WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report (i)

Mar 10, 2024 – 07:55 PM EDT

PDB ID	:	6PZK
EMDB ID	:	EMD-20536
Title	:	Cryo-EM Structure of the Respiratory Syncytial Virus Polymerase (L) Protein Bound by the Tetrameric Phosphoprotein (P)
Authors	:	Gilman, M.S.A.; McLellan, J.S.
Deposited on	:	2019-08-01
Resolution	:	3.20 Å(reported)

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		0
Ramachandran outliers		0
Sidechain outliers		2.4%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
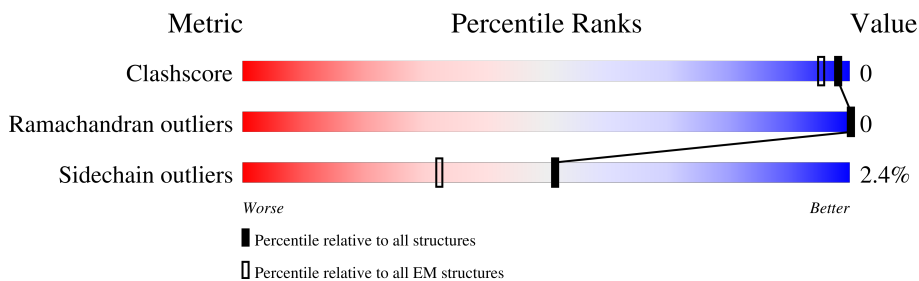
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	2201	58% · 38%
2	B	256	7% 35% · 62%
2	C	256	20% · 78%
2	D	256	11% 20% · 79%
2	E	256	11% 20% · 79%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 13153 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
			Total	C	N	O	S		
1	A	1361	11106	7155	1863	2031	57	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	initiating methionine	UNP P28887
A	-34	GLY	-	expression tag	UNP P28887
A	-33	SER	-	expression tag	UNP P28887
A	-32	TRP	-	expression tag	UNP P28887
A	-31	SER	-	expression tag	UNP P28887
A	-30	HIS	-	expression tag	UNP P28887
A	-29	PRO	-	expression tag	UNP P28887
A	-28	GLN	-	expression tag	UNP P28887
A	-27	PHE	-	expression tag	UNP P28887
A	-26	GLU	-	expression tag	UNP P28887
A	-25	LYS	-	expression tag	UNP P28887
A	-24	GLY	-	expression tag	UNP P28887
A	-23	SER	-	expression tag	UNP P28887
A	-22	GLY	-	expression tag	UNP P28887
A	-21	SER	-	expression tag	UNP P28887
A	-20	GLY	-	expression tag	UNP P28887
A	-19	SER	-	expression tag	UNP P28887
A	-18	SER	-	expression tag	UNP P28887
A	-17	TRP	-	expression tag	UNP P28887
A	-16	SER	-	expression tag	UNP P28887
A	-15	HIS	-	expression tag	UNP P28887
A	-14	PRO	-	expression tag	UNP P28887
A	-13	GLN	-	expression tag	UNP P28887
A	-12	PHE	-	expression tag	UNP P28887
A	-11	GLU	-	expression tag	UNP P28887
A	-10	LYS	-	expression tag	UNP P28887
A	-9	GLY	-	expression tag	UNP P28887
A	-8	SER	-	expression tag	UNP P28887

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP P28887
A	-6	SER	-	expression tag	UNP P28887
A	-5	LEU	-	expression tag	UNP P28887
A	-4	VAL	-	expression tag	UNP P28887
A	-3	PRO	-	expression tag	UNP P28887
A	-2	ARG	-	expression tag	UNP P28887
A	-1	GLY	-	expression tag	UNP P28887
A	0	SER	-	expression tag	UNP P28887

- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	98	Total	C	N	O	S	0	0
			762	462	137	157	6		
2	C	57	Total	C	N	O	S	0	0
			437	269	80	85	3		
2	D	55	Total	C	N	O	S	0	0
			424	260	78	83	3		
2	E	53	Total	C	N	O	S	0	0
			424	261	79	80	4		

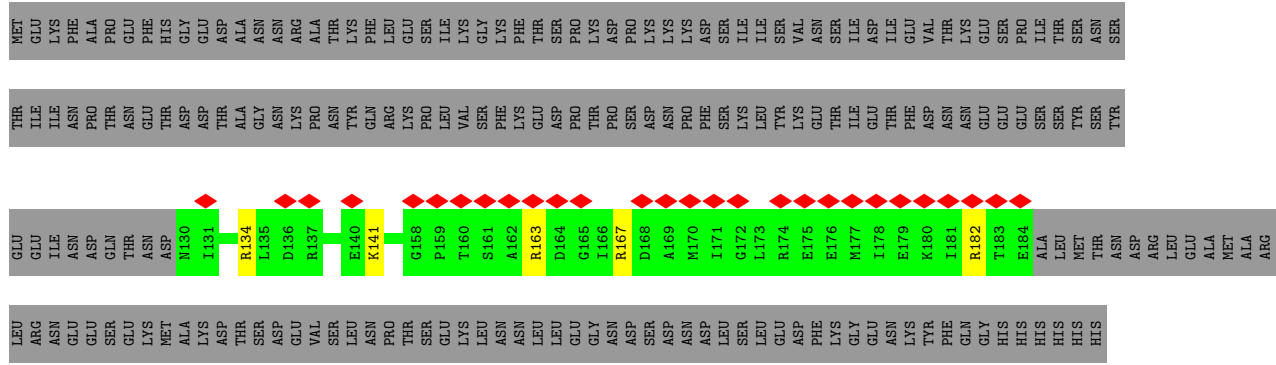There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	242	LYS	-	expression tag	UNP P03421
B	243	GLY	-	expression tag	UNP P03421
B	244	GLU	-	expression tag	UNP P03421
B	245	ASN	-	expression tag	UNP P03421
B	246	LYS	-	expression tag	UNP P03421
B	247	TYR	-	expression tag	UNP P03421
B	248	PHE	-	expression tag	UNP P03421
B	249	GLN	-	expression tag	UNP P03421
B	250	GLY	-	expression tag	UNP P03421
B	251	HIS	-	expression tag	UNP P03421
B	252	HIS	-	expression tag	UNP P03421
B	253	HIS	-	expression tag	UNP P03421
B	254	HIS	-	expression tag	UNP P03421
B	255	HIS	-	expression tag	UNP P03421
B	256	HIS	-	expression tag	UNP P03421
C	242	LYS	-	expression tag	UNP P03421
C	243	GLY	-	expression tag	UNP P03421
C	244	GLU	-	expression tag	UNP P03421

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Chain	Residue	Modelled	Actual	Comment	Reference
C	245	ASN	-	expression tag	UNP P03421
C	246	LYS	-	expression tag	UNP P03421
C	247	TYR	-	expression tag	UNP P03421
C	248	PHE	-	expression tag	UNP P03421
C	249	GLN	-	expression tag	UNP P03421
C	250	GLY	-	expression tag	UNP P03421
C	251	HIS	-	expression tag	UNP P03421
C	252	HIS	-	expression tag	UNP P03421
C	253	HIS	-	expression tag	UNP P03421
C	254	HIS	-	expression tag	UNP P03421
C	255	HIS	-	expression tag	UNP P03421
C	256	HIS	-	expression tag	UNP P03421
D	242	LYS	-	expression tag	UNP P03421
D	243	GLY	-	expression tag	UNP P03421
D	244	GLU	-	expression tag	UNP P03421
D	245	ASN	-	expression tag	UNP P03421
D	246	LYS	-	expression tag	UNP P03421
D	247	TYR	-	expression tag	UNP P03421
D	248	PHE	-	expression tag	UNP P03421
D	249	GLN	-	expression tag	UNP P03421
D	250	GLY	-	expression tag	UNP P03421
D	251	HIS	-	expression tag	UNP P03421
D	252	HIS	-	expression tag	UNP P03421
D	253	HIS	-	expression tag	UNP P03421
D	254	HIS	-	expression tag	UNP P03421
D	255	HIS	-	expression tag	UNP P03421
D	256	HIS	-	expression tag	UNP P03421
E	242	LYS	-	expression tag	UNP P03421
E	243	GLY	-	expression tag	UNP P03421
E	244	GLU	-	expression tag	UNP P03421
E	245	ASN	-	expression tag	UNP P03421
E	246	LYS	-	expression tag	UNP P03421
E	247	TYR	-	expression tag	UNP P03421
E	248	PHE	-	expression tag	UNP P03421
E	249	GLN	-	expression tag	UNP P03421
E	250	GLY	-	expression tag	UNP P03421
E	251	HIS	-	expression tag	UNP P03421
E	252	HIS	-	expression tag	UNP P03421
E	253	HIS	-	expression tag	UNP P03421
E	254	HIS	-	expression tag	UNP P03421
E	255	HIS	-	expression tag	UNP P03421
E	256	HIS	-	expression tag	UNP P03421

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

Chain A:

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

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

LEU TYR ASN HIS ILE ILE ASP ASP GLU LEU THR ILE PRO ALA THR ASP ALA THR ASN ILE THR TRP SER TYR LEU HIS ILE LYS PHE ALA GLU PRO ILE SER LEU PHE VAL CYS ASP ALA GLU LEU SER VAL THR VAL ASN TRP SER LYS ILE ILE ILE GLU TRP

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

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

LYS LEU LYS SER VAL VAL SER GLY ASP ILE LEU SER TYR SER ILE ALA GLY ARG ASN GLU VAL PHE SER ASN LYS LEU ILE ASN HIS LYS HIS MET ASN ILE LEU LYS TRP PHE ASN HIS VAL LEU ASN PHE ARG SER THR GLU LEU ASN TYR ASN HIS LEU TYR MET VAL GLU SER THR

TYR PRO TYR LEU SER GLU LEU ASN LEU LEU ASN SER LEU THR THR ASN GLU GLU LYS LYS LEU ILE LYS LEU THR GLY SER LEU LEU TYR ASN PHE HIS ASN GLU

• Molecule 2: Phosphoprotein

Chain B: 7% / 35% • 62%

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

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

LEU GLU ASP PHE LYS GLY GLU ASN LYS TYR PHE GLN GLY HIS HIS HIS HIS HIS HIS

• Molecule 2: Phosphoprotein

Chain C: 20% • 78%

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

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

SER GLU LYS LEU ASN ASN LEU LEU GLU GLY ASN ASP SER GLU ASP ASN LEU SER LEU GLU ASP PHE LYS GLY GLU ASN LYS TYR PHE GLN GLY HIS HIS HIS HIS HIS HIS

• Molecule 2: Phosphoprotein

Chain D: 11% / 20% • 79%

• Molecule 2: Phosphoprotein

Chain E:

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	196720	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 $(e^-/\text{Å}^2)$	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.980	Depositor
Minimum map value	-2.351	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	275.2, 275.2, 275.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.075, 1.075, 1.075	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	0.63	0/11340	1.06	56/15352 (0.4%)
2	B	0.62	0/764	1.14	5/1024 (0.5%)
2	C	0.63	0/438	1.17	5/587 (0.9%)
2	D	0.65	0/425	1.11	4/569 (0.7%)
2	E	0.61	0/423	1.10	3/563 (0.5%)
All	All	0.63	0/13390	1.07	73/18095 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	378	ARG	NE-CZ-NH2	11.14	125.87	120.30
1	A	302	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	A	468	ARG	NE-CZ-NH1	9.12	124.86	120.30
2	D	163	ARG	NE-CZ-NH2	8.03	124.31	120.30
1	A	1068	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	A	588	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	A	580	ARG	NE-CZ-NH1	7.93	124.27	120.30
2	C	167	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	A	771	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	115	ARG	NE-CZ-NH1	7.63	124.12	120.30
2	B	191	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	A	1164	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	A	353	ARG	NE-CZ-NH1	7.10	123.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	114	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	A	1000	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	A	479	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	A	747	ARG	NE-CZ-NH1	7.00	123.80	120.30
2	B	167	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	A	222	ARG	NE-CZ-NH2	6.95	123.78	120.30
2	E	191	ARG	NE-CZ-NH2	6.93	123.77	120.30
1	A	1409	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	1209	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	A	330	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	A	260	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	462	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	A	929	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	A	1186	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	437	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	A	523	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	581	ARG	NE-CZ-NH1	6.60	123.60	120.30
2	C	163	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	1170	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	B	199	ARG	NE-CZ-NH1	6.49	123.54	120.30
2	D	182	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	1035	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	A	918	ARG	NE-CZ-NH2	6.33	123.46	120.30
1	A	588	ARG	NE-CZ-NH2	-6.29	117.15	120.30
2	B	134	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	A	1286	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	995	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	526	ARG	NE-CZ-NH2	6.09	123.34	120.30
1	A	511	ARG	NE-CZ-NH2	6.08	123.34	120.30
2	C	182	ARG	NE-CZ-NH2	6.02	123.31	120.30
2	D	167	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	1059	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	1370	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	396	ARG	NE-CZ-NH2	5.93	123.26	120.30
2	E	182	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	822	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	637	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	C	137	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	355	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	555	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	1278	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	1345	ARG	NE-CZ-NH1	5.52	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	709	ARG	NE-CZ-NH1	5.47	123.03	120.30
2	E	134	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	1207	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	1444	HIS	CB-CA-C	-5.45	99.49	110.40
1	A	1444	HIS	CA-CB-CG	5.41	122.80	113.60
1	A	51	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	A	427	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	1331	TYR	CB-CG-CD1	-5.23	117.86	121.00
2	C	174	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	A	1068	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	D	134	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	A	1035	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	1357	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	557	TYR	CB-CG-CD2	-5.09	117.95	121.00
1	A	1256	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	B	174	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	A	714	CYS	CA-CB-SG	-5.03	104.95	114.00
1	A	864	ARG	NE-CZ-NH2	5.02	122.81	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1059	ARG	Sidechain
1	A	1164	ARG	Sidechain
1	A	269	PHE	Sidechain
1	A	586	TYR	Sidechain
1	A	606	TYR	Sidechain
1	A	770	TYR	Sidechain
1	A	834	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11106	0	11295	6	0
2	B	762	0	780	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	437	0	459	1	0
2	D	424	0	443	1	0
2	E	424	0	450	0	0
All	All	13153	0	13427	8	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 0.

All (8) 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:1056:THR:HG21	1:A:1211:TRP:CH2	2.34	0.62
1:A:710:TYR:CE2	1:A:714:CYS:SG	3.04	0.49
1:A:121:ASP:OD1	1:A:187:THR:HG22	2.14	0.48
1:A:1056:THR:HG21	1:A:1211:TRP:CZ3	2.53	0.43
1:A:487:ILE:O	2:D:141:LYS:HE2	2.20	0.42
1:A:1065:GLY:HA3	1:A:1211:TRP:CH2	2.54	0.42
2:B:152:LEU:HB3	2:B:171:ILE:HD11	2.01	0.41
2:C:173:LEU:H	2:C:173:LEU:HD12	1.86	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	1353/2201 (62%)	1297 (96%)	56 (4%)	0	100	100
2	B	96/256 (38%)	93 (97%)	3 (3%)	0	100	100
2	C	55/256 (22%)	53 (96%)	2 (4%)	0	100	100
2	D	53/256 (21%)	53 (100%)	0	0	100	100
2	E	49/256 (19%)	49 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1606/3225 (50%)	1545 (96%)	61 (4%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1265/2041 (62%)	1233 (98%)	32 (2%)	47 77
2	B	85/233 (36%)	83 (98%)	2 (2%)	49 77
2	C	47/233 (20%)	46 (98%)	1 (2%)	53 79
2	D	46/233 (20%)	46 (100%)	0	100 100
2	E	46/233 (20%)	46 (100%)	0	100 100
All	All	1489/2973 (50%)	1454 (98%)	35 (2%)	51 77

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	43	ASN
1	A	94	TYR
1	A	268	GLN
1	A	307	ASN
1	A	311	THR
1	A	320	ILE
1	A	378	ARG
1	A	401	LEU
1	A	446	ASN
1	A	536	ILE
1	A	539	ASP
1	A	569	GLU
1	A	577	ASP
1	A	600	CYS
1	A	627	ARG

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Mol	Chain	Res	Type
1	A	699	THR
1	A	700	ASP
1	A	727	GLN
1	A	760	LEU
1	A	869	MET
1	A	876	ASN
1	A	885	LYS
1	A	994	TYR
1	A	1025	LYS
1	A	1177	ILE
1	A	1252	THR
1	A	1284	LYS
1	A	1310	GLU
1	A	1342	VAL
1	A	1403	THR
1	A	1445	MET
2	B	182	ARG
2	B	224	ASN
2	C	137	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	362	ASN
1	A	739	HIS
1	A	1438	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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-20536. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1　Orthogonal projections ⓘ

6.1.1　Primary map

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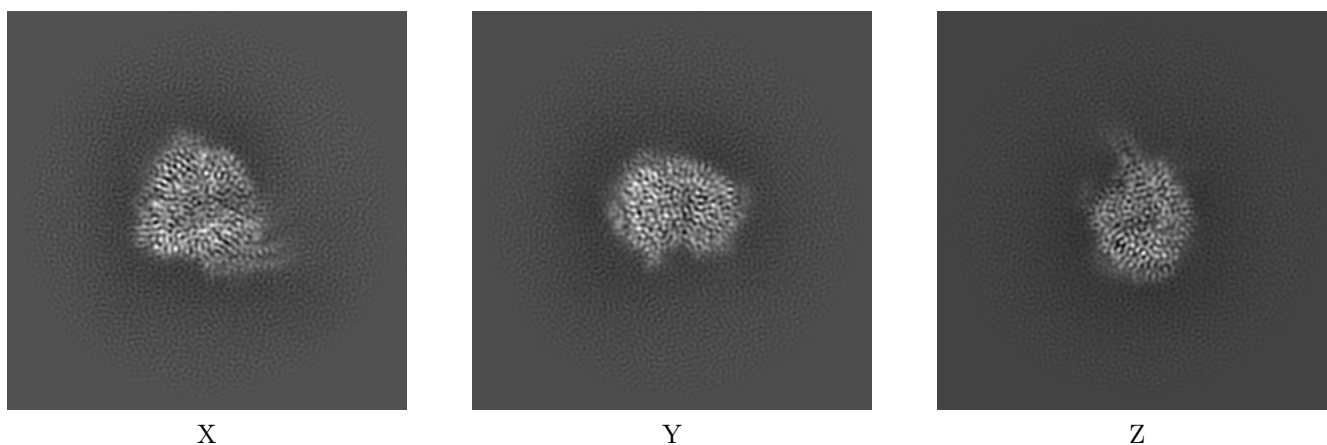
The images above show the map projected in three orthogonal directions.

6.2　Central slices ⓘ

6.2.1　Primary map

| X Index: 128 | Y Index: 128 | Z Index: 128 |
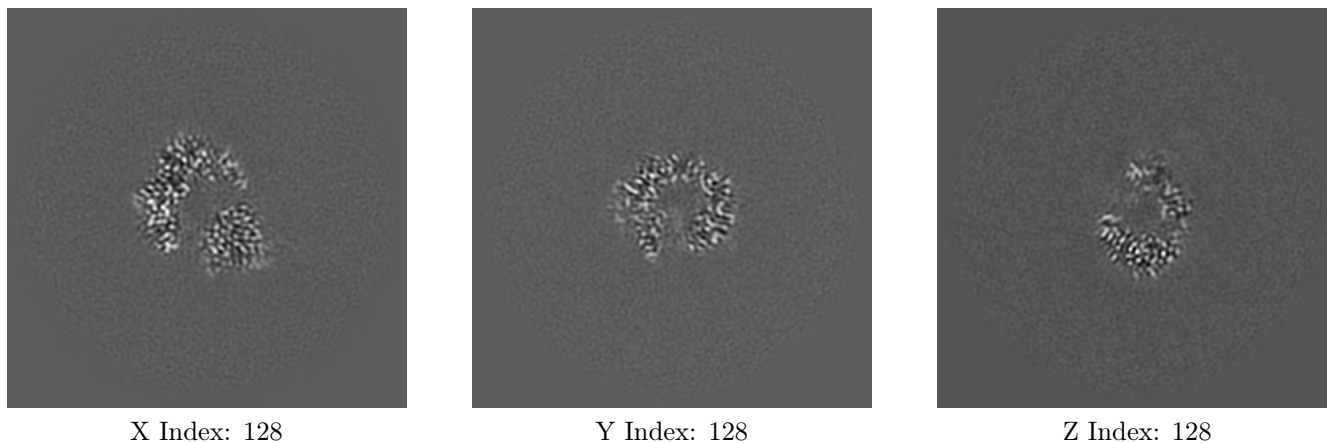
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
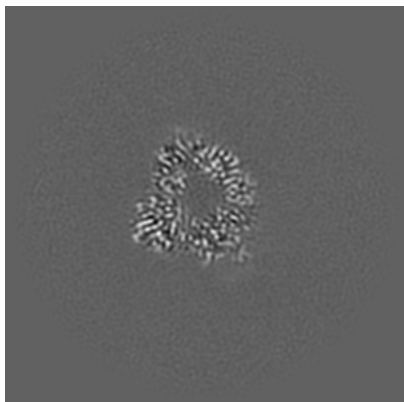
6.3.1 Primary map
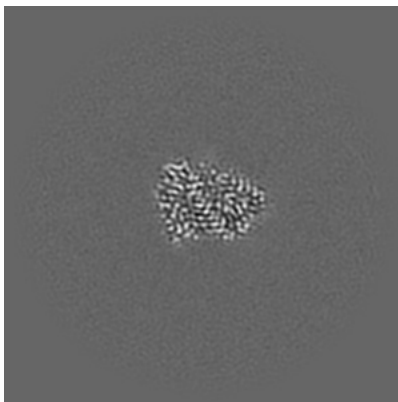
| X Index: 138 | Y Index: 102 | Z Index: 113 |
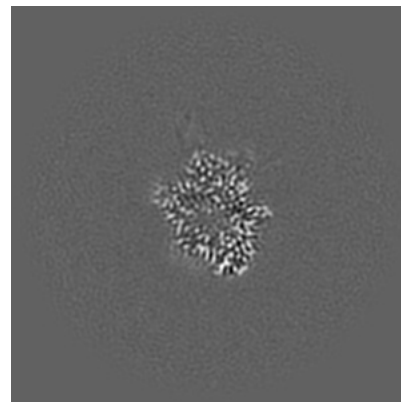
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

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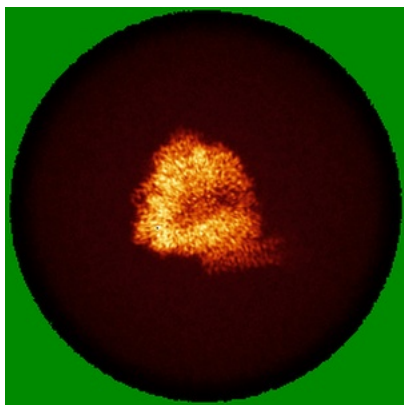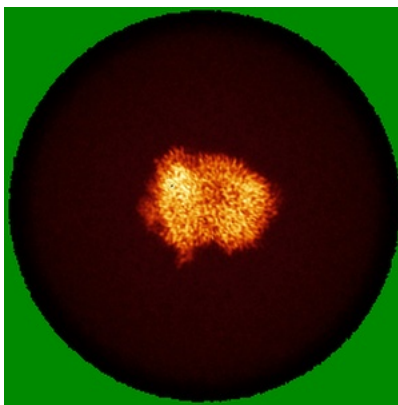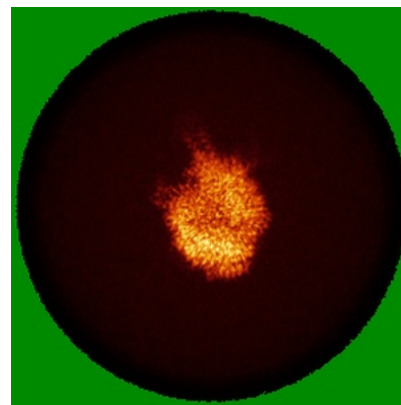
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

| X | Y | Z |
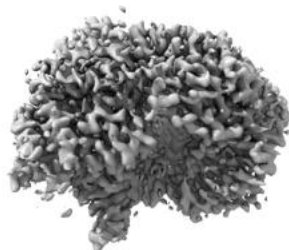
The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation ⓘ

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 ⓘ
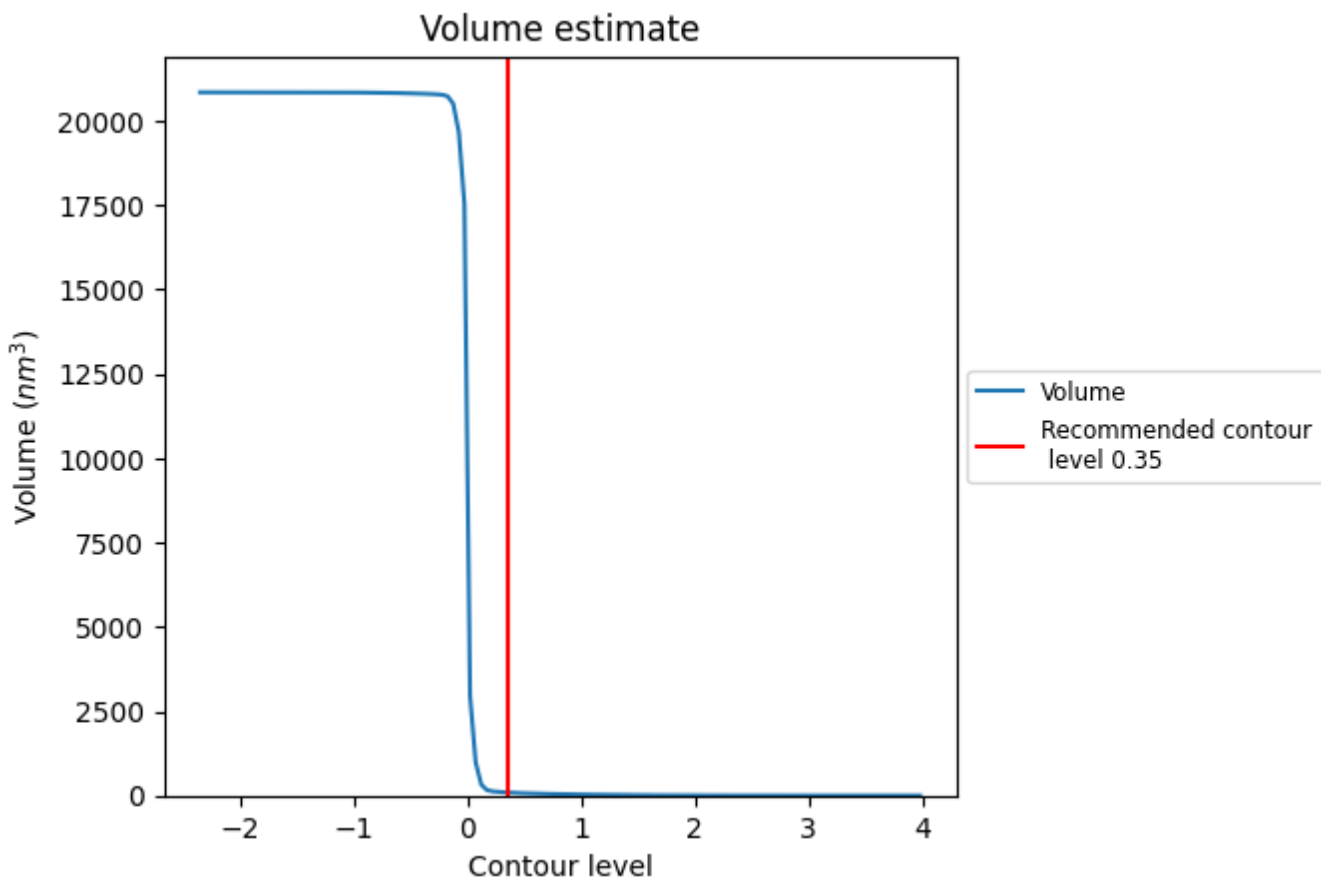
The volume at the recommended contour level is 91 nm^3; this corresponds to an approximate mass of 82 kDa.

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 ⓘ
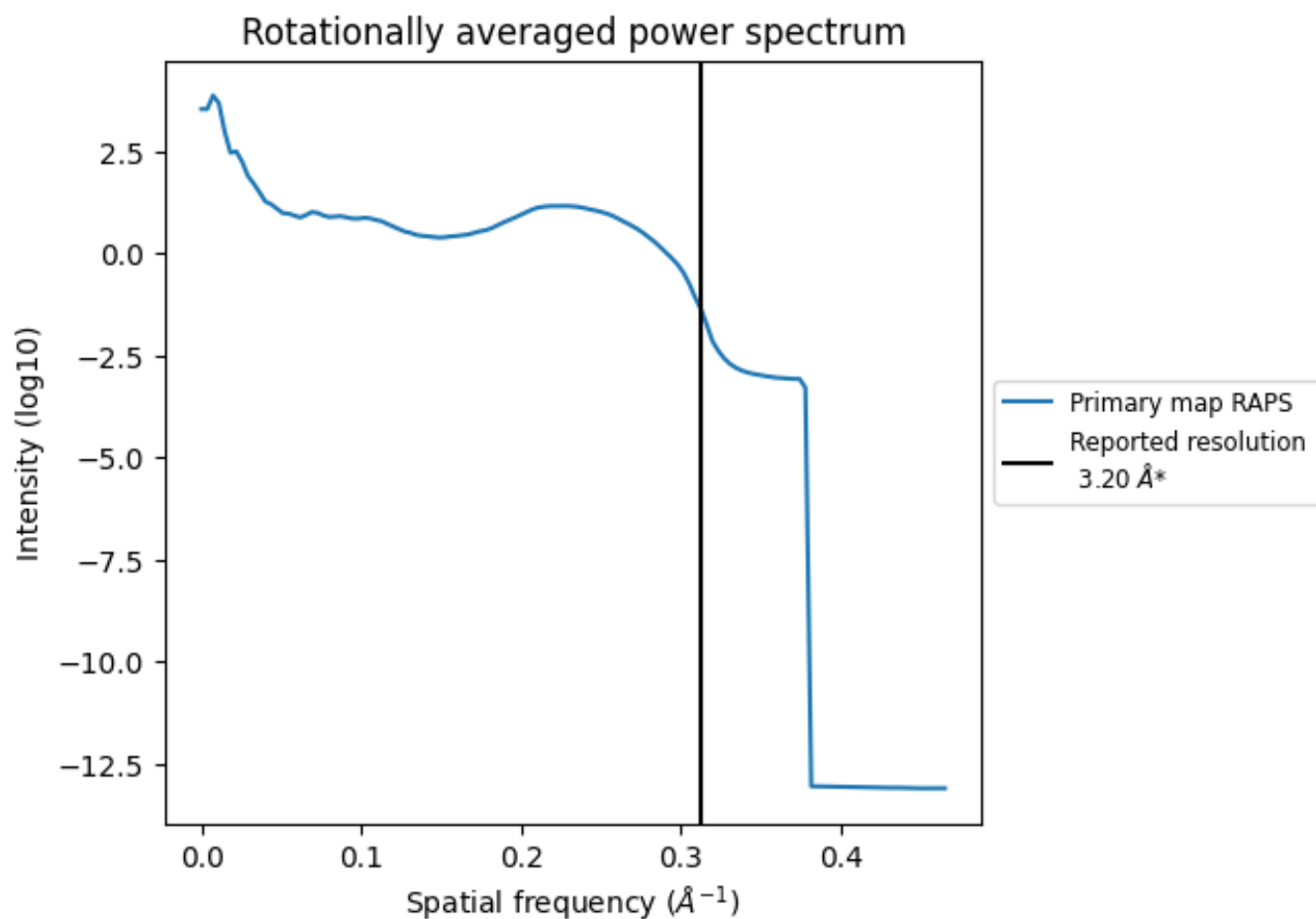
*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8　Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1　FSC ⓘ
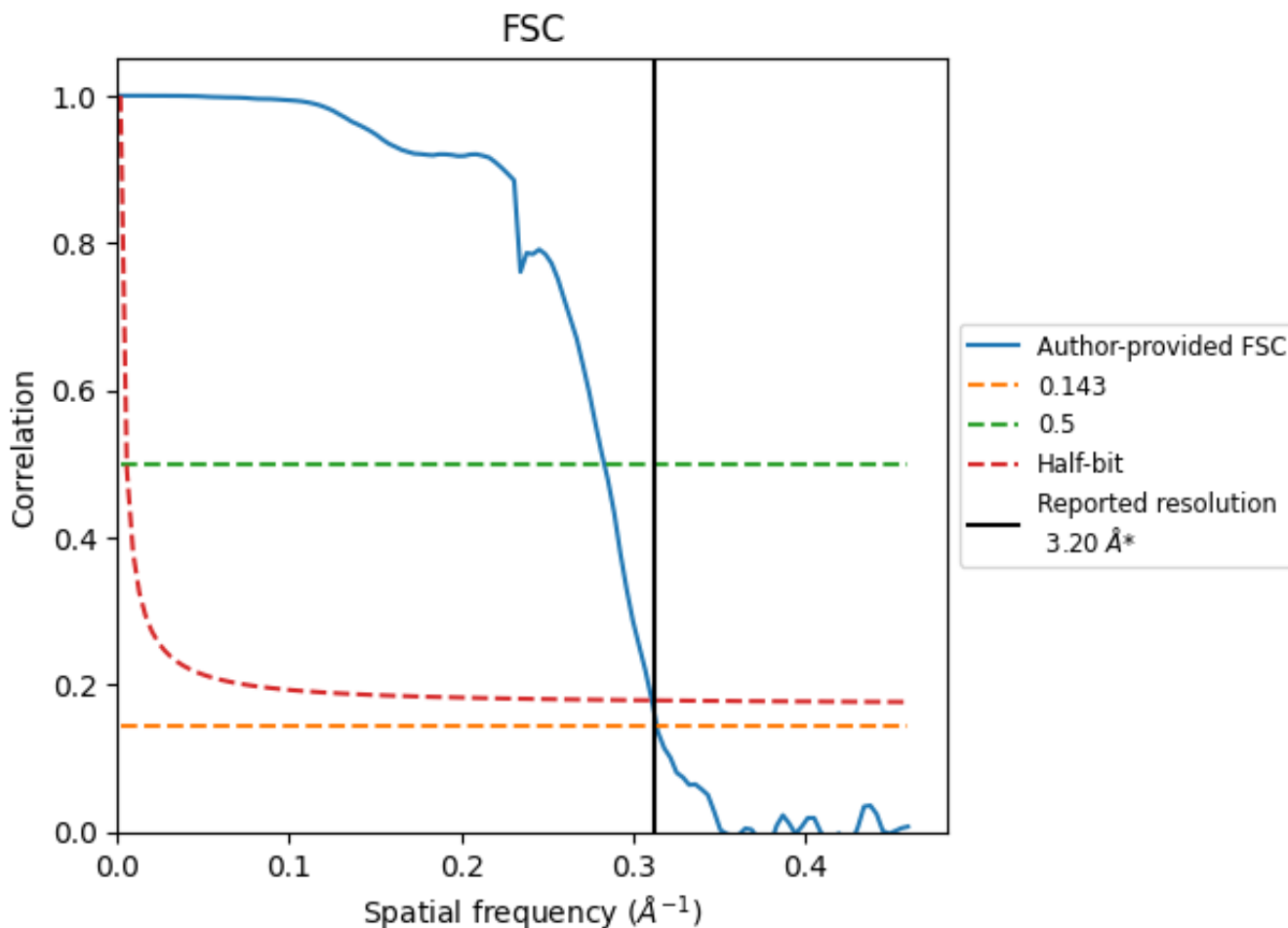
*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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	3.19	3.53	3.22
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-20536 and PDB model 6PZK. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay ⓘ
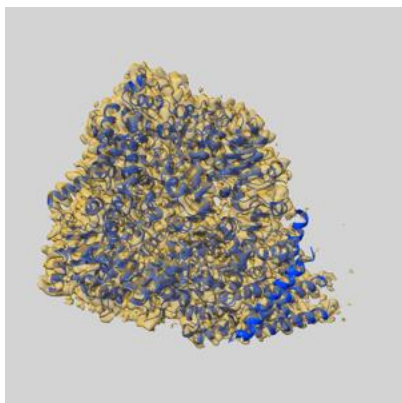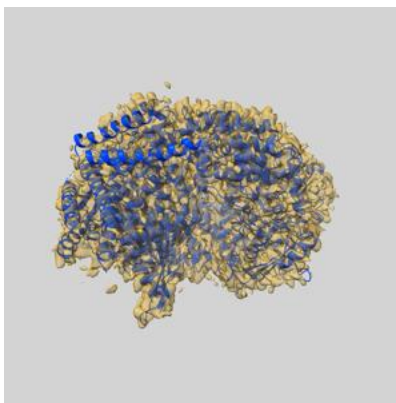
X　　　　　　　　　　　　　Y　　　　　　　　　　　　　Z
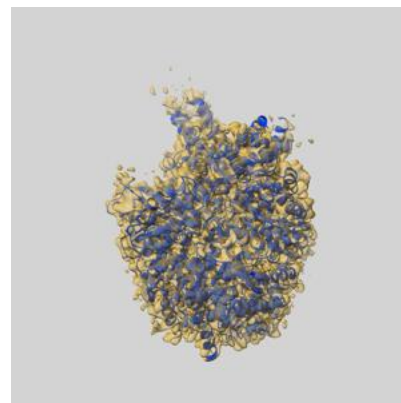
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

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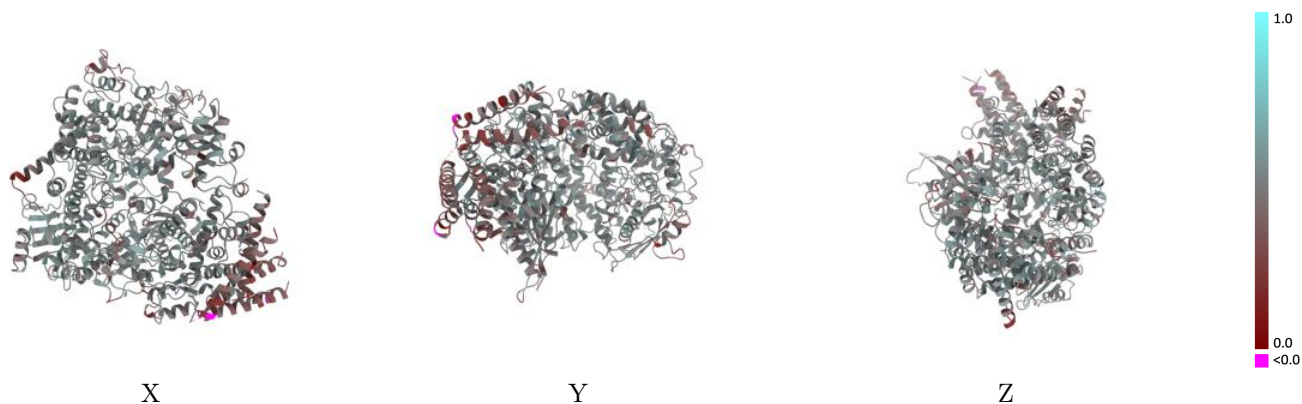
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)

X   Y   Z
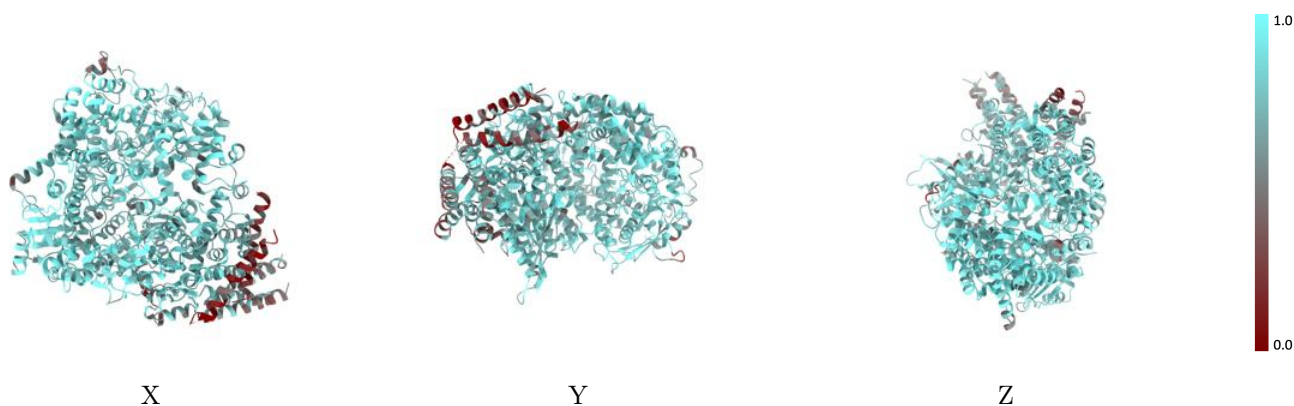
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4　Atom inclusion ⓘ
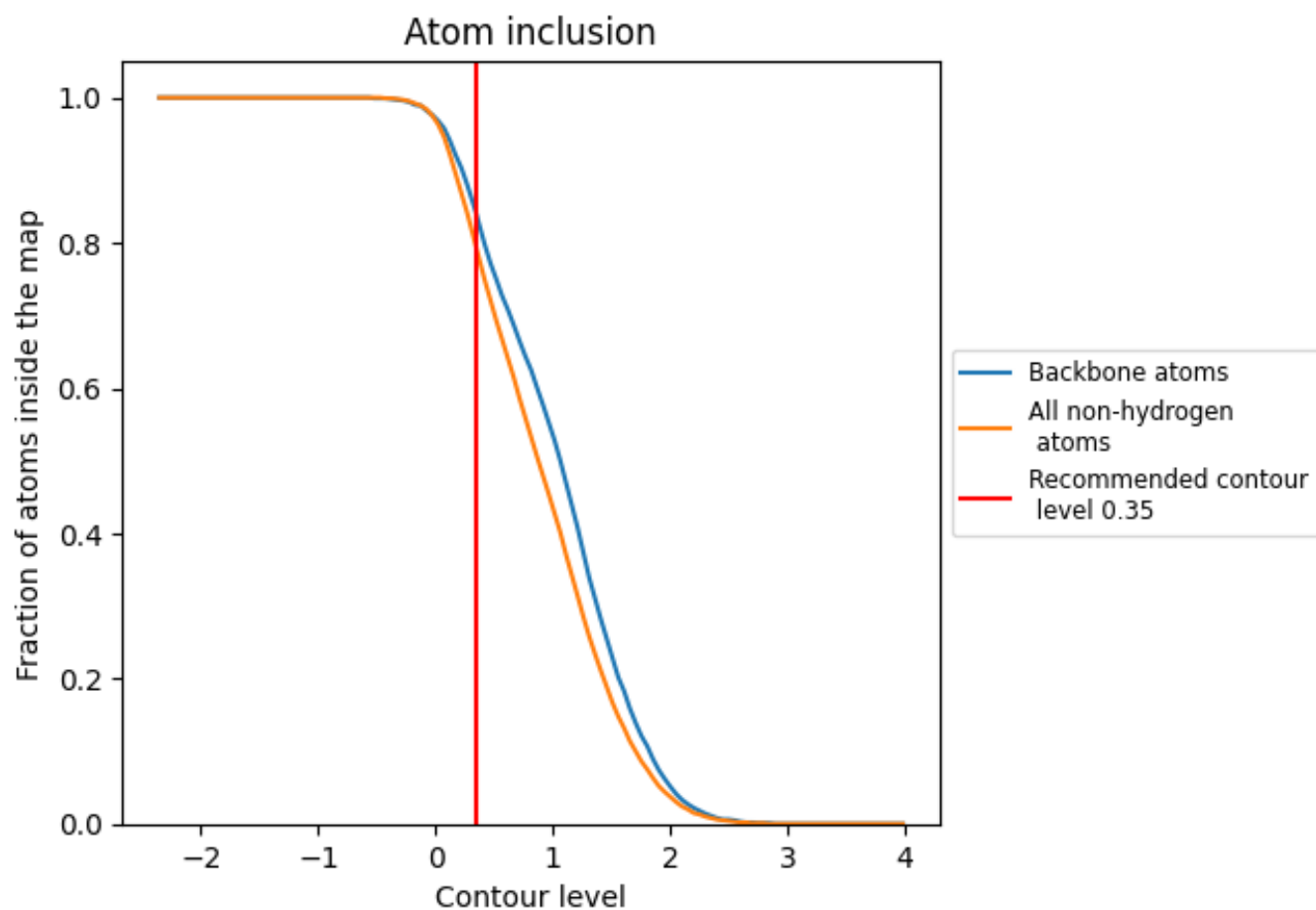
At the recommended contour level, 84% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7920	0.4770
A	0.8340	0.4930
B	0.6460	0.4140
C	0.7130	0.4350
D	0.4150	0.3490
E	0.4020	0.3470

1.0

0.0
<0.0