Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 01:26 pm GMT

PDB ID	:	6QCT
EMDB ID	:	EMD-4512
Title	:	Influenza B polymerase elongation complex
Authors	:	Cusack, S.; Kouba, T.
Deposited on	:	2018-12-30
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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:

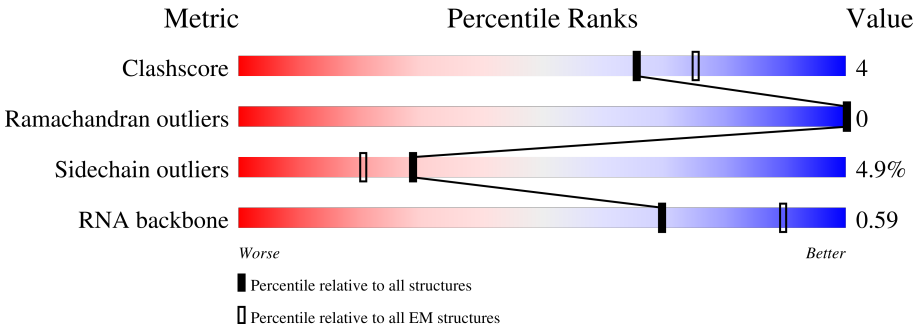
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.20 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	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	12% 83% 13%
2	B	772	82% 12% 5%
3	C	798	15% 77% 14% 9%
4	V	14	50% 29% 14% 7%
5	R	21	5% 43% 14% 5% 38%
6	M	20	5% 45% 20% 35%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18266 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
			Total	C	N	O	S		
1	A	722	5793	3679	970	1104	40	0	0

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	735	Total	C	N	O	S	0	0
			5774	3643	1001	1078	52		

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 basic protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	729	Total	C	N	O	S	0	0
			5832	3707	1021	1064	40		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP Q5V8X3
C	-7	SER	-	expression tag	UNP Q5V8X3
C	-6	GLY	-	expression tag	UNP Q5V8X3
C	-5	SER	-	expression tag	UNP Q5V8X3
C	-4	GLY	-	expression tag	UNP Q5V8X3
C	-3	SER	-	expression tag	UNP Q5V8X3
C	-2	GLY	-	expression tag	UNP Q5V8X3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP Q5V8X3
C	0	GLY	-	expression tag	UNP Q5V8X3
C	771	GLY	-	expression tag	UNP Q5V8X3
C	772	TRP	-	expression tag	UNP Q5V8X3
C	773	SER	-	expression tag	UNP Q5V8X3
C	774	HIS	-	expression tag	UNP Q5V8X3
C	775	PRO	-	expression tag	UNP Q5V8X3
C	776	GLN	-	expression tag	UNP Q5V8X3
C	777	PHE	-	expression tag	UNP Q5V8X3
C	778	GLU	-	expression tag	UNP Q5V8X3
C	779	LYS	-	expression tag	UNP Q5V8X3
C	780	GLY	-	expression tag	UNP Q5V8X3
C	781	SER	-	expression tag	UNP Q5V8X3
C	782	GLY	-	expression tag	UNP Q5V8X3
C	783	SER	-	expression tag	UNP Q5V8X3
C	784	GLU	-	expression tag	UNP Q5V8X3
C	785	ASN	-	expression tag	UNP Q5V8X3
C	786	LEU	-	expression tag	UNP Q5V8X3
C	787	TYR	-	expression tag	UNP Q5V8X3
C	788	PHE	-	expression tag	UNP Q5V8X3
C	789	GLN	-	expression tag	UNP Q5V8X3

- Molecule 4 is a RNA chain called 5 end.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	13	Total	C	N	O	P	0	0
			284	127	57	87	13		

- Molecule 5 is a RNA chain called 3 end.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	13	Total	C	N	O	P	0	0
			268	120	39	96	13		

- Molecule 6 is a RNA chain called capped RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	13	Total	C	N	O	P	0	0
			313	138	62	98	15		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

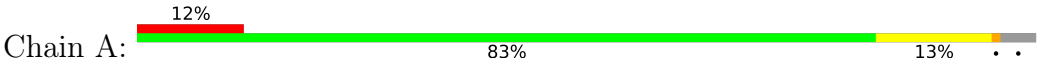
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total Mg 1 1	0
7	B	1	Total Mg 1 1	0

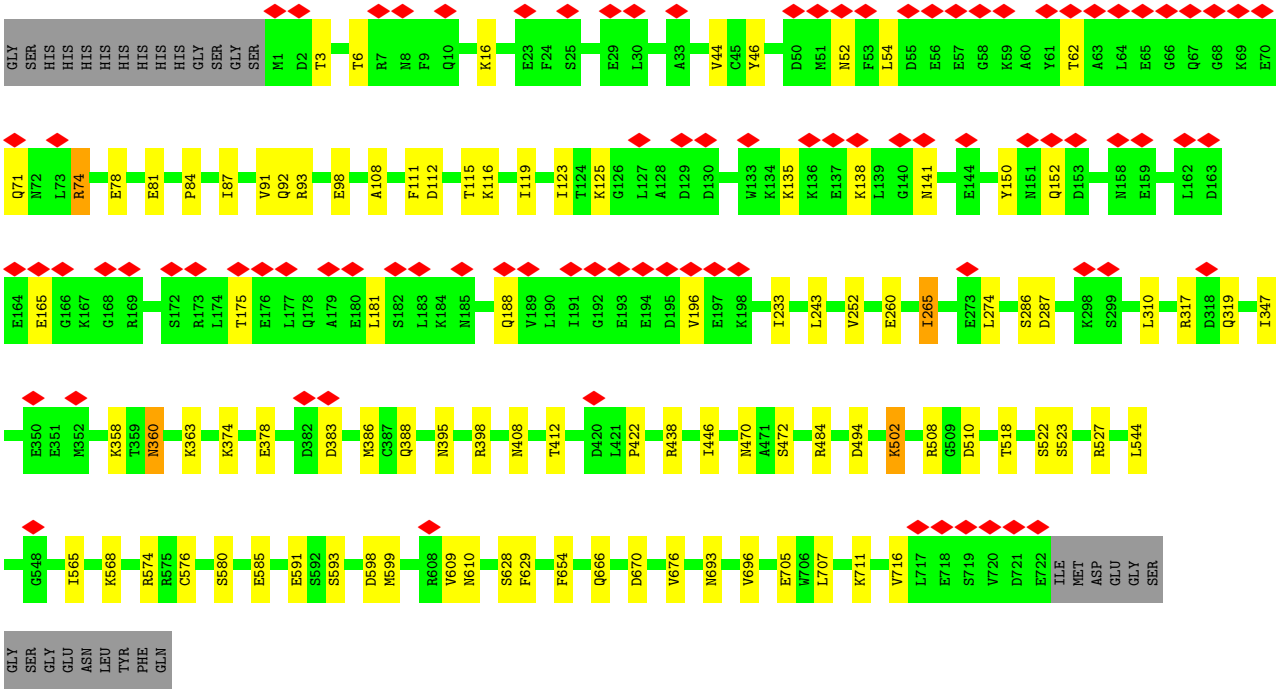
3 Residue-property plots (i)

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

• Molecule 1: Polymerase acidic protein

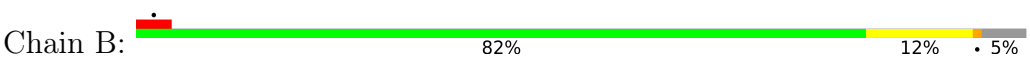
Chain A:

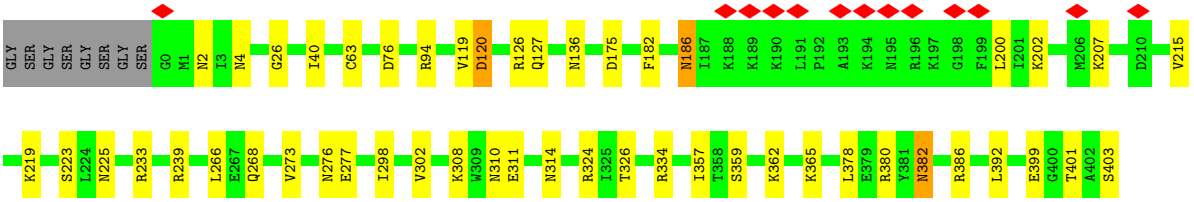


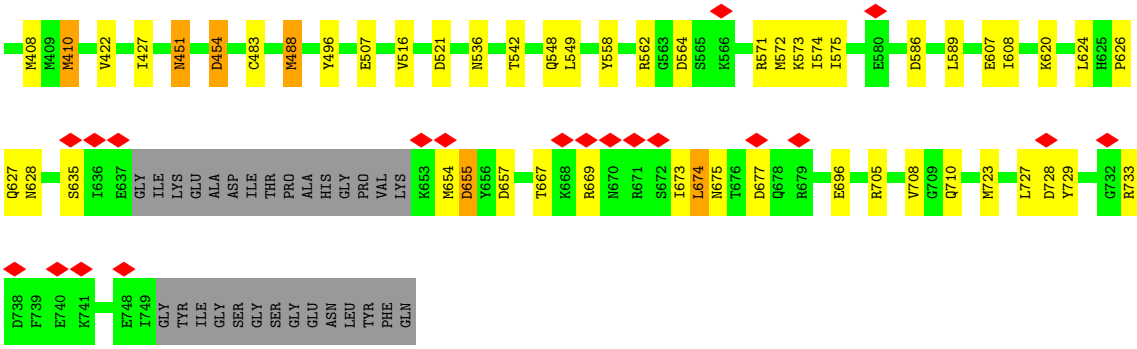


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain B:

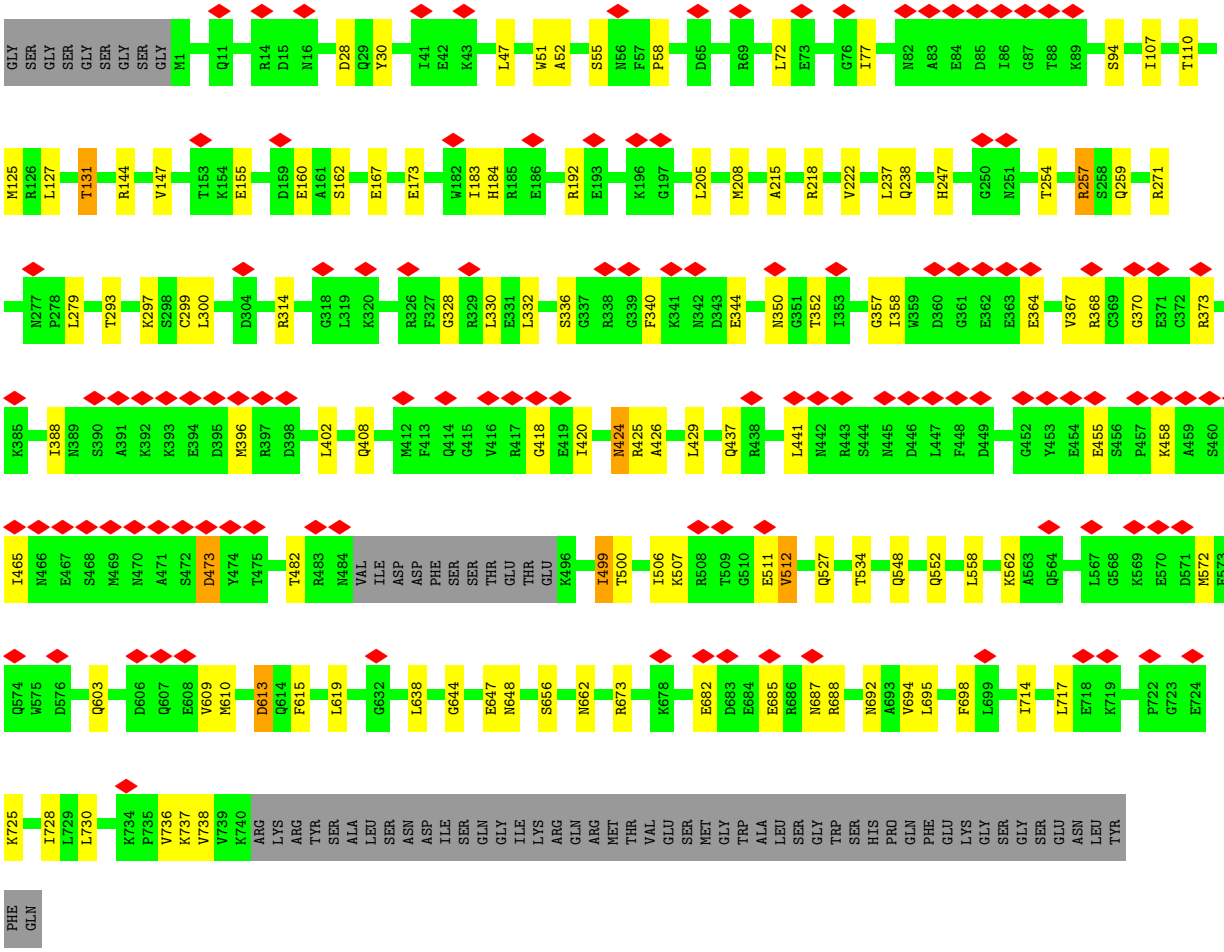






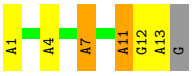
• Molecule 3: Polymerase basic protein 2

Chain C:



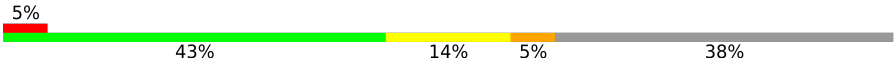
• Molecule 4: 5 end

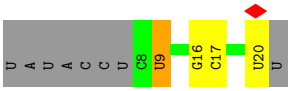
Chain V:



• Molecule 5: 3 end

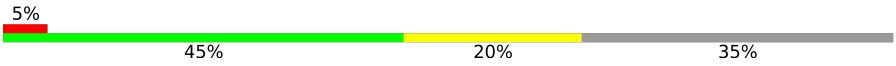
Chain R:





• Molecule 6: capped RNA

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34000	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 ($e^-/Å^2$)	22	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	0.695	Depositor
Minimum map value	-0.222	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	259.3032, 259.3032, 259.3032	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8311, 0.8311, 0.8311	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTG, 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	0.34	0/5910	0.48	0/7970
2	B	0.35	0/5886	0.50	0/7932
3	C	0.31	0/5932	0.49	0/7973
4	V	0.89	1/319 (0.3%)	1.07	1/494 (0.2%)
5	R	0.62	0/296	1.01	1/457 (0.2%)
6	M	0.61	0/292	0.94	0/451
All	All	0.36	1/18635 (0.0%)	0.53	2/25277 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	1	A	OP3-P	-10.79	1.48	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	17	C	C6-N1-C2	-5.56	118.08	120.30
4	V	7	A	O4'-C1'-N9	5.07	112.25	108.20

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	5793	0	5765	49	0
2	B	5774	0	5792	65	0
3	C	5832	0	5995	59	0
4	V	284	0	142	2	0
5	R	268	0	138	2	0
6	M	313	0	158	2	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
All	All	18266	0	17990	148	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 (148) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:488:MET:HA	2:B:496:TYR:O	1.99	0.63
3:C:694:VAL:HG12	3:C:695:LEU:HG	1.80	0.63
1:A:386:MET:HG2	2:B:359:SER:HB2	1.82	0.62
1:A:568:LYS:HB2	3:C:47:LEU:HD13	1.82	0.61
2:B:63:CYS:HB3	2:B:403:SER:HB2	1.83	0.60
1:A:78:GLU:HB2	1:A:111:PHE:HB3	1.84	0.60
1:A:91:VAL:HG22	2:B:723:MET:HG3	1.84	0.58
1:A:54:LEU:HB2	1:A:74:ARG:HG3	1.85	0.58
1:A:274:LEU:O	1:A:398:ARG:NH1	2.37	0.58
1:A:693:ASN:HD22	1:A:696:VAL:H	1.50	0.58
3:C:613:ASP:OD1	3:C:613:ASP:N	2.34	0.58
1:A:438:ARG:NH2	1:A:598:ASP:OD1	2.36	0.58
3:C:609:VAL:HG11	3:C:692:ASN:HD22	1.68	0.58
3:C:638:LEU:HG	3:C:714:ILE:HD11	1.84	0.58
1:A:383:ASP:O	2:B:380:ARG:NH1	2.36	0.57
1:A:16:LYS:NZ	1:A:46:TYR:OH	2.38	0.57
1:A:422:PRO:O	2:B:548:GLN:NE2	2.37	0.57
3:C:507:LYS:HD2	3:C:511:GLU:HG3	1.86	0.57
3:C:205:LEU:HA	3:C:208:MET:HG2	1.86	0.57
2:B:675:ASN:ND2	4:V:12:G:O2'	2.39	0.56
2:B:326:THR:O	2:B:334:ARG:NH1	2.36	0.56
1:A:470:ASN:ND2	3:C:51:TRP:O	2.40	0.55
3:C:155:GLU:HG3	3:C:215:ALA:HB2	1.89	0.55
1:A:508:ARG:NH2	4:V:11:A:N3	2.54	0.55
1:A:705:GLU:OE1	2:B:4:ASN:ND2	2.40	0.55
2:B:454:ASP:N	2:B:454:ASP:OD1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:610:MET:H	3:C:688:ARG:HH11	1.55	0.55
2:B:120:ASP:N	2:B:120:ASP:OD1	2.40	0.55
3:C:603:GLN:NE2	3:C:692:ASN:O	2.39	0.55
2:B:382:ASN:OD1	2:B:382:ASN:N	2.36	0.54
2:B:620:LYS:HG2	3:C:110:THR:HG21	1.89	0.54
2:B:729:TYR:HE1	2:B:736:LYS:HG2	1.73	0.54
2:B:710:GLN:NE2	3:C:28:ASP:OD2	2.40	0.54
3:C:160:GLU:OE2	3:C:184:HIS:NE2	2.38	0.54
2:B:705:ARG:NH1	3:C:162:SER:OG	2.40	0.54
3:C:218:ARG:NH1	5:R:16:G:OP2	2.41	0.54
3:C:328:GLY:HA3	3:C:437:GLN:HE22	1.72	0.54
3:C:344:GLU:HB2	3:C:358:ILE:HD13	1.90	0.53
2:B:310:ASN:ND2	2:B:408:MET:O	2.41	0.53
6:M:1:GTG:H8B	6:M:1:GTG:H5B1	1.90	0.53
2:B:410:MET:SD	2:B:410:MET:N	2.72	0.53
1:A:666:GLN:NE2	1:A:670:ASP:OD1	2.41	0.53
1:A:585:GLU:OE1	2:B:542:THR:OG1	2.27	0.53
3:C:644:GLY:O	3:C:648:ASN:ND2	2.43	0.52
1:A:508:ARG:HD3	2:B:674:LEU:HD13	1.91	0.52
1:A:388:GLN:NE2	2:B:382:ASN:OD1	2.42	0.52
1:A:52:ASN:ND2	1:A:62:THR:OG1	2.43	0.52
2:B:507:GLU:OE1	2:B:536:ASN:ND2	2.41	0.52
1:A:92:GLN:HE22	1:A:108:ALA:H	1.57	0.51
3:C:300:LEU:HD22	3:C:314:ARG:HG3	1.93	0.51
1:A:360:ASN:N	1:A:360:ASN:OD1	2.42	0.51
2:B:26:GLY:O	2:B:233:ARG:NH2	2.43	0.51
3:C:167:GLU:O	3:C:192:ARG:NH2	2.43	0.51
3:C:455:GLU:OE1	3:C:458:LYS:NZ	2.42	0.51
2:B:298:ILE:HD13	2:B:454:ASP:HA	1.93	0.50
2:B:608:ILE:HG21	2:B:624:LEU:HD21	1.93	0.50
3:C:279:LEU:HD13	3:C:499:ILE:HD12	1.92	0.50
3:C:695:LEU:HB2	3:C:698:PHE:HB2	1.94	0.50
3:C:330:LEU:HD11	3:C:367:VAL:HB	1.93	0.50
2:B:302:VAL:HG22	2:B:483:CYS:HB2	1.93	0.50
1:A:112:ASP:HB2	1:A:119:ILE:HD11	1.94	0.49
1:A:374:LYS:HE3	2:B:365:LYS:HE3	1.94	0.49
1:A:599:MET:SD	1:A:610:ASN:ND2	2.85	0.49
2:B:572:MET:HA	2:B:575:ILE:HB	1.95	0.49
2:B:521:ASP:OD2	2:B:558:TYR:OH	2.26	0.49
1:A:408:ASN:HD21	2:B:2:ASN:HA	1.76	0.49
2:B:202:LYS:HE2	2:B:677:ASP:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLN:OE1	1:A:175:THR:OG1	2.30	0.48
1:A:141:ASN:OD1	1:A:141:ASN:N	2.46	0.48
1:A:502:LYS:HB3	1:A:502:LYS:HE3	1.63	0.48
1:A:310:LEU:HB3	1:A:317:ARG:HD3	1.94	0.48
1:A:388:GLN:HB2	2:B:357:ILE:HG22	1.95	0.48
1:A:707:LEU:HG	1:A:711:LYS:HE3	1.96	0.48
3:C:350:ASN:ND2	3:C:418:GLY:O	2.47	0.48
1:A:574:ARG:HB3	2:B:549:LEU:HD22	1.96	0.48
3:C:615:PHE:O	3:C:619:LEU:HB2	2.14	0.48
2:B:728:ASP:OD1	2:B:733:ARG:NH1	2.47	0.47
3:C:332:LEU:HD23	3:C:367:VAL:HG12	1.96	0.47
3:C:368:ARG:NH1	3:C:370:GLY:O	2.40	0.47
3:C:388:ILE:HD12	3:C:396:MET:HG2	1.96	0.47
1:A:84:PRO:HD2	1:A:87:ILE:HD12	1.97	0.47
2:B:378:LEU:HB3	2:B:386:ARG:HG3	1.97	0.47
2:B:451:ASN:OD1	2:B:451:ASN:N	2.46	0.47
2:B:40:ILE:HG23	2:B:392:LEU:HD13	1.97	0.46
3:C:147:VAL:HG11	3:C:222:VAL:HG11	1.97	0.46
1:A:125:LYS:HG2	1:A:150:TYR:HE2	1.79	0.46
1:A:628:SER:OG	1:A:629:PHE:N	2.47	0.46
2:B:586:ASP:N	2:B:586:ASP:OD1	2.43	0.46
3:C:548:GLN:OE1	3:C:673:ARG:NH1	2.49	0.46
2:B:589:LEU:HD22	2:B:607:GLU:HG2	1.97	0.46
2:B:268:GLN:HG3	2:B:422:VAL:HG13	1.98	0.46
3:C:506:ILE:HG22	3:C:512:VAL:HG12	1.96	0.46
1:A:510:ASP:HB3	1:A:565:ILE:HD11	1.97	0.45
3:C:297:LYS:H	3:C:297:LYS:HG2	1.51	0.45
3:C:682:GLU:HB2	3:C:685:GLU:HG3	1.98	0.45
1:A:98:GLU:HG2	2:B:727:LEU:HD22	1.98	0.45
2:B:127:GLN:HG3	5:R:9:U:H5'	1.98	0.45
3:C:58:PRO:HD2	3:C:94:SER:HA	1.99	0.45
2:B:126:ARG:NH1	6:M:15:C:OP2	2.49	0.45
3:C:131:THR:HG23	3:C:247:HIS:HB2	1.98	0.45
1:A:522:SER:OG	1:A:523:SER:N	2.50	0.45
1:A:568:LYS:HD2	3:C:47:LEU:HB2	1.99	0.45
2:B:94:ARG:NH2	2:B:427:ILE:O	2.50	0.45
3:C:473:ASP:N	3:C:473:ASP:OD1	2.49	0.45
2:B:635:SER:HB3	2:B:655:ASP:HB3	1.98	0.44
3:C:254:THR:HG22	3:C:257:ARG:HH12	1.82	0.44
1:A:135:LYS:HD3	1:A:138:LYS:HE3	1.99	0.44
1:A:472:SER:O	1:A:502:LYS:NZ	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:ASP:N	2:B:76:ASP:OD1	2.48	0.44
2:B:573:LYS:HD3	3:C:77:ILE:HD11	2.00	0.44
2:B:696:GLU:OE2	3:C:30:TYR:OH	2.33	0.44
2:B:276:ASN:HB3	3:C:144:ARG:HG2	1.99	0.44
3:C:725:LYS:HD3	3:C:737:LYS:HE3	1.99	0.44
3:C:424:ASN:HD22	3:C:425:ARG:H	1.66	0.44
2:B:266:LEU:HD13	2:B:422:VAL:HG11	2.00	0.43
2:B:308:LYS:HB3	2:B:311:GLU:HB2	2.01	0.43
2:B:219:LYS:O	2:B:223:SER:OG	2.31	0.43
2:B:562:ARG:NH2	2:B:564:ASP:OD2	2.52	0.43
1:A:358:LYS:HB3	1:A:363:LYS:HE3	2.00	0.43
1:A:74:ARG:H	1:A:74:ARG:HG2	1.69	0.42
2:B:626:PRO:HB3	2:B:657:ASP:HB3	2.00	0.42
2:B:627:GLN:HE21	2:B:627:GLN:HB3	1.64	0.42
3:C:558:LEU:O	3:C:562:LYS:HB2	2.20	0.42
3:C:336:SER:OG	3:C:364:GLU:OE1	2.38	0.42
1:A:438:ARG:HD3	1:A:585:GLU:HG3	2.00	0.42
3:C:717:LEU:HD11	3:C:728:ILE:HD11	2.01	0.42
2:B:558:TYR:O	2:B:571:ARG:NH1	2.53	0.42
1:A:44:VAL:HG11	1:A:123:ILE:HD11	2.02	0.42
1:A:93:ARG:NH2	3:C:167:GLU:OE2	2.53	0.42
2:B:200:LEU:HD12	2:B:200:LEU:HA	1.92	0.42
2:B:182:PHE:HB3	2:B:207:LYS:HE2	2.01	0.41
3:C:548:GLN:HE21	3:C:552:GLN:NE2	2.19	0.41
2:B:277:GLU:HG3	3:C:426:ALA:HB2	2.01	0.41
2:B:628:ASN:OD1	2:B:628:ASN:N	2.49	0.41
3:C:52:ALA:O	3:C:55:SER:OG	2.37	0.41
1:A:112:ASP:O	1:A:116:LYS:N	2.53	0.41
3:C:330:LEU:HB2	3:C:402:LEU:HD13	2.03	0.41
3:C:357:GLY:O	3:C:408:GLN:NE2	2.46	0.41
1:A:265:ILE:HD11	1:A:654:PHE:HE1	1.85	0.41
2:B:399:GLU:OE2	2:B:401:THR:OG1	2.39	0.41
3:C:183:ILE:H	3:C:183:ILE:HG12	1.70	0.41
2:B:136:ASN:OD1	2:B:225:ASN:ND2	2.40	0.41
2:B:496:TYR:OH	3:C:647:GLU:OE2	2.38	0.40
2:B:624:LEU:HB2	3:C:110:THR:HG22	2.04	0.40
3:C:725:LYS:HA	3:C:738:VAL:O	2.21	0.40
3:C:694:VAL:HG21	3:C:730:LEU:HD22	2.03	0.40
1:A:576:CYS:O	1:A:580:SER:OG	2.33	0.40
2:B:186:ASN:OD1	2:B:186:ASN:N	2.54	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	720/751 (96%)	686 (95%)	34 (5%)	0	100	100
2	B	731/772 (95%)	706 (97%)	25 (3%)	0	100	100
3	C	725/798 (91%)	675 (93%)	50 (7%)	0	100	100
All	All	2176/2321 (94%)	2067 (95%)	109 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	641/664 (96%)	606 (94%)	35 (6%)	21	57
2	B	632/657 (96%)	608 (96%)	24 (4%)	33	67
3	C	636/694 (92%)	602 (95%)	34 (5%)	22	58
All	All	1909/2015 (95%)	1816 (95%)	93 (5%)	29	61

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	6	THR
1	A	71	GLN
1	A	74	ARG
1	A	81	GLU

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Mol	Chain	Res	Type
1	A	115	THR
1	A	165	GLU
1	A	181	LEU
1	A	188	GLN
1	A	196	VAL
1	A	233	ILE
1	A	243	LEU
1	A	252	VAL
1	A	260	GLU
1	A	265	ILE
1	A	286	SER
1	A	287	ASP
1	A	319	GLN
1	A	347	ILE
1	A	360	ASN
1	A	378	GLU
1	A	395	ASN
1	A	412	THR
1	A	446	ILE
1	A	484	ARG
1	A	494	ASP
1	A	502	LYS
1	A	518	THR
1	A	527	ARG
1	A	544	LEU
1	A	591	GLU
1	A	593	SER
1	A	609	VAL
1	A	676	VAL
1	A	716	VAL
2	B	119	VAL
2	B	120	ASP
2	B	175	ASP
2	B	186	ASN
2	B	215	VAL
2	B	239	ARG
2	B	273	VAL
2	B	314	ASN
2	B	324	ARG
2	B	362	LYS
2	B	382	ASN
2	B	410	MET

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Mol	Chain	Res	Type
2	B	451	ASN
2	B	454	ASP
2	B	488	MET
2	B	516	VAL
2	B	574	ILE
2	B	654	MET
2	B	655	ASP
2	B	667	THR
2	B	669	ARG
2	B	673	ILE
2	B	674	LEU
2	B	708	VAL
3	C	72	LEU
3	C	107	ILE
3	C	125	MET
3	C	127	LEU
3	C	131	THR
3	C	173	GLU
3	C	237	LEU
3	C	238	GLN
3	C	257	ARG
3	C	259	GLN
3	C	271	ARG
3	C	293	THR
3	C	299	CYS
3	C	340	PHE
3	C	352	THR
3	C	373	ARG
3	C	420	ILE
3	C	424	ASN
3	C	429	LEU
3	C	441	LEU
3	C	465	ILE
3	C	473	ASP
3	C	482	THR
3	C	499	ILE
3	C	500	THR
3	C	512	VAL
3	C	527	GLN
3	C	534	THR
3	C	572	MET
3	C	613	ASP

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Mol	Chain	Res	Type
3	C	656	SER
3	C	662	ASN
3	C	687	ASN
3	C	736	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	92	GLN
1	A	222	ASN
1	A	319	GLN
1	A	357	GLN
1	A	388	GLN
1	A	462	HIS
1	A	470	ASN
1	A	566	GLN
1	A	610	ASN
1	A	693	ASN
2	B	47	HIS
2	B	310	ASN
2	B	346	ASN
2	B	475	ASN
2	B	531	ASN
2	B	613	ASN
2	B	627	GLN
2	B	675	ASN
2	B	680	ASN
2	B	710	GLN
3	C	259	GLN
3	C	323	GLN
3	C	389	ASN
3	C	424	ASN
3	C	437	GLN
3	C	442	ASN
3	C	502	ASN
3	C	552	GLN
3	C	587	GLN
3	C	614	GLN
3	C	662	ASN
3	C	727	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	V	12/14 (85%)	4 (33%)	0
5	R	12/21 (57%)	2 (16%)	0
6	M	10/20 (50%)	2 (20%)	0
All	All	34/55 (61%)	8 (23%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	V	4	A
4	V	7	A
4	V	11	A
4	V	13	A
5	R	9	U
5	R	20	U
6	M	4	U
6	M	13	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

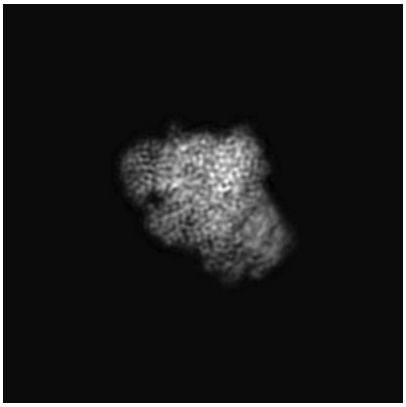
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4512. These allow visual inspection of the internal detail of the map and identification of artifacts.

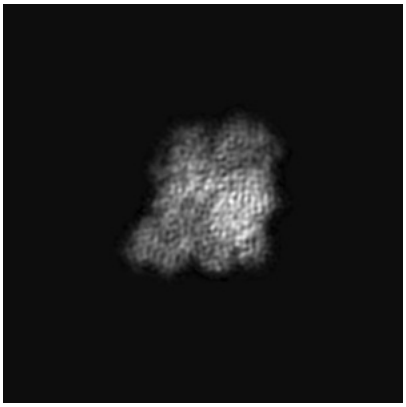
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

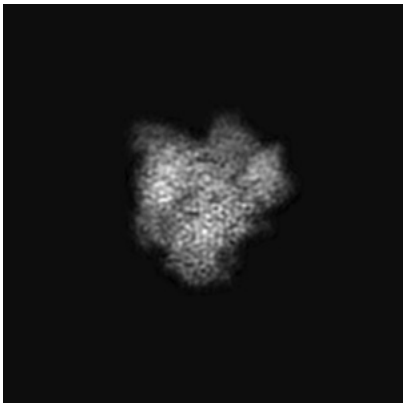
6.1.1 Primary map



X



Y

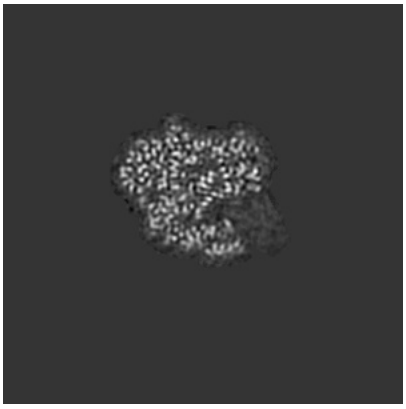


Z

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

6.2 Central slices

6.2.1 Primary map



X Index: 156

Y Index: 156

Z Index: 156

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: 157

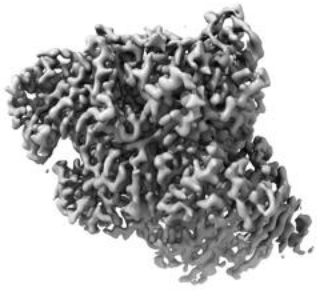
Y Index: 170

Z Index: 189

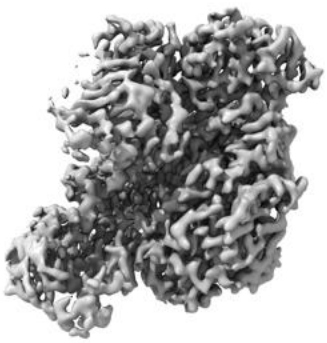
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

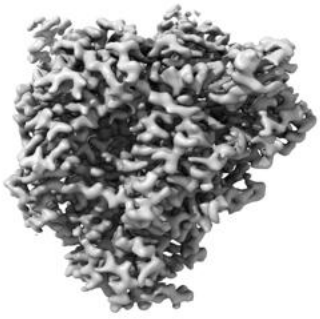
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

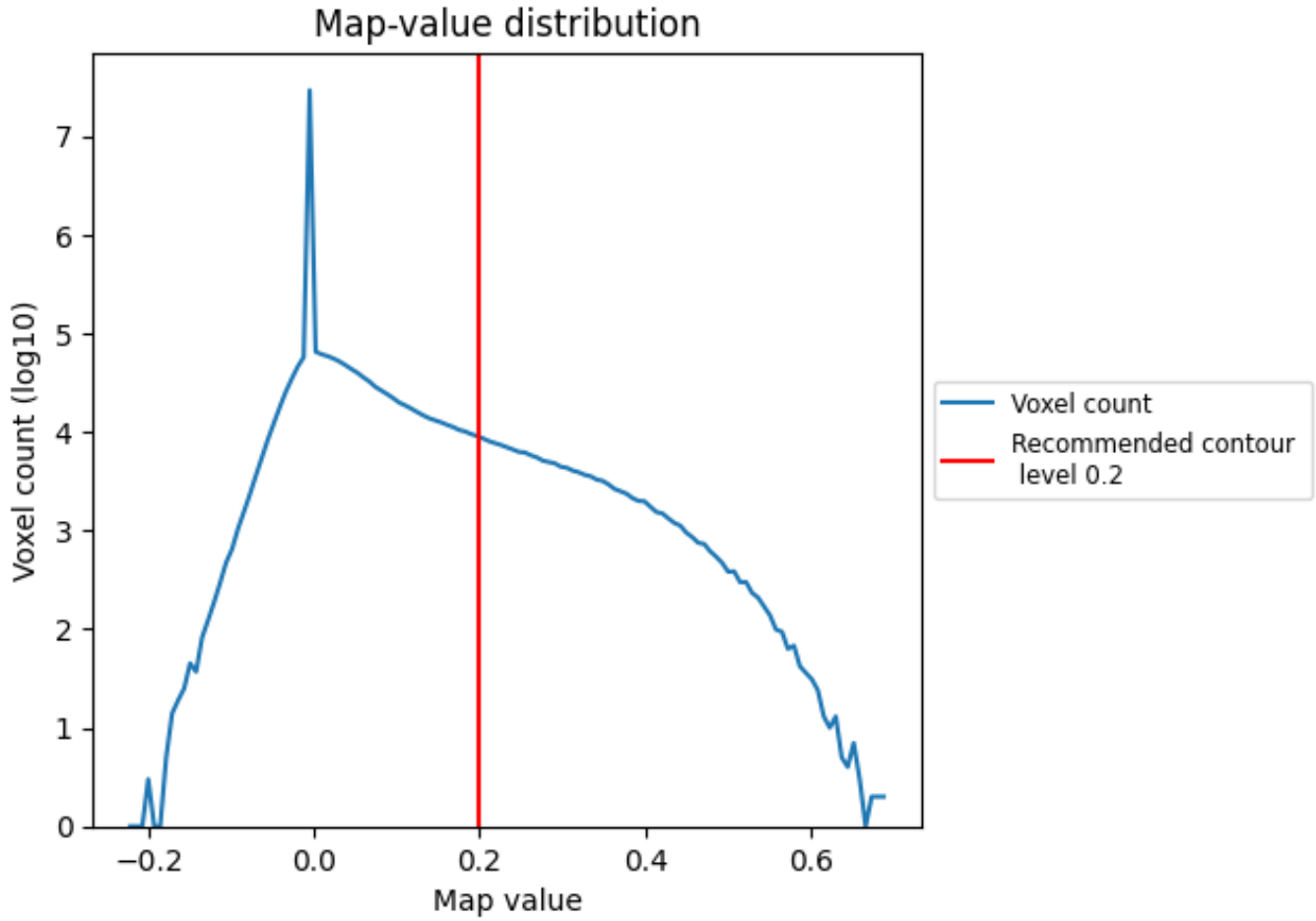
6.5 Mask visualisation (i)

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

7 Map analysis

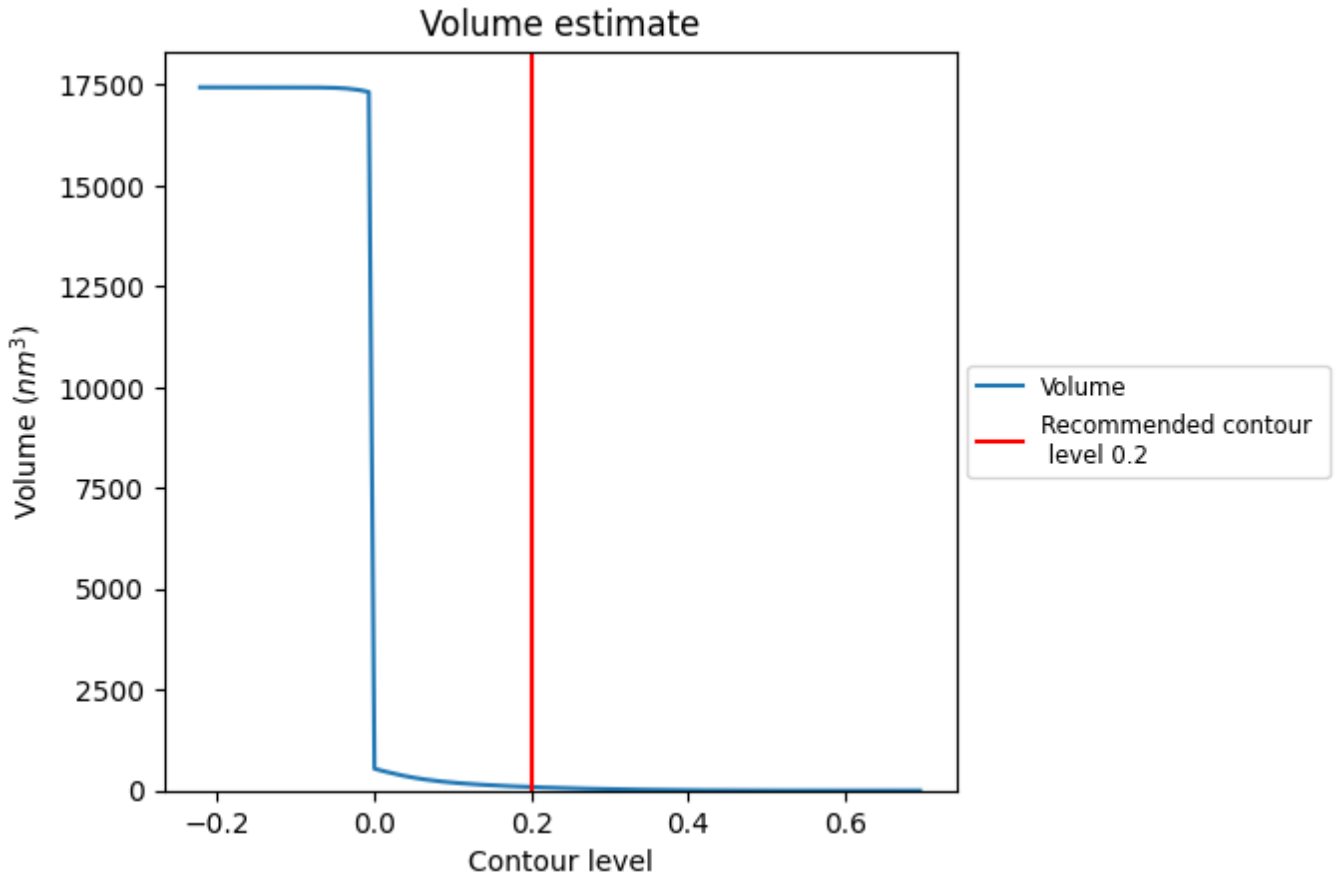
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

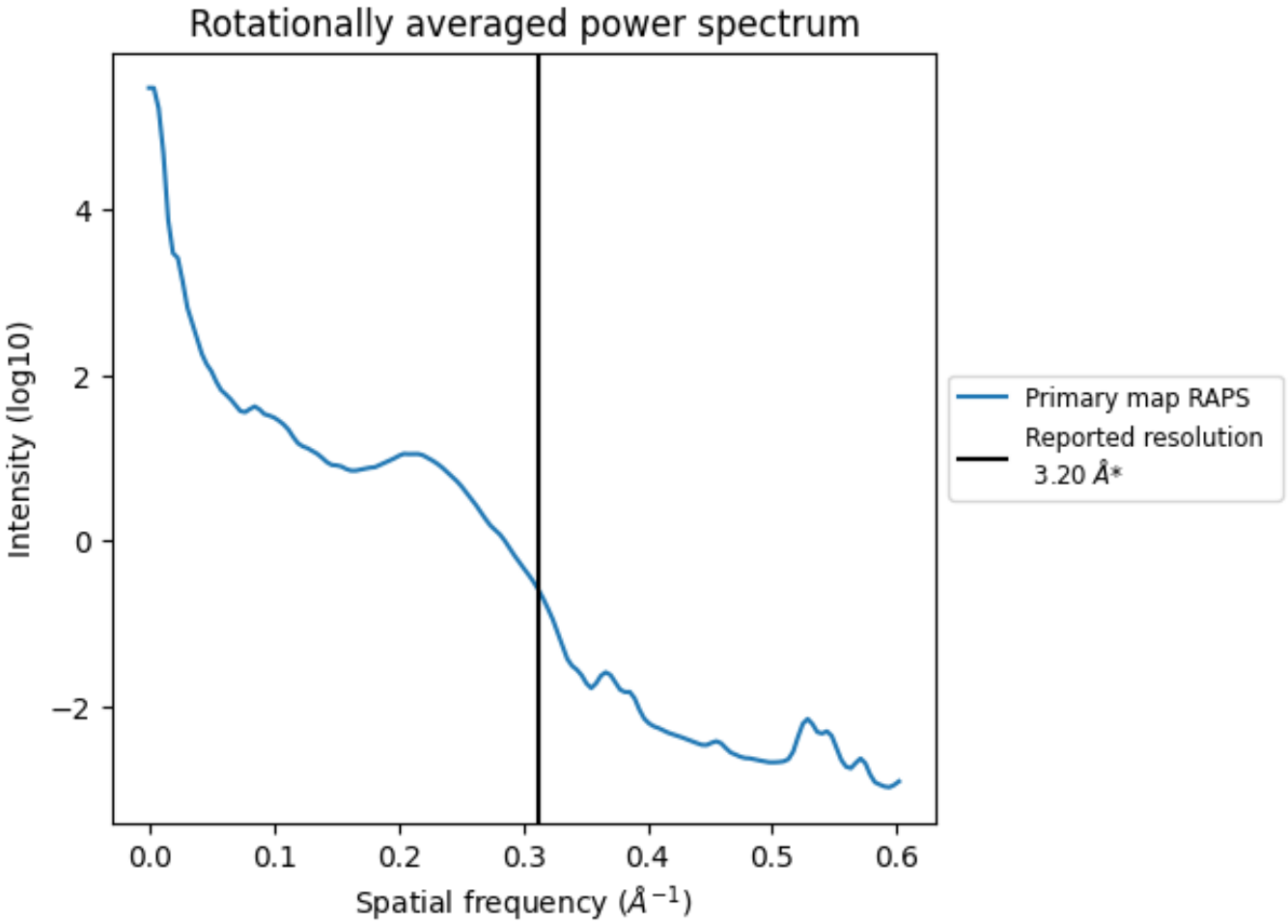
7.2 Volume estimate (i)



The volume at the recommended contour level is 87 nm^3; this corresponds to an approximate mass of 79 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)

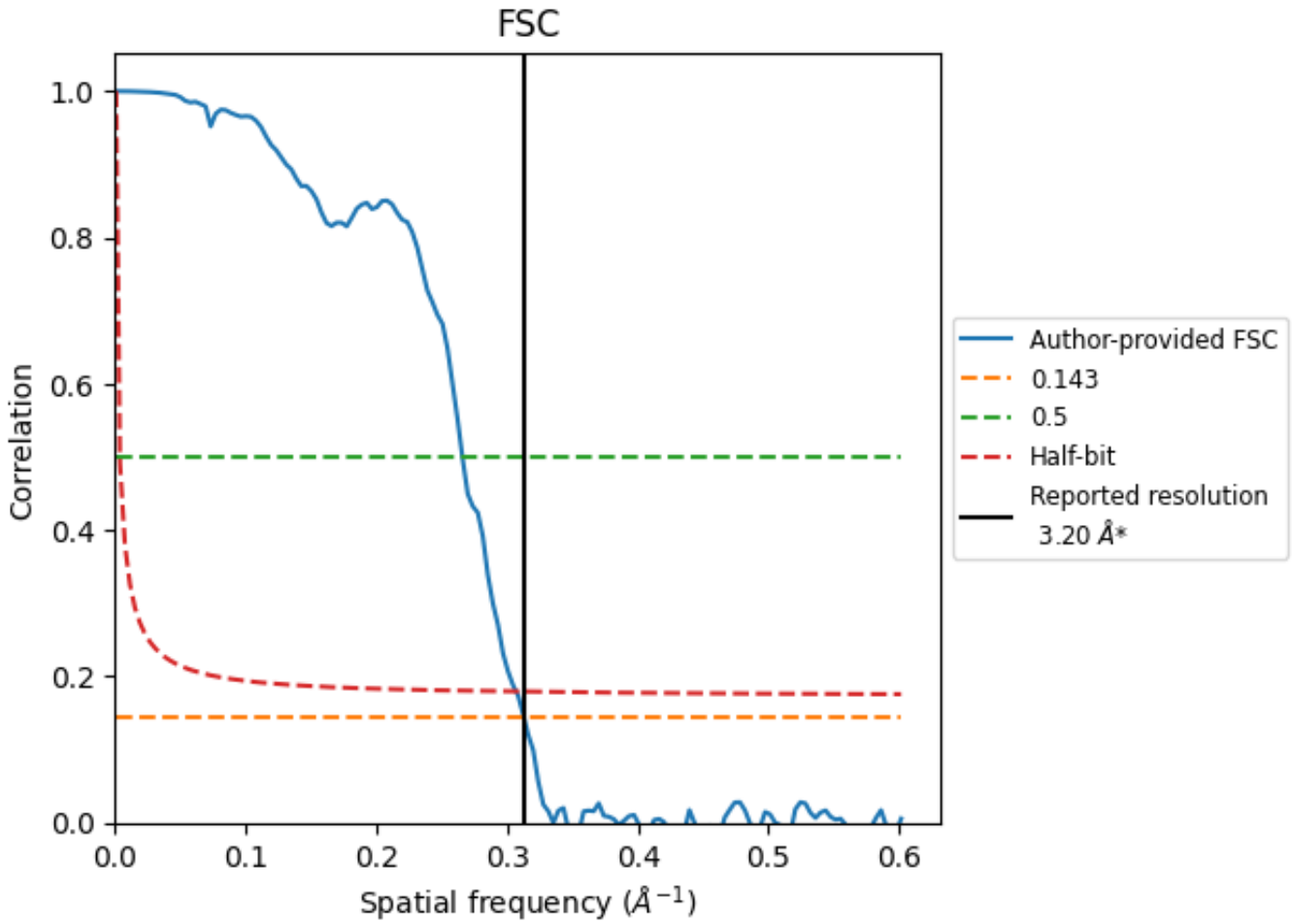


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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)

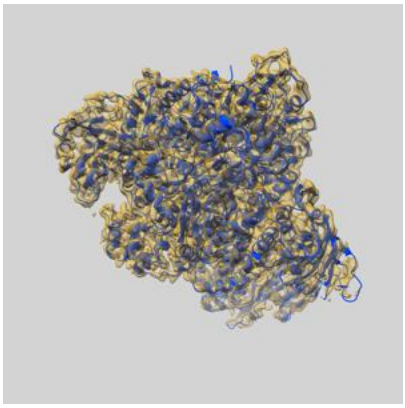
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.76	3.26
Unmasked-calculated*	-	-	-

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

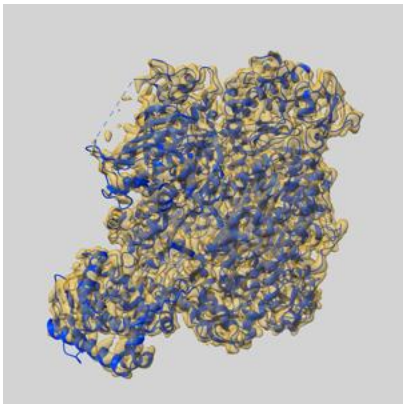
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4512 and PDB model 6QCT. Per-residue inclusion information can be found in section 3 on page 7.

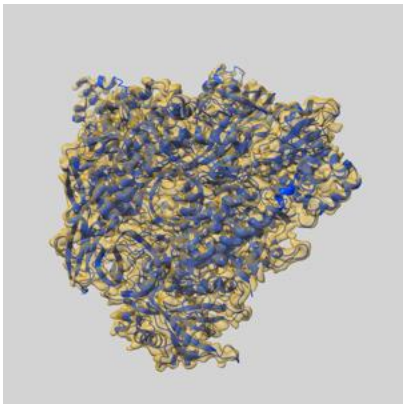
9.1 Map-model overlay



X



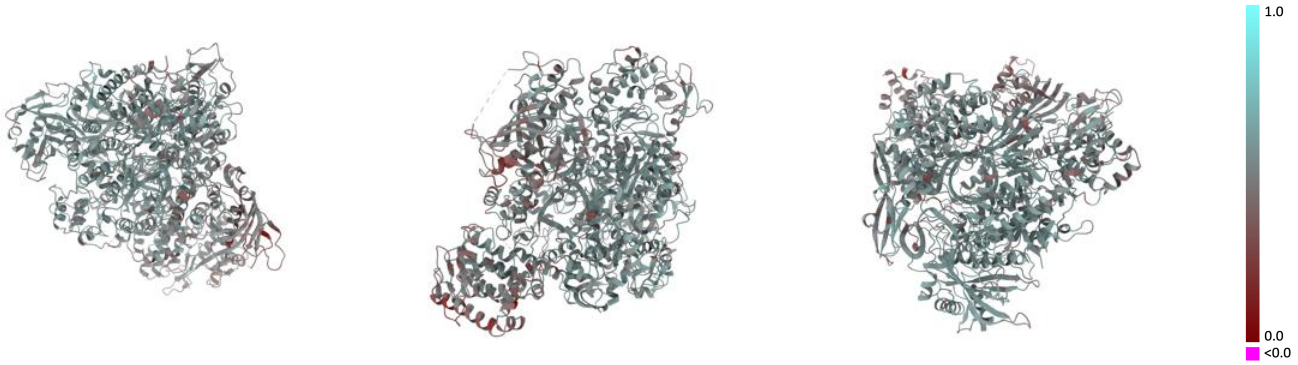
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

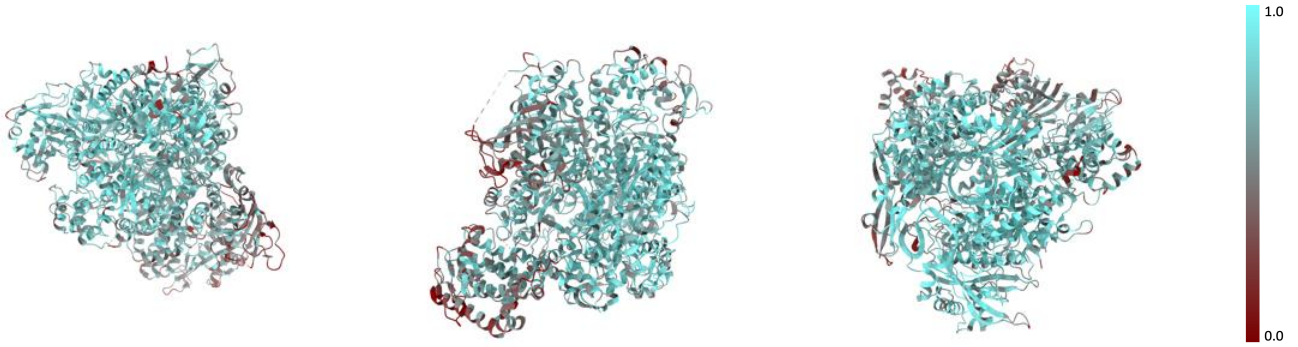
9.2 Q-score mapped to coordinate model



X Y Z

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

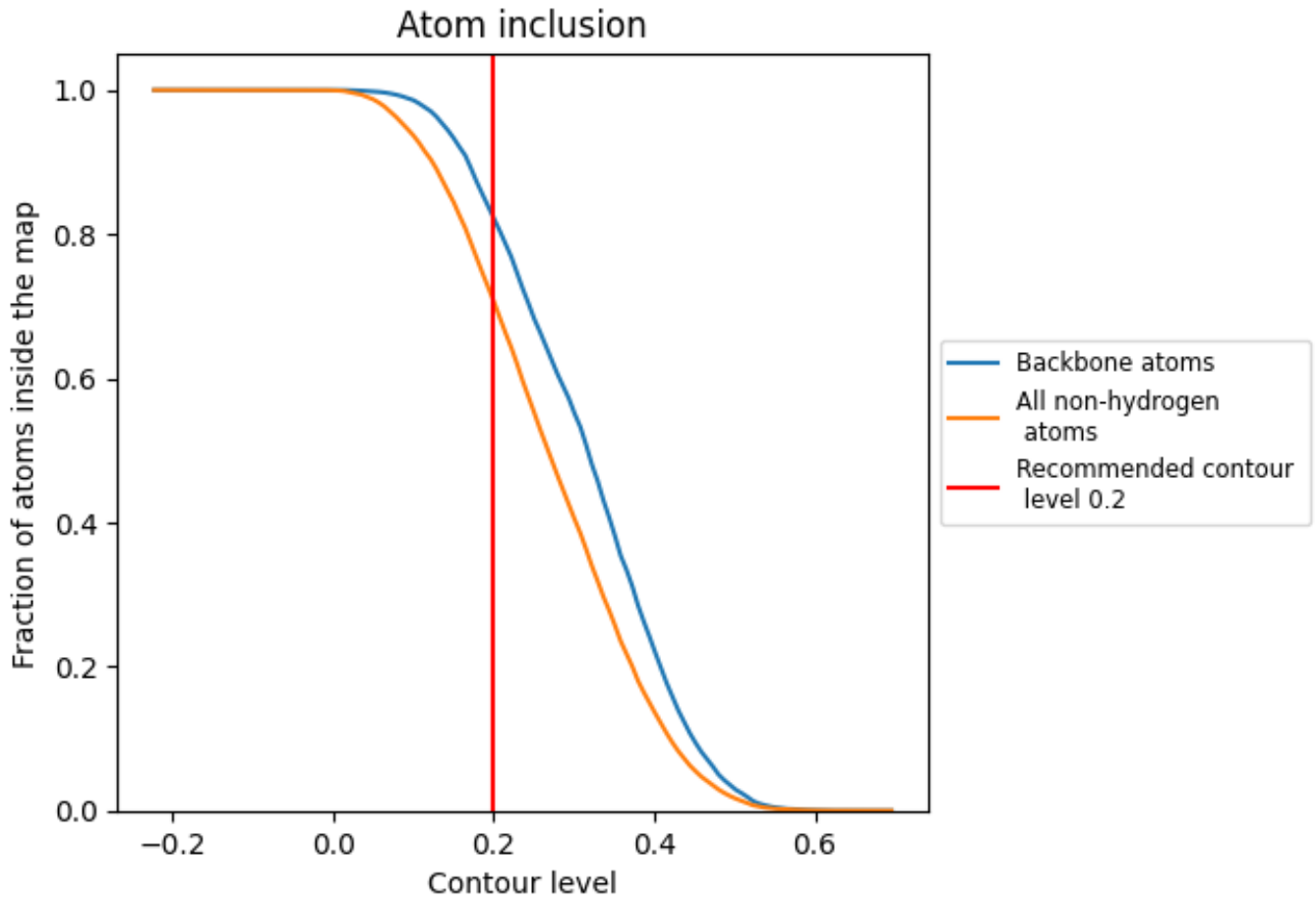
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 71% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7079	0.5210
A	0.6968	0.5190
B	0.7735	0.5440
C	0.6363	0.4980
M	0.7764	0.5190
R	0.8134	0.5450
V	0.8803	0.5460