Full wwPDB EM Validation Report ⓘ

Aug 24, 2026 – 10:15 AM EDT

PDB ID	:	11GP / pdb_000011gp
EMDB ID	:	EMD-75681
Title	:	Cryo-EM structure of the bacteriophage N4 virion RNA polymerase (closed plug state)
Authors	:	Narwal, M.; Shin, Y.; Murakami, K.S.
Deposited on	:	2026-02-23
Resolution	:	3.43 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:

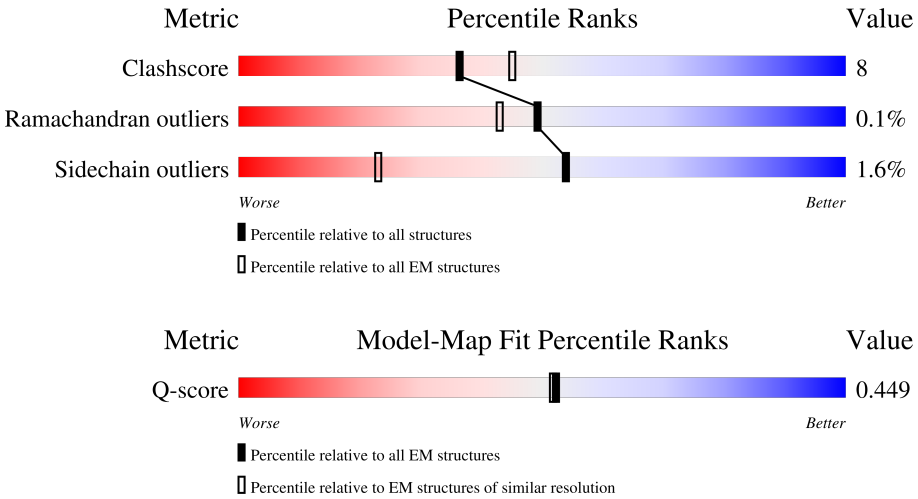
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.43 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	13927 (2.93 - 3.93)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3500	56% 13% 30%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 19068 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
			Total	C	N	O	S		
1	A	2453	19068	11972	3309	3695	92	0	0

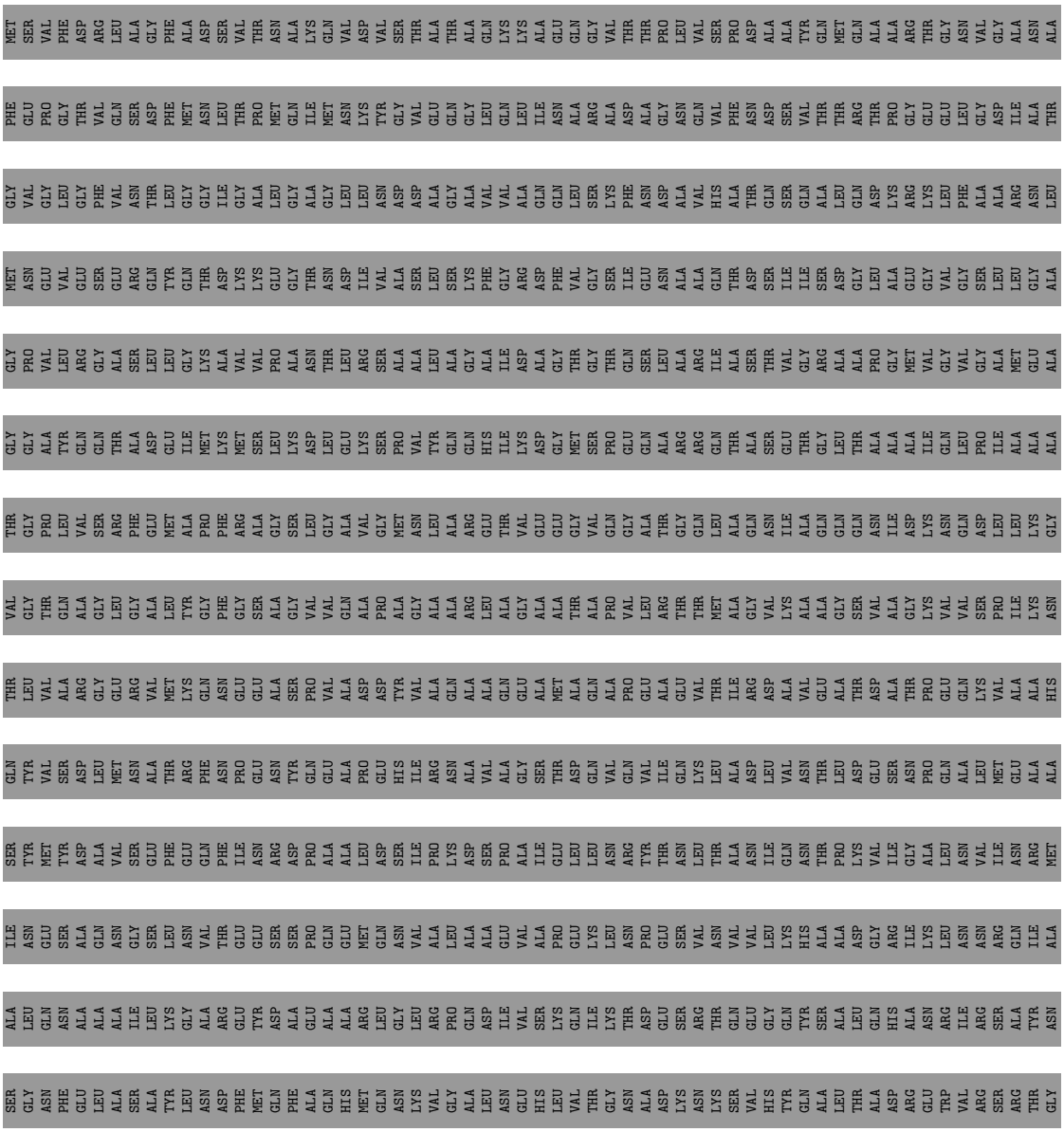
3 Residue-property plots (i)

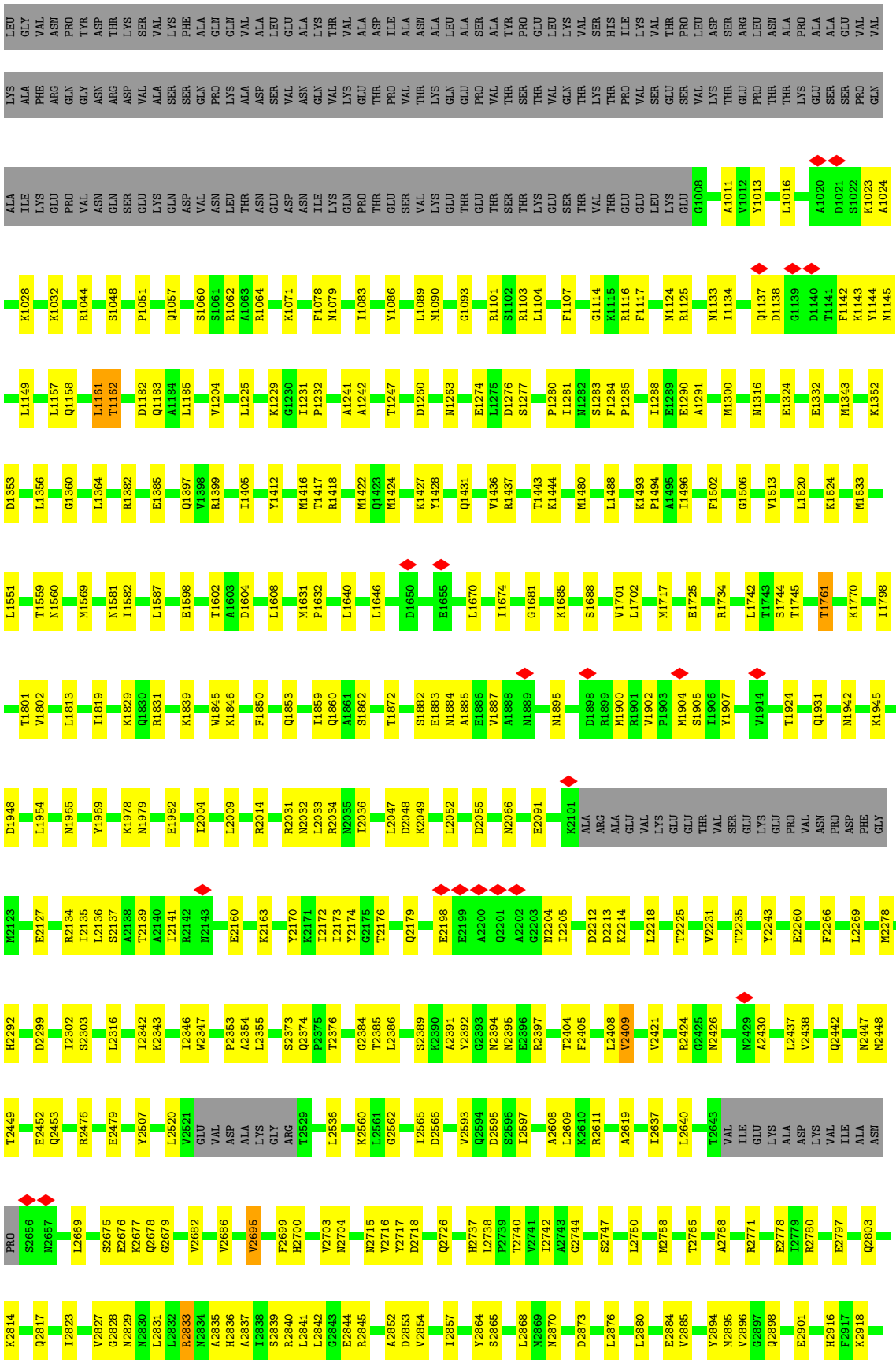
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

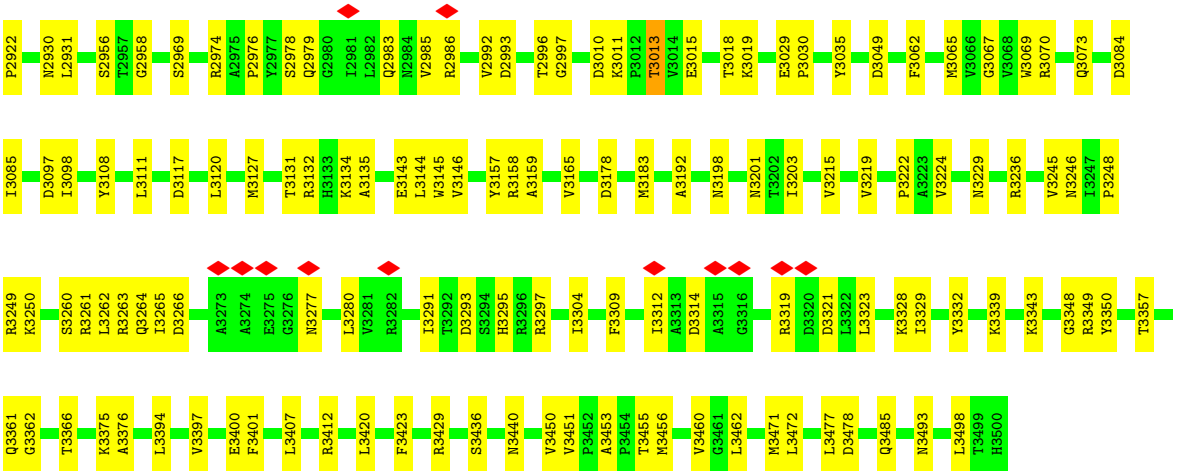
- Molecule 1: Virion DNA-directed RNA polymerase

Chain A:






LEU GLY VAL ASN PRO TYR ASP THR LYS SER VAL LYS PHE ALA GLN GLN VAL ALA LEU GLU ALA LYS VAL THR VAL ALA ASP ILE ALA ASN ALA LEU ASP ALA SER LEU ASN ALA PRO ASN LEU ARG LEU PRO THR HIS ILE LYS VAL THR PRO LEU ASP SER ARG LEU ASN ALA PRO ALA ALA GLU VAL VAL
LYS ALA PHE ARG GLN GLY ASN ARG ASP VAL ALA SER SER GLN PRO LYS ALA ASP SER VAL ASN GLN THR VAL LYS GLU THR PRO VAL THR LYS GLN GLU PRO VAL THR SER THR VAL GLN THR LYS VAL THR PRO VAL SER GLU SER VAL LYS THR GLU PRO THR THR LYS GLU SER PRO GLN
ALA ILE LYS GLU PRO VAL ASN GLN SER GLU LYS GLN ASP VAL ASN LEU THR ASN GLU ASP ASN ILE LYS GLN PRO THR GLU SER VAL LYS GLU THR GLU THR SER THR LYS GLU SER THR VAL THR VAL THR GLU GLU LEU LYS GLU G1008 A1011 V1012 Y1013 L1016 A1020 D1021 S1022 K1023 A1024
K1028 K1032 R1044 S1048 P1051 Q1057 S1060 S1061 R1062 A1063 R1064 K1071 F1078 N1079 I1083 Y1086 L1089 M1090 G1093 R1101 S1102 R1103 L1104 F1107 G1114 K1115 R1116 F1117 N1124 R1125 N1133 I1134 Q1137 D1138 G1139 D1140 T1141 F1142 K1143 Y1144 N1145
L1149 L1157 Q1158 L1161 T1162 D1182 Q1183 A1184 L1185 V1204 L1225 K1229 G1230 I1231 P1232 A1241 A1242 T1247 D1260 N1263 E1274 L1275 D1276 S1277 P1280 I1281 N1282 S1283 F1284 P1285 I1288 E1289 E1290 A1291 M1300 N1316 E1324 E1332 M1343 K1352
D1353 L1356 G1360 L1364 R1382 E1385 Q1397 V1398 R1399 I1405 Y1412 M1416 T1417 R1418 M1422 Q1423 M1424 K1427 Y1428 Q1431 V1436 R1437 T1443 K1444 M1480 L1488 K1493 P1494 A1495 I1496 F1502 G1506 V1513 L1520 K1524 M1533
L1551 T1559 N1560 M1569 N1581 I1582 L1587 E1598 T1602 A1603 D1604 L1608 M1631 P1632 L1640 L1646 D1650 E1655 L1670 I1674 G1681 K1685 S1688 V1701 L1702 M1717 E1725 R1734 L1742 T1743 S1744 T1745 T1761 K1770 I1798
T1801 V1802 L1813 I1819 K1829 Q1830 R1831 K1839 W1845 K1846 F1850 Q1853 I1859 Q1860 A1861 S1862 T1872 S1882 E1883 N1884 A1885 E1886 V1887 A1888 N1889 N1895 D1898 R1899 M1900 R1901 V1902 P1903 M1904 S1905 I1906 Y1907 V1914 T1924 Q1931 N1942 K1945
D1948 L1954 N1965 Y1969 K1978 N1979 E1982 I2004 L2009 R2014 R2031 N2032 L2033 R2034 N2035 I2036 L2047 D2048 K2049 L2052 D2055 N2066 E2091 K2101 ALA ARG ALA GLU VAL LYS GLU GLU THR VAL SER GLU LYS GLU PRO VAL ASN PRO ASP PHE GLY
M2123 E2127 R2134 I2135 L2136 S2137 A2138 T2139 A2140 I2141 R2142 N2143 E2160 K2163 Y2170 K2171 I2172 I2173 Y2174 G2175 T2176 Q2179 E2198 E2199 A2200 Q2201 A2202 G2203 N2204 I2205 D2212 D2213 K2214 L2218 T2225 V2231 T2235 Y2243 E2260 F2266 L2269 M2278
H2292 D2299 I2302 S2303 L2316 I2342 K2343 I2346 W2347 P2353 A2354 L2355 S2373 Q2374 P2375 T2376 G2384 T2385 L2386 S2389 K2390 A2391 Y2392 G2393 N2394 N2395 E2396 R2397 T2404 F2405 L2408 V2409 V2421 R2424 G2425 N2426 N2429 A2430 L2437 V2438 Q2442 N2447 M2448
T2449 E2452 Q2453 R2476 E2479 Y2507 L2520 V2521 GLU VAL ASP ALA LYS GLY ARG T2529 L2536 K2560 L2561 G2562 I2565 D2566 V2593 Q2594 D2595 S2596 I2597 A2608 L2609 K2610 R2611 A2619 I2637 L2640 T2643 VAL ILE GLU LYS ALA ASP LYS VAL ILE ALA ASN
PRO S2656 N2657 L2669 S2675 E2676 K2677 Q2678 G2679 V2682 V2686 V2695 F2699 H2700 V2703 N2704 N2715 V2716 Y2717 D2718 Q2726 H2737 L2738 P2739 T2740 V2741 I2742 A2743 G2744 S2747 L2750 M2758 T2765 A2768 R2771 E2778 I2779 R2780 E2797 Q2803
K2814 Q2817 I2823 V2827 G2828 N2829 N2830 L2831 L2832 R2833 N2834 A2835 H2836 A2837 I2838 S2839 R2840 L2841 L2842 G2843 E2844 R2845 A2852 D2853 V2854 I2857 Y2864 S2865 L2868 M2869 N2870 D2873 L2876 L2880 E2884 V2885 Y2894 M2895 V2896 G2897 Q2898 E2901 H2916 F2917 K2918


P2922 N2930 L2931 S2956 T2957 G2958 S2969 R2974 A2975 P2976 Y2977 S2978 Q2979 G2980 I2981 L2982 Q2983 N2984 V2985 R2986 V2992 D2993 T2996 G2997 D3010 K3011 P3012 T3013 V3014 E3015 T3018 K3019 E3029 P3030 Y3035 D3049 F3062 M3065 V3066 G3067 V3068 W3069 R3070 Q3073 D3084
I3085 D3097 I3098 Y3108 L3111 D3117 L3120 M3127 T3131 R3132 H3133 K3134 A3135 E3143 L3144 W3145 V3146 Y3157 R3158 A3159 V3165 D3178 M3183 A3192 N3198 N3201 T3202 I3203 V3215 V3219 P3222 A3223 V3224 N3229 R3236 V3245 N3246 I3247 P3248
R3249 K3250 S3260 R3261 L3262 R3263 Q3264 I3265 D3266 A3273 A3274 E3275 G3276 N3277 L3280 V3281 R3282 I3291 T3292 D3293 S3294 H3295 R3296 R3297 I3304 F3309 I3312 A3313 D3314 A3315 G3316 R3319 D3320 D3321 L3322 L3323 K3328 I3329 Y3332 K3339 K3343 G3348 R3349 Y3350 T3357
Q3361 G3362 T3366 K3375 A3376 L3394 V3397 E3400 F3401 L3407 R3412 L3420 F3423 R3429 S3436 N3440 V3450 V3451 P3452 A3453 P3454 T3455 M3456 V3460 G3461 L3462 M3471 L3472 L3477 D3478 Q3485 N3493 L3498 T3499 H3500

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50000	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.566	Depositor
Minimum map value	-0.246	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.102	Depositor
Map size (Å)	256.80002, 256.80002, 256.80002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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	0.28	0/19370	0.41	1/26178 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3312	ILE	N-CA-C	-5.21	107.64	112.43

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	19068	0	19173	294	0
All	All	19068	0	19173	294	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 8.

All (294) 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:2922:PRO:HD3	1:A:3069:TRP:HD1	1.40	0.84
1:A:2797:GLU:OE2	1:A:2864:TYR:OH	2.05	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2969:SER:OG	1:A:2974:ARG:NH2	2.18	0.75
1:A:2898:GLN:HB3	1:A:3069:TRP:CZ3	2.23	0.73
1:A:2922:PRO:HD3	1:A:3069:TRP:CD1	2.24	0.72
1:A:2715:ASN:O	1:A:2717:TYR:N	2.18	0.72
1:A:1831:ARG:NH1	1:A:1862:SER:OG	2.23	0.71
1:A:2771:ARG:HG3	1:A:2896:VAL:HG21	1.71	0.71
1:A:2742:ILE:HG12	1:A:2894:TYR:HE2	1.58	0.69
1:A:3117:ASP:OD2	1:A:3158:ARG:NH2	2.26	0.69
1:A:1640:LEU:HA	1:A:1742:LEU:HD11	1.75	0.69
1:A:1646:LEU:HD11	1:A:1734:ARG:HH21	1.58	0.69
1:A:2385:THR:HG23	1:A:2386:LEU:HG	1.75	0.69
1:A:2803:GLN:NE2	1:A:2853:ASP:OD2	2.24	0.68
1:A:2841:LEU:HG	1:A:2852:ALA:HB3	1.75	0.68
1:A:1444:LYS:NZ	1:A:1942:ASN:OD1	2.27	0.68
1:A:2675:SER:OG	1:A:2737:HIS:NE2	2.24	0.68
1:A:2993:ASP:HB3	1:A:2997:GLY:H	1.59	0.67
1:A:3450:VAL:HG13	1:A:3451:VAL:HG23	1.75	0.67
1:A:2814:LYS:HG2	1:A:2833:ARG:HH11	1.58	0.67
1:A:2316:LEU:HD21	1:A:2342:ILE:HD13	1.77	0.67
1:A:1086:TYR:OH	1:A:1284:PHE:O	2.11	0.67
1:A:3304:ILE:HG13	1:A:3309:PHE:CE2	2.30	0.66
1:A:3328:LYS:HG3	1:A:3329:ILE:H	1.60	0.66
1:A:1324:GLU:OE1	1:A:1324:GLU:N	2.27	0.66
1:A:1044:ARG:NH2	1:A:1290:GLU:O	2.28	0.66
1:A:3015:GLU:O	1:A:3019:LYS:NZ	2.22	0.66
1:A:1560:ASN:HD22	1:A:1948:ASP:HB2	1.61	0.66
1:A:2384:GLY:O	1:A:2611:ARG:NH1	2.29	0.66
1:A:2243:TYR:OH	1:A:2260:GLU:OE2	2.13	0.65
1:A:2814:LYS:HG2	1:A:2833:ARG:HD3	1.78	0.65
1:A:2922:PRO:CD	1:A:3069:TRP:HD1	2.08	0.65
1:A:1060:SER:OG	1:A:1064:ARG:NH2	2.28	0.65
1:A:1674:ILE:HD11	1:A:1802:VAL:HG21	1.77	0.65
1:A:2765:THR:OG1	1:A:2865:SER:OG	2.14	0.65
1:A:3264:GLN:HB2	1:A:3291:ILE:HG21	1.80	0.64
1:A:2718:ASP:OD1	1:A:2718:ASP:N	2.30	0.64
1:A:1093:GLY:HA3	1:A:1157:LEU:HD11	1.80	0.64
1:A:2835:ALA:HB3	1:A:2918:LYS:H	1.63	0.63
1:A:3018:THR:OG1	1:A:3019:LYS:NZ	2.31	0.63
1:A:2476:ARG:NH1	1:A:2479:GLU:OE1	2.32	0.62
1:A:1332:GLU:OE2	1:A:1945:LYS:NZ	2.32	0.62
1:A:2676:GLU:OE2	1:A:2678:GLN:N	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:ARG:HD3	1:A:1078:PHE:HD2	1.64	0.62
1:A:1581:ASN:ND2	1:A:1801:THR:O	2.33	0.62
1:A:3293:ASP:HB3	1:A:3297:ARG:HH12	1.65	0.61
1:A:2404:THR:HG23	1:A:2408:LEU:HD12	1.81	0.61
1:A:2009:LEU:O	1:A:2014:ARG:NH2	2.34	0.61
1:A:1204:VAL:HG11	1:A:1902:VAL:HG11	1.82	0.61
1:A:1134:ILE:O	1:A:1145:ASN:ND2	2.34	0.60
1:A:1274:GLU:OE2	1:A:1382:ARG:NH2	2.29	0.60
1:A:3236:ARG:NH1	1:A:3400:GLU:OE1	2.31	0.60
1:A:1604:ASP:OD1	1:A:3412:ARG:NH2	2.23	0.60
1:A:3453:ALA:HB3	1:A:3456:MET:HB2	1.82	0.60
1:A:2346:ILE:HG22	1:A:2347:TRP:CD1	2.37	0.60
1:A:3097:ASP:OD2	1:A:3108:TYR:OH	2.18	0.60
1:A:3198:ASN:OD1	1:A:3201:ASN:N	2.33	0.59
1:A:2703:VAL:HG12	1:A:3085:ILE:HG21	1.84	0.59
1:A:3178:ASP:OD1	1:A:3178:ASP:N	2.33	0.59
1:A:3262:LEU:HD22	1:A:3319:ARG:HG2	1.84	0.58
1:A:1417:THR:OG1	1:A:1418:ARG:N	2.28	0.58
1:A:2204:ASN:ND2	1:A:2205:ILE:O	2.37	0.58
1:A:3215:VAL:HA	1:A:3339:LYS:HZ1	1.69	0.57
1:A:3127:MET:HE3	1:A:3132:ARG:HG2	1.84	0.57
1:A:3117:ASP:HB3	1:A:3120:LEU:HB3	1.86	0.57
1:A:1016:LEU:HD12	1:A:1032:LYS:HE3	1.85	0.57
1:A:1431:GLN:O	1:A:1437:ARG:NH2	2.34	0.57
1:A:2231:VAL:O	1:A:2235:THR:HG23	2.04	0.56
1:A:2780:ARG:HD2	1:A:2885:VAL:HG22	1.86	0.56
1:A:1158:GLN:O	1:A:1162:THR:OG1	2.24	0.56
1:A:2032:ASN:O	1:A:2036:ILE:HG13	2.06	0.56
1:A:1138:ASP:OD2	1:A:1143:LYS:NZ	2.31	0.56
1:A:2170:TYR:CD1	1:A:2214:LYS:HB3	2.41	0.56
1:A:3436:SER:O	1:A:3440:ASN:ND2	2.32	0.55
1:A:1103:ARG:HG2	1:A:1107:PHE:CE2	2.40	0.55
1:A:3229:ASN:OD1	1:A:3429:ARG:NH2	2.39	0.55
1:A:1104:LEU:HD22	1:A:1144:TYR:CZ	2.41	0.55
1:A:1316:ASN:OD1	1:A:1907:TYR:OH	2.11	0.55
1:A:1399:ARG:HE	1:A:1405:ILE:HD11	1.71	0.55
1:A:2437:LEU:HD22	1:A:2520:LEU:HD23	1.88	0.55
1:A:2049:LYS:NZ	1:A:2091:GLU:OE2	2.40	0.55
1:A:2986:ARG:HD3	1:A:3493:ASN:HD22	1.71	0.55
1:A:2448:MET:HB3	1:A:2452:GLU:HB2	1.88	0.55
1:A:3265:ILE:HG23	1:A:3319:ARG:HH21	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2676:GLU:OE2	1:A:2677:LYS:N	2.41	0.54
1:A:2394:ASN:HD22	1:A:2397:ARG:NH1	2.06	0.54
1:A:2682:VAL:HG11	1:A:2894:TYR:HE1	1.73	0.54
1:A:2836:HIS:O	1:A:2839:SER:OG	2.23	0.54
1:A:1831:ARG:HB3	1:A:1859:ILE:HD12	1.90	0.54
1:A:2768:ALA:HB2	1:A:2895:MET:HG3	1.89	0.54
1:A:2814:LYS:HZ2	1:A:2844:GLU:HA	1.73	0.54
1:A:1850:PHE:HZ	1:A:1887:VAL:HG21	1.73	0.53
1:A:1602:THR:HG23	1:A:2619:ALA:HB1	1.89	0.53
1:A:1969:TYR:OH	1:A:2048:ASP:OD1	2.27	0.53
1:A:3471:MET:HE1	1:A:3485:GLN:HB2	1.90	0.53
1:A:2835:ALA:HB1	1:A:2918:LYS:HB3	1.91	0.53
1:A:3263:ARG:NH1	1:A:3266:ASP:OD2	2.42	0.53
1:A:2442:GLN:HE22	1:A:2453:GLN:HG3	1.73	0.53
1:A:1103:ARG:HH22	1:A:1241:ALA:C	2.17	0.53
1:A:3215:VAL:HA	1:A:3339:LYS:NZ	2.24	0.53
1:A:1416:MET:SD	1:A:1422:MET:HG2	2.48	0.52
1:A:2845:ARG:HG2	1:A:3035:TYR:CE1	2.44	0.52
1:A:1978:LYS:NZ	1:A:1982:GLU:OE2	2.34	0.52
1:A:2292:HIS:O	1:A:2303:SER:OG	2.27	0.52
1:A:3246:ASN:OD1	1:A:3249:ARG:NH1	2.42	0.52
1:A:3203:ILE:HG21	1:A:3477:LEU:HD22	1.92	0.52
1:A:2405:PHE:HD1	1:A:2409:VAL:HB	1.75	0.52
1:A:2837:ALA:HA	1:A:2840:ARG:NH1	2.25	0.52
1:A:2978:SER:OG	1:A:2979:GLN:N	2.43	0.52
1:A:3250:LYS:HD2	1:A:3376:ALA:HB1	1.91	0.51
1:A:2845:ARG:N	1:A:2845:ARG:HD2	2.25	0.51
1:A:3260:SER:OG	1:A:3295:HIS:NE2	2.29	0.51
1:A:1089:LEU:HD12	1:A:1281:ILE:HD12	1.92	0.51
1:A:1124:ASN:HD22	1:A:1133:ASN:HD21	1.59	0.51
1:A:1276:ASP:OD1	1:A:1277:SER:N	2.44	0.51
1:A:3277:ASN:HB3	1:A:3280:LEU:HB3	1.92	0.51
1:A:1702:LEU:HD11	1:A:1770:LYS:HA	1.92	0.51
1:A:1965:ASN:ND2	1:A:2055:ASP:HA	2.25	0.51
1:A:2136:LEU:HB2	1:A:2172:ILE:HB	1.93	0.50
1:A:2052:LEU:N	1:A:2066:ASN:OD1	2.40	0.50
1:A:2447:ASN:ND2	1:A:2507:TYR:OH	2.44	0.50
1:A:2127:GLU:OE1	1:A:2134:ARG:NH1	2.45	0.50
1:A:1101:ARG:HD2	1:A:1144:TYR:HD2	1.76	0.50
1:A:1353:ASP:N	1:A:1353:ASP:OD1	2.44	0.50
1:A:1725:GLU:OE2	1:A:2560:LYS:NZ	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2678:GLN:OE1	1:A:2679:GLY:N	2.45	0.50
1:A:1569:MET:HE1	1:A:1813:LEU:HD22	1.94	0.50
1:A:1895:ASN:HB2	1:A:1900:MET:H	1.76	0.49
1:A:2593:VAL:HG12	1:A:2597:ILE:HG12	1.94	0.49
1:A:1137:GLN:HG2	1:A:1142:PHE:CE1	2.47	0.49
1:A:2747:SER:OG	1:A:2884:GLU:OE2	2.23	0.49
1:A:2170:TYR:CE1	1:A:2214:LYS:HB3	2.48	0.49
1:A:2835:ALA:CB	1:A:2918:LYS:H	2.25	0.49
1:A:3362:GLY:O	1:A:3366:THR:HG22	2.12	0.49
1:A:1011:ALA:O	1:A:1013:TYR:N	2.37	0.49
1:A:3015:GLU:O	1:A:3018:THR:OG1	2.29	0.49
1:A:3394:LEU:HA	1:A:3397:VAL:HG12	1.95	0.49
1:A:1062:ARG:NH1	1:A:1078:PHE:O	2.46	0.48
1:A:2700:HIS:O	1:A:2704:ASN:ND2	2.46	0.48
1:A:1079:ASN:O	1:A:1083:ILE:HG12	2.14	0.48
1:A:1853:GLN:O	1:A:1853:GLN:NE2	2.47	0.48
1:A:1300:MET:HG3	1:A:1397:GLN:OE1	2.14	0.48
1:A:2389:SER:HB3	1:A:2391:ALA:O	2.14	0.48
1:A:2343:LYS:NZ	1:A:2354:ALA:O	2.45	0.48
1:A:2347:TRP:CZ3	1:A:2353:PRO:HD3	2.48	0.48
1:A:3314:ASP:OD1	1:A:3314:ASP:N	2.46	0.48
1:A:1103:ARG:HH12	1:A:1242:ALA:N	2.13	0.47
1:A:1352:LYS:NZ	1:A:1385:GLU:HB2	2.29	0.47
1:A:2342:ILE:HG13	1:A:2343:LYS:N	2.29	0.47
1:A:3219:VAL:O	1:A:3222:PRO:HD2	2.14	0.47
1:A:1829:LYS:NZ	1:A:1887:VAL:O	2.35	0.47
1:A:2266:PHE:HA	1:A:2269:LEU:HG	1.95	0.47
1:A:1356:LEU:O	1:A:1360:GLY:N	2.38	0.47
1:A:2715:ASN:H	1:A:2718:ASP:CG	2.23	0.47
1:A:1057:GLN:HA	1:A:1064:ARG:HH21	1.80	0.47
1:A:2213:ASP:OD2	1:A:3361:GLN:NE2	2.47	0.47
1:A:2836:HIS:NE2	1:A:2916:HIS:CE1	2.83	0.47
1:A:2901:GLU:HG3	1:A:3073:GLN:NE2	2.30	0.47
1:A:3304:ILE:HG13	1:A:3309:PHE:HE2	1.77	0.47
1:A:2901:GLU:HG3	1:A:3073:GLN:HE22	1.80	0.47
1:A:3215:VAL:HG22	1:A:3339:LYS:HZ3	1.80	0.47
1:A:2033:LEU:HD23	1:A:2033:LEU:HA	1.77	0.46
1:A:1280:PRO:O	1:A:1283:SER:OG	2.24	0.46
1:A:3065:MET:O	1:A:3069:TRP:HB2	2.16	0.46
1:A:1260:ASP:HB3	1:A:1263:ASN:HB2	1.98	0.46
1:A:2870:ASN:HB3	1:A:2873:ASP:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1412:TYR:CD2	1:A:1424:MET:HE1	2.50	0.46
1:A:1427:LYS:HD2	1:A:1428:TYR:CZ	2.51	0.46
1:A:2160:GLU:O	1:A:2163:LYS:HG3	2.15	0.46
1:A:3460:VAL:HG23	1:A:3462:LEU:HG	1.98	0.46
1:A:1044:ARG:NE	1:A:1291:ALA:O	2.32	0.46
1:A:1701:VAL:HG11	1:A:1717:MET:HG2	1.98	0.46
1:A:1819:ILE:HD12	1:A:2004:ILE:HG23	1.98	0.46
1:A:2136:LEU:HD13	1:A:2141:ILE:HD11	1.98	0.46
1:A:3011:LYS:O	1:A:3015:GLU:HG2	2.16	0.46
1:A:2176:THR:N	1:A:2179:GLN:OE1	2.45	0.45
1:A:2916:HIS:HB3	1:A:2992:VAL:HG22	1.98	0.45
1:A:2424:ARG:NH2	1:A:2595:ASP:OD2	2.50	0.45
1:A:1520:LEU:HD13	1:A:1524:LYS:HA	1.99	0.45
1:A:2983:GLN:HB3	1:A:2985:VAL:HG13	1.99	0.45
1:A:1685:LYS:O	1:A:1688:SER:OG	2.34	0.45
1:A:2394:ASN:CG	1:A:2395:ASN:H	2.23	0.45
1:A:2956:SER:OG	1:A:2958:GLY:N	2.49	0.45
1:A:2686:VAL:HB	1:A:3070:ARG:HH11	1.81	0.45
1:A:2829:ASN:C	1:A:2831:LEU:H	2.25	0.45
1:A:3084:ASP:CG	1:A:3134:LYS:HG2	2.42	0.45
1:A:2565:ILE:HG22	1:A:2566:ASP:H	1.82	0.45
1:A:3111:LEU:HD23	1:A:3111:LEU:HA	1.75	0.45
1:A:2814:LYS:HD2	1:A:2840:ARG:HD3	1.99	0.45
1:A:2640:LEU:HG	1:A:3407:LEU:HD21	1.99	0.45
1:A:3265:ILE:HG23	1:A:3319:ARG:NH2	2.32	0.45
1:A:1285:PRO:HD2	1:A:1397:GLN:HE21	1.82	0.45
1:A:1882:SER:OG	1:A:1883:GLU:N	2.50	0.45
1:A:1048:SER:HB2	1:A:1051:PRO:HG3	1.97	0.44
1:A:2876:LEU:HD23	1:A:2876:LEU:HA	1.86	0.44
1:A:3498:LEU:HA	1:A:3498:LEU:HD23	1.70	0.44
1:A:1182:ASP:HB3	1:A:1185:LEU:HG	1.98	0.44
1:A:2299:ASP:HB3	1:A:2302:ILE:HG12	1.99	0.44
1:A:1231:ILE:HB	1:A:1232:PRO:HD3	2.00	0.44
1:A:2174:TYR:HB3	1:A:2218:LEU:HB2	1.99	0.44
1:A:3321:ASP:C	1:A:3323:LEU:H	2.25	0.44
1:A:1023:LYS:HB2	1:A:1023:LYS:HE2	1.82	0.44
1:A:2342:ILE:O	1:A:2346:ILE:HG12	2.18	0.44
1:A:3029:GLU:OE2	1:A:3049:ASP:HB2	2.17	0.44
1:A:3375:LYS:HG2	1:A:3401:PHE:CE2	2.51	0.44
1:A:1185:LEU:HD13	1:A:1681:GLY:HA3	2.00	0.44
1:A:2918:LYS:HE2	1:A:2918:LYS:HB2	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1829:LYS:HA	1:A:1829:LYS:HD2	1.75	0.44
1:A:1860:GLN:O	1:A:1860:GLN:NE2	2.45	0.43
1:A:2373:SER:OG	1:A:2374:GLN:N	2.51	0.43
1:A:2426:ASN:O	1:A:2430:ALA:HB3	2.18	0.43
1:A:2669:LEU:HD13	1:A:2695:VAL:HG12	2.00	0.43
1:A:2831:LEU:CB	1:A:2833:ARG:HE	2.31	0.43
1:A:3010:ASP:O	1:A:3013:THR:OG1	2.35	0.43
1:A:3192:ALA:HB2	1:A:3332:TYR:HB2	2.00	0.43
1:A:1343:MET:HE1	1:A:1533:MET:HB3	2.00	0.43
1:A:1364:LEU:HD13	1:A:1364:LEU:HA	1.88	0.43
1:A:1885:ALA:HA	1:A:1905:SER:HA	2.01	0.43
1:A:1116:ARG:H	1:A:1116:ARG:HG3	1.62	0.43
1:A:1493:LYS:HB3	1:A:1494:PRO:HD3	2.00	0.43
1:A:2841:LEU:HD21	1:A:2857:ILE:HD12	2.00	0.43
1:A:2842:LEU:HD12	1:A:2842:LEU:HA	1.79	0.43
1:A:1071:LYS:HD2	1:A:1071:LYS:HA	1.82	0.43
1:A:1225:LEU:O	1:A:1229:LYS:N	2.49	0.43
1:A:1144:TYR:CG	1:A:1149:LEU:HG	2.53	0.43
1:A:1182:ASP:OD1	1:A:1183:GLN:N	2.52	0.43
1:A:3348:GLY:O	1:A:3349:ARG:HB3	2.18	0.43
1:A:1480:MET:HE3	1:A:1480:MET:HB3	1.92	0.43
1:A:2930:ASN:OD1	1:A:2931:LEU:N	2.52	0.43
1:A:1057:GLN:O	1:A:1060:SER:OG	2.36	0.43
1:A:2738:LEU:HD23	1:A:3067:GLY:HA2	2.01	0.43
1:A:1103:ARG:HG2	1:A:1107:PHE:CZ	2.54	0.42
1:A:1382:ARG:HD2	1:A:1385:GLU:OE2	2.18	0.42
1:A:2976:PRO:HG2	1:A:3423:PHE:HE2	1.84	0.42
1:A:1024:ALA:O	1:A:1028:LYS:HD2	2.19	0.42
1:A:1125:ARG:NH1	1:A:1846:LYS:HD2	2.34	0.42
1:A:2536:LEU:HD12	1:A:2536:LEU:HA	1.76	0.42
1:A:3157:TYR:O	1:A:3159:ALA:N	2.49	0.42
1:A:2302:ILE:HD11	1:A:3343:LYS:HD3	2.00	0.42
1:A:2993:ASP:OD2	1:A:2996:THR:N	2.53	0.42
1:A:3245:VAL:C	1:A:3248:PRO:HD2	2.45	0.42
1:A:1488:LEU:HD22	1:A:1496:ILE:HD11	2.02	0.42
1:A:1086:TYR:O	1:A:1090:MET:HG2	2.20	0.42
1:A:1502:PHE:O	1:A:1506:GLY:N	2.34	0.42
1:A:2823:ILE:HD11	1:A:2868:LEU:HD23	2.01	0.42
1:A:3224:VAL:HG11	1:A:3472:LEU:HD13	2.02	0.42
1:A:1744:SER:OG	1:A:1745:THR:HG23	2.20	0.42
1:A:3266:ASP:HB2	1:A:3319:ARG:HH12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1872:THR:HG23	1:A:1979:ASN:OD1	2.19	0.42
1:A:2031:ARG:HG2	1:A:2034:ARG:HH21	1.85	0.42
1:A:2047:LEU:HD23	1:A:2047:LEU:HA	1.82	0.42
1:A:2278:MET:HB3	1:A:2278:MET:HE3	1.80	0.42
1:A:2560:LYS:O	1:A:2562:GLY:N	2.51	0.42
1:A:2699:PHE:HE2	1:A:2726:GLN:HE22	1.66	0.42
1:A:1158:GLN:HE21	1:A:1288:ILE:HB	1.83	0.42
1:A:1343:MET:HE2	1:A:1343:MET:HB2	1.85	0.42
1:A:2355:LEU:HD23	1:A:2355:LEU:HA	1.82	0.42
1:A:1551:LEU:HB3	1:A:1954:LEU:HD11	2.02	0.41
1:A:2137:SER:C	1:A:2139:THR:H	2.28	0.41
1:A:2212:ASP:HB3	1:A:3357:THR:HA	2.02	0.41
1:A:2437:LEU:HD23	1:A:2437:LEU:HA	1.88	0.41
1:A:1904:MET:HE3	1:A:1904:MET:HB3	1.77	0.41
1:A:1965:ASN:HD21	1:A:2055:ASP:HA	1.85	0.41
1:A:2814:LYS:NZ	1:A:2833:ARG:HG2	2.36	0.41
1:A:2828:GLY:O	1:A:3030:PRO:HG3	2.21	0.41
1:A:2608:ALA:O	1:A:2611:ARG:HG2	2.20	0.41
1:A:2135:ILE:HG13	1:A:2173:ILE:HG12	2.03	0.41
1:A:1761:THR:O	1:A:1761:THR:OG1	2.36	0.41
1:A:2609:LEU:HD23	1:A:2609:LEU:HA	1.79	0.41
1:A:1062:ARG:HD3	1:A:1078:PHE:CD2	2.50	0.41
1:A:1598:GLU:O	1:A:1602:THR:HB	2.21	0.41
1:A:2391:ALA:O	1:A:2392:TYR:HB3	2.21	0.41
1:A:2394:ASN:CG	1:A:2395:ASN:N	2.78	0.41
1:A:2740:THR:O	1:A:2744:GLY:N	2.54	0.41
1:A:3062:PHE:CG	1:A:3062:PHE:O	2.73	0.41
1:A:3420:LEU:HD23	1:A:3420:LEU:HA	1.81	0.41
1:A:3261:ARG:O	1:A:3265:ILE:HG22	2.21	0.41
1:A:1114:GLY:HA2	1:A:1117:PHE:HB3	2.03	0.40
1:A:2836:HIS:CD2	1:A:2916:HIS:O	2.74	0.40
1:A:1839:LYS:HB3	1:A:1845:TRP:CD2	2.56	0.40
1:A:1931:GLN:HE21	1:A:1931:GLN:HB3	1.73	0.40
1:A:2715:ASN:C	1:A:2717:TYR:N	2.80	0.40
1:A:3183:MET:N	1:A:3183:MET:SD	2.95	0.40
1:A:3321:ASP:HB3	1:A:3323:LEU:HG	2.03	0.40
1:A:1587:LEU:HD11	1:A:2052:LEU:HD13	2.02	0.40
1:A:2750:LEU:HD13	1:A:2758:MET:HE1	2.03	0.40
1:A:3098:ILE:HD13	1:A:3098:ILE:HA	1.90	0.40
1:A:3135:ALA:HB1	1:A:3144:LEU:HD12	2.03	0.40
1:A:1161:LEU:H	1:A:1161:LEU:HG	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3143:GLU:OE2	1:A:3145:TRP:NE1	2.51	0.40
1:A:1582:ILE:HD12	1:A:1582:ILE:HA	1.86	0.40
1:A:1631:MET:N	1:A:1632:PRO:HD2	2.36	0.40
1:A:2373:SER:HB2	1:A:3343:LYS:HD2	2.04	0.40
1:A:3348:GLY:C	1:A:3350:TYR:H	2.29	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	2445/3500 (70%)	2287 (94%)	155 (6%)	3 (0%)	48 78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2716	VAL
1	A	2778	GLU
1	A	2198	GLU

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	2055/2875 (72%)	2023 (98%)	32 (2%)	55 70

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1161	LEU
1	A	1162	THR
1	A	1247	THR
1	A	1436	VAL
1	A	1443	THR
1	A	1513	VAL
1	A	1559	THR
1	A	1608	LEU
1	A	1670	LEU
1	A	1761	THR
1	A	1798	ILE
1	A	1884	ASN
1	A	1924	THR
1	A	2225	THR
1	A	2376	THR
1	A	2409	VAL
1	A	2421	VAL
1	A	2438	VAL
1	A	2449	THR
1	A	2637	ILE
1	A	2695	VAL
1	A	2817	GLN
1	A	2827	VAL
1	A	2833	ARG
1	A	2854	VAL
1	A	2880	LEU
1	A	3013	THR
1	A	3131	THR
1	A	3146	VAL
1	A	3165	VAL
1	A	3455	THR
1	A	3478	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1079	ASN
1	A	1133	ASN
1	A	1147	GLN
1	A	1321	ASN
1	A	1372	ASN

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Mol	Chain	Res	Type
1	A	1390	GLN
1	A	1466	GLN
1	A	1560	ASN
1	A	1814	GLN
1	A	1818	GLN
1	A	1911	GLN
1	A	1965	ASN
1	A	2056	GLN
1	A	2162	GLN
1	A	2340	GLN
1	A	2447	ASN
1	A	2542	ASN
1	A	2581	ASN
1	A	2704	ASN
1	A	2726	GLN
1	A	2759	HIS
1	A	2812	GLN
1	A	2882	GLN
1	A	3060	ASN
1	A	3061	HIS
1	A	3073	GLN
1	A	3128	ASN
1	A	3232	GLN
1	A	3330	HIS
1	A	3459	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.

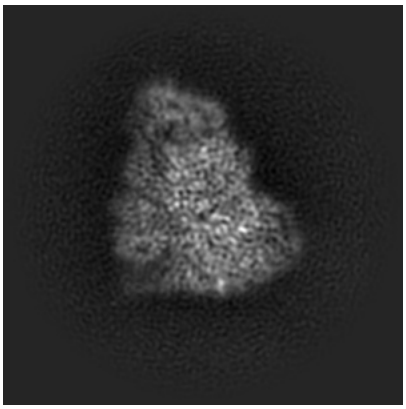
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-75681. These allow visual inspection of the internal detail of the map and identification of artifacts.

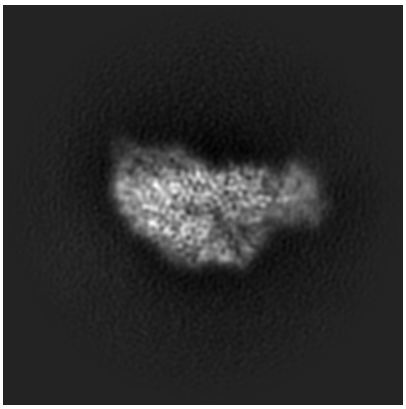
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

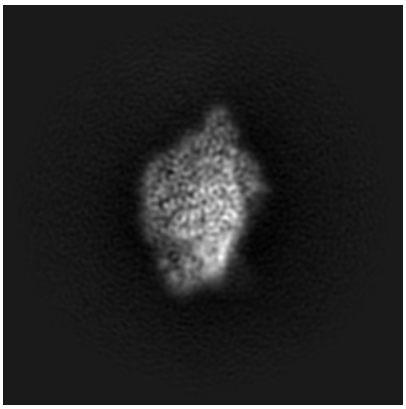
6.1.1 Primary map



X

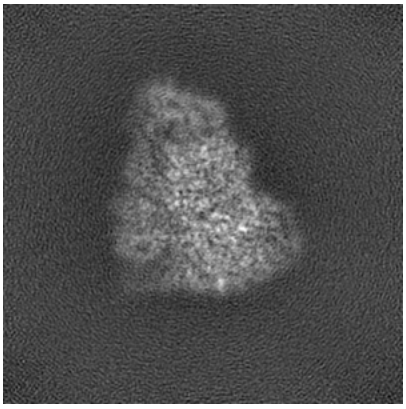


Y

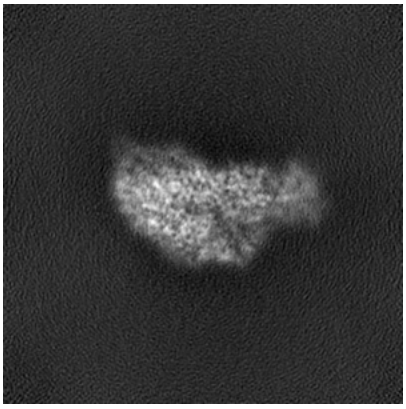


Z

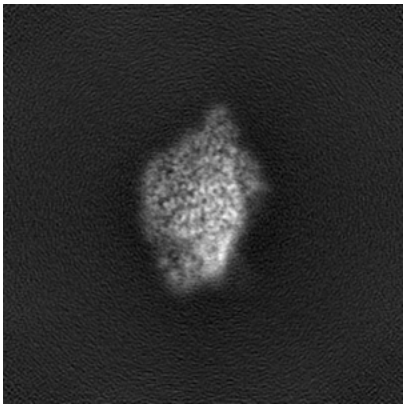
6.1.2 Raw map



X



Y

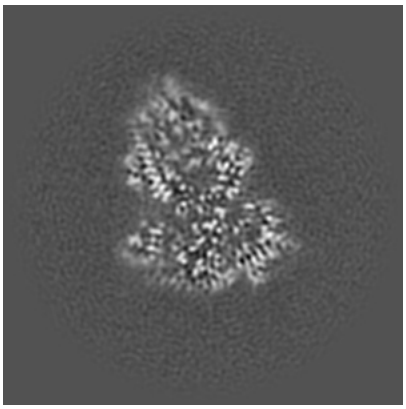


Z

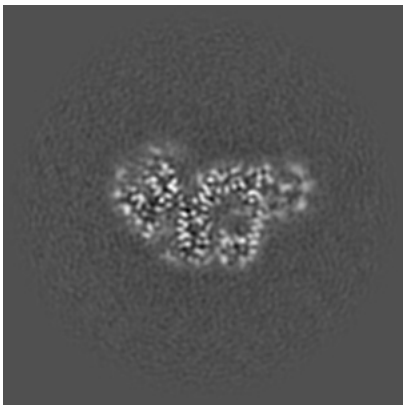
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

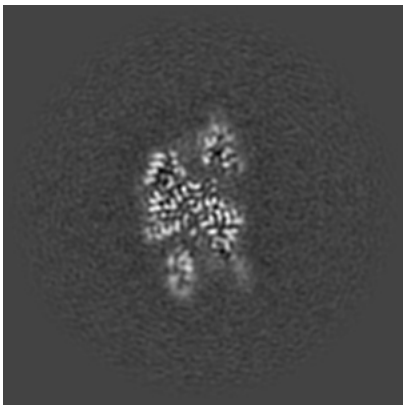
6.2.1 Primary map



X Index: 120

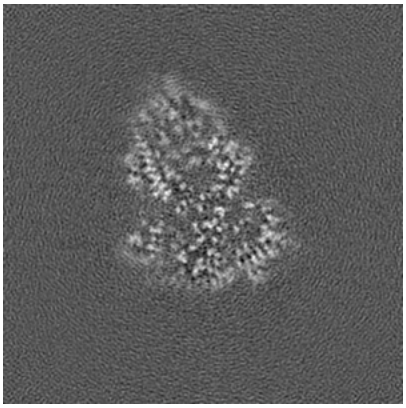


Y Index: 120

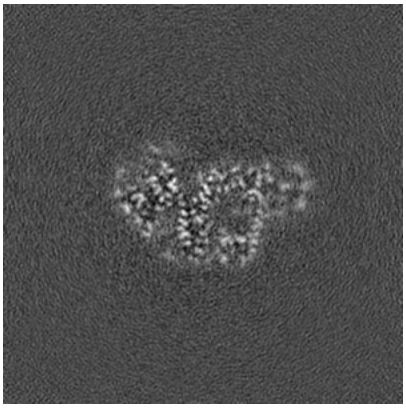


Z Index: 120

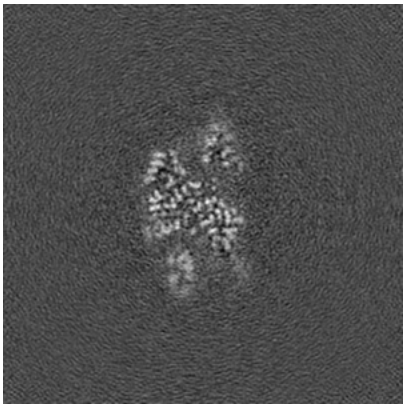
6.2.2 Raw map



X Index: 120



Y Index: 120

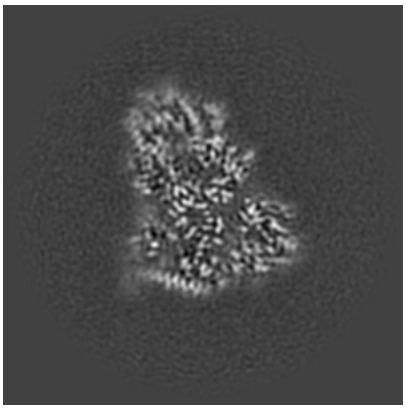


Z Index: 120

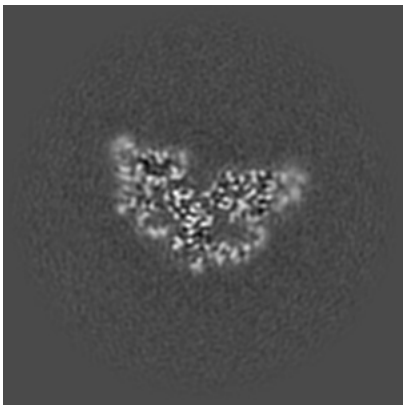
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

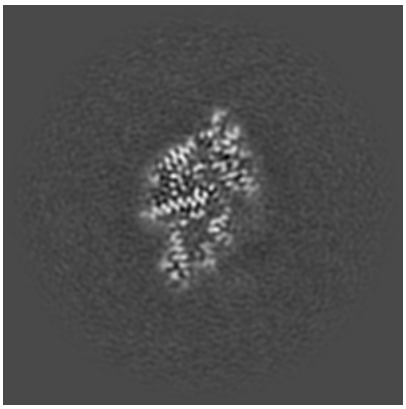
6.3.1 Primary map



X Index: 124

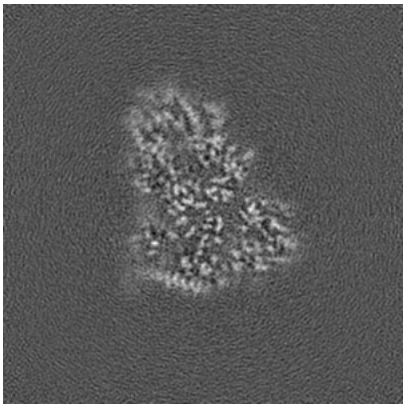


Y Index: 129

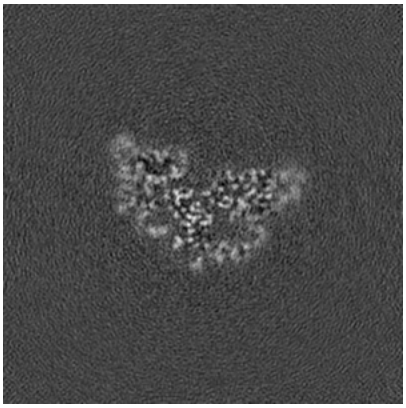


Z Index: 108

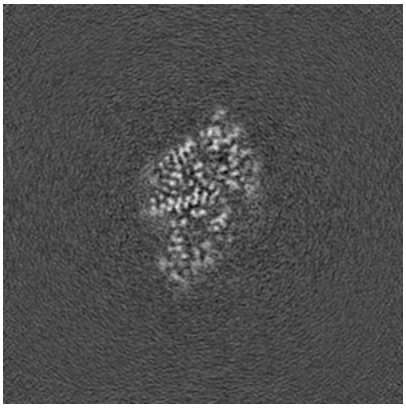
6.3.2 Raw map



X Index: 124



Y Index: 129

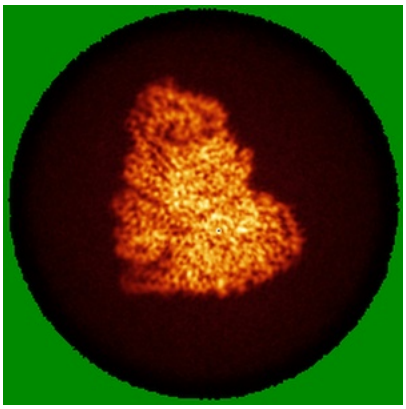


Z Index: 107

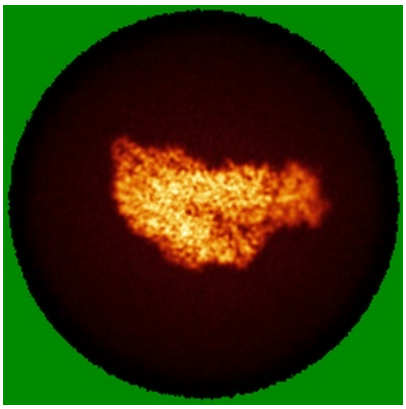
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

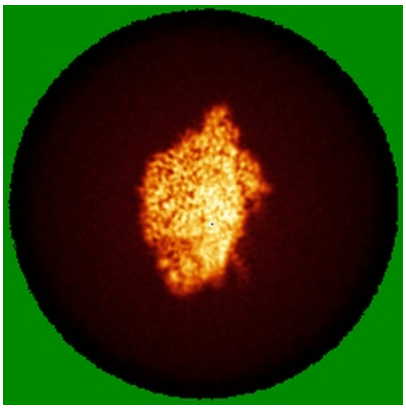
6.4.1 Primary map



X

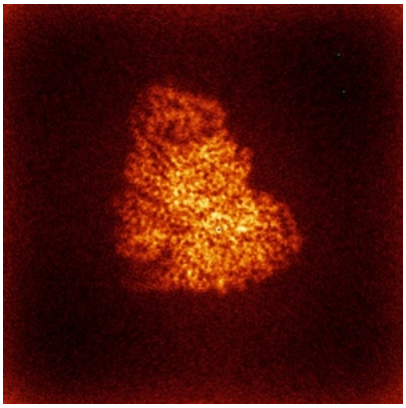


Y

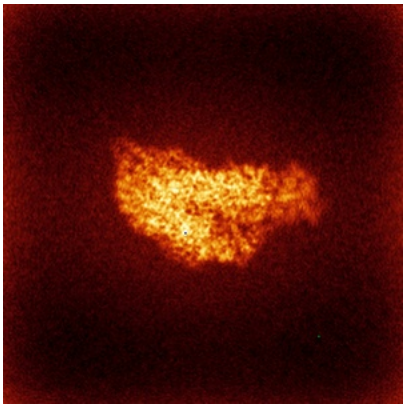


Z

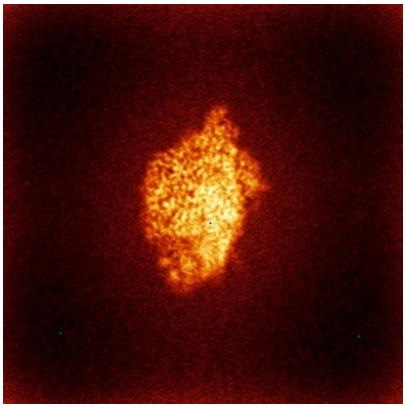
6.4.2 Raw map



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)

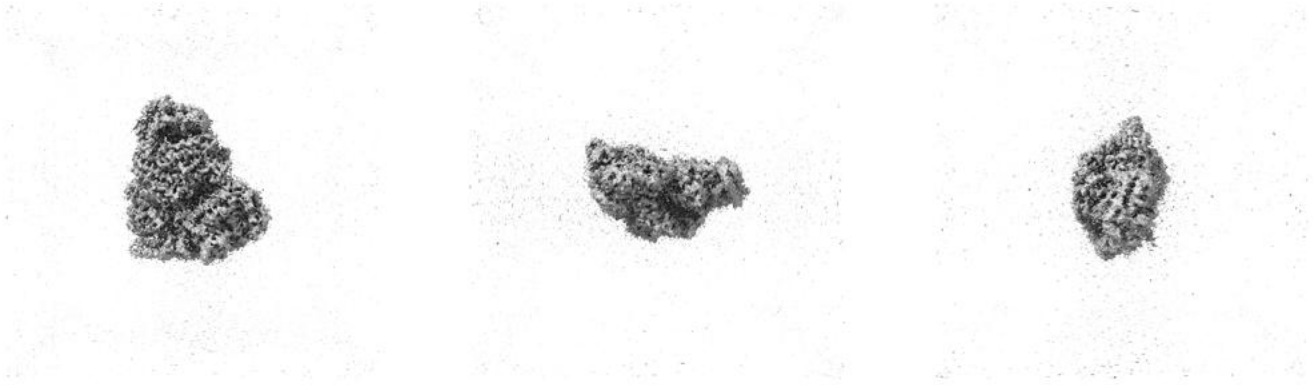
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.102. 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



X Y Z

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

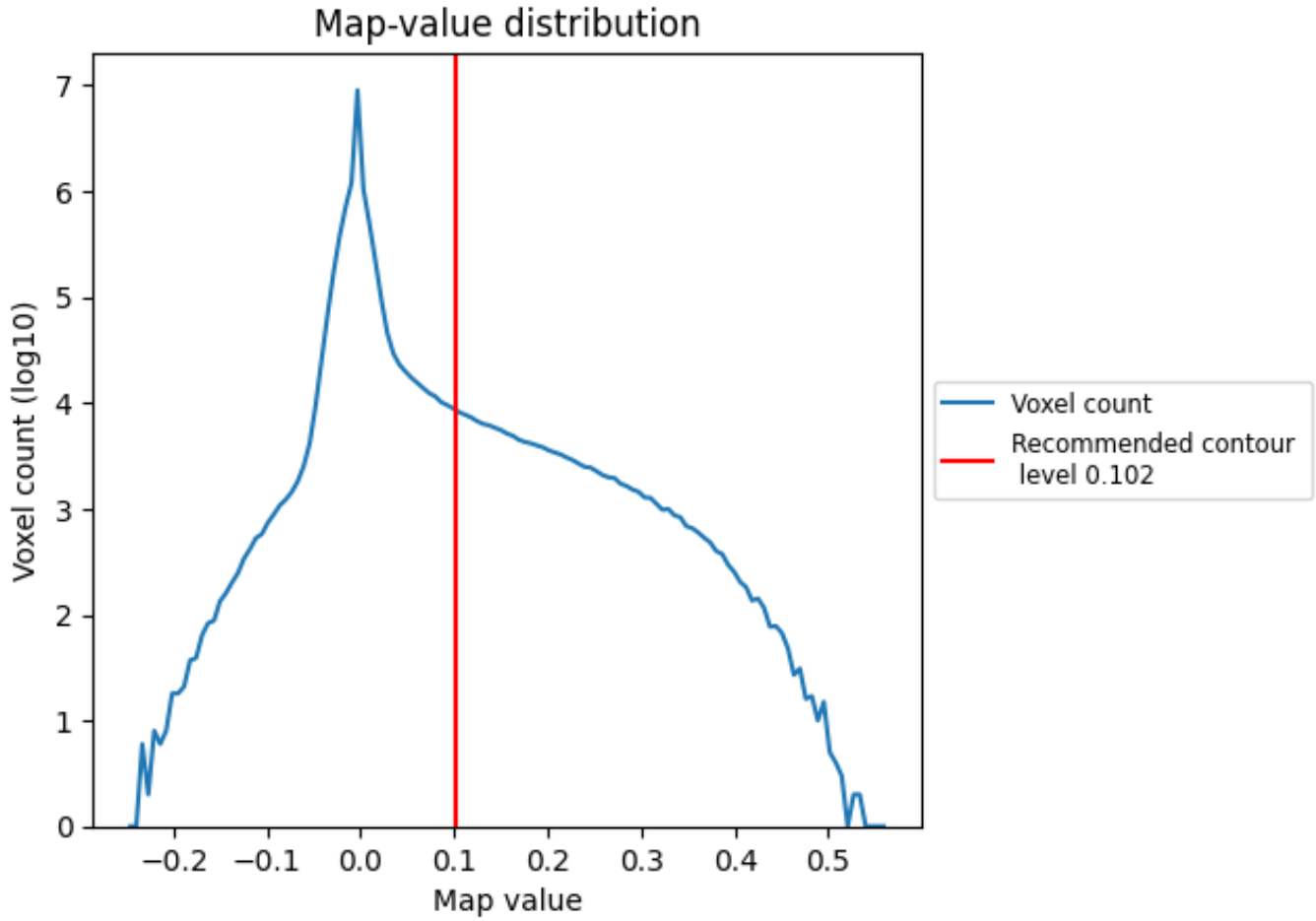
6.6 Mask visualisation (i)

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

7 Map analysis

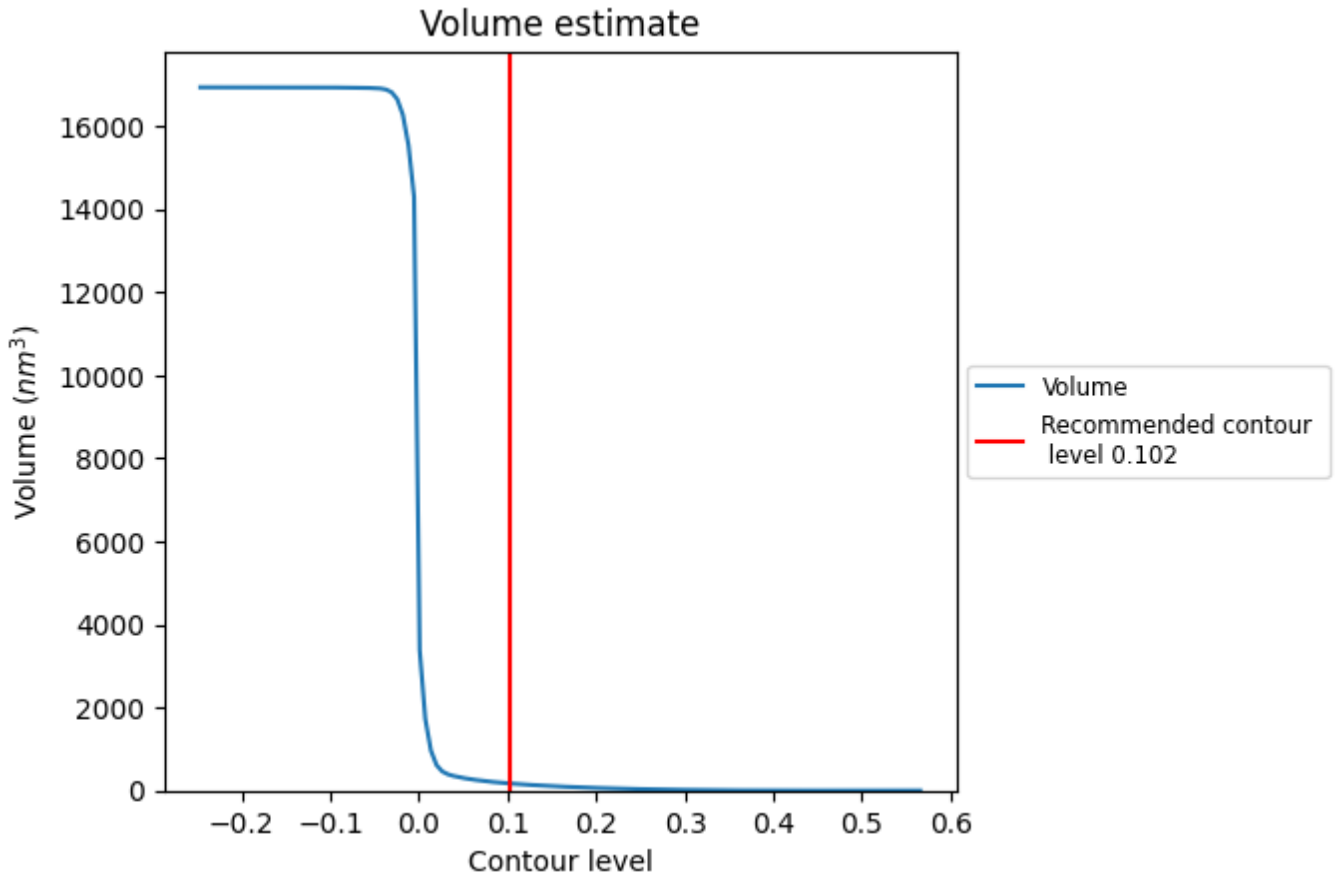
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

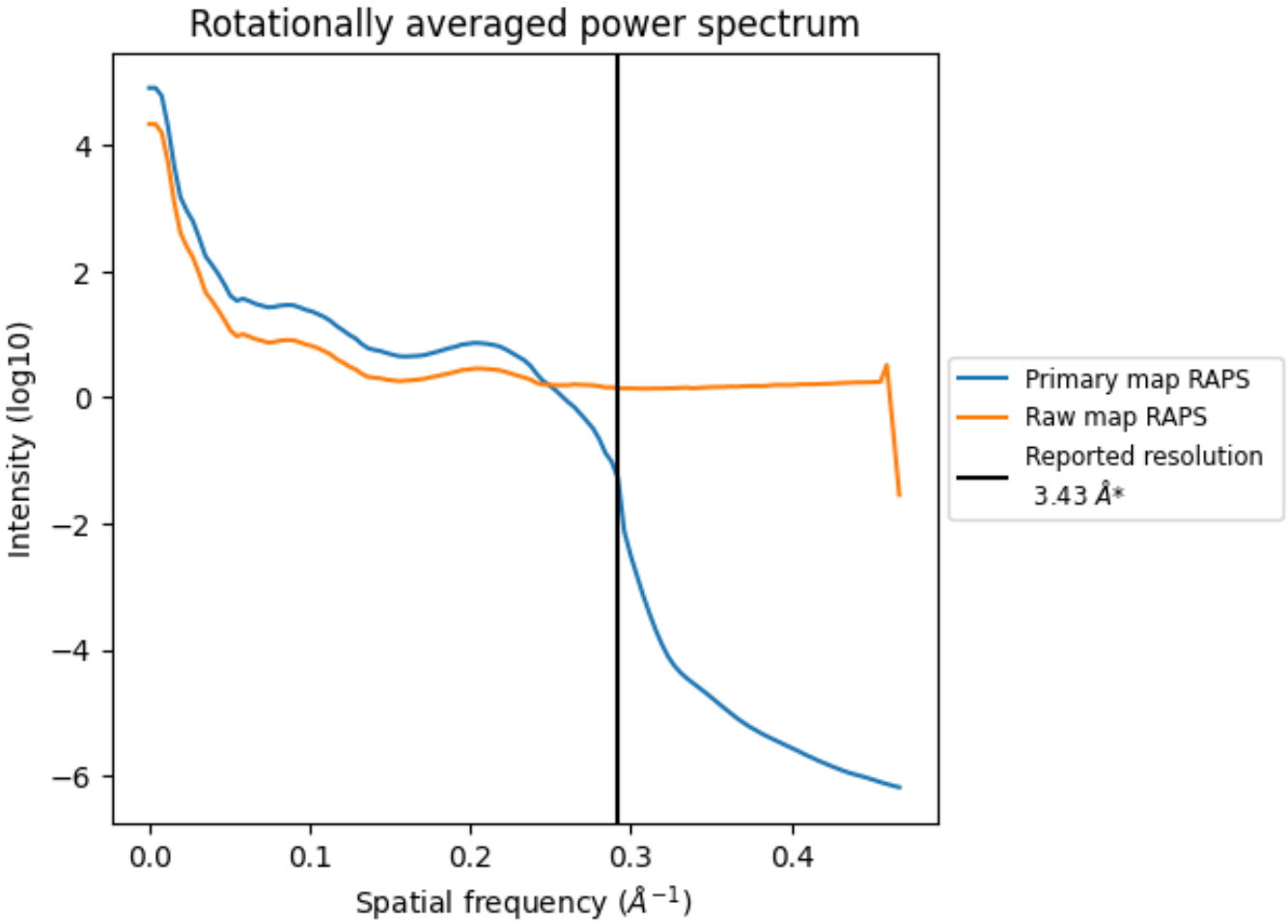
7.2 Volume estimate



The volume at the recommended contour level is 172 nm^3; this corresponds to an approximate mass of 155 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)

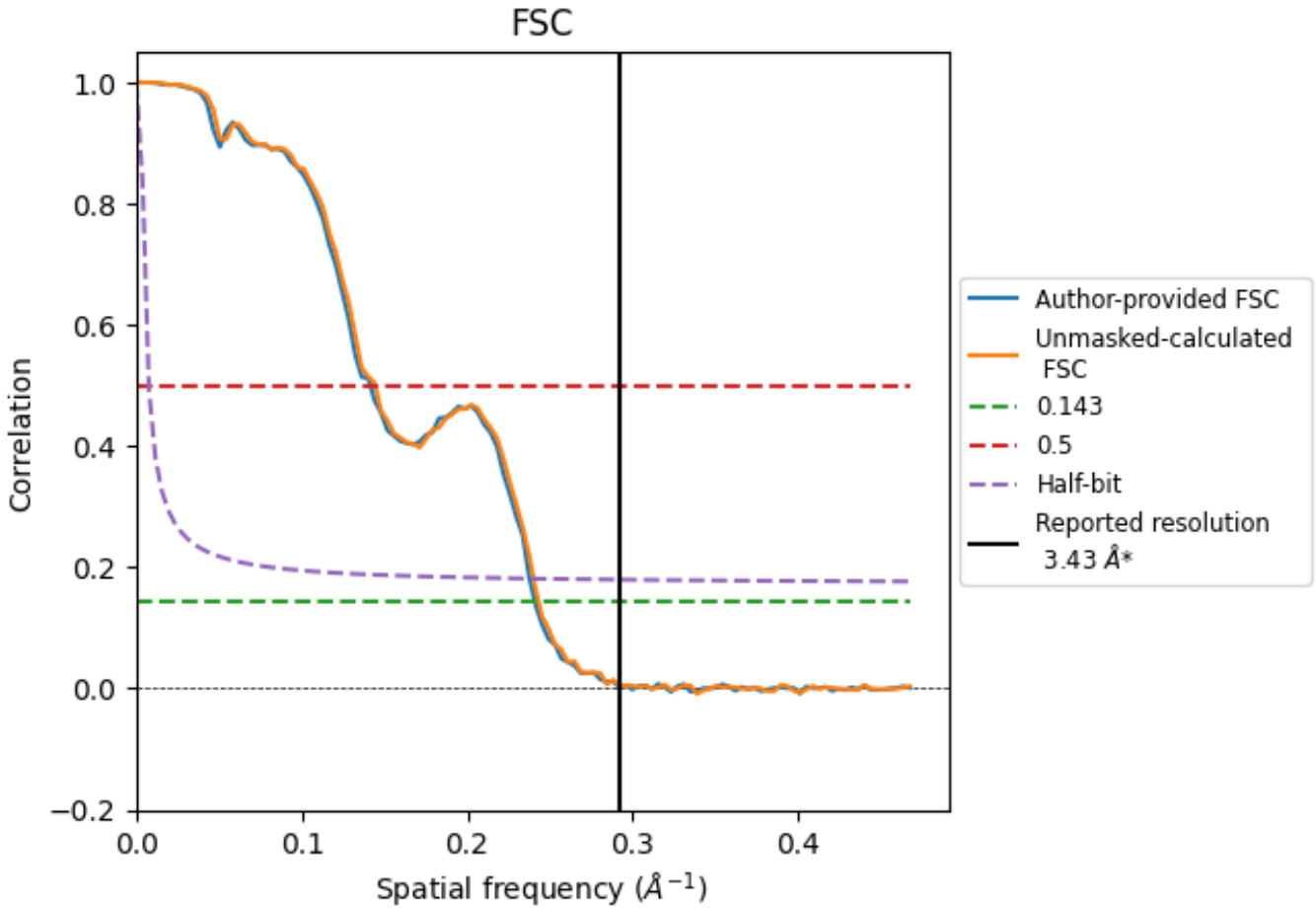


*Reported resolution corresponds to spatial frequency of 0.292 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.292 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.43	-	-
Author-provided FSC curve	4.15	7.07	4.21
Unmasked-calculated*	4.11	6.93	4.16

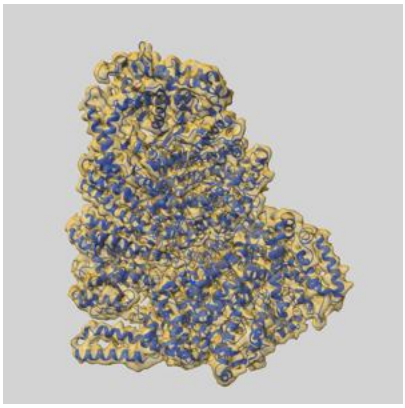
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.43 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.11 differs from the reported value 3.43 by more than 10 %

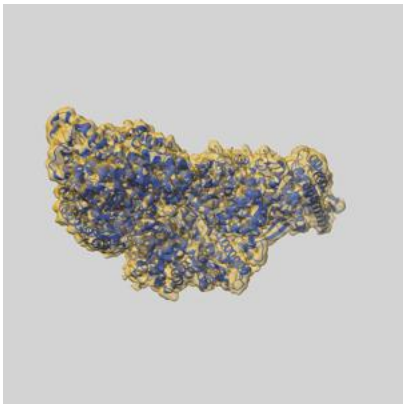
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-75681 and PDB model 11GP. Per-residue inclusion information can be found in section 3 on page 4.

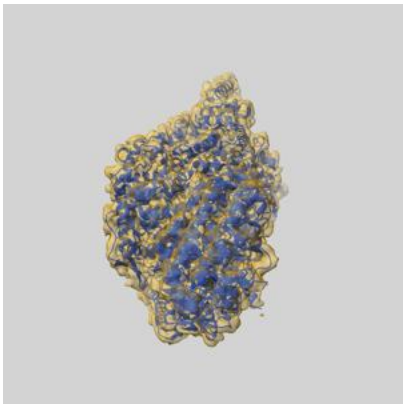
9.1 Map-model overlay



X



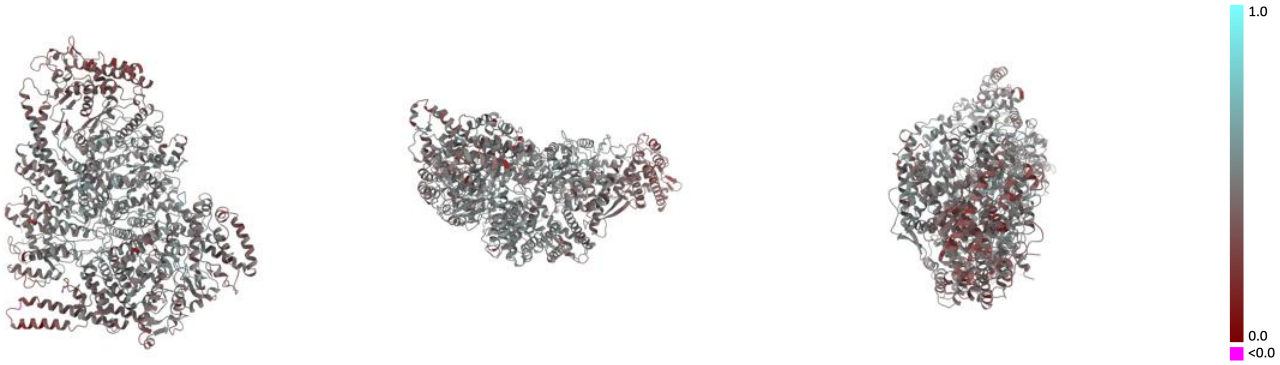
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.102 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.

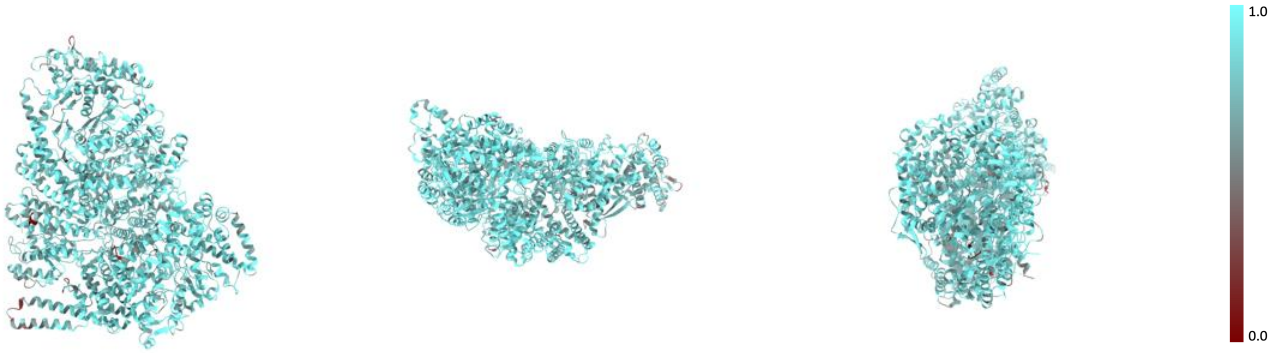
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

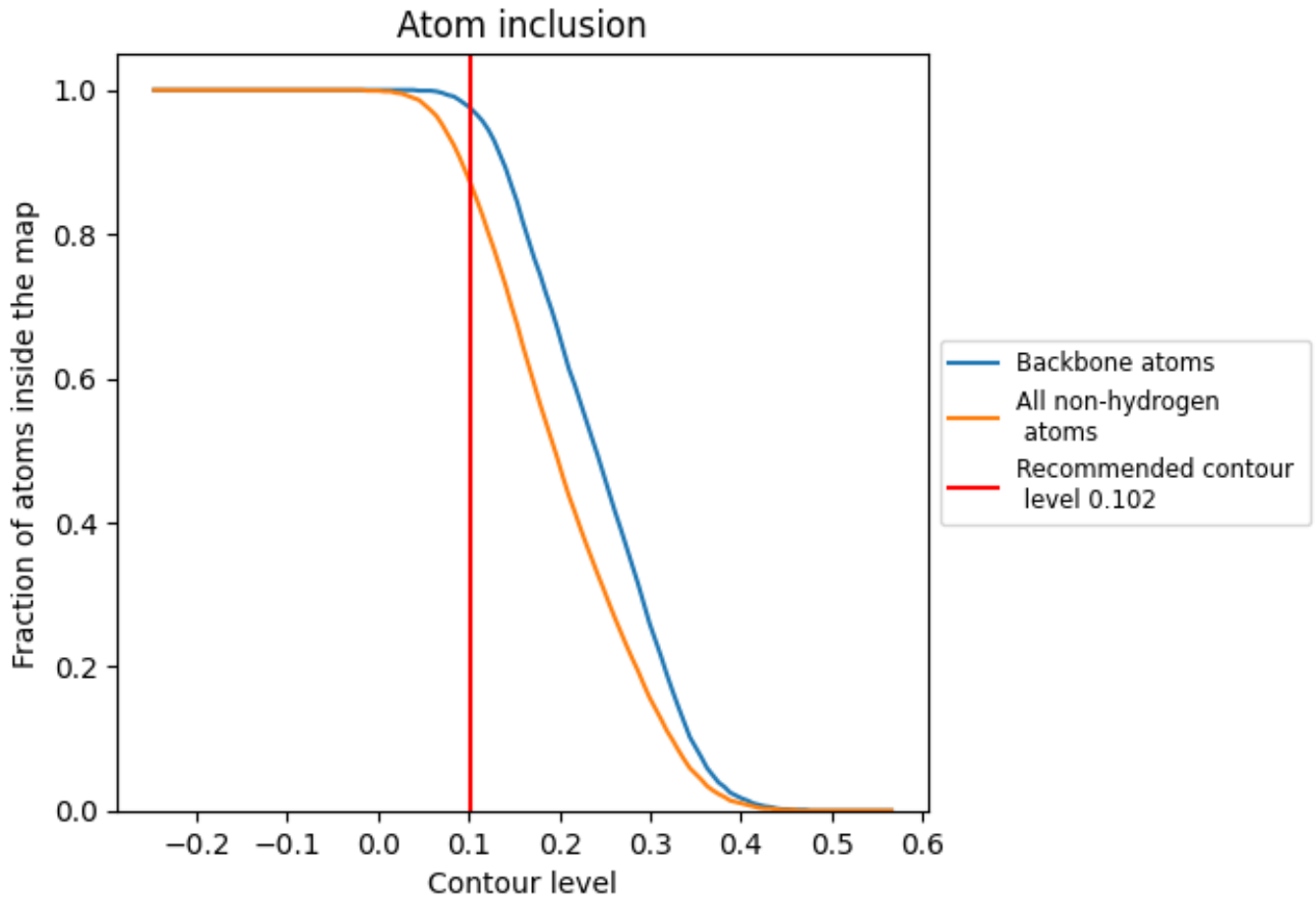
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.102).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 87% 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 (0.102) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.8700	0.4490
A	0.8700	0.4490