W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB EM Validation Report (i)

Dec 12, 2022 – 06:39 am GMT

PDB ID	:	6Y0C
EMDB ID	:	EMD-10667
Title	:	Influenza C virus polymerase in complex with human ANP32A - Subclass 2
Authors	:	Fan, H.; Carrique, L.; Keown, J.R.; Grimes, J.M.; Fodor, E.
Deposited on	:	2020-02-07
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:
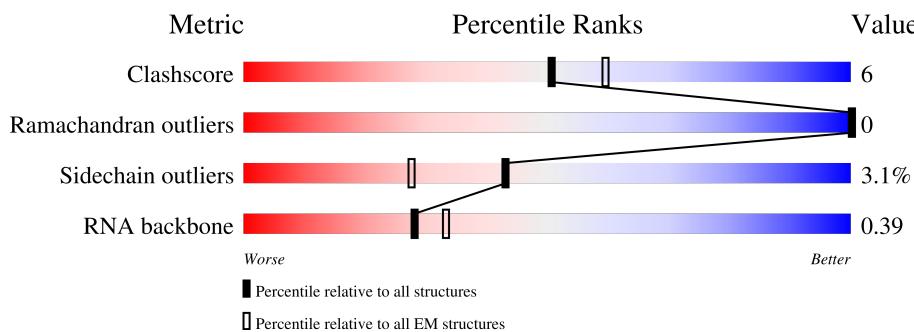
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY
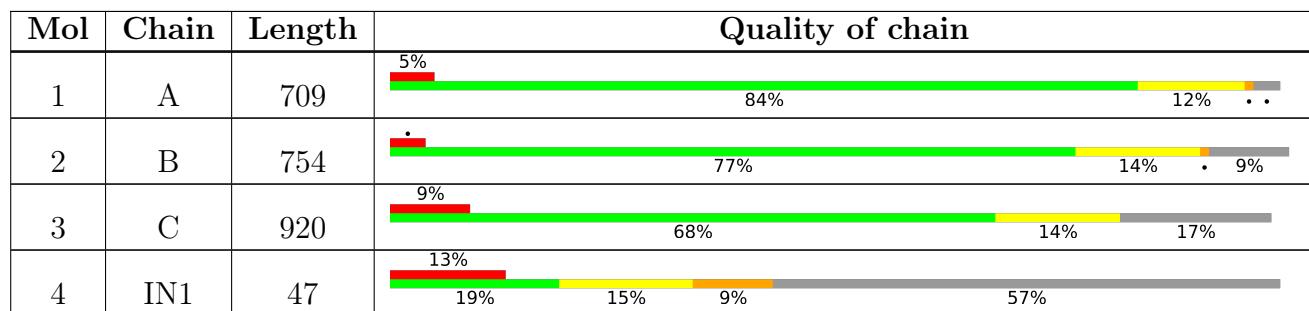
The reported resolution of this entry is 3.20 Å.

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	Percentile Ranks	Value
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		3.1%
RNA backbone		0.39

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures

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	709	5% 84% · · 12% · ·
2	B	754	· 77% 14% · 9%
3	C	920	9% 68% 14% 17%
4	IN1	47	13% 19% 15% 9% 57%

2　Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 34967 atoms, of which 17430 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	688	Total 11153	C 3563	H 5565	N 946	O 1037	S 42	0	0

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	686	Total 10982	C 3474	H 5517	N 913	O 1026	S 52	0	0

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	761	Total 12190	C 3834	H 6132	N 1063	O 1123	S 38	0	0

There are 146 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	775	GLU	-	expression tag	UNP Q9IMP3
C	776	ASN	-	expression tag	UNP Q9IMP3
C	777	LEU	-	expression tag	UNP Q9IMP3
C	778	TYR	-	expression tag	UNP Q9IMP3
C	779	PHE	-	expression tag	UNP Q9IMP3
C	780	GLN	-	expression tag	UNP Q9IMP3
C	781	GLY	-	expression tag	UNP Q9IMP3
C	782	GLU	-	expression tag	UNP Q9IMP3
C	783	LEU	-	expression tag	UNP Q9IMP3
C	784	LYS	-	expression tag	UNP Q9IMP3
C	785	THR	-	expression tag	UNP Q9IMP3
C	786	ALA	-	expression tag	UNP Q9IMP3
C	787	ALA	-	expression tag	UNP Q9IMP3
C	788	LEU	-	expression tag	UNP Q9IMP3
C	789	ALA	-	expression tag	UNP Q9IMP3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	790	GLN	-	expression tag	UNP Q9IMP3
C	791	HIS	-	expression tag	UNP Q9IMP3
C	792	ASP	-	expression tag	UNP Q9IMP3
C	793	GLU	-	expression tag	UNP Q9IMP3
C	794	ALA	-	expression tag	UNP Q9IMP3
C	795	VAL	-	expression tag	UNP Q9IMP3
C	796	ASP	-	expression tag	UNP Q9IMP3
C	797	ASN	-	expression tag	UNP Q9IMP3
C	798	LYS	-	expression tag	UNP Q9IMP3
C	799	PHE	-	expression tag	UNP Q9IMP3
C	800	ASN	-	expression tag	UNP Q9IMP3
C	801	LYS	-	expression tag	UNP Q9IMP3
C	802	GLU	-	expression tag	UNP Q9IMP3
C	803	GLN	-	expression tag	UNP Q9IMP3
C	804	GLN	-	expression tag	UNP Q9IMP3
C	805	ASN	-	expression tag	UNP Q9IMP3
C	806	ALA	-	expression tag	UNP Q9IMP3
C	807	PHE	-	expression tag	UNP Q9IMP3
C	808	TYR	-	expression tag	UNP Q9IMP3
C	809	GLU	-	expression tag	UNP Q9IMP3
C	810	ILE	-	expression tag	UNP Q9IMP3
C	811	LEU	-	expression tag	UNP Q9IMP3
C	812	HIS	-	expression tag	UNP Q9IMP3
C	813	LEU	-	expression tag	UNP Q9IMP3
C	814	PRO	-	expression tag	UNP Q9IMP3
C	815	ASN	-	expression tag	UNP Q9IMP3
C	816	LEU	-	expression tag	UNP Q9IMP3
C	817	ASN	-	expression tag	UNP Q9IMP3
C	818	GLU	-	expression tag	UNP Q9IMP3
C	819	GLU	-	expression tag	UNP Q9IMP3
C	820	GLN	-	expression tag	UNP Q9IMP3
C	821	ARG	-	expression tag	UNP Q9IMP3
C	822	ASN	-	expression tag	UNP Q9IMP3
C	823	ALA	-	expression tag	UNP Q9IMP3
C	824	PHE	-	expression tag	UNP Q9IMP3
C	825	ILE	-	expression tag	UNP Q9IMP3
C	826	GLN	-	expression tag	UNP Q9IMP3
C	827	SER	-	expression tag	UNP Q9IMP3
C	828	LEU	-	expression tag	UNP Q9IMP3
C	829	LYS	-	expression tag	UNP Q9IMP3
C	830	ASP	-	expression tag	UNP Q9IMP3
C	831	ASP	-	expression tag	UNP Q9IMP3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	832	PRO	-	expression tag	UNP Q9IMP3
C	833	SER	-	expression tag	UNP Q9IMP3
C	834	GLN	-	expression tag	UNP Q9IMP3
C	835	SER	-	expression tag	UNP Q9IMP3
C	836	ALA	-	expression tag	UNP Q9IMP3
C	837	ASN	-	expression tag	UNP Q9IMP3
C	838	LEU	-	expression tag	UNP Q9IMP3
C	839	LEU	-	expression tag	UNP Q9IMP3
C	840	ALA	-	expression tag	UNP Q9IMP3
C	841	GLU	-	expression tag	UNP Q9IMP3
C	842	ALA	-	expression tag	UNP Q9IMP3
C	843	LYS	-	expression tag	UNP Q9IMP3
C	844	LYS	-	expression tag	UNP Q9IMP3
C	845	LEU	-	expression tag	UNP Q9IMP3
C	846	ASN	-	expression tag	UNP Q9IMP3
C	847	ASP	-	expression tag	UNP Q9IMP3
C	848	ALA	-	expression tag	UNP Q9IMP3
C	849	GLN	-	expression tag	UNP Q9IMP3
C	850	ALA	-	expression tag	UNP Q9IMP3
C	851	PRO	-	expression tag	UNP Q9IMP3
C	852	LYS	-	expression tag	UNP Q9IMP3
C	853	VAL	-	expression tag	UNP Q9IMP3
C	854	ASP	-	expression tag	UNP Q9IMP3
C	855	ASN	-	expression tag	UNP Q9IMP3
C	856	LYS	-	expression tag	UNP Q9IMP3
C	857	PHE	-	expression tag	UNP Q9IMP3
C	858	ASN	-	expression tag	UNP Q9IMP3
C	859	LYS	-	expression tag	UNP Q9IMP3
C	860	GLU	-	expression tag	UNP Q9IMP3
C	861	GLN	-	expression tag	UNP Q9IMP3
C	862	GLN	-	expression tag	UNP Q9IMP3
C	863	ASN	-	expression tag	UNP Q9IMP3
C	864	ALA	-	expression tag	UNP Q9IMP3
C	865	PHE	-	expression tag	UNP Q9IMP3
C	866	TYR	-	expression tag	UNP Q9IMP3
C	867	GLU	-	expression tag	UNP Q9IMP3
C	868	ILE	-	expression tag	UNP Q9IMP3
C	869	LEU	-	expression tag	UNP Q9IMP3
C	870	HIS	-	expression tag	UNP Q9IMP3
C	871	LEU	-	expression tag	UNP Q9IMP3
C	872	PRO	-	expression tag	UNP Q9IMP3
C	873	ASN	-	expression tag	UNP Q9IMP3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	874	LEU	-	expression tag	UNP Q9IMP3
C	875	ASN	-	expression tag	UNP Q9IMP3
C	876	GLU	-	expression tag	UNP Q9IMP3
C	877	GLU	-	expression tag	UNP Q9IMP3
C	878	GLN	-	expression tag	UNP Q9IMP3
C	879	ARG	-	expression tag	UNP Q9IMP3
C	880	ASN	-	expression tag	UNP Q9IMP3
C	881	ALA	-	expression tag	UNP Q9IMP3
C	882	PHE	-	expression tag	UNP Q9IMP3
C	883	ILE	-	expression tag	UNP Q9IMP3
C	884	GLN	-	expression tag	UNP Q9IMP3
C	885	SER	-	expression tag	UNP Q9IMP3
C	886	LEU	-	expression tag	UNP Q9IMP3
C	887	LYS	-	expression tag	UNP Q9IMP3
C	888	ALA	-	expression tag	UNP Q9IMP3
C	889	ASP	-	expression tag	UNP Q9IMP3
C	890	PRO	-	expression tag	UNP Q9IMP3
C	891	SER	-	expression tag	UNP Q9IMP3
C	892	GLN	-	expression tag	UNP Q9IMP3
C	893	SER	-	expression tag	UNP Q9IMP3
C	894	ALA	-	expression tag	UNP Q9IMP3
C	895	ASN	-	expression tag	UNP Q9IMP3
C	896	LEU	-	expression tag	UNP Q9IMP3
C	897	LEU	-	expression tag	UNP Q9IMP3
C	898	ALA	-	expression tag	UNP Q9IMP3
C	899	GLU	-	expression tag	UNP Q9IMP3
C	900	ALA	-	expression tag	UNP Q9IMP3
C	901	LYS	-	expression tag	UNP Q9IMP3
C	902	LYS	-	expression tag	UNP Q9IMP3
C	903	LEU	-	expression tag	UNP Q9IMP3
C	904	ASN	-	expression tag	UNP Q9IMP3
C	905	GLY	-	expression tag	UNP Q9IMP3
C	906	ALA	-	expression tag	UNP Q9IMP3
C	907	GLN	-	expression tag	UNP Q9IMP3
C	908	ALA	-	expression tag	UNP Q9IMP3
C	909	PRO	-	expression tag	UNP Q9IMP3
C	910	LYS	-	expression tag	UNP Q9IMP3
C	911	VAL	-	expression tag	UNP Q9IMP3
C	912	ASP	-	expression tag	UNP Q9IMP3
C	913	ALA	-	expression tag	UNP Q9IMP3
C	914	ASN	-	expression tag	UNP Q9IMP3
C	915	SER	-	expression tag	UNP Q9IMP3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	916	ALA	-	expression tag	UNP Q9IMP3
C	917	GLY	-	expression tag	UNP Q9IMP3
C	918	LYS	-	expression tag	UNP Q9IMP3
C	919	SER	-	expression tag	UNP Q9IMP3
C	920	THR	-	expression tag	UNP Q9IMP3
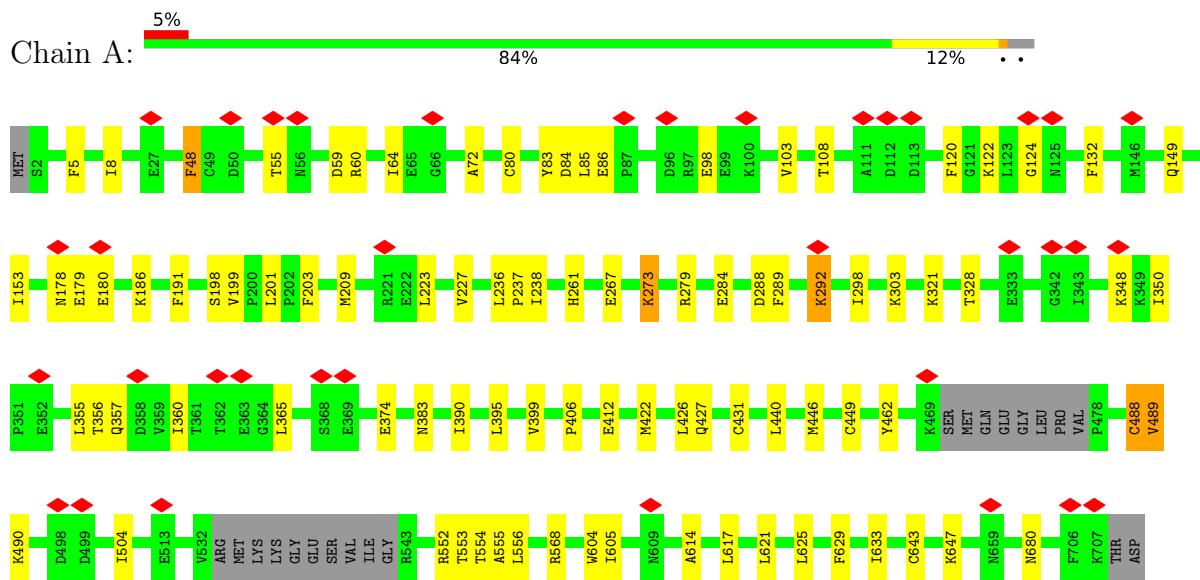
- Molecule 4 is a RNA chain called RNA (5'-R(*AP*GP*UP*AP*GP*AP*AP*AP*CP*AP* AP*GP*GP*GP*CP*CP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
4	IN1	20	642	192	216	79	136	19	0	0
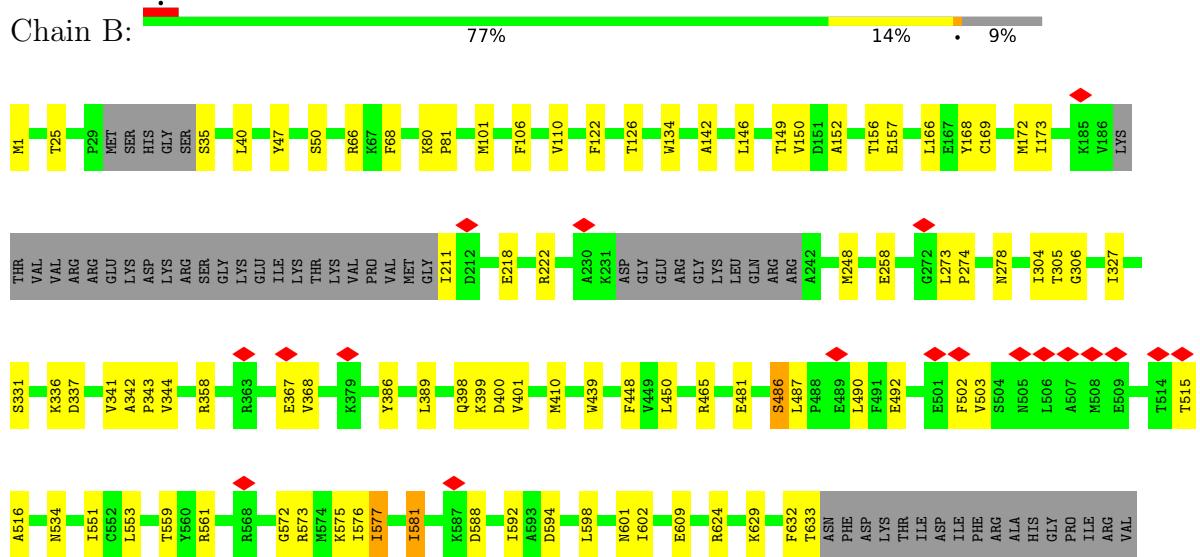
3 Residue-property plots ⓘ
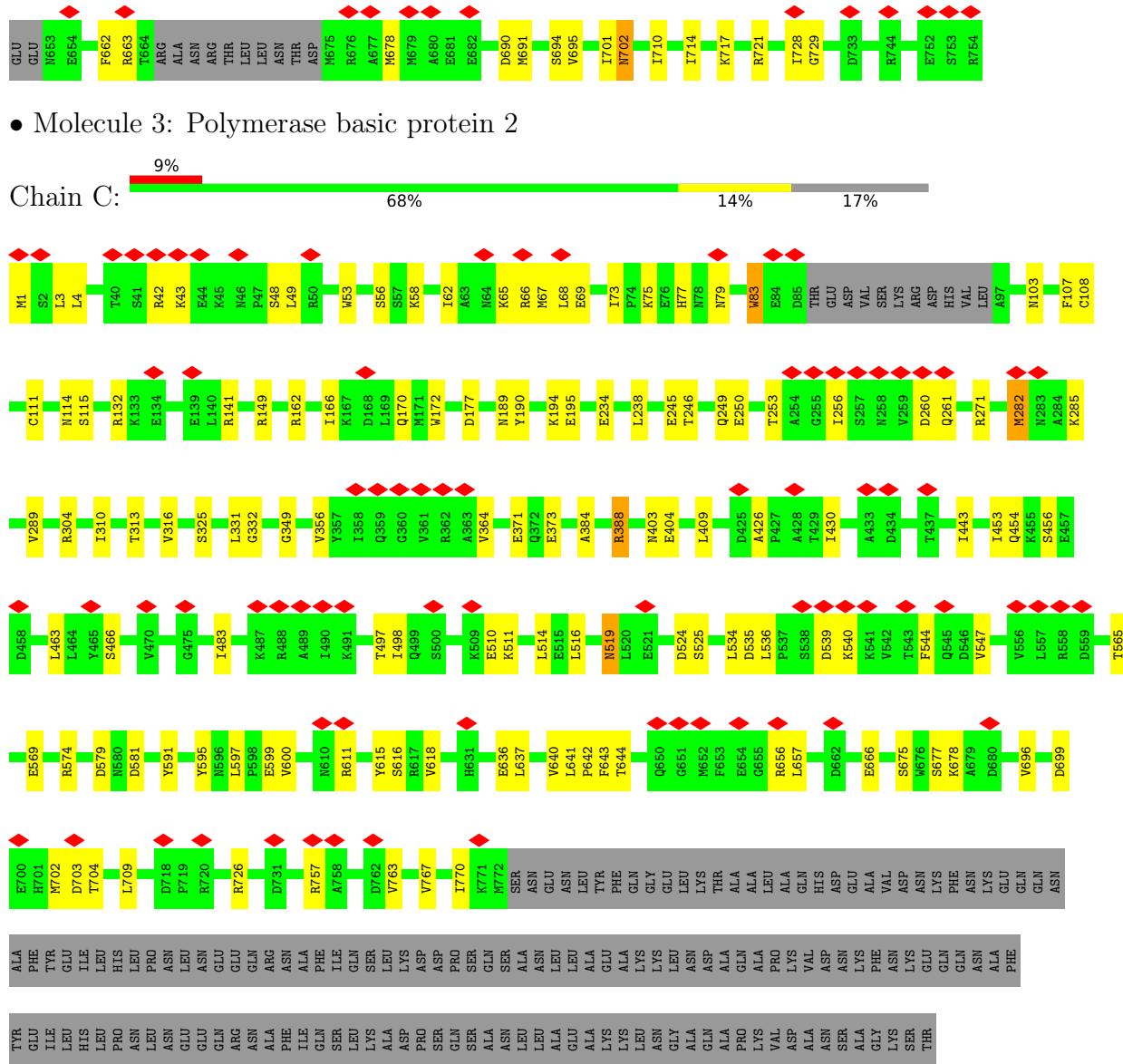
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Polymerase acidic protein

• Molecule 2: RNA-directed RNA polymerase catalytic subunit

GLU GLU N653 E654 F662 R663 T664 ARG ALA ASN ARG THR LEU LEU ASN THR ASP M675 R676 A677 M678 M679 A680 E681 E682 D690 M691 S694 V695 I701 N702 I710 I714 K717 R721 I728 G729 D733 R744 E752 S753 R754

• Molecule 3: Polymerase basic protein 2

Chain C:

9%

68% 14% 17%

M1 S2 L3 L4 T40 S41 R42 K43 E44 K45 N46 P47 S48 L49 R50 W53 S56 S57 K58 I62 A63 N64 K65 R66 M67 L68 E69 I73 P74 K75 E76 H77 N78 N79 W83 E84 D85 THR GLU ASP VAL SER LYS ARG ASP HIS VAL LEU A97 N103 F107 C108

C111 N114 S115 R132 K133 E134 E139 L140 R141 R149 R162 I166 K167 D168 L169 Q170 M171 W172 D177 N189 Y190 K194 E195 E234 L238 E245 T246 Q249 E250 T253 A254 G255 I256 S257 N258 V259 D260 Q261 R271 M282 N283 A284 K285

V289 R304 I310 T313 V316 S325 L331 G332 G349 V356 Y357 I358 Q359 G360 V361 R362 A363 V364 E371 Q372 E373 A384 R388 N403 E404 L409 D425 A426 P427 A428 T429 I430 A433 D434 T437 I443 I453 Q454 K455 S456 E457

D458 L463 L464 Y465 S466 V470 G475 I483 K487 R488 A489 I490 K491 T497 I498 Q499 S500 K509 E510 K511 L514 E515 L516 N519 L520 E521 D524 S525 L534 D535 L536 P537 S538 D539 K540 K541 V542 T543 F544 Q545 D546 V547 V556 L557 R558 D559 T565

E569 R574 D579 N580 D581 Y591 V595 N596 L597 P598 E599 V600 N610 R611 Y615 S616 R617 V618 H631 E636 L637 V640 L641 P642 F643 T644 Q650 G651 M652 F653 E654 G655 R656 L657 D662 E666 S675 W676 S677 K678 A679 D680 V696 D699

E700 H701 M702 D703 T704 L709 D718 P719 R720 R726 D731 R757 A758 D762 V763 V767 I770 K771 M772 SER ASN ASN LEU TYR PHE GLN GLY LEU LEU LYS THR ALA ALA LEU ALA GLN HIS ASP GLU ALA VAL ASP ASN LYS PHE ASN LYS GLU GLN GLN ASN

ALA PHE TYR GLU ILE LEU HIS LEU PRO ASN LEU ASN GLU GLU GLN ARG ASN ALA PHE ILE GLN SER LEU LYS ASP ASP PRO SER GLN SER ALA ASN LEU LEU ALA GLU ALA LYS LYS LEU ASN ASP ALA GLN ALA PRO LYS VAL ASP ASN LYS PHE ASN LYS GLU GLN GLN ASN ALA PHE

TYR GLU ILE LEU HIS LEU PRO ASN LEU ASN GLU GLU GLN ARG ASN ALA PHE ILE GLN SER LEU LYS ASP ASP PRO SER GLN SER ALA ASN LEU LEU ALA GLU ALA LYS LYS LEU ASN ASP ALA GLN ALA PRO LYS VAL ASP ASN SER ALA GLY LYS SER THR

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

Chain IN1:

13%

19% 15% 9% 57%

A1 A4 G5 A6 A7 A8 A11 G14 U A U U U U U C U U U A C U A G U U A C C36 C37 U38 G C U U42 U43 U44 G C U

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	32.1	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.164	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	499.1, 499.1, 499.1	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.085, 1.085, 1.085	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.35	0/5704	0.45	0/7662
2	B	0.35	0/5559	0.47	0/7466
3	C	0.33	0/6167	0.48	0/8299
4	IN1	0.38	0/475	0.91	1/734 (0.1%)
All	All	0.34	0/17905	0.49	1/24161 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	IN1	42	U	P-O3'-C3'	5.47	126.26	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5588	5565	5587	62	0
2	B	5465	5517	5540	71	0
3	C	6058	6132	6172	80	0
4	IN1	426	216	219	10	0
All	All	17537	17430	17518	204	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 6.

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All (204) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:573:ARG:HE	3:C:103:ASN:HD21	1.13	0.91
2:B:573:ARG:NE	3:C:103:ASN:HD21	1.69	0.89
4:IN1:44:U:O2	4:IN1:44:U:H5"	1.78	0.82
3:C:331:LEU:HD11	3:C:514:LEU:HD21	1.62	0.81
3:C:426:ALA:HB1	3:C:430:ILE:HD11	1.66	0.76
1:A:86:GLU:N	1:A:86:GLU:OE1	2.20	0.74
2:B:47:TYR:O	2:B:66:ARG:NH2	2.22	0.72
2:B:624:ARG:NH2	3:C:107:PHE:O	2.24	0.70
3:C:702:MET:O	3:C:704:THR:HG22	1.91	0.69
1:A:643:CYS:O	1:A:647:LYS:NZ	2.25	0.69
3:C:514:LEU:HD12	3:C:514:LEU:O	1.93	0.68
2:B:573:ARG:HG3	3:C:103:ASN:HD22	1.57	0.68
4:IN1:5:G:N2	4:IN1:5:G:OP2	2.28	0.67
1:A:236:LEU:O	2:B:465:ARG:NH2	2.27	0.67
2:B:678:MET:SD	2:B:678:MET:N	2.68	0.66
3:C:189:ASN:HD21	3:C:304:ARG:NE	1.93	0.66
3:C:611:ARG:HA	3:C:611:ARG:HE	1.60	0.66
3:C:245:GLU:HG3	3:C:246:THR:HG23	1.78	0.65
3:C:234:GLU:HB3	3:C:256:ILE:HD12	1.76	0.65
3:C:253:THR:HB	3:C:256:ILE:HD11	1.79	0.65
1:A:390:ILE:HG22	1:A:390:ILE:O	1.97	0.64
1:A:48:PHE:O	1:A:149:GLN:NE2	2.31	0.64
1:A:179:GLU:HG2	1:A:180:GLU:N	2.12	0.64
2:B:573:ARG:HG3	3:C:103:ASN:ND2	2.12	0.64
1:A:5:PHE:HA	1:A:8:ILE:HD12	1.80	0.63
3:C:285:LYS:O	3:C:289:VAL:HG23	1.98	0.63
2:B:481:GLU:OE1	2:B:481:GLU:N	2.31	0.62
2:B:573:ARG:NE	3:C:103:ASN:ND2	2.47	0.61
1:A:488:CYS:SG	1:A:489:VAL:N	2.74	0.61
4:IN1:44:U:O2	4:IN1:44:U:C5'	2.48	0.61
1:A:120:PHE:O	1:A:124:GLY:N	2.34	0.61
3:C:763:VAL:O	3:C:767:VAL:HG23	2.02	0.59
2:B:337:ASP:O	2:B:341:VAL:HG23	2.02	0.59
3:C:3:LEU:HD12	3:C:4:LEU:N	2.18	0.58
1:A:355:LEU:HD21	1:A:360:ILE:HD11	1.84	0.58
2:B:211:ILE:HG22	2:B:211:ILE:O	2.04	0.58
2:B:572:GLY:O	2:B:576:ILE:HG23	2.04	0.57
3:C:767:VAL:HA	3:C:770:ILE:HD12	1.87	0.57
3:C:310:ILE:O	3:C:313:THR:HG22	2.04	0.57
3:C:565:THR:HG22	3:C:569:GLU:OE2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:691:MET:O	2:B:694:SER:OG	2.20	0.57
3:C:316:VAL:O	3:C:316:VAL:HG23	2.05	0.57
3:C:597:LEU:O	3:C:600:VAL:HG22	2.05	0.56
2:B:25:THR:HG22	2:B:25:THR:O	2.06	0.56
2:B:134:TRP:HZ2	2:B:149:THR:HG1	1.53	0.56
3:C:194:LYS:NZ	3:C:678:LYS:O	2.39	0.56
2:B:400:ASP:O	2:B:401:VAL:HG13	2.07	0.55
2:B:341:VAL:O	2:B:344:VAL:HG22	2.06	0.55
2:B:695:VAL:O	2:B:721:ARG:NH2	2.40	0.54
3:C:636:GLU:O	3:C:640:VAL:HG22	2.07	0.54
1:A:191:PHE:CZ	2:B:341:VAL:HG22	2.42	0.54
1:A:328:THR:HG23	1:A:328:THR:O	2.08	0.54
3:C:637:LEU:O	3:C:641:LEU:HG	2.07	0.54
1:A:431:CYS:SG	1:A:625:LEU:HD23	2.48	0.54
2:B:577:ILE:HG23	2:B:581:ILE:HD12	1.89	0.54
3:C:282:MET:SD	3:C:282:MET:N	2.81	0.54
4:IN1:5:G:O2'	4:IN1:6:A:O4'	2.25	0.53
1:A:553:THR:HG23	1:A:553:THR:O	2.08	0.53
3:C:68:LEU:HD13	3:C:83:TRP:CE3	2.43	0.53
3:C:384:ALA:HB2	3:C:409:LEU:HD21	1.91	0.53
1:A:406:PRO:O	2:B:601:ASN:ND2	2.41	0.53
2:B:576:ILE:HG13	2:B:577:ILE:N	2.24	0.53
3:C:615:TYR:O	3:C:618:VAL:HG12	2.09	0.52
2:B:410:MET:SD	2:B:410:MET:N	2.83	0.52
2:B:515:THR:O	3:C:48:SER:HB3	2.10	0.52
1:A:629:PHE:CE1	1:A:633:ILE:HD11	2.45	0.52
3:C:599:GLU:N	3:C:599:GLU:OE1	2.43	0.52
4:IN1:7:A:O2'	4:IN1:8:A:OP2	2.22	0.52
2:B:398:GLN:HB3	2:B:401:VAL:HG23	1.92	0.51
2:B:516:ALA:O	3:C:48:SER:N	2.43	0.51
3:C:331:LEU:HD12	3:C:332:GLY:O	2.10	0.51
2:B:399:LYS:O	2:B:401:VAL:HG22	2.11	0.51
1:A:178:ASN:OD1	1:A:179:GLU:N	2.44	0.50
1:A:604:TRP:CE3	1:A:614:ALA:HB2	2.46	0.50
1:A:261:HIS:O	1:A:552:ARG:NH2	2.44	0.50
1:A:355:LEU:HD23	1:A:356:THR:N	2.26	0.50
3:C:516:LEU:HD23	3:C:516:LEU:N	2.26	0.50
1:A:350:ILE:HB	2:B:368:VAL:HG22	1.94	0.50
1:A:103:VAL:HG13	1:A:103:VAL:O	2.12	0.50
2:B:702:ASN:O	2:B:702:ASN:ND2	2.44	0.50
3:C:49:LEU:O	3:C:49:LEU:HD12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:373:GLU:OE1	3:C:388:ARG:NH2	2.45	0.50
2:B:273:LEU:HB3	2:B:274:PRO:HD3	1.94	0.49
2:B:553:LEU:HD22	2:B:598:LEU:HD13	1.93	0.49
3:C:483:ILE:HD12	3:C:483:ILE:N	2.27	0.49
1:A:412:GLU:OE2	2:B:602:ILE:N	2.41	0.49
1:A:298:ILE:O	1:A:321:LYS:NZ	2.45	0.49
2:B:66:ARG:HB3	2:B:68:PHE:HE1	1.76	0.49
2:B:503:VAL:HG13	2:B:503:VAL:O	2.12	0.49
1:A:440:LEU:HD23	1:A:462:TYR:CE2	2.48	0.49
1:A:374:GLU:N	1:A:374:GLU:OE1	2.46	0.48
3:C:591:TYR:HD1	3:C:595:TYR:HH	1.60	0.48
2:B:592:ILE:HD12	2:B:609:GLU:OE1	2.14	0.48
3:C:73:ILE:O	3:C:73:ILE:HD12	2.13	0.48
2:B:106:PHE:HB3	2:B:327:ILE:HG23	1.96	0.47
3:C:574:ARG:NH2	3:C:581:ASP:OD1	2.47	0.47
1:A:399:VAL:HG13	1:A:427:GLN:HE22	1.78	0.47
3:C:249:GLN:NE2	3:C:250:GLU:O	2.44	0.47
1:A:605:ILE:C	1:A:605:ILE:HD12	2.35	0.47
1:A:186:LYS:O	2:B:173:ILE:HG21	2.14	0.47
3:C:535:ASP:OD1	3:C:536:LEU:HD12	2.14	0.47
1:A:267:GLU:OE1	1:A:267:GLU:N	2.47	0.47
3:C:641:LEU:N	3:C:642:PRO:CD	2.78	0.47
2:B:50:SER:HG	2:B:66:ARG:HH21	1.62	0.47
4:IN1:44:U:O2	4:IN1:44:U:O4'	2.30	0.47
3:C:271:ARG:HG3	3:C:536:LEU:HD23	1.98	0.46
3:C:166:ILE:HG22	3:C:170:GLN:OE1	2.15	0.46
3:C:172:TRP:CH2	3:C:709:LEU:HD11	2.50	0.46
2:B:701:ILE:HG13	2:B:702:ASN:H	1.80	0.46
1:A:223:LEU:O	1:A:227:VAL:HG23	2.15	0.46
3:C:331:LEU:HD21	3:C:514:LEU:HD11	1.97	0.46
4:IN1:7:A:O2'	4:IN1:8:A:P	2.73	0.46
1:A:504:ILE:HD13	1:A:556:LEU:HD12	1.99	0.45
1:A:629:PHE:CZ	1:A:633:ILE:HD11	2.50	0.45
1:A:383:ASN:ND2	2:B:1:MET:O	2.40	0.45
2:B:40:LEU:HB2	2:B:389:LEU:HD21	1.97	0.45
3:C:260:ASP:OD2	3:C:261:GLN:N	2.49	0.45
3:C:611:ARG:HA	3:C:611:ARG:NE	2.30	0.45
3:C:656:ARG:HG2	3:C:666:GLU:HG2	1.98	0.45
1:A:64:ILE:HD11	1:A:72:ALA:O	2.17	0.45
3:C:325:SER:OG	3:C:514:LEU:HD12	2.16	0.45
1:A:680:ASN:ND2	1:A:680:ASN:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:MET:SD	2:B:248:MET:O	2.75	0.45
2:B:305:THR:HG22	2:B:492:GLU:H	1.82	0.45
1:A:83:TYR:HB2	1:A:85:LEU:HD23	1.98	0.45
1:A:199:VAL:HG13	1:A:209:MET:CE	2.47	0.45
2:B:306:GLY:HA3	2:B:448:PHE:CZ	2.52	0.45
1:A:360:ILE:CG1	1:A:365:LEU:HD12	2.47	0.45
2:B:166:LEU:HD12	2:B:166:LEU:O	2.17	0.45
1:A:554:THR:OG1	1:A:555:ALA:N	2.48	0.44
2:B:168:TYR:O	2:B:172:MET:HG2	2.17	0.44
3:C:757:ARG:NE	3:C:757:ARG:HA	2.32	0.44
3:C:331:LEU:HD11	3:C:514:LEU:CD2	2.41	0.44
3:C:524:ASP:O	3:C:525:SER:OG	2.25	0.44
2:B:331:SER:O	2:B:336:LYS:HE3	2.17	0.44
2:B:106:PHE:O	2:B:110:VAL:HG13	2.17	0.44
2:B:152:ALA:O	2:B:156:THR:OG1	2.35	0.44
3:C:1:MET:O	3:C:4:LEU:N	2.51	0.44
4:IN1:4:A:O2'	4:IN1:5:G:O4'	2.29	0.44
2:B:358:ARG:NH1	2:B:367:GLU:OE2	2.50	0.43
3:C:65:LYS:O	3:C:69:GLU:HG2	2.19	0.43
4:IN1:42:U:O2	4:IN1:42:U:O4'	2.34	0.43
1:A:84:ASP:C	1:A:85:LEU:HD22	2.39	0.43
2:B:35:SER:HB3	4:IN1:7:A:H4'	2.00	0.43
3:C:42:ARG:NE	3:C:43:LYS:O	2.49	0.43
1:A:199:VAL:HG12	1:A:203:PHE:HB2	2.01	0.43
1:A:356:THR:HG22	1:A:357:GLN:N	2.34	0.43
1:A:426:LEU:HD22	1:A:625:LEU:HD22	1.99	0.43
2:B:146:LEU:O	2:B:150:VAL:HG23	2.19	0.43
1:A:59:ASP:OD1	1:A:60:ARG:N	2.52	0.43
2:B:218:GLU:OE2	2:B:222:ARG:NH2	2.52	0.43
3:C:699:ASP:O	3:C:703:ASP:HB2	2.19	0.43
1:A:132:PHE:CZ	1:A:153:ILE:HD13	2.54	0.42
2:B:40:LEU:CB	2:B:389:LEU:HD21	2.49	0.42
2:B:572:GLY:O	2:B:575:LYS:HG2	2.19	0.42
2:B:717:LYS:NZ	3:C:177:ASP:O	2.52	0.42
1:A:55:THR:HG23	1:A:98:GLU:OE2	2.19	0.42
3:C:349:GLY:HA2	3:C:371:GLU:HB2	2.01	0.42
3:C:510:GLU:O	3:C:511:LYS:NZ	2.48	0.42
3:C:544:PHE:HB3	3:C:547:VAL:HG21	2.01	0.42
3:C:699:ASP:O	3:C:703:ASP:N	2.52	0.42
2:B:126:THR:O	2:B:142:ALA:HB3	2.20	0.42
3:C:595:TYR:N	3:C:595:TYR:CD1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:403:ASN:OD1	3:C:404:GLU:N	2.53	0.42
2:B:577:ILE:HG23	2:B:581:ILE:CD1	2.49	0.42
1:A:446:MET:HA	1:A:449:CYS:SG	2.59	0.42
2:B:342:ALA:HB3	2:B:343:PRO:HD3	2.02	0.42
3:C:539:ASP:OD1	3:C:540:LYS:N	2.53	0.42
3:C:463:LEU:O	3:C:466:SER:HB2	2.19	0.42
2:B:169:CYS:O	2:B:173:ILE:HG12	2.20	0.42
2:B:304:ILE:HD12	2:B:450:LEU:HD23	2.02	0.42
2:B:439:TRP:CD1	2:B:439:TRP:O	2.73	0.42
3:C:497:THR:O	3:C:498:ILE:HD13	2.20	0.42
1:A:355:LEU:HD23	1:A:355:LEU:C	2.39	0.41
2:B:68:PHE:N	2:B:68:PHE:CD1	2.86	0.41
1:A:422:MET:HE3	1:A:426:LEU:HD11	2.01	0.41
3:C:519:ASN:OD1	3:C:519:ASN:N	2.52	0.41
2:B:710:ILE:HG22	2:B:714:ILE:HD12	2.02	0.41
1:A:629:PHE:O	1:A:633:ILE:HG12	2.21	0.41
1:A:279:ARG:HA	1:A:284:GLU:OE1	2.20	0.41
1:A:279:ARG:NH1	1:A:288:ASP:OD2	2.54	0.41
2:B:278:ASN:HB3	3:C:149:ARG:HD3	2.03	0.41
3:C:616:SER:OG	3:C:644:THR:HA	2.21	0.41
1:A:237:PRO:O	1:A:238:ILE:HD13	2.20	0.41
1:A:390:ILE:O	1:A:390:ILE:CG2	2.67	0.41
1:A:568:ARG:HD2	2:B:551:ILE:HD12	2.01	0.41
3:C:453:ILE:HG13	3:C:454:GLN:N	2.36	0.41
1:A:289:PHE:O	1:A:292:LYS:HG2	2.20	0.41
2:B:80:LYS:HB3	2:B:81:PRO:CD	2.51	0.41
3:C:643:PHE:CE2	3:C:657:LEU:HB3	2.56	0.41
1:A:273:LYS:HG2	1:A:289:PHE:CZ	2.56	0.41
1:A:446:MET:HA	1:A:449:CYS:HG	1.85	0.41
2:B:486:SER:OG	2:B:487:LEU:N	2.54	0.41
3:C:443:ILE:HG23	3:C:534:LEU:HD13	2.02	0.41
1:A:108:THR:HG23	1:A:108:THR:O	2.21	0.40
2:B:559:THR:O	2:B:561:ARG:NE	2.54	0.40
2:B:728:ILE:HG23	2:B:729:GLY:N	2.35	0.40
3:C:696:VAL:O	3:C:696:VAL:HG12	2.22	0.40
3:C:83:TRP:CD1	3:C:83:TRP:N	2.90	0.40
3:C:162:ARG:O	3:C:166:ILE:HD12	2.20	0.40
3:C:356:VAL:HG12	3:C:364:VAL:O	2.22	0.40
1:A:48:PHE:CD1	1:A:48:PHE:C	2.95	0.40
1:A:617:LEU:O	1:A:621:LEU:HD13	2.21	0.40
3:C:238:LEU:C	3:C:238:LEU:HD12	2.42	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	682/709 (96%)	653 (96%)	29 (4%)	0	100	100
2	B	674/754 (89%)	637 (94%)	37 (6%)	0	100	100
3	C	757/920 (82%)	714 (94%)	43 (6%)	0	100	100
All	All	2113/2383 (89%)	2004 (95%)	109 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	613/631 (97%)	600 (98%)	13 (2%)	53	79
2	B	609/669 (91%)	589 (97%)	20 (3%)	38	71
3	C	666/801 (83%)	640 (96%)	26 (4%)	32	67
All	All	1888/2101 (90%)	1829 (97%)	59 (3%)	43	72

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	PHE
1	A	80	CYS

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Mol	Chain	Res	Type
1	A	122	LYS
1	A	198	SER
1	A	201	LEU
1	A	273	LYS
1	A	292	LYS
1	A	303	LYS
1	A	348	LYS
1	A	395	LEU
1	A	488	CYS
1	A	489	VAL
1	A	490	LYS
2	B	101	MET
2	B	122	PHE
2	B	157	GLU
2	B	258	GLU
2	B	386	TYR
2	B	486	SER
2	B	490	LEU
2	B	502	PHE
2	B	534	ASN
2	B	577	ILE
2	B	581	ILE
2	B	588	ASP
2	B	594	ASP
2	B	629	LYS
2	B	632	PHE
2	B	633	THR
2	B	662	PHE
2	B	663	ARG
2	B	690	ASP
2	B	702	ASN
3	C	53	TRP
3	C	56	SER
3	C	58	LYS
3	C	62	ILE
3	C	66	ARG
3	C	67	MET
3	C	75	LYS
3	C	77	HIS
3	C	79	ASN
3	C	83	TRP
3	C	108	CYS

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Mol	Chain	Res	Type
3	C	111	CYS
3	C	114	ASN
3	C	115	SER
3	C	132	ARG
3	C	141	ARG
3	C	190	TYR
3	C	195	GLU
3	C	282	MET
3	C	388	ARG
3	C	456	SER
3	C	519	ASN
3	C	579	ASP
3	C	675	SER
3	C	677	SER
3	C	726	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	HIS
1	A	315	ASN
1	A	319	GLN
1	A	417	HIS
1	A	494	HIS
1	A	615	GLN
2	B	147	GLN
2	B	315	GLN
2	B	414	ASN
2	B	702	ASN
3	C	46	ASN
3	C	79	ASN
3	C	103	ASN
3	C	189	ASN
3	C	202	ASN
3	C	212	HIS
3	C	264	ASN
3	C	764	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	IN1	17/47 (36%)	7 (41%)	0

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	IN1	6	A
4	IN1	8	A
4	IN1	11	A
4	IN1	14	G
4	IN1	37	C
4	IN1	43	U
4	IN1	44	U

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.
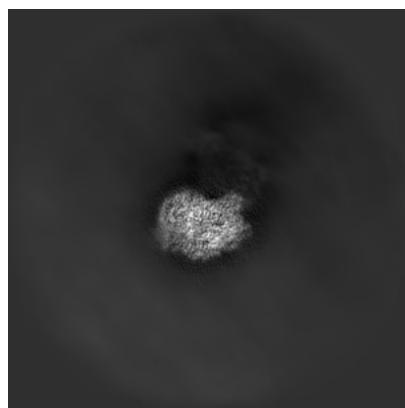
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-10667. These allow visual inspection of the internal detail of the map and identification of artifacts.
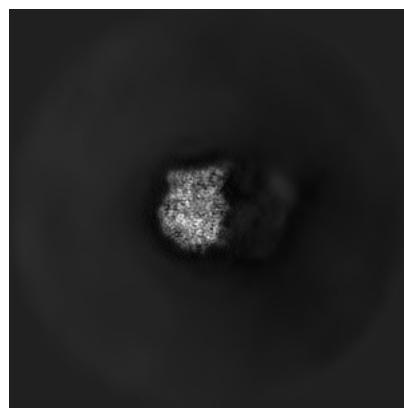
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ
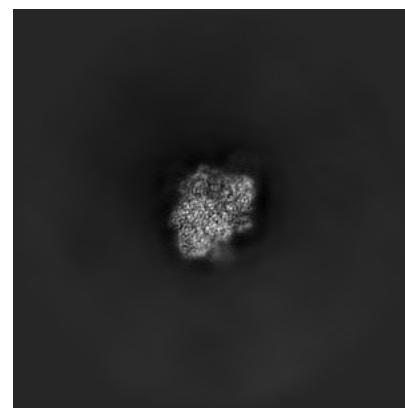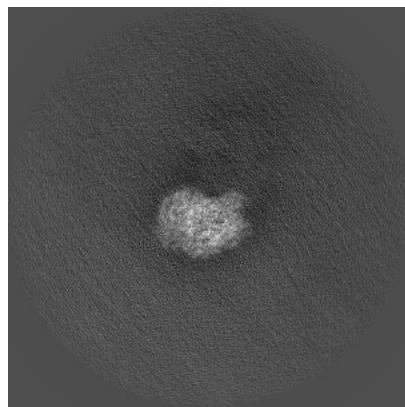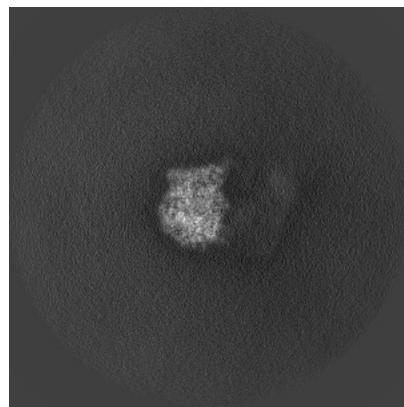
6.1.1 Primary map

X	Y	Z
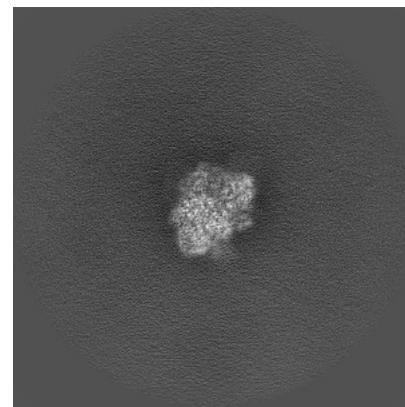
6.1.2 Raw map

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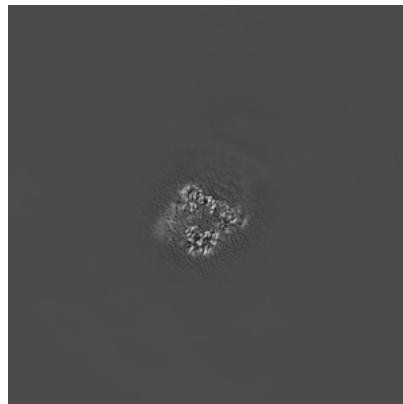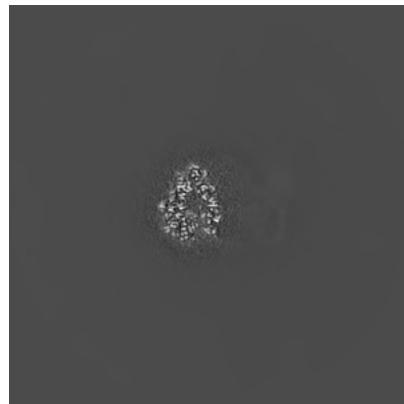
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
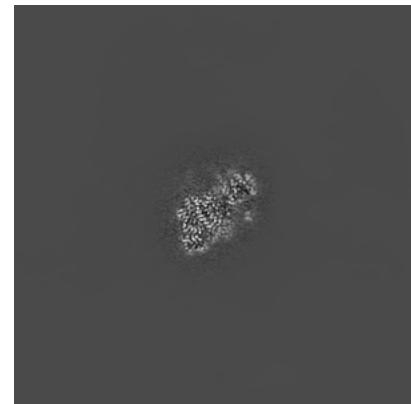
6.2.1 Primary map
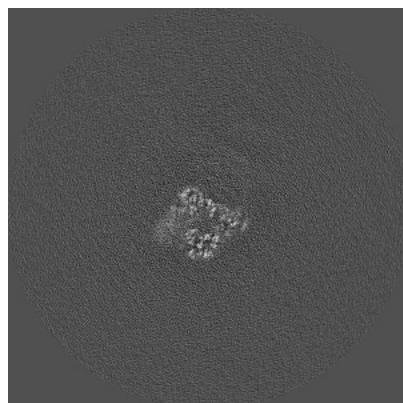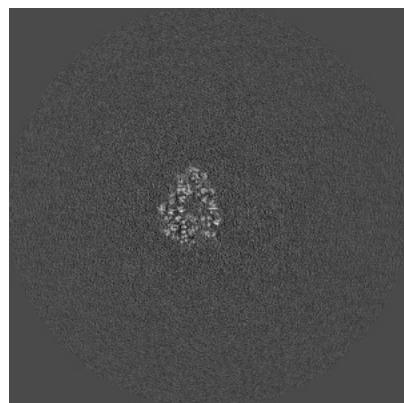
| X Index: 230 | Y Index: 230 | Z Index: 230 |
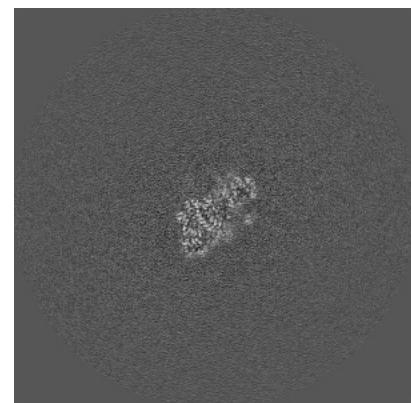
6.2.2 Raw map
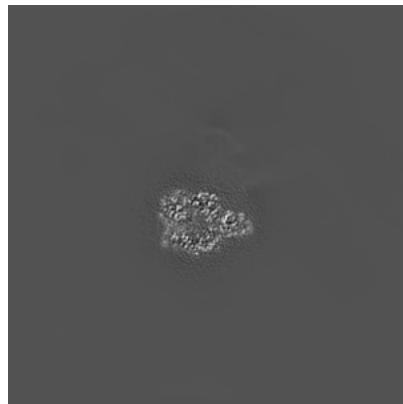
| X Index: 230 | Y Index: 230 | Z Index: 230 |
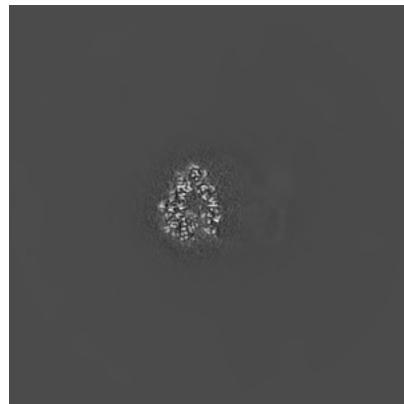
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
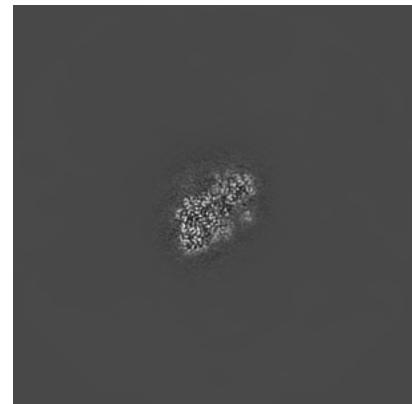
6.3.1 Primary map
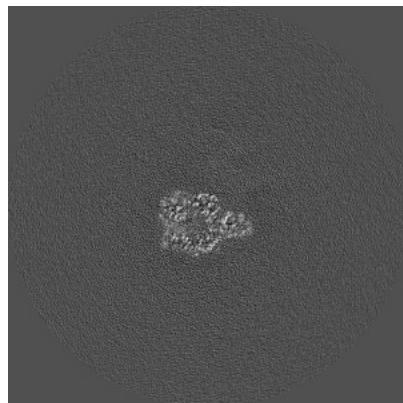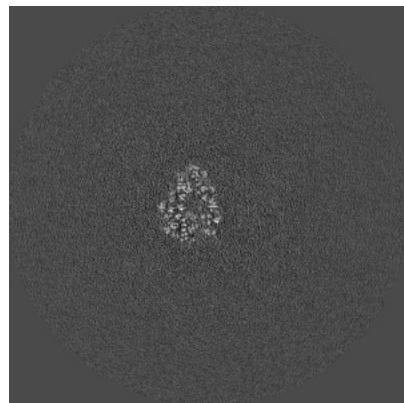
| X Index: 217 | Y Index: 230 | Z Index: 229 |
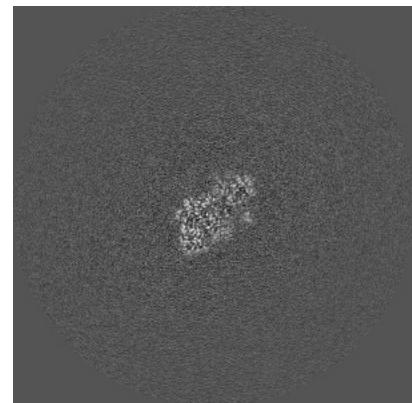
6.3.2 Raw map
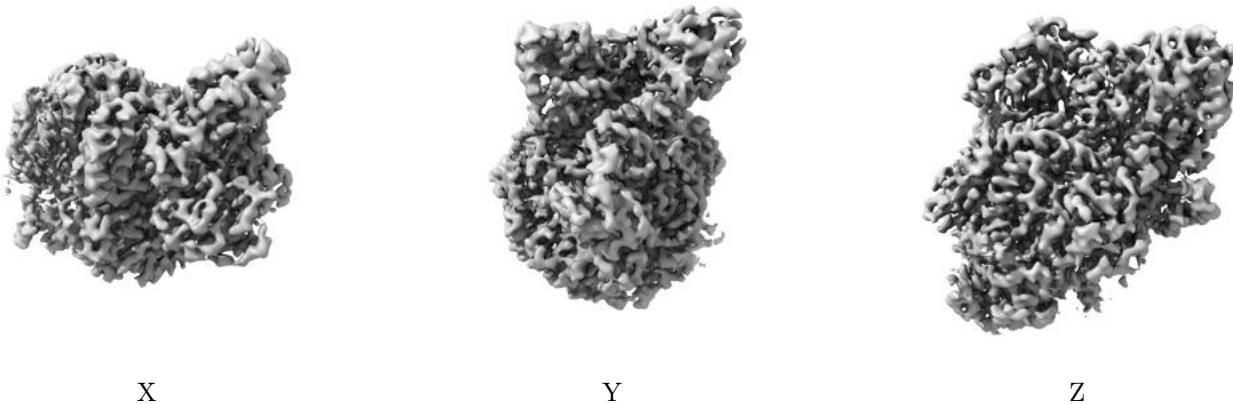
| X Index: 217 | Y Index: 230 | Z Index: 229 |

The images above show the largest variance slices of the map in three orthogonal directions.
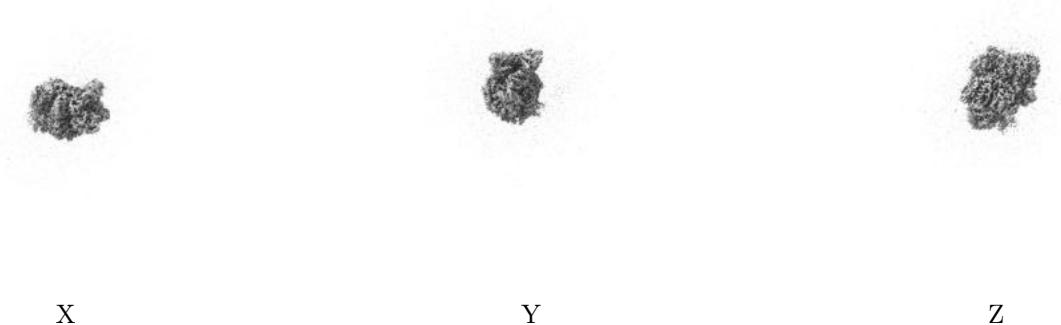
6.4 Orthogonal surface views (i)

6.4.1 Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.
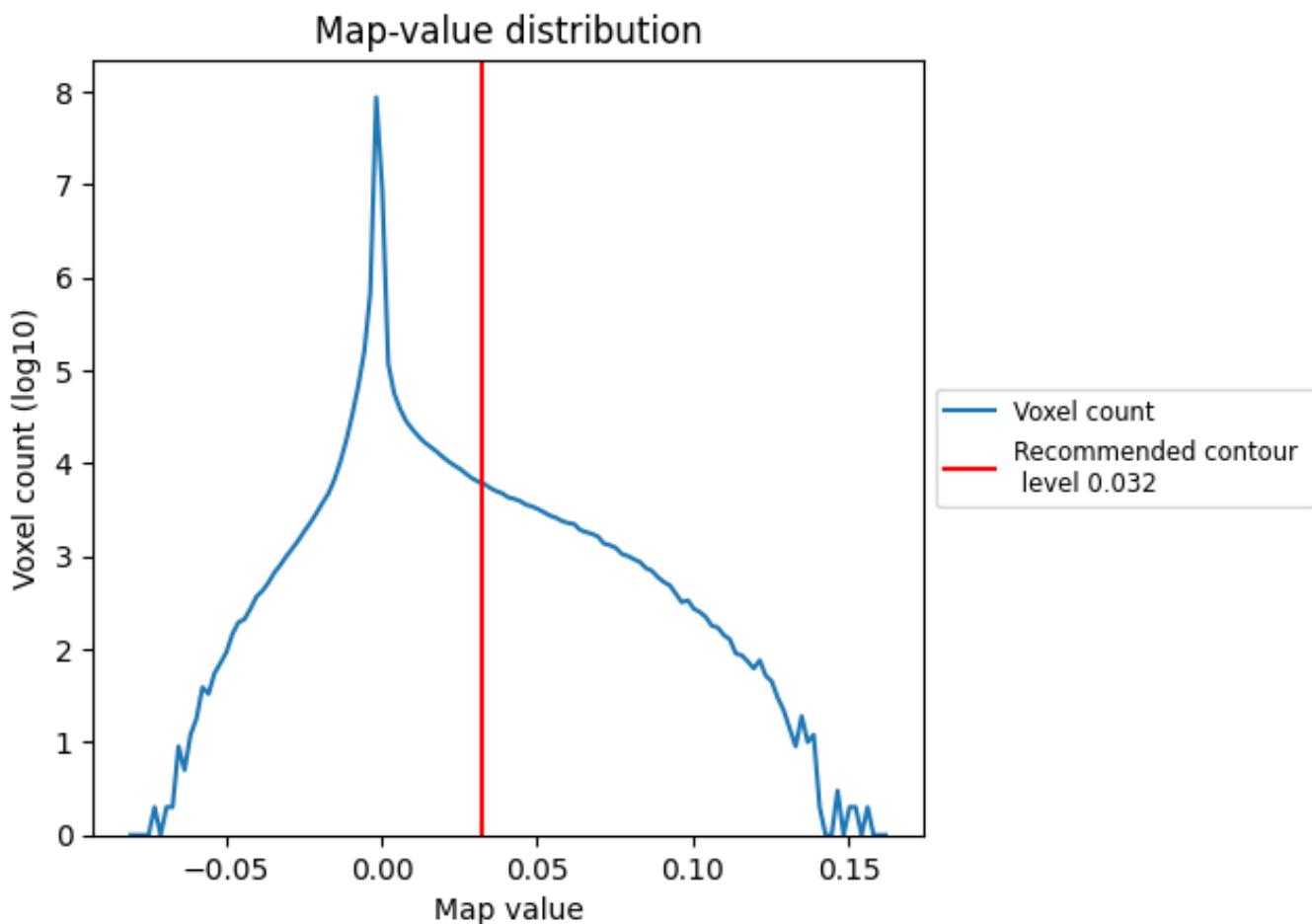
6.5 Mask visualisation (i)

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

7 Map analysis ⓘ
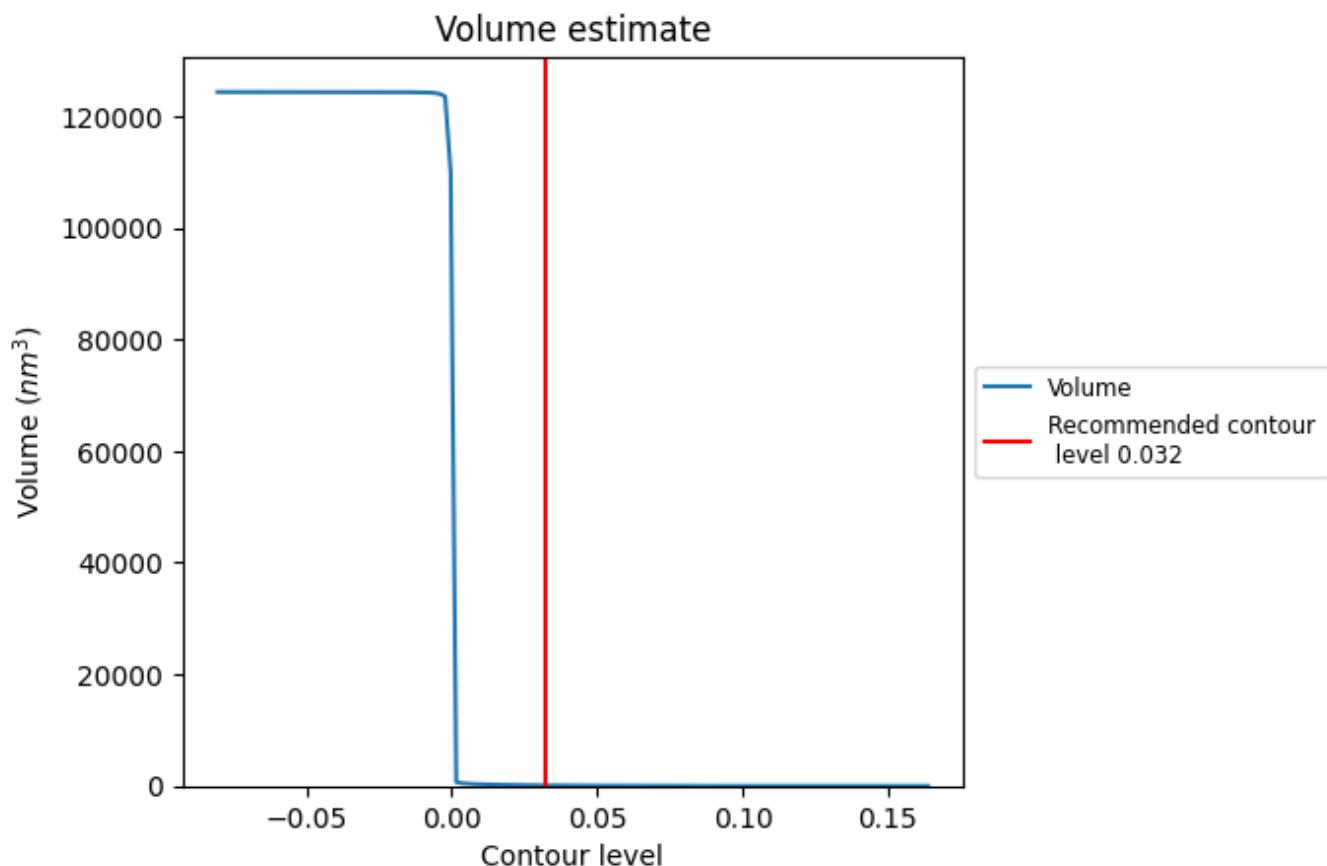
This section contains the results of statistical analysis of the map.

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.
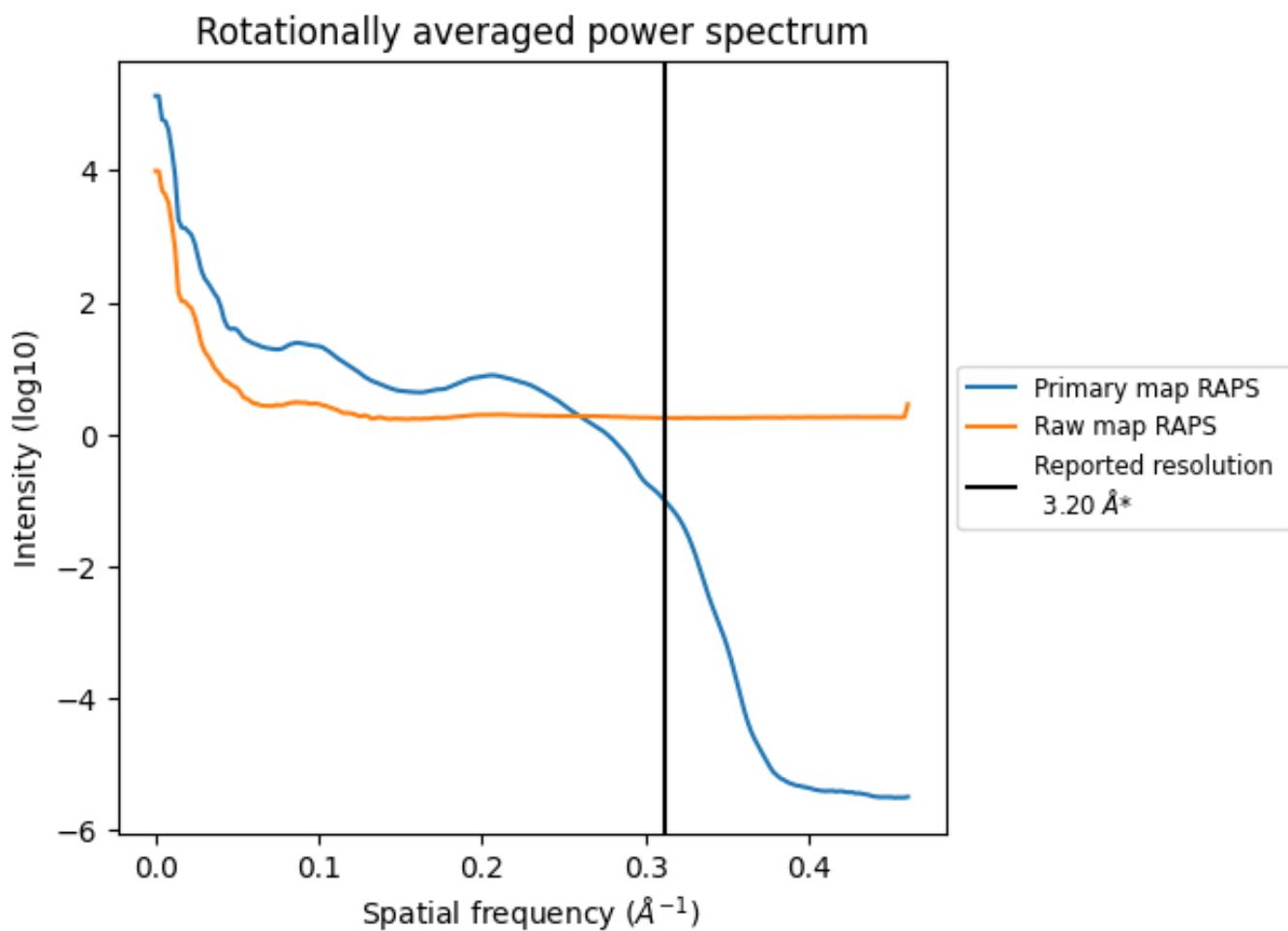
7.2   Volume estimate ⓘ

The volume at the recommended contour level is 106 nm^3; this corresponds to an approximate mass of 96 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 ⓘ
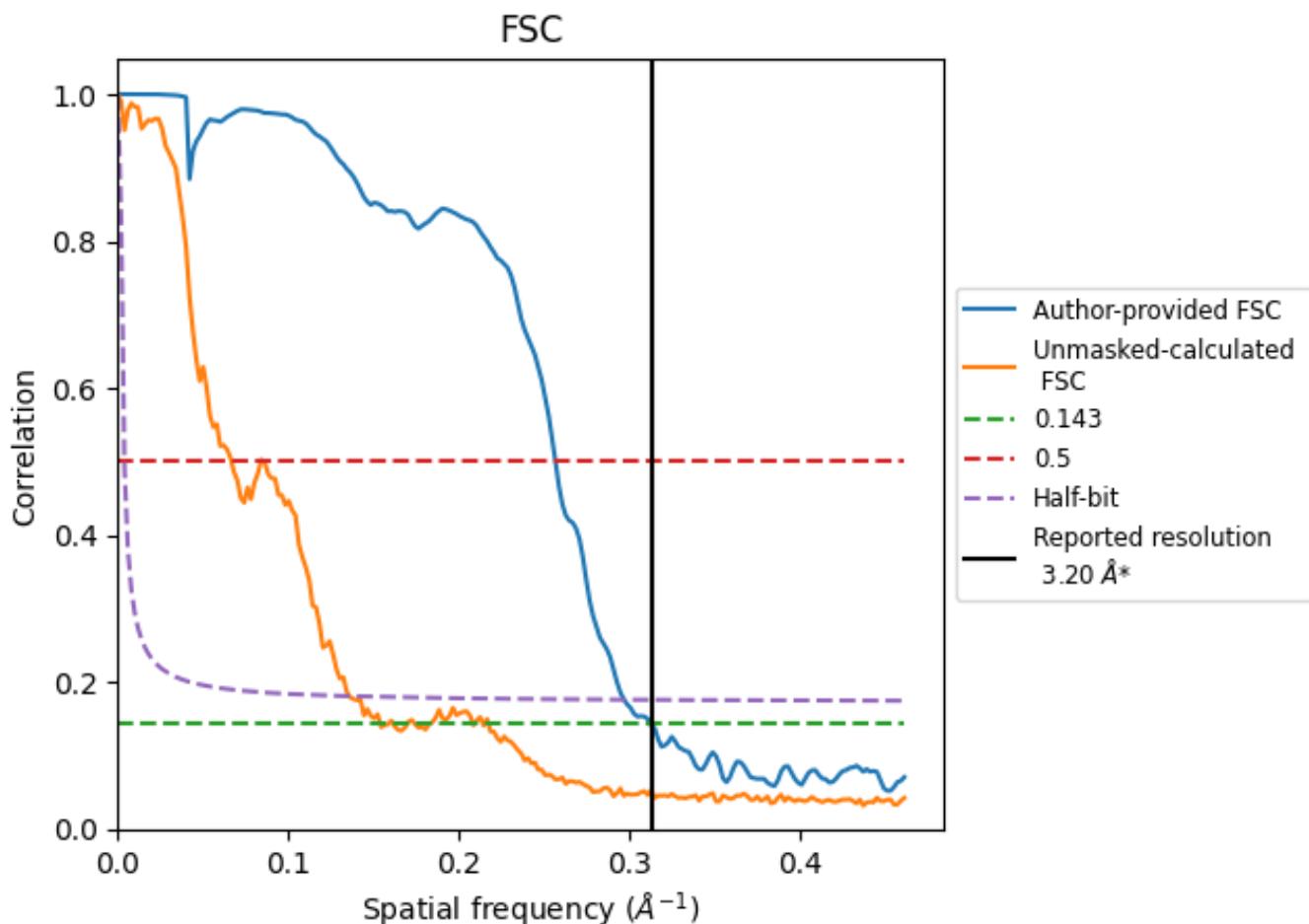
*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2   Resolution estimates (i)
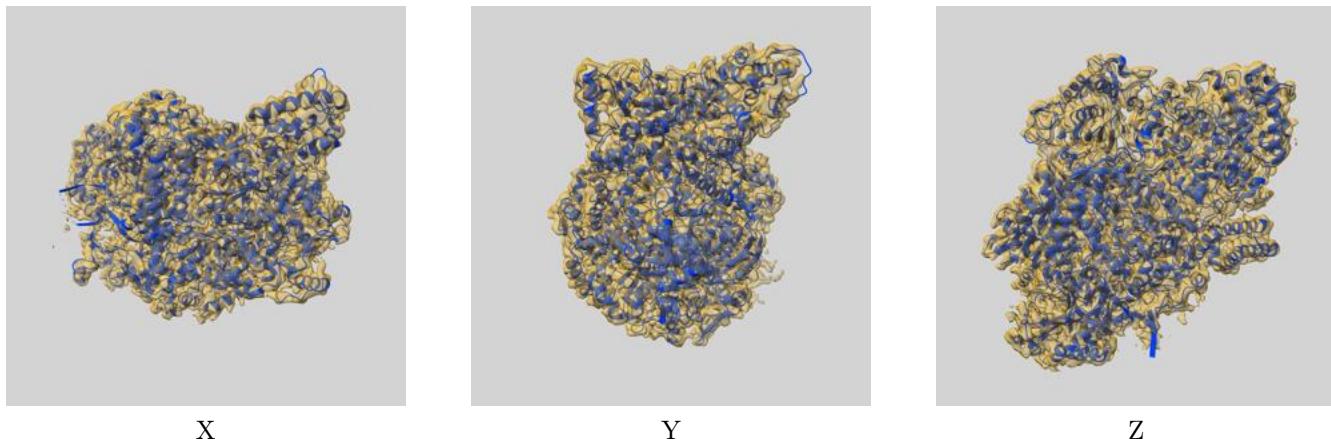
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.21	3.90	3.37
Unmasked-calculated*	6.51	15.02	7.36

*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 6.51 differs from the reported value 3.2 by more than 10 %

9 Map-model fit ⓘ
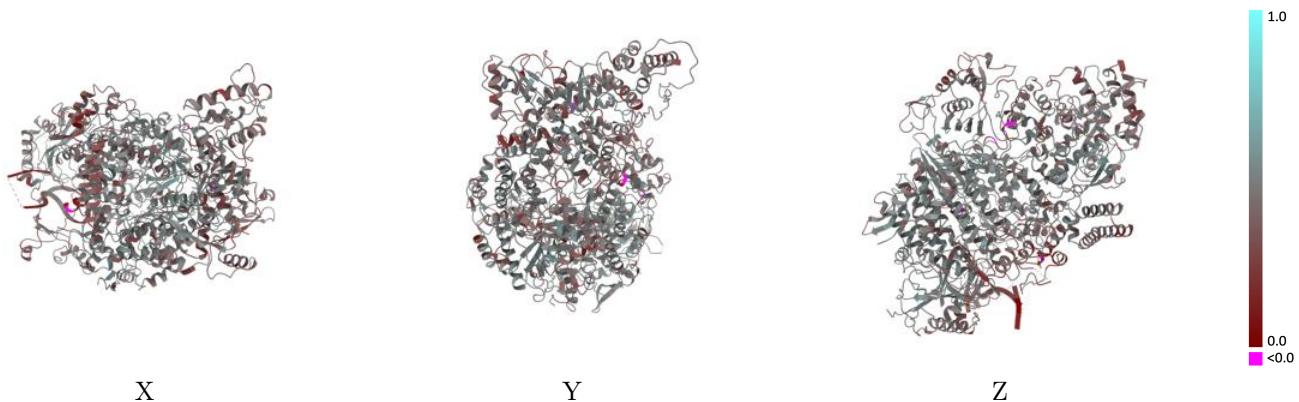
This section contains information regarding the fit between EMDB map EMD-10667 and PDB model 6Y0C. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay ⓘ

X　　　　　　　　　　　　　Y　　　　　　　　　　　　　Z
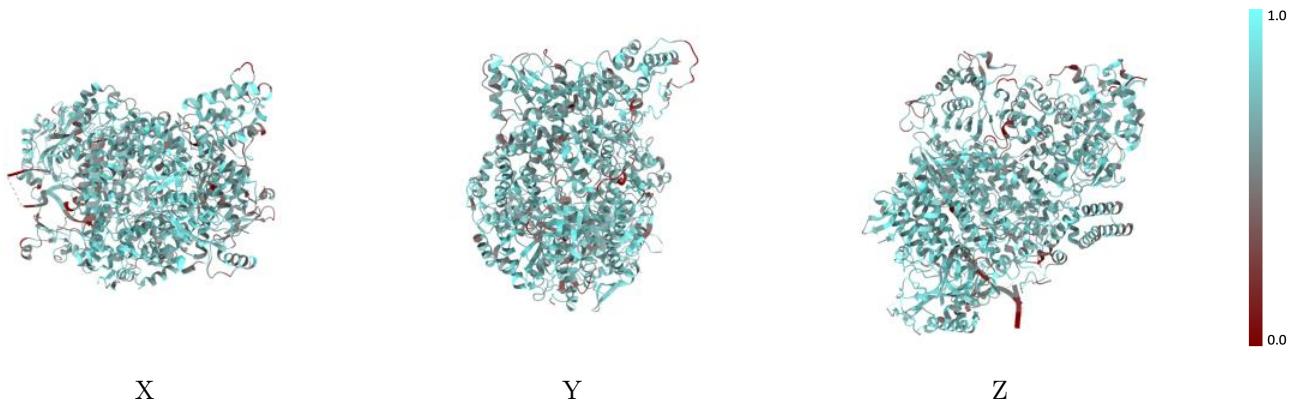
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ

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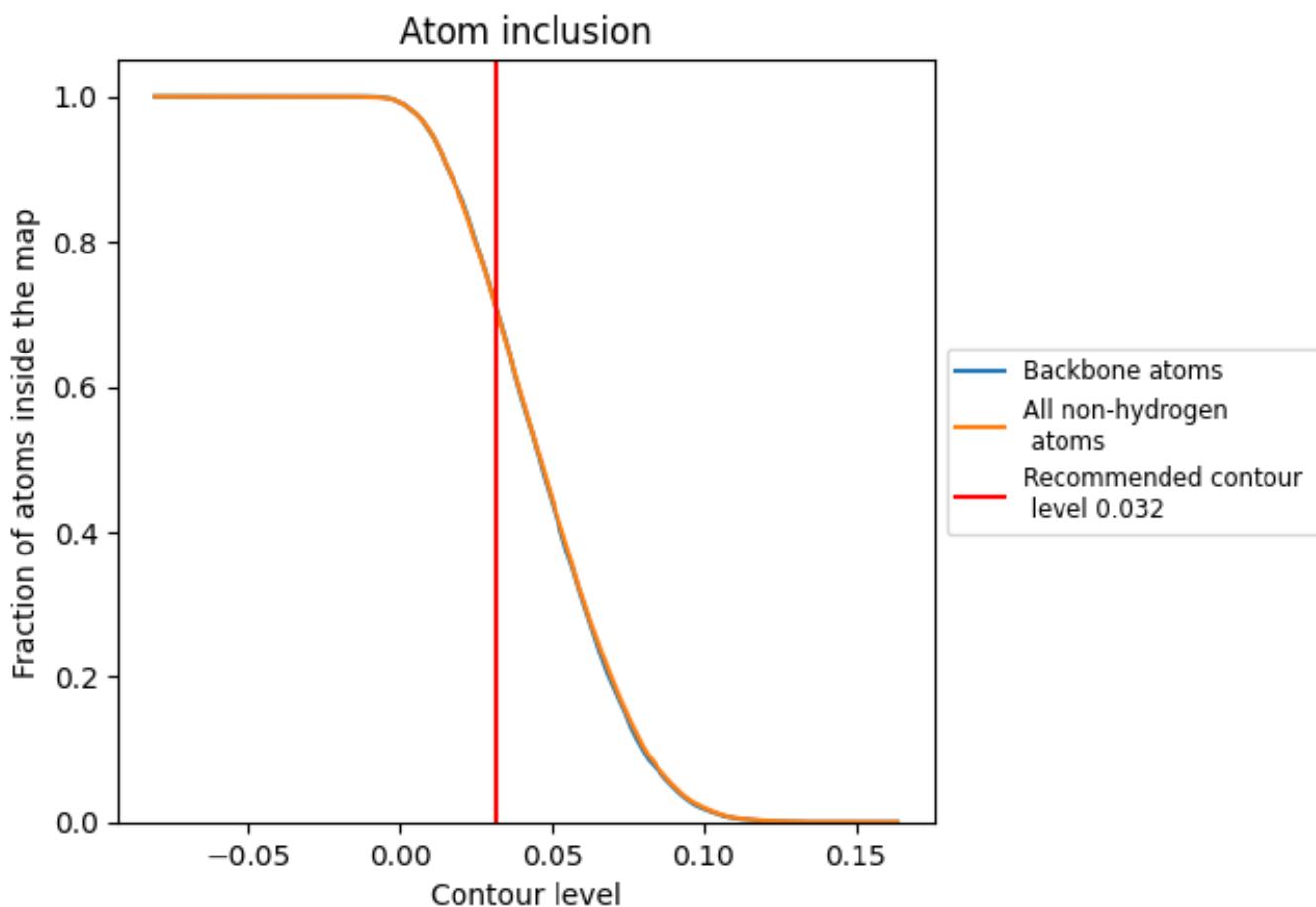
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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 (0.032).

9.4   Atom inclusion ⓘ

At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.032) and Q-score for the entire model and for each chain.

1.0

Chain	Atom inclusion	Q-score
All	0.7039	0.4400
A	0.7403	0.4520
B	0.7367	0.4510
C	0.6885	0.4290
IN1	0.4437	0.2800

0.0
<0.0