



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 11:07 AM UTC

PDB ID : 8YQQ / pdb_00008yqq
EMDB ID : EMD-39502
Title : Structure of HKU1B RBD with TMPRSS2
Authors : Gao, X.; Cui, S.; Ding, W.; Zhu, K.; Shang, K.; Zhu, H.
Deposited on : 2024-03-19
Resolution : 3.95 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

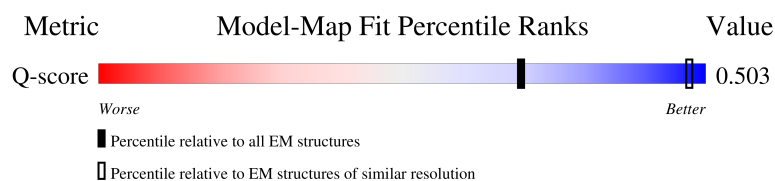
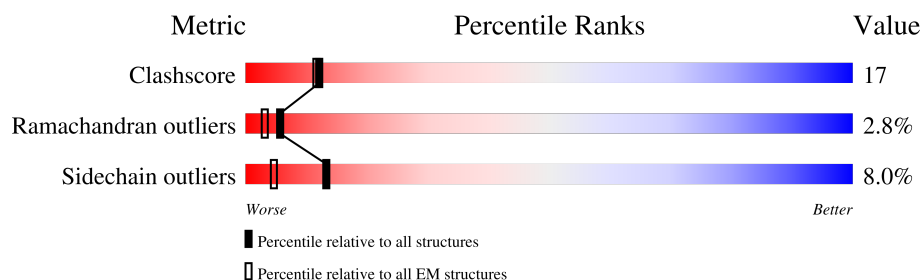
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

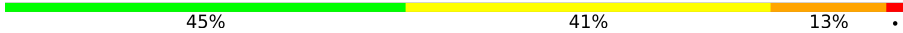
The reported resolution of this entry is 3.95 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7707 (3.45 - 4.45)

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	285	 45% 41% 13% .
2	B	384	 80% 15% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	502	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5231 atoms, of which 90 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 Spike protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	285	Total	C	N	O	S	0	0
			2218	1384	381	431	22		

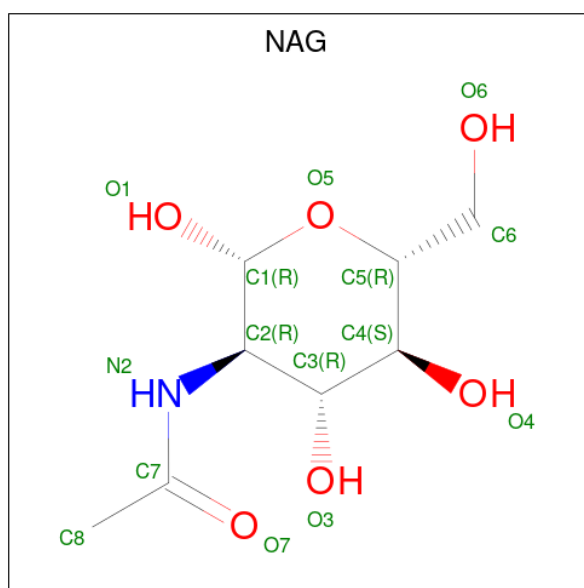
- Molecule 2 is a protein called Transmembrane protease serine 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	364	Total	C	N	O	S	0	0
			2833	1785	496	527	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	441	ALA	SER	conflict	UNP O15393

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	N	O	0
			30	8	15	1	6	
3	A	1	Total	C	H	N	O	0
			30	8	15	1	6	
3	A	1	Total	C	H	N	O	0
			30	8	15	1	6	
3	A	1	Total	C	H	N	O	0
			30	8	15	1	6	
3	B	1	Total	C	H	N	O	0
			30	8	15	1	6	
3	B	1	Total	C	H	N	O	0
			30	8	15	1	6	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	709482	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.857	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	252.72, 252.72, 252.72	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.81, 0.81, 0.81	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.79	0/2276	1.14	8/3097 (0.3%)
2	B	0.17	0/2910	0.49	0/3956
All	All	0.54	0/5186	0.84	8/7053 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	ARG	N-CA-C	-8.44	103.12	113.50
1	A	475	PRO	N-CA-C	-6.35	104.29	113.75
1	A	602	THR	CB-CA-C	-6.20	103.25	111.74
1	A	559	GLN	N-CA-C	-6.07	106.01	113.41
1	A	562	HIS	CA-CB-CG	5.53	119.33	113.80
1	A	490	PRO	CB-CA-C	5.23	117.30	110.92
1	A	574	GLY	N-CA-C	-5.18	107.65	114.95
1	A	530	PRO	N-CA-C	-5.09	108.09	114.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	446	ARG	Sidechain
1	A	447	ARG	Sidechain
1	A	502	ARG	Sidechain
1	A	517	ARG	Sidechain
1	A	585	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2218	0	2073	126	0
2	B	2833	0	2710	46	0
3	A	60	60	60	4	0
3	B	30	30	29	14	0
All	All	5141	90	4872	172	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 17.

All (172) 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:355:ASN:ND2	3:A:703:NAG:O1	1.79	1.15
3:B:501:NAG:O4	3:B:502:NAG:H1	1.44	1.14
1:A:605:ASN:O	1:A:607:LEU:N	1.91	1.02
2:B:226:TYR:HB3	3:B:502:NAG:C8	1.89	1.02
1:A:510:LEU:HD23	2:B:419:LEU:HD21	1.48	0.94
2:B:226:TYR:CG	3:B:502:NAG:H81	2.03	0.93
2:B:226:TYR:CB	3:B:502:NAG:C8	2.53	0.86
2:B:226:TYR:HB3	3:B:502:NAG:H82	1.56	0.86
1:A:563:SER:HB2	1:A:566:PHE:CZ	2.11	0.85
1:A:605:ASN:C	1:A:607:LEU:H	1.87	0.82
2:B:226:TYR:CD2	3:B:502:NAG:H81	2.14	0.81
2:B:226:TYR:CB	3:B:502:NAG:H81	2.15	0.77
1:A:431:LEU:HD11	1:A:581:ILE:HG23	1.70	0.73
1:A:552:ASN:HB3	1:A:555:LYS:HG3	1.71	0.73
1:A:355:ASN:HD22	3:A:703:NAG:HO1	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:PRO:HG2	1:A:499:THR:HG21	1.71	0.72
1:A:563:SER:HB2	1:A:566:PHE:HZ	1.54	0.71
3:B:501:NAG:O4	3:B:502:NAG:C1	2.31	0.70
1:A:416:ILE:HG23	1:A:591:ASN:ND2	2.07	0.69
1:A:355:ASN:ND2	3:A:703:NAG:HO1	1.90	0.69
1:A:447:ARG:HG3	1:A:448:TYR:CD1	2.28	0.68
2:B:226:TYR:CD2	3:B:502:NAG:C8	2.77	0.67
1:A:582:SER:O	1:A:583:ASN:C	2.37	0.67
1:A:454:ASN:O	1:A:455:LEU:HG	1.96	0.66
1:A:522:PRO:HD3	2:B:414:TYR:OH	1.97	0.64
3:B:501:NAG:C4	3:B:502:NAG:H1	2.23	0.63
1:A:582:SER:HB2	1:A:587:ASN:HD21	1.64	0.63
2:B:152:TYR:HB3	2:B:157:ILE:HG23	1.80	0.63
2:B:226:TYR:CG	3:B:502:NAG:C8	2.80	0.63
2:B:226:TYR:CB	3:B:502:NAG:H82	2.25	0.62
1:A:434:VAL:HB	1:A:458:TYR:OH	2.00	0.62
1:A:444:TRP:CE3	1:A:469:VAL:HG21	2.35	0.62
1:A:383:PHE:CZ	1:A:594:PHE:HE2	2.18	0.61
1:A:487:LYS:HE3	1:A:512:VAL:HG11	1.81	0.61
2:B:373:LEU:HD11	2:B:456:ILE:HD13	1.81	0.61
1:A:496:PRO:HG2	1:A:499:THR:CG2	2.32	0.59
2:B:285:ILE:HG22	2:B:291:ILE:HG12	1.85	0.59
1:A:558:THR:HG23	1:A:566:PHE:CE1	2.38	0.59
1:A:580:CYS:O	1:A:586:CYS:HA	2.03	0.59
1:A:373:LEU:HD11	1:A:597:ILE:HD13	1.86	0.58
1:A:444:TRP:CD1	1:A:548:GLY:HA3	2.38	0.58
1:A:448:TYR:O	1:A:567:CYS:HB2	2.04	0.57
1:A:474:CYS:SG	1:A:476:CYS:HB2	2.43	0.57
1:A:517:ARG:HB2	1:A:517:ARG:HH21	1.69	0.57
1:A:571:ALA:O	1:A:573:LEU:HG	2.05	0.57
2:B:147:ARG:NH1	2:B:220:ASP:OD1	2.37	0.57
1:A:454:ASN:C	1:A:455:LEU:HG	2.30	0.57
1:A:449:GLY:O	1:A:572:PHE:HZ	1.88	0.56
1:A:495:CYS:HB3	1:A:496:PRO:HD2	1.86	0.56
2:B:253:GLN:OE1	2:B:267:TRP:NE1	2.38	0.56
2:B:268:PRO:HB2	2:B:362:LYS:H	1.71	0.56
3:B:501:NAG:H83	3:B:502:NAG:H62	1.87	0.56
1:A:444:TRP:NE1	1:A:548:GLY:HA3	2.21	0.56
1:A:355:ASN:ND2	1:A:357:SER:OG	2.39	0.56
1:A:441:PRO:O	1:A:442:SER:HB3	2.07	0.55
2:B:178:GLU:OE1	2:B:197:SER:OG	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:LEU:HD11	1:A:581:ILE:CG2	2.37	0.55
1:A:533:CYS:SG	1:A:535:GLN:HB2	2.47	0.55
1:A:591:ASN:O	1:A:592:PHE:C	2.50	0.54
1:A:605:ASN:C	1:A:607:LEU:N	2.51	0.54
1:A:482:VAL:C	1:A:484:SER:H	2.16	0.54
1:A:387:THR:HB	1:A:593:ILE:HG22	1.90	0.54
1:A:444:TRP:HE1	1:A:548:GLY:HA3	1.73	0.54
1:A:417:ASP:N	1:A:417:ASP:OD1	2.41	0.53
1:A:438:ASN:OD1	1:A:461:VAL:HG23	2.07	0.53
1:A:523:ASP:OD2	1:A:525:ILE:HG22	2.08	0.53
1:A:424:GLN:HB3	1:A:589:PHE:HE1	1.74	0.53
1:A:425:LEU:HB3	1:A:590:SER:OG	2.07	0.53
1:A:606:ASP:O	1:A:607:LEU:HB2	2.08	0.53
1:A:467:PHE:CZ	1:A:525:ILE:HD13	2.44	0.53
1:A:527:THR:HG21	1:A:533:CYS:HB2	1.91	0.53
1:A:473:PHE:CZ	1:A:475:PRO:HA	2.43	0.53
1:A:519:SER:O	1:A:520:CYS:C	2.52	0.53
2:B:402:VAL:HB	2:B:428:GLY:HA2	1.91	0.53
1:A:522:PRO:HB2	1:A:526:SER:OG	2.09	0.52
1:A:582:SER:CB	1:A:587:ASN:HD21	2.23	0.52
2:B:367:PRO:HG3	2:B:454:TRP:HB3	1.92	0.51
3:B:501:NAG:C8	3:B:502:NAG:H62	2.41	0.51
2:B:299:GLU:OE2	2:B:337:TYR:OH	2.26	0.51
1:A:520:CYS:SG	1:A:534:PRO:HD2	2.51	0.51
1:A:447:ARG:HG3	1:A:448:TYR:CE1	2.45	0.51
2:B:329:GLU:HB3	2:B:352:GLN:HG3	1.93	0.50
1:A:495:CYS:HB3	1:A:496:PRO:CD	2.41	0.50
1:A:589:PHE:CG	1:A:590:SER:N	2.79	0.50
2:B:295:ALA:N	2:B:345:ASP:OD1	2.40	0.50
1:A:524:PRO:HG2	1:A:551:ILE:H	1.77	0.50
1:A:346:ARG:NH2	1:A:543:GLY:HA2	2.26	0.50
1:A:467:PHE:HZ	1:A:525:ILE:HD13	1.76	0.50
1:A:541:GLY:O	1:A:542:ILE:C	2.54	0.50
1:A:424:GLN:HB3	1:A:589:PHE:CE1	2.47	0.50
1:A:371:ASN:OD1	1:A:424:GLN:NE2	2.36	0.49
1:A:494:ILE:O	1:A:494:ILE:HG12	2.11	0.49
2:B:229:ASP:N	2:B:229:ASP:OD1	2.41	0.49
1:A:450:PHE:CG	1:A:451:GLY:N	2.80	0.49
2:B:332:ILE:HB	2:B:348:LEU:HB2	1.93	0.49
1:A:525:ILE:CD1	1:A:537:LYS:HE3	2.43	0.49
1:A:584:ASN:O	1:A:585:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:PHE:CE2	1:A:594:PHE:HE2	2.30	0.49
2:B:255:ARG:HB3	2:B:398:ASN:HA	1.94	0.48
1:A:373:LEU:CD1	1:A:597:ILE:HD13	2.43	0.48
2:B:376:GLU:HG2	2:B:403:LEU:HD13	1.95	0.48
1:A:339:PRO:HG2	1:A:391:PHE:HA	1.95	0.48
1:A:329:ILE:HB	1:A:359:LEU:HD11	1.95	0.48
1:A:355:ASN:HD22	1:A:358:THR:HG23	1.78	0.48
1:A:473:PHE:CE1	1:A:475:PRO:HA	2.48	0.47
1:A:505:ASP:O	1:A:506:LEU:C	2.57	0.47
1:A:482:VAL:C	1:A:484:SER:N	2.73	0.47
1:A:507:ASP:CB	1:A:517:ARG:HH22	2.28	0.47
1:A:352:CYS:H	1:A:602:THR:HG23	1.78	0.47
1:A:392:ALA:HA	1:A:588:ILE:HA	1.97	0.47
1:A:509:THR:O	1:A:512:VAL:HG23	2.16	0.46
2:B:213:ASN:HB3	2:B:226:TYR:HE2	1.80	0.46
1:A:445:ASN:HD21	1:A:551:ILE:HD11	1.80	0.46
1:A:513:LYS:O	1:A:514:ASN:C	2.58	0.46
1:A:487:LYS:HB3	1:A:515:TRP:CD1	2.51	0.46
2:B:253:GLN:HG2	2:B:262:ALA:HA	1.98	0.46
1:A:451:GLY:O	1:A:452:SER:C	2.57	0.46
1:A:477:ALA:HA	1:A:502:ARG:HG2	1.97	0.46
1:A:560:LEU:HD23	1:A:560:LEU:HA	1.79	0.45
1:A:477:ALA:HB2	1:A:502:ARG:NE	2.32	0.45
2:B:170:PRO:HG2	2:B:209:PHE:HD1	1.82	0.45
1:A:397:ARG:HB3	1:A:409:LEU:HD11	1.99	0.45
2:B:449:LYS:HB3	2:B:454:TRP:HE1	1.81	0.45
1:A:438:ASN:HD22	1:A:438:ASN:H	1.65	0.45
2:B:433:ASN:HA	2:B:466:ALA:HB1	1.98	0.45
1:A:517:ARG:HB2	1:A:517:ARG:NH2	2.31	0.44
1:A:433:ASN:HD21	3:A:701:NAG:H1	1.82	0.44
1:A:520:CYS:HB2	1:A:553:GLU:CD	2.42	0.44
1:A:394:PRO:HB2	1:A:397:ARG:HB2	1.99	0.44
1:A:477:ALA:HB2	1:A:502:ARG:CZ	2.47	0.44
2:B:346:ILE:HD12	2:B:346:ILE:HA	1.88	0.44
1:A:329:ILE:O	1:A:333:LEU:HD12	2.18	0.43
1:A:378:ILE:HG23	1:A:383:PHE:HZ	1.84	0.43
1:A:496:PRO:HD2	1:A:499:THR:OG1	2.19	0.43
1:A:521:LEU:HB3	1:A:522:PRO:CD	2.48	0.43
1:A:510:LEU:CD2	2:B:419:LEU:HD21	2.34	0.43
1:A:476:CYS:SG	1:A:493:ALA:HB3	2.58	0.43
1:A:370:CYS:HA	1:A:423:CYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:THR:HB	1:A:593:ILE:CG2	2.49	0.42
1:A:525:ILE:HD12	1:A:537:LYS:HE3	2.01	0.42
1:A:525:ILE:HD12	1:A:525:ILE:HA	1.73	0.42
2:B:132:TRP:HH2	2:B:147:ARG:HB2	1.83	0.42
1:A:416:ILE:HG23	1:A:591:ASN:CG	2.45	0.42
2:B:268:PRO:HB2	2:B:362:LYS:N	2.33	0.42
1:A:507:ASP:HB3	1:A:517:ARG:HH22	1.84	0.42
1:A:453:PHE:HE1	1:A:575:TRP:CD2	2.38	0.42
1:A:480:SER:O	1:A:481:VAL:C	2.63	0.41
1:A:506:LEU:HD23	1:A:506:LEU:HA	1.92	0.41
1:A:527:THR:HG23	2:B:469:TYR:OH	2.20	0.41
2:B:408:GLN:OE1	2:B:408:GLN:N	2.43	0.41
1:A:442:SER:HB2	1:A:547:PRO:O	2.20	0.41
1:A:450:PHE:HD1	1:A:572:PHE:CZ	2.37	0.41
1:A:591:ASN:O	1:A:593:ILE:N	2.53	0.41
1:A:472:ASP:OD2	1:A:500:LYS:HG3	2.21	0.41
2:B:203:ASP:N	2:B:203:ASP:OD1	2.54	0.41
1:A:434:VAL:HG12	1:A:458:TYR:HE1	1.85	0.41
1:A:507:ASP:CG	2:B:470:ARG:HH12	2.28	0.41
2:B:310:ALA:O	2:B:326:TYR:N	2.45	0.41
2:B:371:MET:HE2	2:B:371:MET:HB3	1.98	0.41
2:B:374:GLN:HG2	2:B:377:GLN:HB2	2.02	0.41
1:A:338:VAL:HG21	1:A:434:VAL:HG13	2.03	0.41
1:A:382:CYS:CB	1:A:603:CYS:HA	2.51	0.41
1:A:474:CYS:O	1:A:475:PRO:C	2.62	0.41
1:A:597:ILE:O	1:A:598:ASN:C	2.63	0.41
2:B:253:GLN:NE2	2:B:263:LEU:H	2.19	0.41
1:A:453:PHE:HB3	1:A:455:LEU:HD12	2.03	0.41
1:A:597:ILE:HD12	1:A:597:ILE:HA	1.92	0.40
2:B:256:ILE:HG22	2:B:257:VAL:H	1.86	0.40
1:A:520:CYS:O	1:A:553:GLU:HB2	2.21	0.40
1:A:593:ILE:HD12	1:A:593:ILE:HA	1.83	0.40
1:A:487:LYS:HB3	1:A:487:LYS:HZ2	1.87	0.40
2:B:152:TYR:CE1	2:B:370:GLY:HA3	2.57	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	283/285 (99%)	216 (76%)	49 (17%)	18 (6%)	1	15
2	B	362/384 (94%)	347 (96%)	15 (4%)	0	100	100
All	All	645/669 (96%)	563 (87%)	64 (10%)	18 (3%)	6	27

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	562	HIS
1	A	584	ASN
1	A	606	ASP
1	A	465	HIS
1	A	510	LEU
1	A	522	PRO
1	A	592	PHE
1	A	595	ASN
1	A	454	ASN
1	A	458	TYR
1	A	520	CYS
1	A	583	ASN
1	A	598	ASN
1	A	486	ALA
1	A	497	ALA
1	A	540	VAL
1	A	472	ASP
1	A	542	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	265/265 (100%)	219 (83%)	46 (17%)	2	12
2	B	308/325 (95%)	308 (100%)	0	100	100
All	All	573/590 (97%)	527 (92%)	46 (8%)	13	35

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	436	ILE
1	A	444	TRP
1	A	445	ASN
1	A	446	ARG
1	A	452	SER
1	A	457	SER
1	A	458	TYR
1	A	465	HIS
1	A	469	VAL
1	A	479	PRO
1	A	481	VAL
1	A	482	VAL
1	A	487	LYS
1	A	488	SER
1	A	494	ILE
1	A	503	HIS
1	A	504	CYS
1	A	509	THR
1	A	510	LEU
1	A	511	TYR
1	A	512	VAL
1	A	513	LYS
1	A	516	CYS
1	A	517	ARG
1	A	519	SER
1	A	521	LEU
1	A	523	ASP
1	A	525	ILE
1	A	531	ASN
1	A	532	THR
1	A	536	LYS
1	A	537	LYS
1	A	538	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	555	LYS
1	A	556	CYS
1	A	566	PHE
1	A	568	SER
1	A	573	LEU
1	A	577	PHE
1	A	578	ASP
1	A	581	ILE
1	A	585	ARG
1	A	593	ILE
1	A	601	THR
1	A	602	THR
1	A	604	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	ASN
1	A	353	ASN
1	A	355	ASN
1	A	440	ASN
1	A	445	ASN
1	A	465	HIS
1	A	483	ASN
1	A	531	ASN
1	A	561	ASN
1	A	562	HIS
1	A	587	ASN
1	A	605	ASN
2	B	146	ASN
2	B	159	GLN
2	B	177	ASN
2	B	227	HIS
2	B	270	GLN
2	B	374	GLN

5.3.3 RNA ⓘ

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](#)

6 ligands are modelled in this entry.

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	$\# Z > 2$
3	NAG	A	702	-	15,15,15	0.21	0	21,21,21	0.79	1 (4%)
3	NAG	A	703	-	15,15,15	0.22	0	21,21,21	0.38	0
3	NAG	A	701	-	15,15,15	0.29	0	21,21,21	0.94	1 (4%)
3	NAG	B	501	-	15,15,15	0.21	0	21,21,21	0.76	0
3	NAG	A	704	-	15,15,15	0.23	0	21,21,21	0.78	1 (4%)
3	NAG	B	502	-	15,15,15	0.23	0	21,21,21	0.71	1 (4%)

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
3	NAG	A	702	-	-	2/6/26/26	0/1/1/1
3	NAG	A	703	-	-	2/6/26/26	0/1/1/1
3	NAG	A	701	-	-	4/6/26/26	0/1/1/1
3	NAG	B	501	-	-	4/6/26/26	0/1/1/1
3	NAG	A	704	-	-	3/6/26/26	0/1/1/1
3	NAG	B	502	-	-	4/6/26/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	NAG	O5-C1-C2	3.45	112.98	109.52
3	A	702	NAG	O5-C1-C2	3.10	112.63	109.52
3	A	704	NAG	O5-C1-C2	3.07	112.60	109.52
3	B	502	NAG	O5-C1-C2	2.62	112.15	109.52

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	NAG	C8-C7-N2-C2
3	A	701	NAG	O7-C7-N2-C2
3	A	702	NAG	C8-C7-N2-C2
3	A	702	NAG	O7-C7-N2-C2
3	A	703	NAG	C8-C7-N2-C2
3	A	703	NAG	O7-C7-N2-C2
3	A	704	NAG	C8-C7-N2-C2
3	A	704	NAG	O7-C7-N2-C2
3	B	501	NAG	C8-C7-N2-C2
3	B	501	NAG	O7-C7-N2-C2
3	B	502	NAG	C8-C7-N2-C2
3	B	502	NAG	O7-C7-N2-C2
3	B	501	NAG	C4-C5-C6-O6
3	B	501	NAG	O5-C5-C6-O6
3	A	701	NAG	O5-C5-C6-O6
3	A	701	NAG	C4-C5-C6-O6
3	B	502	NAG	C4-C5-C6-O6
3	A	704	NAG	O5-C5-C6-O6
3	B	502	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	NAG	3	0
3	A	701	NAG	1	0
3	B	501	NAG	5	0
3	B	502	NAG	14	0

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.

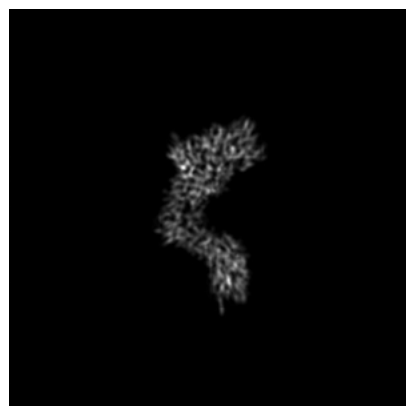
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39502. These allow visual inspection of the internal detail of the map and identification of artifacts.

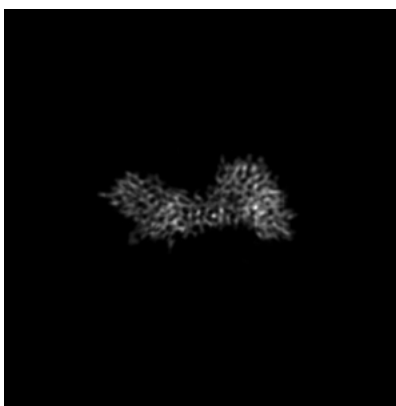
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

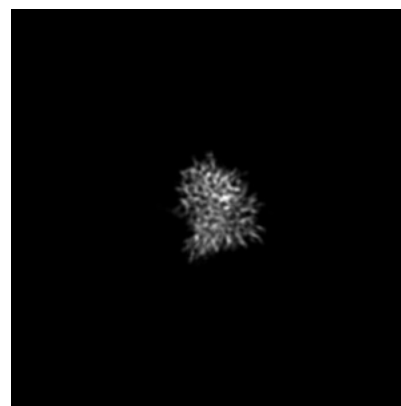
6.1.1 Primary map



X

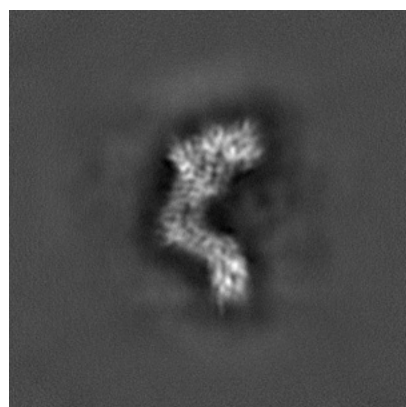


Y

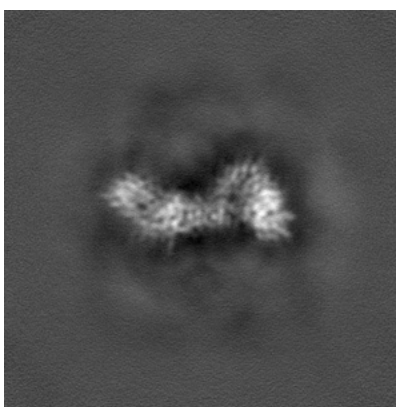


Z

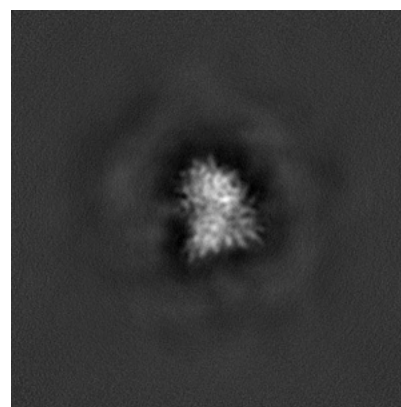
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

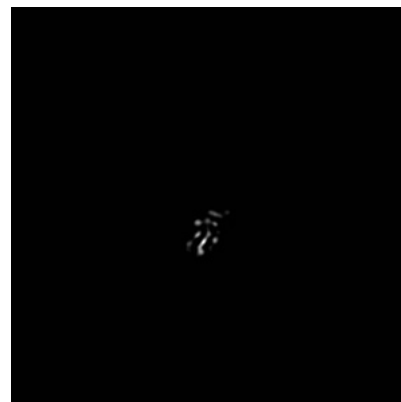
6.2.1 Primary map



X Index: 156

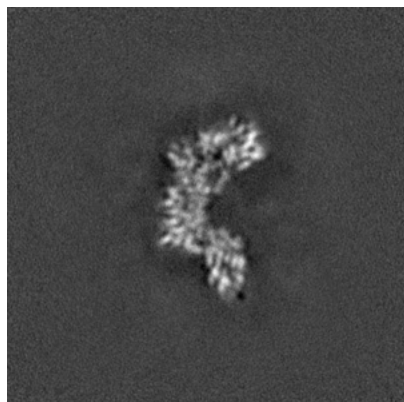


Y Index: 156

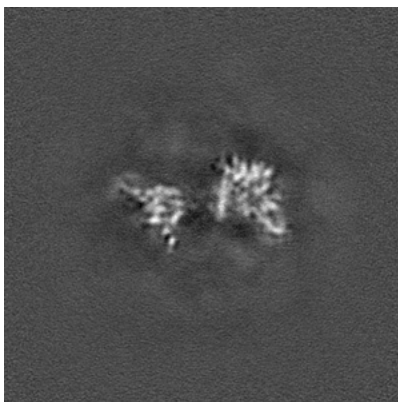


Z Index: 156

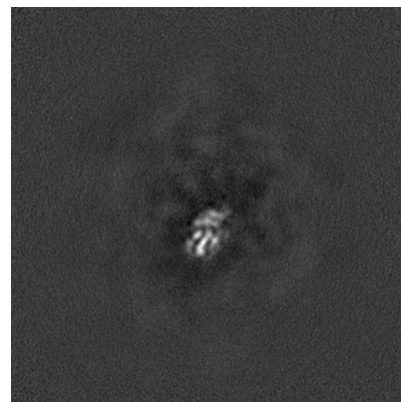
6.2.2 Raw map



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: 157

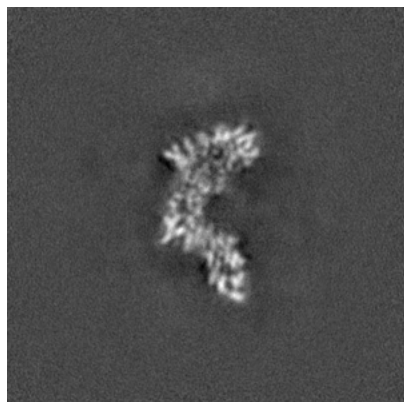


Y Index: 165

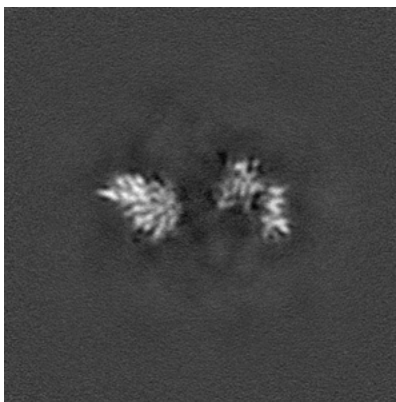


Z Index: 196

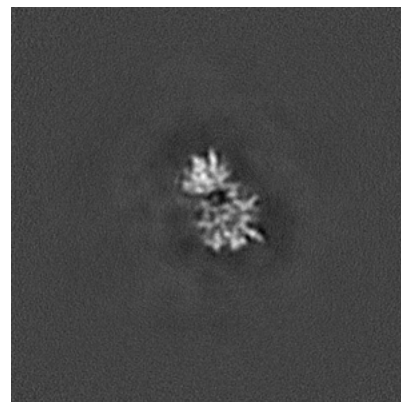
6.3.2 Raw map



X Index: 159



Y Index: 164

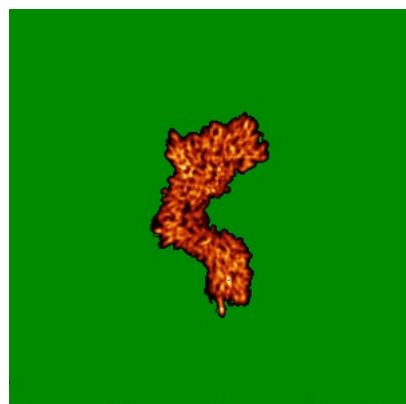


Z Index: 197

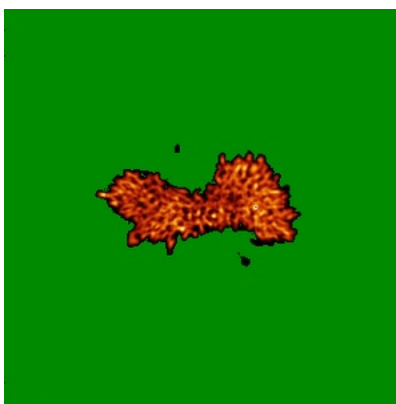
The images above show the largest variance slices of the map in three orthogonal directions.

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

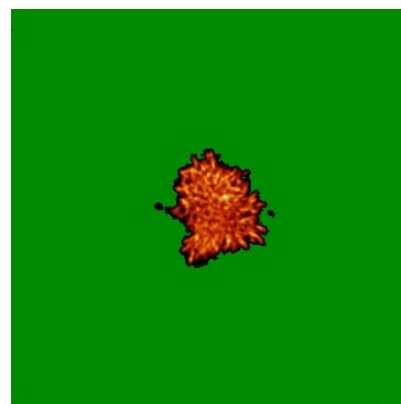
6.4.1 Primary map



X

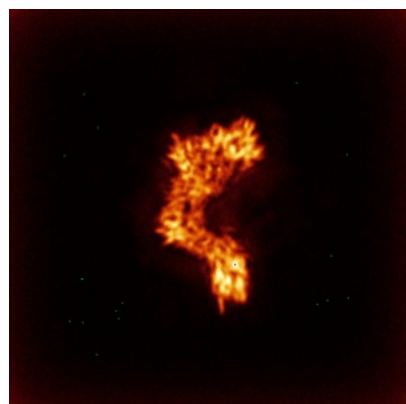


Y

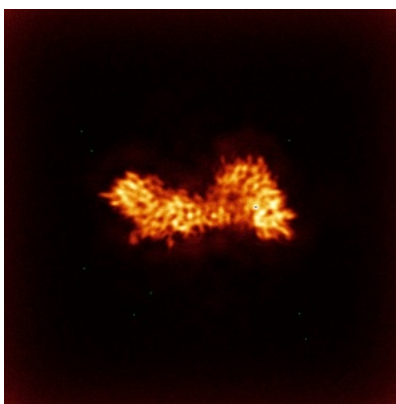


Z

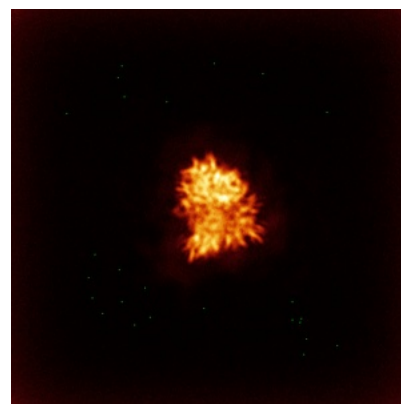
6.4.2 Raw map



X



Y

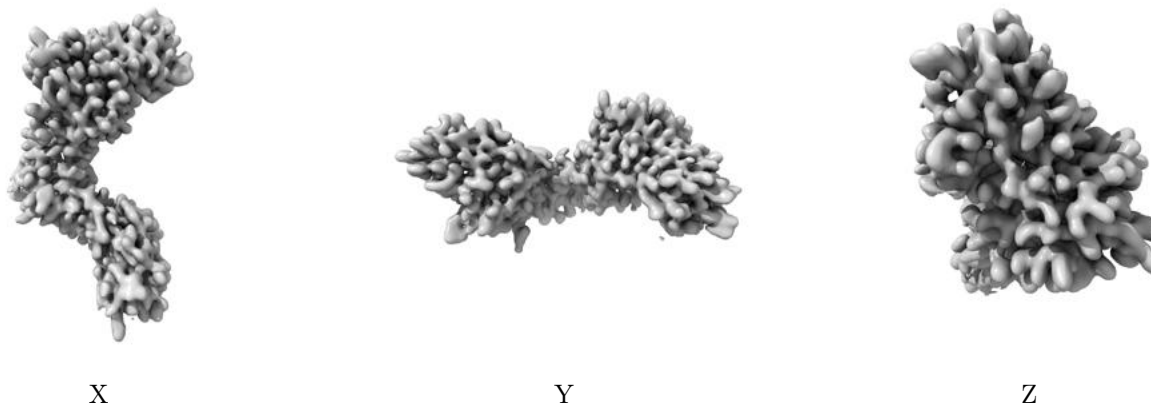


Z

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

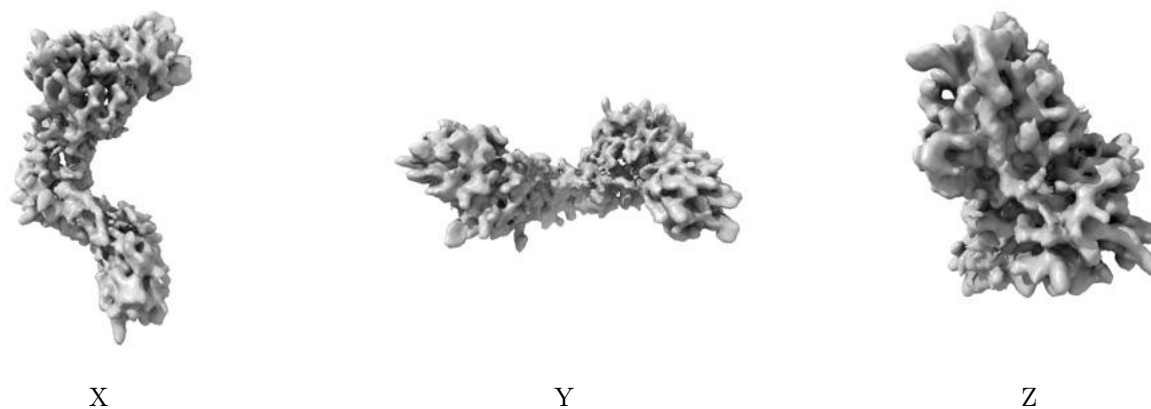
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

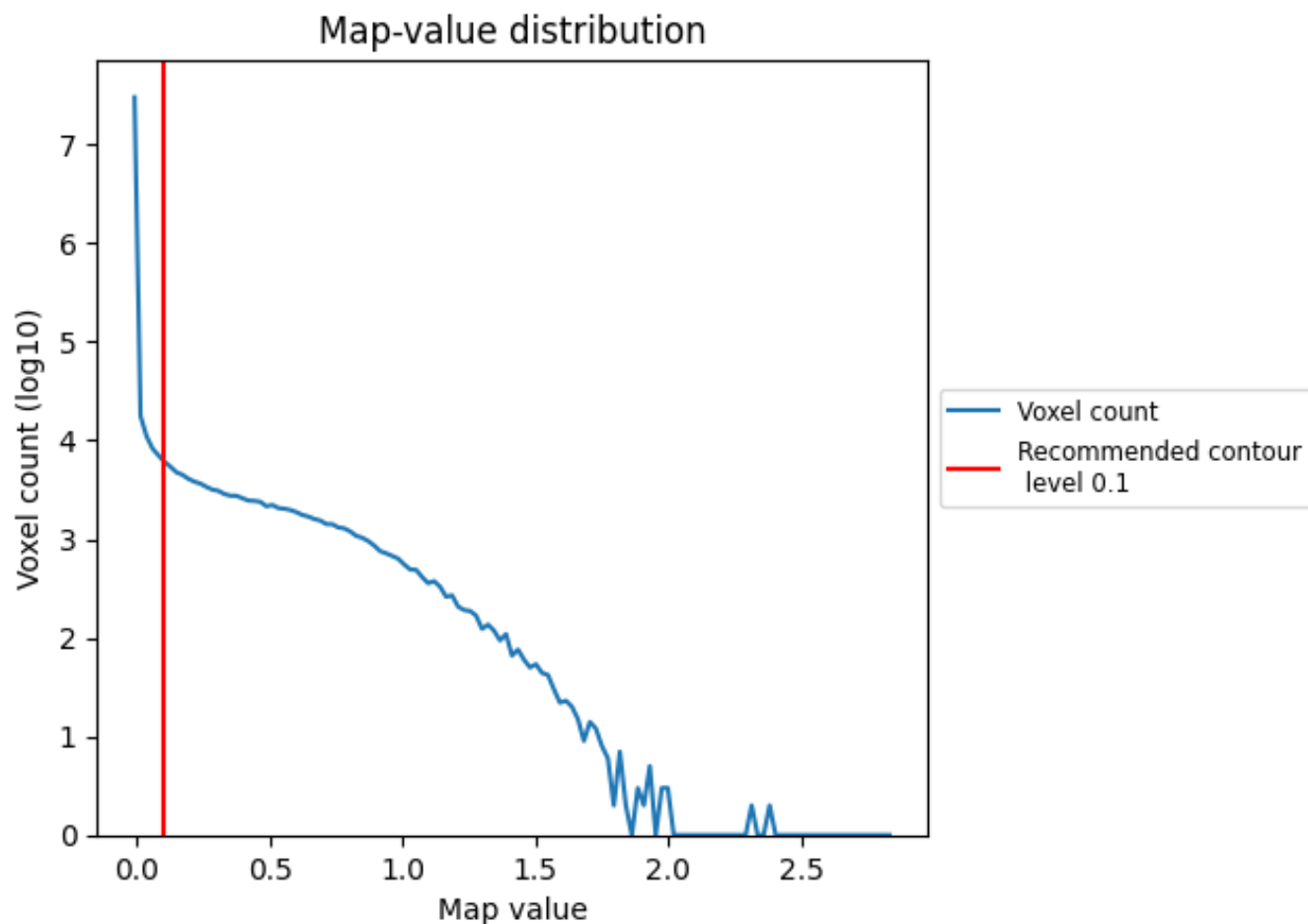
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

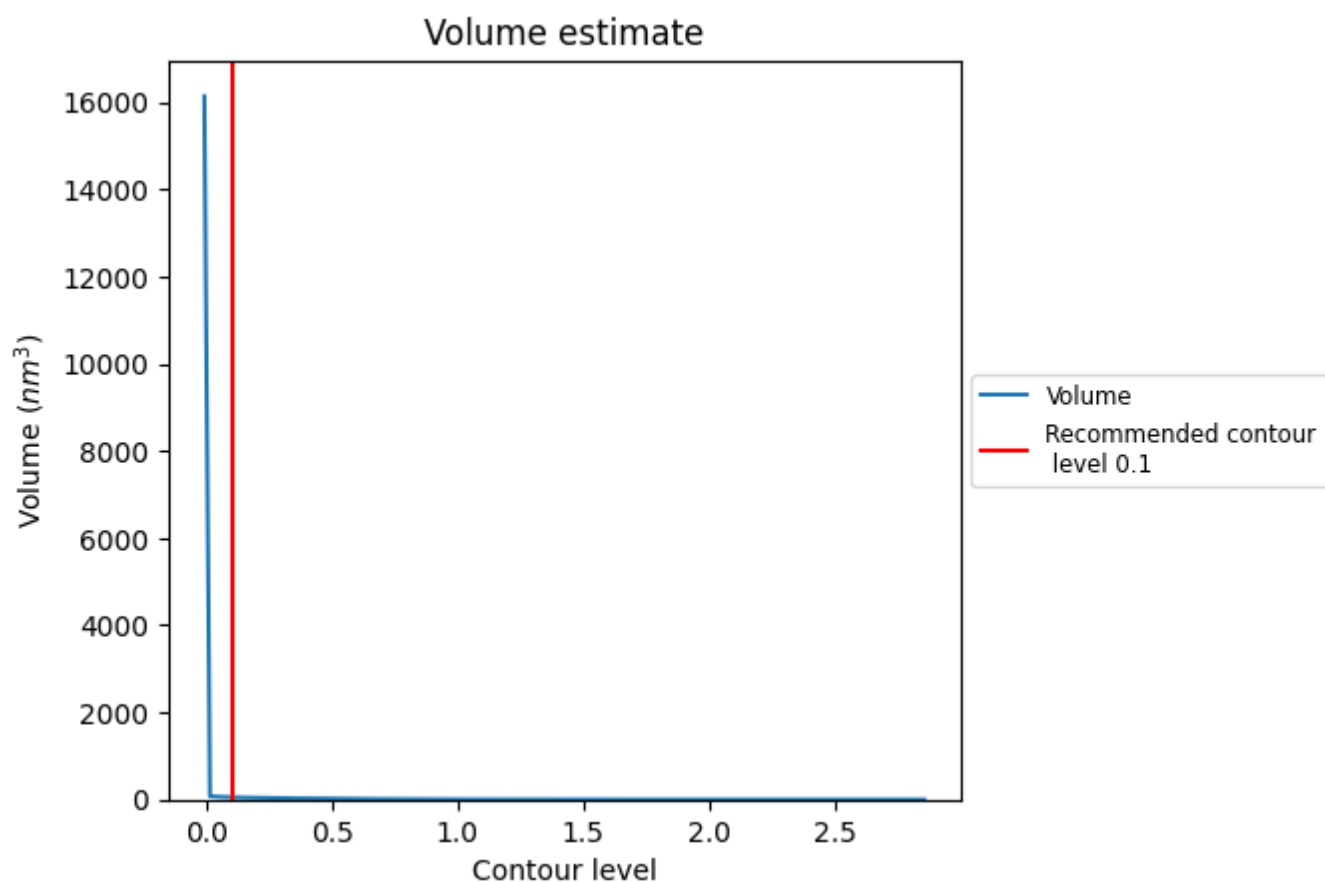
This section contains the results of statistical analysis of the map.

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.

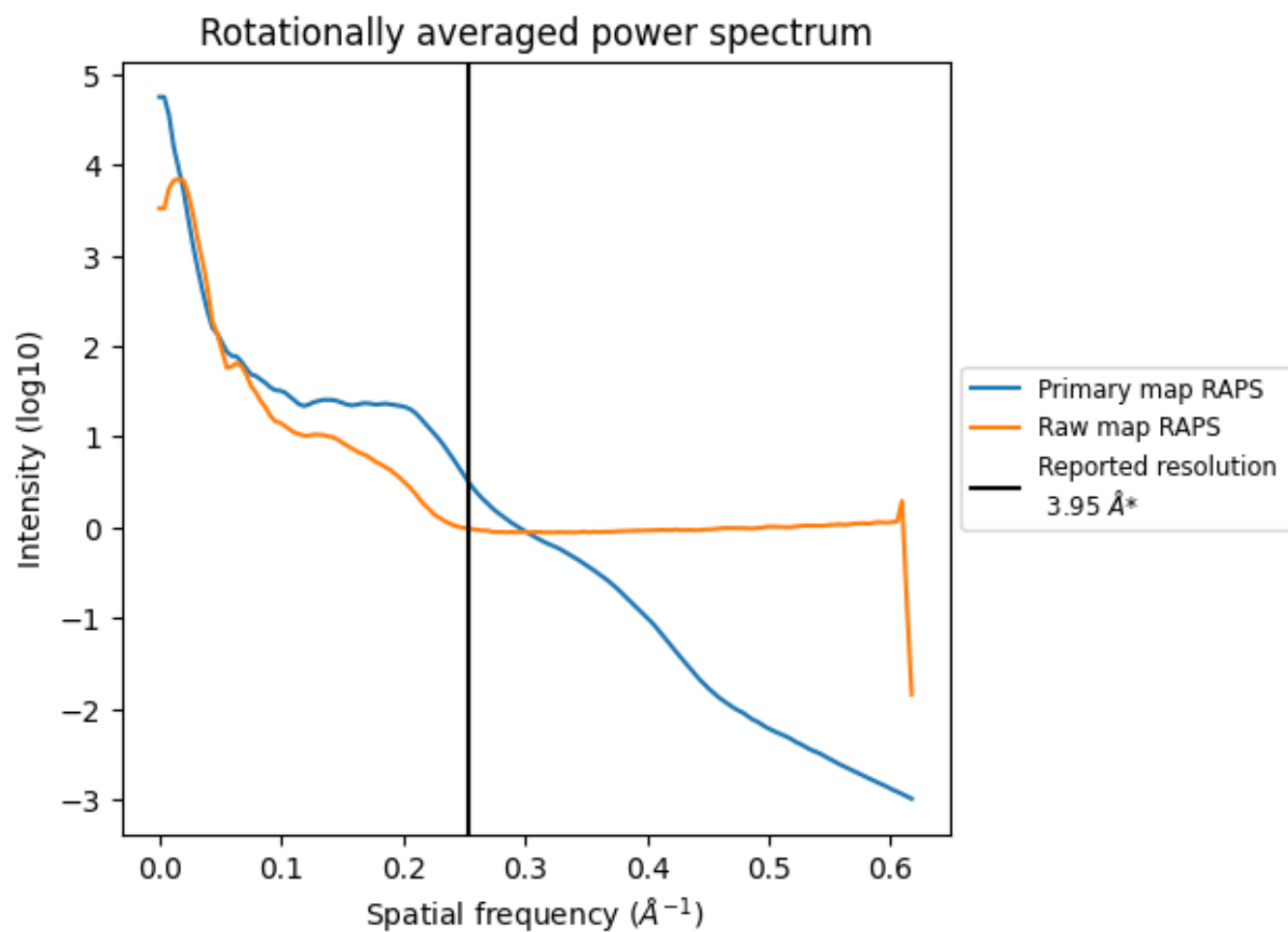
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 53 nm^3 ; this corresponds to an approximate mass of 48 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

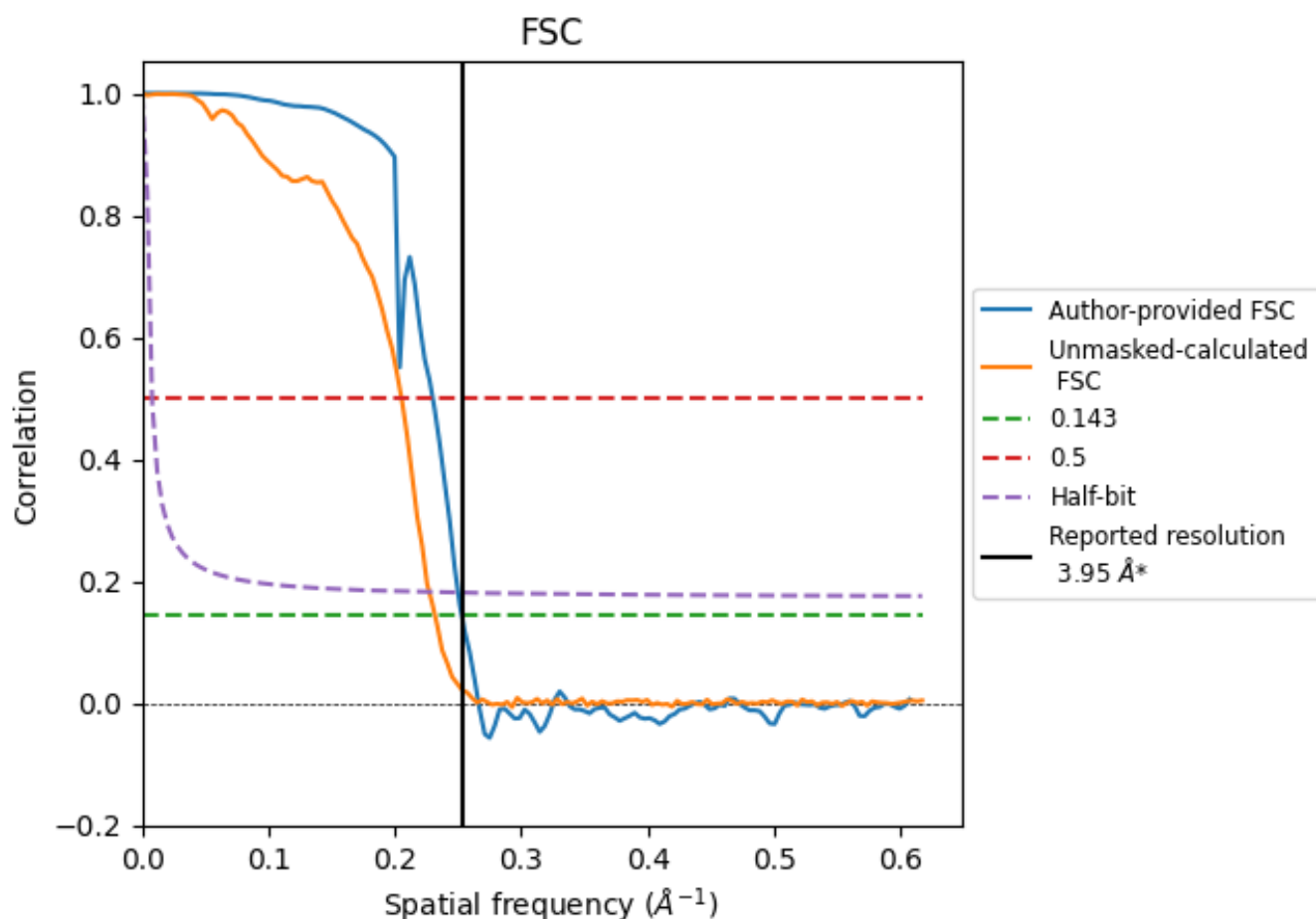


*Reported resolution corresponds to spatial frequency of 0.253 Å⁻¹

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 0.253 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

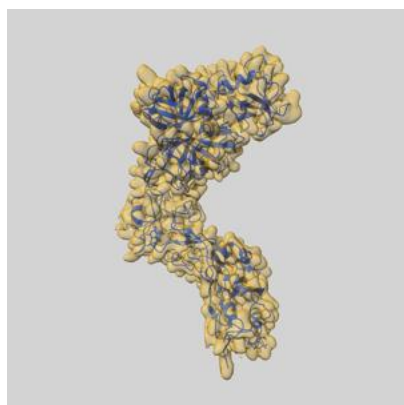
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.95	-	-
Author-provided FSC curve	3.95	4.35	4.00
Unmasked-calculated*	4.32	4.87	4.40

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

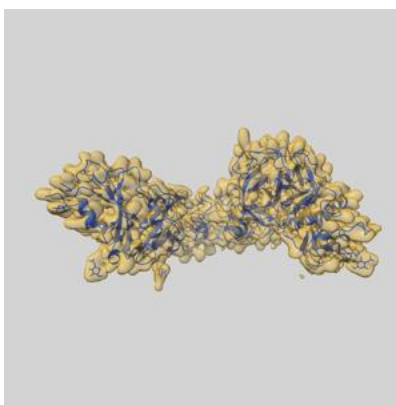
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39502 and PDB model 8YQQ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

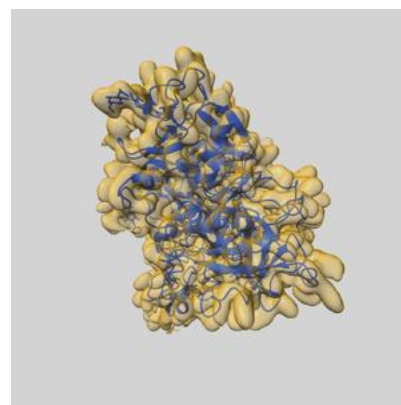
9.1 Map-model overlay [i](#)



X



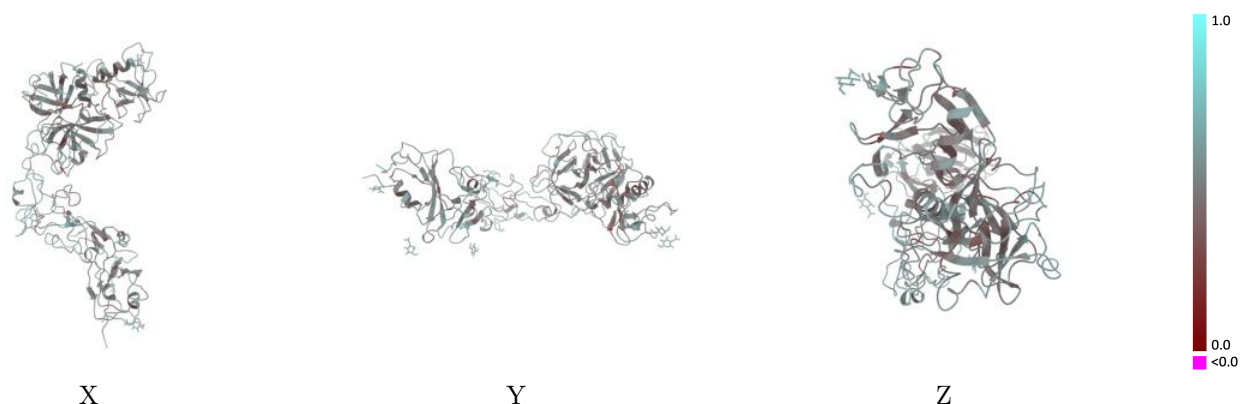
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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](#)

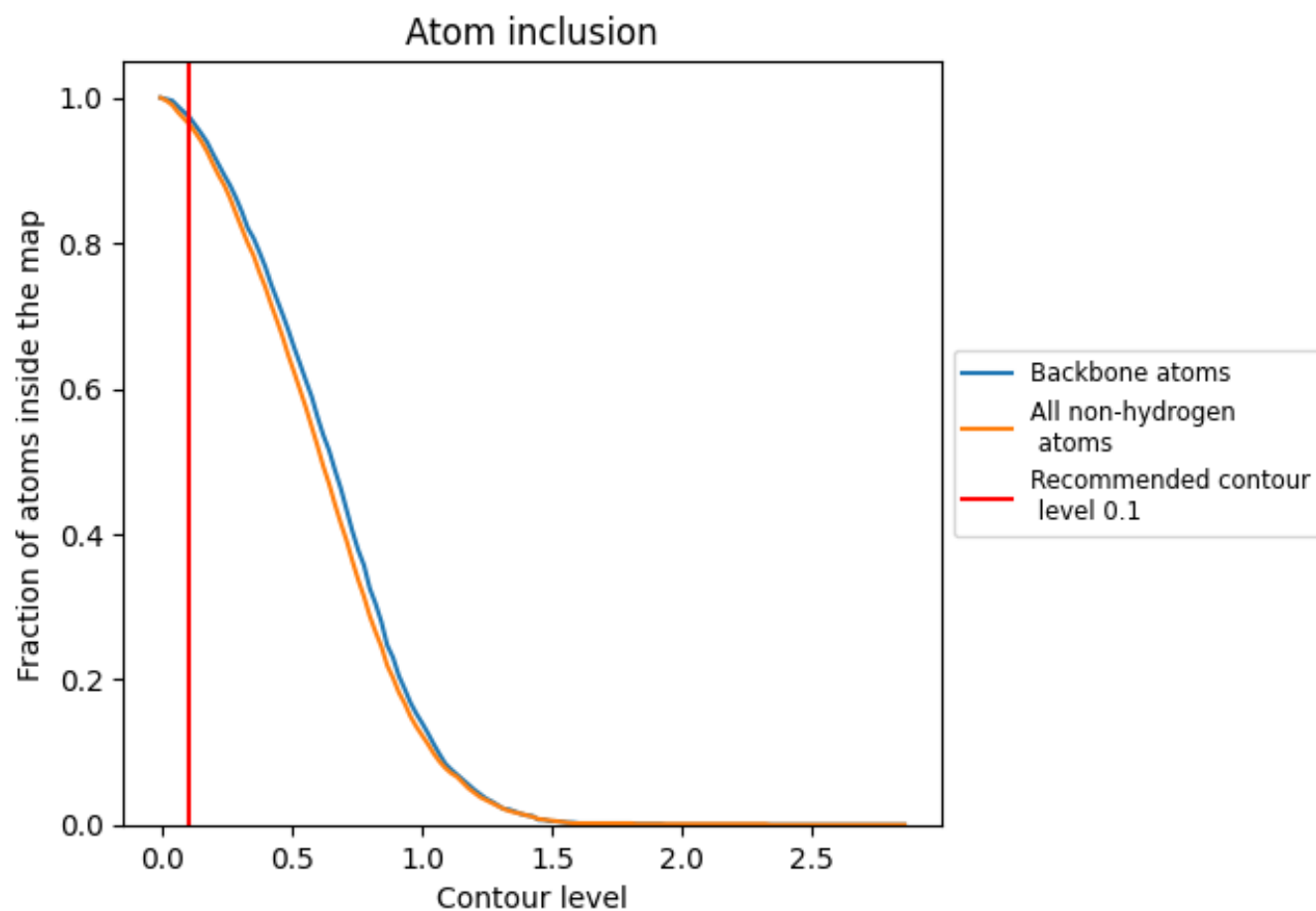


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9640	0.5030
A	0.9600	0.5140
B	0.9670	0.4950

