



Full wwPDB EM Validation Report ⓘ

Sep 4, 2024 – 04:43 pm BST

PDB ID : 8RN9
EMDB ID : EMD-19391
Title : Influenza B polymerase, replicase (from "Influenza B polymerase apo-trimer"
| Local refinement)
Authors : Arragain, B.; Cusack, S.
Deposited on : 2024-01-09
Resolution : 3.31 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.dev112
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

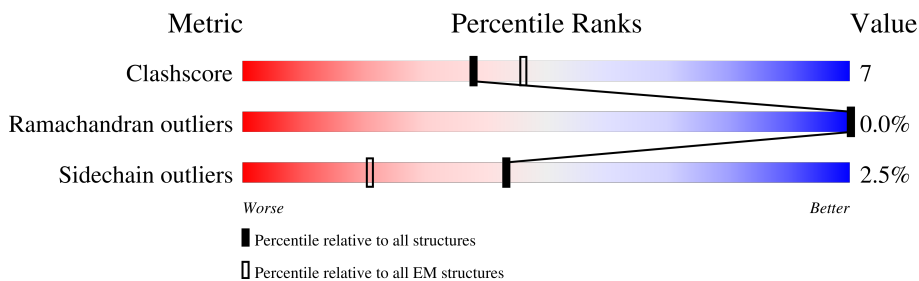
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.31 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	726	22% (red), 82% (green), 17% (yellow), 5% (grey)
1	E	726	96% (grey), 4% (red), 5% (yellow)
2	B	752	12% (red), 76% (green), 19% (yellow), 5% (grey)
2	D	752	97% (grey), 3% (red), 5% (yellow)
3	C	799	39% (red), 78% (green), 16% (yellow), 5% (grey)

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 35902 atoms, of which 18026 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	H	N	O	S		
1	A	716	Total	C	H	N	O	S	0	0
			11470	3651	5724	964	1091	40		
1	E	29	Total	C	H	N	O	S	0	0
			446	143	218	35	47	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	718	Total	C	H	N	O	S	0	0
			11272	3558	5636	968	1059	51		
2	D	23	Total	C	H	N	O	S	0	0
			379	118	198	31	30	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	760	Total	C	H	N	O	S	0	0
			12335	3859	6250	1068	1116	42		

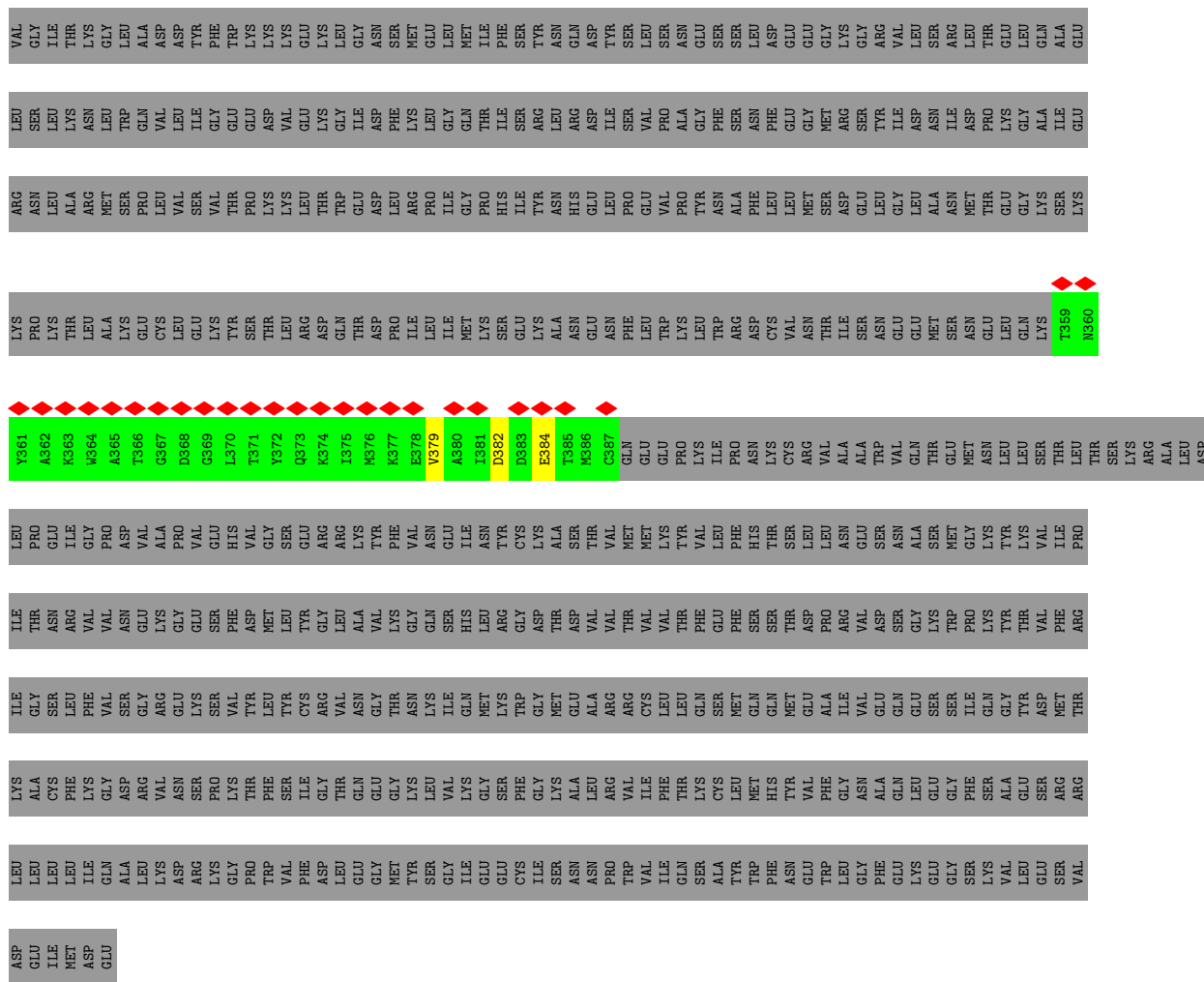
There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	GLY	-	expression tag	UNP Q5V8X3

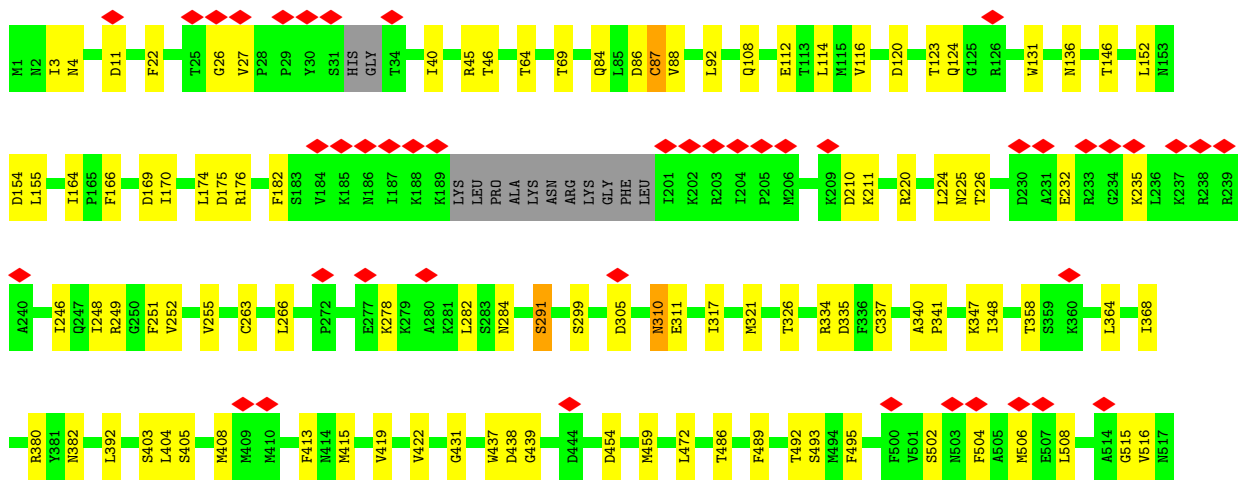
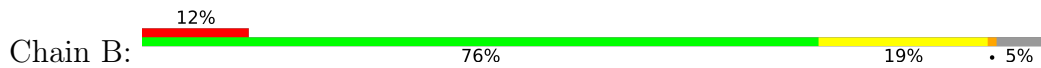
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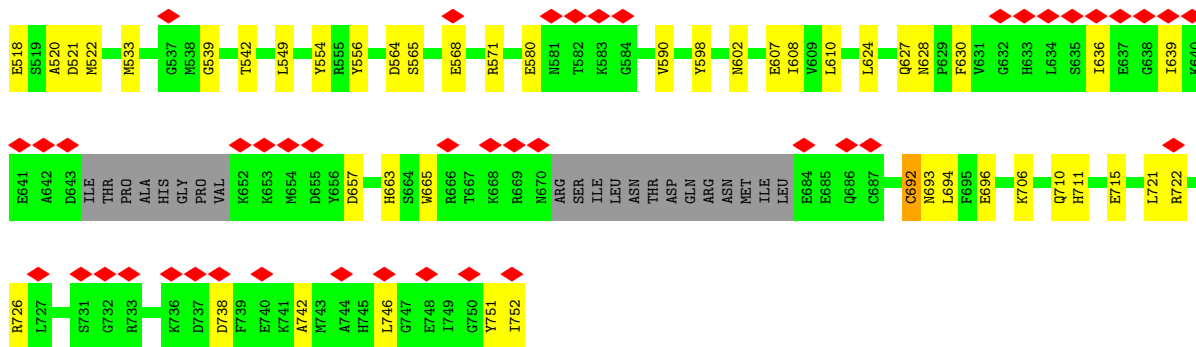
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Chain	Residue	Modelled	Actual	Comment	Reference
C	782	GLY	-	expression tag	UNP Q5V8X3
C	783	SER	-	expression tag	UNP Q5V8X3
C	784	GLY	-	expression tag	UNP Q5V8X3
C	785	GLY	-	expression tag	UNP Q5V8X3
C	786	GLY	-	expression tag	UNP Q5V8X3
C	787	SER	-	expression tag	UNP Q5V8X3
C	788	GLY	-	expression tag	UNP Q5V8X3
C	789	GLY	-	expression tag	UNP Q5V8X3
C	790	SER	-	expression tag	UNP Q5V8X3
C	791	ALA	-	expression tag	UNP Q5V8X3
C	792	TRP	-	expression tag	UNP Q5V8X3
C	793	SER	-	expression tag	UNP Q5V8X3
C	794	HIS	-	expression tag	UNP Q5V8X3
C	795	PRO	-	expression tag	UNP Q5V8X3
C	796	GLN	-	expression tag	UNP Q5V8X3
C	797	PHE	-	expression tag	UNP Q5V8X3
C	798	GLU	-	expression tag	UNP Q5V8X3
C	799	LYS	-	expression tag	UNP Q5V8X3



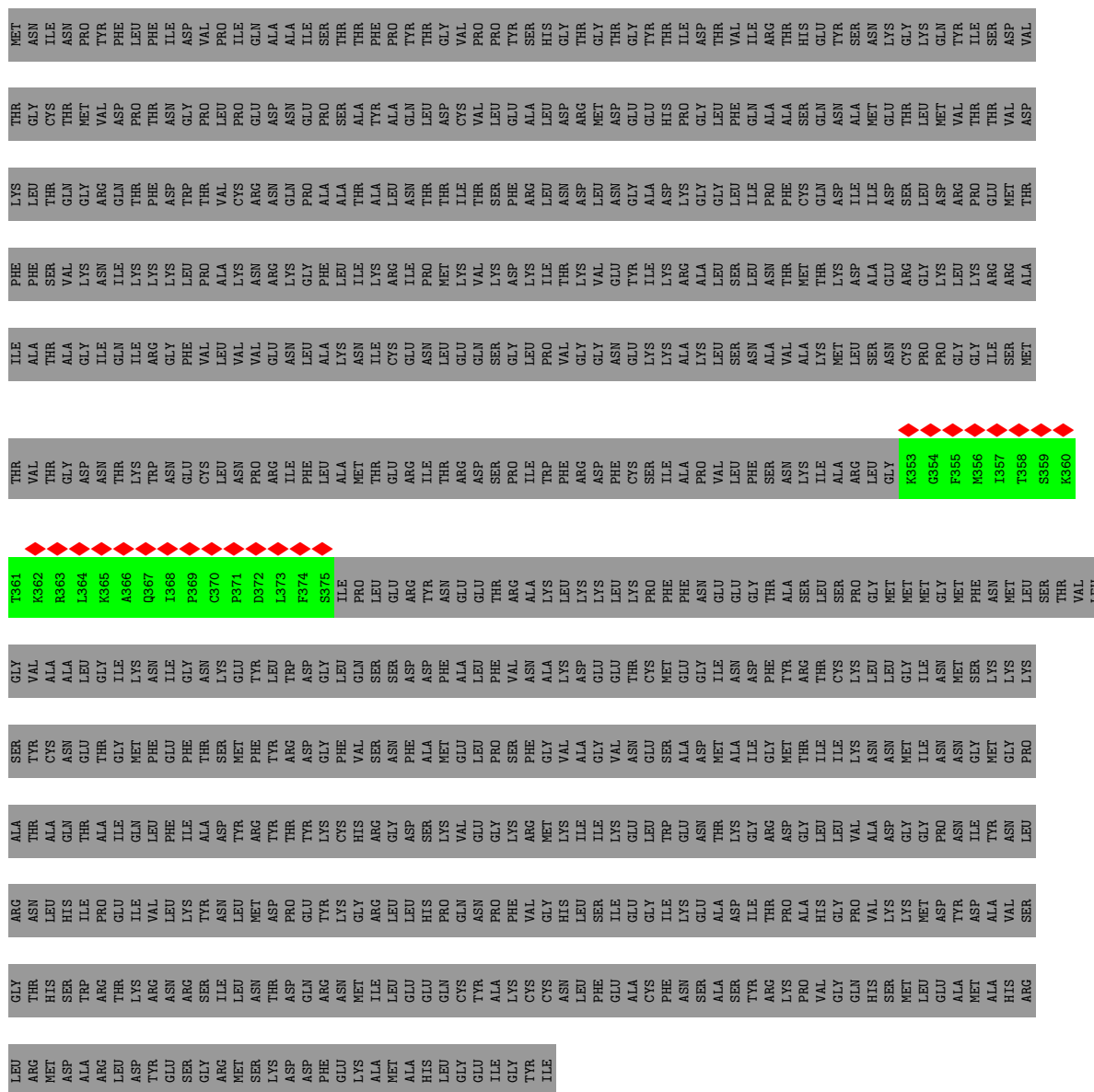
• Molecule 2: RNA-directed RNA polymerase catalytic subunit



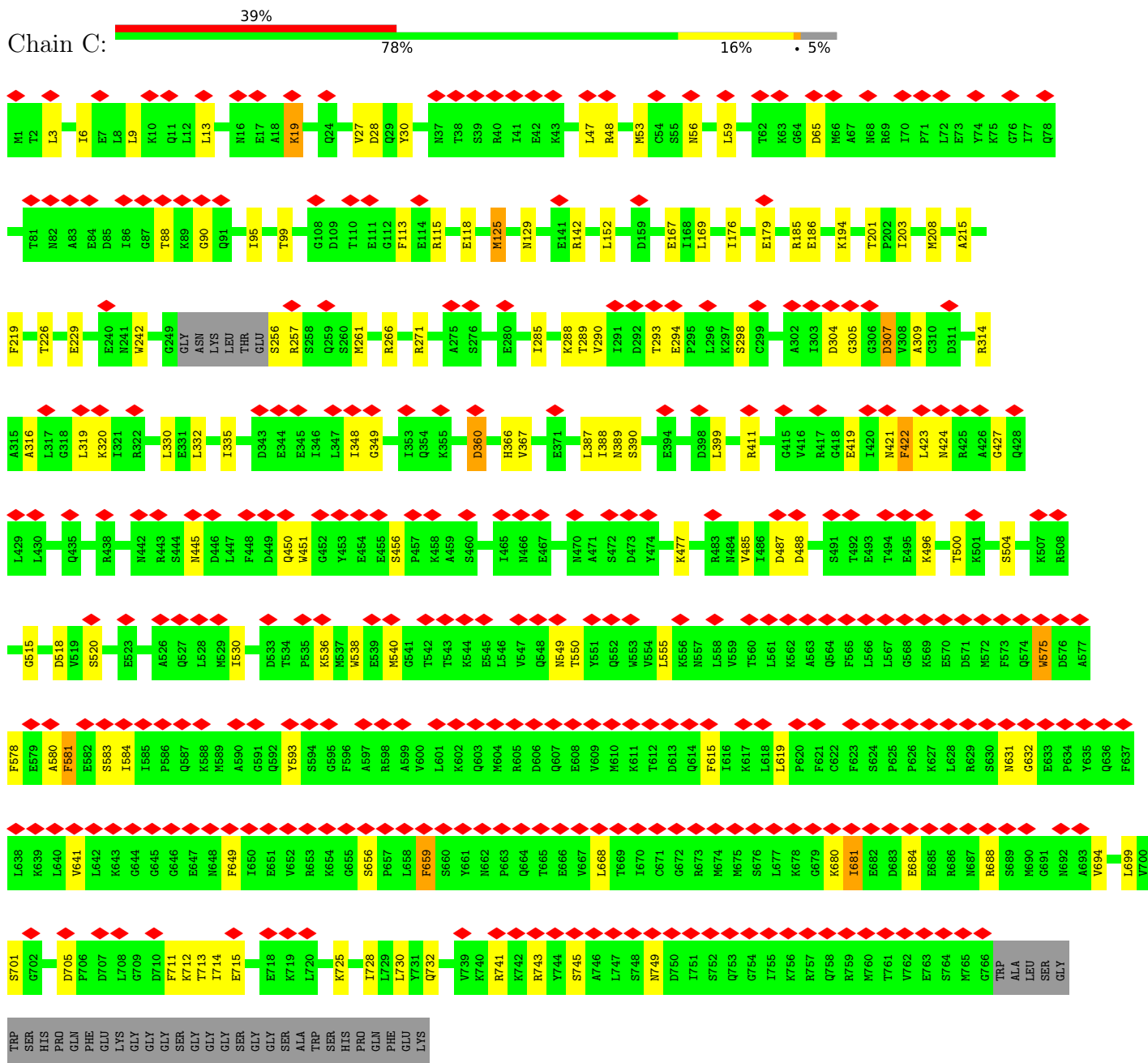


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain D:  97%



• Molecule 3: Polymerase basic protein 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24051	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.970	Depositor
Minimum map value	-2.031	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.086	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	430.08, 430.08, 430.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.26	0/5863	0.46	0/7906
1	E	0.24	0/231	0.41	0/311
2	B	0.27	0/5743	0.49	0/7735
2	D	0.24	0/184	0.47	0/244
3	C	0.25	0/6187	0.51	0/8312
All	All	0.26	0/18208	0.49	0/24508

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	722	ARG	Sidechain

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	5746	5724	5724	96	0
1	E	228	218	218	3	0
2	B	5636	5636	5635	118	0
2	D	181	198	198	0	0
3	C	6085	6250	6250	100	0
All	All	17876	18026	18025	259	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 7.

All (259) 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:187:TRP:NE1	2:B:710:GLN:OE1	1.79	1.14
1:A:187:TRP:CE2	2:B:710:GLN:OE1	2.25	0.88
2:B:146:THR:HG21	2:B:246:ILE:HG21	1.57	0.87
3:C:186:GLU:OE1	3:C:293:THR:OG1	1.93	0.86
3:C:185:ARG:NH2	3:C:688:ARG:O	2.10	0.83
2:B:154:ASP:O	2:B:176:ARG:NH2	2.12	0.81
3:C:580:ALA:O	3:C:583:SER:OG	1.99	0.80
1:A:207:THR:OG1	2:B:175:ASP:OD1	1.99	0.80
3:C:125:MET:SD	3:C:129:ASN:ND2	2.55	0.80
2:B:746:LEU:HG	3:C:6:ILE:HD11	1.64	0.79
1:A:277:VAL:HG21	1:A:697:ILE:HD13	1.62	0.79
1:A:298:LYS:NZ	2:B:568:GLU:OE2	2.17	0.78
2:B:266:LEU:HD13	2:B:422:VAL:HG11	1.66	0.78
3:C:285:ILE:O	3:C:289:THR:OG1	2.02	0.78
1:A:229:TYR:OH	2:B:86:ASP:OD2	2.03	0.76
2:B:124:GLN:O	2:B:249:ARG:NH2	2.17	0.76
1:A:284:LEU:O	1:A:457:LYS:NZ	2.18	0.76
2:B:299:SER:O	2:B:486:THR:OG1	2.04	0.76
2:B:284:ASN:ND2	3:C:488:ASP:OD1	2.20	0.75
2:B:251:PHE:O	2:B:255:VAL:HG23	1.86	0.75
1:A:644:TYR:CD1	2:B:26:GLY:HA2	2.22	0.74
1:A:700:ALA:O	1:A:704:ASN:ND2	2.21	0.74
2:B:738:ASP:HB3	3:C:3:LEU:HD11	1.69	0.73
1:A:566:GLN:HG2	2:B:27:VAL:HG11	1.70	0.72
1:A:484:ARG:NH2	1:A:494:ASP:OD2	2.22	0.72
2:B:210:ASP:OD1	2:B:211:LYS:N	2.22	0.72
2:B:284:ASN:ND2	3:C:487:ASP:O	2.22	0.71
1:A:423:GLU:N	1:A:423:GLU:OE1	2.25	0.69
3:C:549:ASN:OD1	3:C:550:THR:N	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:THR:HG21	2:B:404:LEU:HD11	1.72	0.69
3:C:229:GLU:N	3:C:229:GLU:OE1	2.26	0.68
2:B:146:THR:HG21	2:B:246:ILE:CG2	2.24	0.68
3:C:9:LEU:HD12	3:C:13:LEU:HD23	1.77	0.67
1:A:445:GLU:OE2	1:A:634:ARG:NE	2.26	0.67
2:B:438:ASP:OD1	2:B:439:GLY:N	2.27	0.67
3:C:615:PHE:CE1	3:C:619:LEU:HD12	2.30	0.67
1:A:324:LEU:HD22	1:A:333:GLU:OE1	1.95	0.67
3:C:332:LEU:HD23	3:C:367:VAL:HG12	1.76	0.66
1:A:582:GLN:HA	2:B:542:THR:HG21	1.77	0.66
3:C:288:LYS:NZ	3:C:749:ASN:OD1	2.29	0.66
1:A:644:TYR:HD1	2:B:26:GLY:HA2	1.58	0.66
2:B:136:ASN:OD1	2:B:225:ASN:ND2	2.28	0.66
2:B:515:GLY:N	2:B:521:ASP:OD2	2.29	0.65
3:C:142:ARG:O	3:C:485:VAL:HG11	1.95	0.65
3:C:332:LEU:CD2	3:C:367:VAL:HG12	2.27	0.65
2:B:738:ASP:CB	3:C:3:LEU:HD11	2.26	0.65
3:C:266:ARG:NH1	3:C:520:SER:O	2.31	0.64
1:A:279:TYR:OH	1:A:283:LEU:O	2.15	0.64
1:A:319:GLN:O	1:A:341:ARG:NH1	2.32	0.63
2:B:746:LEU:CG	3:C:6:ILE:HD11	2.30	0.62
3:C:305:GLY:O	3:C:314:ARG:NH2	2.31	0.62
3:C:500:THR:HG22	3:C:504:SER:O	1.99	0.62
1:A:149:SER:OG	1:A:153:ASP:OD1	2.04	0.61
1:A:388:GLN:OE1	2:B:382:ASN:ND2	2.33	0.61
2:B:627:GLN:OE1	2:B:628:ASN:N	2.34	0.60
1:A:187:TRP:CD1	2:B:710:GLN:OE1	2.53	0.60
1:A:570:GLY:HA2	1:A:644:TYR:OH	2.01	0.60
2:B:326:THR:O	2:B:334:ARG:NH1	2.32	0.60
3:C:176:ILE:CD1	3:C:730:LEU:HD21	2.32	0.60
1:A:240:GLU:OE2	2:B:431:GLY:N	2.34	0.60
1:A:324:LEU:HD21	1:A:327:LYS:HB2	1.83	0.59
2:B:636:ILE:HG23	2:B:639:ILE:HD12	1.83	0.59
1:A:411:SER:O	1:A:631:LYS:NZ	2.35	0.59
2:B:665:TRP:CG	3:C:59:LEU:HD11	2.37	0.59
1:A:36:PHE:O	1:A:40:VAL:HG23	2.02	0.59
1:A:293:ASN:ND2	1:A:308:GLU:OE1	2.35	0.59
2:B:696:GLU:OE2	3:C:30:TYR:OH	2.21	0.59
1:A:507:LEU:HD13	1:A:512:ASP:HB2	1.85	0.58
3:C:530:ILE:HG23	3:C:530:ILE:O	2.03	0.58
2:B:746:LEU:HG	3:C:6:ILE:CD1	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:631:ASN:OD1	3:C:632:GLY:N	2.36	0.58
2:B:45:ARG:NH1	2:B:311:GLU:OE1	2.36	0.58
2:B:64:THR:O	2:B:403:SER:OG	2.19	0.58
3:C:118:GLU:OE1	3:C:194:LYS:NZ	2.21	0.58
1:A:11:THR:OG1	3:C:316:ALA:O	2.09	0.58
3:C:515:GLY:N	3:C:518:ASP:OD2	2.36	0.58
3:C:335:ILE:HD11	3:C:366:HIS:CE1	2.38	0.58
2:B:154:ASP:O	2:B:154:ASP:OD1	2.22	0.57
2:B:706:LYS:NZ	3:C:28:ASP:O	2.37	0.57
3:C:266:ARG:NH1	3:C:520:SER:OG	2.38	0.57
1:A:411:SER:O	1:A:411:SER:OG	2.20	0.57
2:B:726:ARG:NH2	3:C:711:PHE:O	2.37	0.57
3:C:593:TYR:OH	3:C:641:VAL:HG12	2.05	0.57
2:B:266:LEU:HD13	2:B:422:VAL:CG1	2.35	0.56
1:A:507:LEU:HD22	1:A:512:ASP:HB3	1.87	0.56
2:B:492:THR:O	2:B:493:SER:OG	2.22	0.56
1:A:483:ASN:OD1	1:A:484:ARG:N	2.38	0.56
1:A:599:MET:O	1:A:602:ALA:N	2.39	0.55
2:B:415:MET:O	2:B:419:VAL:HG23	2.05	0.55
2:B:746:LEU:CD2	3:C:6:ILE:HD11	2.36	0.55
2:B:564:ASP:OD1	2:B:565:SER:N	2.40	0.54
1:A:334:ASN:ND2	1:E:384:GLU:OE2	2.41	0.54
2:B:694:LEU:HD21	3:C:9:LEU:HD13	1.89	0.54
1:A:296:GLU:N	1:A:296:GLU:OE1	2.40	0.54
1:A:501:VAL:HG22	1:A:517:VAL:HB	1.90	0.54
1:A:574:ARG:HD2	2:B:549:LEU:HD22	1.89	0.54
2:B:166:PHE:O	2:B:169:ASP:OD1	2.25	0.54
1:A:399:VAL:HA	1:A:697:ILE:HD12	1.90	0.54
1:A:693:ASN:O	1:A:697:ILE:HG23	2.07	0.53
2:B:715:GLU:HB2	2:B:751:TYR:CD1	2.43	0.53
2:B:636:ILE:HD11	3:C:201:THR:HG21	1.89	0.53
1:A:421:LEU:HD22	2:B:549:LEU:HD23	1.91	0.53
2:B:84:GLN:O	2:B:88:VAL:HG23	2.09	0.53
1:A:87:ILE:O	1:A:91:VAL:HG23	2.09	0.53
1:A:359:THR:HG22	1:A:359:THR:O	2.08	0.52
1:A:660:ARG:NH1	2:B:305:ASP:OD2	2.42	0.52
1:A:332:ASN:ND2	1:E:382:ASP:O	2.39	0.52
2:B:87:CYS:SG	2:B:472:LEU:HD21	2.49	0.52
3:C:732:GLN:N	3:C:732:GLN:OE1	2.43	0.52
1:A:387:CYS:O	2:B:358:THR:N	2.40	0.52
1:A:277:VAL:CG2	1:A:697:ILE:HD13	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:LEU:N	2:B:348:ILE:O	2.42	0.51
3:C:307:ASP:OD1	3:C:309:ALA:N	2.40	0.51
1:A:506:HIS:O	1:A:506:HIS:ND1	2.41	0.51
2:B:504:PHE:CE2	2:B:506:MET:HB3	2.45	0.51
2:B:518:GLU:OE1	2:B:663:HIS:ND1	2.41	0.51
1:A:368:ASP:OD2	1:A:476:TYR:OH	2.13	0.51
2:B:602:ASN:ND2	2:B:610:LEU:HD11	2.25	0.51
3:C:411:ARG:O	3:C:450:GLN:NE2	2.44	0.51
2:B:742:ALA:HB2	3:C:3:LEU:HD23	1.93	0.51
2:B:232:GLU:OE2	2:B:235:LYS:NZ	2.34	0.51
1:A:487:ASN:OD1	1:A:491:GLU:N	2.41	0.50
1:A:381:ILE:HD11	2:B:368:ILE:HD12	1.94	0.50
2:B:711:HIS:O	3:C:27:VAL:HG23	2.12	0.50
1:A:468:GLU:OE2	1:A:477:LYS:NZ	2.37	0.50
2:B:22:PHE:CD1	2:B:504:PHE:CE1	2.99	0.50
3:C:419:GLU:OE2	3:C:421:ASN:ND2	2.45	0.49
1:A:507:LEU:HD22	1:A:512:ASP:CB	2.42	0.49
3:C:256:SER:OG	3:C:257:ARG:N	2.46	0.49
3:C:615:PHE:CZ	3:C:619:LEU:HD12	2.48	0.49
1:A:62:THR:HG21	3:C:743:ARG:NH1	2.28	0.49
3:C:705:ASP:OD1	3:C:725:LYS:NZ	2.29	0.49
1:A:84:PRO:HG2	1:A:87:ILE:HD12	1.96	0.48
2:B:340:ALA:HB3	2:B:341:PRO:HD3	1.95	0.48
3:C:9:LEU:HD12	3:C:13:LEU:CD2	2.41	0.48
2:B:291:SER:HB3	3:C:387:LEU:HD12	1.95	0.48
1:A:354:ASN:ND2	1:A:468:GLU:OE2	2.43	0.48
1:A:222:ASN:N	1:A:222:ASN:OD1	2.47	0.48
2:B:88:VAL:HG22	2:B:472:LEU:HD22	1.96	0.48
2:B:120:ASP:O	2:B:123:THR:HG22	2.14	0.48
2:B:539:GLY:O	2:B:542:THR:OG1	2.25	0.48
3:C:713:THR:HG22	3:C:714:ILE:H	1.77	0.48
1:A:624:LEU:HD23	1:A:624:LEU:H	1.79	0.48
3:C:53:MET:CE	3:C:95:ILE:HD13	2.44	0.48
1:A:327:LYS:HA	1:A:537:THR:HG23	1.96	0.47
1:A:565:ILE:HG22	2:B:27:VAL:HG13	1.96	0.47
1:A:675:TRP:HB2	2:B:459:MET:HE1	1.96	0.47
3:C:152:LEU:HD11	3:C:215:ALA:HA	1.96	0.47
2:B:282:LEU:HD11	2:B:489:PHE:CE2	2.49	0.47
3:C:179:GLU:O	3:C:179:GLU:OE1	2.31	0.47
1:A:414:THR:N	1:A:448:TYR:O	2.39	0.47
1:A:257:LEU:HD23	1:A:664:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LEU:HD23	1:A:567:MET:SD	2.54	0.47
2:B:225:ASN:OD1	2:B:226:THR:N	2.47	0.47
1:A:51:MET:HG2	1:A:62:THR:HG23	1.96	0.47
1:A:439:ARG:O	1:A:443:VAL:HG22	2.14	0.47
3:C:88:THR:HG23	3:C:90:GLY:H	1.79	0.47
3:C:179:GLU:O	3:C:179:GLU:CD	2.53	0.47
3:C:167:GLU:OE1	3:C:694:VAL:HG12	2.15	0.47
3:C:257:ARG:NH1	3:C:294:GLU:OE2	2.47	0.47
3:C:581:PHE:CD1	3:C:584:ILE:HD11	2.50	0.47
1:A:446:ILE:HD11	1:A:633:LEU:HG	1.97	0.46
2:B:69:THR:HG23	2:B:317:ILE:HD11	1.95	0.46
2:B:715:GLU:HB2	2:B:751:TYR:CE1	2.50	0.46
3:C:289:THR:HG22	3:C:290:VAL:H	1.81	0.46
2:B:310:ASN:OD1	2:B:310:ASN:N	2.49	0.46
1:A:136:LYS:O	1:A:140:GLY:N	2.45	0.46
3:C:257:ARG:O	3:C:261:MET:HG2	2.15	0.46
3:C:741:ARG:NH2	3:C:745:SER:OG	2.48	0.46
2:B:282:LEU:HD11	2:B:489:PHE:CZ	2.51	0.46
3:C:208:MET:HA	3:C:208:MET:HE2	1.96	0.46
1:A:584:MET:HG3	1:A:633:LEU:HD13	1.98	0.45
1:A:694:PRO:O	1:A:697:ILE:HG12	2.16	0.45
2:B:742:ALA:HB2	3:C:3:LEU:CD2	2.46	0.45
2:B:738:ASP:O	3:C:3:LEU:HD21	2.16	0.45
2:B:746:LEU:HB3	2:B:752:ILE:HD11	1.98	0.45
3:C:424:ASN:OD1	3:C:427:GLY:N	2.50	0.45
2:B:636:ILE:HG22	2:B:636:ILE:O	2.15	0.45
1:A:250:VAL:O	1:A:251:SER:OG	2.30	0.45
2:B:152:LEU:HD11	2:B:182:PHE:CZ	2.51	0.45
1:A:227:ARG:NH2	2:B:335:ASP:OD1	2.46	0.45
2:B:624:LEU:HD22	3:C:113:PHE:CZ	2.52	0.45
1:A:222:ASN:ND2	1:A:224:GLU:OE2	2.50	0.45
1:A:663:LEU:HD11	2:B:495:PHE:HE2	1.83	0.44
3:C:289:THR:O	3:C:290:VAL:HG23	2.17	0.44
2:B:114:LEU:HG	2:B:164:ILE:HD11	2.00	0.44
1:A:525:ASP:O	1:A:528:VAL:HG12	2.17	0.44
2:B:40:ILE:HG23	2:B:392:LEU:HD22	1.99	0.44
2:B:516:VAL:HG23	2:B:520:ALA:HB3	1.99	0.44
1:A:538:VAL:HG12	1:A:556:TYR:HA	1.99	0.44
2:B:571:ARG:NE	3:C:99:THR:OG1	2.51	0.44
3:C:578:PHE:CZ	3:C:619:LEU:HD22	2.53	0.44
2:B:131:TRP:O	2:B:220:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:692:CYS:SG	2:B:693:ASN:N	2.91	0.43
3:C:48:ARG:O	3:C:48:ARG:HD3	2.17	0.43
2:B:252:VAL:HG23	2:B:413:PHE:CE1	2.53	0.43
2:B:608:ILE:HD12	2:B:608:ILE:H	1.83	0.43
2:B:454:ASP:OD1	2:B:454:ASP:N	2.51	0.43
2:B:746:LEU:HB3	2:B:752:ILE:CD1	2.48	0.43
2:B:752:ILE:O	2:B:752:ILE:HG22	2.17	0.43
2:B:116:VAL:HG12	2:B:116:VAL:O	2.19	0.43
1:A:616:SER:N	2:B:11:ASP:OD2	2.51	0.42
1:A:389:GLU:HG2	2:B:358:THR:HG22	2.00	0.42
2:B:248:ILE:O	2:B:248:ILE:HG22	2.19	0.42
1:A:295:THR:OG1	1:A:494:ASP:OD1	2.28	0.42
2:B:170:ILE:O	2:B:174:LEU:HD12	2.20	0.42
2:B:580:GLU:OE1	2:B:580:GLU:N	2.43	0.42
1:A:339:LEU:HD21	1:A:501:VAL:HG21	2.02	0.42
1:A:431:VAL:HG21	3:C:242:TRP:CZ3	2.54	0.42
1:A:501:VAL:O	1:A:501:VAL:HG23	2.19	0.42
1:A:624:LEU:H	1:A:624:LEU:CD2	2.33	0.42
3:C:445:ASN:O	3:C:445:ASN:ND2	2.52	0.42
1:A:364:TRP:CD1	1:E:379:VAL:HG11	2.55	0.42
1:A:568:LYS:HB2	3:C:47:LEU:HD21	2.01	0.42
2:B:358:THR:OG1	2:B:364:LEU:O	2.19	0.42
2:B:154:ASP:C	2:B:155:LEU:HD22	2.40	0.42
3:C:226:THR:O	3:C:226:THR:HG22	2.20	0.41
3:C:330:LEU:HD21	3:C:399:LEU:HD12	2.02	0.41
1:A:584:MET:CG	1:A:633:LEU:HD13	2.51	0.41
1:A:168:GLY:HA2	3:C:701:SER:HG	1.85	0.41
1:A:253:THR:O	1:A:253:THR:OG1	2.33	0.41
3:C:271:ARG:NH2	3:C:536:LYS:O	2.52	0.41
2:B:92:LEU:HD11	2:B:321:MET:HG2	2.02	0.41
2:B:291:SER:CB	3:C:387:LEU:HD12	2.51	0.41
2:B:347:LYS:NZ	2:B:405:SER:O	2.53	0.41
3:C:555:LEU:HD22	3:C:688:ARG:HH22	1.84	0.41
3:C:680:LYS:O	3:C:681:ILE:HB	2.21	0.41
3:C:728:ILE:HD12	3:C:728:ILE:HA	1.96	0.41
1:A:265:ILE:N	1:A:704:ASN:OD1	2.54	0.41
2:B:46:THR:CG2	2:B:404:LEU:HD11	2.46	0.41
2:B:408:MET:HE1	2:B:413:PHE:HB2	2.03	0.41
2:B:554:TYR:CE1	2:B:590:VAL:HG23	2.56	0.41
3:C:451:TRP:NE1	3:C:477:LYS:HB3	2.36	0.41
1:A:169:ARG:HA	3:C:699:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:388:ILE:HG22	3:C:389:ASN:N	2.36	0.41
3:C:659:PHE:CE1	3:C:668:LEU:HD11	2.55	0.41
1:A:62:THR:HG21	3:C:743:ARG:CZ	2.50	0.41
2:B:522:MET:CE	2:B:607:GLU:OE1	2.68	0.41
3:C:13:LEU:HD12	3:C:19:LYS:HG3	2.01	0.41
2:B:3:ILE:HG22	2:B:4:ASN:N	2.36	0.41
3:C:314:ARG:HD3	3:C:319:LEU:HD13	2.03	0.41
3:C:348:ILE:HG22	3:C:349:GLY:N	2.36	0.41
3:C:360:ASP:OD1	3:C:360:ASP:N	2.54	0.40
1:A:383:ASP:O	2:B:380:ARG:NH2	2.53	0.40
1:A:431:VAL:HG13	1:A:432:GLU:N	2.36	0.40
2:B:108:GLN:O	2:B:112:GLU:HG3	2.22	0.40
2:B:636:ILE:HG21	3:C:203:ILE:CG2	2.51	0.40
2:B:721:LEU:HD13	3:C:6:ILE:HD12	2.03	0.40
3:C:9:LEU:O	3:C:13:LEU:HD23	2.21	0.40
3:C:422:PHE:O	3:C:423:LEU:HD23	2.21	0.40
3:C:575:TRP:HA	3:C:575:TRP:CE3	2.55	0.40
3:C:656:SER:N	3:C:659:PHE:O	2.40	0.40
1:A:12:THR:O	1:A:16:LYS:HG2	2.21	0.40
1:A:517:VAL:HG22	1:A:559:VAL:HG12	2.04	0.40
2:B:299:SER:O	2:B:299:SER:OG	2.39	0.40
1:A:53:PHE:CD1	1:A:63:ALA:HB3	2.56	0.40
3:C:619:LEU:HD23	3:C:619:LEU:O	2.22	0.40
1:A:163:ASP:OD1	1:A:163:ASP:N	2.55	0.40
3:C:575:TRP:HA	3:C:575:TRP:HE3	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	714/726 (98%)	683 (96%)	31 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	27/726 (4%)	27 (100%)	0	0	100	100
2	B	708/752 (94%)	677 (96%)	31 (4%)	0	100	100
2	D	21/752 (3%)	21 (100%)	0	0	100	100
3	C	756/799 (95%)	710 (94%)	45 (6%)	1 (0%)	48	77
All	All	2226/3755 (59%)	2118 (95%)	107 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	681	ILE

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	635/645 (98%)	625 (98%)	10 (2%)	58	76
1	E	24/645 (4%)	24 (100%)	0	100	100
2	B	616/645 (96%)	601 (98%)	15 (2%)	44	68
2	D	21/645 (3%)	21 (100%)	0	100	100
3	C	666/693 (96%)	641 (96%)	25 (4%)	28	56
All	All	1962/3273 (60%)	1912 (98%)	50 (2%)	43	67

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	SER
1	A	360	ASN
1	A	376	MET
1	A	449	CYS
1	A	464	SER
1	A	492	SER
1	A	494	ASP

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Mol	Chain	Res	Type
1	A	543	SER
1	A	592	SER
1	A	595	GLN
2	B	87	CYS
2	B	263	CYS
2	B	278	LYS
2	B	291	SER
2	B	310	ASN
2	B	337	CYS
2	B	437	TRP
2	B	502	SER
2	B	508	LEU
2	B	533	MET
2	B	556	TYR
2	B	598	TYR
2	B	630	PHE
2	B	657	ASP
2	B	692	CYS
3	C	19	LYS
3	C	56	ASN
3	C	65	ASP
3	C	115	ARG
3	C	125	MET
3	C	169	LEU
3	C	219	PHE
3	C	298	SER
3	C	304	ASP
3	C	307	ASP
3	C	320	LYS
3	C	360	ASP
3	C	390	SER
3	C	422	PHE
3	C	456	SER
3	C	496	LYS
3	C	538	TRP
3	C	540	MET
3	C	575	TRP
3	C	581	PHE
3	C	649	PHE
3	C	659	PHE
3	C	684	GLU
3	C	712	LYS

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Mol	Chain	Res	Type
3	C	715	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	583	GLN
2	B	503	ASN
2	B	710	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

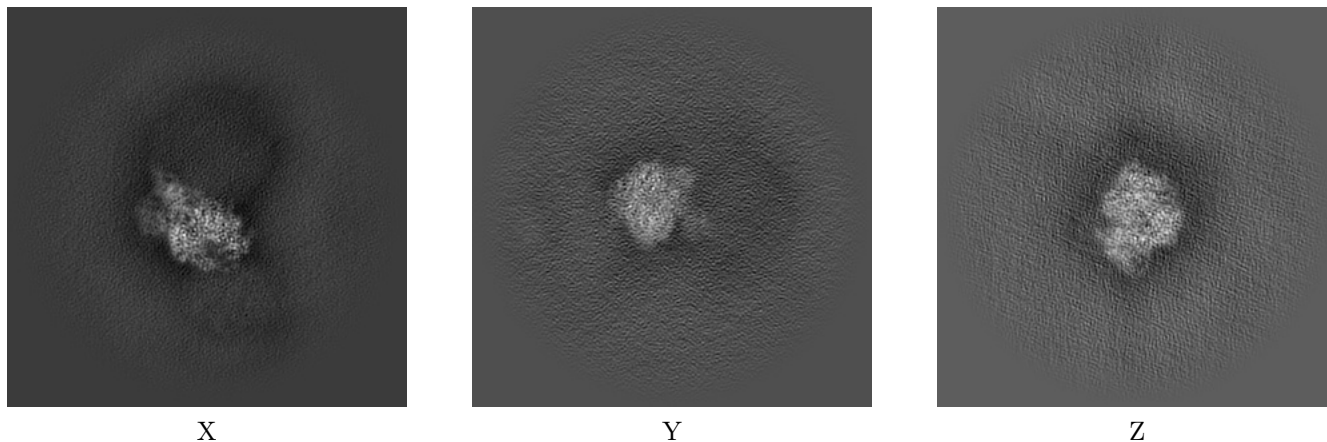
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19391. These allow visual inspection of the internal detail of the map and identification of artifacts.

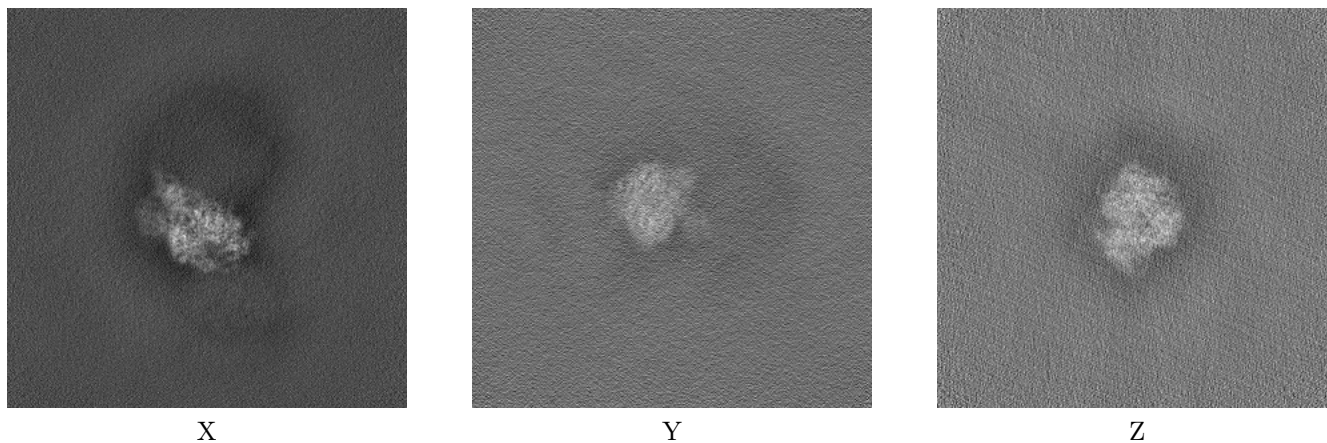
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



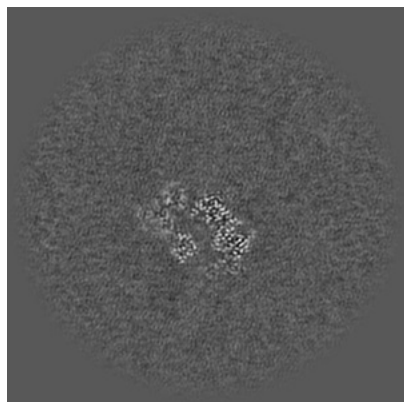
6.1.2 Raw map



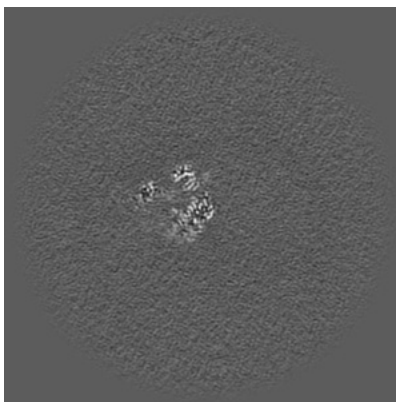
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

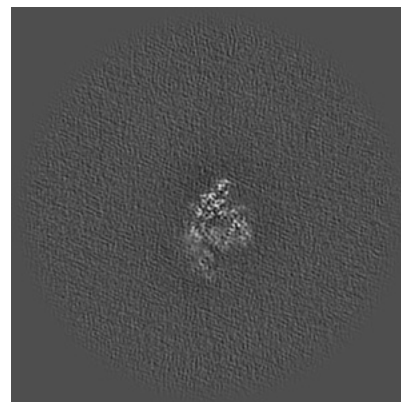
6.2.1 Primary map



X Index: 256

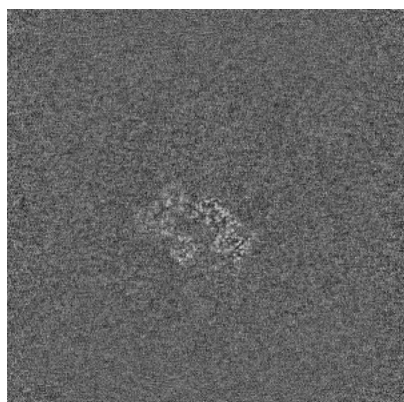


Y Index: 256

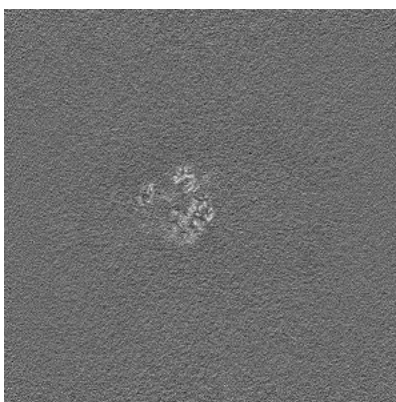


Z Index: 256

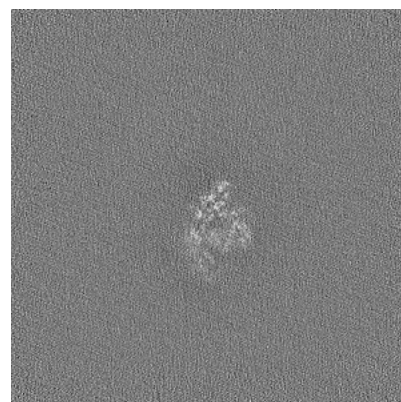
6.2.2 Raw map



X Index: 256



Y Index: 256

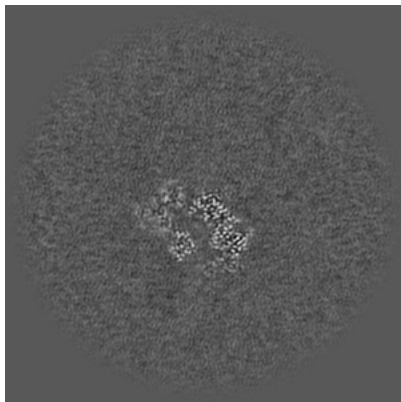


Z Index: 256

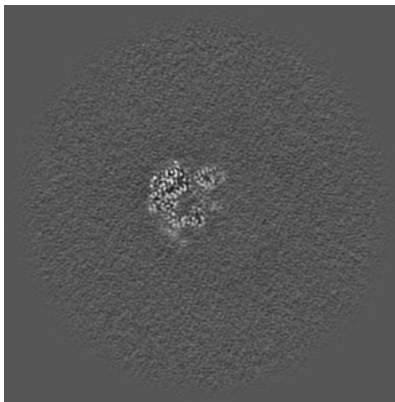
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

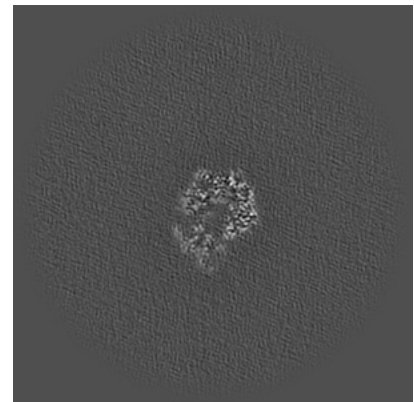
6.3.1 Primary map



X Index: 256

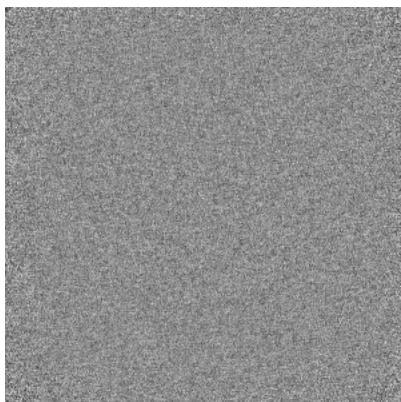


Y Index: 227

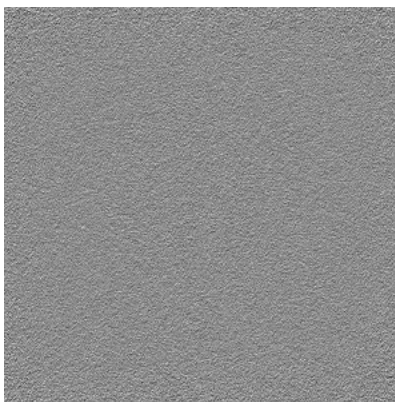


Z Index: 231

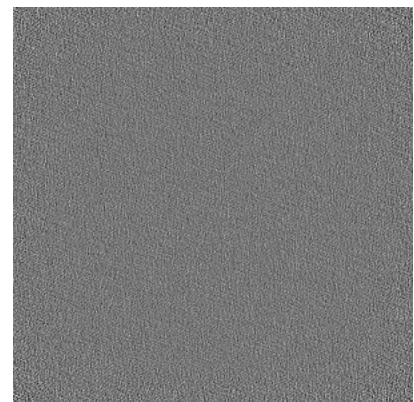
6.3.2 Raw map



X Index: 0



Y Index: 0

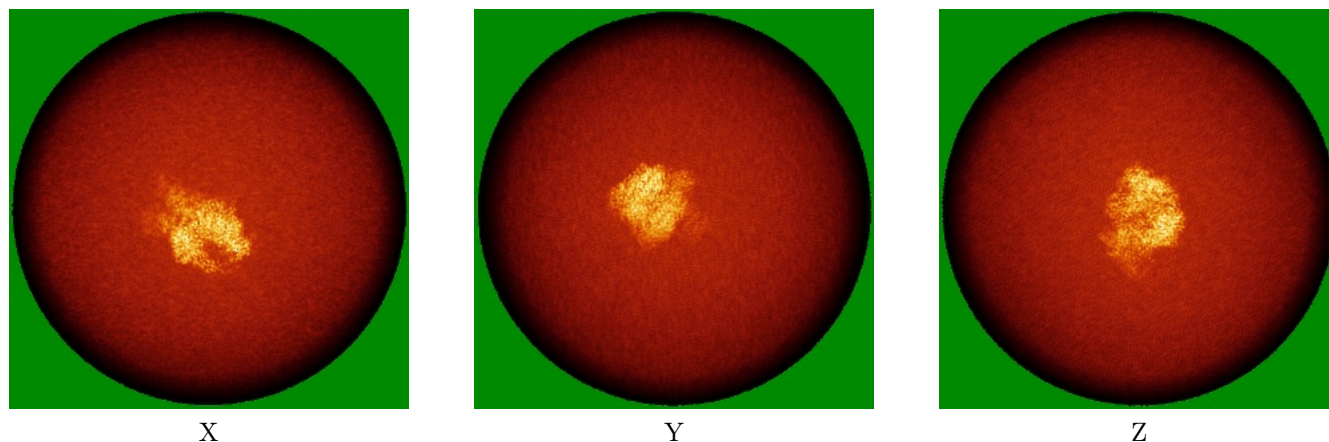


Z Index: 0

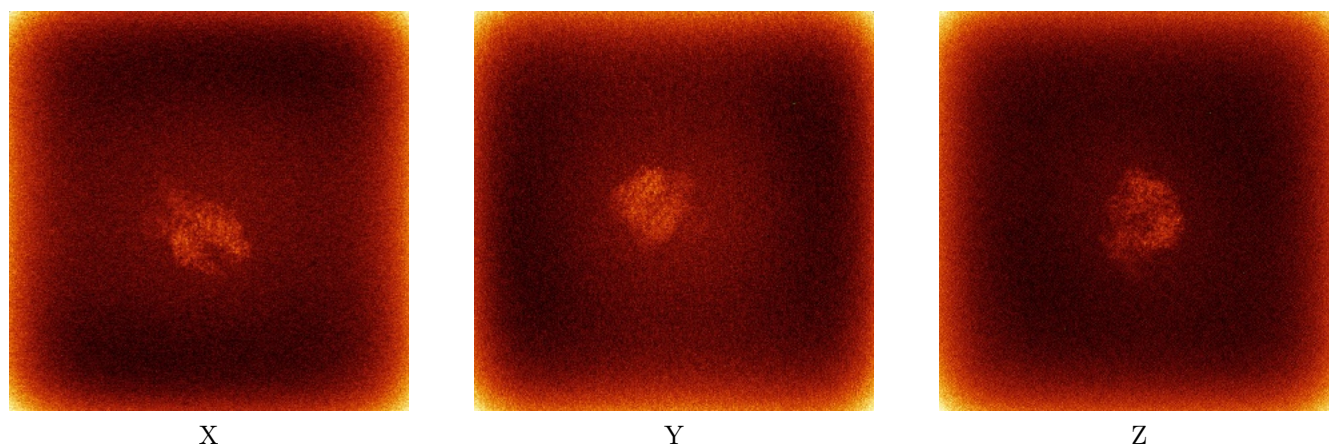
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



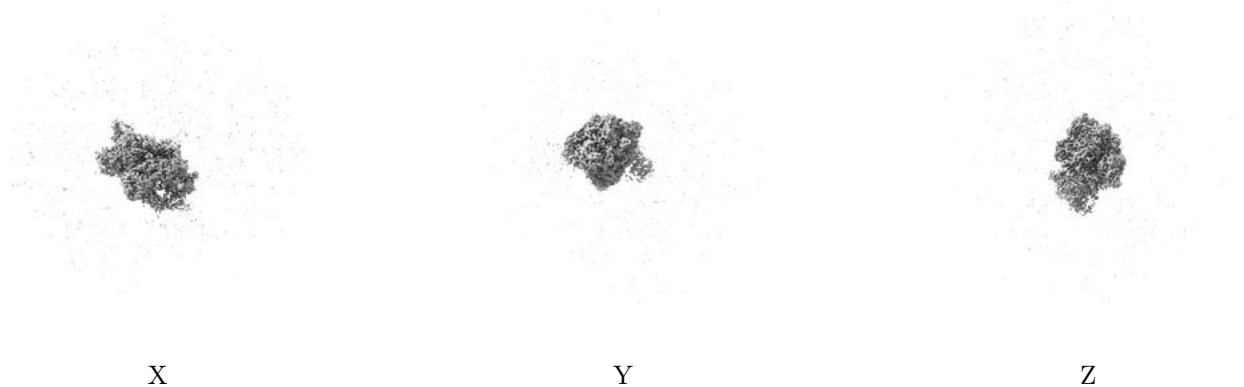
6.4.2 Raw map



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

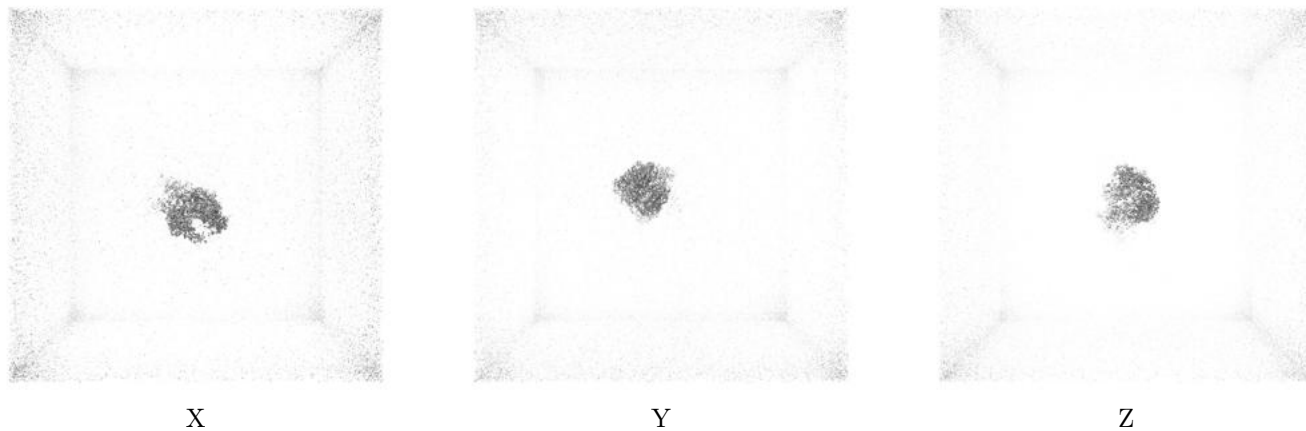
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

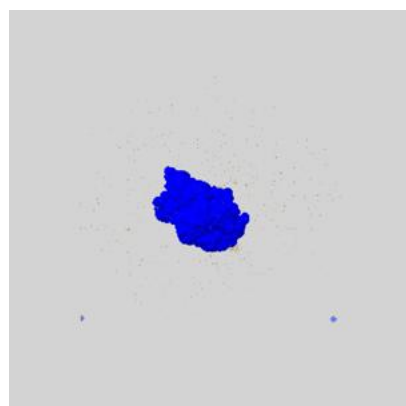
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

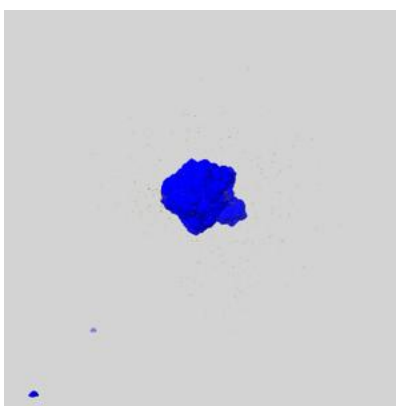
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

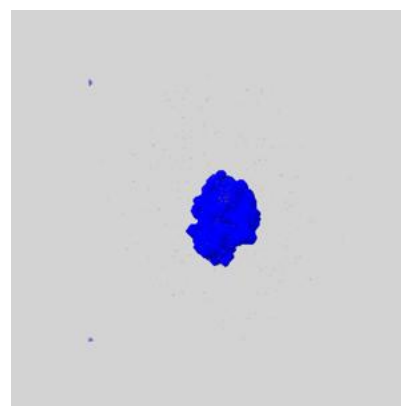
6.6.1 emd_19391_msk_1.map [i](#)



X



Y

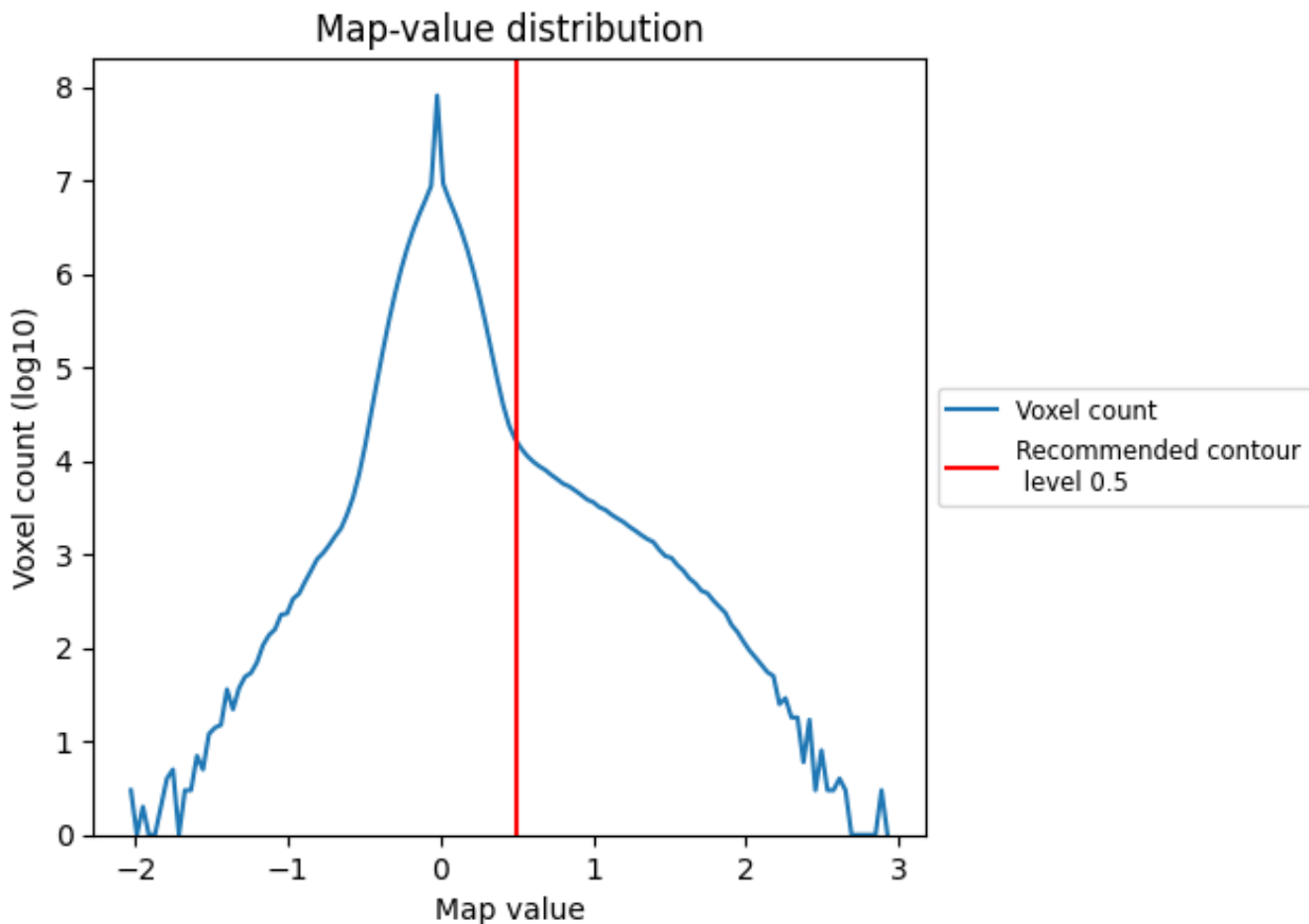


Z

7 Map analysis [i](#)

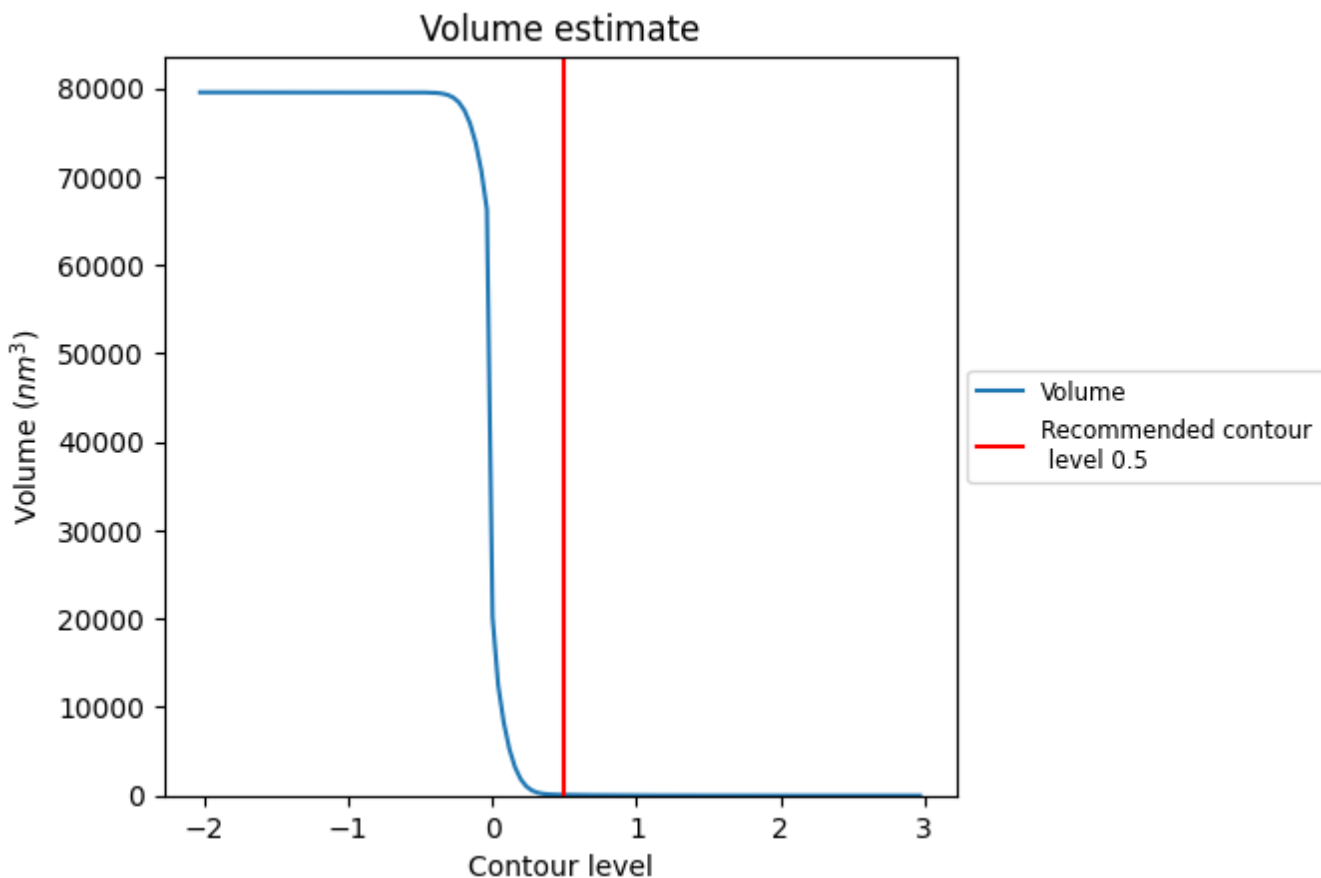
This section contains the results of statistical analysis of the map.

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.

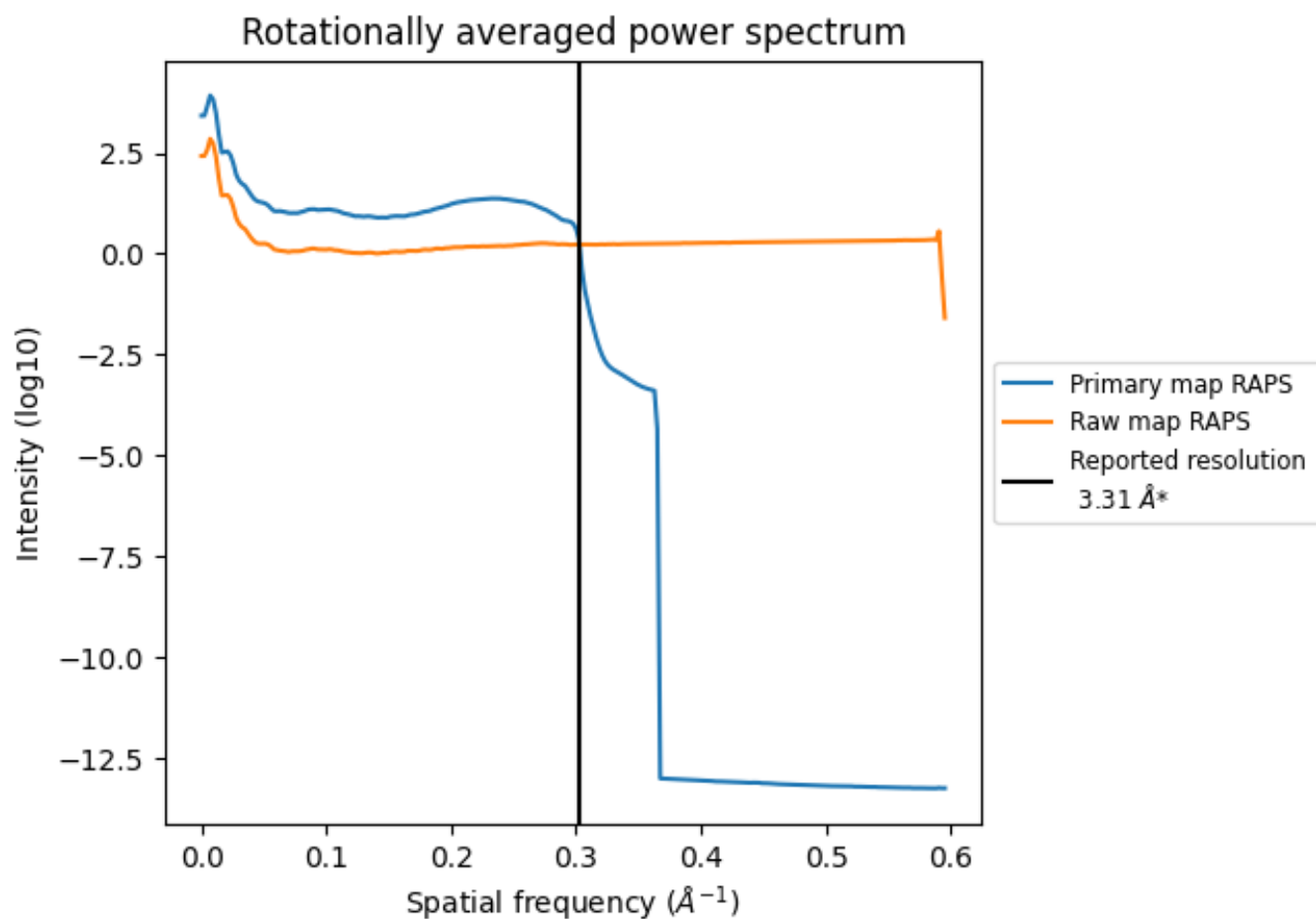
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 nm³; this corresponds to an approximate mass of 72 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](#)

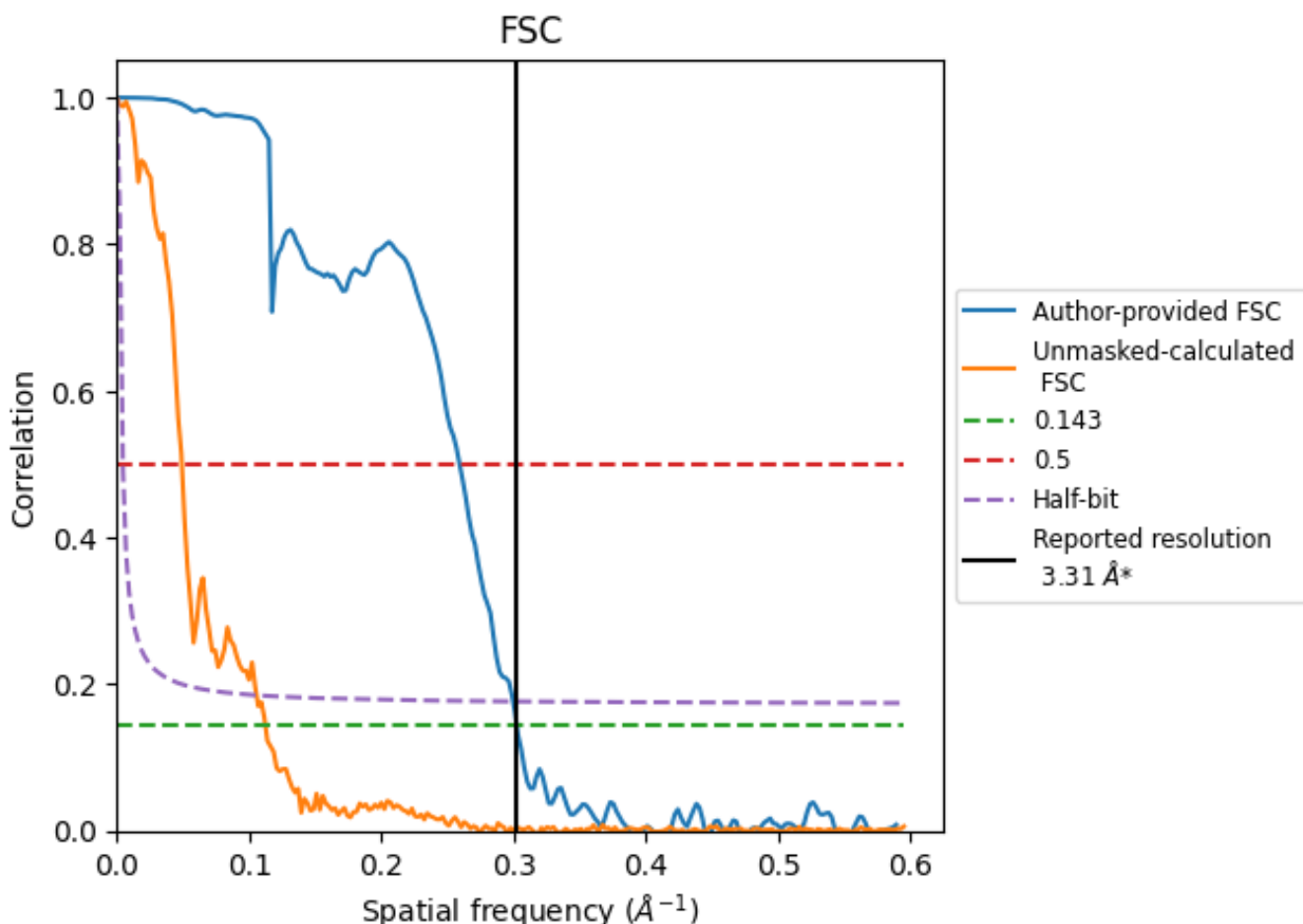


*Reported resolution corresponds to spatial frequency of 0.302 Å⁻¹

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 0.302 Å⁻¹

8.2 Resolution estimates [i](#)

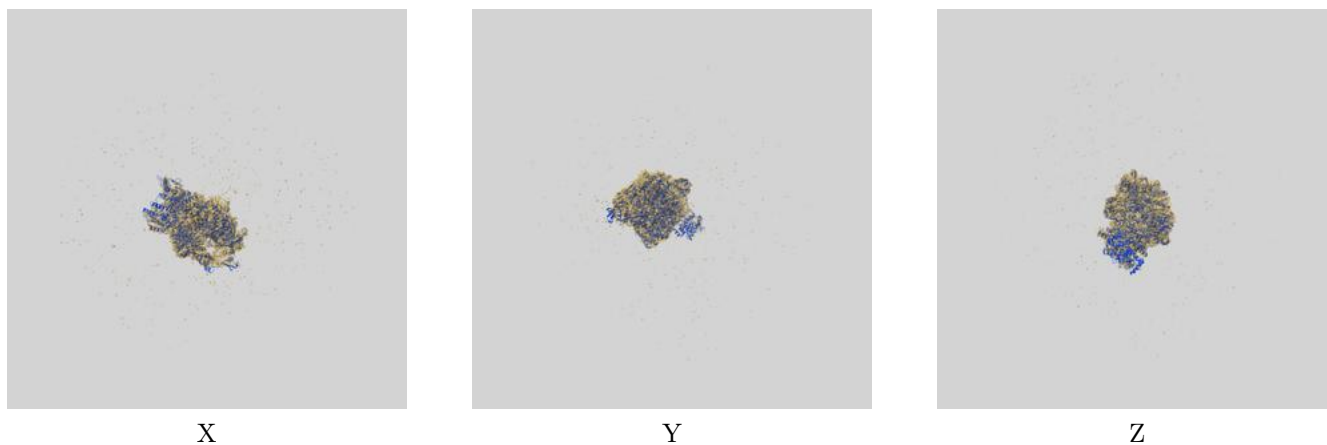
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.31	-	-
Author-provided FSC curve	3.31	3.86	3.34
Unmasked-calculated*	8.90	20.33	9.46

*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 8.90 differs from the reported value 3.31 by more than 10 %

9 Map-model fit [i](#)

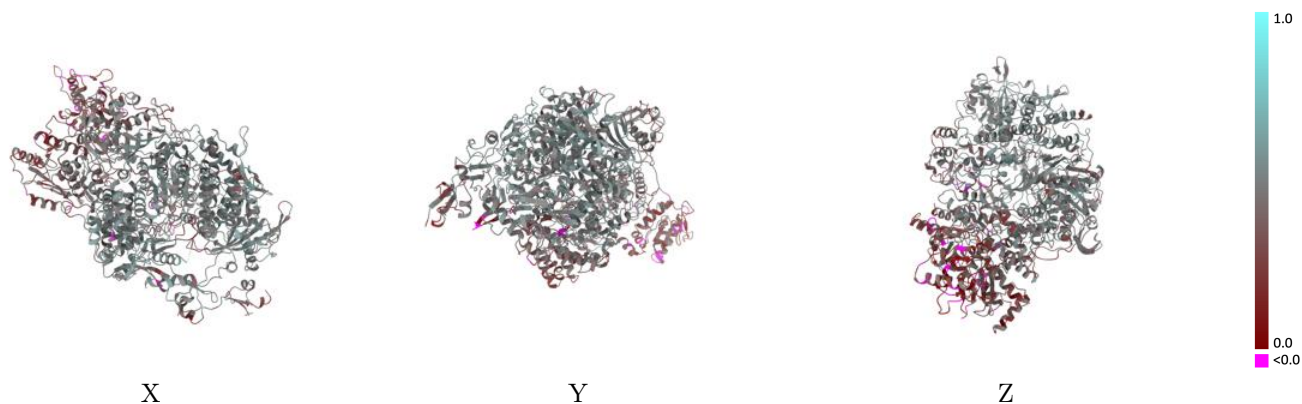
This section contains information regarding the fit between EMDB map EMD-19391 and PDB model 8RN9. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



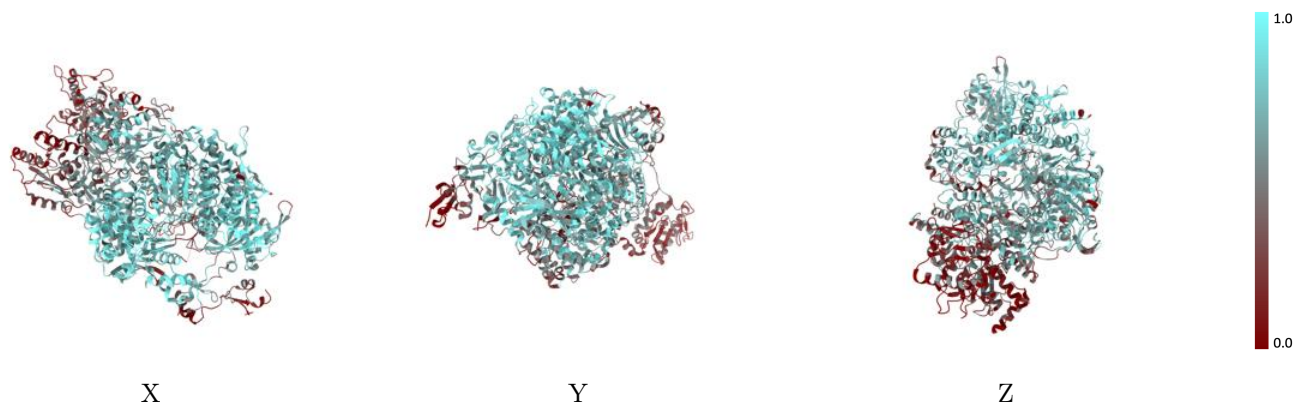
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



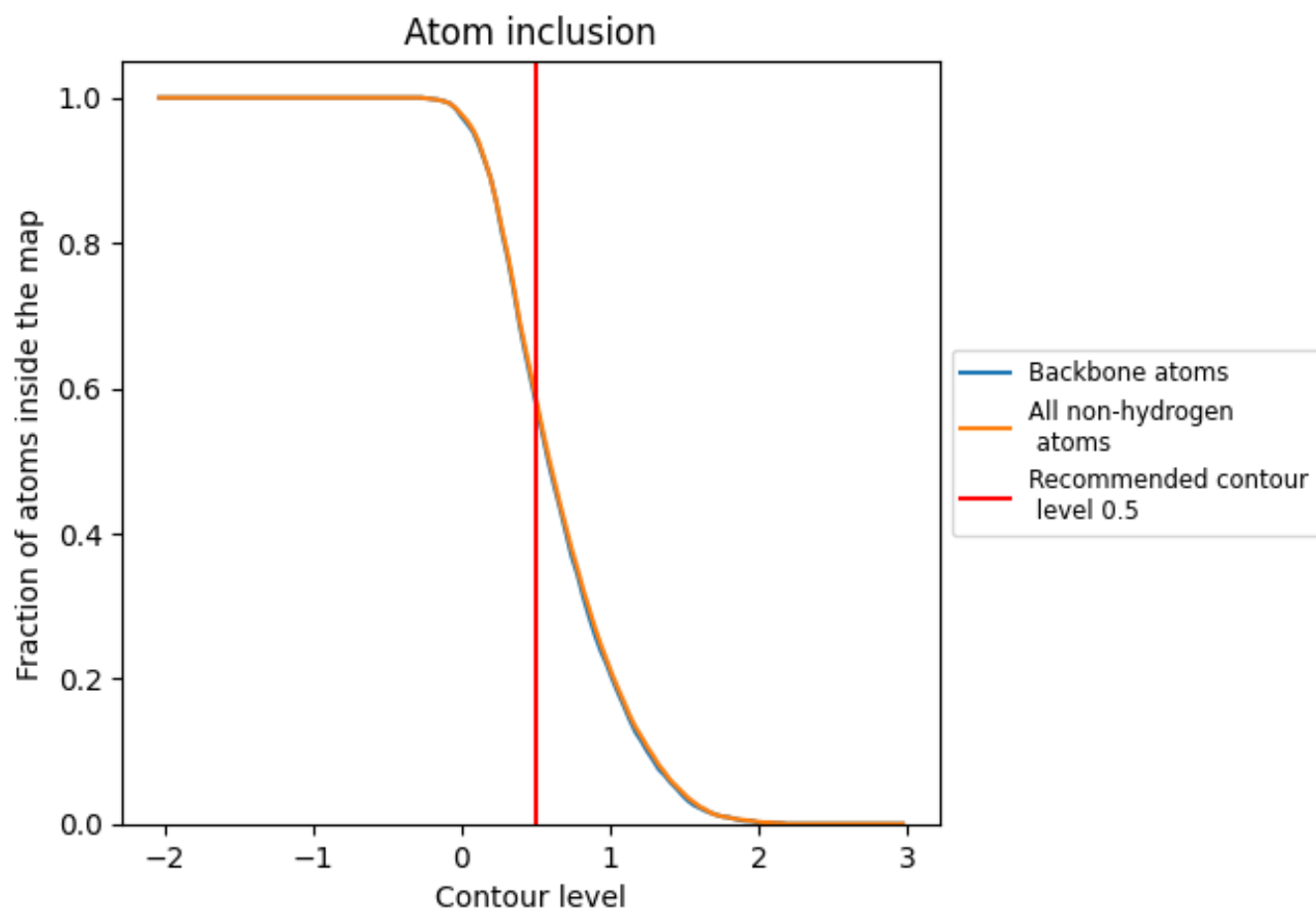
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).













9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 59% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5860	 0.4330
A	 0.6300	 0.4550
B	 0.7090	 0.4720
C	 0.4650	 0.3800
D	 0.1290	 0.3570
E	 0.1910	 0.3970

