



Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 03:52 am GMT

PDB ID : 6TW1
EMDB ID : EMD-10603
Title : Bat Influenza A polymerase termination complex with pyrophosphate using 44-mer vRNA template with mutated oligo(U) sequence
Authors : Wandzik, J.M.; Kouba, T.; Cusack, S.
Deposited on : 2020-01-11
Resolution : 2.70 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:

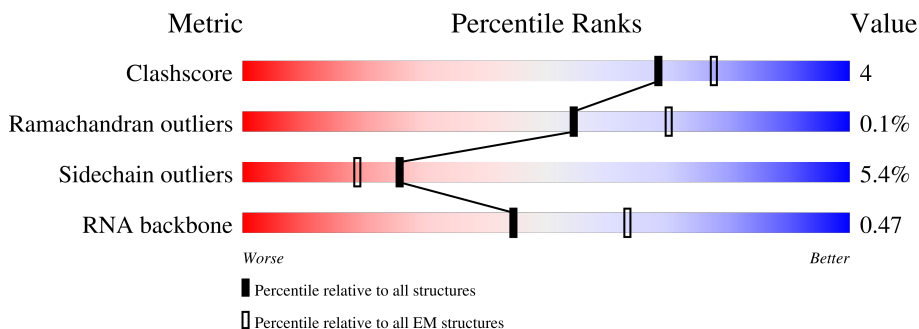
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	738	 13% 83% 11% • 5%
2	B	776	 • 83% 12% • 5%
3	C	809	 44% 75% 15% • 9%
4	V	44	 7% 50% 25% 25%
5	M	10	 80% 20%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18627 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	703	5733	3646	967	1083	37	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	GLY	-	expression tag	UNP H6QM92
A	-12	SER	-	expression tag	UNP H6QM92
A	-11	HIS	-	expression tag	UNP H6QM92
A	-10	HIS	-	expression tag	UNP H6QM92
A	-9	HIS	-	expression tag	UNP H6QM92
A	-8	HIS	-	expression tag	UNP H6QM92
A	-7	HIS	-	expression tag	UNP H6QM92
A	-6	HIS	-	expression tag	UNP H6QM92
A	-5	HIS	-	expression tag	UNP H6QM92
A	-4	HIS	-	expression tag	UNP H6QM92
A	-3	GLY	-	expression tag	UNP H6QM92
A	-2	SER	-	expression tag	UNP H6QM92
A	-1	GLY	-	expression tag	UNP H6QM92
A	0	SER	-	expression tag	UNP H6QM92
A	714	GLY	-	expression tag	UNP H6QM92
A	715	SER	-	expression tag	UNP H6QM92
A	716	GLY	-	expression tag	UNP H6QM92
A	717	SER	-	expression tag	UNP H6QM92
A	718	GLY	-	expression tag	UNP H6QM92
A	719	GLU	-	expression tag	UNP H6QM92
A	720	ASN	-	expression tag	UNP H6QM92
A	721	LEU	-	expression tag	UNP H6QM92
A	722	TYR	-	expression tag	UNP H6QM92
A	723	PHE	-	expression tag	UNP H6QM92
A	724	GLN	-	expression tag	UNP H6QM92

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	740	5925	3725	1056	1105	39	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP H6QM91
B	-7	SER	-	expression tag	UNP H6QM91
B	-6	GLY	-	expression tag	UNP H6QM91
B	-5	SER	-	expression tag	UNP H6QM91
B	-4	GLY	-	expression tag	UNP H6QM91
B	-3	SER	-	expression tag	UNP H6QM91
B	-2	GLY	-	expression tag	UNP H6QM91
B	-1	SER	-	expression tag	UNP H6QM91
B	0	GLY	-	expression tag	UNP H6QM91
B	757	GLY	-	expression tag	UNP H6QM91
B	758	SER	-	expression tag	UNP H6QM91
B	759	GLY	-	expression tag	UNP H6QM91
B	760	SER	-	expression tag	UNP H6QM91
B	761	GLY	-	expression tag	UNP H6QM91
B	762	GLU	-	expression tag	UNP H6QM91
B	763	ASN	-	expression tag	UNP H6QM91
B	764	LEU	-	expression tag	UNP H6QM91
B	765	TYR	-	expression tag	UNP H6QM91
B	766	PHE	-	expression tag	UNP H6QM91
B	767	GLN	-	expression tag	UNP H6QM91

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	740	5879	3708	1040	1099	32	0	0

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP H6QM90
C	-7	SER	-	expression tag	UNP H6QM90
C	-6	GLY	-	expression tag	UNP H6QM90
C	-5	SER	-	expression tag	UNP H6QM90
C	-4	GLY	-	expression tag	UNP H6QM90
C	-3	SER	-	expression tag	UNP H6QM90
C	-2	GLY	-	expression tag	UNP H6QM90

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP H6QM90
C	0	GLY	-	expression tag	UNP H6QM90
C	761	GLY	-	expression tag	UNP H6QM90
C	762	TRP	-	expression tag	UNP H6QM90
C	763	SER	-	expression tag	UNP H6QM90
C	764	HIS	-	expression tag	UNP H6QM90
C	765	PRO	-	expression tag	UNP H6QM90
C	766	GLN	-	expression tag	UNP H6QM90
C	767	PHE	-	expression tag	UNP H6QM90
C	768	GLU	-	expression tag	UNP H6QM90
C	769	LYS	-	expression tag	UNP H6QM90
C	770	GLY	-	expression tag	UNP H6QM90
C	771	GLY	-	expression tag	UNP H6QM90
C	772	GLY	-	expression tag	UNP H6QM90
C	773	SER	-	expression tag	UNP H6QM90
C	774	GLY	-	expression tag	UNP H6QM90
C	775	GLY	-	expression tag	UNP H6QM90
C	776	GLY	-	expression tag	UNP H6QM90
C	777	SER	-	expression tag	UNP H6QM90
C	778	GLY	-	expression tag	UNP H6QM90
C	779	GLY	-	expression tag	UNP H6QM90
C	780	SER	-	expression tag	UNP H6QM90
C	781	ALA	-	expression tag	UNP H6QM90
C	782	TRP	-	expression tag	UNP H6QM90
C	783	SER	-	expression tag	UNP H6QM90
C	784	HIS	-	expression tag	UNP H6QM90
C	785	PRO	-	expression tag	UNP H6QM90
C	786	GLN	-	expression tag	UNP H6QM90
C	787	PHE	-	expression tag	UNP H6QM90
C	788	GLU	-	expression tag	UNP H6QM90
C	789	LYS	-	expression tag	UNP H6QM90
C	790	GLY	-	expression tag	UNP H6QM90
C	791	ARG	-	expression tag	UNP H6QM90
C	792	SER	-	expression tag	UNP H6QM90
C	793	GLY	-	expression tag	UNP H6QM90
C	794	GLY	-	expression tag	UNP H6QM90
C	795	GLU	-	expression tag	UNP H6QM90
C	796	ASN	-	expression tag	UNP H6QM90
C	797	LEU	-	expression tag	UNP H6QM90
C	798	TYR	-	expression tag	UNP H6QM90
C	799	PHE	-	expression tag	UNP H6QM90
C	800	GLN	-	expression tag	UNP H6QM90

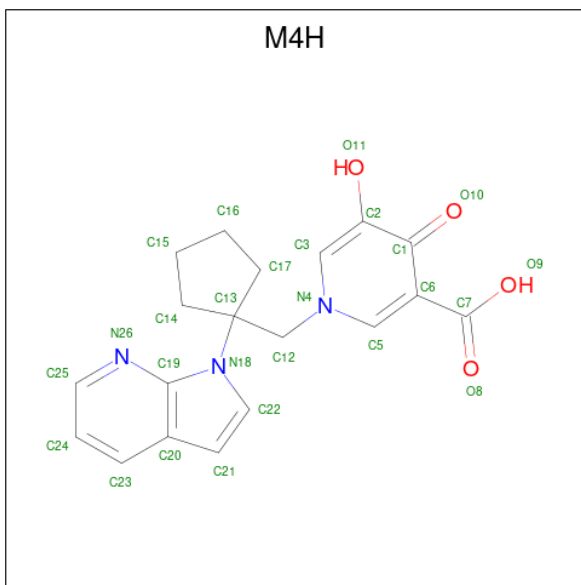
- Molecule 4 is a RNA chain called vRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	V	33	703	314	124	232	33	0	0

- Molecule 5 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	M	10	214	96	41	67	10	0	0

- Molecule 6 is 5-oxidanyl-4-oxidanylidene-1-[(1-pyrrolo[2,3-b]pyridin-1-ylcyclopentyl)methyl]pyridine-3-carboxylic acid (three-letter code: M4H) (formula: C₁₉H₁₉N₃O₄).

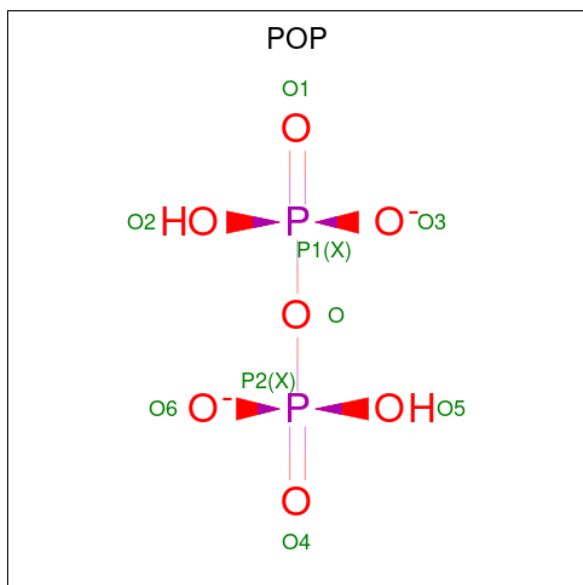


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	26	19	3	4	0

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
7	A	2	2	2	0
7	B	2	2	2	0

- Molecule 8 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms			AltConf
8	B	1	Total	O	P	0
			9	7	2	

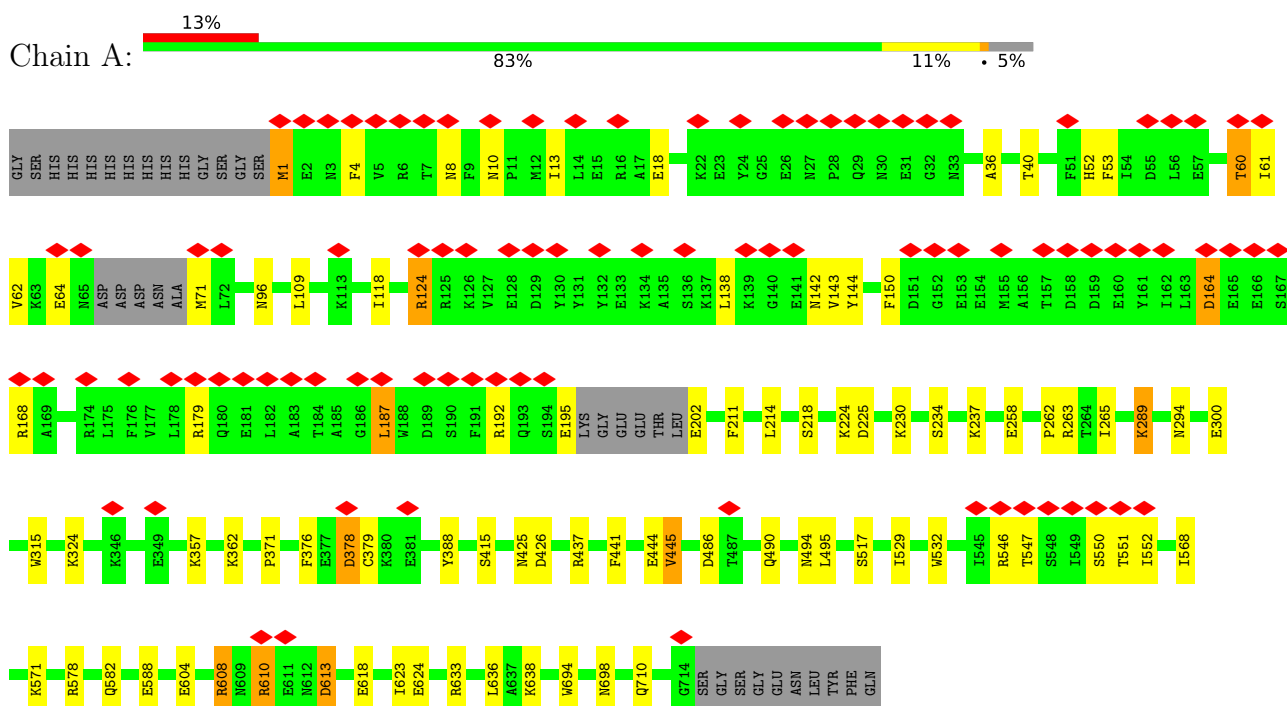
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	45	Total	O	0
			45	45	
9	B	59	Total	O	0
			59	59	
9	C	6	Total	O	0
			6	6	
9	V	20	Total	O	0
			20	20	
9	M	4	Total	O	0
			4	4	

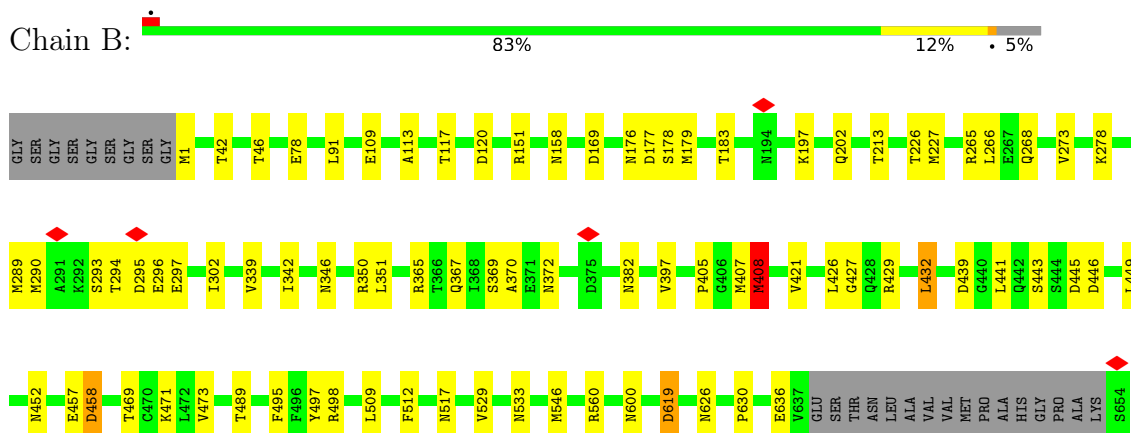
3 Residue-property plots i

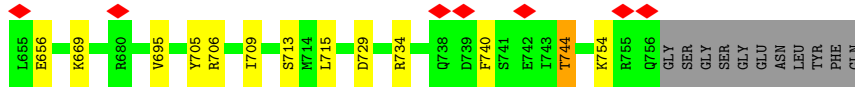
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

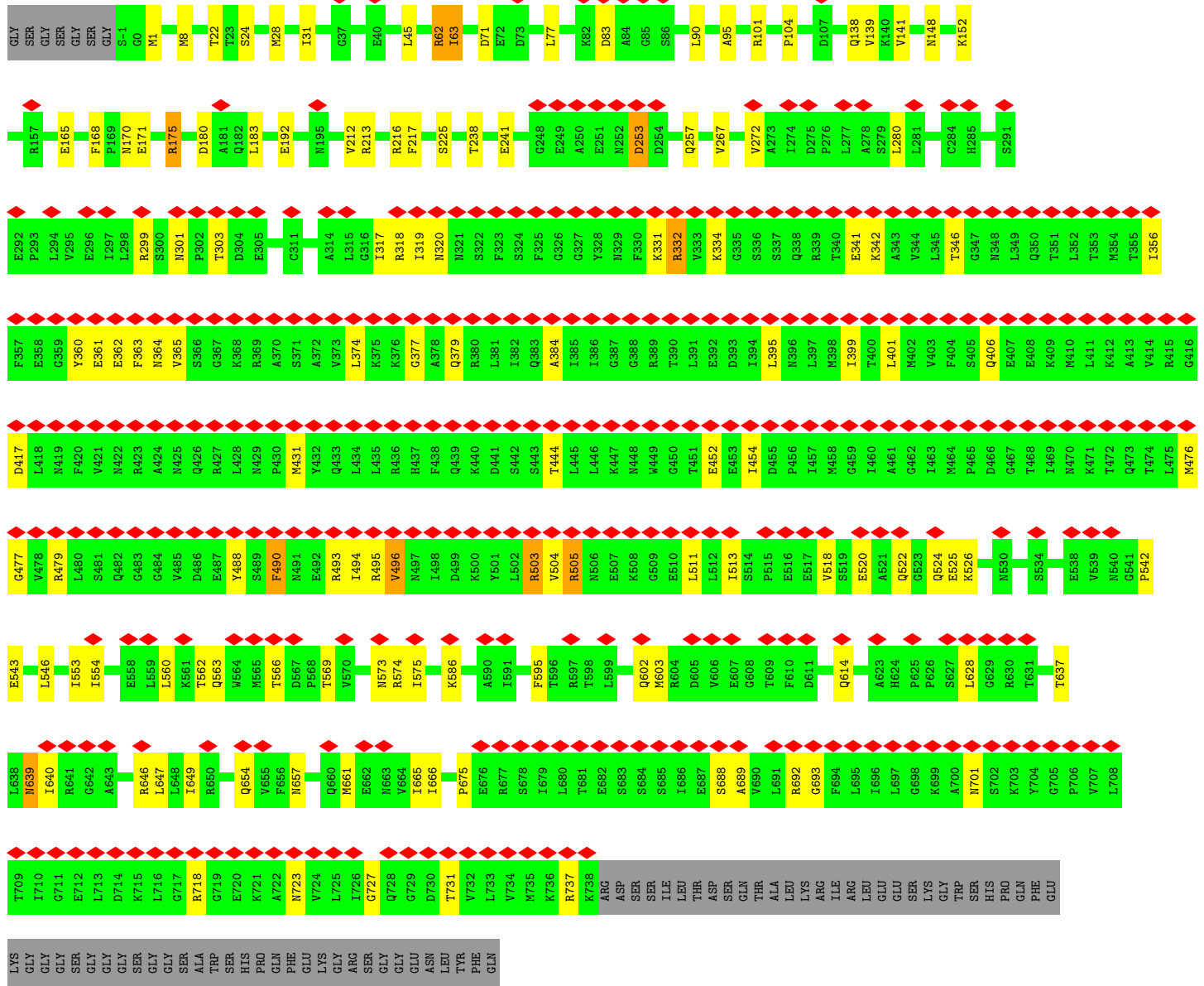
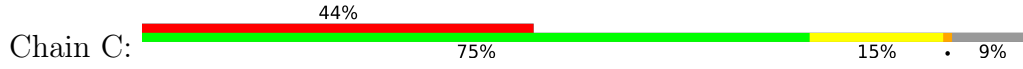


- Molecule 2: RNA-directed RNA polymerase catalytic subunit






• Molecule 3: Polymerase basic protein 2

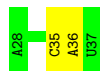


• Molecule 4: vRNA



- Molecule 5: mRNA

Chain M:  80% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101612	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 ($e^-/\text{\AA}^2$)	46	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	0.156	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	253.5624, 253.5624, 253.5624	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8127, 0.8127, 0.8127	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: M4H, MG, POP

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	0.42	0/5855	0.49	0/7883
2	B	0.43	0/6039	0.53	0/8145
3	C	0.33	0/5981	0.51	0/8075
4	V	0.94	1/784 (0.1%)	0.98	1/1215 (0.1%)
5	M	0.84	0/239	0.97	0/370
All	All	0.44	1/18898 (0.0%)	0.55	1/25688 (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	-11.27	1.47	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	7	A	O4'-C1'-N9	6.67	113.54	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5733	0	5652	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5925	0	5938	48	0
3	C	5879	0	5998	62	0
4	V	703	0	356	1	0
5	M	214	0	110	1	0
6	A	26	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	B	9	0	0	0	0
9	A	45	0	0	1	0
9	B	59	0	0	0	0
9	C	6	0	0	0	0
9	M	4	0	0	0	0
9	V	20	0	0	0	0
All	All	18627	0	18054	140	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 (140) 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)
3:C:505:ARG:HH21	3:C:511:LEU:HB2	1.61	0.66
3:C:454:ILE:HD13	3:C:479:ARG:HH21	1.63	0.64
1:A:694:TRP:O	1:A:698:ASN:ND2	2.36	0.59
1:A:571:LYS:HB2	3:C:45:LEU:HD13	1.85	0.59
2:B:630:PRO:HB2	3:C:63:ILE:HG13	1.84	0.58
2:B:489:THR:HG22	2:B:498:ARG:HA	1.84	0.58
2:B:342:ILE:O	2:B:346:ASN:ND2	2.33	0.58
2:B:729:ASP:OD1	2:B:734:ARG:NH1	2.36	0.58
3:C:299:ARG:HG2	3:C:317:ILE:HG12	1.87	0.57
2:B:295:ASP:OD1	3:C:646:ARG:NH1	2.37	0.57
2:B:740:PHE:O	2:B:744:THR:OG1	2.24	0.56
1:A:444:GLU:OE1	1:A:633:ARG:NH1	2.39	0.56
2:B:290:MET:SD	3:C:654:GLN:NE2	2.79	0.56
2:B:705:TYR:O	2:B:706:ARG:NH2	2.38	0.56
1:A:138:LEU:HD23	1:A:143:VAL:HG21	1.87	0.56
3:C:320:ASN:HB2	3:C:493:ARG:HG2	1.88	0.55
3:C:614:GLN:NE2	3:C:649:ILE:O	2.38	0.55
1:A:578:ARG:NH2	2:B:512:PHE:O	2.36	0.55
1:A:582:GLN:HB2	2:B:509:LEU:HD11	1.87	0.55
1:A:96:ASN:ND2	3:C:170:ASN:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:656:GLU:OE1	3:C:62:ARG:NH1	2.40	0.55
1:A:124:ARG:NH1	1:A:195:GLU:OE1	2.41	0.54
2:B:369:SER:OG	2:B:372:ASN:ND2	2.41	0.54
1:A:546:ARG:NH1	1:A:547:THR:O	2.39	0.54
3:C:71:ASP:OD1	3:C:101:ARG:NH2	2.41	0.53
2:B:176:ASN:ND2	2:B:179:MET:SD	2.81	0.53
3:C:553:ILE:HG23	3:C:560:LEU:HD12	1.90	0.53
3:C:503:ARG:HB2	3:C:511:LEU:HD11	1.91	0.53
3:C:614:GLN:NE2	3:C:689:ALA:O	2.42	0.53
2:B:529:VAL:O	2:B:533:ASN:ND2	2.38	0.52
2:B:158:ASN:ND2	2:B:169:ASP:OD2	2.40	0.52
2:B:626:ASN:ND2	3:C:104:PRO:O	2.42	0.52
2:B:715:LEU:HD23	2:B:754:LYS:HG3	1.91	0.52
1:A:618:GLU:HG3	1:A:623:ILE:HD13	1.92	0.52
3:C:406:GLN:NE2	3:C:431:MET:SD	2.82	0.52
2:B:268:GLN:NE2	2:B:439:ASP:OD1	2.36	0.52
2:B:151:ARG:HH22	3:C:22:THR:HB	1.75	0.52
3:C:301:ASN:ND2	3:C:303:THR:OG1	2.44	0.51
2:B:458:ASP:N	2:B:458:ASP:OD1	2.43	0.51
1:A:294:ASN:ND2	1:A:490:GLN:OE1	2.41	0.50
3:C:225:SER:HB3	3:C:526:LYS:HB3	1.92	0.50
3:C:718:ARG:NH1	3:C:737:ARG:O	2.42	0.50
2:B:351:LEU:HB2	2:B:370:ALA:HB1	1.94	0.50
1:A:613:ASP:N	1:A:613:ASP:OD1	2.44	0.49
2:B:713:SER:HA	3:C:24:SER:HA	1.94	0.49
3:C:332:ARG:NH1	3:C:361:GLU:OE2	2.45	0.49
1:A:437:ARG:NH1	1:A:588:GLU:OE2	2.38	0.49
3:C:452:GLU:HB2	3:C:476:MET:HG2	1.95	0.49
2:B:78:GLU:O	2:B:471:LYS:NZ	2.46	0.49
3:C:267:VAL:HG11	3:C:518:VAL:HG21	1.94	0.49
2:B:113:ALA:O	2:B:117:THR:OG1	2.26	0.48
2:B:266:LEU:HD13	2:B:421:VAL:HG11	1.96	0.48
3:C:152:LYS:NZ	3:C:253:ASP:OD1	2.44	0.48
3:C:569:THR:O	3:C:573:ASN:ND2	2.38	0.48
1:A:263:ARG:HA	1:A:710:GLN:HG2	1.95	0.48
1:A:371:PRO:HB2	2:B:365:ARG:HG2	1.95	0.47
2:B:46:THR:HG22	2:B:405:PRO:HG2	1.97	0.47
1:A:426:ASP:OD1	2:B:600:ASN:ND2	2.44	0.47
1:A:142:ASN:OD1	1:A:142:ASN:N	2.42	0.47
1:A:378:ASP:N	1:A:378:ASP:OD1	2.48	0.47
3:C:319:ILE:HD12	3:C:496:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ILE:HG23	1:A:144:TYR:HD2	1.80	0.47
3:C:28:MET:HA	3:C:31:ILE:HG12	1.96	0.47
3:C:168:PHE:HB3	3:C:171:GLU:HG3	1.96	0.47
3:C:342:LYS:NZ	3:C:379:GLN:OE1	2.47	0.47
3:C:331:LYS:HD3	3:C:490:PHE:HD1	1.78	0.47
1:A:109:LEU:HB2	1:A:118:ILE:HB	1.97	0.47
1:A:388:TYR:O	2:B:382:ASN:ND2	2.48	0.47
3:C:148:ASN:ND2	3:C:212:VAL:O	2.48	0.47
1:A:376:PHE:HA	1:A:379:CYS:HB2	1.96	0.47
2:B:489:THR:HA	2:B:497:TYR:O	2.15	0.47
1:A:150:PHE:HB3	1:A:179:ARG:HB2	1.97	0.46
1:A:53:PHE:O	1:A:60:THR:HA	2.16	0.45
1:A:4:PHE:O	1:A:8:ASN:ND2	2.50	0.45
1:A:357:LYS:HB3	1:A:362:LYS:HE3	1.98	0.45
3:C:504:VAL:HB	3:C:513:ILE:HB	1.99	0.45
1:A:300:GLU:O	4:V:42:G:N2	2.49	0.45
3:C:360:TYR:HA	3:C:377:GLY:HA2	1.99	0.45
1:A:445:VAL:HG22	1:A:636:LEU:HD22	1.98	0.45
2:B:226:THR:OG1	2:B:350:ARG:O	2.32	0.45
3:C:77:LEU:HB3	3:C:95:ALA:HB2	1.99	0.45
3:C:374:LEU:HD22	3:C:401:LEU:HD22	1.98	0.44
1:A:164:ASP:O	1:A:168:ARG:NE	2.51	0.44
3:C:657:ASN:HD22	3:C:666:ILE:HB	1.83	0.44
3:C:334:LYS:H	3:C:362:GLU:HB3	1.83	0.44
3:C:356:ILE:HG21	3:C:379:GLN:HG2	1.98	0.44
1:A:441:PHE:O	1:A:445:VAL:HB	2.18	0.44
1:A:604:GLU:O	1:A:608:ARG:HB2	2.18	0.44
3:C:417:ASP:OD1	3:C:417:ASP:N	2.51	0.43
1:A:230:LYS:O	1:A:234:SER:OG	2.29	0.43
2:B:302:ILE:HD12	2:B:449:LEU:HD23	1.99	0.43
2:B:407:MET:HG3	2:B:408:MET:H	1.84	0.43
2:B:619:ASP:OD1	2:B:619:ASP:N	2.41	0.43
2:B:91:LEU:HD12	2:B:473:VAL:HG11	1.99	0.43
3:C:554:ILE:HD11	3:C:665:ILE:HD12	2.00	0.43
2:B:706:ARG:HD3	2:B:706:ARG:HA	1.88	0.43
2:B:427:GLY:HA2	2:B:432:LEU:HD22	2.01	0.42
1:A:638:LYS:NZ	9:A:909:HOH:O	2.43	0.42
2:B:293:SER:OG	2:B:452:ASN:ND2	2.52	0.42
3:C:520:GLU:OE2	3:C:586:LYS:NZ	2.51	0.42
1:A:547:THR:OG1	1:A:550:SER:O	2.32	0.42
1:A:624:GLU:HG3	2:B:1:MET:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASN:HB2	1:A:13:ILE:HG12	2.01	0.42
1:A:52:HIS:HD2	1:A:62:VAL:HG22	1.83	0.42
1:A:324:LYS:NZ	1:A:532:TRP:O	2.43	0.42
3:C:318:ARG:HB2	3:C:493:ARG:HB3	2.02	0.42
3:C:542:PRO:HB2	3:C:640:ILE:HG13	2.01	0.42
1:A:1:MET:HB2	1:A:187:LEU:HD22	2.01	0.42
1:A:211:PHE:CZ	2:B:339:VAL:HG13	2.55	0.42
3:C:332:ARG:HA	3:C:363:PHE:HD1	1.85	0.42
3:C:595:PHE:HE1	3:C:692:ARG:HB2	1.85	0.42
5:M:35:C:H2'	5:M:36:A:C8	2.55	0.42
1:A:262:PRO:HA	1:A:265:ILE:HG12	2.01	0.42
2:B:669:LYS:HD3	3:C:90:LEU:HD22	2.02	0.42
3:C:384:ALA:N	3:C:477:GLY:O	2.51	0.41
2:B:636:GLU:HG3	2:B:656:GLU:HG2	2.01	0.41
1:A:289:LYS:HA	1:A:495:LEU:O	2.20	0.41
2:B:432:LEU:HD12	2:B:432:LEU:HA	1.95	0.41
3:C:602:GLN:HE22	3:C:693:GLY:H	1.68	0.41
1:A:187:LEU:H	1:A:187:LEU:HG	1.57	0.41
3:C:342:LYS:HE3	3:C:356:ILE:HD12	2.01	0.41
1:A:36:ALA:O	1:A:40:THR:OG1	2.30	0.41
1:A:214:LEU:O	1:A:218:SER:OG	2.32	0.41
2:B:296:GLU:HA	3:C:727:GLY:HA2	2.01	0.41
3:C:639:ASN:N	3:C:639:ASN:OD1	2.51	0.41
3:C:399:ILE:HD13	3:C:399:ILE:HA	1.88	0.41
1:A:289:LYS:HB3	1:A:494:ASN:HB3	2.02	0.41
3:C:138:GLN:HE22	3:C:241:GLU:HB2	1.86	0.41
3:C:180:ASP:HA	3:C:183:LEU:HD12	2.02	0.41
2:B:109:GLU:OE2	2:B:265:ARG:NH2	2.50	0.41
2:B:278:LYS:HD3	2:B:495:PHE:HE2	1.85	0.41
2:B:296:GLU:H	2:B:296:GLU:HG2	1.64	0.41
3:C:701:ASN:H	3:C:723:ASN:HD21	1.68	0.41
2:B:426:LEU:HD22	2:B:469:THR:HG21	2.03	0.40
3:C:363:PHE:HB3	3:C:365:VAL:HG23	2.03	0.40
3:C:595:PHE:HD1	3:C:692:ARG:HD2	1.86	0.40
3:C:139:VAL:HG11	3:C:543:GLU:HB3	2.03	0.40
3:C:165:GLU:OE1	3:C:175:ARG:NH2	2.54	0.40
3:C:563:GLN:HE22	3:C:574:ARG:HH21	1.70	0.40
1:A:610:ARG:HD2	1:A:610:ARG:HA	1.98	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	697/738 (94%)	674 (97%)	23 (3%)	0	100	100
2	B	736/776 (95%)	719 (98%)	16 (2%)	1 (0%)	51	78
3	C	738/809 (91%)	698 (95%)	39 (5%)	1 (0%)	51	78
All	All	2171/2323 (94%)	2091 (96%)	78 (4%)	2 (0%)	54	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	408	MET
3	C	675	PRO

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	629/657 (96%)	599 (95%)	30 (5%)	25	53
2	B	652/676 (96%)	621 (95%)	31 (5%)	25	53
3	C	655/706 (93%)	611 (93%)	44 (7%)	16	37
All	All	1936/2039 (95%)	1831 (95%)	105 (5%)	26	47

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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Mol	Chain	Res	Type
1	A	18	GLU
1	A	60	THR
1	A	61	ILE
1	A	64	GLU
1	A	71	MET
1	A	124	ARG
1	A	164	ASP
1	A	187	LEU
1	A	192	ARG
1	A	202	GLU
1	A	224	LYS
1	A	225	ASP
1	A	237	LYS
1	A	258	GLU
1	A	289	LYS
1	A	315	TRP
1	A	378	ASP
1	A	415	SER
1	A	425	ASN
1	A	445	VAL
1	A	486	ASP
1	A	517	SER
1	A	529	ILE
1	A	551	THR
1	A	552	ILE
1	A	568	ILE
1	A	608	ARG
1	A	610	ARG
1	A	613	ASP
2	B	42	THR
2	B	120	ASP
2	B	177	ASP
2	B	178	SER
2	B	183	THR
2	B	197	LYS
2	B	202	GLN
2	B	213	THR
2	B	227	MET
2	B	273	VAL
2	B	289	MET
2	B	294	THR
2	B	297	GLU

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Mol	Chain	Res	Type
2	B	367	GLN
2	B	397	VAL
2	B	408	MET
2	B	429	ARG
2	B	432	LEU
2	B	441	LEU
2	B	443	SER
2	B	445	ASP
2	B	446	ASP
2	B	457	GLU
2	B	458	ASP
2	B	517	ASN
2	B	546	MET
2	B	560	ARG
2	B	619	ASP
2	B	695	VAL
2	B	709	ILE
2	B	744	THR
3	C	1	MET
3	C	8	MET
3	C	62	ARG
3	C	63	ILE
3	C	83	ASP
3	C	141	VAL
3	C	175	ARG
3	C	192	GLU
3	C	213	ARG
3	C	216	ARG
3	C	217	PHE
3	C	238	THR
3	C	253	ASP
3	C	257	GLN
3	C	272	VAL
3	C	280	LEU
3	C	332	ARG
3	C	341	GLU
3	C	346	THR
3	C	364	ASN
3	C	395	LEU
3	C	444	THR
3	C	488	TYR
3	C	490	PHE

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Mol	Chain	Res	Type
3	C	494	ILE
3	C	495	ARG
3	C	496	VAL
3	C	503	ARG
3	C	505	ARG
3	C	522	GLN
3	C	524	GLN
3	C	525	GLU
3	C	546	LEU
3	C	562	THR
3	C	566	THR
3	C	575	ILE
3	C	603	MET
3	C	628	LEU
3	C	637	THR
3	C	639	ASN
3	C	647	LEU
3	C	661	MET
3	C	688	SER
3	C	731	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	256	GLN
2	B	127	GLN
2	B	186	GLN
2	B	216	ASN
2	B	310	ASN
2	B	372	ASN
2	B	454	HIS
2	B	567	ASN
2	B	745	ASN
3	C	138	GLN
3	C	148	ASN
3	C	301	ASN
3	C	588	ASN
3	C	614	GLN
3	C	654	GLN
3	C	659	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	V	31/44 (70%)	8 (25%)	0
5	M	9/10 (90%)	0	0
All	All	40/54 (74%)	8 (20%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	V	4	A
4	V	6	U
4	V	8	A
4	V	11	A
4	V	14	G
4	V	15	C
4	V	40	C
4	V	44	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](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	POP	B	803	7	6,8,8	1.02	0	13,13,13	1.06	1 (7%)
6	M4H	A	801	7	27,29,29	1.27	1 (3%)	33,43,43	2.05	11 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	POP	B	803	7	-	4/6/6/6	-
6	M4H	A	801	7	-	5/8/24/24	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	M4H	C22-N18	-4.52	1.35	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	M4H	C17-C13-C12	-5.50	107.21	113.80
6	A	801	M4H	C22-N18-C13	-4.53	120.74	124.18
6	A	801	M4H	C5-C6-C1	-4.04	117.26	120.26
6	A	801	M4H	C25-N26-C19	3.00	120.50	116.77
6	A	801	M4H	C14-C13-C17	2.99	107.61	102.20
6	A	801	M4H	C3-N4-C5	2.80	122.31	119.30
6	A	801	M4H	C7-C6-C1	2.63	125.51	121.53
8	B	803	POP	O3-P1-O	2.60	113.35	104.64
6	A	801	M4H	C16-C17-C13	2.32	107.64	104.37
6	A	801	M4H	C21-C20-C19	2.24	111.66	105.30
6	A	801	M4H	O11-C2-C1	2.21	121.44	117.89
6	A	801	M4H	C21-C20-C23	-2.09	129.41	136.72

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	803	POP	P2-O-P1-O3
6	A	801	M4H	C1-C6-C7-O8
6	A	801	M4H	C1-C6-C7-O9

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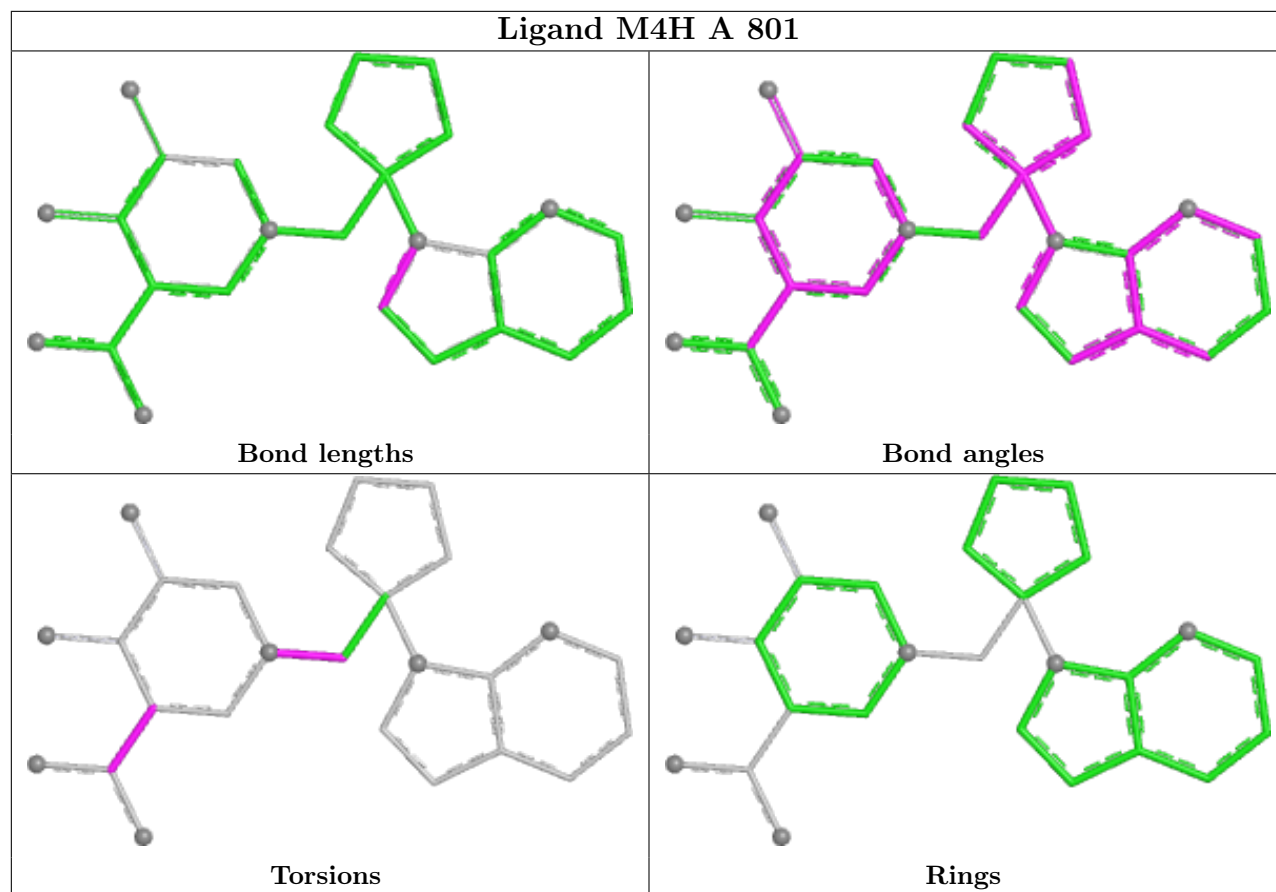
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Mol	Chain	Res	Type	Atoms
6	A	801	M4H	C5-C6-C7-O8
6	A	801	M4H	C5-C6-C7-O9
6	A	801	M4H	C13-C12-N4-C3
8	B	803	POP	P2-O-P1-O1
8	B	803	POP	P2-O-P1-O2
8	B	803	POP	P1-O-P2-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

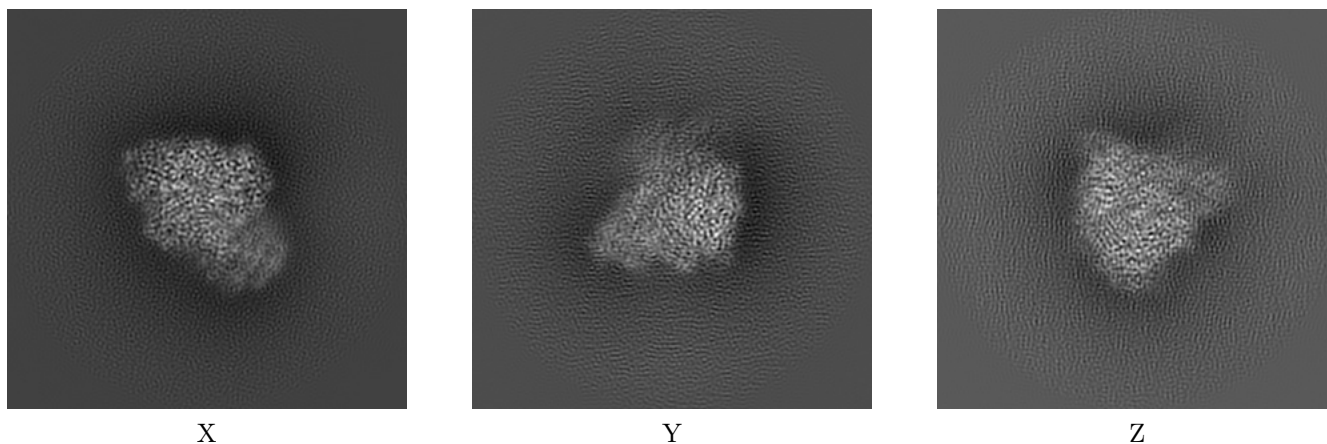
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10603. These allow visual inspection of the internal detail of the map and identification of artifacts.

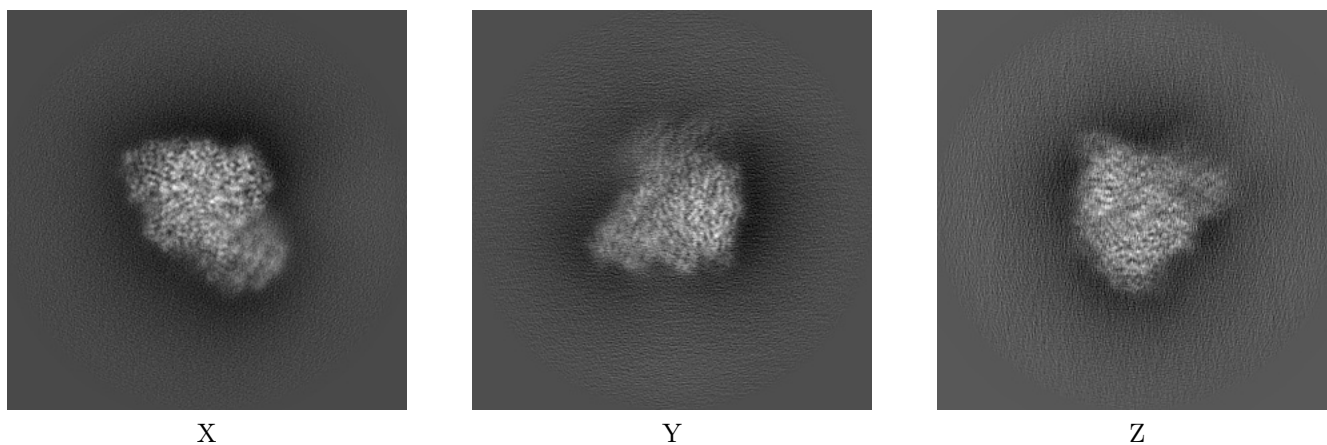
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



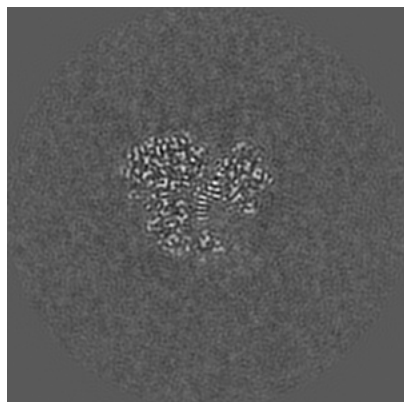
6.1.2 Raw map



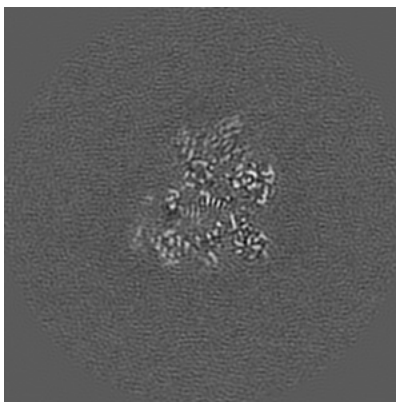
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

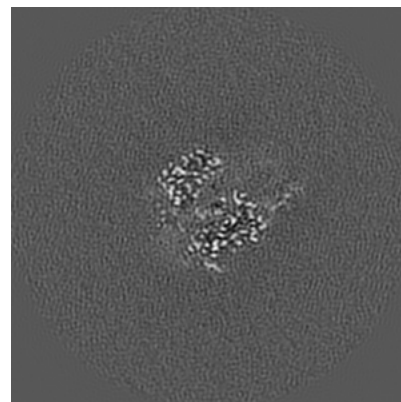
6.2.1 Primary map



X Index: 156

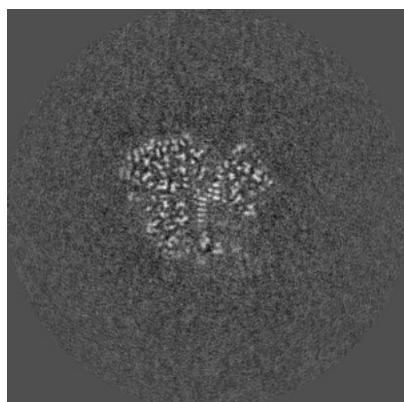


Y Index: 156

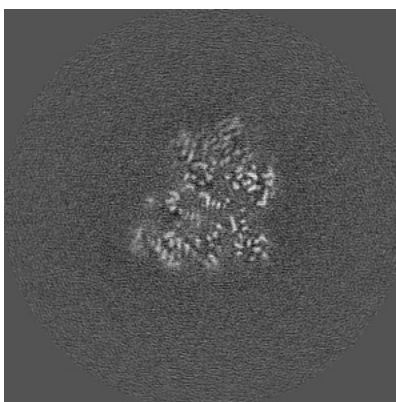


Z Index: 156

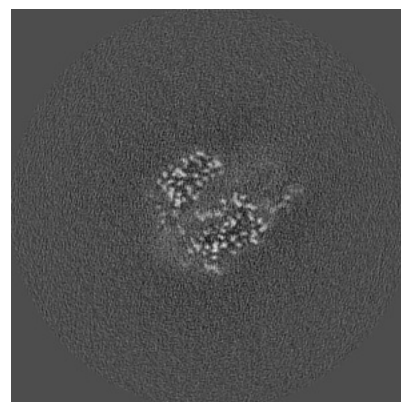
6.2.2 Raw map



X Index: 156



Y Index: 156

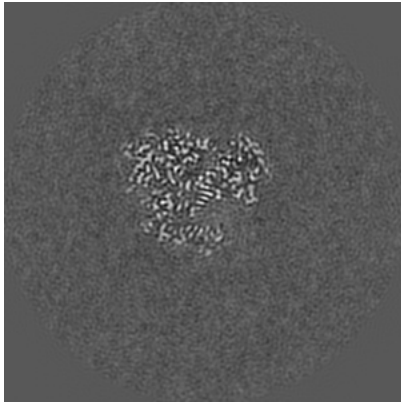


Z Index: 156

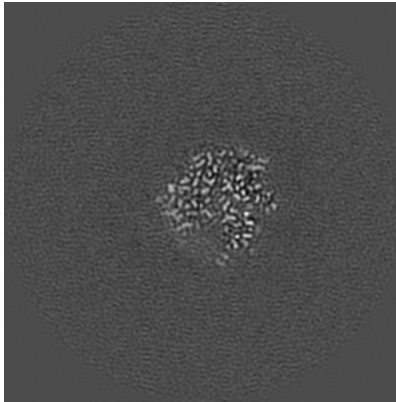
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

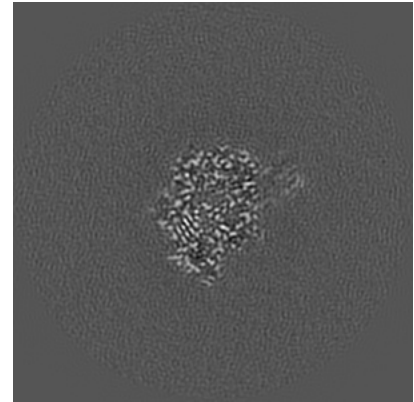
6.3.1 Primary map



X Index: 160

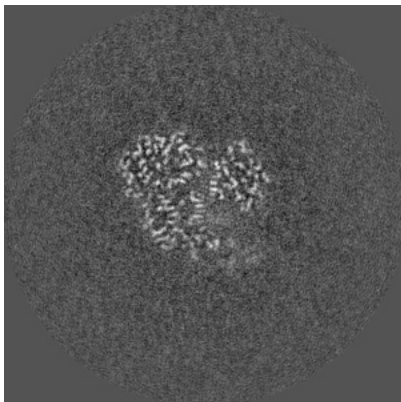


Y Index: 133

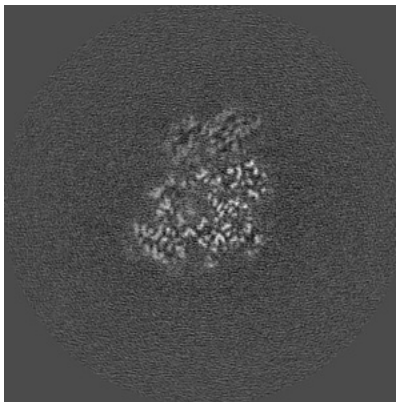


Z Index: 190

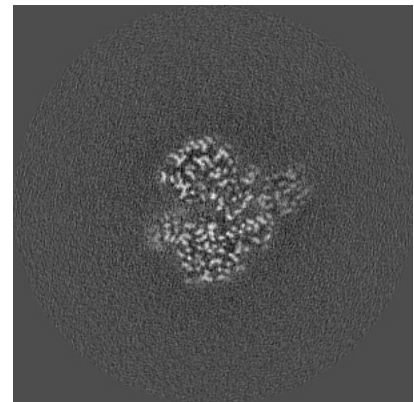
6.3.2 Raw map



X Index: 154



Y Index: 165



Z Index: 174

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

6.4 Orthogonal surface views [i](#)

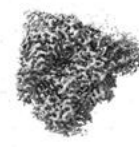
6.4.1 Primary map



X



Y



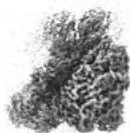
Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

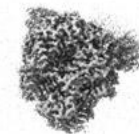
6.4.2 Raw map



X



Y



Z

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

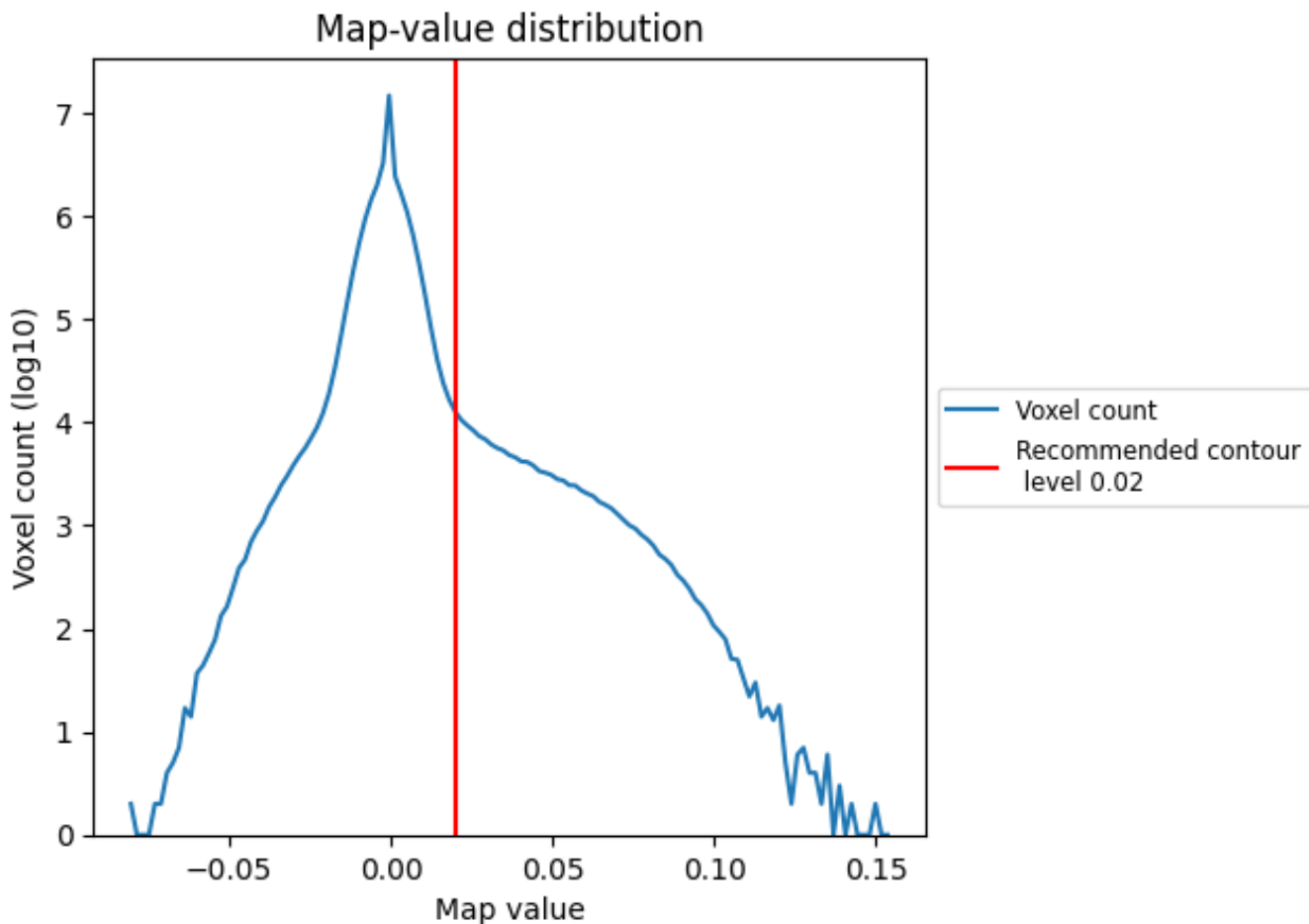
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

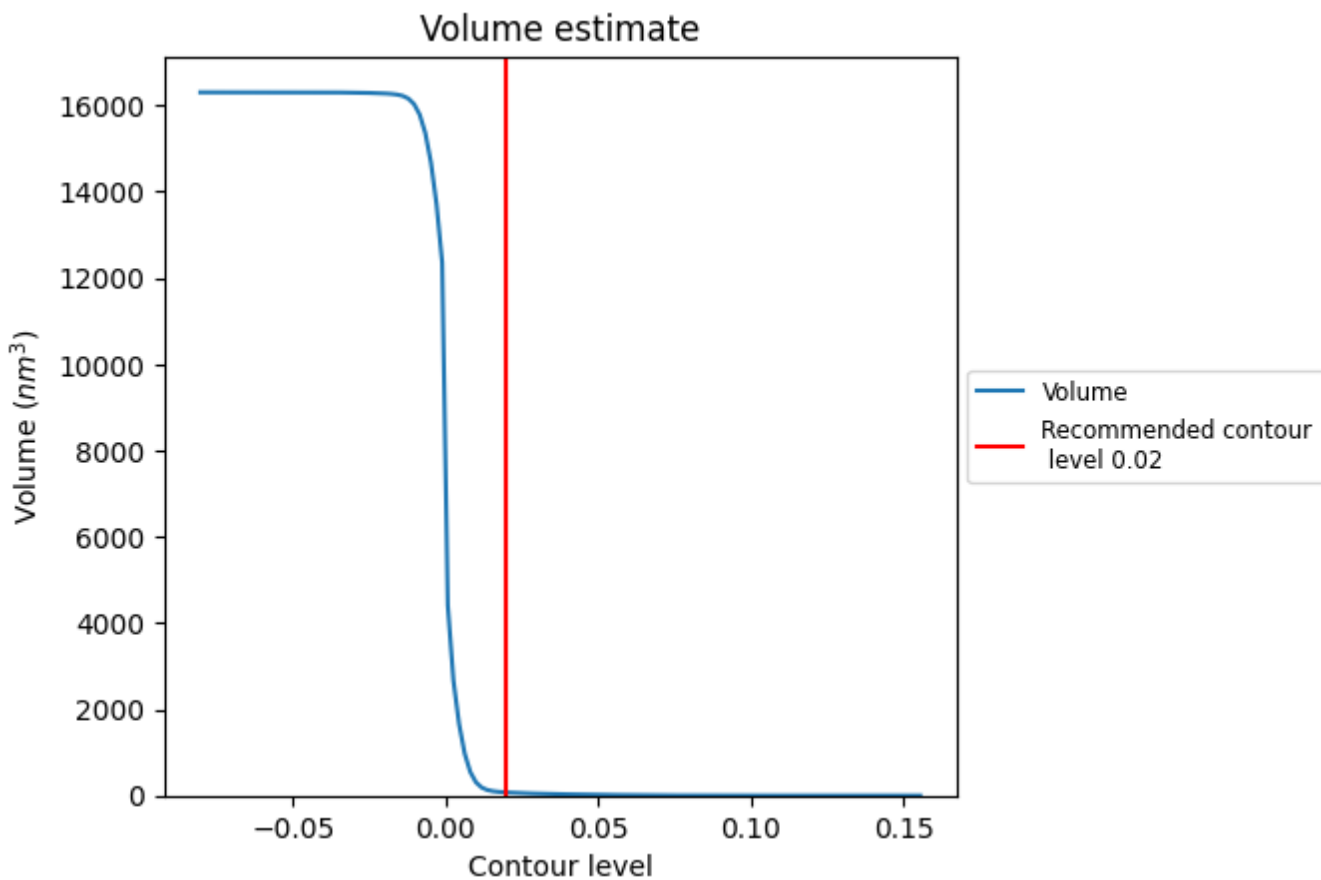
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

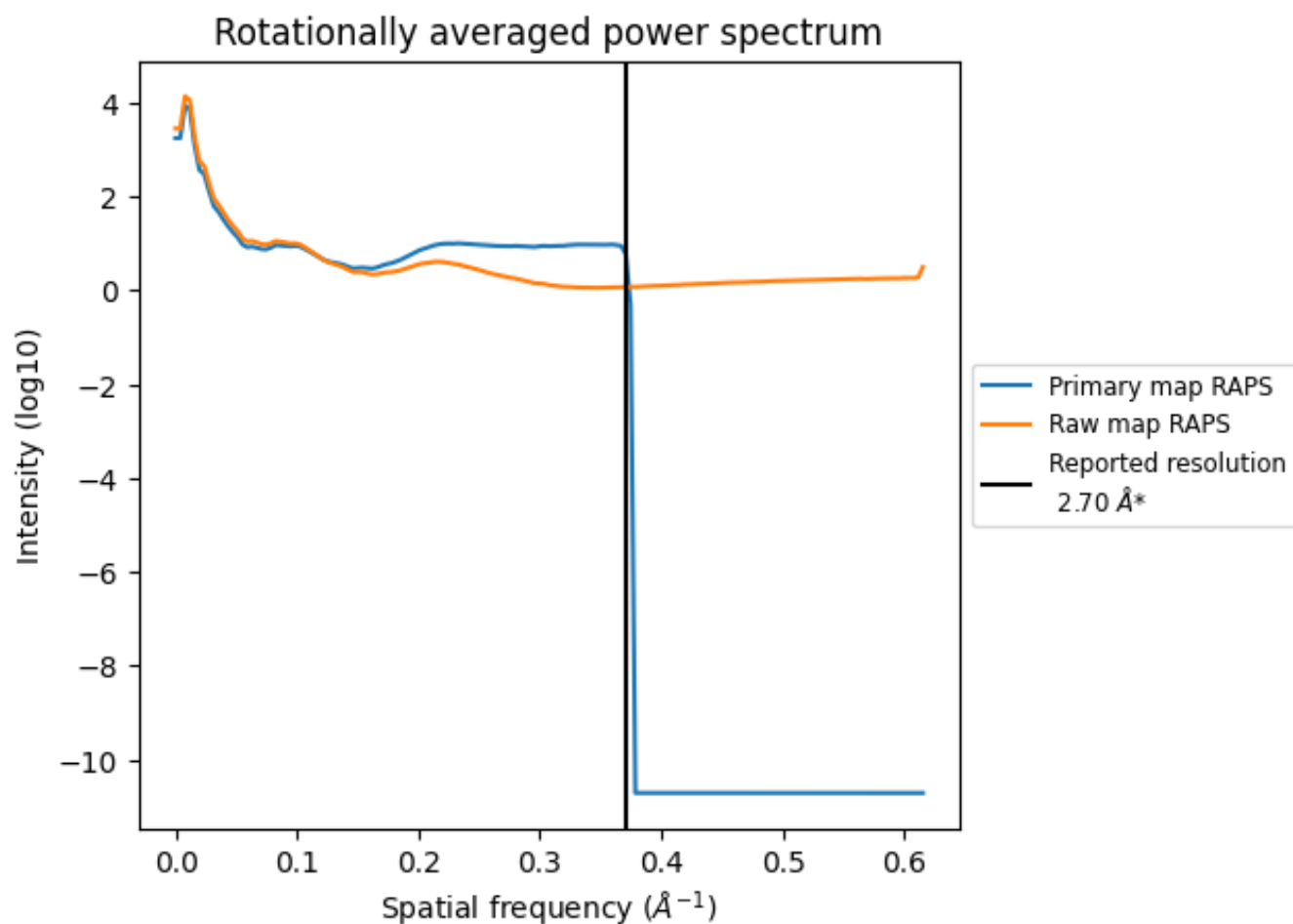
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 72 nm³; this corresponds to an approximate mass of 65 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

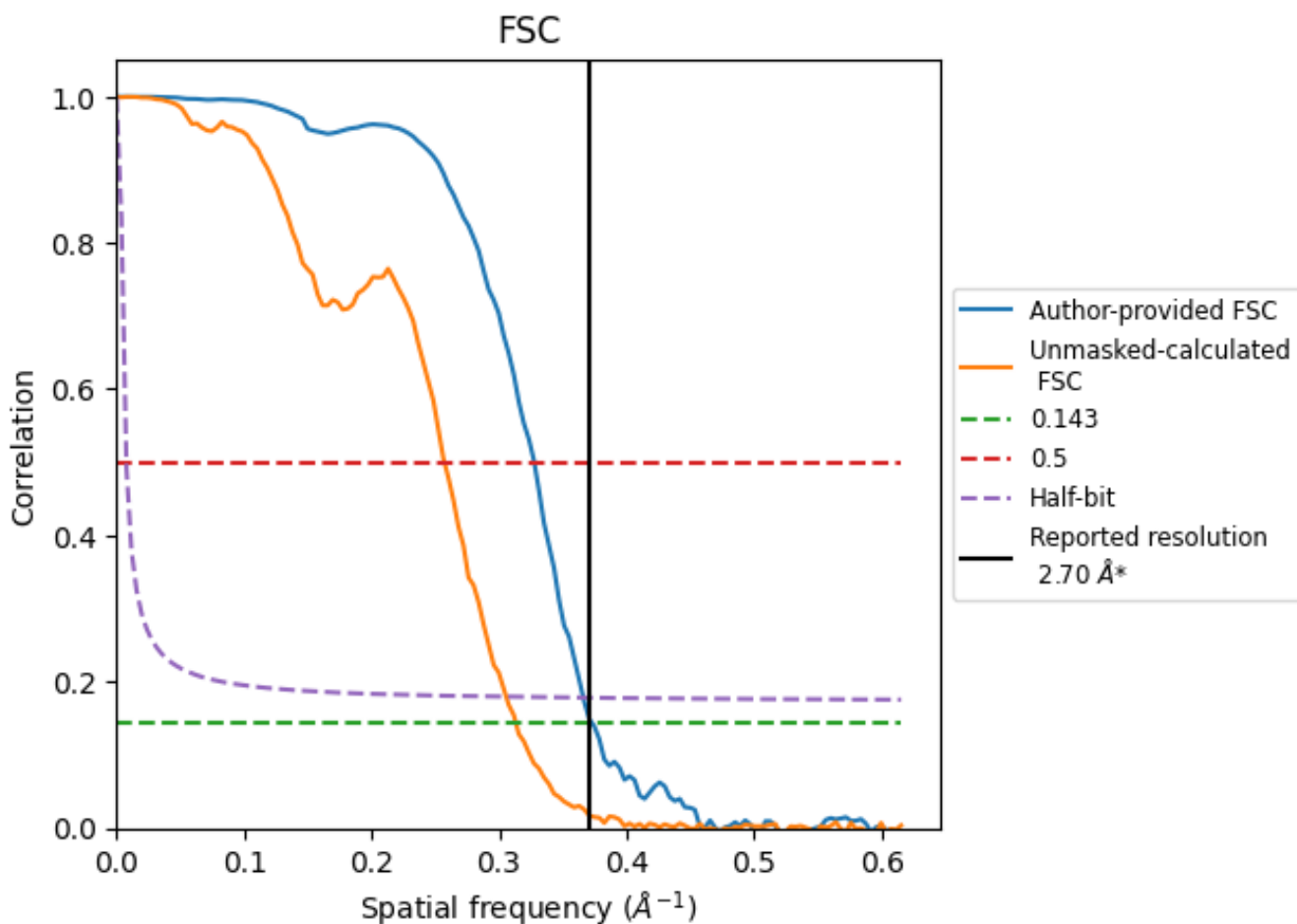


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

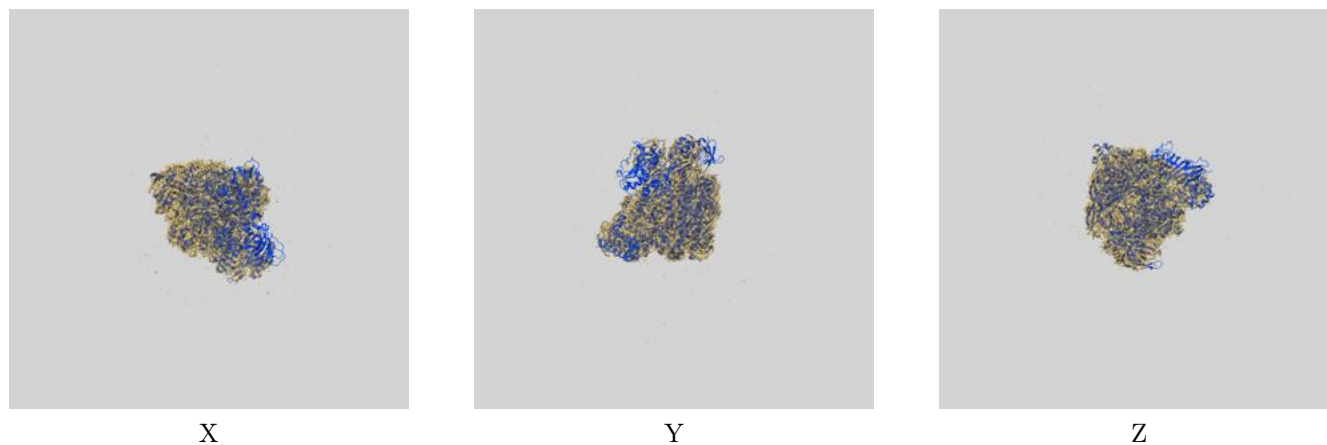
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.68	3.05	2.73
Unmasked-calculated*	3.19	3.89	3.27

*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 3.19 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

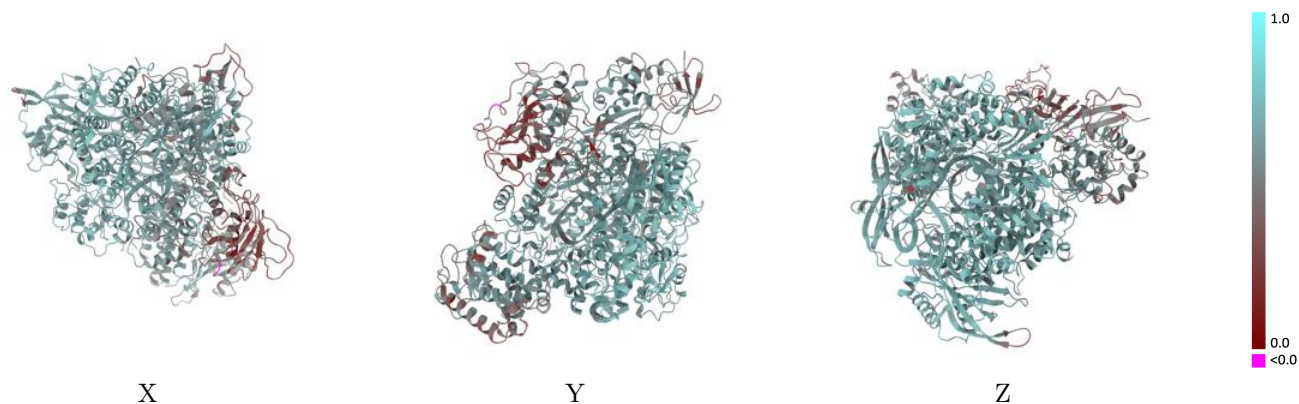
This section contains information regarding the fit between EMDB map EMD-10603 and PDB model 6TW1. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



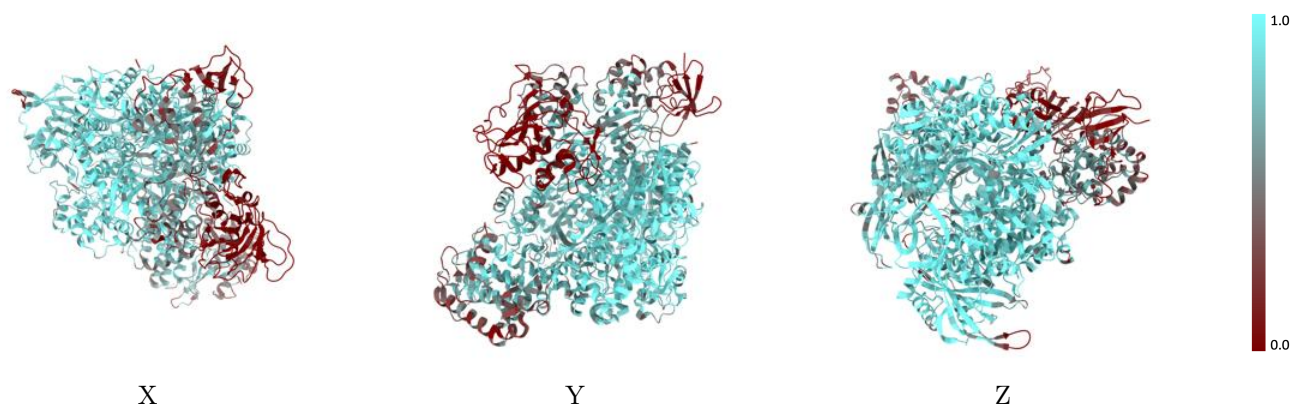
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



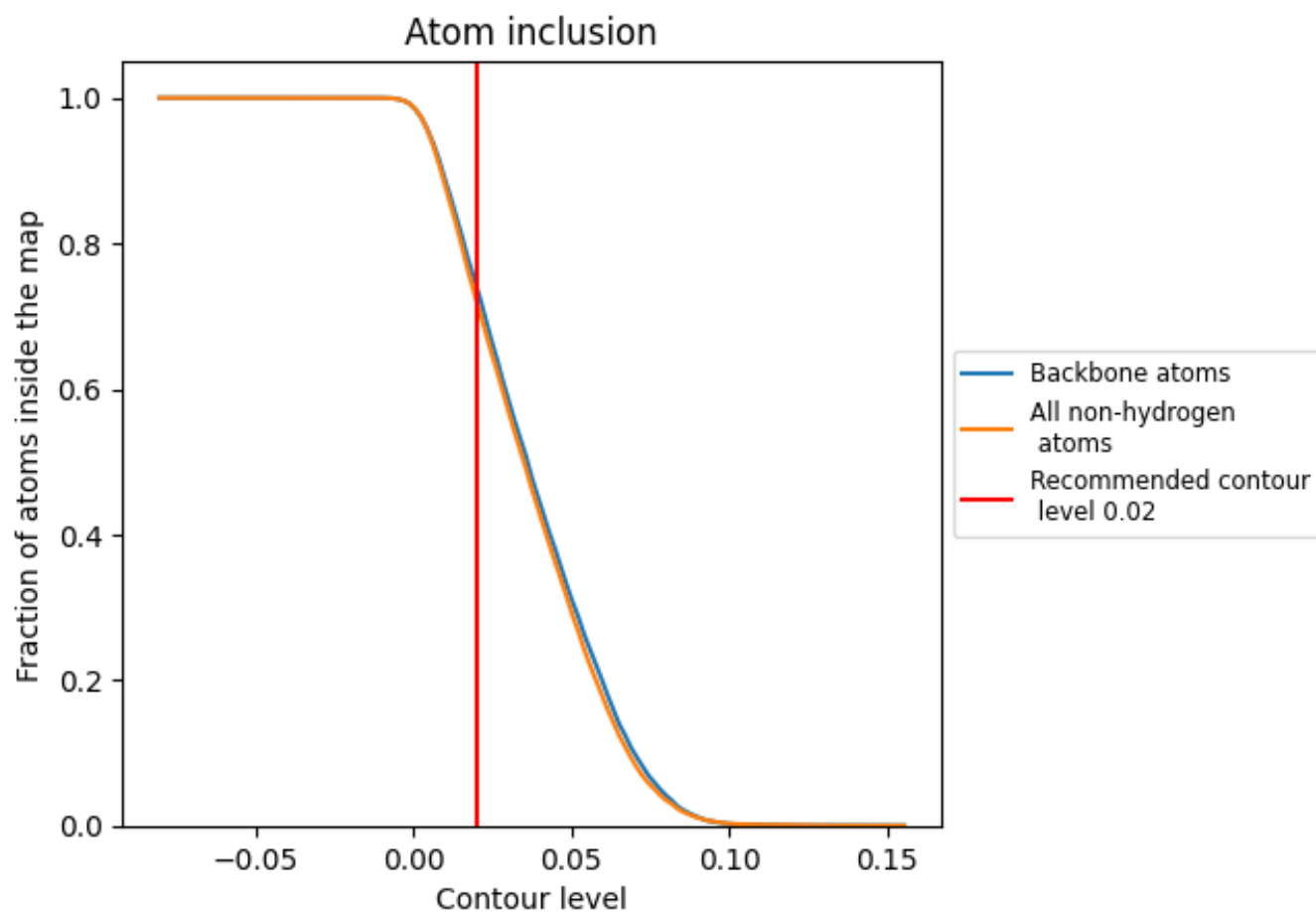
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).













9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7202	 0.5910
A	 0.7891	 0.6120
B	 0.8962	 0.6470
C	 0.4587	 0.5080
M	 0.8925	 0.6290
V	 0.8805	 0.6300

