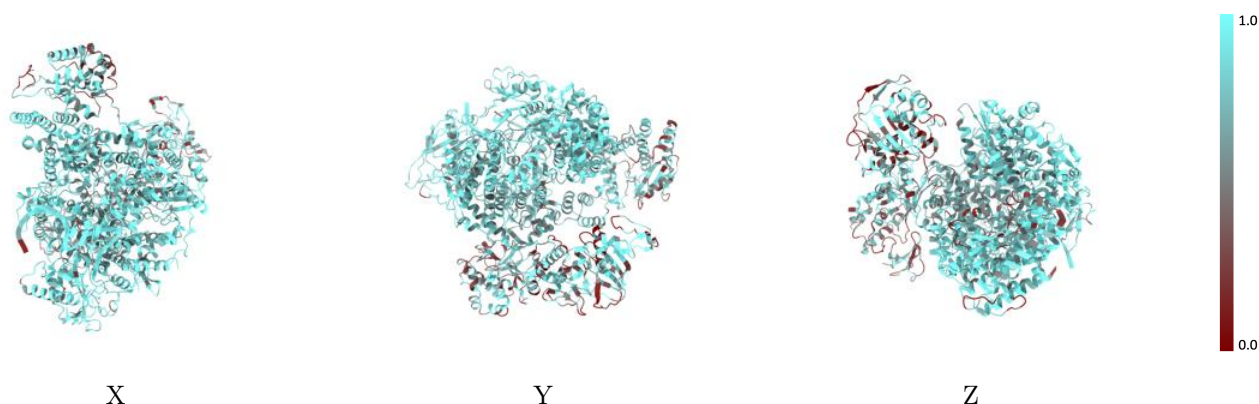
The images above show the 3D surface view of the map at the recommended contour level 0.144 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



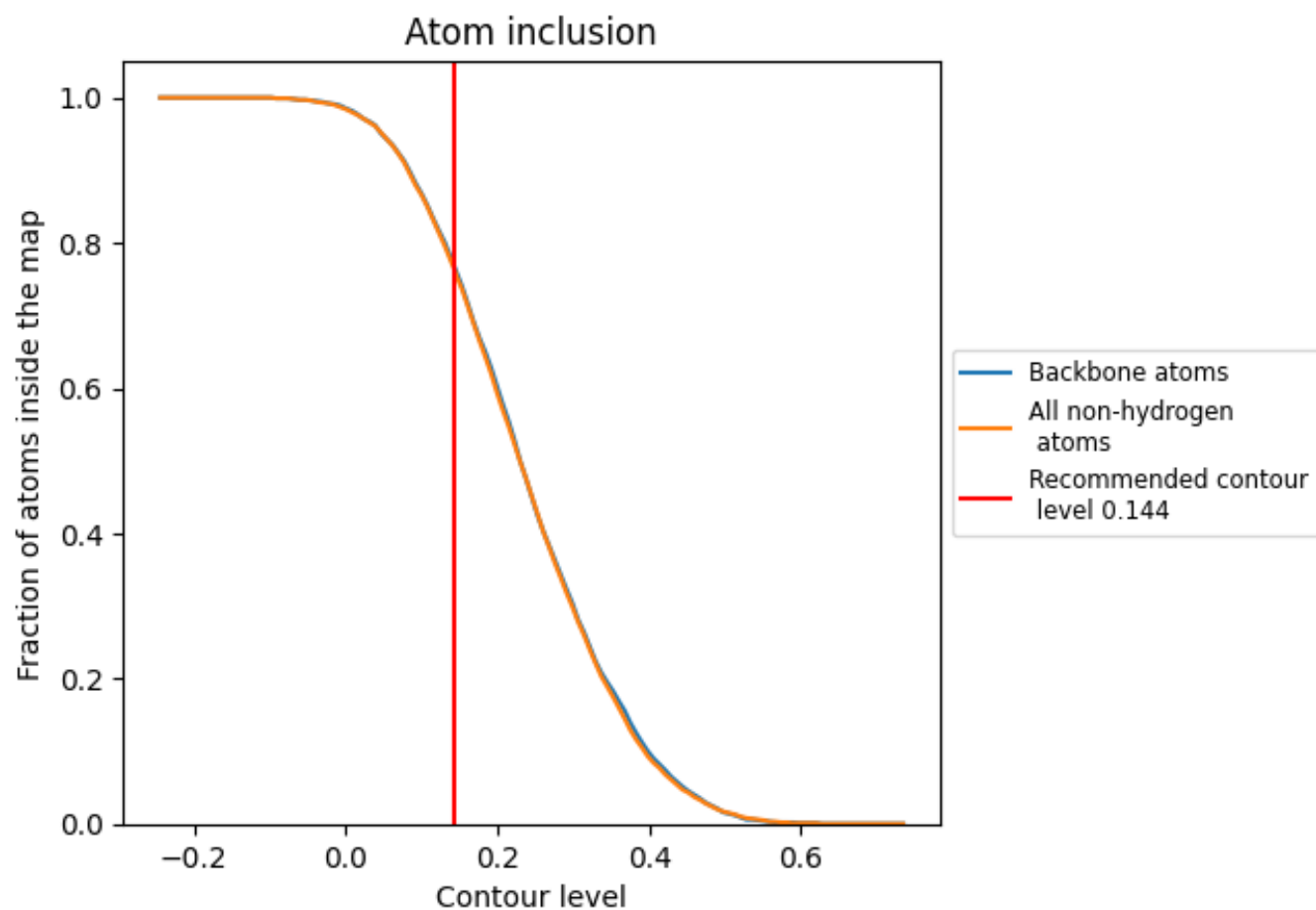
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.144).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.144) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7610	0.1800
A	0.7900	0.1830
B	0.8370	0.2160
C	0.6570	0.1400
D	0.9510	0.1870
E	0.7460	0.1740
X	0.8190	0.2220

1.0

0.0

<0.0