Full wwPDB EM Validation Report ⓘ

Mar 18, 2024 – 01:57 pm GMT

PDB ID	:	8R65
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:

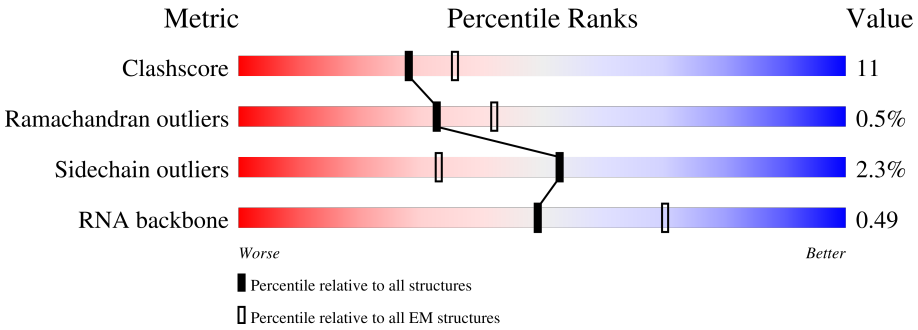
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	7% 83% 16%
2	C	905	19% 61% 19% 19%
3	D	15	47% 47% 7%
4	E	17	6% 29% 18% 53%
5	X	28	32% 39% 18% 11%
6	B	757	80% 15% 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 11519	C 3670	H 5724	N 985	O 1100	S 40	0	0

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 11651	C 3670	H 5805	N 1052	O 1084	S 40	0	0

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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.

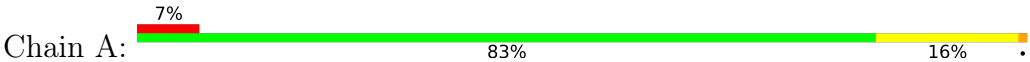
Mol	Chain	Residues	Atoms						AltConf	Trace
6	B	718	Total	C	H	N	O	S	0	0
			11428	3614	5682	1005	1083	44		

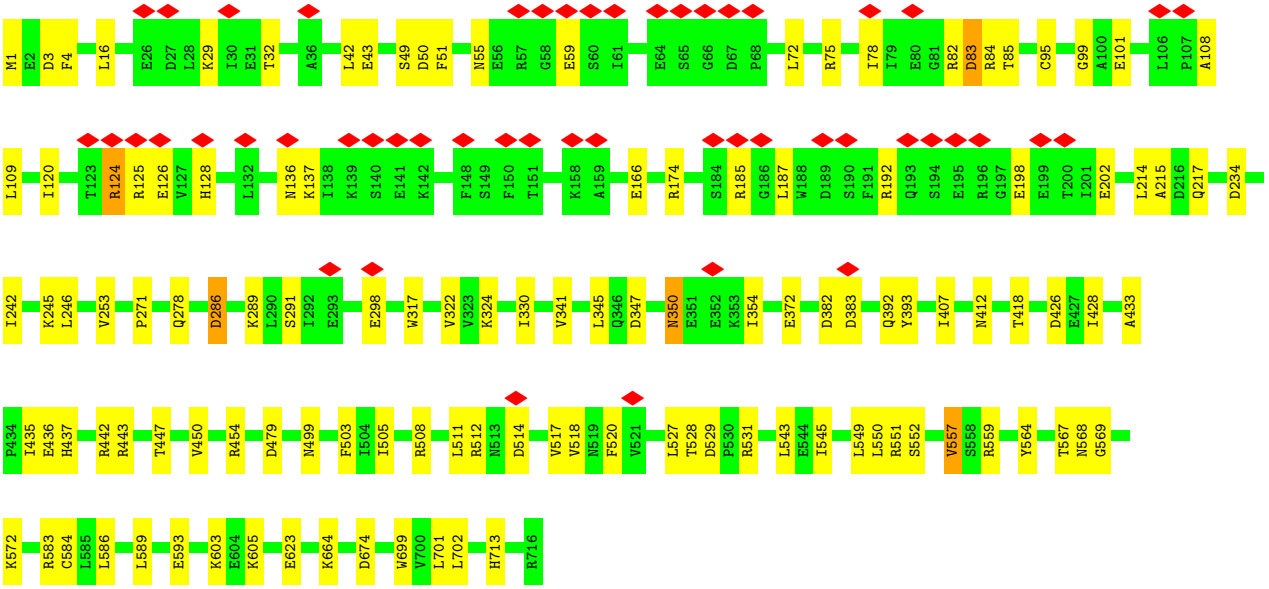
3 Residue-property plots (i)

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

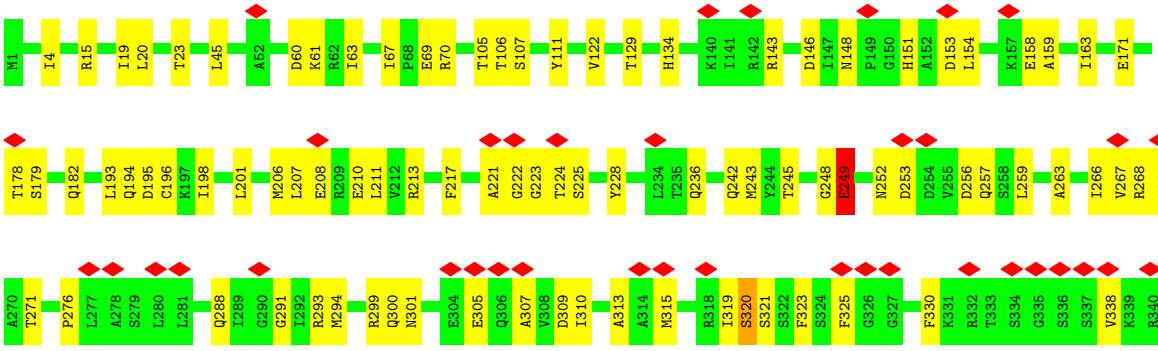
Chain A:

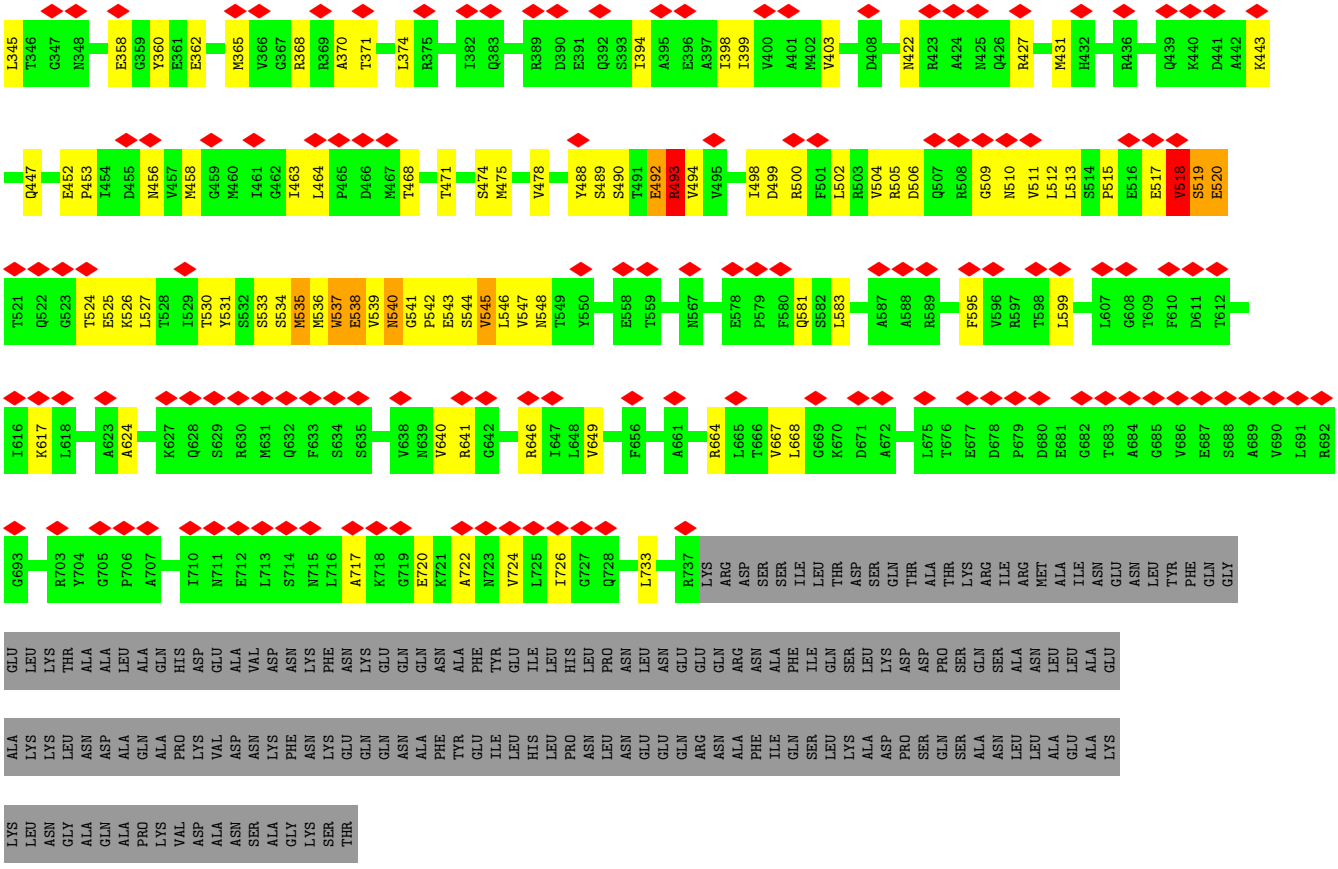




• Molecule 2: Polymerase basic protein 2

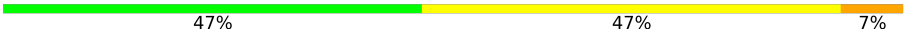
Chain C:

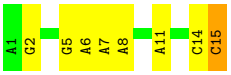




• Molecule 3: RNA (5'-R(P*AP*GP*UP*AP*GP*AP*AP*AP*CP*AP*AP*GP*GP*CP*C)-3')

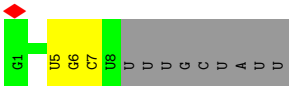
Chain D:





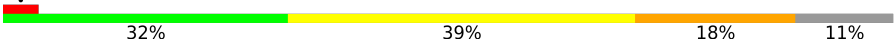
• Molecule 4: RNA (5'-R(P*GP*GP*CP*CP*UP*GP*CP*U)-3')

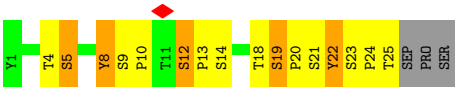
Chain E:



• Molecule 5: RNA polymerase II 4 repeat peptide with serine5 phosphorylation

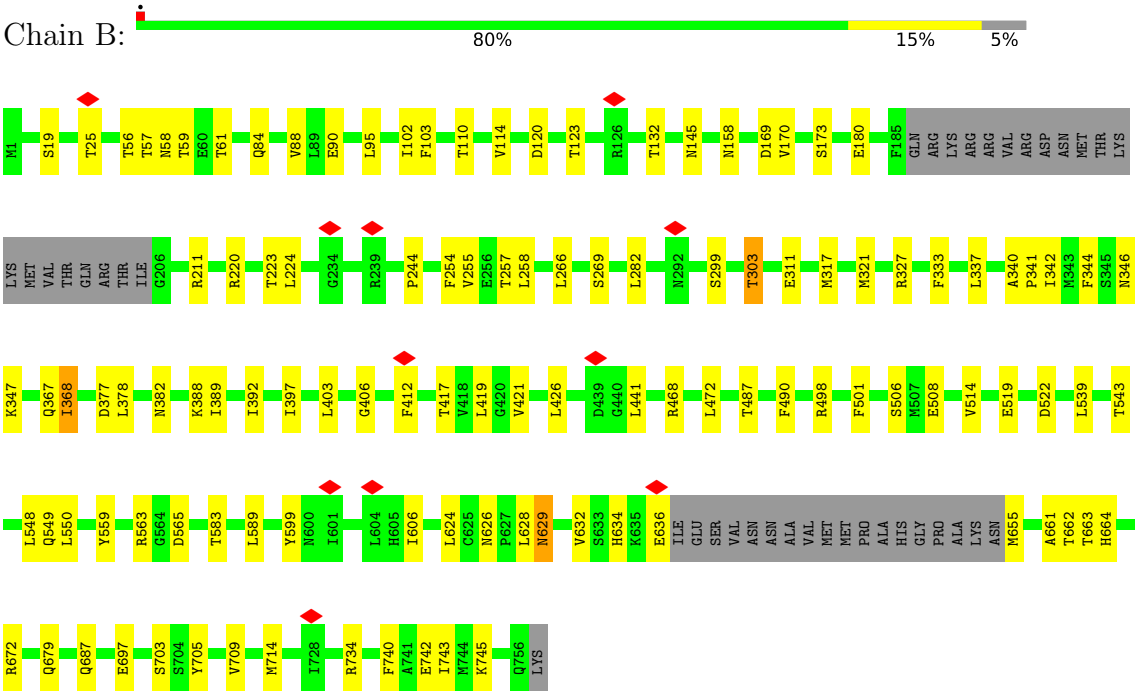
Chain X:





• Molecule 6: RNA-directed RNA polymerase catalytic subunit

Chain B:


80%
15%
5%
M1 S19 T25 T56 T57 N58 T59 E60 T61 Q84 V88 L89 E90 L95 I102 F103 T110 V114 D120 T123 R126 T132 N145 N158 D169 V170 S173 E180 F185 GLN ARG LYS ARG ARG VAL ARG ASP ASN MET THR LYS
LYS MET VAL THR GLN ARG THR ILE G206 R211 R220 T223 L224 G234 R239 P244 F254 V255 E256 T257 L258 L266 S269 L282 N292 S299 T303 E311 M317 M321 R327 F333 L337 A340 P341 I342 M343 F344 S345 N346
K347 Q367 I368 D377 L378 N382 K388 I389 I392 I397 L403 G406 F412 T417 V418 L419 G420 V421 L426 D439 G440 L441 R468 L472 T487 F490 R498 F501 S506 M507 E508 V514 E519 D522 L539 T543
L548 Q549 L550 Y559 R563 G564 D565 T583 L589 Y599 N600 I601 L604 H605 I606 L624 C625 N626 P627 L628 N629 V632 S633 H634 K635 E636 ILE GLU SER VAL ASN ASN ALA VAL MET MET PRO ALA HIS GLY PRO ALA LYS ASN M655 A661 T662 T663 H664
R672 Q679 Q687 E697 S703 S704 Y705 V709 M714 I728 R734 F740 A741 E742 I743 M744 K745 Q756 LYS

4 Experimental information (i)

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 ($e^-/Å^2$)	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	0.29	0/5918	0.48	0/7975
2	C	0.33	0/5944	0.59	0/8017
3	D	0.48	0/366	0.73	0/569
4	E	0.30	0/187	0.72	0/289
5	X	0.30	0/174	0.38	0/237
6	B	0.30	0/5858	0.50	0/7897
All	All	0.31	0/18447	0.53	0/24984

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

There are no bond length outliers.

There are no bond angle outliers.

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 (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	5795	5724	5733	91	0
2	C	5846	5805	5964	214	0
3	D	326	165	165	5	0
4	E	169	86	87	3	0
5	X	197	0	161	14	0
6	B	5746	5682	5721	92	0
All	All	18079	17462	17831	380	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 11.

All (380) 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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:299:SER:HG	6:B:487:THR:HG1	0.78	0.77
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: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: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:628:LEU:HD23	6:B:628:LEU:O	1.93	0.69
1:A:392:GLN:NE2	6:B:382:ASN:OD1	2.26	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:347:LYS:NZ	6:B:406:GLY:O	2.27	0.65
6:B:508:GLU:N	6:B:508:GLU:OE1	2.30	0.65
2:C:222:GLY:C	2:C:525:GLU:OE2	2.35	0.65
2:C:4:ILE:CD1	6:B:743:ILE:HD11	2.23	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
6:B:347:LYS:NZ	6:B:403:LEU:O	2.26	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
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
2:C:518:VAL:O	2:C:519:SER:C	2.39	0.61
6:B:110:THR:HG21	6:B:258:LEU:HA	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:B:321:MET:HE2	6:B:419:LEU:HD13	1.88	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: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:321:MET:CE	6:B:419:LEU:HD13	2.38	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
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
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: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
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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:344:VAL:CG1	2:C:345:LEU:N	2.73	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:544:SER:O	2:C:545:VAL:C	2.49	0.51
2:C:143:ARG:NH1	2:C:524:THR:CB	2.71	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:518:VAL:HG13	1:A:518:VAL:O	2.11	0.50
1:A:242:ILE:HD13	6:B:426:LEU:HD21	1.92	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: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:193:LEU:HD12	2:C:193:LEU:O	2.12	0.50
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: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: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
2:C:542:PRO:C	2:C:544:SER:N	2.63	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:110:THR:HG1	6:B:333:PHE:HZ	1.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:20:LEU:HD13	6:B:714:MET:HE3	1.96	0.48
6:B:255:VAL:HG11	6:B:412:PHE:CE2	2.48	0.48
1:A:108:ALA:C	1:A:109:LEU:HD12	2.35	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
2:C:547:VAL:CG2	2:C:667:VAL:CG1	2.93	0.47
1:A:49:SER:OG	1:A:78:ILE:HD11	2.15	0.47
2:C:543:GLU:C	2:C:547:VAL:HB	2.36	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
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: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:105:THR:O	2:C:106:THR:OG1	2.21	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:45:LEU:HD23	2:C:45:LEU:O	2.16	0.45
2:C:537:TRP:O	2:C:538:GLU:C	2.54	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:248:GLY:O	2:C:249:GLU:C	2.53	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
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
1:A:528:THR:O	1:A:564:TYR:OH	2.28	0.44
2:C:143:ARG:HH12	2:C:524:THR:HG1	1.50	0.44
2:C:223:GLY:C	2:C:224:THR:HG1	2.10	0.44
2:C:343:GLU:C	2:C:344:VAL:HG23	2.37	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
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
6:B:102:ILE:HG23	6:B:103:PHE:N	2.32	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
2:C:463:ILE:HD11	2:C:478:VAL:C	2.38	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:B:539:LEU:HD11	6:B:543:THR:HG22	1.99	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
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: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
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
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:HG23	6:B:514:VAL:O	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:540:ASN:C	2:C:544:SER:HB3	2.40	0.41
2:C:548:ASN:HD22	2:C:548:ASN:N	2.18	0.41
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
2:C:531:TYR:O	2:C:535:MET:CE	2.68	0.41
1:A:3:ASP:OD1	1:A:4:PHE:N	2.53	0.41
1:A:529:ASP:OD1	1:A:531:ARG:NE	2.40	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: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:541:GLY:C	2:C:544:SER:H	2.24	0.41
2:C:547:VAL:HA	2:C:667:VAL:HG11	2.03	0.41
6:B:25:THR:HG22	6:B:25:THR:O	2.20	0.41
6:B:120:ASP:O	6:B:123:THR:OG1	2.30	0.41
6:B:321:MET:HE1	6:B:419:LEU:HB2	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
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
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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	714/716 (100%)	669 (94%)	44 (6%)	1 (0%)	51 85
2	C	735/905 (81%)	668 (91%)	58 (8%)	9 (1%)	13 50
5	X	20/28 (71%)	17 (85%)	2 (10%)	1 (5%)	2 23
6	B	712/757 (94%)	669 (94%)	43 (6%)	0	100 100
All	All	2181/2406 (91%)	2023 (93%)	147 (7%)	11 (0%)	32 68

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	639/639 (100%)	623 (98%)	16 (2%)	47 68
2	C	646/788 (82%)	627 (97%)	19 (3%)	42 64
5	X	22/24 (92%)	21 (96%)	1 (4%)	27 54
6	B	634/669 (95%)	626 (99%)	8 (1%)	69 82
All	All	1941/2120 (92%)	1897 (98%)	44 (2%)	53 70

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	75	ARG
1	A	124	ARG
1	A	278	GLN
1	A	286	ASP
1	A	324	LYS
1	A	350	ASN
1	A	393	TYR
1	A	412	ASN
1	A	479	ASP
1	A	514	ASP
1	A	549	LEU
1	A	551	ARG
1	A	557	VAL
1	A	583	ARG
1	A	664	LYS
2	C	15	ARG
2	C	69	GLU
2	C	70	ARG
2	C	206	MET
2	C	210	GLU
2	C	217	PHE
2	C	249	GLU
2	C	299	ARG
2	C	309	ASP
2	C	320	SER
2	C	427	ARG
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	640	VAL
5	X	8	TYR
6	B	303	THR
6	B	344	PHE
6	B	368	ILE
6	B	441	LEU
6	B	629	ASN
6	B	687	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	B	734	ARG
6	B	740	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	217	GLN
1	A	392	GLN
1	A	412	ASN
1	A	437	HIS
2	C	75	GLN
2	C	100	ASN
2	C	127	HIS
2	C	134	HIS
2	C	182	GLN
2	C	540	ASN
2	C	548	ASN
6	B	136	ASN
6	B	567	GLN

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 (i)

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	19	5	8,9,10	1.49	1 (12%)	8,12,14	1.63	2 (25%)
5	SEP	X	12	5	8,9,10	1.56	1 (12%)	8,12,14	1.65	2 (25%)
5	SEP	X	5	5	8,9,10	1.51	1 (12%)	8,12,14	1.66	2 (25%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	X	12	SEP	P-O1P	3.41	1.61	1.50
5	X	5	SEP	P-O1P	3.32	1.61	1.50
5	X	19	SEP	P-O1P	3.26	1.61	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
5	X	19	SEP	P-OG-CB	-2.88	110.36	118.30
5	X	5	SEP	P-OG-CB	-2.80	110.58	118.30
5	X	12	SEP	P-OG-CB	-2.69	110.89	118.30

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	X	5	SEP	N-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	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	19	SEP	1	0
5	X	12	SEP	3	0
5	X	5	SEP	2	0

5.5 Carbohydrates (i)

There are no monosaccharides 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.

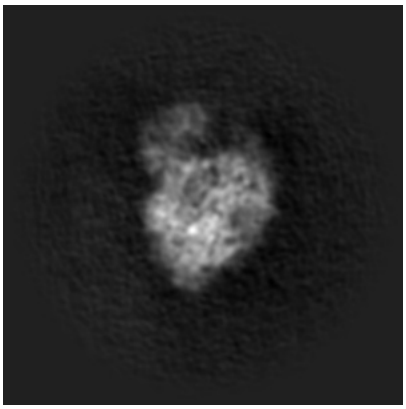
6 Map visualisation

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.

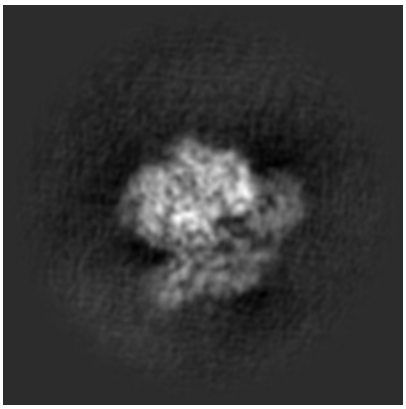
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

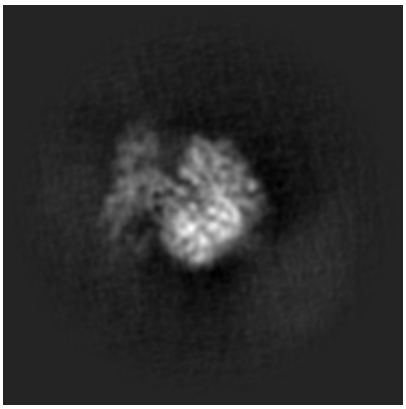
6.1.1 Primary map



X

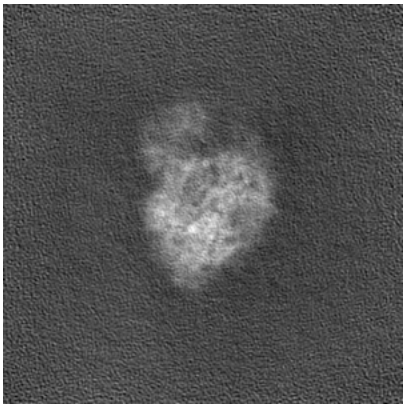


Y

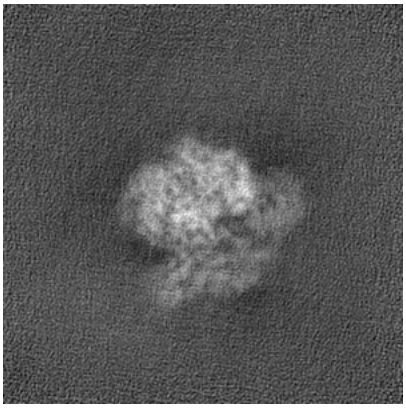


Z

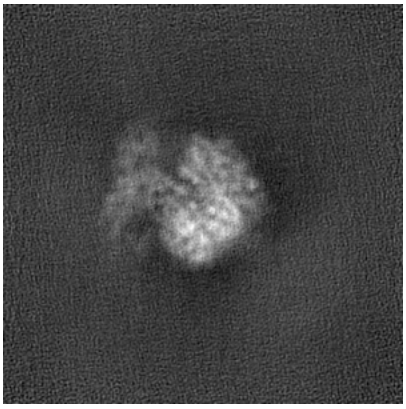
6.1.2 Raw map



X



Y

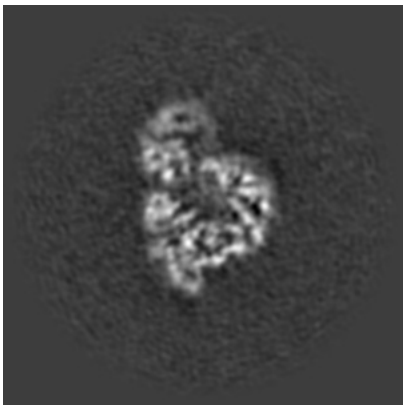


Z

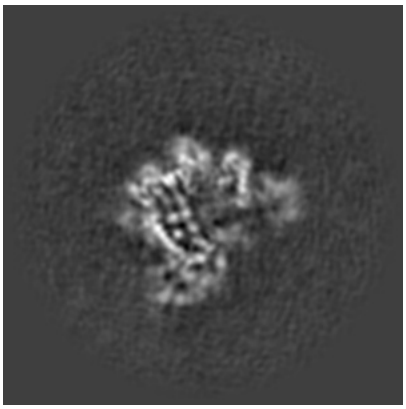
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

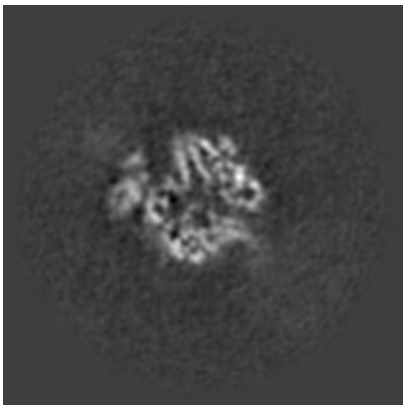
6.2.1 Primary map



X Index: 128

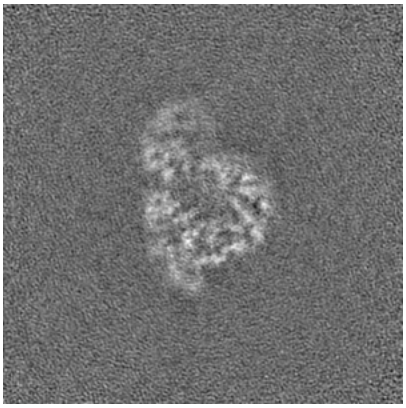


Y Index: 128

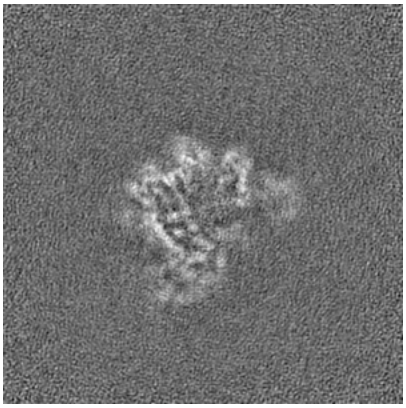


Z Index: 128

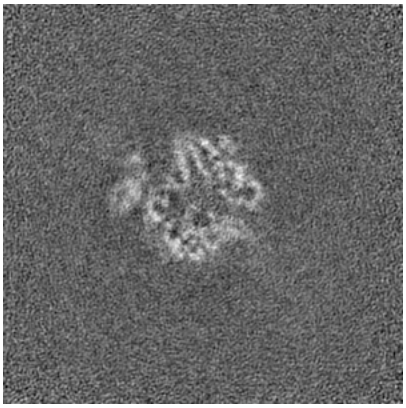
6.2.2 Raw map



X Index: 128



Y Index: 128

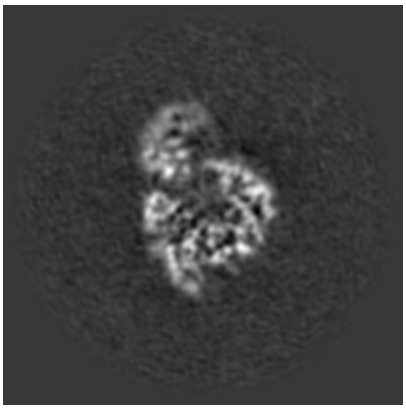


Z Index: 128

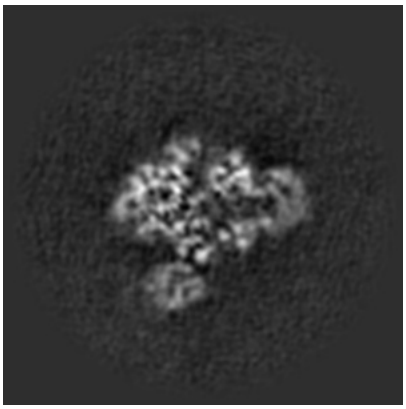
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

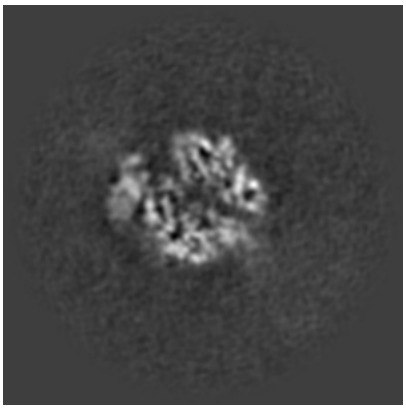
6.3.1 Primary map



X Index: 126

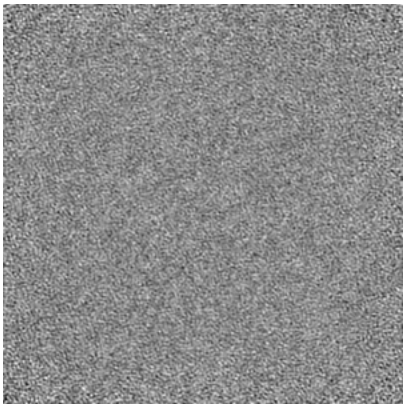


Y Index: 121

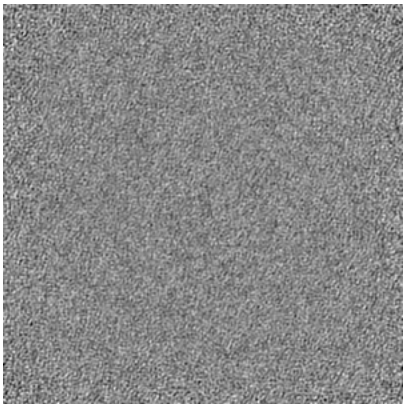


Z Index: 126

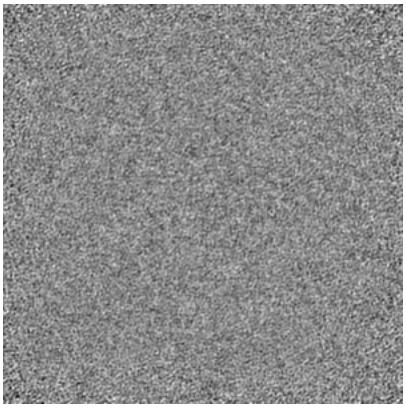
6.3.2 Raw map



X Index: 0



Y Index: 0

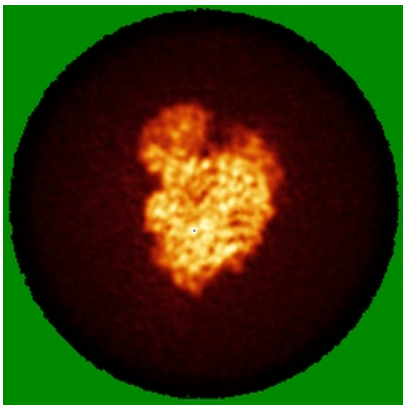


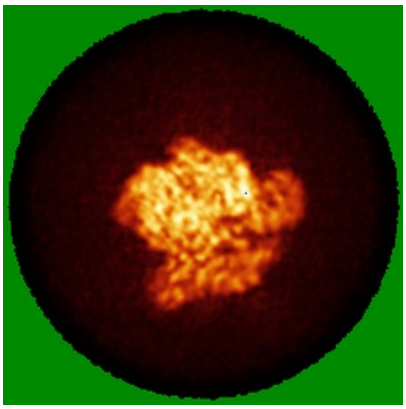
Z Index: 0

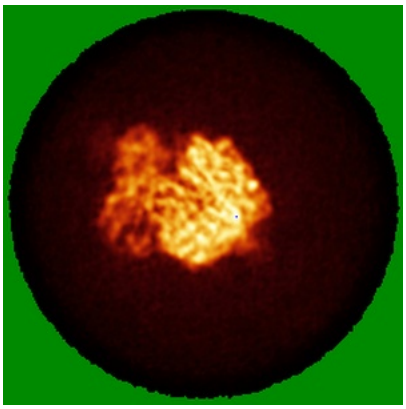
The images above show the largest variance slices of the map in three orthogonal directions.

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

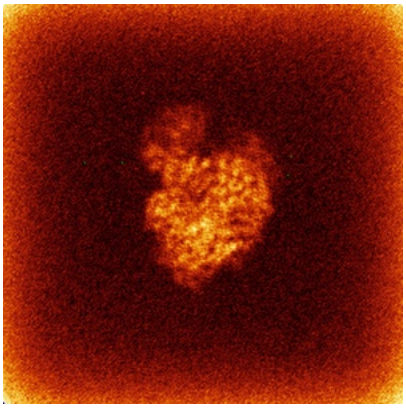
6.4.1 Primary map

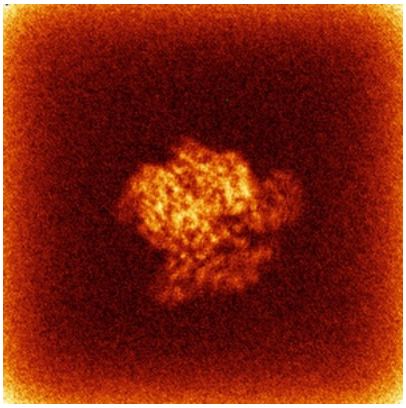

X

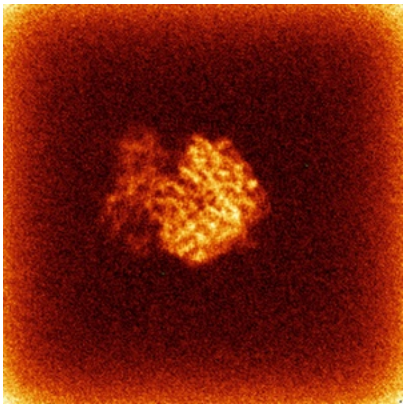

Y


Z

6.4.2 Raw map


X

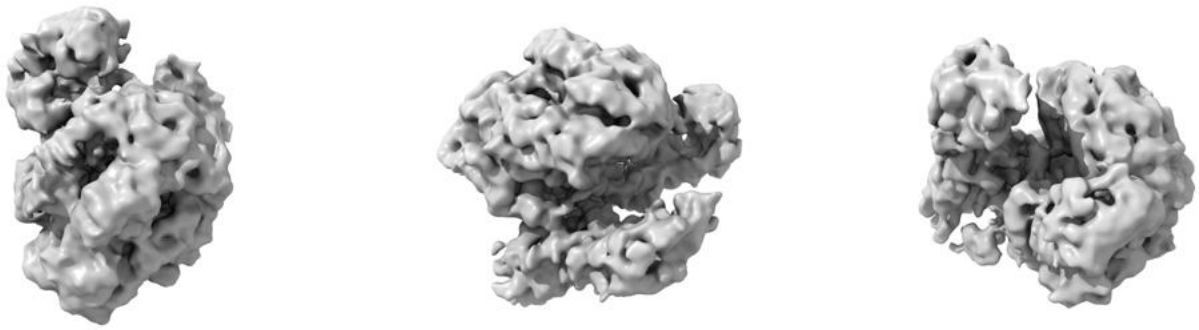

Y


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)

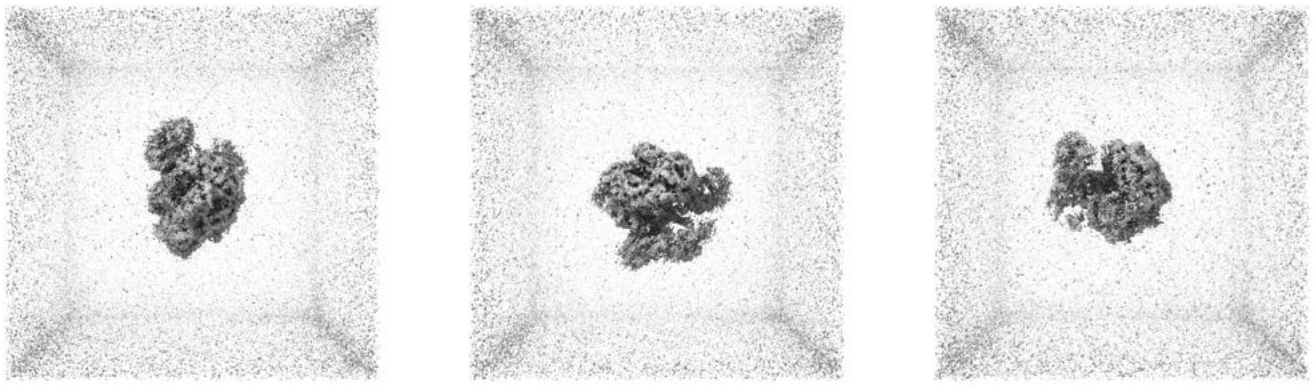
6.5.1 Primary map



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.

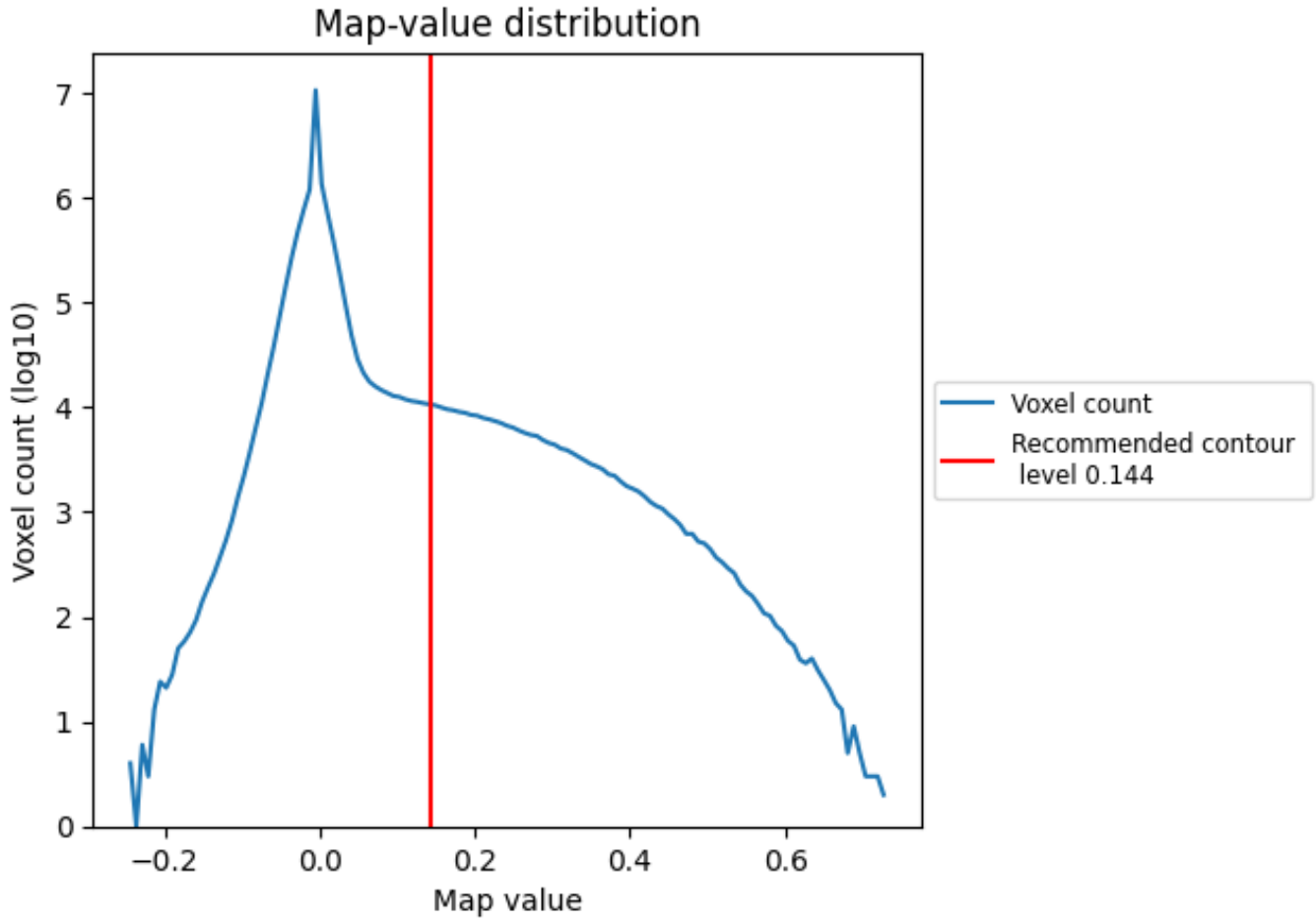
6.6 Mask visualisation (i)

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

7 Map analysis

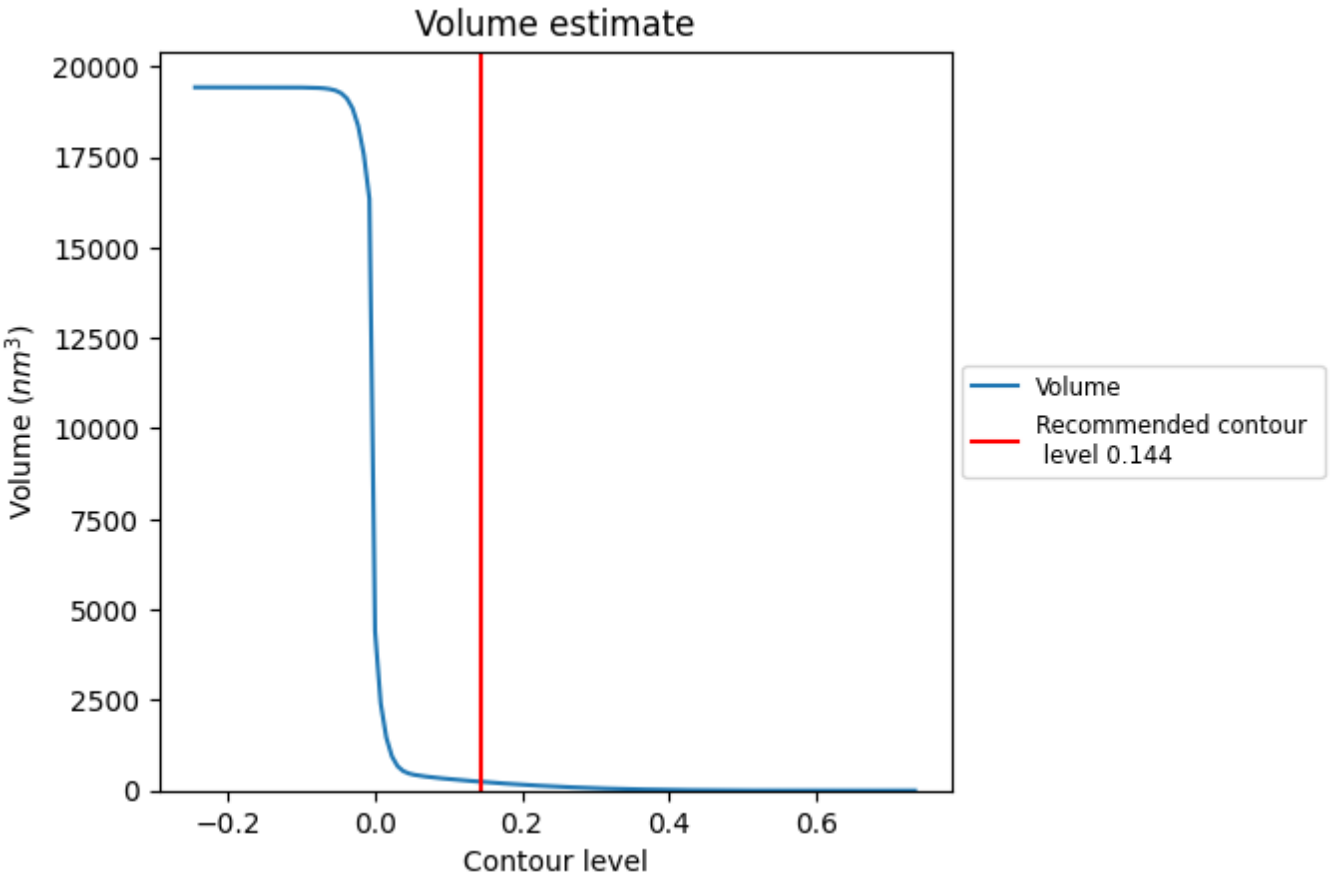
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

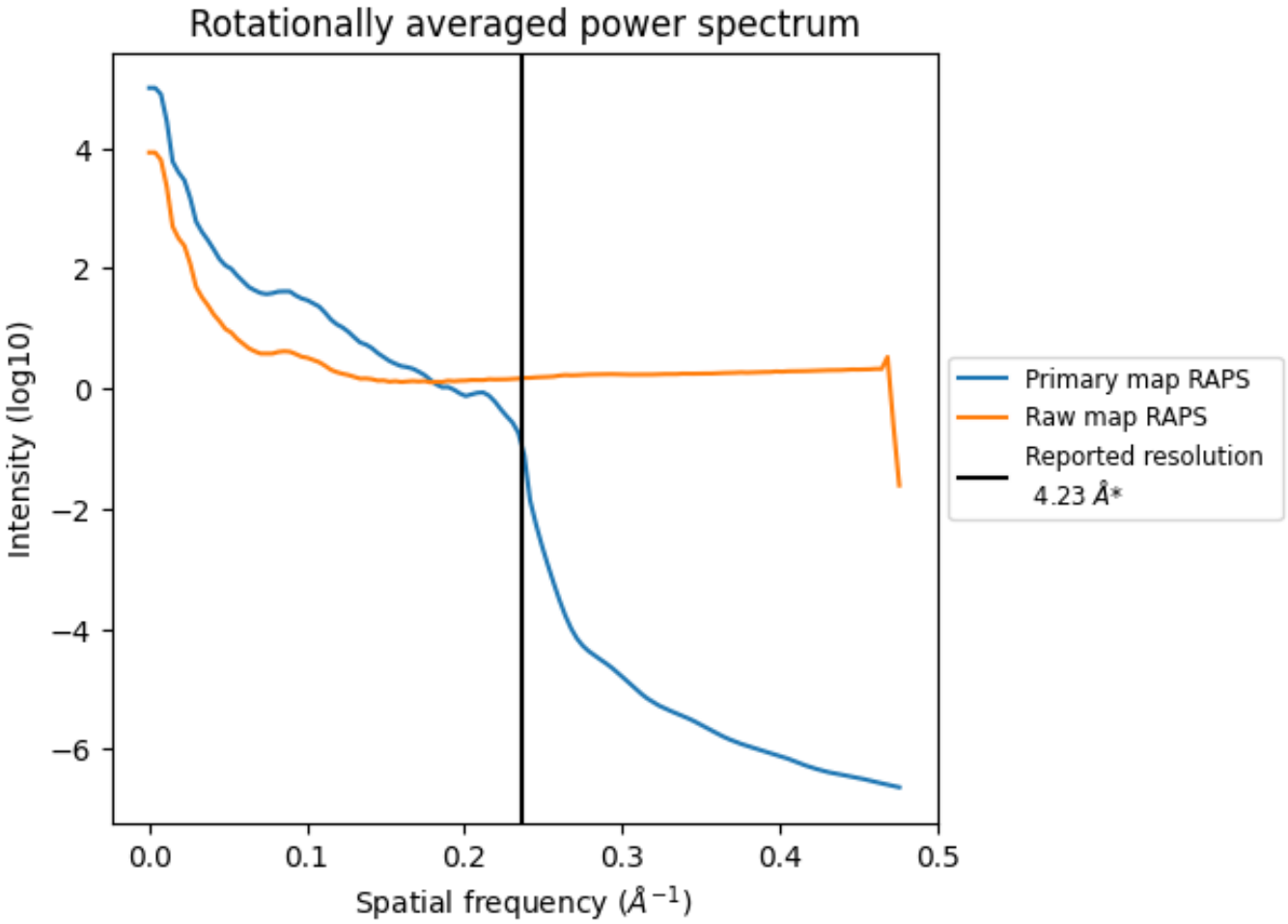
7.2 Volume estimate



The volume at the recommended contour level is 243 nm^3; 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 (i)

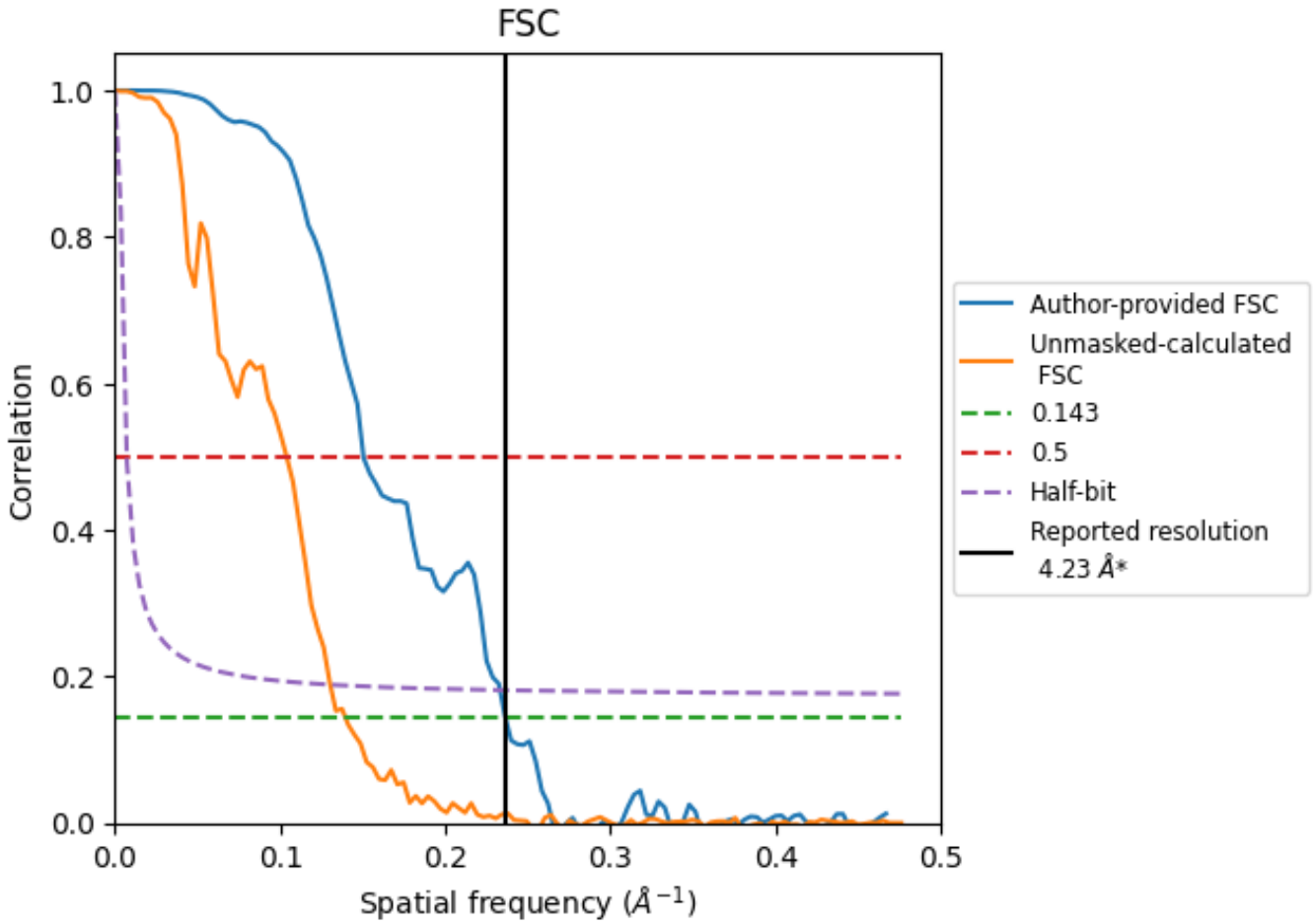


*Reported resolution corresponds to spatial frequency of 0.236 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.236 $Å^{-1}$

8.2 Resolution estimates (i)

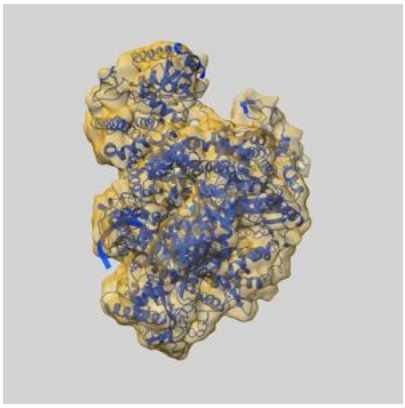
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.23	-	-
Author-provided FSC curve	4.23	6.64	4.29
Unmasked-calculated*	7.15	9.62	7.66

*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 %

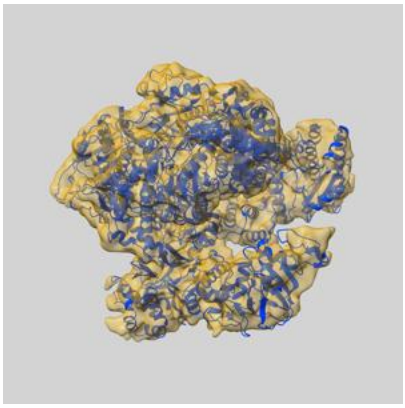
9 Map-model fit

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 8.

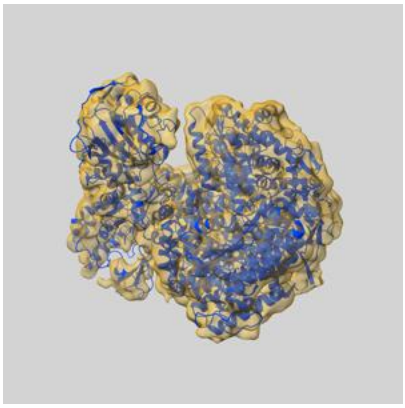
9.1 Map-model overlay



X



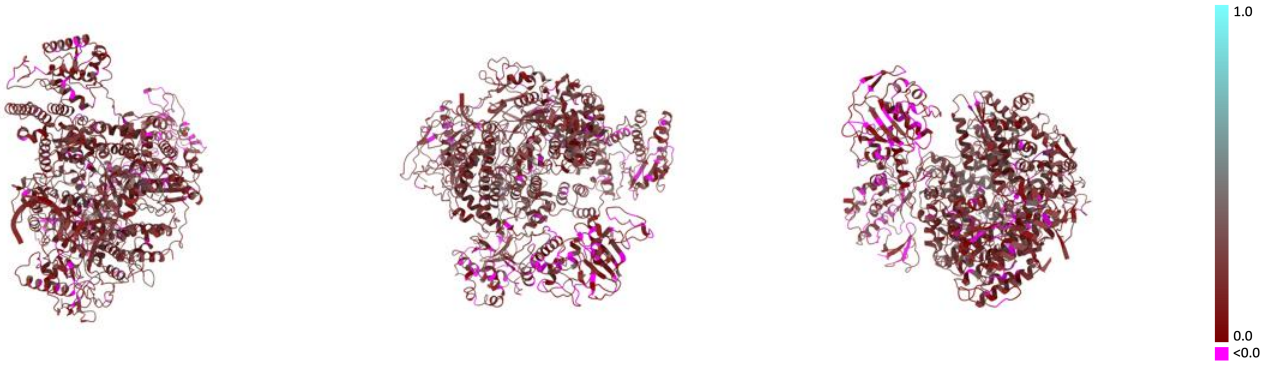
Y



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.

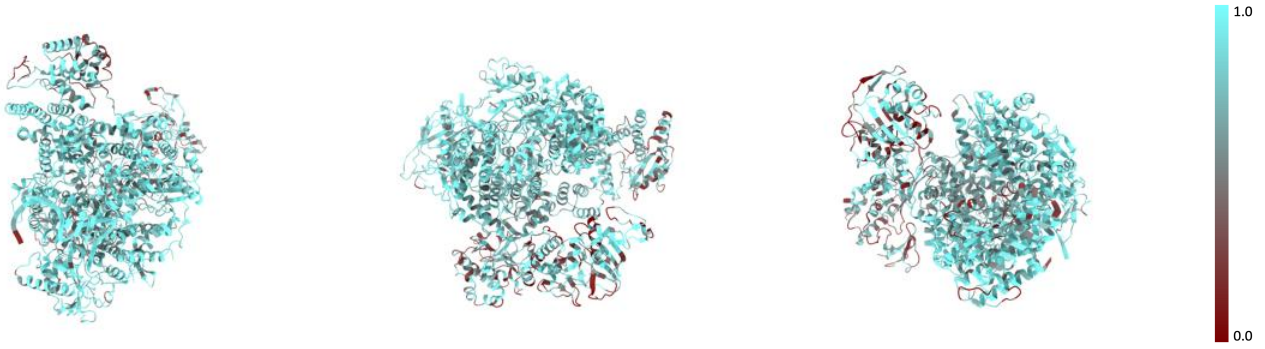
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

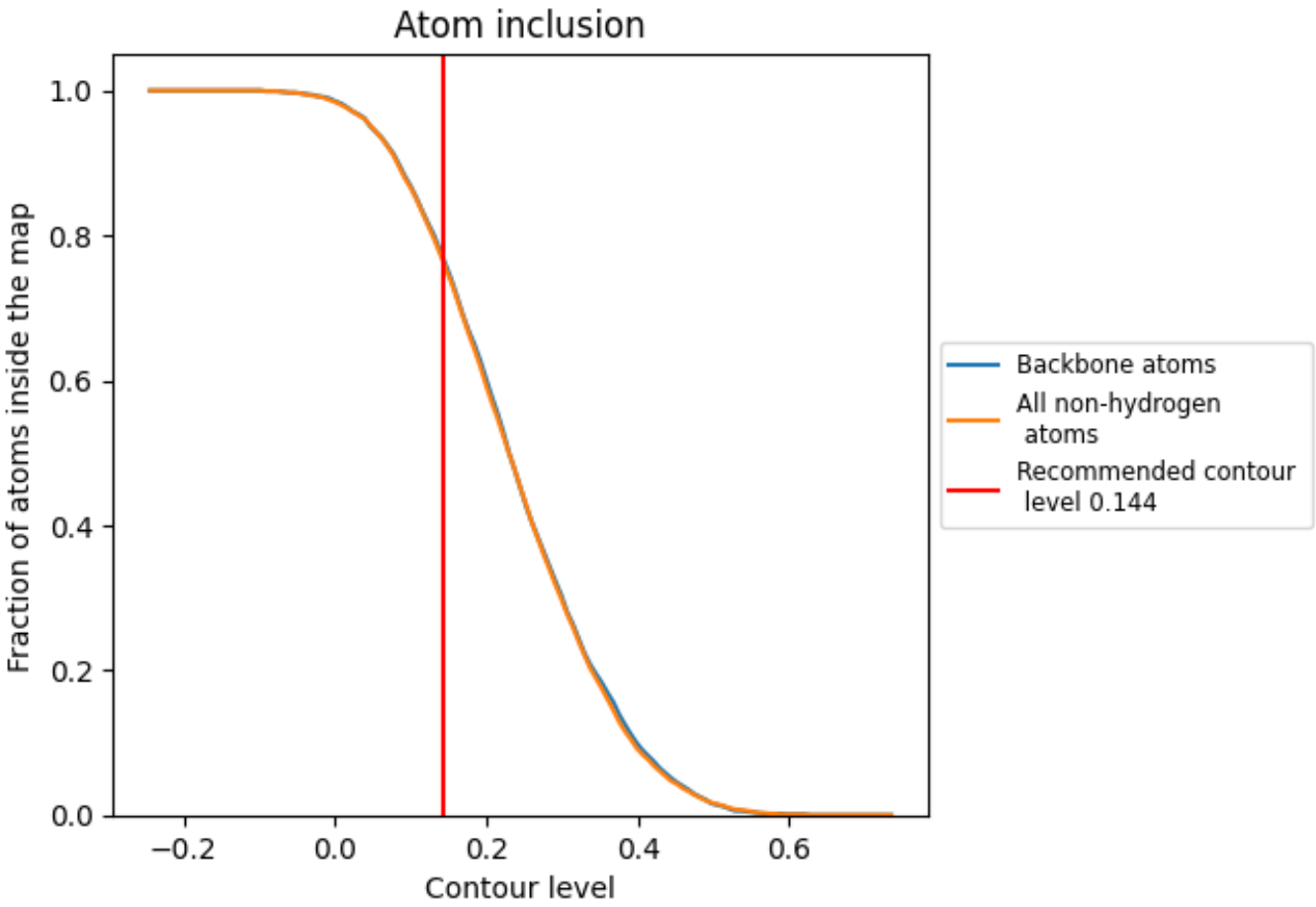
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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