



Full wwPDB EM Validation Report ⓘ

Dec 1, 2025 – 01:39 PM EST

PDB ID : 9PNR / pdb_00009pnr
EMDB ID : EMD-71769
Title : N4 vRNAP gp50 - Closed Complex
Authors : Bellis, N.F.; Lokareddy, R.K.; Cingolani, G.
Deposited on : 2025-07-21
Resolution : 2.80 Å (reported)
Based on initial model : 4FF3

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.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

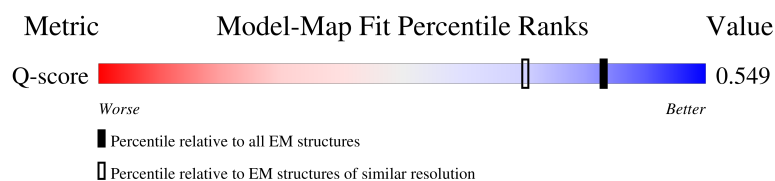
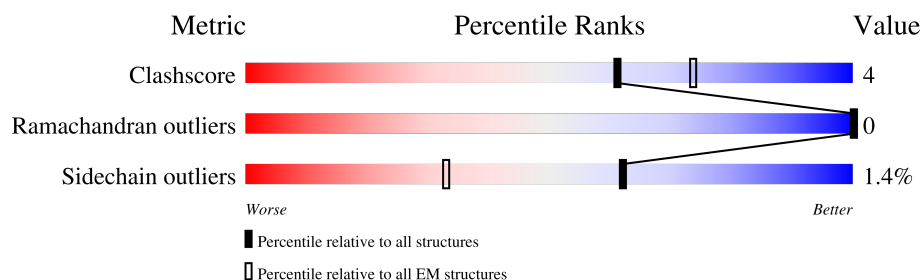
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	3500	 62% 8% 30%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 19000 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 Virion DNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2443	Total	C	N	O	S	0	0
			19000	11931	3297	3681	91		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3218	ALA	SER	conflict	UNP Q859P9

N3346	N3347	G3348	R3349	Y3350	A3351	T3357	F3360	Q3364	K3384	K3387	D3405	M3421	M3437	I3438	R3439	P3442	V3443	H3444	P3452	F3457	V3460	L3477	L3481	Q3485	G3486	N3493	F3496	N3497	H3500																			
I3214	V3215	V3219	V3240	N3255	I3258	S3259	S3260	R3261	I3265	E3268	A3269	E3270	L3271	R3272	A3273	A3274	E3275	G3276	N3277	P3278	N3279	L3280	V3281	R3282	K3283	L3284	K3285	H3295	K3301	I3304	E3305	F3309	S3310	S3311	I3312	G3316	I3317	V3319	V3320	E3331	Y3332	M3333						
Y2953	K2964	Q2983	N2987	D2993	T2996	A3005	G3006	R3007	R3016	K3019	P3030	Q3046	S3047	A3079	N3083	D3097	Y3108	D3117	L3120	I3124	N3125	L3126	M3127	F3139	E3143	M3150	N3169	S3170	R3171	S3175	V3195	V3196	Q3204															
S2272	S2294	K2304	K2326	R2327	R2349	Q2351	A2352	L2355	G2356	E2357	V2421	E2422	R2423	R2424	M2458	E2491	D2498	R2505	V2521	VAL	ALA	ALA	LYS	GLY	T2529	S2530	L2531	K2556	E2502	T2503	L2504	E2642	THR	VAL	ILE	GLU	LYS	ALA	ASP	VAL	ILE							
SER	GLU	LYS	GLU	PRO	VAL	ASN	ASN	ASP	PHE	GLY	MET	V2124	G2125	R2126	V2133	R2134	I2135	L2136	S2137	A2138	I2141	R2142	N2143	L2144	A2145	K2146	I2147	L2150	Q2154	L2158	I2173	E2196	M2197	E2198	E2199	A2200	Q2201	A2202	G2203	N2210	F2211	D2212	D2213	K2214	M2223	E2247	D2270	L2271
D1826	M1827	F1828	K1829	Q1830	Q1831	R1832	D1849	Q1853	M1857	E1886	M1895	R1899	M1930	M1936	K1945	K1963	E1966	M1988	D2012	L2028	L2047	N2051	E1541	E1542	K1544	V1553	M1567	M1596	D1607	N1656	L1659	T1271	I1272	A1291	E1298													
M1343	K1352	D1353	R1354	M1359	N1365	L1369	A1374	V1384	E1385	T1417	R1418	V1419	R1420	R1421	M1424	Q1431	S1432	A1433	M1498	E1501	T1505	L1508	M1530	A1541	E1542	K1544	V1553	M1567	M1596	D1607	N1656	L1659	T1271	I1272	A1291	E1298												
K1130	L1131	L1132	M1133	T1134	V1135	Q1136	Q1137	D1138	G1139	D1140	T1141	F1142	K1143	E1146	L1157	R1160	E1066	L1067	F1068	T1069	E1070	K1071	E1072	T1073	A1074	M1079	I1083	K1084	R1085	Y1086	K1087	M1090	G1093	I1096	I1099	L1100	R1101	L1104	D1112	K1115	R1116	F1117	R1125	W1126	V1127			
G1026	I1027	K1028	N1029	Y1030	L1033	L1037	P1038	E1039	E1040	Q1041	K1042	S1043	R1044	K1053	R1064	Y1065	L1066	L1067	F1068	T1069	E1070	K1071	E1072	T1073	A1074	M1079	I1083	K1084	R1085	Y1086	K1087	M1090	G1093	I1096	I1099	L1100	R1101	L1104	D1112	K1115	R1116	F1117	R1125	W1126	V1127			
LYS	ALA	PHE	ARG	GLN	GLY	ASN	ARG	ASP	VAL	ALA	VAL	GLN	ALA	ASP	SER	ASN	ASN	VAL	GLU	THR	GLU	PRO	VAL	THR	GLN	GLU	PRO	THR	TYR	SER	PRO	GLY	THR	VAL	GLN	THR	LYS	PRO	VAL	SER	GLU	THR	PRO	GLN				
LEU	GLY	VAL	ASN	GLY	TYR	ASP	THR	LYS	SER	THR	LYS	VAL	PHE	ALA	GLN	PRO	LYS	GLN	ALA	VAL	ALA	ASP	SER	LEU	GLU	ALA	ALA	VAL	TYR	SER	PRO	GLY	THR	VAL	GLN	THR	LYS	PRO	VAL	SER	GLU	THR	PRO	GLN				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	221813	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.437	Depositor
Minimum map value	-0.194	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0646	Depositor
Map size (\AA)	389.44, 389.44, 389.44	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.217, 1.217, 1.217	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	0.08	0/19302	0.22	0/26087

There are no bond length outliers.

There are no bond angle outliers.

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	19000	0	19100	161	0
All	All	19000	0	19100	161	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 (161) 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:1359:MET:HB3	1:A:1659:LEU:HD21	1.67	0.76
1:A:1197:GLY:HA3	1:A:1269:LEU:HB3	1.75	0.69
1:A:2223:MET:HA	1:A:2223:MET:HE2	1.74	0.68
1:A:3331:GLU:OE1	1:A:3331:GLU:N	2.27	0.64
1:A:3342:GLU:OE2	1:A:3346:ASN:ND2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1424:MET:HE3	1:A:1431:GLN:HB2	1.80	0.63
1:A:3493:ASN:HB3	1:A:3496:PHE:HB3	1.82	0.61
1:A:3258:ILE:HD12	1:A:3258:ILE:H	1.64	0.61
1:A:1238:GLU:OE2	1:A:1895:ASN:ND2	2.32	0.61
1:A:1182:ASP:HB3	1:A:1185:LEU:HD12	1.83	0.60
1:A:2210:ASN:ND2	1:A:2213:ASP:OD1	2.34	0.60
1:A:2807:ASN:OD1	1:A:2845:ARG:NH1	2.35	0.60
1:A:2909:ASP:HB3	1:A:2912:THR:HG22	1.84	0.59
1:A:3261:ARG:HD2	1:A:3265:ILE:HD13	1.84	0.59
1:A:1826:ASP:OD2	1:A:1830:GLN:NE2	2.36	0.59
1:A:1022:SER:HA	1:A:1033:LEU:HD21	1.84	0.59
1:A:2423:ARG:NH2	1:A:2602:GLU:OE2	2.36	0.59
1:A:3260:SER:OG	1:A:3295:HIS:NE2	2.30	0.58
1:A:3485:GLN:OE1	1:A:3486:GLY:N	2.36	0.58
1:A:2351:GLN:NE2	1:A:2352:ALA:O	2.35	0.57
1:A:3030:PRO:O	1:A:3047:SER:OG	2.23	0.57
1:A:2135:ILE:HG13	1:A:2173:ILE:HG12	1.85	0.57
1:A:2498:ASP:OD1	1:A:2498:ASP:N	2.38	0.57
1:A:3301:TRP:NE1	1:A:3305:GLU:OE2	2.37	0.56
1:A:1104:LEU:HD21	1:A:1143:LYS:HA	1.87	0.55
1:A:2012:ASP:HB2	1:A:2272:SER:HB3	1.89	0.55
1:A:1041:GLN:HE22	1:A:1044:ARG:HA	1.70	0.54
1:A:1066:GLU:HA	1:A:1071:LYS:HZ1	1.72	0.54
1:A:3169:ASN:O	1:A:3171:ARG:NH1	2.41	0.54
1:A:3384:LYS:O	1:A:3387:LYS:NZ	2.41	0.54
1:A:1101:ARG:NH2	1:A:1146:GLU:OE2	2.41	0.53
1:A:3493:ASN:O	1:A:3497:ASN:ND2	2.42	0.53
1:A:3214:ILE:HD11	1:A:3351:ALA:HB3	1.90	0.53
1:A:2424:ARG:NH1	1:A:2424:ARG:HB3	2.25	0.52
1:A:1853:GLN:NE2	1:A:1857:ASN:OD1	2.43	0.52
1:A:2424:ARG:HB3	1:A:2424:ARG:HH11	1.74	0.52
1:A:1210:LYS:NZ	1:A:1298:GLU:OE2	2.40	0.51
1:A:1343:MET:HE3	1:A:1530:MET:HA	1.93	0.51
1:A:2146:LYS:N	1:A:2146:LYS:HD3	2.25	0.51
1:A:3016:ARG:HA	1:A:3019:LYS:HE3	1.92	0.51
1:A:3310:SER:O	1:A:3310:SER:OG	2.27	0.51
1:A:1021:ASP:O	1:A:1028:LYS:NZ	2.37	0.50
1:A:1044:ARG:NH1	1:A:1291:ALA:O	2.44	0.50
1:A:2270:ASP:OD1	1:A:2270:ASP:N	2.42	0.50
1:A:1498:MET:HE3	1:A:1508:LEU:HD22	1.92	0.50
1:A:1417:THR:HG22	1:A:1421:ARG:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2458:MET:HE2	1:A:2604:ILE:HG23	1.94	0.50
1:A:1093:GLY:HA3	1:A:1157:LEU:HD11	1.93	0.50
1:A:2142:ARG:HB2	1:A:2142:ARG:NH1	2.26	0.50
1:A:2196:GLU:O	1:A:2200:ALA:N	2.41	0.50
1:A:3139:PHE:HB3	1:A:3143:GLU:HB2	1.92	0.49
1:A:1064:ARG:NH1	1:A:1064:ARG:O	2.45	0.49
1:A:3347:ALA:HB3	1:A:3351:ALA:HB2	1.94	0.49
1:A:3364:GLN:NE2	1:A:3405:ASP:OD1	2.46	0.49
1:A:1656:ASN:OD1	1:A:1656:ASN:N	2.45	0.48
1:A:3357:THR:HG23	1:A:3360:PHE:H	1.78	0.48
1:A:1160:ARG:HD2	1:A:1272:ILE:HD11	1.95	0.48
1:A:1242:ALA:HA	1:A:1245:GLU:HB2	1.95	0.48
1:A:1250:VAL:HG12	1:A:1271:THR:HB	1.94	0.47
1:A:1137:GLN:OE1	1:A:1137:GLN:N	2.48	0.47
1:A:2126:ARG:HD2	1:A:3265:ILE:HG13	1.95	0.47
1:A:3117:ASP:HB3	1:A:3120:LEU:HB3	1.96	0.47
1:A:2071:ASP:OD1	1:A:2073:SER:OG	2.28	0.47
1:A:2911:ARG:O	1:A:2915:ASN:ND2	2.42	0.47
1:A:1352:LYS:NZ	1:A:1385:GLU:OE1	2.36	0.47
1:A:1012:VAL:HG22	1:A:1013:TYR:CD2	2.49	0.47
1:A:2012:ASP:N	1:A:2012:ASP:OD1	2.44	0.47
1:A:3097:ASP:OD2	1:A:3108:TYR:OH	2.33	0.47
1:A:3150:MET:HE1	1:A:3442:PRO:HD2	1.97	0.47
1:A:1823:VAL:O	1:A:1827:MET:HG2	2.15	0.47
1:A:1936:MET:HE1	1:A:1966:GLU:HG2	1.97	0.47
1:A:1541:ALA:O	1:A:1544:LYS:NZ	2.46	0.46
1:A:1715:MET:HE2	1:A:1715:MET:HA	1.98	0.46
1:A:2150:LEU:HD12	1:A:2154:GLN:HG3	1.96	0.46
1:A:1027:ILE:HD11	1:A:1117:PHE:CE1	2.50	0.46
1:A:1417:THR:HG23	1:A:1419:VAL:H	1.80	0.46
1:A:1501:GLU:OE2	1:A:1505:THR:OG1	2.29	0.46
1:A:1136:GLU:N	1:A:1143:LYS:O	2.47	0.46
1:A:2847:THR:HG22	1:A:2849:GLY:H	1.81	0.46
1:A:2996:THR:HG22	1:A:3126:LEU:HD13	1.98	0.46
1:A:1017:VAL:HG23	1:A:1137:GLN:HB3	1.98	0.46
1:A:1037:LEU:HD22	1:A:1038:PRO:HD2	1.98	0.46
1:A:2213:ASP:OD1	1:A:2213:ASP:N	2.39	0.46
1:A:1030:TYR:OH	1:A:1125:ARG:NH2	2.49	0.46
1:A:2796:LEU:HD21	1:A:2859:LYS:HB3	1.98	0.46
1:A:3079:ALA:O	1:A:3083:ASN:ND2	2.47	0.45
1:A:1085:ARG:HA	1:A:1085:ARG:HD2	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1607:ASP:OD1	1:A:1607:ASP:N	2.43	0.45
1:A:1988:MET:HA	1:A:1988:MET:HE2	1.98	0.45
1:A:1079:ASN:O	1:A:1083:ILE:HD13	2.16	0.45
1:A:2137:SER:OG	1:A:2138:ALA:N	2.50	0.45
1:A:2993:ASP:OD2	1:A:2996:THR:OG1	2.29	0.45
1:A:2211:PHE:O	1:A:2214:LYS:NZ	2.33	0.45
1:A:3204:GLN:OE1	1:A:3349:ARG:NH2	2.49	0.45
1:A:1365:ASN:OD1	1:A:1365:ASN:N	2.48	0.44
1:A:2797:GLU:OE2	1:A:2864:TYR:OH	2.29	0.44
1:A:2799:GLU:OE2	1:A:2803:GLN:NE2	2.48	0.44
1:A:2196:GLU:HB2	1:A:2199:GLU:HG2	1.99	0.44
1:A:1090:MET:HE3	1:A:1090:MET:HB2	1.80	0.44
1:A:1130:LYS:NZ	1:A:1226:GLY:O	2.42	0.44
1:A:2700:HIS:O	1:A:2704:ASN:ND2	2.51	0.44
1:A:1071:LYS:NZ	1:A:1074:ALA:HB2	2.33	0.44
1:A:1112:ASP:HB2	1:A:1115:LYS:HD3	2.00	0.44
1:A:2529:THR:HG23	1:A:2531:LEU:H	1.83	0.44
1:A:2697:GLN:HB3	1:A:2698:PRO:HD3	1.99	0.44
1:A:3005:ALA:HB3	1:A:3046:GLN:HB2	1.99	0.44
1:A:2761:GLY:O	1:A:2765:THR:OG1	2.26	0.43
1:A:1369:LEU:HB3	1:A:1374:ALA:HB2	2.00	0.43
1:A:1010:ASP:OD1	1:A:1010:ASP:N	2.49	0.43
1:A:3304:ILE:HD13	1:A:3309:PHE:HB3	1.99	0.43
1:A:1254:VAL:HG12	1:A:1267:ILE:H	1.84	0.43
1:A:3255:ASN:C	1:A:3255:ASN:OD1	2.61	0.43
1:A:1053:LYS:HA	1:A:1053:LYS:HD3	1.92	0.43
1:A:1353:ASP:OD1	1:A:1354:ARG:N	2.52	0.43
1:A:2491:GLU:OE2	1:A:2505:ARG:NH2	2.51	0.43
1:A:3332:TYR:CZ	1:A:3336:LEU:HD11	2.54	0.43
1:A:3452:PRO:HA	1:A:3457:PHE:CE1	2.54	0.43
1:A:1567:MET:HB3	1:A:1567:MET:HE3	1.78	0.42
1:A:2125:GLY:O	1:A:2134:ARG:NH1	2.50	0.42
1:A:1066:GLU:HA	1:A:1071:LYS:NZ	2.34	0.42
1:A:2067:ASN:O	1:A:2067:ASN:ND2	2.45	0.42
1:A:2705:ASP:O	1:A:3439:ARG:NH2	2.52	0.42
1:A:3007:ARG:NH2	1:A:3460:VAL:O	2.50	0.42
1:A:1384:VAL:HG21	1:A:1659:LEU:HD22	2.02	0.42
1:A:2304:LYS:HE2	1:A:2304:LYS:HB2	1.91	0.42
1:A:1596:MET:N	1:A:2055:ASP:OD2	2.50	0.42
1:A:1135:VAL:CG1	1:A:1142:PHE:HB3	2.50	0.42
1:A:2834:ASN:OD1	1:A:2834:ASN:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3317:ILE:HD13	1:A:3317:ILE:HA	1.89	0.42
1:A:1030:TYR:H	1:A:1133:ASN:HD21	1.65	0.42
1:A:1849:ASP:OD1	1:A:1849:ASP:N	2.53	0.42
1:A:3215:VAL:O	1:A:3219:VAL:HG23	2.20	0.42
1:A:1264:LYS:HD3	1:A:1264:LYS:HA	1.85	0.42
1:A:1930:MET:HE2	1:A:1945:LYS:HB2	2.01	0.42
1:A:3196:VAL:HG13	1:A:3481:LEU:HD12	2.02	0.42
1:A:2051:ASN:OD1	1:A:2051:ASN:N	2.53	0.41
1:A:1096:ILE:HA	1:A:1099:ILE:HD12	2.03	0.41
1:A:2987:ASN:OD1	1:A:2987:ASN:N	2.53	0.41
1:A:1069:THR:HB	1:A:1071:LYS:HE3	2.03	0.41
1:A:1083:ILE:O	1:A:1087:LYS:HG2	2.19	0.41
1:A:3421:MET:HE2	1:A:3421:MET:HB3	1.79	0.41
1:A:2072:LEU:HD23	1:A:2072:LEU:HA	1.91	0.41
1:A:2814:LYS:HD3	1:A:2814:LYS:HA	1.86	0.41
1:A:3437:MET:HE3	1:A:3444:HIS:CD2	2.56	0.41
1:A:1432:SER:OG	1:A:1433:ALA:N	2.53	0.41
1:A:2196:GLU:H	1:A:2199:GLU:HB2	1.85	0.41
1:A:2530:SER:O	1:A:2530:SER:OG	2.33	0.41
1:A:2953:TYR:HB3	1:A:2964:LYS:HB2	2.03	0.41
1:A:1041:GLN:NE2	1:A:1043:SER:O	2.54	0.40
1:A:1899:ARG:O	1:A:1899:ARG:NH1	2.54	0.40
1:A:2197:MET:O	1:A:2201:GLN:NE2	2.54	0.40
1:A:3219:VAL:HG22	1:A:3333:MET:HG3	2.03	0.40
1:A:1132:LEU:HA	1:A:1135:VAL:HG23	2.02	0.40
1:A:3477:LEU:HD23	1:A:3477:LEU:HA	1.90	0.40
1:A:2047:LEU:HD23	1:A:2047:LEU:HA	1.92	0.40
1:A:3258:ILE:HD12	1:A:3258:ILE:N	2.34	0.40
1:A:1828:PHE:O	1:A:1832:VAL:HG13	2.22	0.40
1:A:1084:LYS:HE3	1:A:1084:LYS:HB3	1.97	0.40
1:A:2136:LEU:HD12	1:A:2136:LEU:HA	1.80	0.40
1:A:2158:LEU:HD13	1:A:2158:LEU:HA	1.93	0.40
1:A:3124:ILE:O	1:A:3127:MET:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	2435/3500 (70%)	2388 (98%)	47 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	2047/2874 (71%)	2019 (99%)	28 (1%)	62	87

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1067	LEU
1	A	1127	VAL
1	A	1243	PHE
1	A	1359	MET
1	A	1505	THR
1	A	1542	GLU
1	A	1553	VAL
1	A	1963	LYS
1	A	2028	LEU
1	A	2124	VAL
1	A	2133	VAL
1	A	2141	ILE
1	A	2144	LEU

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Mol	Chain	Res	Type
1	A	2158	LEU
1	A	2247	GLU
1	A	2294	SER
1	A	2421	VAL
1	A	2556	LYS
1	A	2769	VAL
1	A	2894	TYR
1	A	2923	VAL
1	A	2983	GLN
1	A	2987	ASN
1	A	3127	MET
1	A	3175	SER
1	A	3195	VAL
1	A	3240	VAL
1	A	3485	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1041	GLN
1	A	1193	GLN
1	A	1453	ASN
1	A	1503	ASN
1	A	1636	GLN
1	A	1830	GLN
1	A	1895	ASN
1	A	1979	ASN
1	A	2024	ASN
1	A	2149	ASN
1	A	2154	GLN
1	A	2201	GLN
1	A	2318	ASN
1	A	2394	ASN
1	A	2510	GLN
1	A	2519	ASN
1	A	2665	HIS
1	A	2704	ASN
1	A	2759	HIS
1	A	2836	HIS
1	A	3194	HIS
1	A	3277	ASN
1	A	3396	GLN

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Mol	Chain	Res	Type
1	A	3467	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

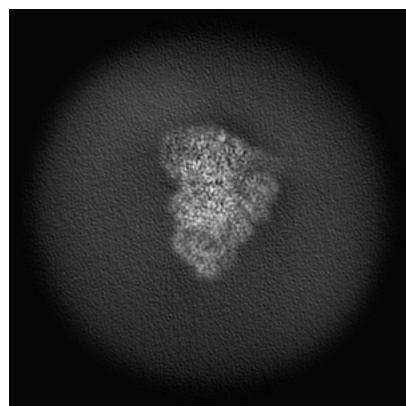
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71769. These allow visual inspection of the internal detail of the map and identification of artifacts.

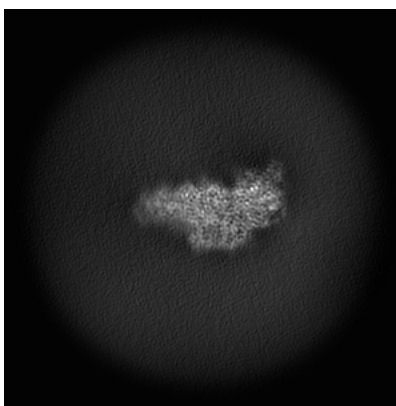
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

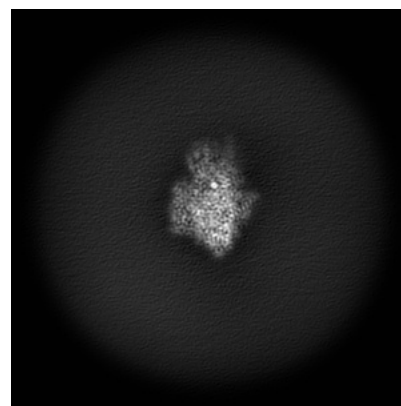
6.1.1 Primary map



X

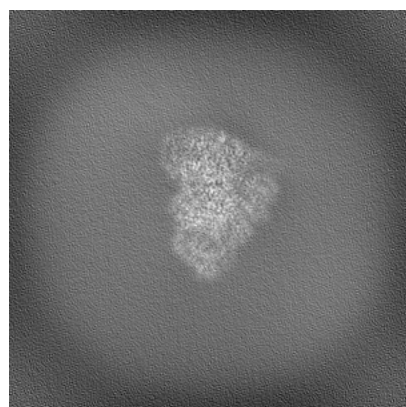


Y

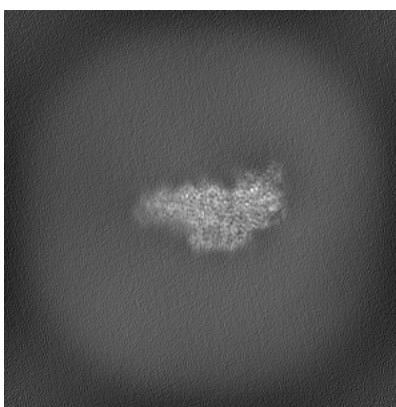


Z

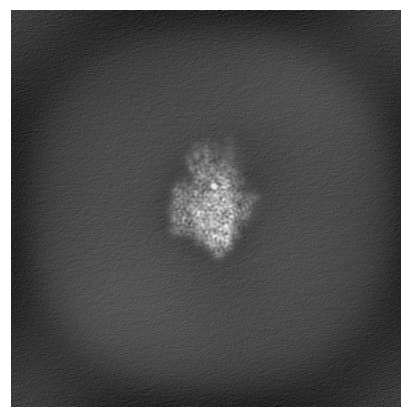
6.1.2 Raw map



X



Y

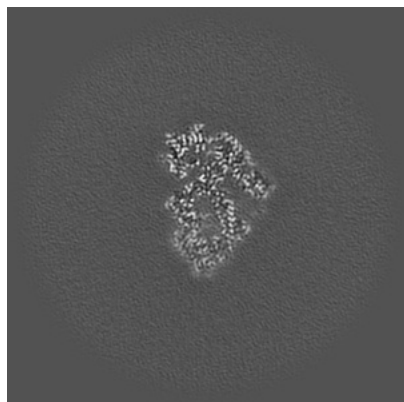


Z

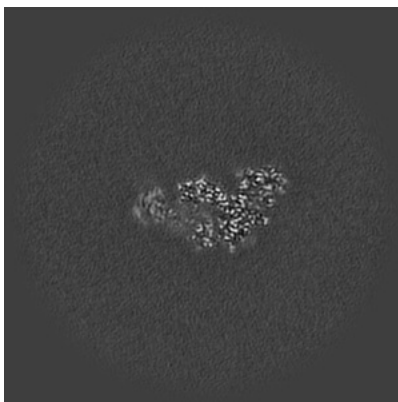
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

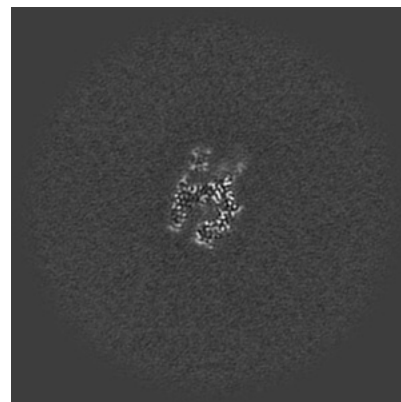
6.2.1 Primary map



X Index: 160

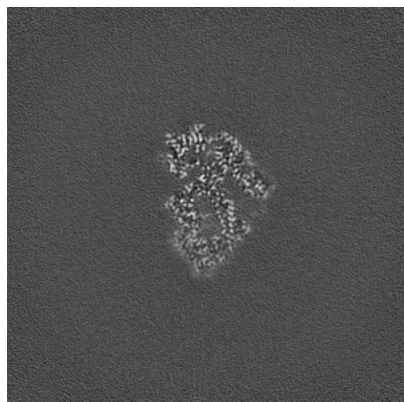


Y Index: 160

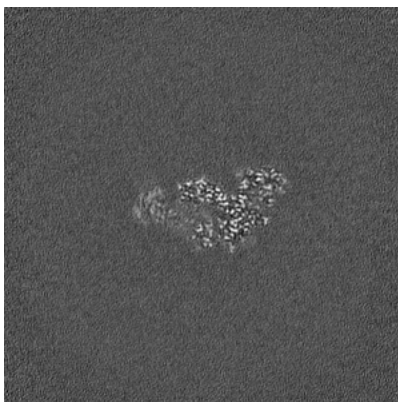


Z Index: 160

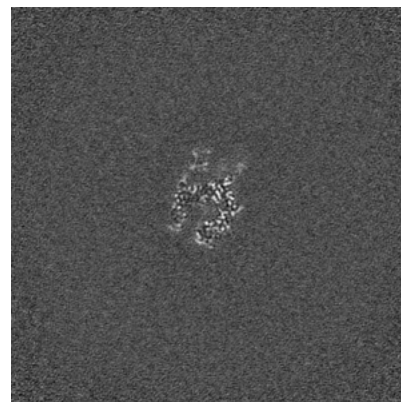
6.2.2 Raw map



X Index: 160



Y Index: 160

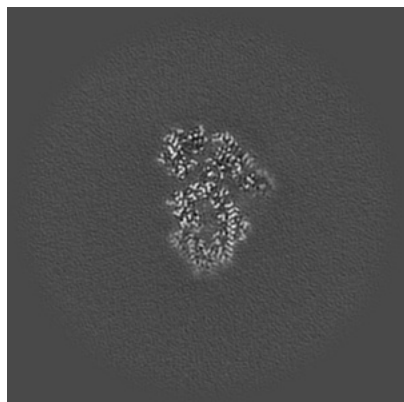


Z Index: 160

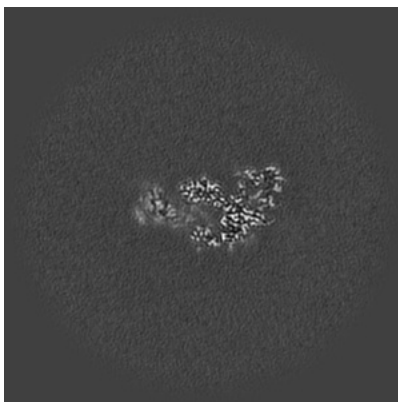
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

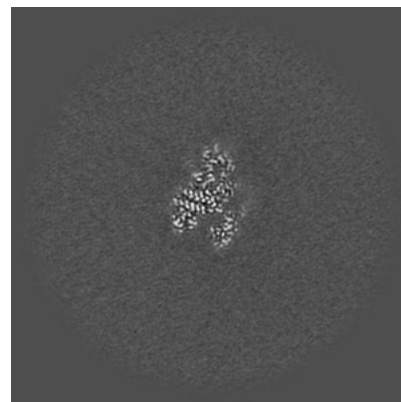
6.3.1 Primary map



X Index: 162

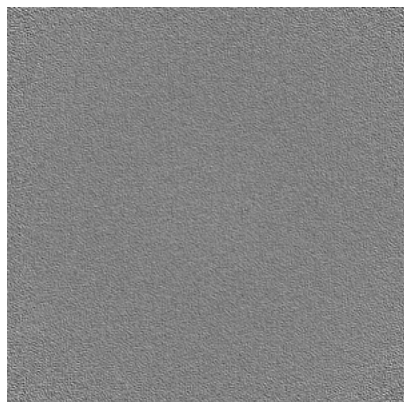


Y Index: 158

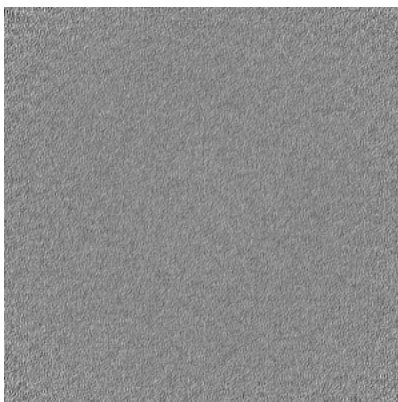


Z Index: 185

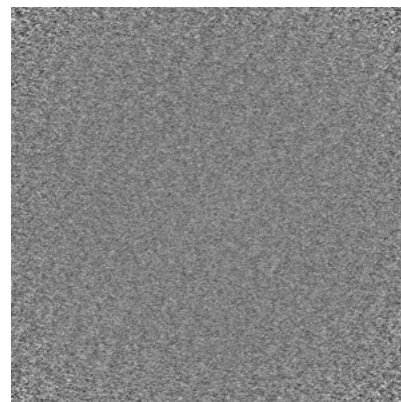
6.3.2 Raw map



X Index: 0



Y Index: 0

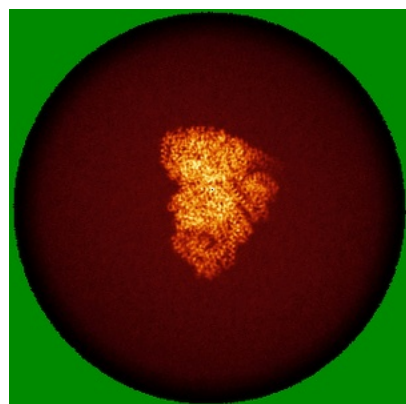


Z Index: 0

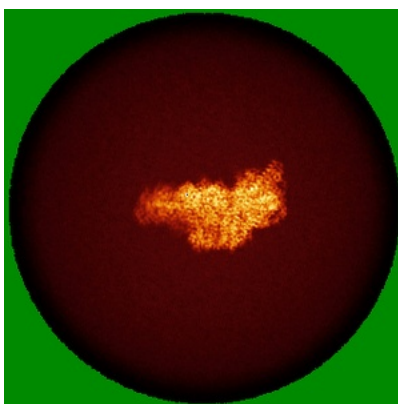
The images above show the largest variance slices of the map in three orthogonal directions.

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

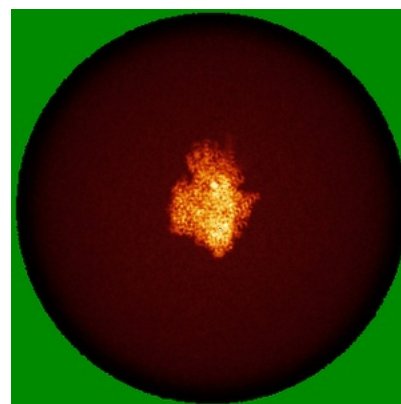
6.4.1 Primary map



X

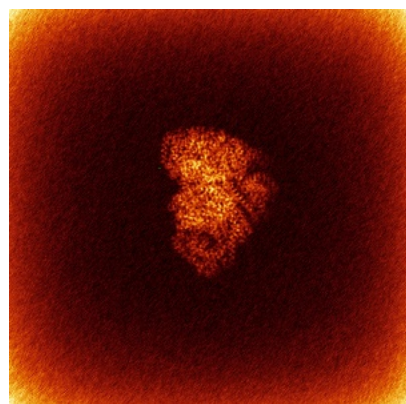


Y

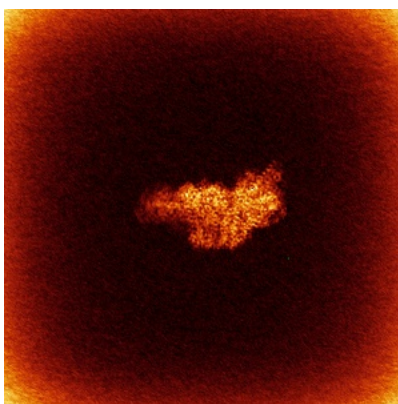


Z

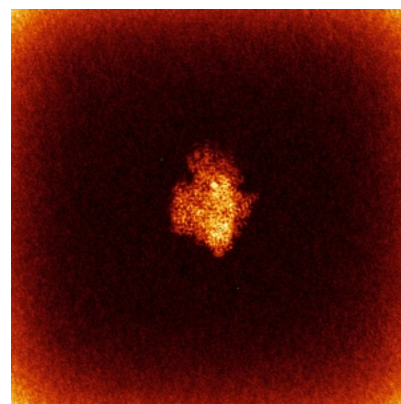
6.4.2 Raw map



X



Y

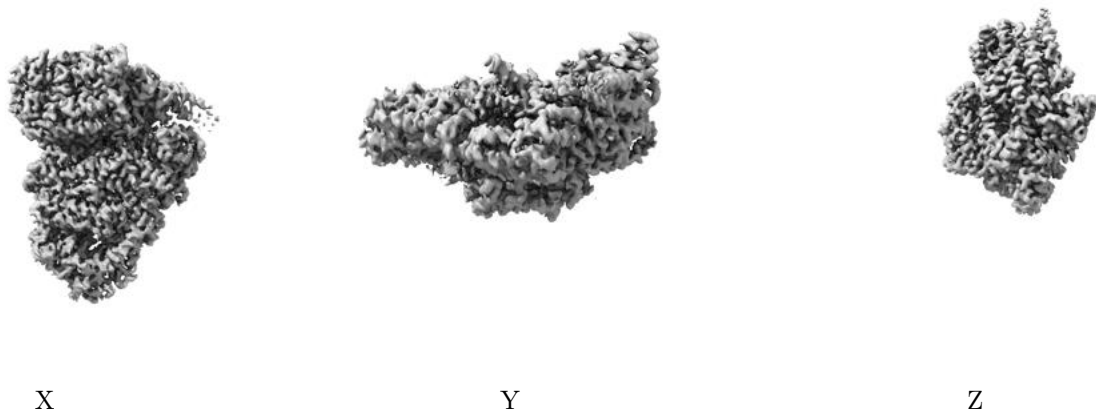


Z

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.

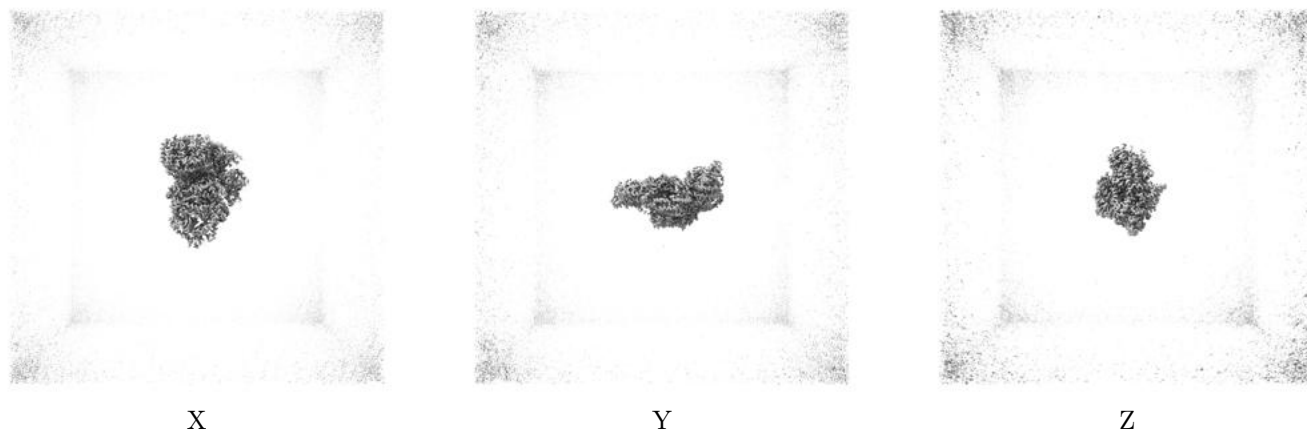
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0646. 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.

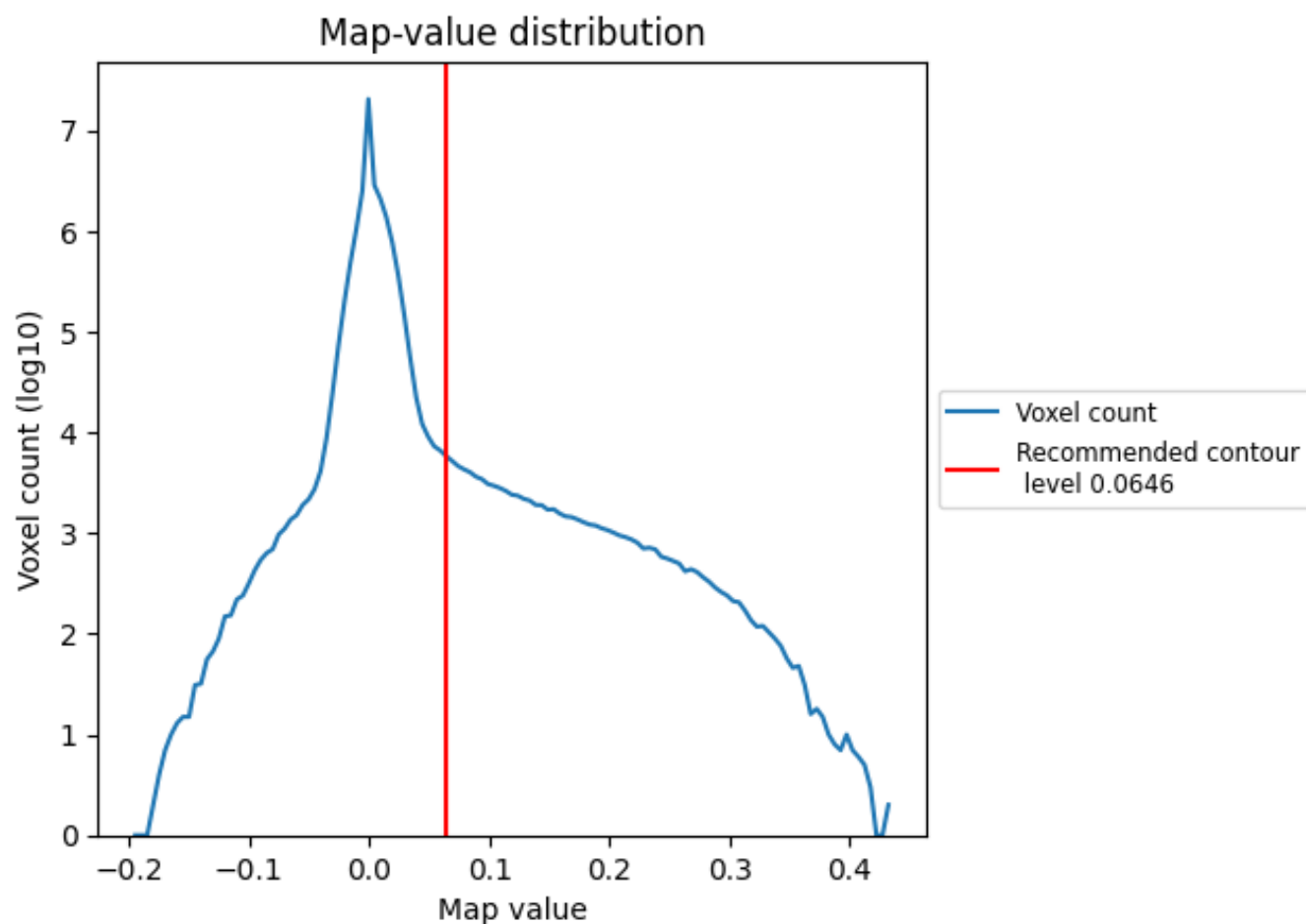
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

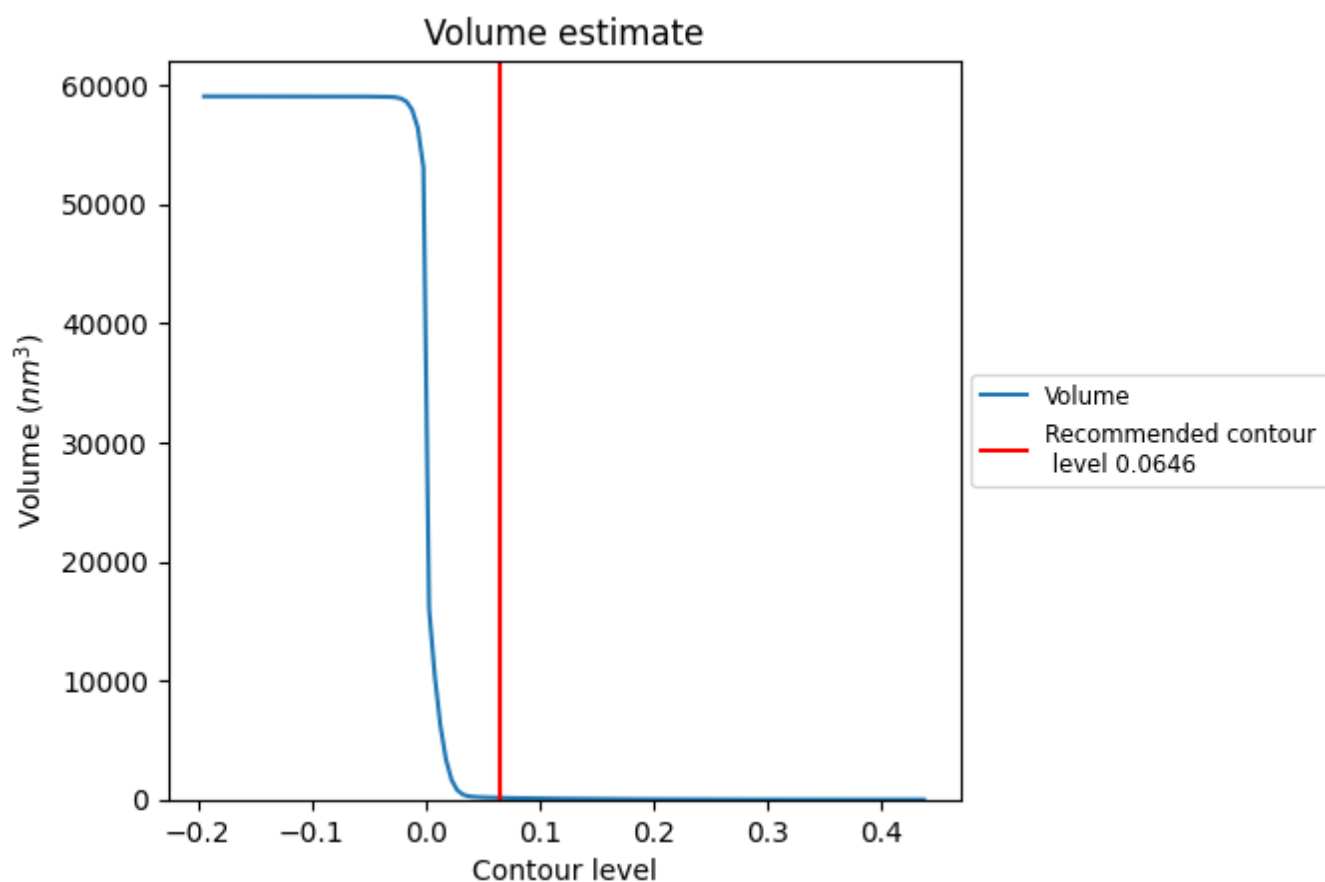
This section contains the results of statistical analysis of the map.

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.

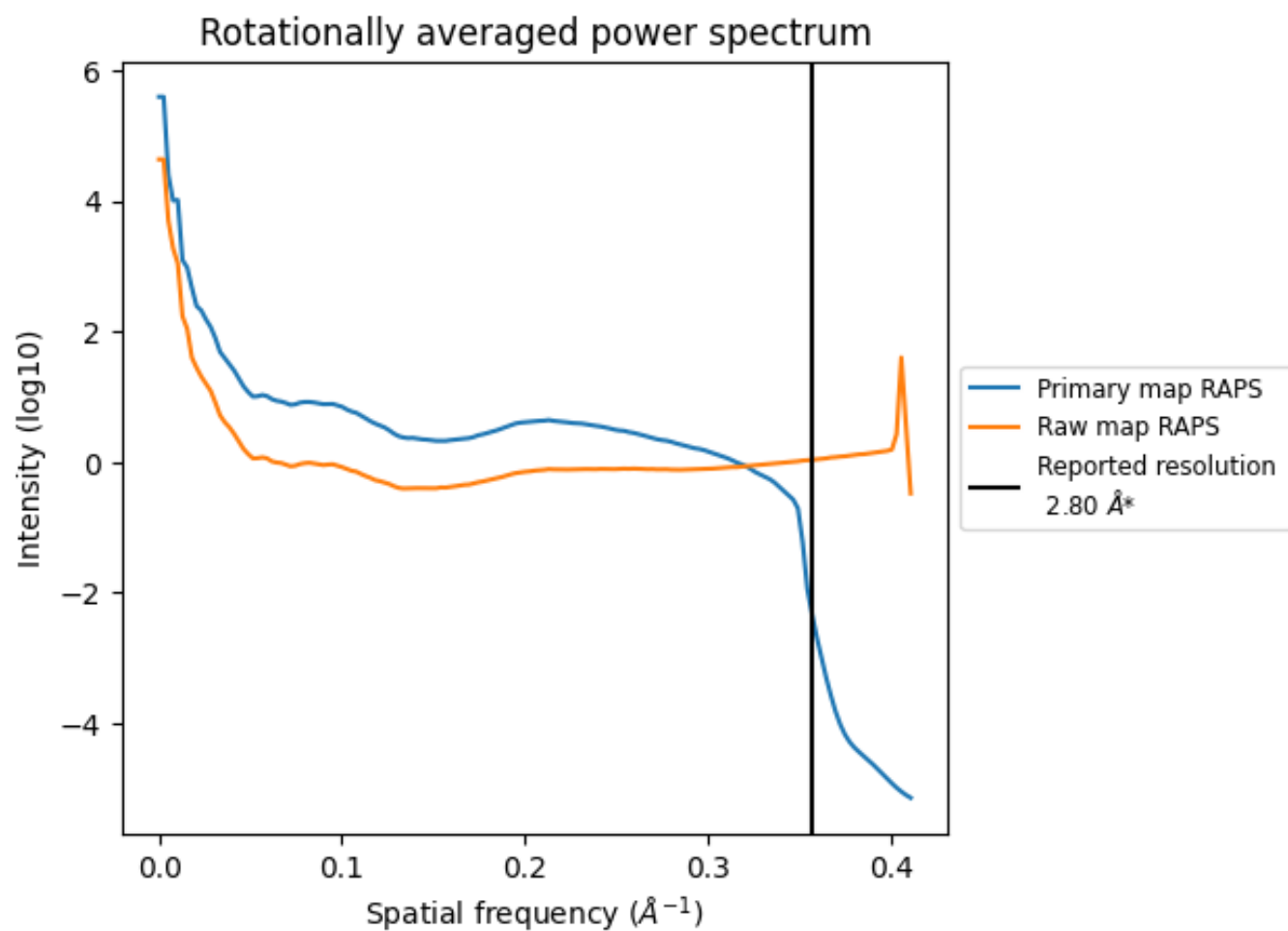
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 150 nm³; this corresponds to an approximate mass of 136 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 ⓘ

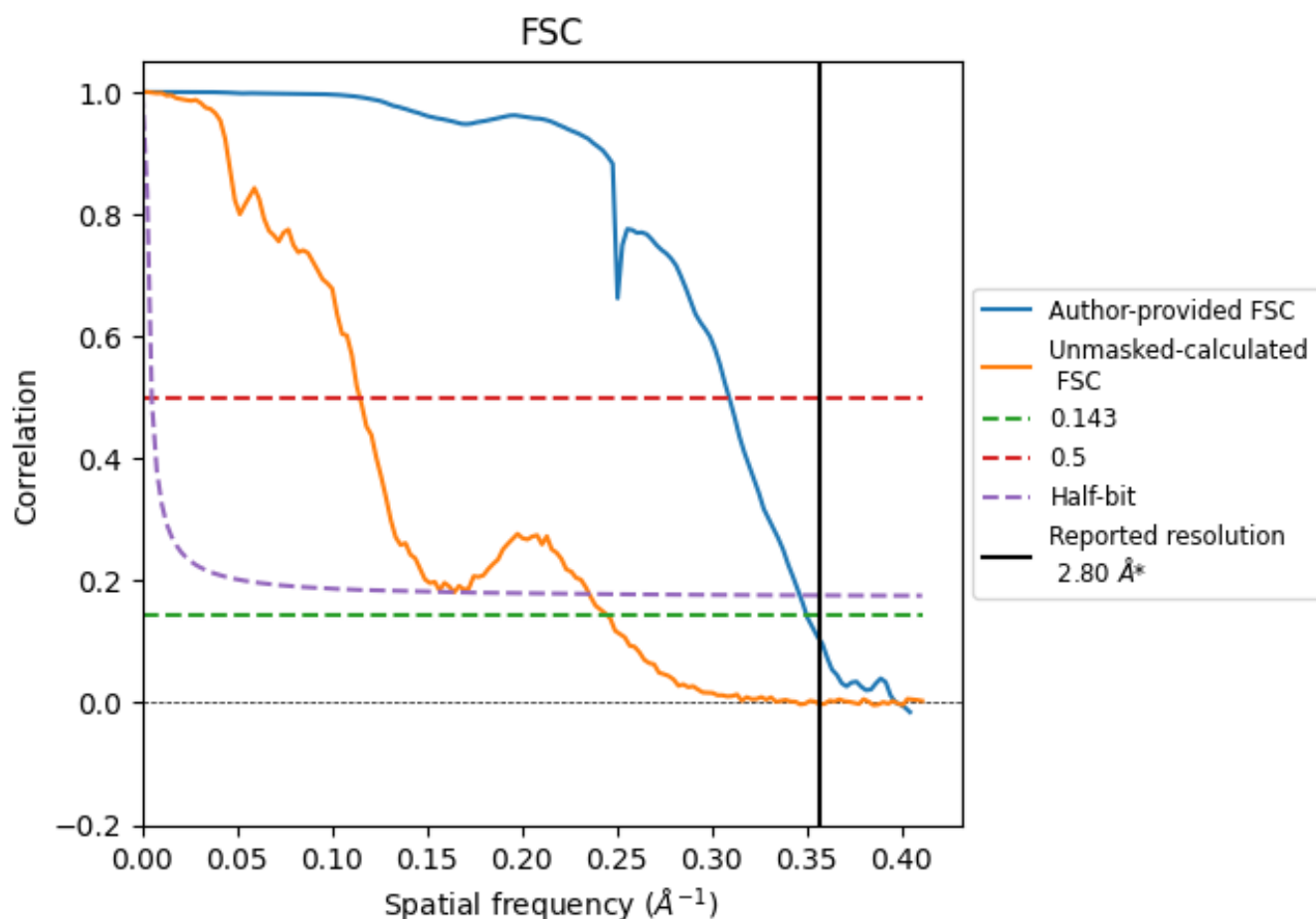


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

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 0.357 \AA^{-1}

8.2 Resolution estimates [i](#)

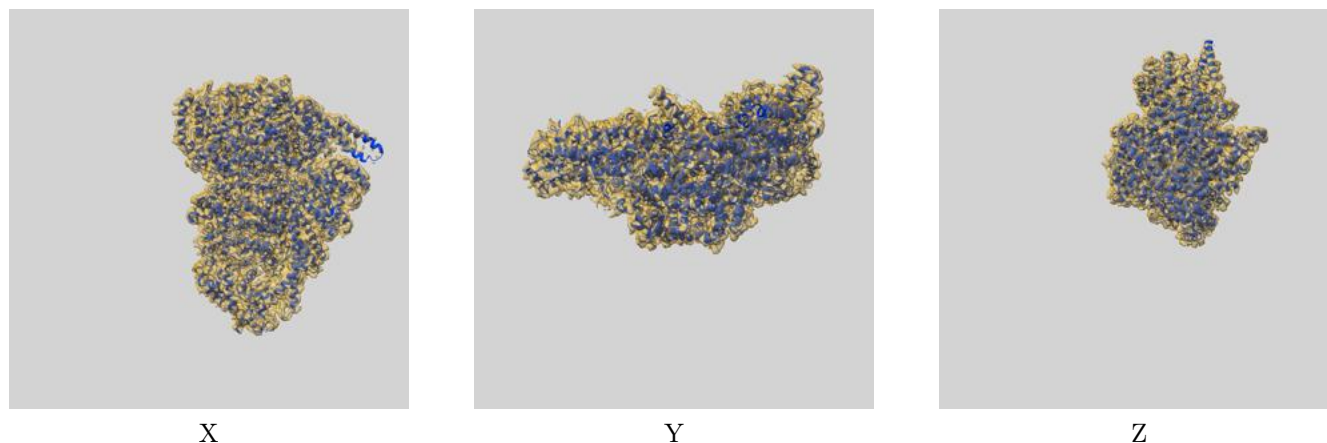
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.86	3.24	2.89
Unmasked-calculated*	4.08	8.73	6.09

*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 4.08 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

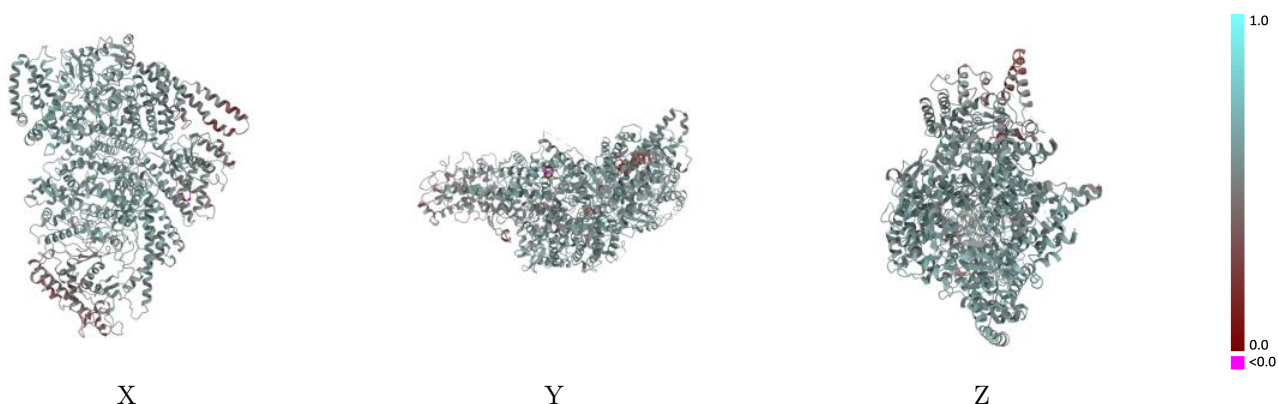
This section contains information regarding the fit between EMDB map EMD-71769 and PDB model 9PNR. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



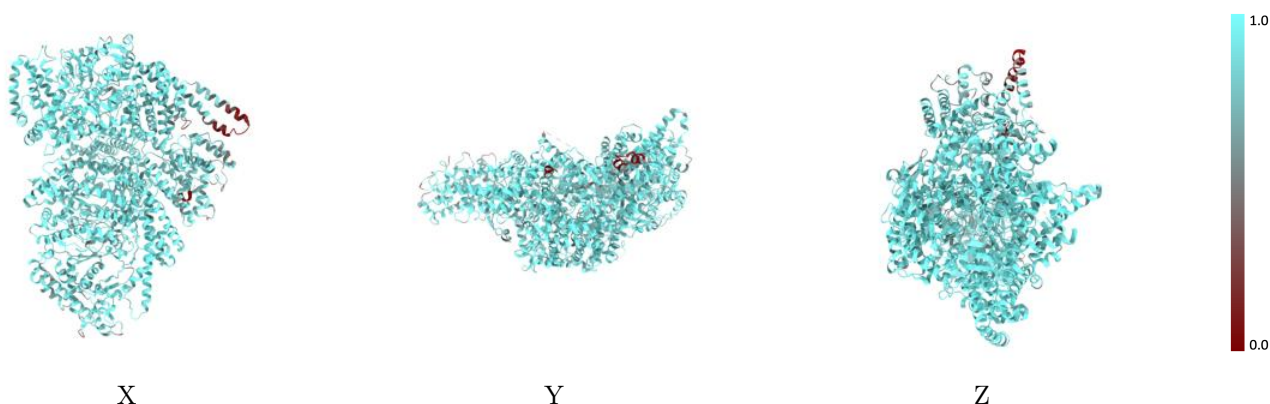
The images above show the 3D surface view of the map at the recommended contour level 0.0646 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



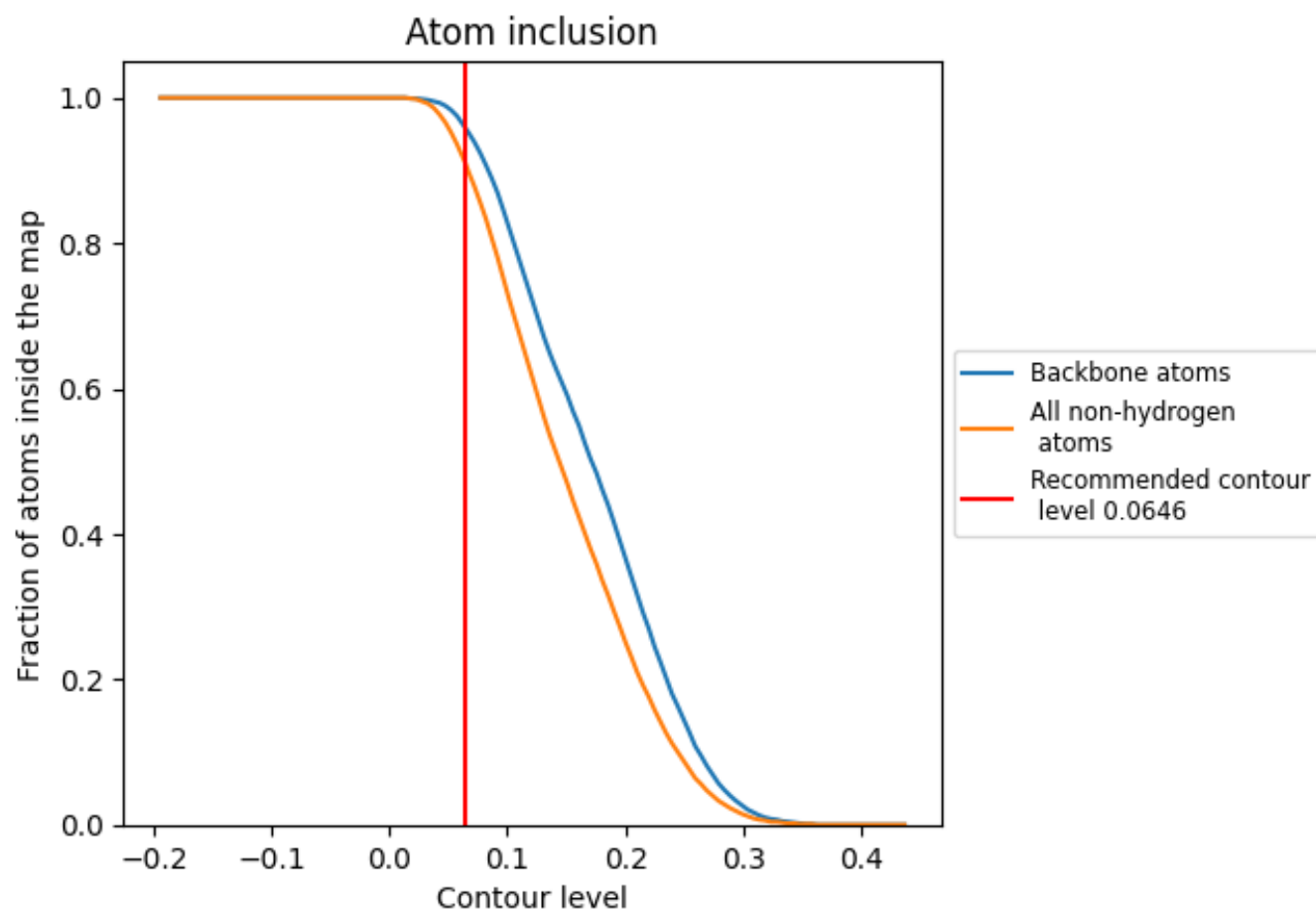
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0646).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 91% 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 (0.0646) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9090	<div><div></div></div> 0.5490
A	<div><div></div></div> 0.9090	<div><div></div></div> 0.5490

