Full wwPDB EM Validation Report ⓘ

May 12, 2024 – 04:30 pm BST

PDB ID	:	6T0W
EMDB ID	:	EMD-10361
Title	:	Human Influenza B polymerase recycling complex
Authors	:	Wandzik, J.M.; Kouba, T.; Karuppasamy, M.; Cusack, S.
Deposited on	:	2019-10-03
Resolution	:	3.18 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:

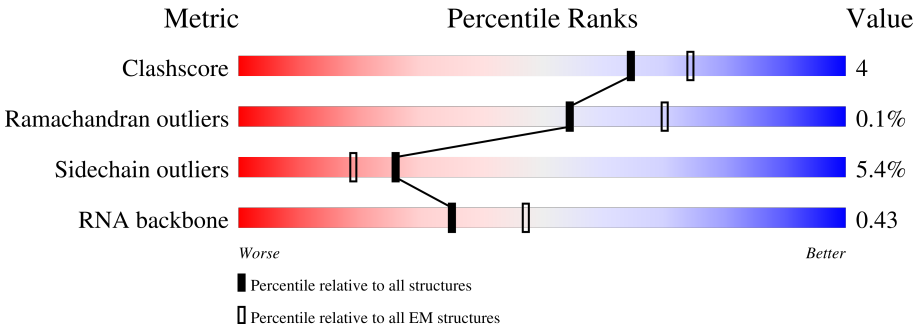
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.18 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	751	5% 60% 8% · 31%
2	B	772	13% 72% 13% · 14%
3	C	799	8% 9% · 89%
4	V	34	24% 53% 18% · 26%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10556 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	521	Total	C	N	O	S	0	0
			4161	2644	707	780	30		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	GLY	-	expression tag	UNP Q5V8Z9
A	-12	SER	-	expression tag	UNP Q5V8Z9
A	-11	HIS	-	expression tag	UNP Q5V8Z9
A	-10	HIS	-	expression tag	UNP Q5V8Z9
A	-9	HIS	-	expression tag	UNP Q5V8Z9
A	-8	HIS	-	expression tag	UNP Q5V8Z9
A	-7	HIS	-	expression tag	UNP Q5V8Z9
A	-6	HIS	-	expression tag	UNP Q5V8Z9
A	-5	HIS	-	expression tag	UNP Q5V8Z9
A	-4	HIS	-	expression tag	UNP Q5V8Z9
A	-3	GLY	-	expression tag	UNP Q5V8Z9
A	-2	SER	-	expression tag	UNP Q5V8Z9
A	-1	GLY	-	expression tag	UNP Q5V8Z9
A	0	SER	-	expression tag	UNP Q5V8Z9
A	727	GLY	-	expression tag	UNP Q5V8Z9
A	728	SER	-	expression tag	UNP Q5V8Z9
A	729	GLY	-	expression tag	UNP Q5V8Z9
A	730	SER	-	expression tag	UNP Q5V8Z9
A	731	GLY	-	expression tag	UNP Q5V8Z9
A	732	GLU	-	expression tag	UNP Q5V8Z9
A	733	ASN	-	expression tag	UNP Q5V8Z9
A	734	LEU	-	expression tag	UNP Q5V8Z9
A	735	TYR	-	expression tag	UNP Q5V8Z9
A	736	PHE	-	expression tag	UNP Q5V8Z9
A	737	GLN	-	expression tag	UNP Q5V8Z9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	661	Total	C	N	O	S	0	0
			5174	3279	886	967	42		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP Q5V8Y6
B	-7	SER	-	expression tag	UNP Q5V8Y6
B	-6	GLY	-	expression tag	UNP Q5V8Y6
B	-5	SER	-	expression tag	UNP Q5V8Y6
B	-4	GLY	-	expression tag	UNP Q5V8Y6
B	-3	SER	-	expression tag	UNP Q5V8Y6
B	-2	GLY	-	expression tag	UNP Q5V8Y6
B	-1	SER	-	expression tag	UNP Q5V8Y6
B	0	GLY	-	expression tag	UNP Q5V8Y6
B	753	GLY	-	expression tag	UNP Q5V8Y6
B	754	SER	-	expression tag	UNP Q5V8Y6
B	755	GLY	-	expression tag	UNP Q5V8Y6
B	756	SER	-	expression tag	UNP Q5V8Y6
B	757	GLY	-	expression tag	UNP Q5V8Y6
B	758	GLU	-	expression tag	UNP Q5V8Y6
B	759	ASN	-	expression tag	UNP Q5V8Y6
B	760	LEU	-	expression tag	UNP Q5V8Y6
B	761	TYR	-	expression tag	UNP Q5V8Y6
B	762	PHE	-	expression tag	UNP Q5V8Y6
B	763	GLN	-	expression tag	UNP Q5V8Y6

- Molecule 3 is a protein called Polymerase PB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	86	Total	C	N	O	S	0	0
			688	438	118	125	7		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP A0A4Y5WMY1
C	-7	SER	-	expression tag	UNP A0A4Y5WMY1
C	-6	GLY	-	expression tag	UNP A0A4Y5WMY1
C	-5	SER	-	expression tag	UNP A0A4Y5WMY1
C	-4	GLY	-	expression tag	UNP A0A4Y5WMY1
C	-3	SER	-	expression tag	UNP A0A4Y5WMY1
C	-2	GLY	-	expression tag	UNP A0A4Y5WMY1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP A0A4Y5WMY1
C	0	GLY	-	expression tag	UNP A0A4Y5WMY1
C	771	GLY	-	expression tag	UNP A0A4Y5WMY1
C	772	TRP	-	expression tag	UNP A0A4Y5WMY1
C	773	SER	-	expression tag	UNP A0A4Y5WMY1
C	774	HIS	-	expression tag	UNP A0A4Y5WMY1
C	775	PRO	-	expression tag	UNP A0A4Y5WMY1
C	776	GLN	-	expression tag	UNP A0A4Y5WMY1
C	777	PHE	-	expression tag	UNP A0A4Y5WMY1
C	778	GLU	-	expression tag	UNP A0A4Y5WMY1
C	779	LYS	-	expression tag	UNP A0A4Y5WMY1
C	780	GLY	-	expression tag	UNP A0A4Y5WMY1
C	781	ARG	-	expression tag	UNP A0A4Y5WMY1
C	782	SER	-	expression tag	UNP A0A4Y5WMY1
C	783	GLY	-	expression tag	UNP A0A4Y5WMY1
C	784	GLY	-	expression tag	UNP A0A4Y5WMY1
C	785	GLU	-	expression tag	UNP A0A4Y5WMY1
C	786	ASN	-	expression tag	UNP A0A4Y5WMY1
C	787	LEU	-	expression tag	UNP A0A4Y5WMY1
C	788	TYR	-	expression tag	UNP A0A4Y5WMY1
C	789	PHE	-	expression tag	UNP A0A4Y5WMY1
C	790	GLN	-	expression tag	UNP A0A4Y5WMY1

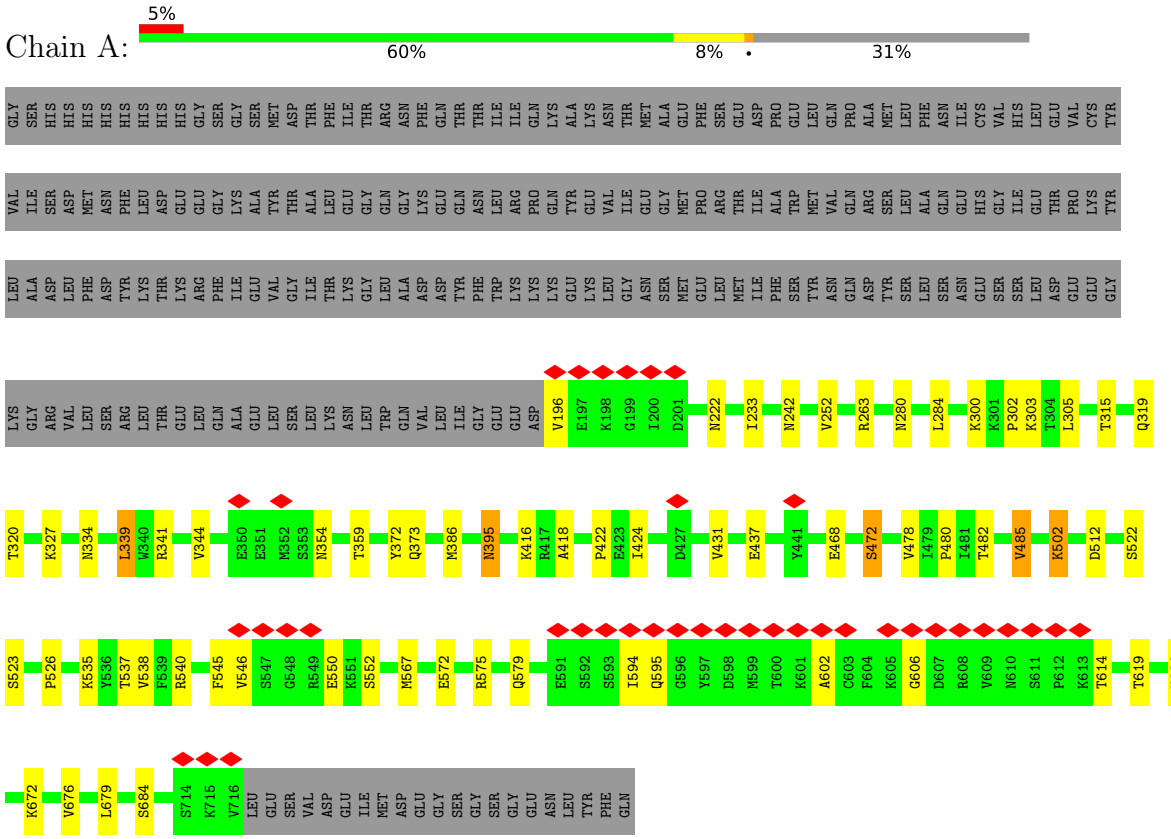
- Molecule 4 is a RNA chain called vRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	25	Total	C	N	O	P	0	0
			533	238	95	175	25		

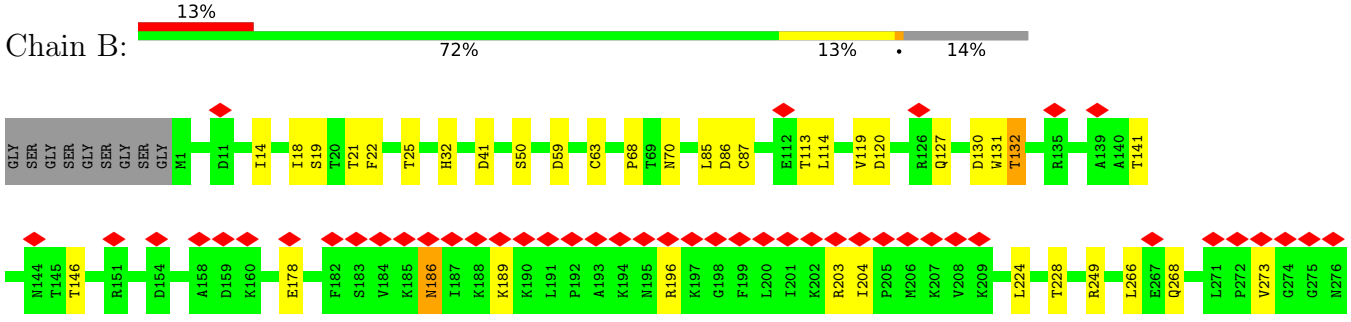
3 Residue-property plots (i)

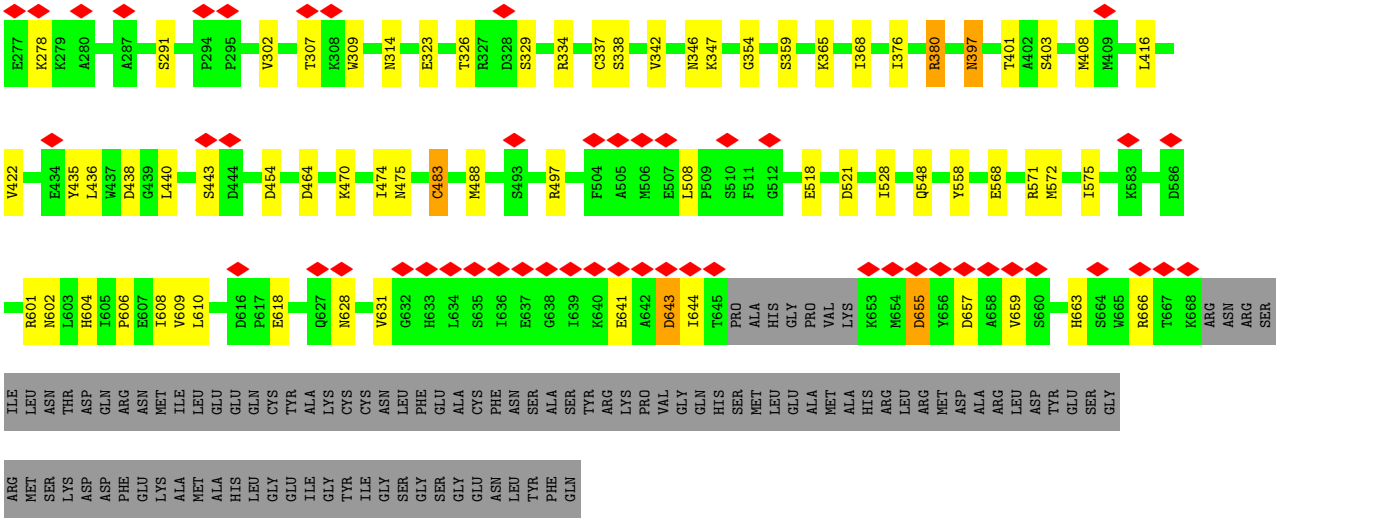
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Polymerase acidic protein

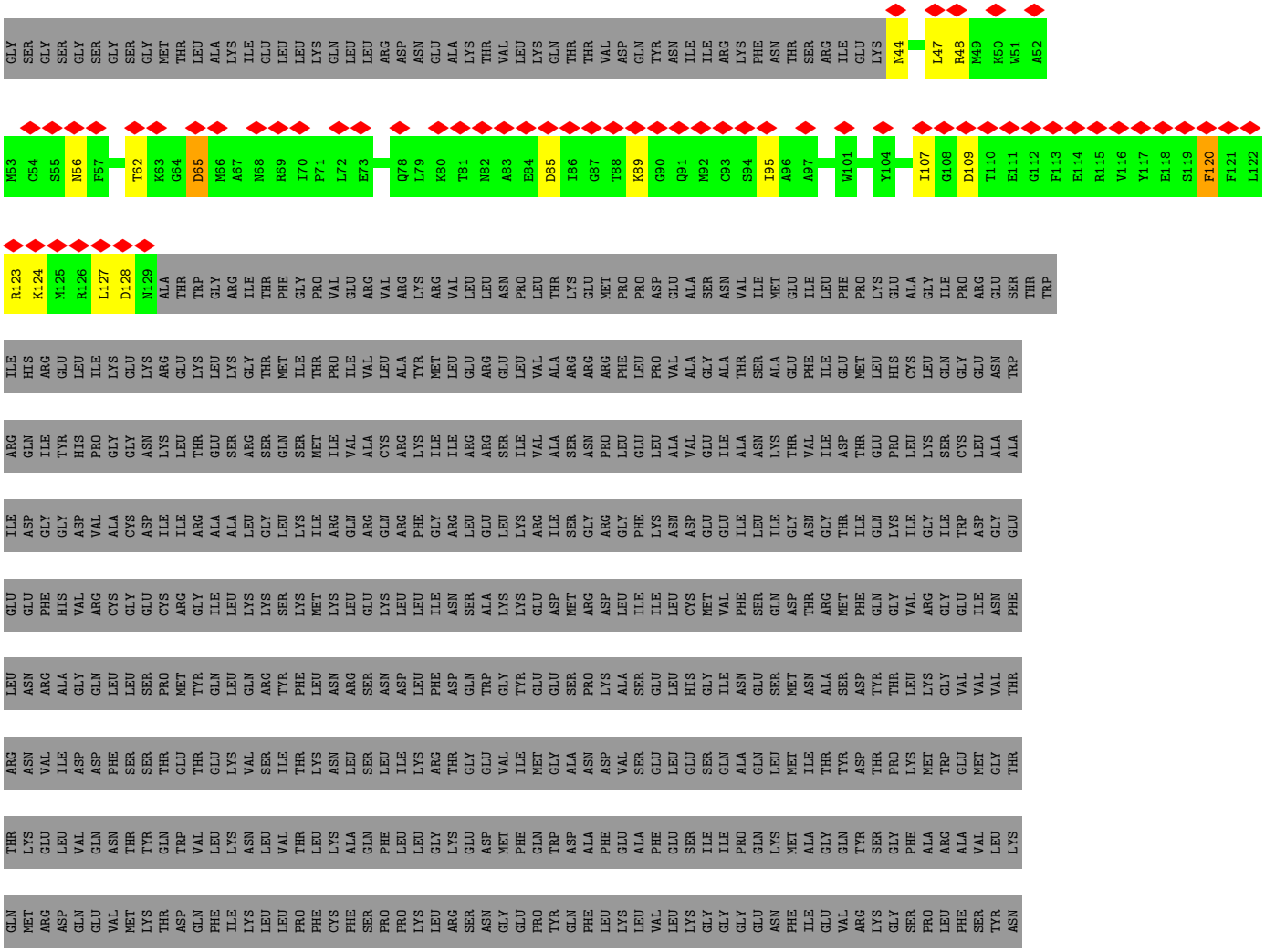


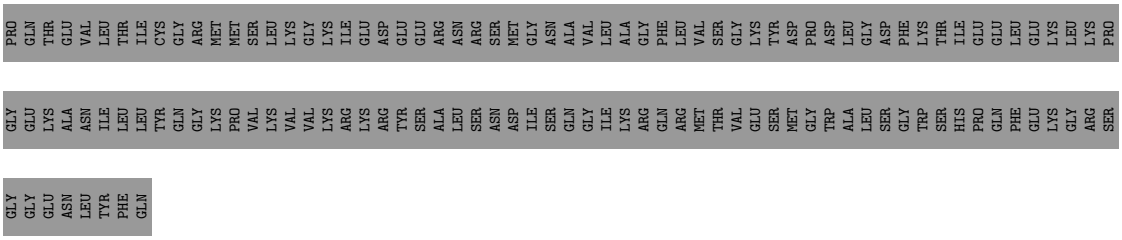
• Molecule 2: RNA-directed RNA polymerase catalytic subunit





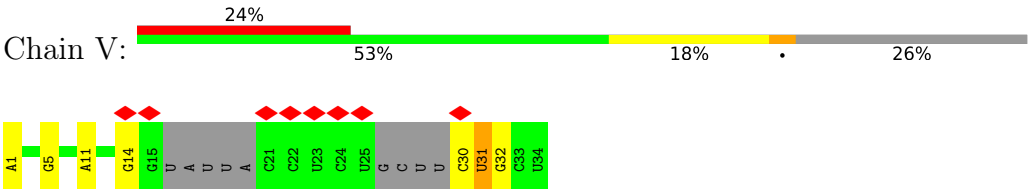
• Molecule 3: Polymerase PB2





- Molecule 4: vRNA

Chain V:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68333	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.234	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	184.90561, 184.90561, 184.90561	wwPDB
Map dimensions	176, 176, 176	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0506, 1.0506, 1.0506	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	0.44	0/4248	0.50	0/5729
2	B	0.39	0/5276	0.52	0/7119
3	C	0.29	0/704	0.47	0/949
4	V	0.82	1/593 (0.2%)	0.96	0/915
All	All	0.44	1/10821 (0.0%)	0.55	0/14712

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	1	A	OP3-P	-10.86	1.48	1.61

There are no bond angle outliers.

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	4161	0	4166	34	0
2	B	5174	0	5216	57	0
3	C	688	0	679	10	0
4	V	533	0	272	4	0
All	All	10556	0	10333	88	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 4.

All (88) 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:305:LEU:HD22	1:A:482:THR:HG21	1.47	0.95
1:A:305:LEU:HD22	1:A:482:THR:CG2	2.05	0.85
2:B:268:GLN:NE2	2:B:438:ASP:OD1	2.35	0.60
2:B:273:VAL:HG23	2:B:278:LYS:HG2	1.83	0.59
1:A:672:LYS:HE3	2:B:488:MET:HB2	1.84	0.59
1:A:395:ASN:N	1:A:395:ASN:OD1	2.36	0.59
2:B:518:GLU:OE1	2:B:663:HIS:ND1	2.37	0.58
2:B:326:THR:O	2:B:334:ARG:NH1	2.36	0.58
2:B:568:GLU:OE1	4:V:32:G:N2	2.37	0.58
2:B:609:VAL:HG11	3:C:120:PHE:HB2	1.86	0.57
2:B:604:HIS:O	3:C:123:ARG:NH1	2.38	0.57
2:B:618:GLU:HG3	3:C:107:ILE:HD11	1.87	0.56
1:A:242:ASN:ND2	2:B:87:CYS:SG	2.78	0.56
1:A:572:GLU:OE1	1:A:575:ARG:NH2	2.39	0.56
2:B:655:ASP:N	2:B:655:ASP:OD1	2.37	0.56
1:A:319:GLN:O	1:A:341:ARG:NH1	2.39	0.55
2:B:302:VAL:HG22	2:B:483:CYS:HB2	1.88	0.55
1:A:386:MET:O	2:B:380:ARG:NH1	2.39	0.55
2:B:602:ASN:N	2:B:602:ASN:OD1	2.40	0.55
2:B:521:ASP:OD2	2:B:558:TYR:OH	2.25	0.55
1:A:545:PHE:HE1	1:A:550:GLU:HG2	1.72	0.54
2:B:70:ASN:HD21	2:B:85:LEU:HB2	1.70	0.54
1:A:594:ILE:HG22	1:A:595:GLN:HG3	1.88	0.54
2:B:628:ASN:HD21	2:B:631:VAL:HG23	1.72	0.54
1:A:659:ARG:NH1	2:B:21:THR:O	2.40	0.53
2:B:342:VAL:O	2:B:346:ASN:ND2	2.39	0.53
2:B:643:ASP:OD1	2:B:643:ASP:N	2.40	0.53
1:A:472:SER:O	1:A:502:LYS:NZ	2.41	0.53
2:B:606:PRO:HG3	2:B:657:ASP:HB2	1.90	0.53
3:C:56:ASN:ND2	4:V:30:C:O2'	2.42	0.52
3:C:44:ASN:HD22	3:C:47:LEU:HG	1.74	0.52
1:A:386:MET:HG2	2:B:359:SER:HB2	1.90	0.52
2:B:470:LYS:NZ	2:B:475:ASN:OD1	2.42	0.52
3:C:85:ASP:H	3:C:89:LYS:HA	1.74	0.52
1:A:327:LYS:HA	1:A:537:THR:HG23	1.92	0.52
2:B:323:GLU:OE1	2:B:334:ARG:NH2	2.43	0.52
2:B:59:ASP:OD1	2:B:59:ASP:N	2.42	0.51
2:B:186:ASN:N	2:B:186:ASN:OD1	2.43	0.51
2:B:454:ASP:N	2:B:454:ASP:OD1	2.44	0.51
1:A:468:GLU:OE2	4:V:31:U:N3	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:ASP:OD1	3:C:65:ASP:N	2.45	0.50
2:B:266:LEU:HD13	2:B:422:VAL:HG11	1.94	0.49
1:A:280:ASN:HB3	1:A:535:LYS:HE3	1.92	0.49
1:A:372:TYR:HB2	2:B:365:LYS:HD3	1.95	0.49
1:A:666:GLN:HB2	2:B:14:ILE:HD12	1.95	0.48
2:B:309:TRP:HZ3	2:B:474:ILE:HG23	1.78	0.48
1:A:418:ALA:HB2	1:A:485:VAL:HG23	1.94	0.48
1:A:354:ASN:ND2	1:A:478:VAL:O	2.45	0.48
2:B:397:ASN:ND2	2:B:401:THR:O	2.47	0.47
2:B:608:ILE:HD12	2:B:659:VAL:HB	1.96	0.47
2:B:488:MET:HG3	2:B:497:ARG:HG3	1.97	0.46
1:A:614:THR:OG1	1:A:626:LYS:NZ	2.48	0.46
2:B:224:LEU:HD22	2:B:347:LYS:HD2	1.97	0.46
2:B:291:SER:O	2:B:291:SER:OG	2.30	0.46
2:B:571:ARG:HD2	3:C:95:ILE:HD12	1.97	0.46
3:C:124:LYS:NZ	3:C:128:ASP:OD2	2.47	0.46
2:B:127:GLN:O	2:B:249:ARG:NH2	2.48	0.45
2:B:601:ARG:HG3	3:C:127:LEU:HD11	1.98	0.45
2:B:120:ASP:N	2:B:120:ASP:OD1	2.49	0.45
1:A:222:ASN:OD1	1:A:222:ASN:N	2.49	0.45
1:A:540:ARG:NH2	1:A:552:SER:OG	2.42	0.45
1:A:512:ASP:N	1:A:512:ASP:OD1	2.49	0.45
2:B:435:TYR:OH	2:B:464:ASP:OD2	2.35	0.45
2:B:572:MET:HA	2:B:575:ILE:HB	1.98	0.44
4:V:5:G:OP2	4:V:5:G:N2	2.47	0.44
1:A:602:ALA:HA	1:A:606:GLY:HA2	1.99	0.44
1:A:422:PRO:O	2:B:548:GLN:NE2	2.50	0.44
2:B:18:ILE:O	2:B:21:THR:OG1	2.28	0.44
1:A:575:ARG:HG3	2:B:25:THR:HG22	1.99	0.44
1:A:676:VAL:HG21	1:A:679:LEU:HD13	1.98	0.44
1:A:339:LEU:HD23	1:A:339:LEU:HA	1.90	0.43
2:B:130:ASP:OD1	2:B:132:THR:OG1	2.36	0.43
1:A:522:SER:OG	1:A:523:SER:N	2.51	0.43
2:B:19:SER:HA	2:B:22:PHE:HD2	1.84	0.43
2:B:50:SER:HB2	2:B:68:PRO:HB3	2.01	0.42
1:A:526:PRO:HG3	1:A:538:VAL:HG11	2.01	0.42
1:A:502:LYS:HE3	1:A:502:LYS:HB3	1.63	0.42
2:B:338:SER:O	2:B:338:SER:OG	2.32	0.42
2:B:189:LYS:HB2	2:B:204:ILE:HD12	2.02	0.42
2:B:354:GLY:HA3	2:B:368:ILE:O	2.19	0.42
2:B:416:LEU:HD12	2:B:416:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:528:ILE:HD11	2:B:644:ILE:HG21	2.02	0.41
2:B:63:CYS:HB3	2:B:403:SER:HB2	2.02	0.41
2:B:131:TRP:HE1	2:B:146:THR:HG23	1.85	0.41
2:B:508:LEU:HD23	2:B:508:LEU:HA	1.93	0.41
1:A:302:PRO:HB2	1:A:480:PRO:HG2	2.03	0.41
1:A:567:MET:HB2	1:A:567:MET:HE3	1.91	0.40
2:B:470:LYS:HA	2:B:470:LYS:HD3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	519/751 (69%)	496 (96%)	23 (4%)	0	100	100
2	B	657/772 (85%)	614 (94%)	42 (6%)	1 (0%)	47	78
3	C	84/799 (10%)	78 (93%)	6 (7%)	0	100	100
All	All	1260/2322 (54%)	1188 (94%)	71 (6%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	443	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	461/664 (69%)	435 (94%)	26 (6%)	21	54
2	B	568/657 (86%)	539 (95%)	29 (5%)	24	57
3	C	73/694 (10%)	68 (93%)	5 (7%)	16	47
All	All	1102/2015 (55%)	1042 (95%)	60 (5%)	26	55

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	VAL
1	A	233	ILE
1	A	252	VAL
1	A	263	ARG
1	A	284	LEU
1	A	300	LYS
1	A	303	LYS
1	A	315	THR
1	A	320	THR
1	A	334	ASN
1	A	339	LEU
1	A	344	VAL
1	A	359	THR
1	A	373	GLN
1	A	395	ASN
1	A	416	LYS
1	A	424	ILE
1	A	431	VAL
1	A	437	GLU
1	A	472	SER
1	A	485	VAL
1	A	502	LYS
1	A	546	VAL
1	A	579	GLN
1	A	619	THR
1	A	684	SER
2	B	32	HIS
2	B	41	ASP
2	B	86	ASP
2	B	113	THR
2	B	114	LEU
2	B	119	VAL
2	B	132	THR
2	B	141	THR

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Mol	Chain	Res	Type
2	B	178	GLU
2	B	186	ASN
2	B	196	ARG
2	B	203	ARG
2	B	228	THR
2	B	307	THR
2	B	314	ASN
2	B	329	SER
2	B	337	CYS
2	B	376	ILE
2	B	380	ARG
2	B	397	ASN
2	B	408	MET
2	B	436	LEU
2	B	440	LEU
2	B	483	CYS
2	B	610	LEU
2	B	641	GLU
2	B	643	ASP
2	B	655	ASP
2	B	666	ARG
3	C	48	ARG
3	C	62	THR
3	C	65	ASP
3	C	109	ASP
3	C	120	PHE

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

Mol	Chain	Res	Type
1	A	467	ASN
1	A	666	GLN
2	B	47	HIS
2	B	70	ASN
2	B	104	GLN
2	B	156	ASN
2	B	268	GLN
2	B	314	ASN
2	B	367	GLN
2	B	484	ASN
2	B	548	GLN
3	C	44	ASN

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Mol	Chain	Res	Type
3	C	56	ASN
3	C	68	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	V	22/34 (64%)	3 (13%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	V	11	A
4	V	14	G
4	V	31	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

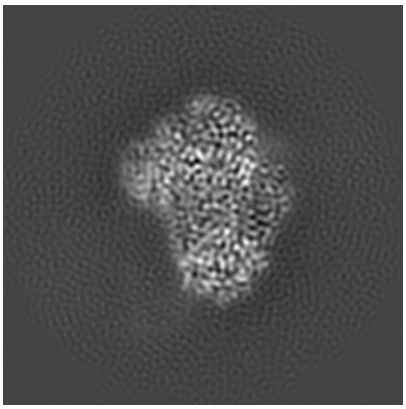
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10361. These allow visual inspection of the internal detail of the map and identification of artifacts.

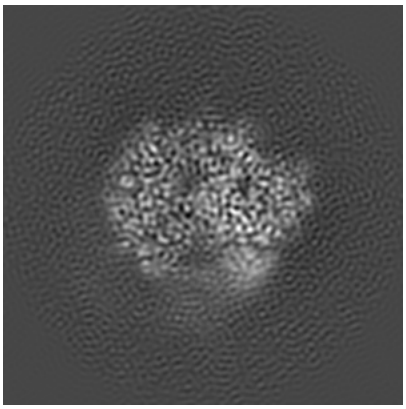
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

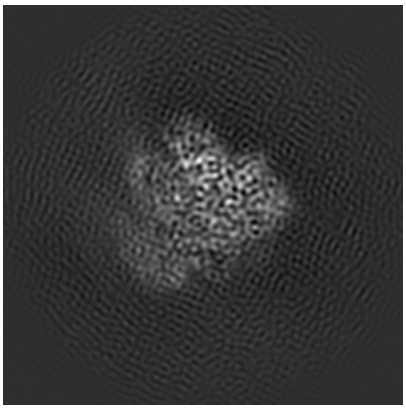
6.1.1 Primary map



X

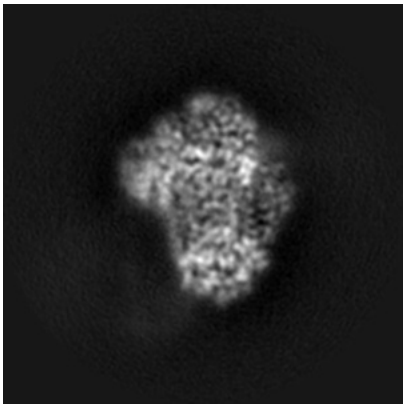


Y

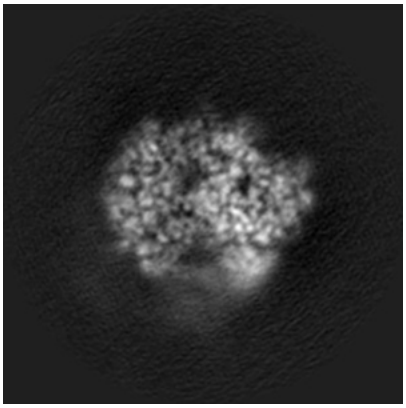


Z

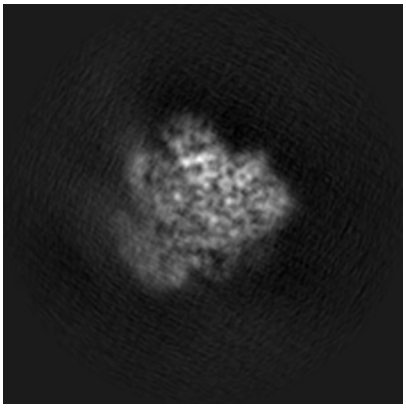
6.1.2 Raw map



X



Y

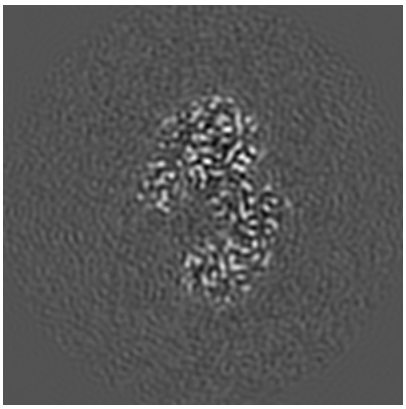


Z

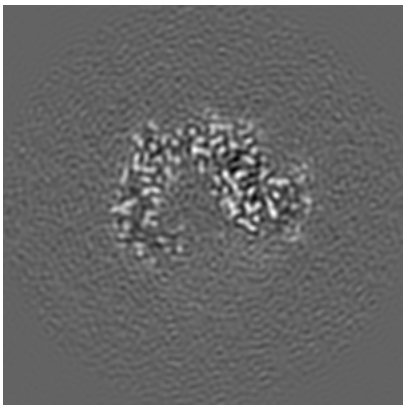
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

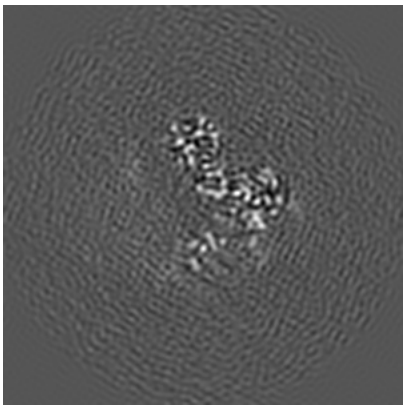
6.2.1 Primary map



X Index: 88

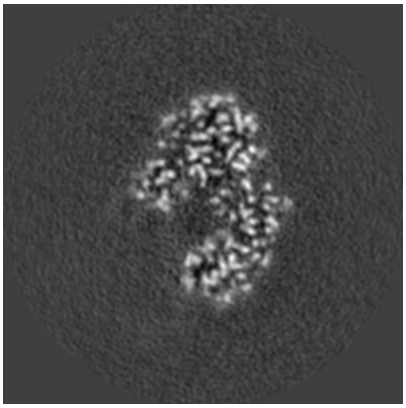


Y Index: 88

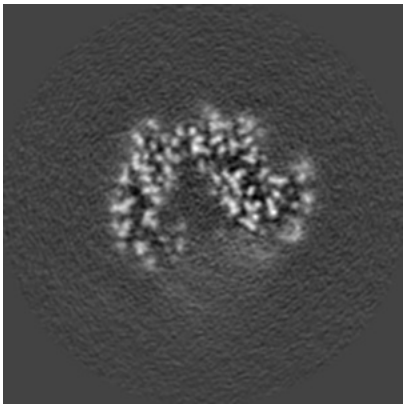


Z Index: 88

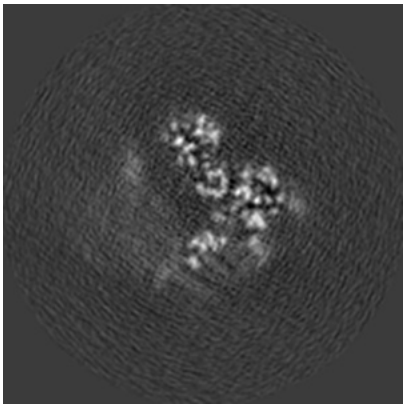
6.2.2 Raw map



X Index: 88



Y Index: 88

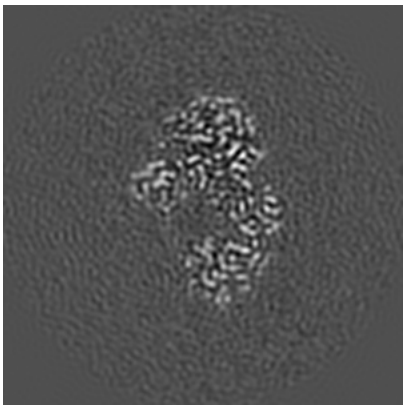


Z Index: 88

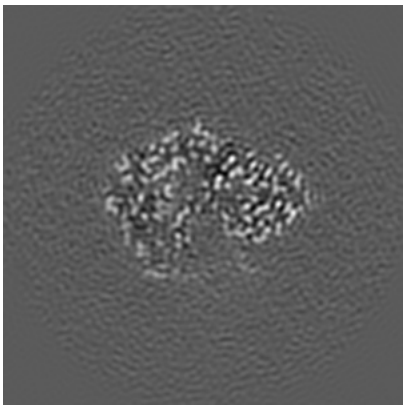
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

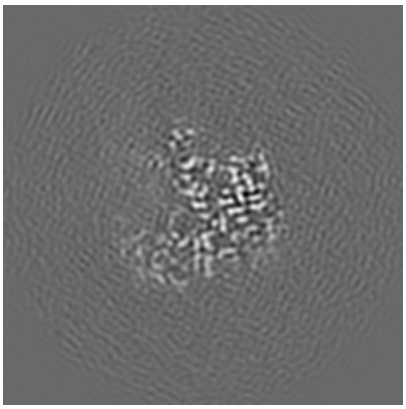
6.3.1 Primary map



X Index: 89

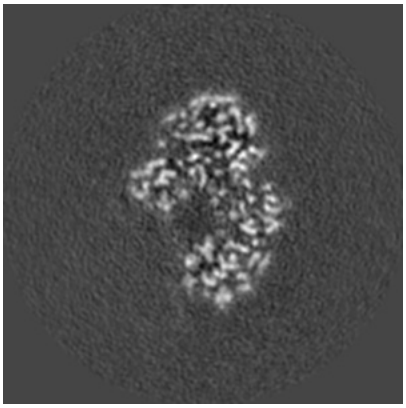


Y Index: 98

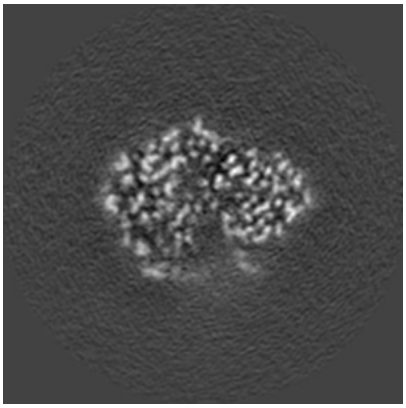


Z Index: 101

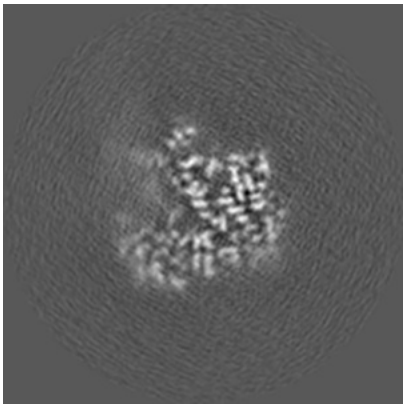
6.3.2 Raw map



X Index: 89



Y Index: 98

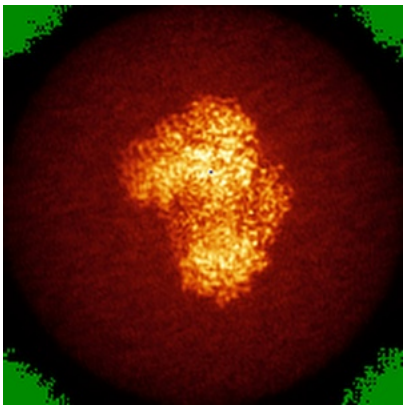


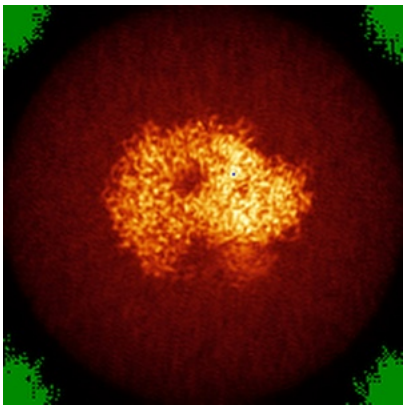
Z Index: 101

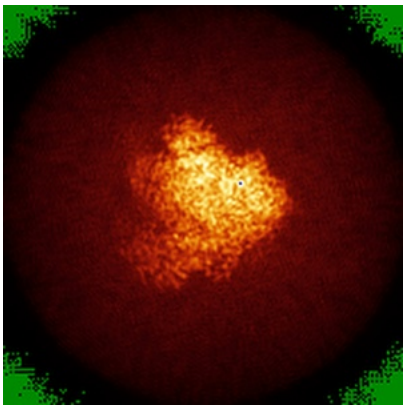
The images above show the largest variance slices of the map in three orthogonal directions.

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

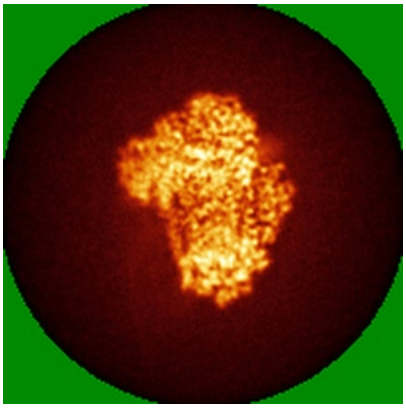
6.4.1 Primary map

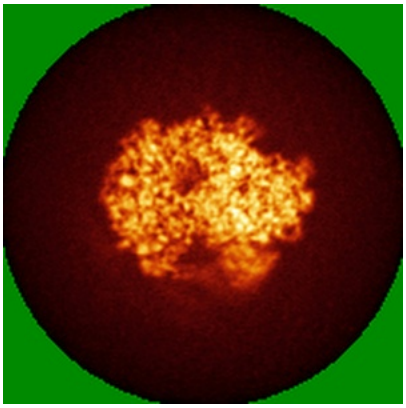

X

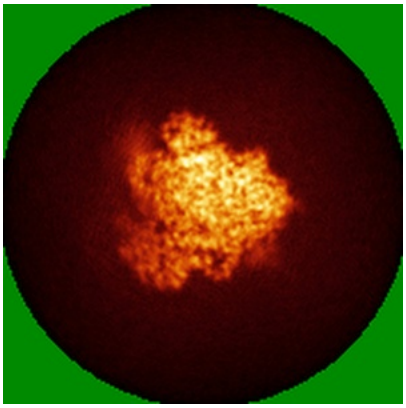

Y


Z

6.4.2 Raw map


X


Y


Z

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

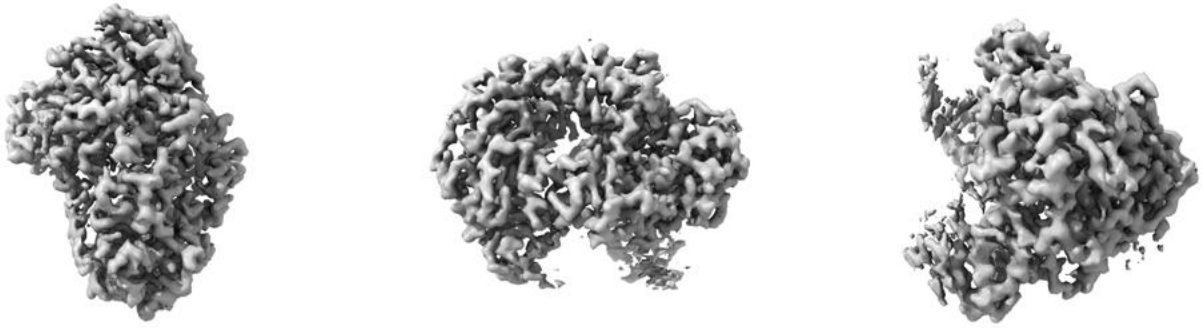
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

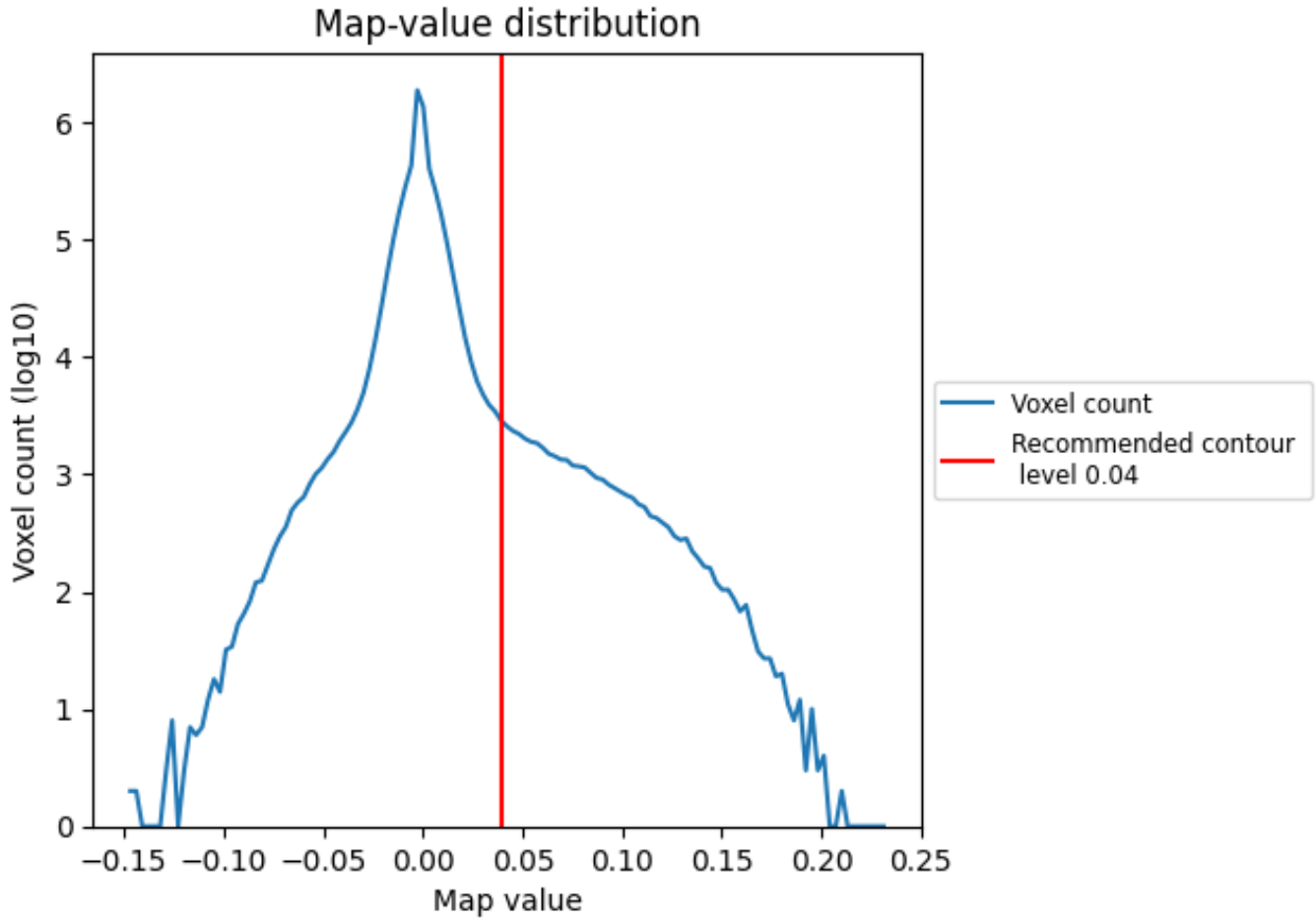
6.6 Mask visualisation (i)

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

7 Map analysis

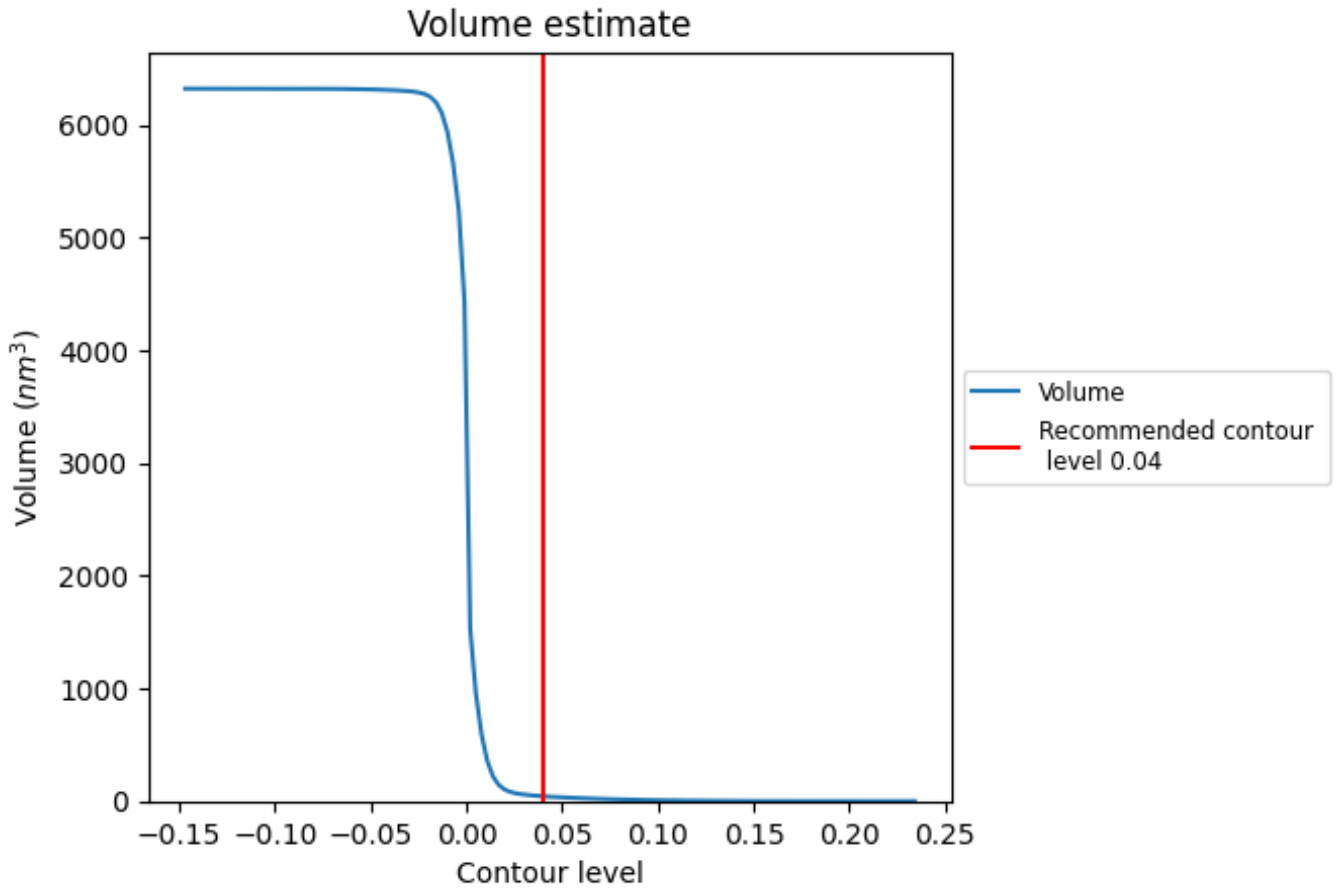
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

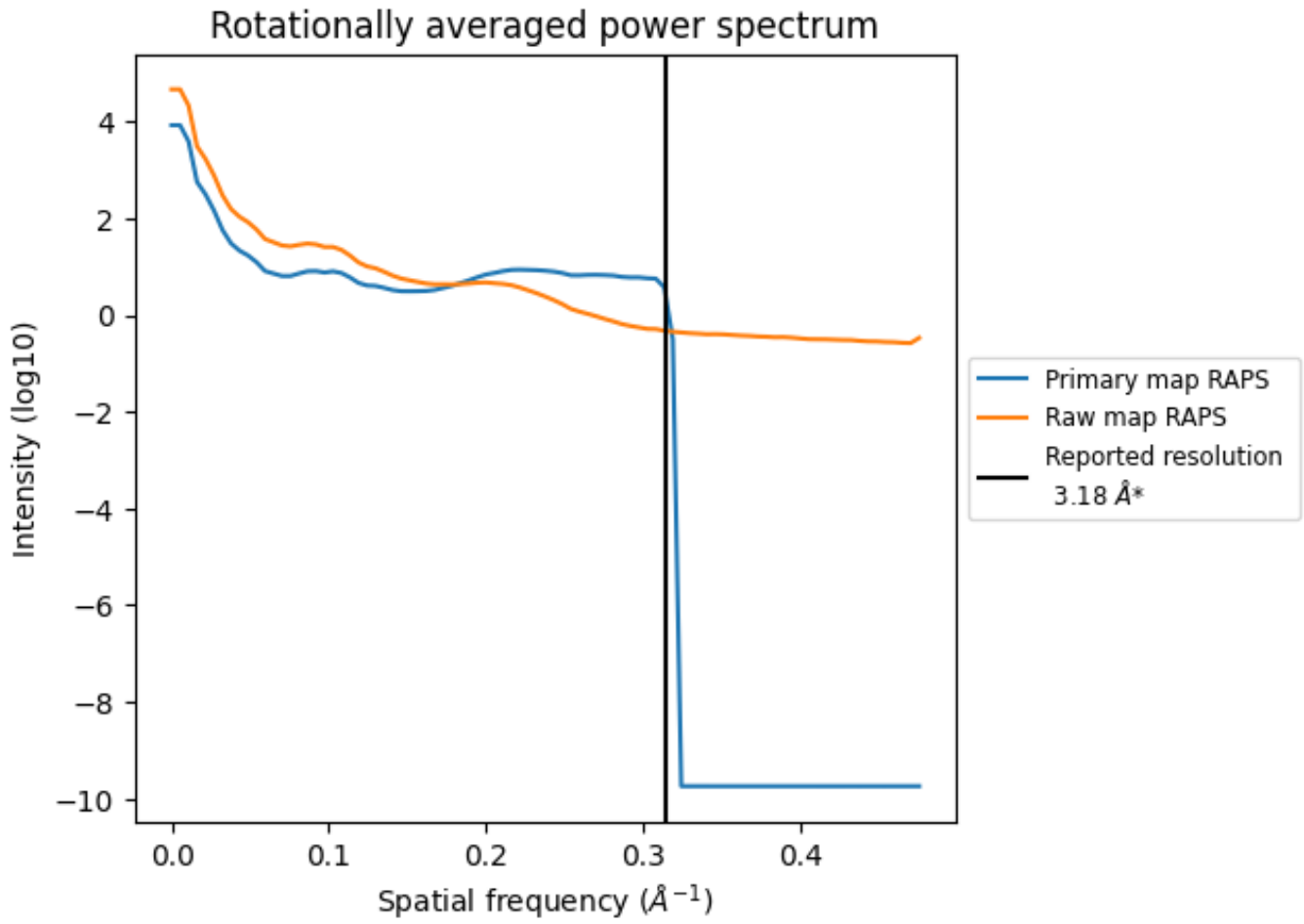
7.2 Volume estimate



The volume at the recommended contour level is 43 nm^3; this corresponds to an approximate mass of 39 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

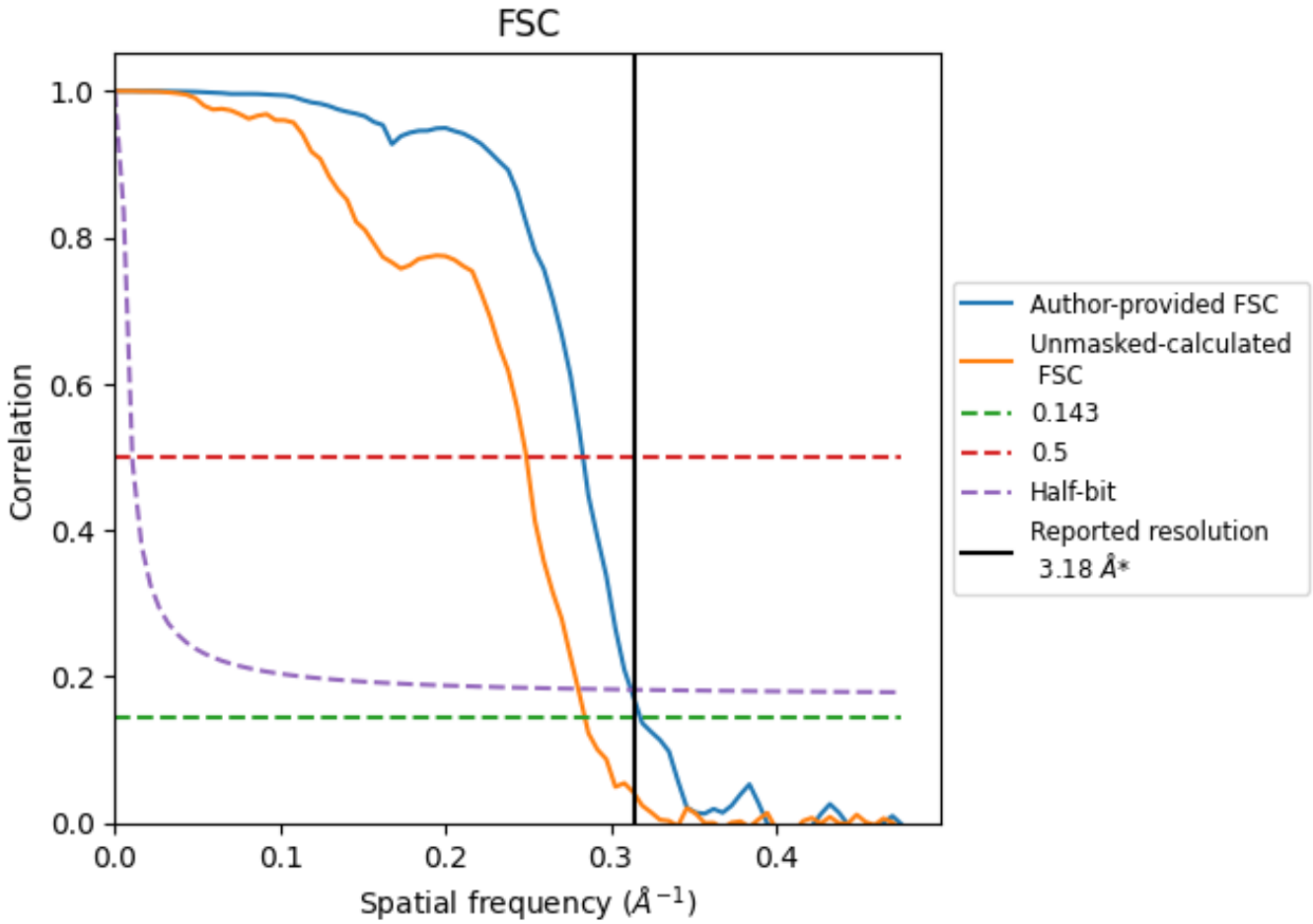


*Reported resolution corresponds to spatial frequency of 0.314 Å^{-1}

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 0.314 Å^{-1}

8.2 Resolution estimates (i)

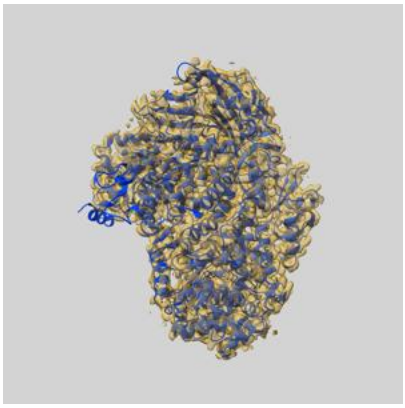
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	3.14	3.53	3.20
Unmasked-calculated*	3.51	4.02	3.57

*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 3.51 differs from the reported value 3.18 by more than 10 %

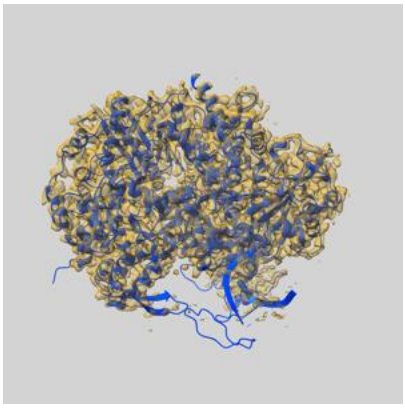
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10361 and PDB model 6T0W. Per-residue inclusion information can be found in section 3 on page 6.

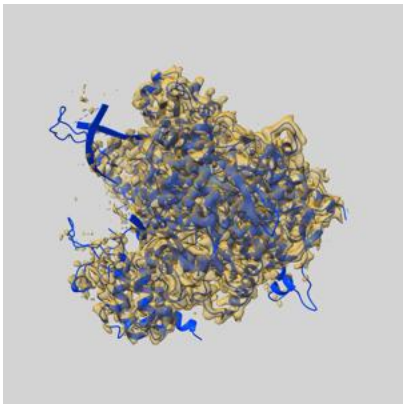
9.1 Map-model overlay



X



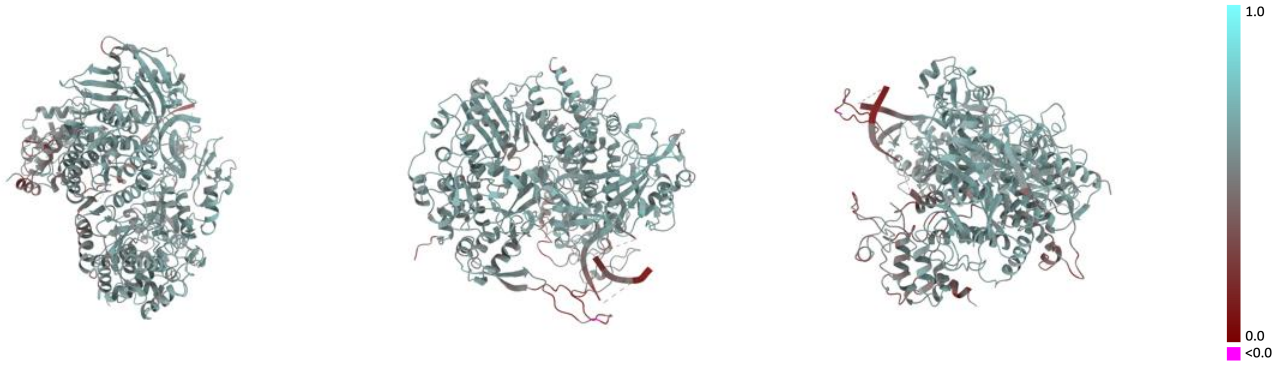
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

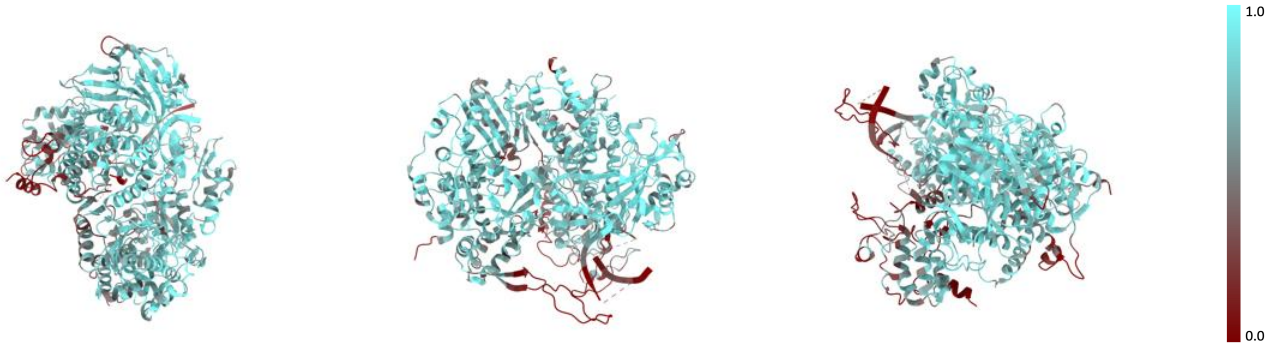
9.2 Q-score mapped to coordinate model (i)



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.

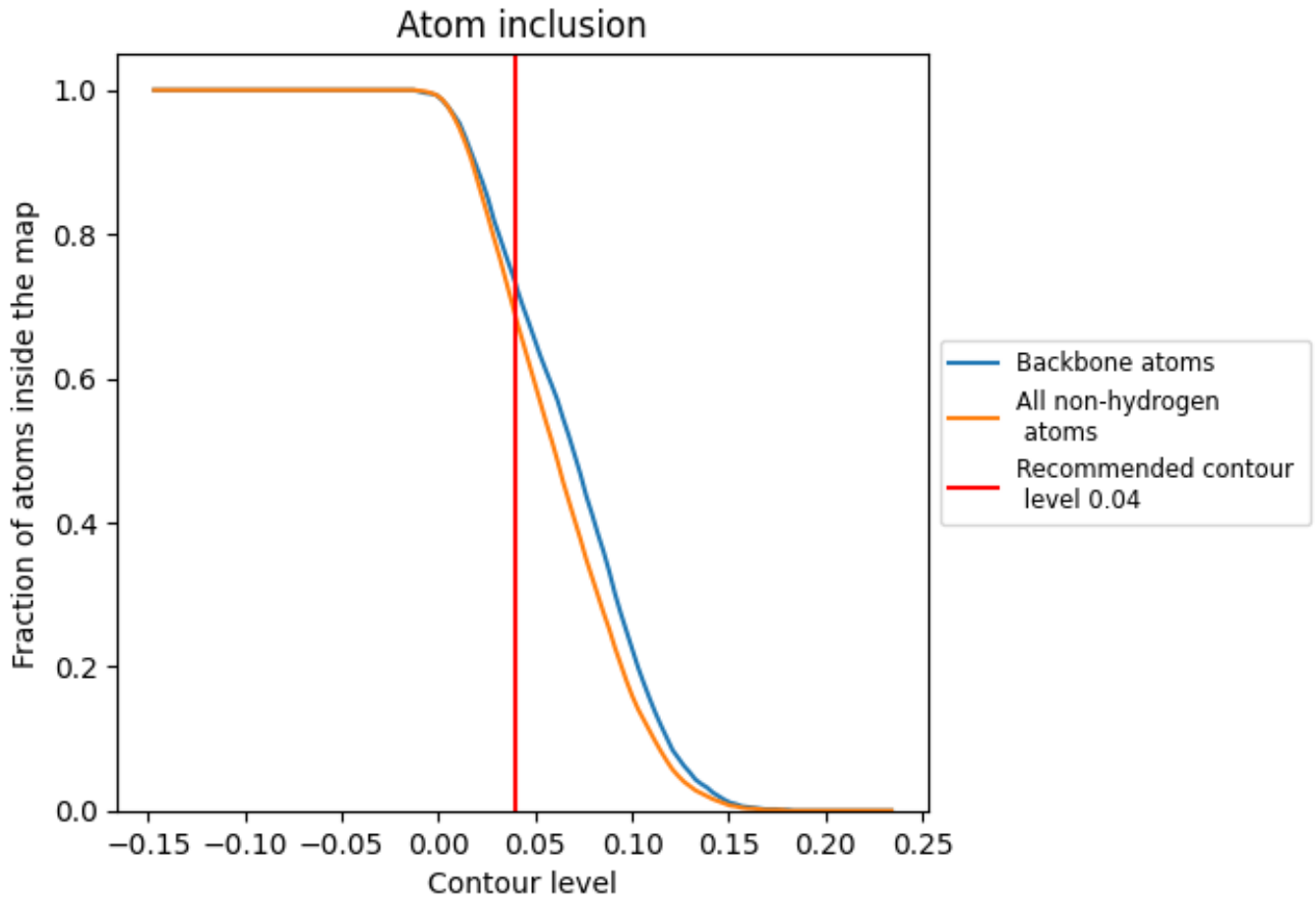
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 68% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6850	0.5460
A	0.7670	0.5750
B	0.6820	0.5460
C	0.2500	0.4180
V	0.6400	0.4900