



Full wwPDB EM Validation Report ⓘ

Jul 8, 2026 – 08:27 AM EDT

PDB ID : 9PFR / pdb_00009pfr
EMDB ID : EMD-71611
Title : Cryo-EM structure of the respiratory syncytial virus polymerase (L:P) in NTP-bound elongation state
Authors : Cao, D.; Chen, Z.; Gao, Y.; Roesler, C.; Gooneratne, I.; Liang, B.
Deposited on : 2025-07-06
Resolution : 3.08 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 ⓘ 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:

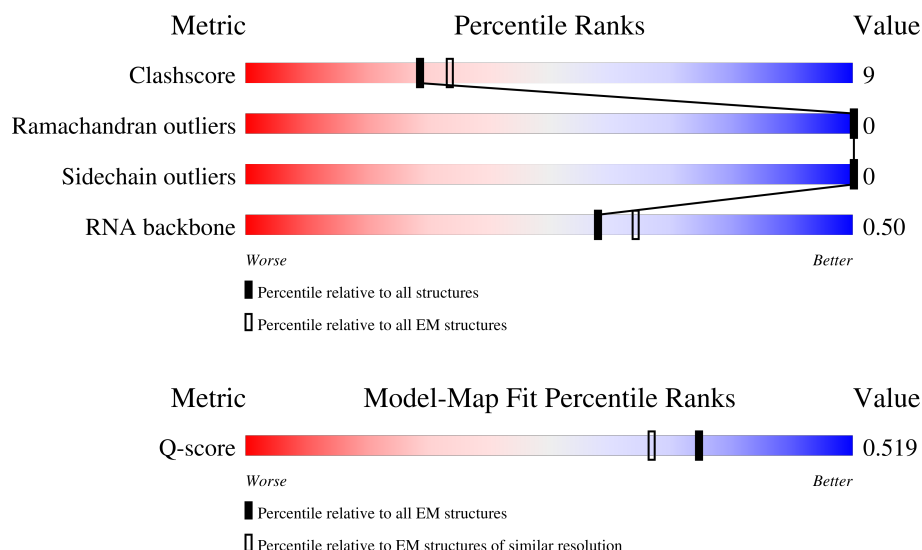
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.08 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14000 (2.58 - 3.58)

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

Mol	Chain	Length	Quality of chain
1	A	2165	
2	B	241	
2	C	241	

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Mol	Chain	Length	Quality of chain
2	D	241	21%75%
2	E	241	39%6%55%
3	P	3	33%67%
4	T	12	8%42%50%8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18533 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1959	Total	C	N	O	S	0	0
			16030	10373	2680	2895	82		

- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	58	Total	C	N	O	S	0	0
			444	273	81	86	4		
2	C	56	Total	C	N	O	S	0	0
			430	262	80	85	3		
2	D	60	Total	C	N	O	S	0	0
			470	289	88	89	4		
2	E	108	Total	C	N	O	S	0	0
			839	508	149	176	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	3	Total	C	N	O	P	0	0
			65	29	13	20	3		

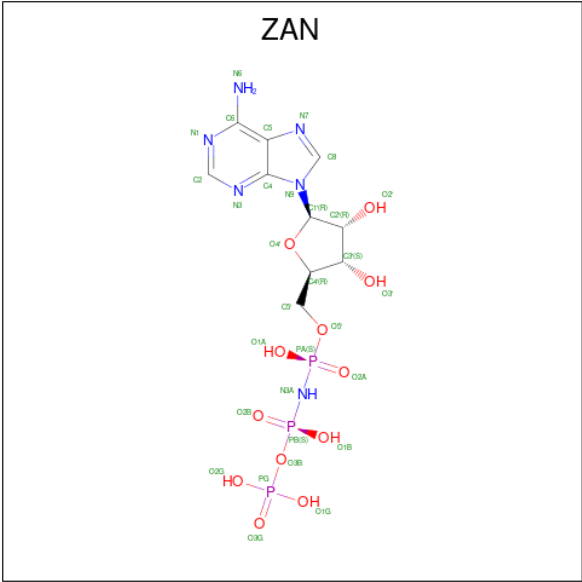
- Molecule 4 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*UP*CP*UP*CP*GP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	11	Total	C	N	O	P	0	0
			223	100	27	85	11		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	

- Molecule 6 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]adenosine (CCD ID: ZAN) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).

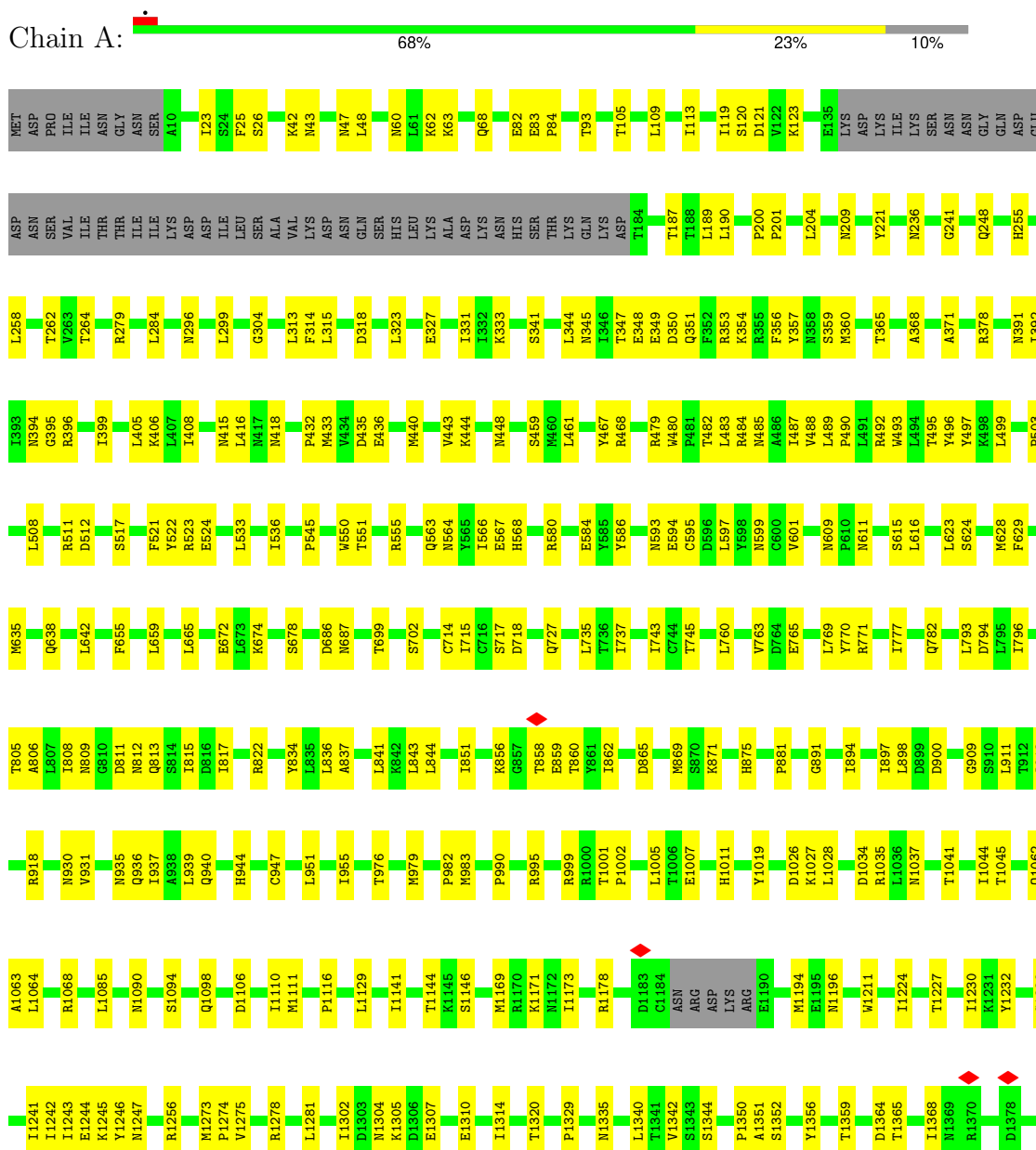


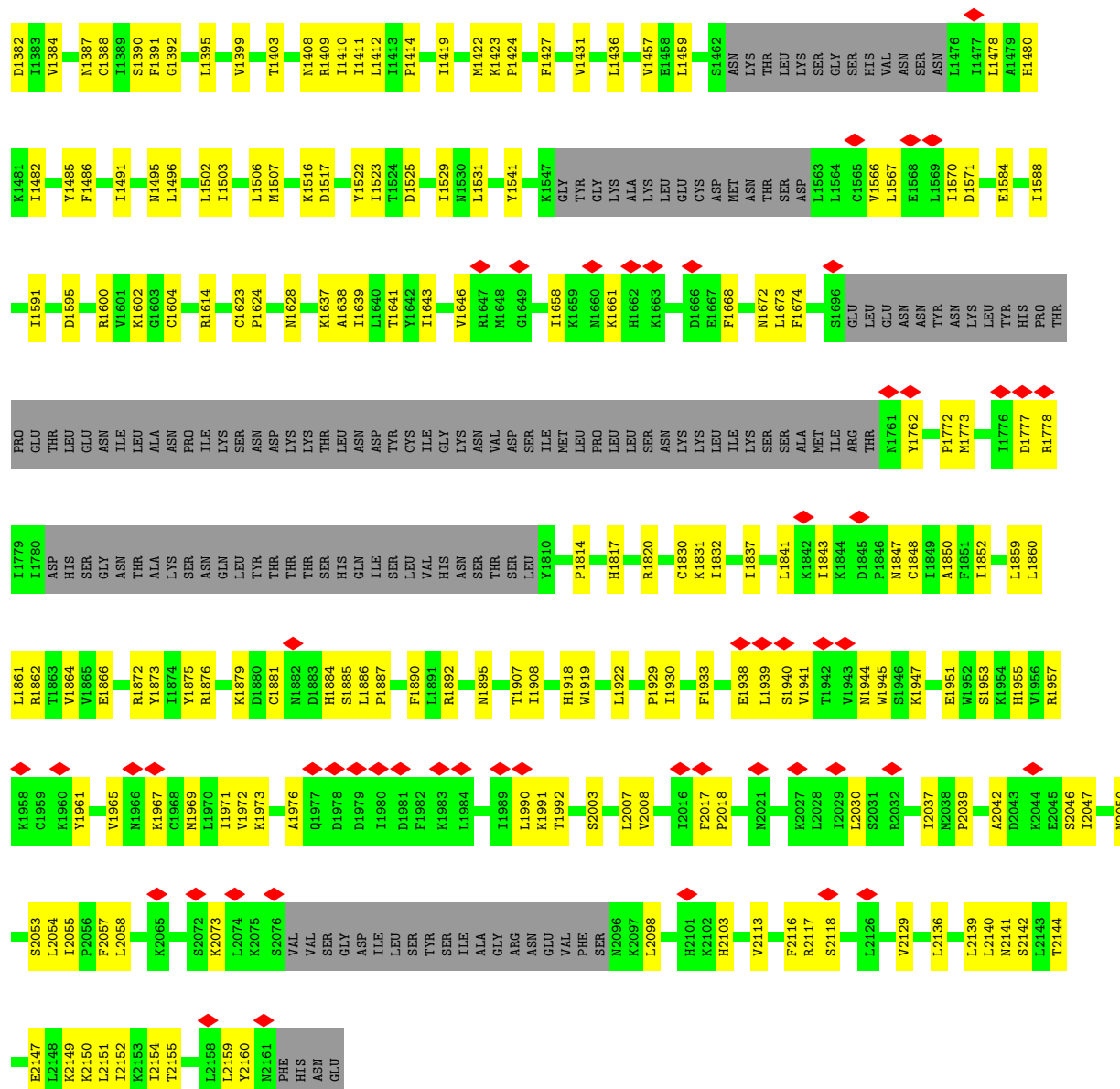
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

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.

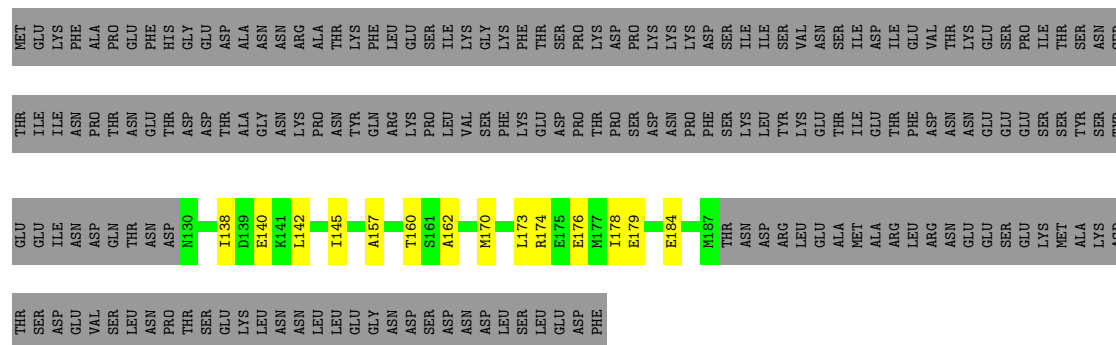
• Molecule 1: RNA-directed RNA polymerase L





• Molecule 2: Phosphoprotein

Chain B:  18% 6% 76%



• Molecule 2: Phosphoprotein



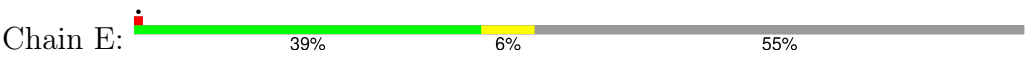
LYS	ASP	THR	SER	ASP	GLU	VAL	SER	LEU	ASN	PRO	THR	SER	GLU	LYS	LEU	ASN	ASN	LEU	LEU	GLY	ASN	ASP	SER	ASP	ASN	ASP	LEU	LEU	GLU	GLU	ASP	PHE																	
THR	SER	GLU	GLU	VAL	THR	THR	GLU	THR	ASP	GLY	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN																	
GLU	GLU	ILE	ASN	ASP	GLN	THR	N128	D129	L135	K141	L149	P159	R163	D164	G165	I166	R167	D168	A169	M170	R174	M177	I178	E179	K180	I181	R182	T183	GLU	ALA	LEU	MET	THR	ASN	ASP	ARG	LEU	GLU	ARG	ASN	GLU	GLU	SER	GLU	GLU	LYS			
THR	ILE	ASN	PRO	PRO	THR	ASN	GLU	THR	ASP	ALA	GLY	ASN	LYS	PRO	ASN	ASN	TYR	GLN	ARG	LYS	PRO	THR	PRO	SER	ASP	ASN	PRO	PHE	LYS	GLU	ASP	ASP	THR	ILE	ILE	VAL	ASN	SER	THR	LYS	GLU	SER	PRO	PRO	THR	THR	SER	SER	
MET	GLU	LYS	PHE	ALA	PRO	GLU	PHE	HIS	GLY	GLU	ASP	ALA	ASN	ASN	ARG	ALA	THR	LYS	PHE	LEU	GLU	SER	GLY	ILE	LYS	THR	THR	PRO	LYS	LYS	LYS	ASP	SER	SER	ILE	ILE	VAL	ASN	SER	THR	LYS	GLU	SER	PRO	PRO	THR	THR	SER	SER

• Molecule 2: Phosphoprotein



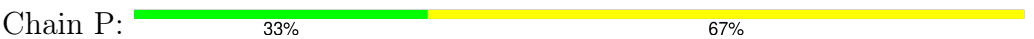
PRO	THR	SER	GLU	LYS	LEU	ASN	ASN	LEU	LEU	GLU	GLY	ASN	ASP	SER	ASN	ASP	ASP	LEU	SER	GLU	ASP	PHE																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
GLU	THR	ILE	ASN	ASP	GLN	THR	ASN	ASP	N130	I131	T132	A133	R134	M148	L149	H150	T151	L152	A157	G158	P159	THR	SER	ALA	ARG	ASP	GLY	ILE	ARG	ASP	ALA	MET	V171	R174	R197	L198	R199	N200	GLU	GLU	SER	GLU	LYS	MET	ALA	LYS	THR	THR	ASP	GLU	VAL	SER	ASN	LEU	ASN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
THR	ILE	ASN	PRO	THR	ASN	GLU	THR	ASP	GLY	ASN	ALA	GLY	LYS	PRO	ASN	GLN	ARG	LYS	PRO	LEU	VAL	SER	PHE	LYS	GLU	ASP	PRO	THR	THR	PRO	ASN	PHE	PRO	ASP	LYS	LYS	LYS	ASP	SER	ILE	ILE	LYS	THR	TYR	GLU	GLU	THR	PHE	ASN	ASN	THR	VAL	GLU	SER	THR	ILE	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER	ASN	SER	THR	TYR	SER

• Molecule 2: Phosphoprotein



MET	GLU	LYS	PHE	ALA	PRO	PRO	GLU	PHE	HIS	GLY	ASP	GLU	ASP	ALA	ASN	ASN	ARG	ALA	THR	LYS	PHE	LEU	GLU	SER	ILE	LYS	GLY	PHE	THR	PRO	PRO	LYS	LYS	ASP	PRO	LYS	LYS	ASP	SER	ILE	ILE	VAL	ASN	SER	THR	LYS	GLU	SER	PRO	THR	ILE	THR	SER	ASN	SER	TYR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
THR	ILE	ASN	ASN	PRO	THR	THR	GLU	THR	THR	ASP	THR	THR	THR	ALA	GLY	ASN	LYS	PRO	ASN	TYR	GLN	ARG	LYS	PRO	LEU	LEU	VAL	PHE	LYS	GLU	ASP	PRO	THR	THR	SER	ASP	ASN	PRO	PHE	SER	LYS	TYR	LYS	LEU	THR	LYS	GLU	THR	PHE	ASN	ASN	GLU	GLU	SER	GLU	SER	THR	SER	TYR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
GLU	GLU	ASN	ASP	ASP	THR	ASN	ASN	ASN	D129	R134	L142	R163	D164	D168	I178	R182	R191	M195	E204	K208	D209	T210	S220	L227	N230	ASP	SER	ASP	ASN	ASP	L236	D240	F241																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	

• Molecule 3: RNA (5'-R(P*AP*CP*G)-3')



A1	C2	G3
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• Molecule 4: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*CP*UP*CP*GP*U)-3')





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21615	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.81	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.893	Depositor
Minimum map value	-1.202	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	236.99199, 236.99199, 236.99199	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.16	0/16384	0.38	0/22176
2	B	0.13	0/445	0.34	0/596
2	C	0.14	0/431	0.36	0/578
2	D	0.11	0/470	0.24	0/628
2	E	0.14	0/841	0.37	0/1127
3	P	0.07	0/72	0.15	0/110
4	T	0.07	0/245	0.19	0/377
All	All	0.16	0/18888	0.37	0/25592

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	16030	0	16308	325	0
2	B	444	0	466	13	0
2	C	430	0	445	9	0
2	D	470	0	495	9	0
2	E	839	0	842	16	0
3	P	65	0	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	T	223	0	114	3	0
5	A	1	0	0	0	0
6	A	31	0	15	0	0
All	All	18533	0	18719	349	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 9.

All (349) 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:1342:VAL:HG12	1:A:1344:SER:H	1.53	0.73
1:A:1028:LEU:HB3	1:A:1194:MET:HB3	1.70	0.72
1:A:1862:ARG:NH1	1:A:1866:GLU:OE1	2.23	0.71
1:A:1990:LEU:HD23	1:A:1991:LYS:HG3	1.74	0.70
1:A:1919:TRP:CD1	1:A:1951:GLU:HB3	2.28	0.69
1:A:900:ASP:HA	1:A:1169:MET:HE2	1.74	0.69
1:A:1238:SER:HB2	1:A:1411:ILE:HG21	1.74	0.68
1:A:983:MET:HE2	1:A:990:PRO:HA	1.76	0.67
1:A:1302:ILE:HG22	1:A:1304:ASN:H	1.60	0.67
1:A:1246:TYR:HA	1:A:1908:ILE:HD12	1.76	0.67
2:C:149:LEU:HB3	2:D:148:MET:HG2	1.77	0.67
1:A:1034:ASP:OD1	1:A:1037:ASN:ND2	2.27	0.66
1:A:1820:ARG:HH12	1:A:1831:LYS:HE3	1.61	0.66
1:A:2116:PHE:HE2	1:A:2129:VAL:HG22	1.59	0.66
1:A:1938:GLU:HG3	1:A:1973:LYS:NZ	2.11	0.65
1:A:1242:ILE:HB	1:A:1364:ASP:HB3	1.77	0.65
1:A:1762:TYR:H	1:A:1895:ASN:HD21	1.44	0.64
1:A:487:ILE:O	2:C:141:LYS:NZ	2.25	0.64
1:A:1861:LEU:HB2	1:A:1890:PHE:HD1	1.63	0.64
1:A:760:LEU:O	1:A:771:ARG:NH1	2.31	0.63
1:A:1600:ARG:HB3	1:A:1892:ARG:HA	1.80	0.63
1:A:1002:PRO:O	1:A:1062:GLN:NE2	2.32	0.63
1:A:659:LEU:HD13	1:A:869:MET:HE2	1.81	0.62
1:A:492:ARG:NH1	1:A:512:ASP:OD2	2.33	0.62
1:A:808:ILE:HD12	1:A:813:GLN:HG2	1.81	0.62
1:A:1879:LYS:HB2	1:A:1908:ILE:HG12	1.82	0.62
1:A:2055:ILE:O	1:A:2055:ILE:HG13	1.99	0.62
1:A:765:GLU:HG2	1:A:770:TYR:HA	1.82	0.61
1:A:856:LYS:HD3	1:A:859:GLU:HB3	1.82	0.61
1:A:545:PRO:HB3	1:A:611:ASN:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:GLY:O	1:A:418:ASN:ND2	2.34	0.61
1:A:2139:LEU:HD21	1:A:2151:LEU:HD21	1.83	0.61
1:A:62:LYS:O	1:A:68:GLN:NE2	2.34	0.60
1:A:1944:ASN:HA	1:A:1947:LYS:HE2	1.82	0.60
1:A:2117:ARG:HG2	1:A:2118:SER:H	1.66	0.60
1:A:2117:ARG:NH2	1:A:2160:TYR:O	2.32	0.60
2:D:132:THR:OG1	2:E:134:ARG:NH1	2.35	0.60
1:A:1302:ILE:HB	1:A:1305:LYS:HB2	1.84	0.59
1:A:255:HIS:HD2	1:A:258:LEU:HB2	1.67	0.59
1:A:480:TRP:NE1	1:A:496:TYR:O	2.34	0.59
1:A:1171:LYS:O	1:A:1178:ARG:NH2	2.36	0.59
1:A:1919:TRP:HZ3	1:A:1933:PHE:HE2	1.49	0.59
1:A:1028:LEU:HD13	1:A:1194:MET:HG2	1.83	0.59
1:A:1368:ILE:HD11	1:A:1414:PRO:HG3	1.83	0.59
1:A:345:ASN:HA	1:A:353:ARG:HB2	1.85	0.59
1:A:1938:GLU:CG	1:A:1973:LYS:HE2	2.33	0.59
1:A:735:LEU:HD22	2:B:162:ALA:HB2	1.83	0.58
1:A:1602:LYS:HD2	1:A:1886:LEU:HD22	1.83	0.58
1:A:396:ARG:HH22	2:E:236:LEU:HD13	1.69	0.58
1:A:672:GLU:OE2	1:A:1256:ARG:NH1	2.36	0.58
1:A:1837:ILE:HD13	1:A:1971:ILE:HG12	1.85	0.58
1:A:1485:TYR:HE2	1:A:1668:PHE:CE2	2.22	0.57
1:A:284:LEU:HD21	1:A:931:VAL:HG11	1.85	0.57
1:A:1281:LEU:HD21	1:A:1459:LEU:HD11	1.87	0.57
1:A:2136:LEU:O	1:A:2140:LEU:HD13	2.04	0.57
1:A:555:ARG:O	1:A:563:GLN:NE2	2.38	0.57
1:A:533:LEU:HD13	1:A:536:ILE:HD11	1.87	0.56
1:A:563:GLN:O	1:A:567:GLU:HG2	2.05	0.56
1:A:935:ASN:HA	1:A:939:LEU:HD12	1.88	0.56
1:A:881:PRO:HB3	1:A:918:ARG:HB3	1.87	0.56
2:B:184:GLU:OE2	2:C:174:ARG:NH1	2.38	0.56
1:A:1965:VAL:HG22	1:A:1967:LYS:H	1.70	0.56
1:A:1887:PRO:HB2	1:A:1890:PHE:HB3	1.88	0.56
1:A:468:ARG:NH1	1:A:794:ASP:OD2	2.39	0.56
1:A:586:TYR:O	1:A:1090:ASN:ND2	2.37	0.56
1:A:1275:VAL:HG13	1:A:1628:ASN:HA	1.88	0.56
1:A:1340:LEU:HG	1:A:1342:VAL:HG23	1.88	0.56
1:A:1588:ILE:HA	1:A:1591:ILE:HG22	1.88	0.55
1:A:1940:SER:O	1:A:1941:VAL:CG2	2.54	0.55
1:A:1111:MET:HG2	1:A:1431:VAL:HG13	1.88	0.55
1:A:1232:TYR:HD1	1:A:1410:ILE:HG12	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:LEU:HD13	1:A:1637:LYS:HD3	1.90	0.54
1:A:523:ARG:NH1	2:B:176:GLU:OE2	2.40	0.54
1:A:1772:PRO:HB3	1:A:2039:PRO:HD3	1.89	0.54
1:A:119:ILE:HA	1:A:976:THR:HG23	1.88	0.54
1:A:483:LEU:HA	1:A:521:PHE:HA	1.88	0.54
1:A:327:GLU:OE1	1:A:378:ARG:NH2	2.40	0.54
1:A:1242:ILE:HG23	1:A:1409:ARG:HD3	1.90	0.54
1:A:601:VAL:HG21	1:A:642:LEU:HD23	1.88	0.54
1:A:1273:MET:HE2	1:A:1278:ARG:HD3	1.90	0.54
1:A:1382:ASP:HB3	1:A:1422:MET:HB2	1.88	0.54
1:A:468:ARG:HH21	1:A:655:PHE:HA	1.73	0.54
2:B:157:ALA:HA	2:B:170:MET:HE1	1.90	0.54
1:A:440:MET:HA	1:A:443:VAL:HG12	1.90	0.54
1:A:597:LEU:HD21	1:A:642:LEU:HB2	1.90	0.53
1:A:674:LYS:NZ	1:A:805:THR:O	2.40	0.53
2:C:170:MET:HA	2:C:170:MET:HE2	1.89	0.53
1:A:1940:SER:O	1:A:1941:VAL:HG23	2.08	0.53
1:A:1502:LEU:O	1:A:1506:LEU:HG	2.09	0.53
1:A:595:CYS:O	1:A:599:ASN:ND2	2.41	0.53
1:A:955:ILE:HD11	1:A:1173:ILE:HD12	1.91	0.53
2:C:149:LEU:HD13	2:D:148:MET:HB3	1.91	0.53
1:A:809:ASN:HB3	1:A:812:ASN:HB3	1.91	0.53
1:A:344:LEU:HA	1:A:347:THR:HG22	1.90	0.52
1:A:550:TRP:HB2	1:A:566:ILE:HD12	1.90	0.52
1:A:1778:ARG:HH12	1:A:1992:THR:H	1.56	0.52
1:A:1595:ASP:OD2	1:A:1614:ARG:NH1	2.42	0.52
1:A:1604:CYS:SG	1:A:1884:HIS:NE2	2.81	0.52
1:A:2144:THR:HG22	1:A:2147:GLU:HG2	1.92	0.52
1:A:1242:ILE:O	1:A:1364:ASP:N	2.42	0.52
1:A:121:ASP:OD1	1:A:187:THR:OG1	2.22	0.52
1:A:1938:GLU:HG2	1:A:1973:LYS:HE2	1.91	0.52
1:A:345:ASN:OD1	1:A:354:LYS:NZ	2.42	0.52
1:A:837:ALA:HB1	1:A:862:ILE:HD12	1.92	0.52
1:A:1531:LEU:HD21	1:A:1591:ILE:HD11	1.90	0.52
1:A:405:LEU:HB2	2:E:227:LEU:HD21	1.92	0.51
1:A:415:ASN:HB3	1:A:418:ASN:HB2	1.92	0.51
1:A:796:ILE:HG21	1:A:844:LEU:HD12	1.92	0.51
1:A:1224:ILE:HG21	1:A:1388:CYS:HA	1.92	0.51
1:A:1063:ALA:O	1:A:1211:TRP:NE1	2.39	0.51
1:A:189:LEU:HD21	1:A:299:LEU:HD21	1.93	0.51
1:A:1356:TYR:O	1:A:1359:THR:OG1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:182:ARG:HA	2:E:191:ARG:HH21	1.75	0.51
1:A:241:GLY:O	1:A:255:HIS:ND1	2.44	0.51
1:A:1939:LEU:HD13	1:A:1944:ASN:HB2	1.92	0.51
1:A:484:ARG:NH1	1:A:521:PHE:O	2.44	0.51
1:A:327:GLU:HB3	1:A:371:ALA:HB1	1.93	0.51
1:A:597:LEU:HD13	1:A:638:GLN:HB3	1.93	0.51
1:A:714:CYS:HA	1:A:717:SER:HB2	1.93	0.51
1:A:1541:TYR:OH	1:A:1624:PRO:O	2.28	0.51
1:A:580:ARG:NH2	4:T:7:U:OP1	2.42	0.50
1:A:1817:HIS:HE1	1:A:2149:LYS:HD3	1.75	0.50
1:A:806:ALA:HB2	1:A:815:ILE:HG23	1.93	0.50
2:B:160:THR:HG21	2:E:168:ASP:HA	1.92	0.50
1:A:1106:ASP:O	1:A:1110:ILE:HG13	2.12	0.50
1:A:1351:ALA:HA	1:A:1390:SER:HB3	1.93	0.50
1:A:221:TYR:OH	1:A:248:GLN:N	2.45	0.49
1:A:1522:TYR:HB3	1:A:1525:ASP:HB2	1.93	0.49
1:A:2155:THR:O	1:A:2159:LEU:HD12	2.13	0.49
1:A:416:LEU:HD21	1:A:875:HIS:NE2	2.27	0.49
1:A:743:ILE:HD12	1:A:760:LEU:HD21	1.94	0.49
1:A:2098:LEU:H	1:A:2098:LEU:HD12	1.76	0.49
1:A:313:LEU:HD11	1:A:408:ILE:HG13	1.95	0.49
1:A:461:LEU:HD22	1:A:851:ILE:HD11	1.94	0.49
1:A:1381:ILE:HD12	1:A:1419:ILE:HG21	1.95	0.49
1:A:897:ILE:HG13	1:A:898:LEU:HD12	1.95	0.49
1:A:1335:ASN:HA	1:A:1424:PRO:HG3	1.94	0.49
1:A:1668:PHE:O	1:A:1672:ASN:HB2	2.12	0.49
1:A:459:SER:O	1:A:517:SER:OG	2.28	0.49
1:A:523:ARG:NH2	2:B:179:GLU:OE2	2.39	0.49
1:A:42:LYS:O	1:A:47:ASN:ND2	2.46	0.48
1:A:1523:ILE:HD12	1:A:1584:GLU:HG3	1.95	0.48
1:A:348:GLU:O	1:A:353:ARG:NH2	2.46	0.48
2:D:148:MET:HA	2:D:151:THR:HG22	1.95	0.48
1:A:686:ASP:OD1	1:A:687:ASN:N	2.41	0.48
1:A:461:LEU:HD23	1:A:715:ILE:HD11	1.95	0.48
1:A:737:ILE:HG21	1:A:777:ILE:HD11	1.96	0.48
1:A:1243:ILE:HD13	1:A:1392:GLY:HA3	1.96	0.48
1:A:1879:LYS:HA	1:A:1885:SER:HB3	1.96	0.48
1:A:841:LEU:HB3	2:E:210:THR:HG23	1.95	0.48
1:A:1876:ARG:HB3	1:A:1918:HIS:HE2	1.79	0.48
1:A:356:PHE:CE1	1:A:360:MET:HE3	2.48	0.48
1:A:1352:SER:O	1:A:1352:SER:OG	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1478:LEU:HD22	1:A:1673:LEU:HB3	1.96	0.48
1:A:665:LEU:HD21	1:A:1350:PRO:HB3	1.95	0.48
1:A:279:ARG:NH1	1:A:318:ASP:OD2	2.32	0.48
1:A:718:ASP:OD1	2:B:174:ARG:NH2	2.45	0.48
1:A:1496:LEU:HD13	1:A:1529:ILE:HD12	1.95	0.48
1:A:811:ASP:HA	1:A:813:GLN:HE21	1.77	0.48
1:A:1384:VAL:HG12	1:A:1387:ASN:H	1.79	0.48
1:A:1832:ILE:HG13	1:A:1859:LEU:HD13	1.94	0.48
1:A:1848:CYS:SG	1:A:1930:ILE:HG12	2.54	0.48
1:A:1953:SER:O	1:A:1957:ARG:HG2	2.14	0.48
1:A:436:GLU:HA	1:A:628:MET:HE1	1.96	0.47
1:A:467:TYR:OH	1:A:503:PRO:O	2.29	0.47
1:A:1224:ILE:HG13	1:A:1387:ASN:HB3	1.95	0.47
1:A:1945:TRP:HH2	1:A:2017:PHE:HE2	1.62	0.47
1:A:1307:GLU:HA	1:A:1310:GLU:HB2	1.96	0.47
1:A:1491:ILE:O	1:A:1495:ASN:ND2	2.46	0.47
1:A:333:LYS:HD3	1:A:624:SER:HA	1.97	0.47
1:A:1129:LEU:HD21	1:A:1436:LEU:HD12	1.96	0.47
1:A:793:LEU:HD23	1:A:796:ILE:HD12	1.97	0.47
1:A:1938:GLU:HG3	1:A:1973:LYS:HZ1	1.77	0.47
1:A:2054:LEU:HD12	1:A:2154:ILE:HD12	1.97	0.47
1:A:702:SER:HB3	1:A:856:LYS:HE3	1.97	0.47
1:A:871:LYS:HD2	3:P:2:C:H5"	1.96	0.47
1:A:350:ASP:OD1	1:A:351:GLN:N	2.47	0.47
1:A:394:ASN:OD1	1:A:395:GLY:N	2.48	0.47
1:A:533:LEU:HA	1:A:536:ILE:HG12	1.97	0.47
1:A:1245:LYS:HG2	1:A:1247:ASN:H	1.81	0.47
1:A:1773:MET:HB2	1:A:2037:ILE:HG21	1.97	0.47
1:A:909:GLY:O	1:A:913:GLN:HG3	2.15	0.46
1:A:1541:TYR:CZ	1:A:1623:CYS:HB3	2.50	0.46
1:A:2042:ALA:HB1	1:A:2047:ILE:HD11	1.98	0.46
1:A:43:ASN:HA	1:A:47:ASN:HD21	1.80	0.46
1:A:120:SER:OG	1:A:930:ASN:ND2	2.45	0.46
2:B:142:LEU:HD23	2:B:145:ILE:HD12	1.97	0.46
1:A:511:ARG:NH1	2:B:140:GLU:OE1	2.49	0.46
1:A:1820:ARG:HG3	1:A:1830:CYS:SG	2.55	0.46
1:A:1847:ASN:O	1:A:1872:ARG:NH2	2.48	0.46
1:A:584:GLU:OE2	4:T:5:U:N3	2.49	0.46
1:A:699:THR:HA	1:A:860:THR:HG22	1.96	0.46
1:A:564:ASN:O	1:A:568:HIS:ND1	2.38	0.46
1:A:1881:CYS:O	1:A:1884:HIS:ND1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2046:SER:O	1:A:2050:ASN:ND2	2.48	0.46
1:A:323:LEU:HD11	1:A:391:ASN:HB2	1.98	0.46
1:A:1482:ILE:HB	1:A:1674:PHE:HB3	1.98	0.46
1:A:1486:PHE:HB2	1:A:1491:ILE:HD11	1.98	0.46
1:A:1423:LYS:HE3	1:A:1423:LYS:HB3	1.70	0.46
1:A:1852:ILE:HG23	1:A:1918:HIS:CE1	2.51	0.46
1:A:84:PRO:HG3	1:A:264:THR:HG22	1.97	0.45
1:A:341:SER:HB2	1:A:357:TYR:HA	1.98	0.45
1:A:365:THR:HG21	2:E:220:SER:HA	1.97	0.45
1:A:1041:THR:O	1:A:1045:THR:HG22	2.16	0.45
1:A:1110:ILE:HG22	1:A:1111:MET:HG3	1.97	0.45
1:A:1639:ILE:O	1:A:1643:ILE:HG12	2.16	0.45
1:A:1241:ILE:HB	1:A:1412:LEU:HB2	1.97	0.45
1:A:765:GLU:OE2	2:E:163:ARG:NH2	2.48	0.45
1:A:1230:ILE:HG12	1:A:1395:LEU:HD21	1.98	0.45
1:A:1814:PRO:O	1:A:2152:ILE:HG21	2.17	0.45
1:A:1638:ALA:O	1:A:1641:THR:OG1	2.26	0.45
1:A:1485:TYR:HE2	1:A:1668:PHE:HE2	1.62	0.45
1:A:727:GLN:HG2	2:B:174:ARG:HB2	1.99	0.44
1:A:796:ILE:HG23	1:A:843:LEU:HB3	1.99	0.44
1:A:1860:LEU:HD13	1:A:1875:TYR:HD1	1.82	0.44
1:A:123:LYS:HE2	1:A:1011:HIS:HE1	1.82	0.44
1:A:489:LEU:HB3	1:A:493:TRP:HB2	2.00	0.44
1:A:1929:PRO:HG3	1:A:1961:TYR:O	2.17	0.44
2:C:135:LEU:HB3	2:D:134:ARG:HE	1.81	0.44
1:A:913:GLN:HE22	1:A:995:ARG:HD3	1.82	0.44
1:A:1516:LYS:HG3	1:A:1517:ASP:N	2.33	0.44
1:A:1945:TRP:HE1	1:A:1972:VAL:CG2	2.31	0.44
1:A:2113:VAL:HG12	1:A:2113:VAL:O	2.17	0.44
1:A:296:ASN:HB3	1:A:299:LEU:HB2	2.00	0.44
1:A:1778:ARG:HH12	1:A:1992:THR:N	2.15	0.44
1:A:60:ASN:HA	1:A:63:LYS:HE3	2.00	0.44
1:A:551:THR:HG23	1:A:566:ILE:HD11	2.00	0.44
1:A:982:PRO:HD3	1:A:1011:HIS:HD2	1.82	0.44
1:A:432:PRO:HD3	1:A:623:LEU:HD13	2.00	0.44
1:A:448:ASN:ND2	2:E:163:ARG:HH12	2.15	0.44
1:A:47:ASN:OD1	1:A:48:LEU:N	2.51	0.44
2:D:149:LEU:HD12	2:D:152:LEU:HD23	2.00	0.44
1:A:1001:THR:HG21	1:A:1007:GLU:HG3	1.99	0.44
1:A:1778:ARG:NH1	1:A:1991:LYS:HB3	2.32	0.44
1:A:93:THR:HG22	1:A:315:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ARG:NH2	1:A:524:GLU:OE1	2.51	0.43
1:A:2007:LEU:HD21	1:A:2018:PRO:HG2	2.00	0.43
1:A:951:LEU:HD11	1:A:1169:MET:HB3	1.99	0.43
1:A:763:VAL:HG11	1:A:769:LEU:HD21	2.00	0.43
1:A:2053:SER:HB2	1:A:2150:LYS:HD3	2.01	0.43
1:A:26:SER:OG	1:A:436:GLU:OE1	2.26	0.43
1:A:1041:THR:HA	1:A:1044:ILE:HG22	2.01	0.43
2:B:138:ILE:HG23	2:E:142:LEU:HD11	2.00	0.43
1:A:894:ILE:HD12	1:A:911:LEU:HD12	1.99	0.43
1:A:1027:LYS:NZ	1:A:1196:ASN:OD1	2.50	0.43
1:A:1224:ILE:HA	1:A:1227:THR:HG22	2.00	0.43
1:A:119:ILE:HD13	1:A:979:MET:HE2	2.00	0.43
1:A:399:ILE:HG21	2:E:236:LEU:HD23	2.01	0.43
1:A:484:ARG:HG2	1:A:522:TYR:CZ	2.53	0.43
1:A:495:THR:O	1:A:499:LEU:HG	2.19	0.43
1:A:485:ASN:HB2	1:A:488:VAL:HG13	2.01	0.43
1:A:1778:ARG:NH1	1:A:1992:THR:O	2.52	0.43
1:A:2054:LEU:HD11	1:A:2150:LYS:HB3	2.01	0.42
1:A:323:LEU:HG	1:A:392:ILE:HD11	2.01	0.42
1:A:349:GLU:HB2	1:A:834:TYR:HE2	1.84	0.42
1:A:1457:VAL:HG11	2:D:199:ARG:HB2	2.01	0.42
1:A:1976:ALA:HB3	1:A:2003:SER:HB2	2.00	0.42
1:A:359:SER:OG	1:A:858:THR:O	2.37	0.42
1:A:593:ASN:OD1	1:A:594:GLU:N	2.52	0.42
1:A:1408:ASN:HB3	1:A:1907:THR:HG21	2.01	0.42
1:A:1864:VAL:HG22	1:A:1873:TYR:CE2	2.54	0.42
1:A:23:ILE:HG22	1:A:433:MET:HG3	2.01	0.42
1:A:121:ASP:HA	1:A:190:LEU:HD12	2.02	0.42
1:A:782:GLN:NE2	3:P:3:G:N3	2.68	0.42
1:A:891:GLY:H	1:A:894:ILE:HG21	1.84	0.42
1:A:1094:SER:O	1:A:1098:GLN:HG3	2.19	0.42
1:A:1116:PRO:HG2	1:A:1427:PHE:CD1	2.54	0.42
1:A:1940:SER:C	1:A:1941:VAL:HG23	2.44	0.42
1:A:678:SER:OG	1:A:865:ASP:OD1	2.31	0.42
1:A:1969:MET:SD	1:A:2008:VAL:HG22	2.60	0.42
2:E:178:ILE:HG23	2:E:195:MET:HE3	2.02	0.42
1:A:200:PRO:HA	1:A:201:PRO:HD3	1.82	0.42
1:A:1144:THR:HG22	1:A:1146:SER:H	1.85	0.42
1:A:1365:THR:O	1:A:1368:ILE:HG22	2.19	0.42
2:C:163:ARG:HA	2:C:166:ILE:HD12	2.01	0.42
1:A:82:GLU:C	1:A:262:THR:HG22	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:TRP:NE1	1:A:497:TYR:HA	2.35	0.42
1:A:503:PRO:HG2	1:A:508:LEU:HD13	2.02	0.42
1:A:944:HIS:HB3	1:A:947:CYS:O	2.19	0.42
1:A:1085:LEU:HD11	1:A:1141:ILE:HD12	2.01	0.42
1:A:1391:PHE:O	1:A:1395:LEU:HB2	2.19	0.42
1:A:1399:VAL:O	1:A:1403:THR:OG1	2.34	0.42
1:A:105:THR:OG1	1:A:209:ASN:ND2	2.48	0.42
1:A:468:ARG:HA	1:A:468:ARG:HD2	1.79	0.42
1:A:1422:MET:HE2	1:A:1422:MET:HB3	1.92	0.42
1:A:936:GLN:HA	1:A:940:GLN:HB2	2.02	0.42
1:A:937:ILE:HD12	1:A:979:MET:SD	2.60	0.42
1:A:2136:LEU:HG	1:A:2140:LEU:HD13	2.01	0.42
1:A:105:THR:HG21	1:A:209:ASN:HB2	2.00	0.41
1:A:1028:LEU:HD23	1:A:1028:LEU:HA	1.88	0.41
1:A:1658:ILE:HG22	1:A:1661:LYS:H	1.85	0.41
1:A:1777:ASP:HB2	1:A:2030:LEU:HD11	2.01	0.41
1:A:1850:ALA:HB2	1:A:1930:ILE:HD13	2.00	0.41
2:E:164:ASP:OD1	2:E:164:ASP:N	2.53	0.41
1:A:482:THR:HG22	1:A:522:TYR:HD2	1.85	0.41
1:A:1244:GLU:OE2	1:A:1907:THR:HA	2.20	0.41
1:A:1566:VAL:HG23	1:A:1567:LEU:HD12	2.01	0.41
1:A:1841:LEU:HB3	1:A:1843:ILE:HG12	2.01	0.41
1:A:2055:ILE:HD12	1:A:2058:LEU:HD13	2.02	0.41
1:A:2141:ASN:O	1:A:2142:SER:C	2.64	0.41
1:A:822:ARG:NH2	1:A:2141:ASN:OD1	2.52	0.41
1:A:995:ARG:HH21	1:A:999:ARG:HB3	1.85	0.41
1:A:1232:TYR:CD1	1:A:1410:ILE:HG12	2.54	0.41
1:A:109:LEU:HD21	1:A:204:LEU:HG	2.01	0.41
1:A:279:ARG:HG2	1:A:314:PHE:CD2	2.55	0.41
1:A:354:LYS:HA	1:A:354:LYS:HD3	1.88	0.41
1:A:1643:ILE:HA	1:A:1646:VAL:HG12	2.02	0.41
1:A:83:GLU:OE2	1:A:378:ARG:NH1	2.43	0.41
1:A:255:HIS:CD2	1:A:258:LEU:HB2	2.53	0.41
1:A:609:ASN:HD22	1:A:635:MET:HE1	1.86	0.41
1:A:1274:PRO:HD3	1:A:1329:PRO:HA	2.03	0.41
1:A:2057:PHE:HE2	1:A:2103:HIS:CD2	2.39	0.41
1:A:25:PHE:HB3	1:A:435:ASP:HA	2.03	0.41
1:A:331:ILE:HD11	1:A:368:ALA:HA	2.01	0.41
1:A:1026:ASP:OD1	1:A:1027:LYS:N	2.46	0.41
1:A:1480:HIS:HB3	1:A:1674:PHE:HD1	1.85	0.41
1:A:113:ILE:HD11	1:A:284:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:HG12	1:A:976:THR:HA	2.03	0.41
1:A:236:ASN:OD1	1:A:236:ASN:N	2.53	0.41
1:A:350:ASP:OD1	1:A:351:GLN:HG2	2.20	0.41
1:A:406:LYS:HG3	2:E:227:LEU:HD23	2.03	0.41
1:A:1571:ASP:OD1	1:A:1571:ASP:N	2.54	0.41
1:A:1852:ILE:HG23	1:A:1918:HIS:HE1	1.85	0.41
2:D:197:ARG:HA	2:D:197:ARG:HD2	1.80	0.41
2:E:204:GLU:O	2:E:208:LYS:HG3	2.20	0.41
2:B:174:ARG:O	2:B:178:ILE:HG12	2.21	0.41
2:D:171:VAL:HG23	2:D:174:ARG:HH21	1.85	0.41
1:A:490:PRO:HD2	1:A:493:TRP:HD1	1.85	0.40
1:A:616:LEU:HD13	1:A:628:MET:HB3	2.02	0.40
1:A:793:LEU:HD23	1:A:793:LEU:HA	1.86	0.40
1:A:1005:LEU:HD22	1:A:1064:LEU:HD11	2.03	0.40
1:A:1566:VAL:O	1:A:1570:ILE:HG12	2.21	0.40
2:C:164:ASP:HA	2:C:167:ARG:HE	1.86	0.40
1:A:444:LYS:HB2	1:A:770:TYR:CE1	2.56	0.40
1:A:490:PRO:HD2	1:A:493:TRP:CD1	2.57	0.40
1:A:615:SER:HB2	1:A:745:THR:OG1	2.21	0.40
1:A:817:ILE:HG22	1:A:836:LEU:HD21	2.02	0.40
1:A:1019:TYR:O	1:A:1035:ARG:NH2	2.54	0.40
1:A:1841:LEU:HD13	1:A:1843:ILE:HD11	2.02	0.40
1:A:2073:LYS:HB3	1:A:2073:LYS:HE2	1.94	0.40
1:A:629:PHE:HB2	4:T:9:U:C2	2.56	0.40
1:A:1922:LEU:HD12	1:A:1955:HIS:CE1	2.56	0.40
1:A:1314:ILE:HD11	1:A:1320:THR:HG22	2.02	0.40
1:A:1503:ILE:HG23	1:A:1507:MET:HE3	2.02	0.40
1:A:1938:GLU:HG3	1:A:1973:LYS:CE	2.51	0.40
2:B:173:LEU:HB3	2:B:178:ILE:HD11	2.03	0.40
2:E:210:THR:HG22	2:E:210:THR:O	2.21	0.40
1:A:1068:ARG:HA	1:A:1068:ARG:HD2	1.84	0.40
2:C:177:MET:O	2:C:181:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1943/2165 (90%)	1927 (99%)	16 (1%)	0	100	100
2	B	56/241 (23%)	55 (98%)	1 (2%)	0	100	100
2	C	54/241 (22%)	54 (100%)	0	0	100	100
2	D	56/241 (23%)	56 (100%)	0	0	100	100
2	E	104/241 (43%)	104 (100%)	0	0	100	100
All	All	2213/3129 (71%)	2196 (99%)	17 (1%)	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	1822/2012 (91%)	1822 (100%)	0	100	100
2	B	48/220 (22%)	48 (100%)	0	100	100
2	C	47/220 (21%)	47 (100%)	0	100	100
2	D	51/220 (23%)	51 (100%)	0	100	100
2	E	94/220 (43%)	94 (100%)	0	100	100
All	All	2062/2892 (71%)	2062 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	209	ASN
1	A	248	GLN

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Mol	Chain	Res	Type
1	A	296	ASN
1	A	381	HIS
1	A	417	ASN
1	A	431	HIS
1	A	438	GLN
1	A	632	GLN
1	A	640	GLN
1	A	706	GLN
1	A	748	HIS
1	A	813	GLN
1	A	829	HIS
1	A	831	GLN
1	A	935	ASN
1	A	1062	GLN
1	A	1215	ASN
1	A	1338	HIS
1	A	1677	ASN
1	A	1690	HIS
1	A	1816	HIS
1	A	1817	HIS
1	A	1895	ASN
1	A	1975	HIS
1	A	1986	ASN
2	B	130	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	2/3 (66%)	0	0
4	T	10/12 (83%)	3 (30%)	0
All	All	12/15 (80%)	3 (25%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	T	3	U
4	T	4	U
4	T	6	U

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ZAN	A	2202	5	32,33,33	1.67	7 (21%)	46,52,52	2.15	13 (28%)

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
6	ZAN	A	2202	5	-	4/19/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2202	ZAN	C5-C4	4.78	1.47	1.39
6	A	2202	ZAN	PB-O2B	3.53	1.51	1.46
6	A	2202	ZAN	PA-O2A	3.47	1.51	1.46
6	A	2202	ZAN	C5-C6	2.57	1.48	1.41
6	A	2202	ZAN	C5-N7	-2.40	1.34	1.39
6	A	2202	ZAN	C8-N7	2.25	1.36	1.31
6	A	2202	ZAN	PB-O1B	-2.01	1.51	1.56

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2202	ZAN	C5-C4-N3	-6.02	118.42	126.72
6	A	2202	ZAN	O1A-PA-O2A	5.07	120.73	109.87
6	A	2202	ZAN	N3-C4-N9	4.94	135.56	127.17
6	A	2202	ZAN	O1B-PB-O2B	4.88	120.34	109.87
6	A	2202	ZAN	C2-N3-C4	3.74	120.96	111.83
6	A	2202	ZAN	C4-C5-N7	-3.20	106.92	110.58
6	A	2202	ZAN	N3-C2-N1	-3.20	123.74	128.58
6	A	2202	ZAN	C4-N9-C8	2.55	108.42	105.74
6	A	2202	ZAN	C3'-C2'-C1'	2.52	106.24	101.46
6	A	2202	ZAN	O5'-PA-O2A	-2.43	107.05	114.27
6	A	2202	ZAN	C5-N7-C8	2.40	107.22	103.45
6	A	2202	ZAN	O3B-PB-N3A	-2.26	100.32	106.59
6	A	2202	ZAN	O2A-PA-N3A	-2.01	108.81	111.77

There are no chirality outliers.

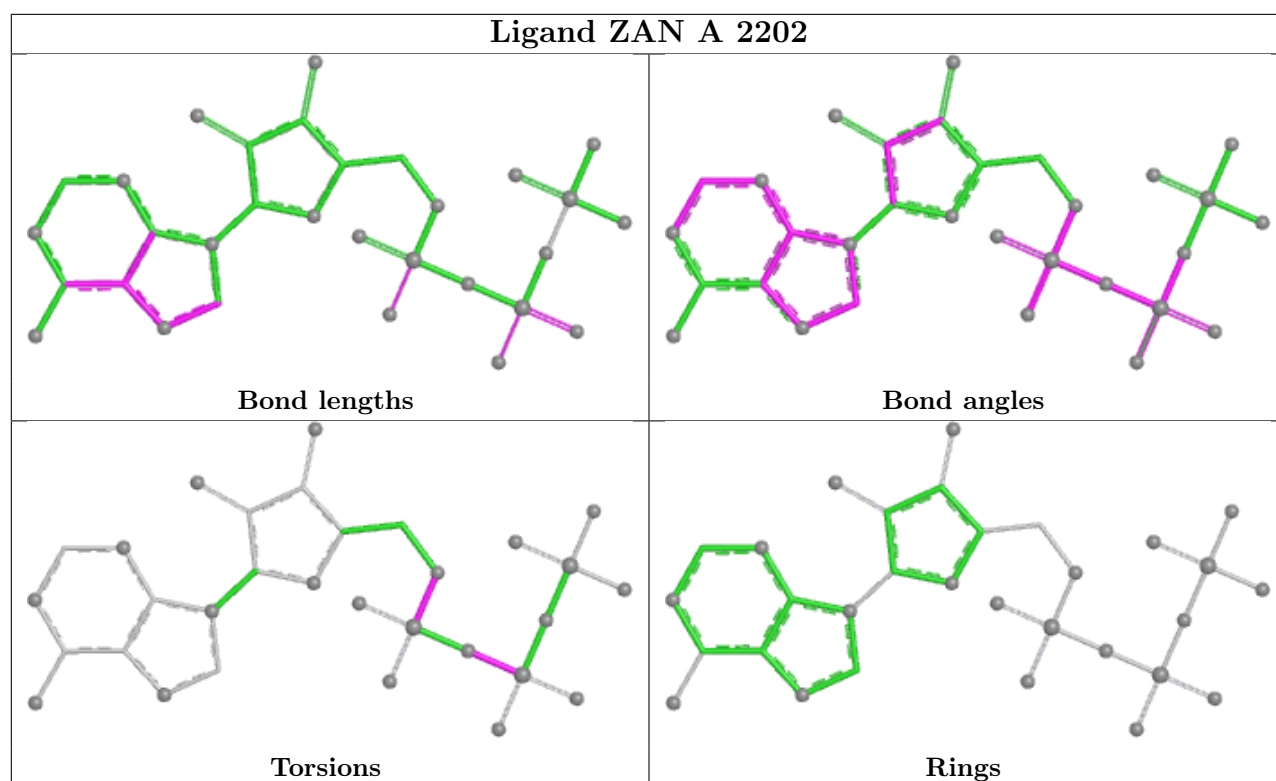
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2202	ZAN	C5'-O5'-PA-O1A
6	A	2202	ZAN	PA-N3A-PB-O2B
6	A	2202	ZAN	C5'-O5'-PA-O2A
6	A	2202	ZAN	C5'-O5'-PA-N3A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

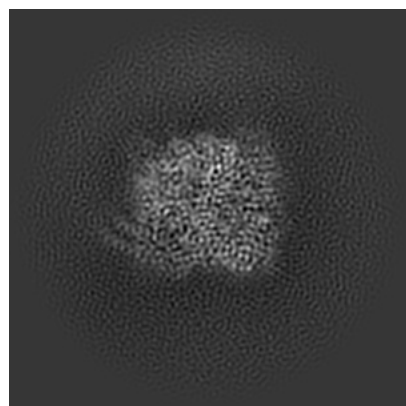
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71611. These allow visual inspection of the internal detail of the map and identification of artifacts.

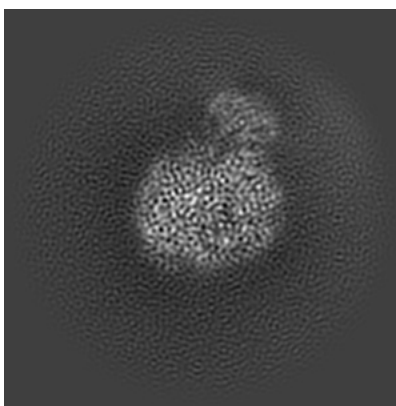
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

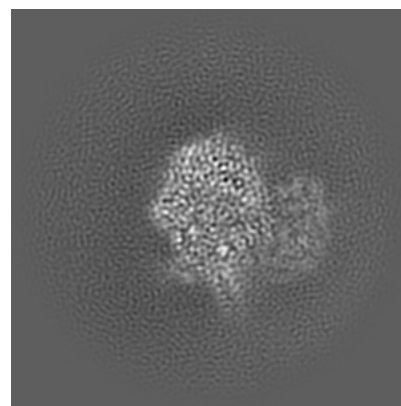
6.1.1 Primary map



X

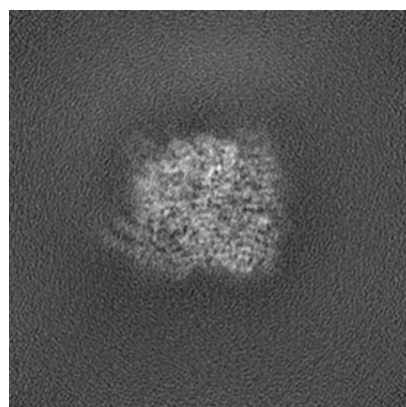


Y

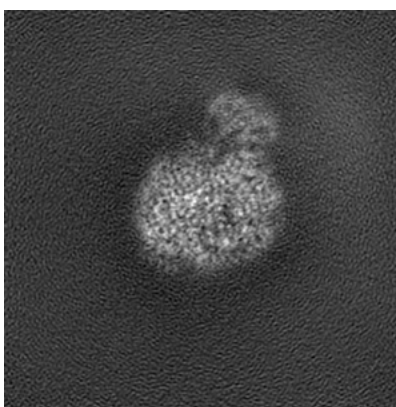


Z

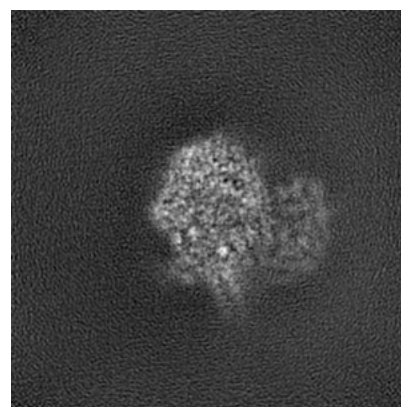
6.1.2 Raw map



X



Y

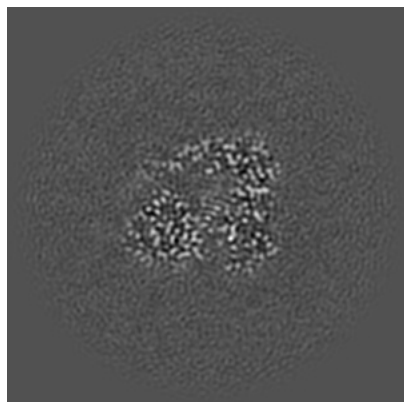


Z

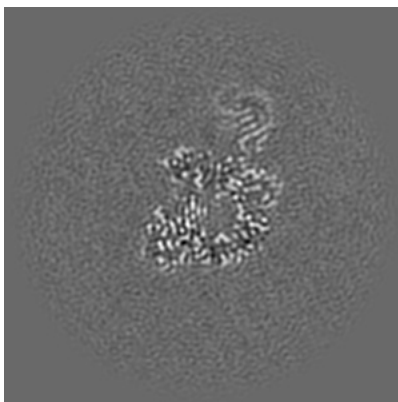
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

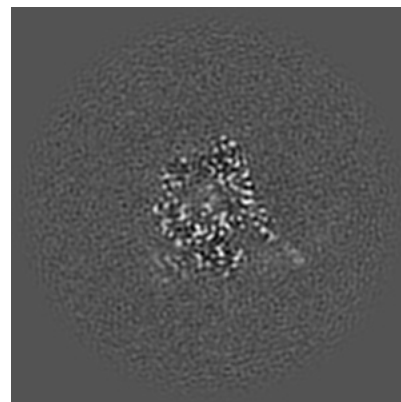
6.2.1 Primary map



X Index: 112

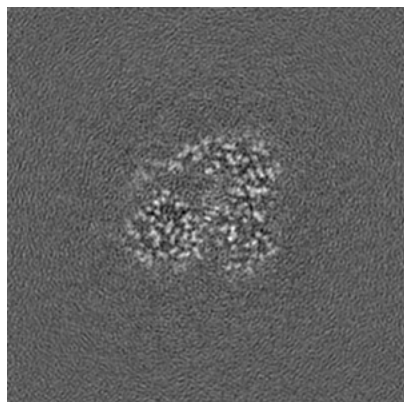


Y Index: 112

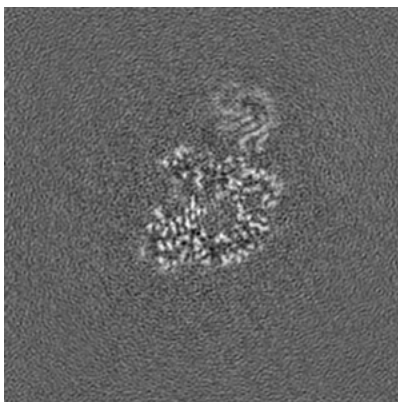


Z Index: 112

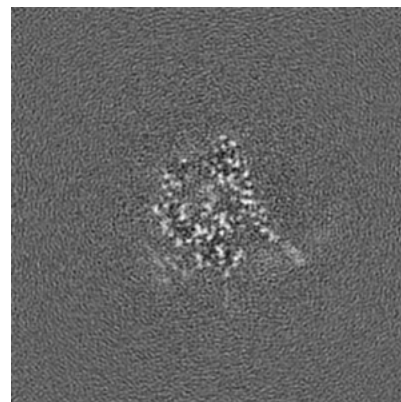
6.2.2 Raw map



X Index: 112



Y Index: 112

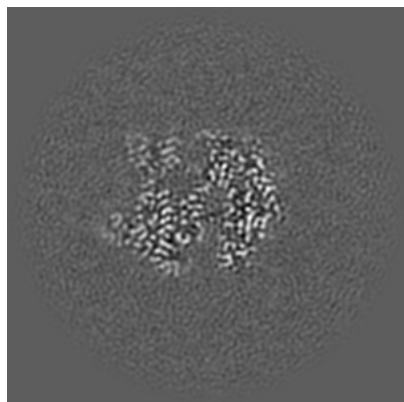


Z Index: 112

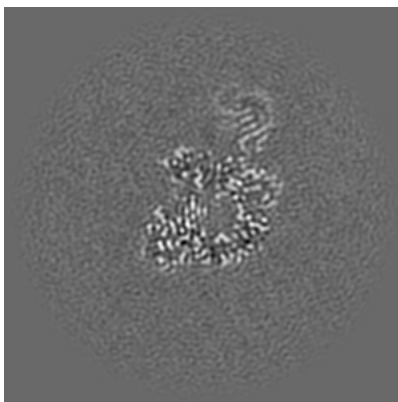
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

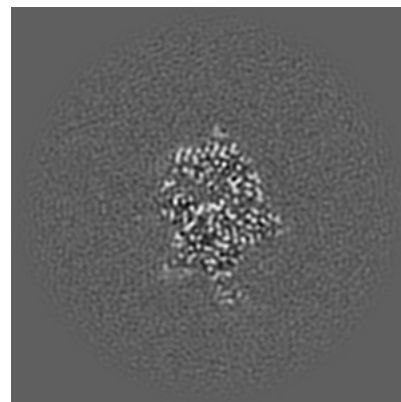
6.3.1 Primary map



X Index: 119

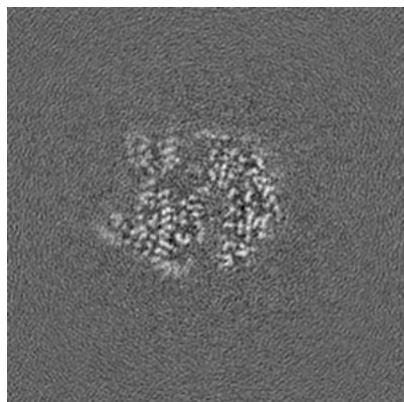


Y Index: 112

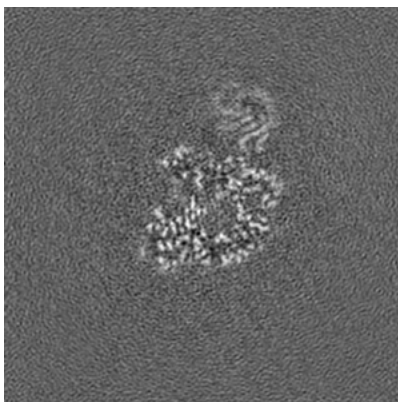


Z Index: 105

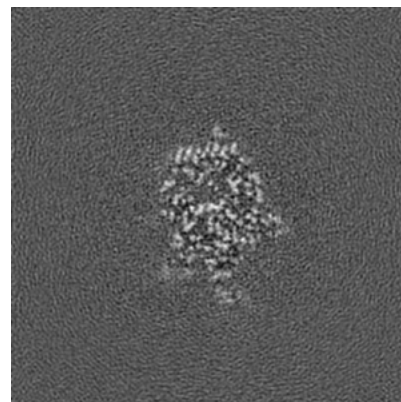
6.3.2 Raw map



X Index: 119



Y Index: 112

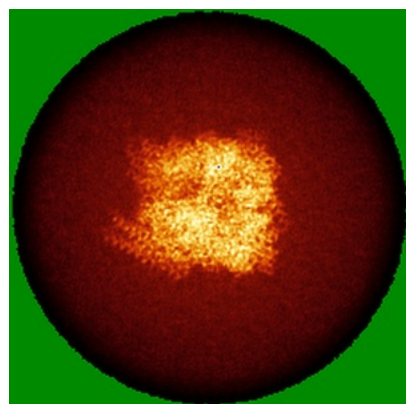


Z Index: 105

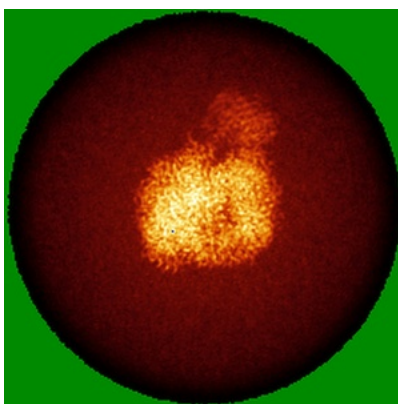
The images above show the largest variance slices of the map in three orthogonal directions.

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

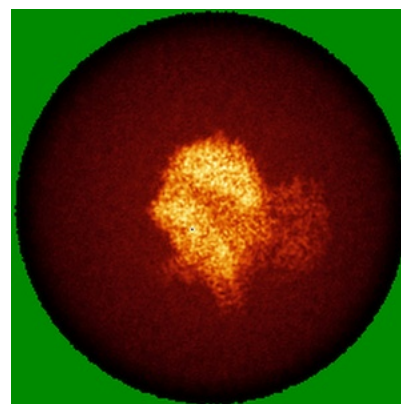
6.4.1 Primary map



X

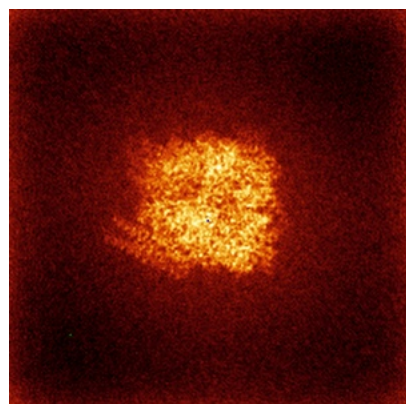


Y

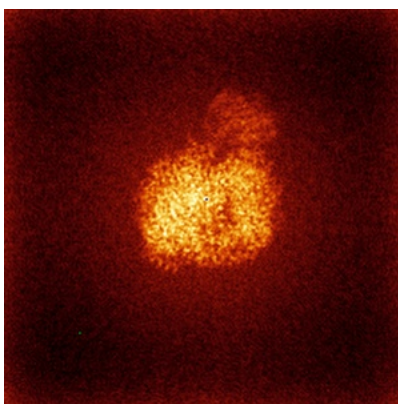


Z

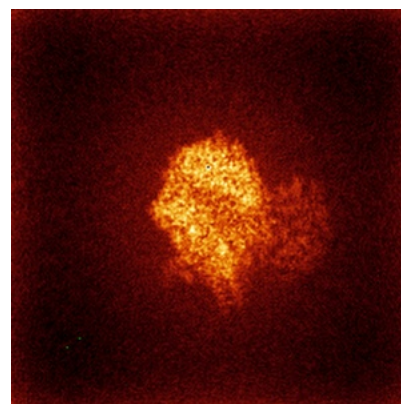
6.4.2 Raw map



X



Y

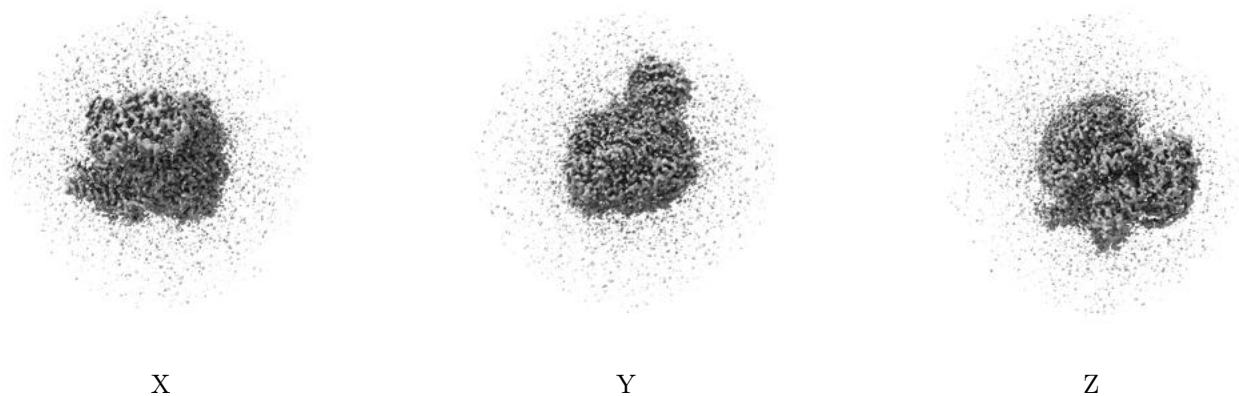


Z

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

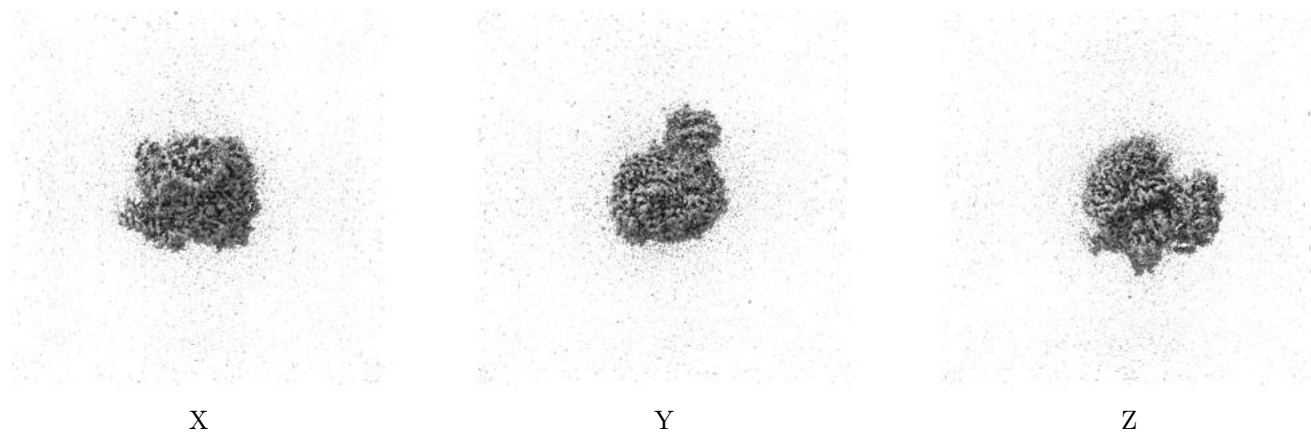
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

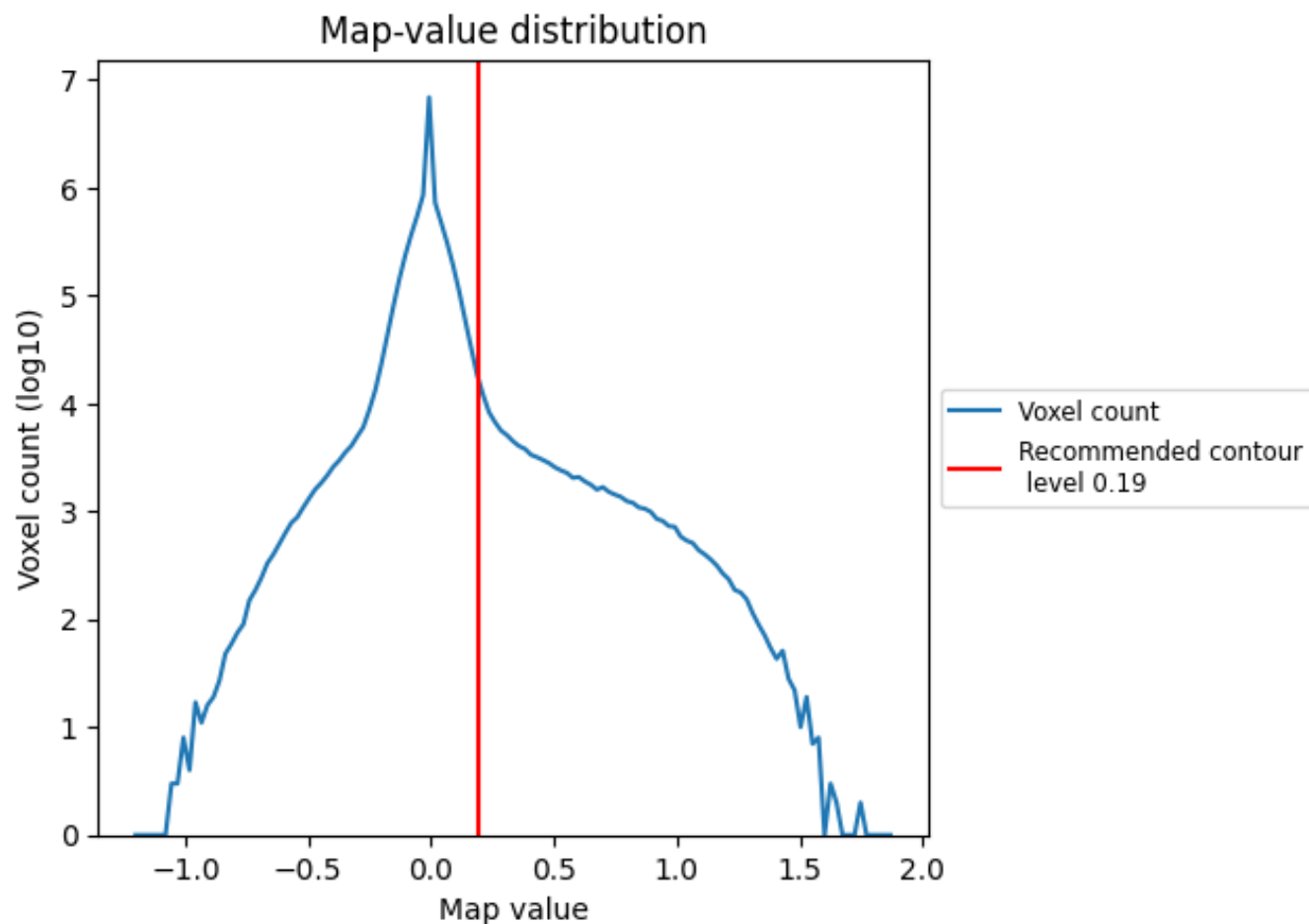
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

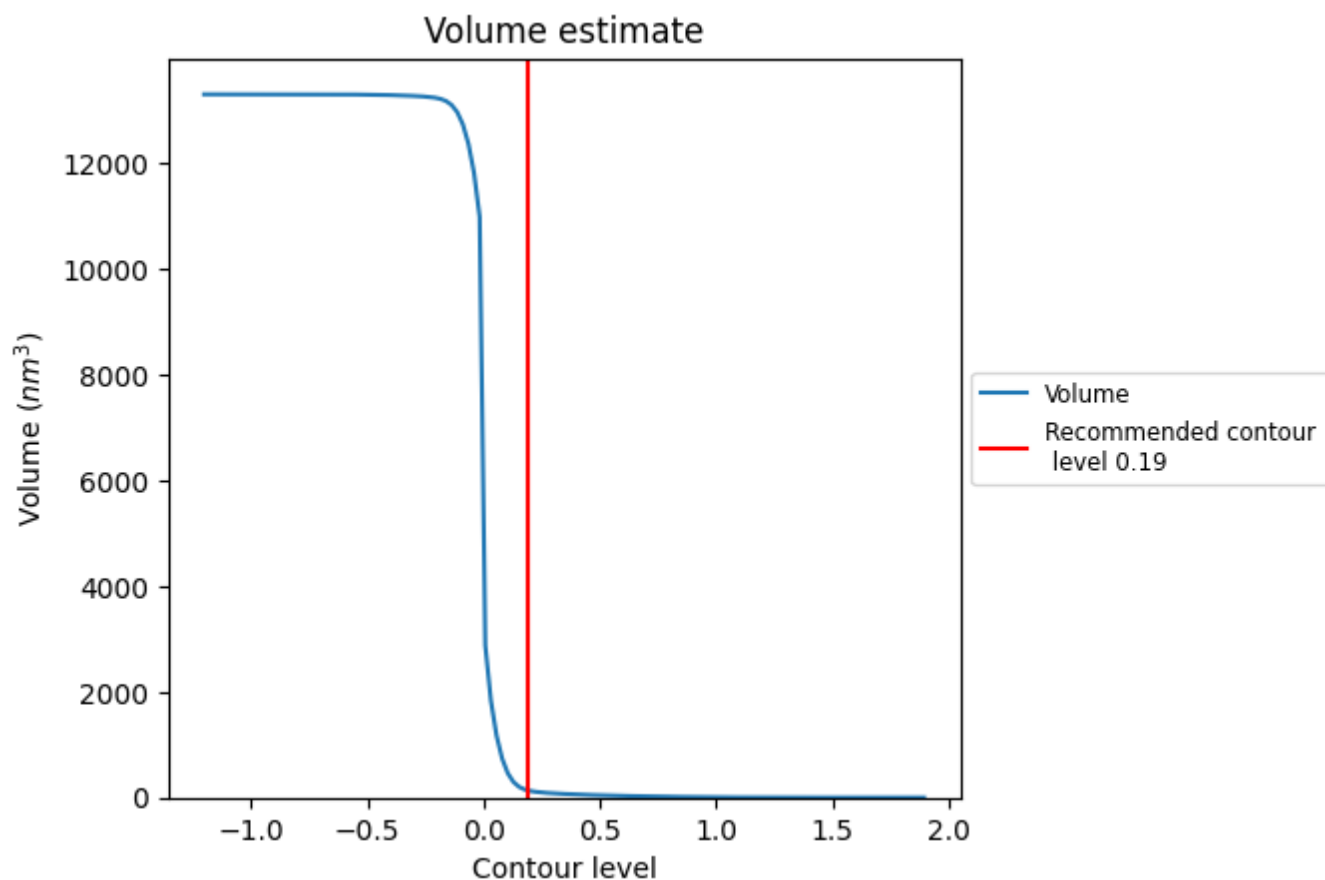
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

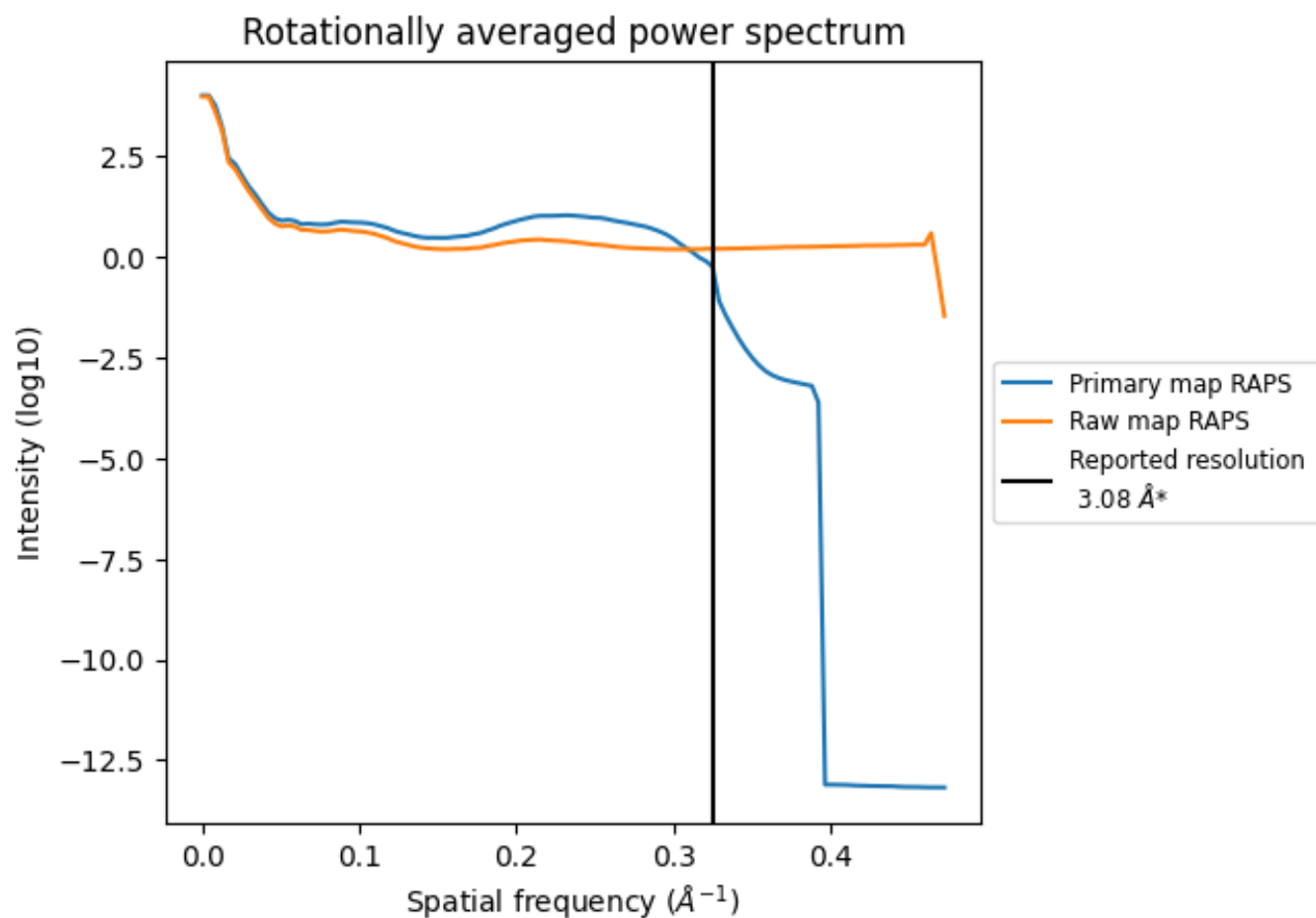
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 137 nm³; this corresponds to an approximate mass of 123 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 ⓘ

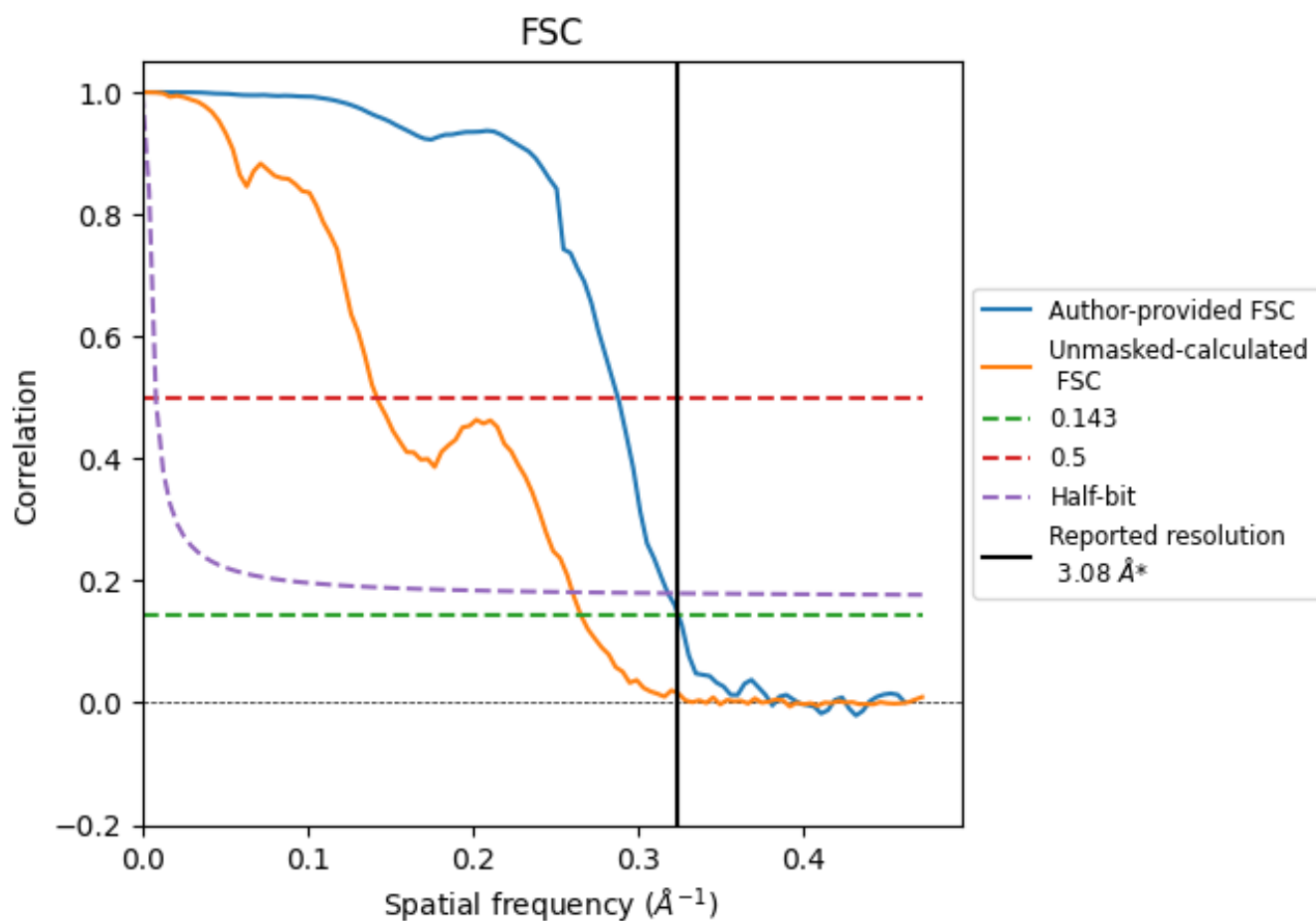


*Reported resolution corresponds to spatial frequency of 0.325 Å⁻¹

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 0.325 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

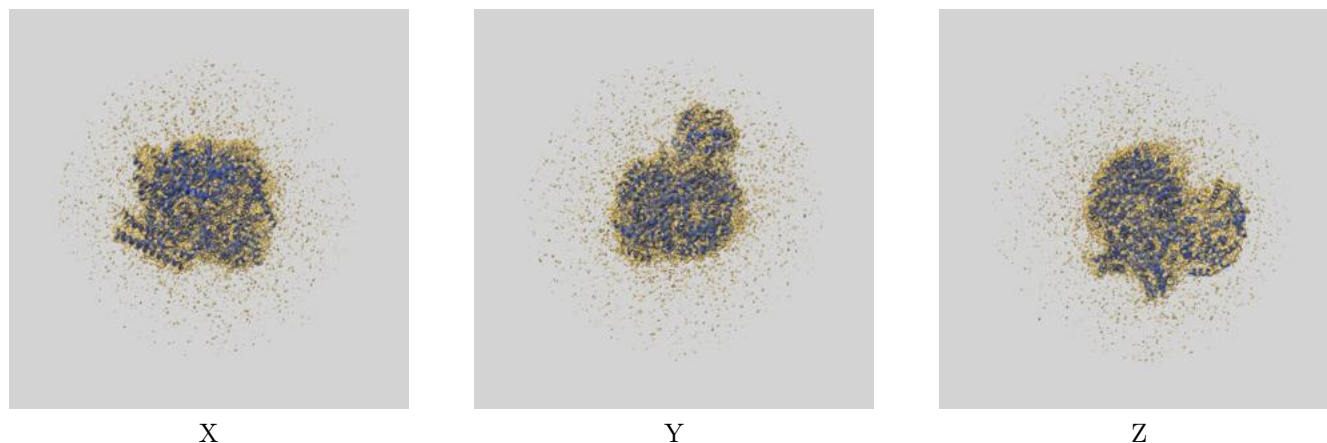
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.08	3.47	3.14
Unmasked-calculated*	3.76	7.03	3.84

*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 3.76 differs from the reported value 3.08 by more than 10 %

9 Map-model fit [i](#)

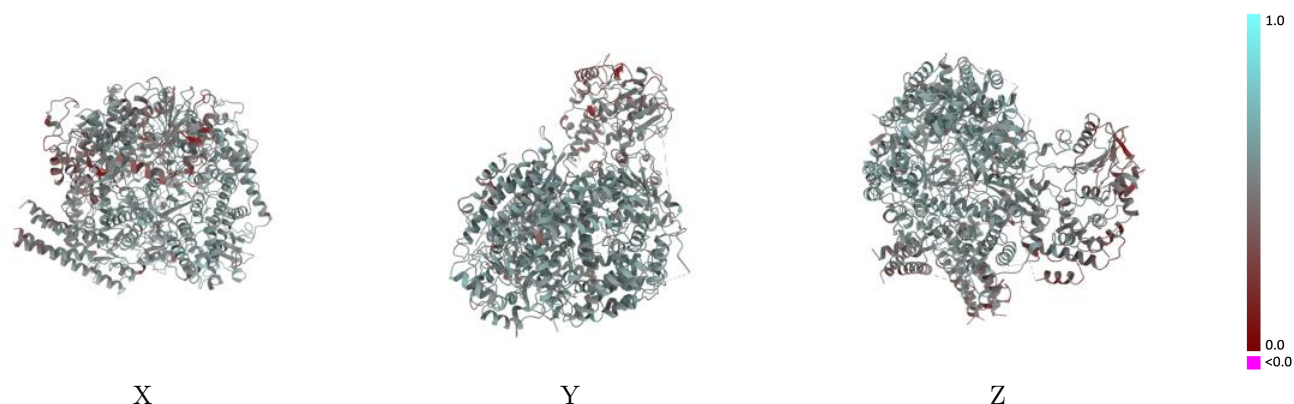
This section contains information regarding the fit between EMDB map EMD-71611 and PDB model 9PFR. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



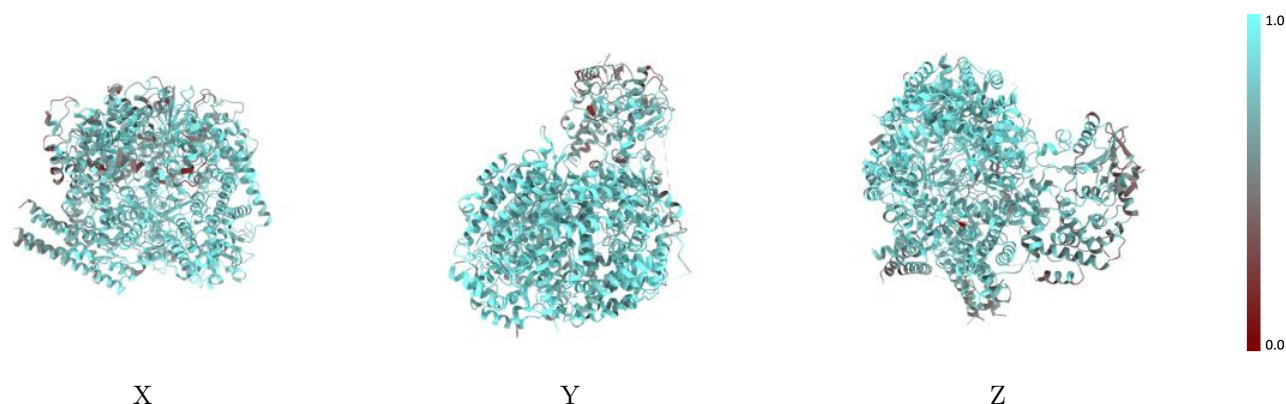
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



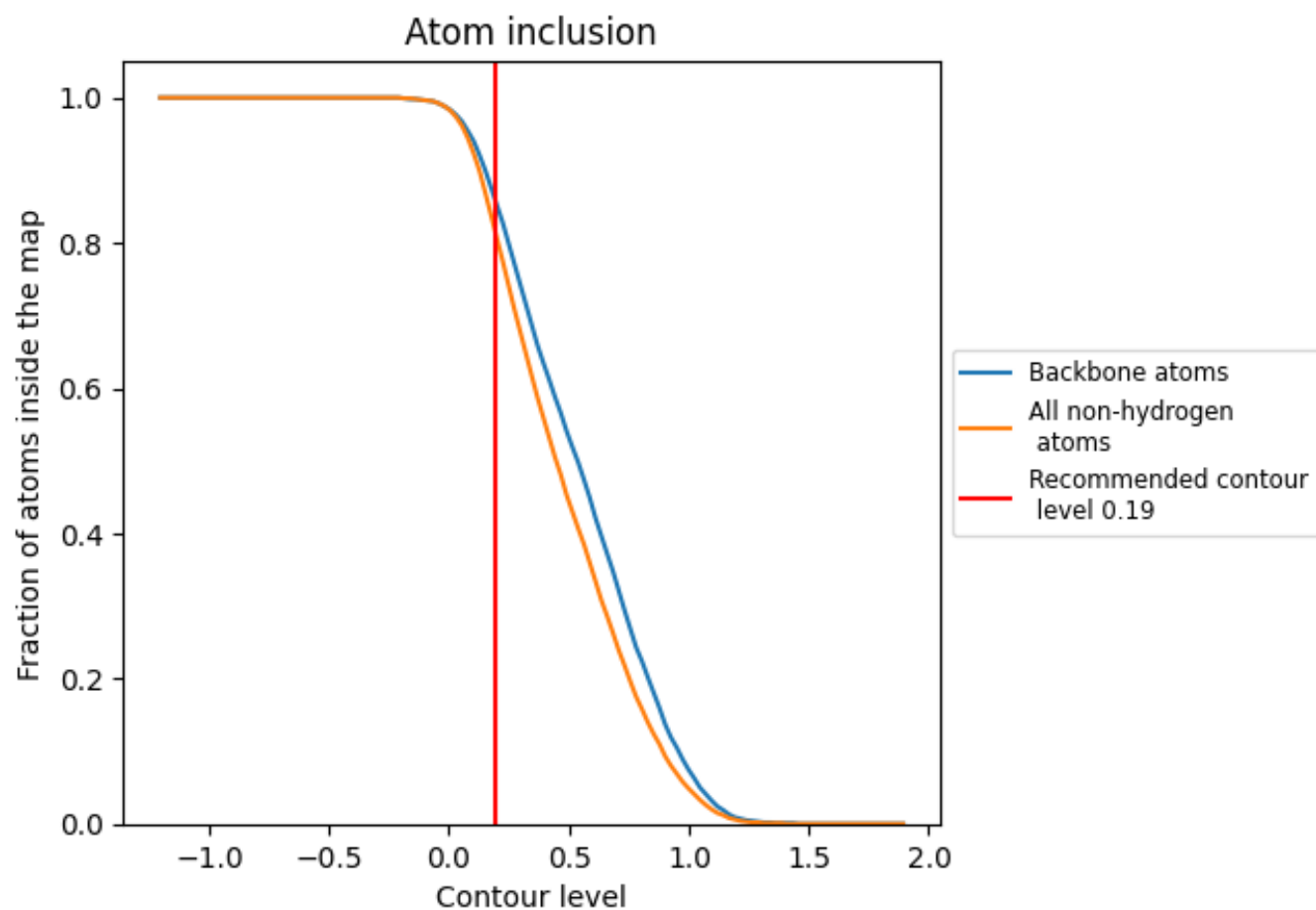
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.19).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 82% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8200	0.5190
A	0.8270	0.5220
B	0.8400	0.5210
C	0.7130	0.4740
D	0.6780	0.4480
E	0.7900	0.5030
P	0.9540	0.5530
T	0.8610	0.5270

1.0

0.0

<0.0