wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 10:21 am GMT

PDB ID	:	6I26
EMDB ID	:	EMD-0328
Title	:	Rea1 Wild type AMPPNP state
Authors	:	Sosnowski, P.; Urnavicius, L.; Boland, A.; Fagiewicz, R.; Busselez, J.; Papai, G.; Schmidt, H.
Deposited on	:	2018-10-31
Resolution	:	4.30 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:

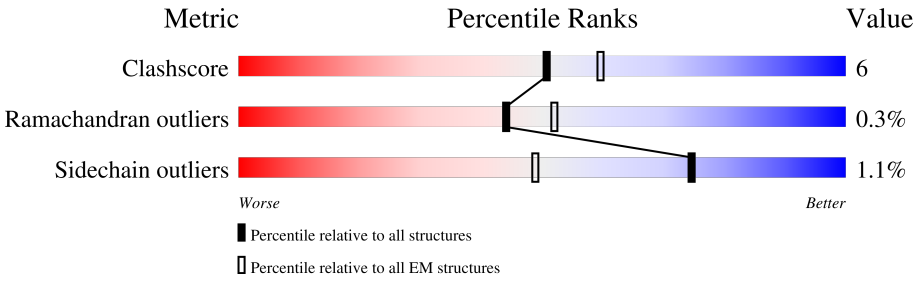
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

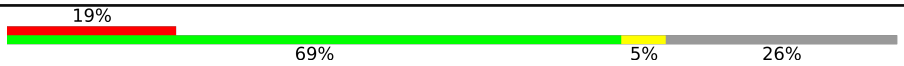
The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	4854	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 22765 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 Midasin,Midasin,Midasin,Midasin.

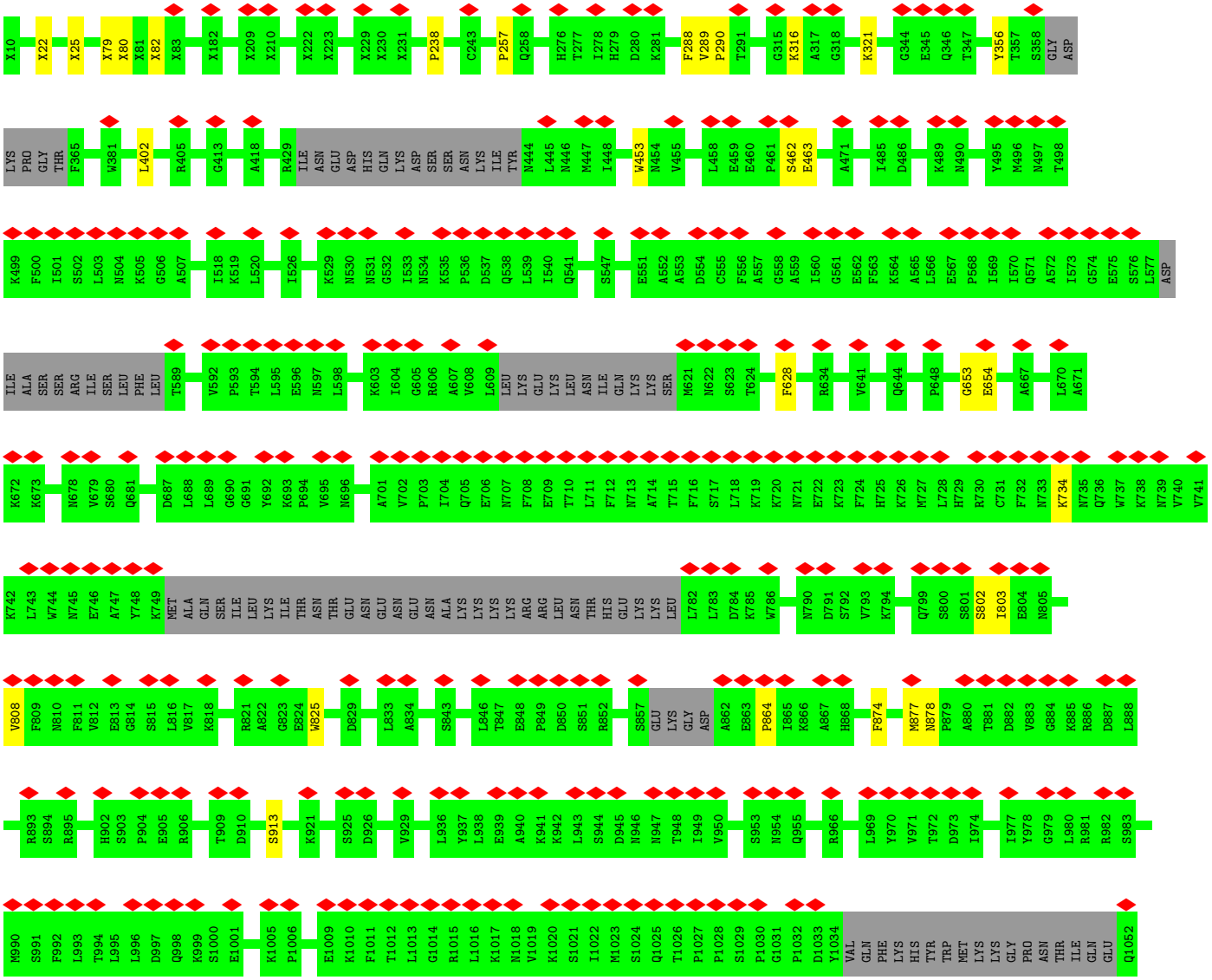
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3587	22765	14329	4101	4303	32	0	0

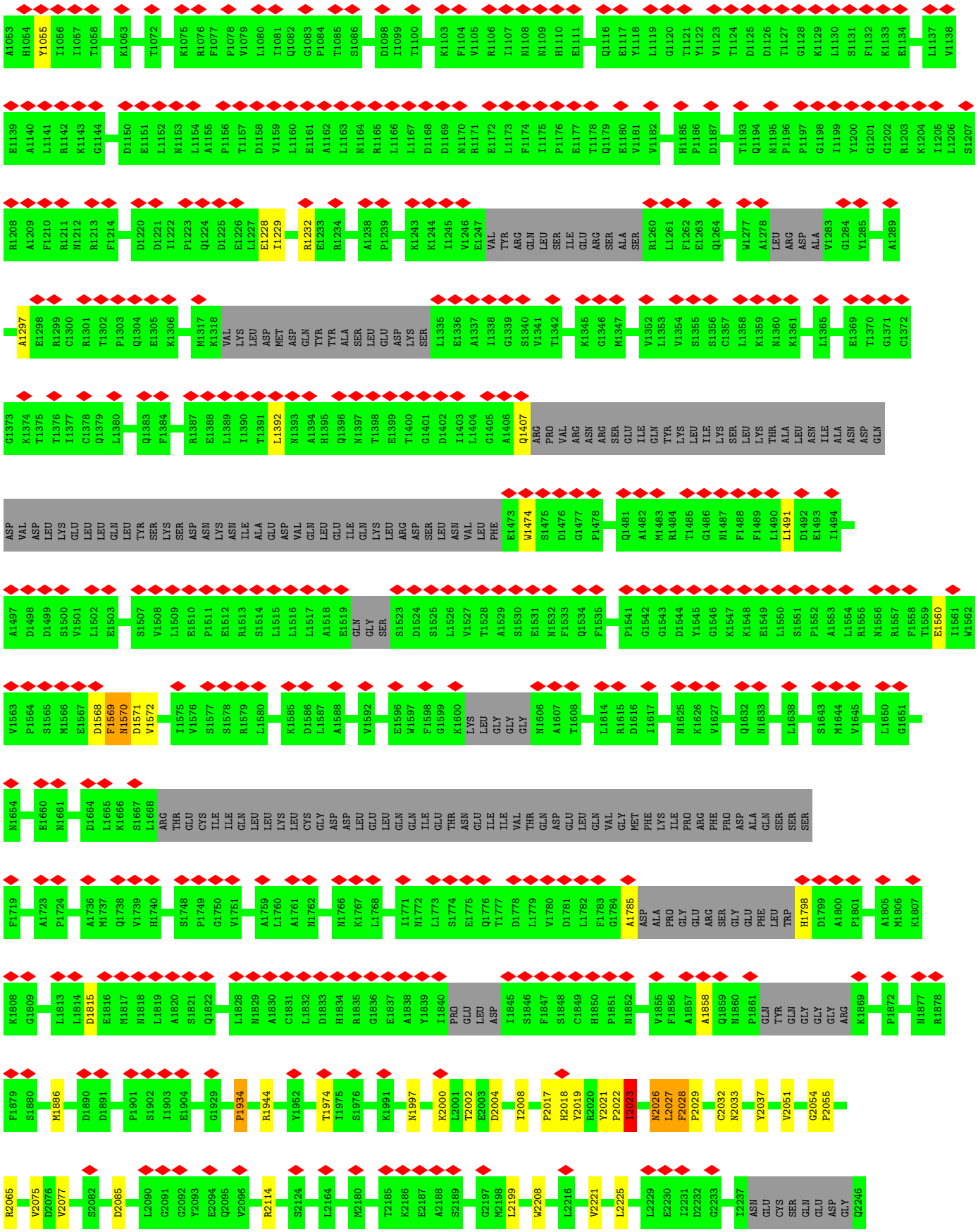
3 Residue-property plots (i)

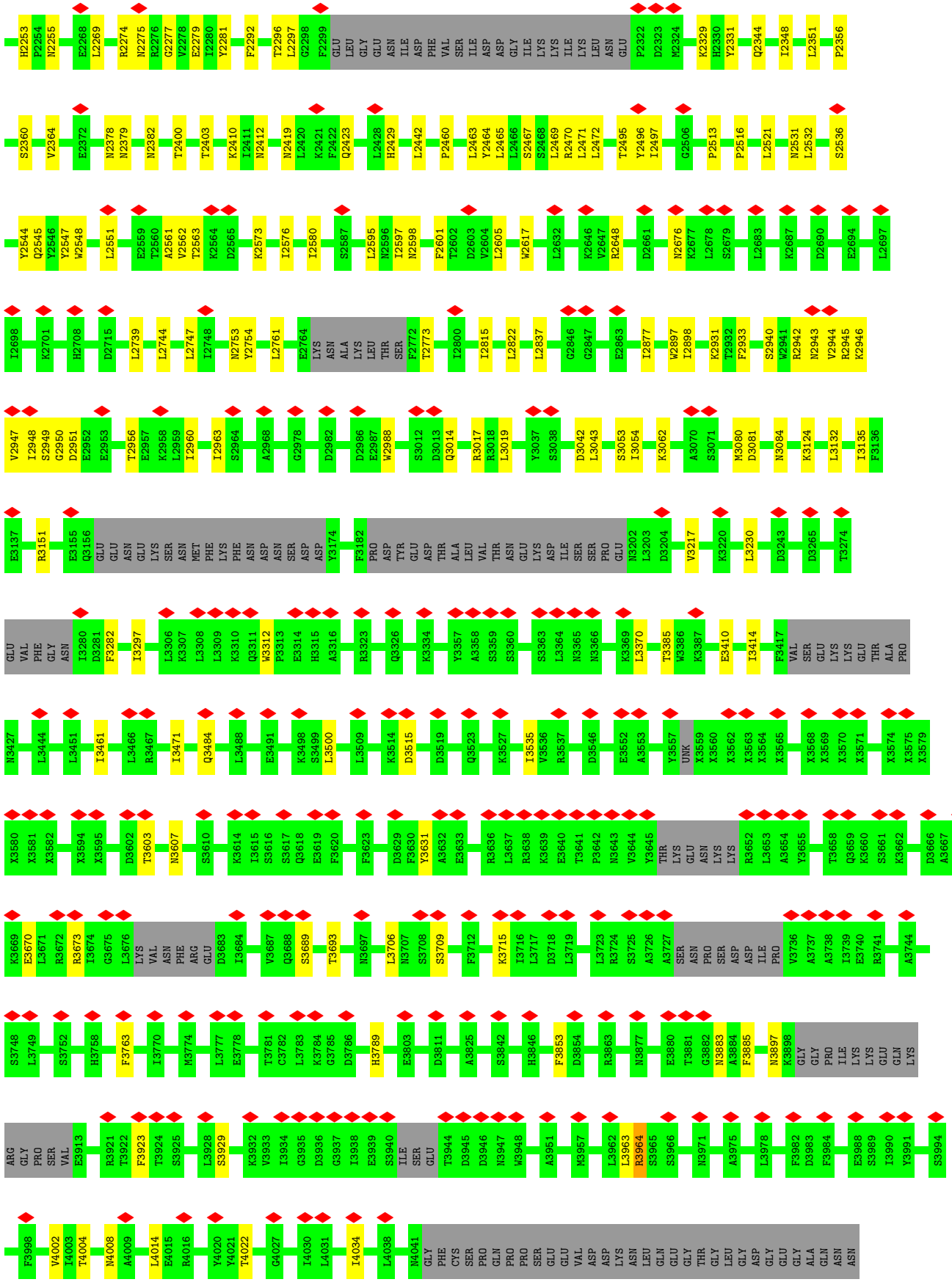
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A: 19% 69% 5% 26%




A1053 H1054 Y1055 I1056 I1057 T1058 K1063 T1072 K1075 R1076 F1077 P1078 V1079 L1080 I1081 Q1082 G1083 P1084 T1085 S1086 D1098 I1099 T1100 K1103 F1104 V1105 R1106 I1107 N1108 N1109 H1110 E1111 Q1116 E1117 Y1118 L1119 G1120 T1121 Y1122 V1123 T1124 D1125 D1126 T1127 G1128 K1129 L1130 S1131 F1132 K1133 E1134 L1137 V1138
E1139 A1140 L1141 R1142 K1143 G1144 D1150 E1151 L1152 N1153 L1154 A1155 P1156 T1157 D1158 V1159 L1160 E1161 A1162 L1163 N1164 R1165 L1166 L1167 D1168 D1169 N1170 R1171 E1172 L1173 F1174 I1175 P1176 E1177 T1178 Q1179 E1180 V1181 V1182 H1185 P1186 D1187 T1193 Q1194 N1195 P1196 P1197 G1198 I1199 Y1200 G1201 G1202 R1203 K1204 I1205 L1206 S1207
R1208 A1209 F1210 R1211 N1212 R1213 F1214 D1220 D1221 I1222 P1223 Q1224 D1225 E1226 L1227 E1228 I1229 R1232 E1233 R1234 A1238 P1239 K1243 K1244 I1245 V1246 E1247 VAL TYR ARG GLN LEU SER ILE GLU ARG SER ALA SER R1260 L1261 F1262 E1263 Q1264 W1277 A1278 LEU ARG ASP ALA V1283 G1284 Y1285 A1289
A1297 E1298 R1299 C1300 R1301 T1302 P1303 Q1304 E1305 K1306 M1317 K1318 VAL LYS LEU ASP MET ASP GLN TYR TYR ALA SER LEU GLU ASP LYS SER L1335 E1336 A1337 I1338 G1339 S1340 V1341 T1342 K1345 G1346 M1347 V1352 L1353 V1354 S1355 S1356 C1357 L1358 K1359 N1360 K1361 L1365 E1369 T1370 G1371 C1372
G1373 K1374 T1375 T1376 I1377 C1378 Q1379 L1380 Q1383 F1384 R1387 E1388 L1389 I1390 T1391 L1392 N1393 A1394 H1395 Q1396 N1397 T1398 E1399 T1400 G1401 D1402 I1403 L1404 G1405 A1406 Q1407 ARG PRO VAL ARG ASN ARG SER GLU ILE GLN TYR LYS LEU ILE LYS SER LEU LYS THR ALA LEU ASN ILE ALA ASN ASP GLN
ASP VAL ASP LEU LYS GLU LEU LEU GLN LEU TYR SER LYS SER ASP ASN LYS ASN ILE ALA GLU ASP VAL GLN LEU GLU ILE GLN LYS LEU ARG ASP SER LEU ASN VAL LEU PHE E1473 W1474 S1475 D1476 G1477 P1478 Q1481 A1482 M1483 R1484 T1485 G1486 N1487 F1488 F1489 L1490 L1491 D1492 E1493 I1494
A1497 D1498 D1499 S1500 V1501 L1502 E1503 S1507 V1508 L1509 E1510 P1511 E1512 R1513 S1514 L1515 L1516 L1517 A1518 E1519 GLN GLY SER S1523 D1524 S1525 L1526 V1527 T1528 A1529 S1530 E1531 N1532 F1533 Q1534 F1535 P1541 G1542 G1543 D1544 Y1545 G1546 K1547 K1548 E1549 L1550 S1551 P1552 A1553 L1554 R1555 N1556 R1557 F1558 T1559 E1560 I1561 W1562
V1563 P1564 S1565 M1566 E1567 D1568 F1569 N1570 D1571 V1572 I1575 V1576 S1577 S1578 R1579 L1580 K1585 D1586 L1587 A1588 V1592 E1596 W1597 F1598 G1599 K1600 LYS LEU GLY GLY GLY N1606 A1607 T1608 L1614 R1615 D1616 I1617 N1625 K1626 V1627 Q1632 N1633 L1638 S1643 M1644 V1645 L1650 G1651
N1654 E1660 N1661 D1664 L1665 K1666 S1667 L1668 ARG THR GLU CYS ILE ILE GLN LEU LEU LYS LEU CYS GLY ASP ASP LEU GLU LEU GLN GLN ILE GLU THR ASN GLU ILE ILE VAL THR GLN ASP GLU LEU GLN VAL GLY MET PHE LYS ILE PRO ARG PHE PRO ASP ALA GLN SER SER SER
F1719 A1723 P1724 A1736 M1737 Q1738 V1739 H1740 S1748 P1749 G1750 V1751 A1759 L1760 A1761 N1762 N1766 K1767 L1768 I1771 N1772 L1773 S1774 E1775 Q1776 T1777 D1778 L1779 V1780 D1781 L1782 F1783 G1784 A1785 ASP ALA PRO GLY GLU ARG SER GLY GLU PHE LEU TRP H1798 D1799 A1800 P1801 A1805 M1806 K1807
K1808 G1809 L1813 L1814 D1815 E1816 M1817 N1818 L1819 A1820 S1821 Q1822 L1828 N1829 A1830 C1831 L1832 D1833 H1834 R1835 G1836 E1837 A1838 Y1839 I1840 PRO GLU LEU ASP I1845 S1846 F1847 S1848 C1849 H1850 P1851 N1852 V1855 F1856 A1857 A1858 Q1859 N1860 P1861 GLN TYR GLN GLY GLY GLY ARG K1869 P1872 N1877 R1878
F1879 S1880 M1886 D1890 D1891 P1901 S1902 I1903 E1904 G1929 P1934 R1944 Y1962 T1974 I1975 S1976 K1991 N1997 K2000 L2001 T2002 E2003 D2004 I2008 P2017 H2018 Y2019 R2020 Y2021 P2022 I2023 N2026 L2027 F2028 P2029 C2032 N2033 Y2037 V2051 G2054 P2055
R2065 V2075 D2076 V2077 S2082 D2085 L2090 G2091 G2092 Y2093 E2094 Q2095 V2096 R2114 S2124 L2164 M2180 T2185 K2186 E2187 A2188 S2189 G2197 W2198 L2199 W2208 L2216 V2221 L2225 L2229 E2230 I2231 D2232 G2233 I2237 ASN GLU CYS SER GLN GLU ASP GLY Q2246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S2360 V2364 E2372 N2378 N2379 N2382 T2400 T2403 K2410 I2411 N2412 N2419 L2420 K2421 F2422 Q2423 L2428 H2429 L2442 P2460 L2463 Y2464 L2465 L2466 S2467 S2468 L2469 R2470 L2471 L2472 T2495 Y2496 I2497 G2506 P2513 P2516 L2521 N2531 L2532 S2536
Y2544 Q2545 Y2546 Y2547 W2548 L2551 E2559 T2560 A2561 V2562 T2563 K2564 D2565 K2573 I2576 I2580 S2587 L2595 W2596 I2597 N2598 F2601 T2602 D2603 V2604 L2605 W2617 L2632 K2646 V2647 R2648 D2661 N2676 K2677 L2678 S2679 L2683 K2687 D2690 E2694 L2697
I2698 K2701 H2708 D2715 L2739 L2744 L2747 I2748 N2753 Y2754 L2761 E2764 LYS ASN ALA LYS LEU THR SER F2772 T2773 I2800 I2815 L2822 L2837 G2846 G2847 E2863 I2877 W2897 I2898 K2931 T2932 F2933 S2940 W2941 R2942 N2943 V2944 R2945 K2946
V2947 I2948 S2949 G2950 D2951 E2952 E2953 T2956 E2957 K2958 L2959 I2960 I2963 S2964 A2968 G2978 D2982 D2986 E2987 W2988 S3012 D3013 Q3014 R3017 R3018 L3019 Y3037 S3038 D3042 L3043 S3053 I3054 K3062 A3070 S3071 M3080 D3081 N3084 K3124 L3132 I3135 F3136
E3137 R3151 E3155 Q3156 GLU GLU ASN GLU LYS SER ASN MET PHE LYS PHE ASN ASP ASN SER ASP ASP Y3174 F3182 PRO ASP TYR GLU ASP THR ALA LEU VAL THR ASN GLU LYS ASP ILE SER SER PRO GLU N3202 L3203 D3204 V3217 K3220 L3230 D3243 D3265 T3274
GLU VAL PHE GLY ASN I3280 D3281 F3282 I3297 L3306 K3307 L3308 L3309 K3310 Q3311 W3312 P3313 E3314 H3315 A3316 R3323 Q3326 K3334 Y3357 A3358 S3359 S3360 S3363 L3364 N3365 M3366 K3369 L3370 T3385 W3386 K3387 E3410 I3414 F3417 VAL SER GLU LYS LYS GLU THR ALA PRO
N3427 L3444 L3451 I3461 L3466 R3467 I3471 Q3484 L3488 E3491 K3498 S3499 L3500 L3509 K3514 D3515 D3519 Q3523 K3527 I3535 V3536 R3537 D3546 E3552 A3553 Y3557 UNK X3559 X3560 X3562 X3563 X3564 X3565 X3568 X3569 X3570 X3571 X3574 X3575 X3579
X3580 X3581 X3582 X3594 X3595 D3602 T3603 N3607 S3610 K3614 I3615 S3616 S3617 Q3618 E3619 F3620 F3623 D3629 F3630 Y3631 A3632 E3633 R3636 L3637 R3638 K3639 E3640 T3641 P3642 N3643 V3644 Y3645 THR LYS GLU ASN LYS LYS R3652 L3653 A3654 Y3655 T3658 Q3659 I3739 K3660 S3661 K3662 D3666 A3667 L3668
K3669 E3670 L3671 R3672 R3673 I3674 G3675 L3676 LYS VAL ASN PHE ARG GLU D3683 I3684 V3687 Q3688 S3689 T3693 N3697 L3706 N3707 S3708 S3709 F3712 K3715 I3716 L3717 D3718 L3719 L3723 R3724 S3725 A3726 A3727 SER ASN PRO SER ASP ASP ILE PRO V3736 A3737 A3738 I3739 E3740 R3741 A3744
S3748 L3749 S3752 H3758 F3763 I3770 M3774 L3777 E3778 T3781 C3782 L3783 K3784 G3785 D3786 H3789 E3803 D3811 A3825 S3842 H3846 F3853 D3854 R3863 N3877 E3880 T3881 G3882 N3883 A3884 F3885 N3897 K3898 GLY GLY PRO ILE LYS LYS GLU GLN LYS
ARG GLY PRO SER VAL E3913 R3921 T3922 F3923 T3924 S3925 L3928 S3929 K3932 V3933 I3934 G3935 D3936 G3937 I3938 E3939 S3940 ILE SER GLU T3944 D3945 D3946 N3947 W3948 A3951 M3957 L3962 L3963 R3964 S3965 S3966 N3971 A3975 L3978 F3982 D3983 F3984 E3988 S3989 I3990 Y3991 S3994
F3998 V4002 I4003 T4004 N4008 A4009 L4014 E4015 R4016 Y4020 Y4021 T4022 G4027 I4030 L4031 I4034 L4038 N4041 GLY PHE CYS SER PRO GLN PRO PRO SER GLU GLU VAL ASP ASP LYS ASN LEU GLN GLU GLY THR GLY LEU GLY ASP GLY GLU GLY ALA GLN ASN ASN

ASN LYS ASP VAL GLU GLN ASP GLU ASP LEU THR GLU ASP ALA GLN ASN GLU ASN LYS GLU GLN GLN ASP LYS ASP GLU ARG ASP ASP GLU ASN GLU ASP ASP ALA VAL GLU MET GLU GLY ASP MET ALA GLY GLU LEU GLU ASP LEU SER ASN GLY GLU GLU ASN ASP ASP GLU ASP THR

ASP SER GLU GLU GLU GLU LEU ASP GLU GLU ILE ASP ASP LEU ASN GLU ASP ASP PRO ASN ALA ILE ASP ASP LYS MET TRP ASP ASP LYS ALA SER ASP ASN SER LYS GLU LYS ASP THR ASP GLN ASN LEU ASP GLY LYS ASN GLN GLU GLU ASP VAL GLN ALA ALA GLU ASN ASP GLU

GLN GLN ARG ASP ASN LYS GLU GLY GLY ASP GLU ASP PRO ASN ALA PRO GLU ASP GLY ASP GLU GLU ILE GLU ASN ASP GLU ASN ALA GLU GLU GLU ASN ASP VAL GLY GLU GLN GLU ASP GLU VAL LYS ASP GLU GLU GLY GLU ASP LEU GLU ALA ASN VAL PRO GLU ILE GLU THR LEU

ASP LEU PRO GLU ASP MET ASN LEU ASP SER GLU HIS GLU GLU SER ASP GLU ASP VAL ASP MET SER ASP GLY MET PRO ASP ASP LEU ASN LYS GLU GLU VAL GLY ASN GLU ASP GLU GLU VAL LYS GLN GLU SER GLY ILE GLU SER ASP ASN GLU ASN ASP GLU PRO GLY PRO GLU GLU

ASP ALA GLY GLU THR GLU THR ALA LEU ASP GLU GLU GLU GLY ALA GLU GLU ASP VAL ASP MET THR ASN ASP GLU GLY LYS GLU ASP GLU GLU ASN GLY PRO GLU GLU GLN ALA MET SER ASP GLU GLU GLU LEU LYS GLN ASP ALA ALA MET GLU GLU ASN LYS GLU LYS GLY GLY GLU

GLN ASN THR GLU GLY LEU ASP GLY VAL GLU GLU LYS ALA ASP THR GLU ASP ILE ASP GLN GLU ALA ALA VAL GLN GLN ASP SER GLY SER LYS GLY ALA GLY ALA ASP ALA THR ASP THR GLN GLU GLN ASP ASP VAL GLY GLY SER GLY THR THR GLN ASN THR TYR GLU GLU ASP GLN

GLU ASP VAL THR LYS ASN ASN GLU GLU SER ARG GLU GLU ALA THR ALA ALA LEU LYS GLN LEU GLY ASP SER MET LYS GLU TYR HIS ARG ARG ARG GLN ASP ILE LYS GLU ALA GLN THR ASN GLY GLU GLU ASP GLU ASN LEU GLU LYS ASN ASN GLU ARG PRO ASP GLU PHE GLU HIS

VAL GLU GLY ALA ASN THR GLU THR ASP THR GLN ALA LEU GLY SER ALA THR GLN ASP GLN LEU GLN THR ILE ASP GLU ASP MET ALA ILE ASP ASP ASP ARG GLU GLU GLN GLU VAL ASP GLN LYS GLU LEU VAL GLU ASP ALA ASP ASP GLU LYS MET ASP ILE ASP GLU GLU GLU MET

LEU SER ASP ILE ASP ALA HIS ASP ALA ASN ASN ASP VAL ASP SER LYS LYS SER GLY PHE ILE GLY LYS ARG LYS SER GLU GLU ASP PHE GLU ASN GLU LEU SER ASN GLU HIS PHE SER ALA ASP GLN GLU ASP ASP SER GLU ILE GLN SER LEU ILE GLU ASN ILE GLU ASP ASN PRO

PRO ASP ALA SER ALA SER LEU THR PRO GLU ARG SER LEU GLU GLU SER ARG GLU LEU TRP HIS LYS SER GLU ILE SER THR ALA ASP LEU VAL SER ARG LEU GLY GLU GLN LEU ARG LEU ILE LEU GLU PRO THR LEU ALA THR LYS LEU LYS GLY ASP TYR LYS THR GLY LYS ARG LEU

ASN MET LYS ARG ILE ILE PRO TYR ILE ALA SER GLN PHE ARG LYS ASP LYS ILE TRP LEU ARG ARG THR LYS PRO SER LYS ARG GLN TYR GLN ILE MET ILE ALA LEU ASP ASP SER LYS SER MET SER GLU SER LYS CYS VAL LYS LEU ALA PHE ASP SER LEU CYS LEU VAL SER LYS

THR LEU THR GLN LEU GLU ALA GLY GLY LEU SER ILE VAL LYS PHE GLY GLU ASN ILE LYS GLU VAL HIS SER PHE ASP GLN GLN PHE SER ASN GLU SER GLY ALA ARG ALA PHE GLN TRP PHE GLY PHE GLN GLU THR LYS THR ASP VAL LYS LYS LEU VAL ALA GLU SER THR LYS ILE

PHE GLU ARG ALA ARG ALA MET VAL HIS ASN ASP GLN TRP GLN LEU GLU ILE VAL ILE SER ASP GLY ILE CYS GLU ASP HIS GLU THR ILE GLN LYS LEU VAL ARG ARG ALA ARG GLU ASN LYS ILE MET LEU VAL PHE VAL ILE ILE ASP GLY ILE THR SER ASN GLU SER ILE LEU ASP

MET SER GLN VAL ASN TYR ILE PRO ASP GLN TYR GLY ASN PRO GLN LEU LYS ILE THR LYS TYR LEU ASP THR PHE PRO PHE GLU PHE TYR VAL VAL VAL HIS ASP ILE SER GLU LEU PRO GLU MET LEU SER LEU ILE LEU ARG GLN TYR PHE THR ASP LEU ALA SER SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	55442	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0156	Depositor
Map size (Å)	418.56, 418.56, 418.56	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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	0.30	2/21930 (0.0%)	0.56	8/30028 (0.0%)

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	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	462	SER	C-N	17.86	1.75	1.34
1	A	1934	PRO	C-N	-14.43	1.00	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	462	SER	O-C-N	-43.22	53.55	122.70
1	A	1934	PRO	O-C-N	-18.52	93.06	122.70
1	A	1934	PRO	CA-C-N	11.05	141.51	117.20
1	A	1934	PRO	C-N-CA	9.52	145.51	121.70
1	A	2595	LEU	CA-CB-CG	6.03	129.16	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1934	PRO	Mainchain
1	A	3312	TRP	Peptide
1	A	3515	ASP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	734	LYS	Peptide

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	22765	0	17093	235	0
All	All	22765	0	17093	235	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 6.

The worst 5 of 235 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:2344:GLN:OE1	1:A:2947:VAL:CG1	1.67	1.39
1:A:2410:LYS:HE3	1:A:2536:SER:CB	1.51	1.39
1:A:2351:LEU:HD21	1:A:2942:ARG:NH1	1.40	1.34
1:A:2410:LYS:CE	1:A:2536:SER:CB	2.11	1.28
1:A:2344:GLN:CD	1:A:2947:VAL:HG13	1.53	1.28

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	3305/4854 (68%)	3081 (93%)	213 (6%)	11 (0%)	41 76

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	PRO
1	A	1570	ASN
1	A	2516	PRO
1	A	864	PRO
1	A	2023	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	1413/4180 (34%)	1397 (99%)	16 (1%)	73 85

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3897	ASN
1	A	3706	LEU
1	A	2412	ASN
1	A	3151	ARG
1	A	2382	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3618	GLN
1	A	3897	ASN
1	A	3883	ASN
1	A	2598	ASN
1	A	3262	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	7

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	31:UNK	C	70:UNK	N	16.07
1	A	3575:UNK	C	3579:UNK	N	7.33
1	A	3587:UNK	C	3591:UNK	N	5.27
1	A	3596:UNK	C	3599:ARG	N	5.16
1	A	3560:UNK	C	3562:UNK	N	3.64

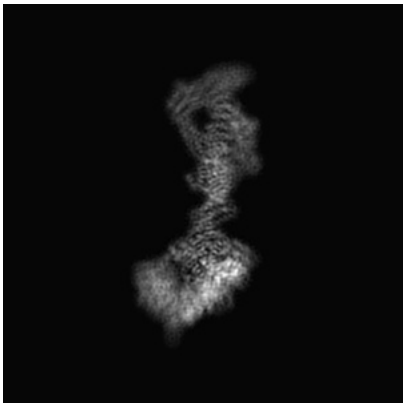
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0328. These allow visual inspection of the internal detail of the map and identification of artifacts.

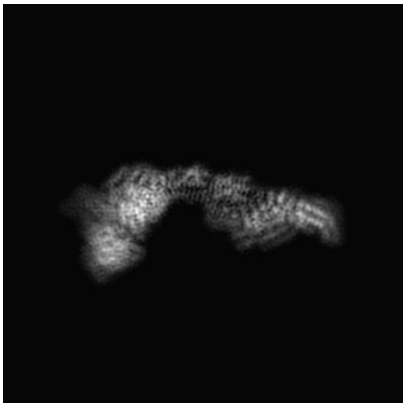
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

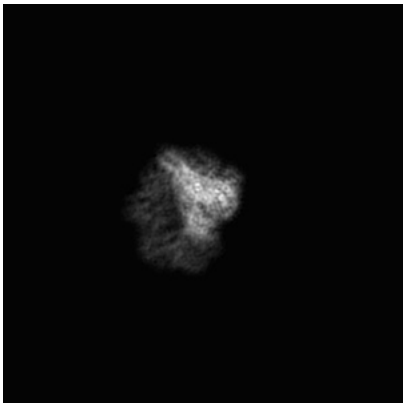
6.1.1 Primary map



X



Y

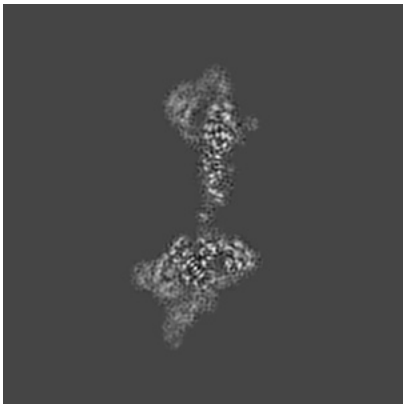


Z

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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 192

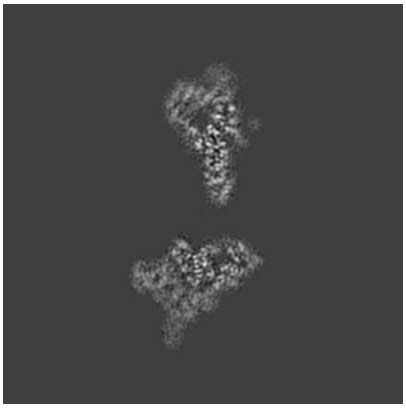
Y Index: 192

Z Index: 192

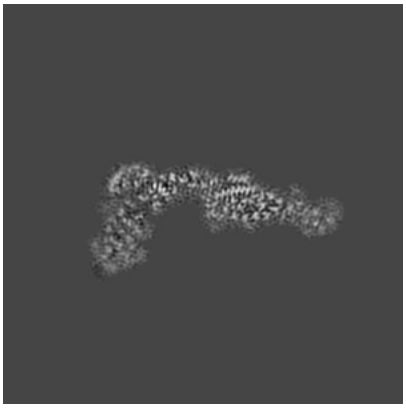
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 186



Y Index: 203

Z Index: 133

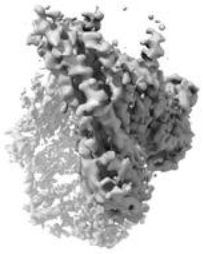
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0156. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

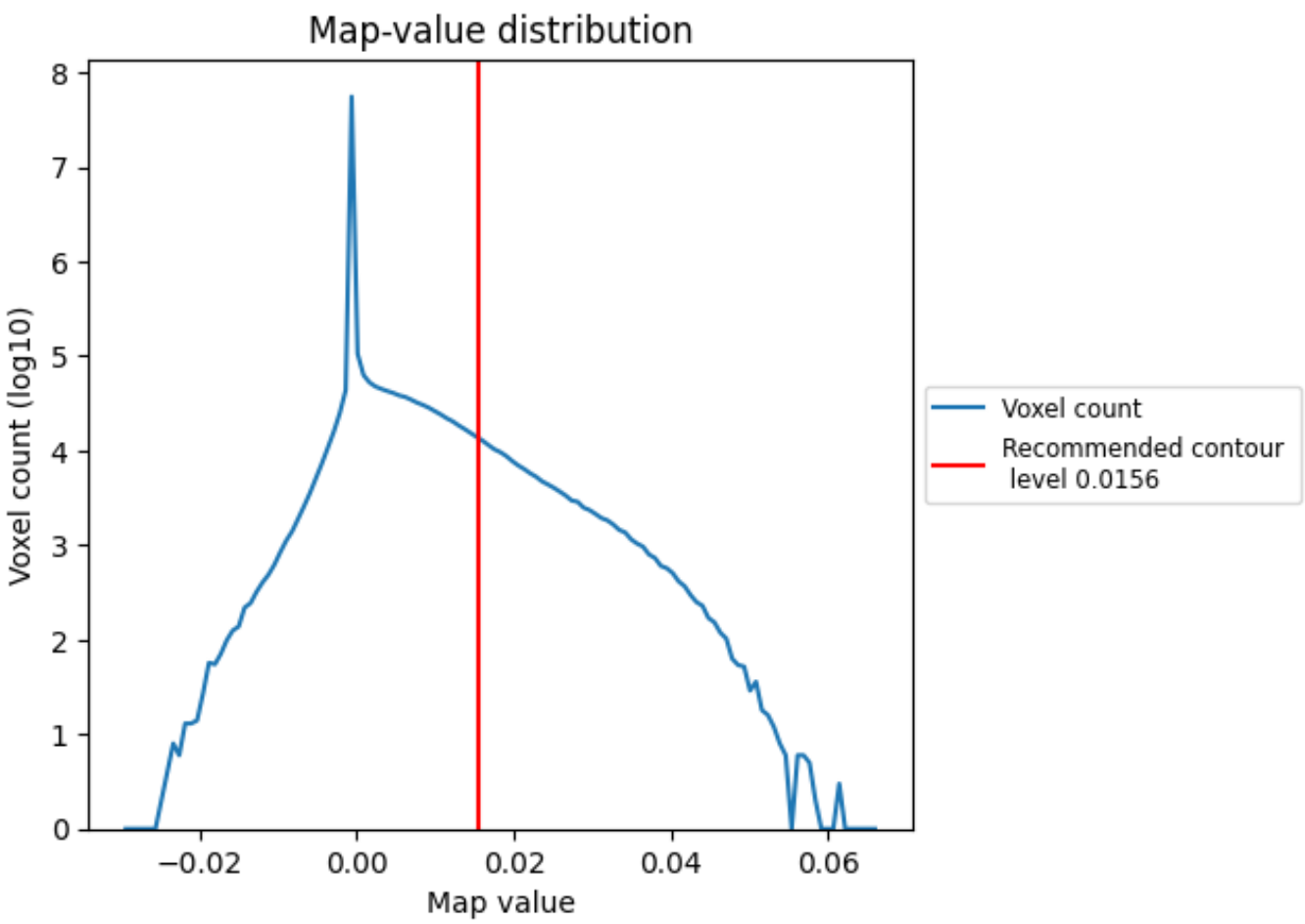
6.5 Mask visualisation (i)

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

7 Map analysis (i)

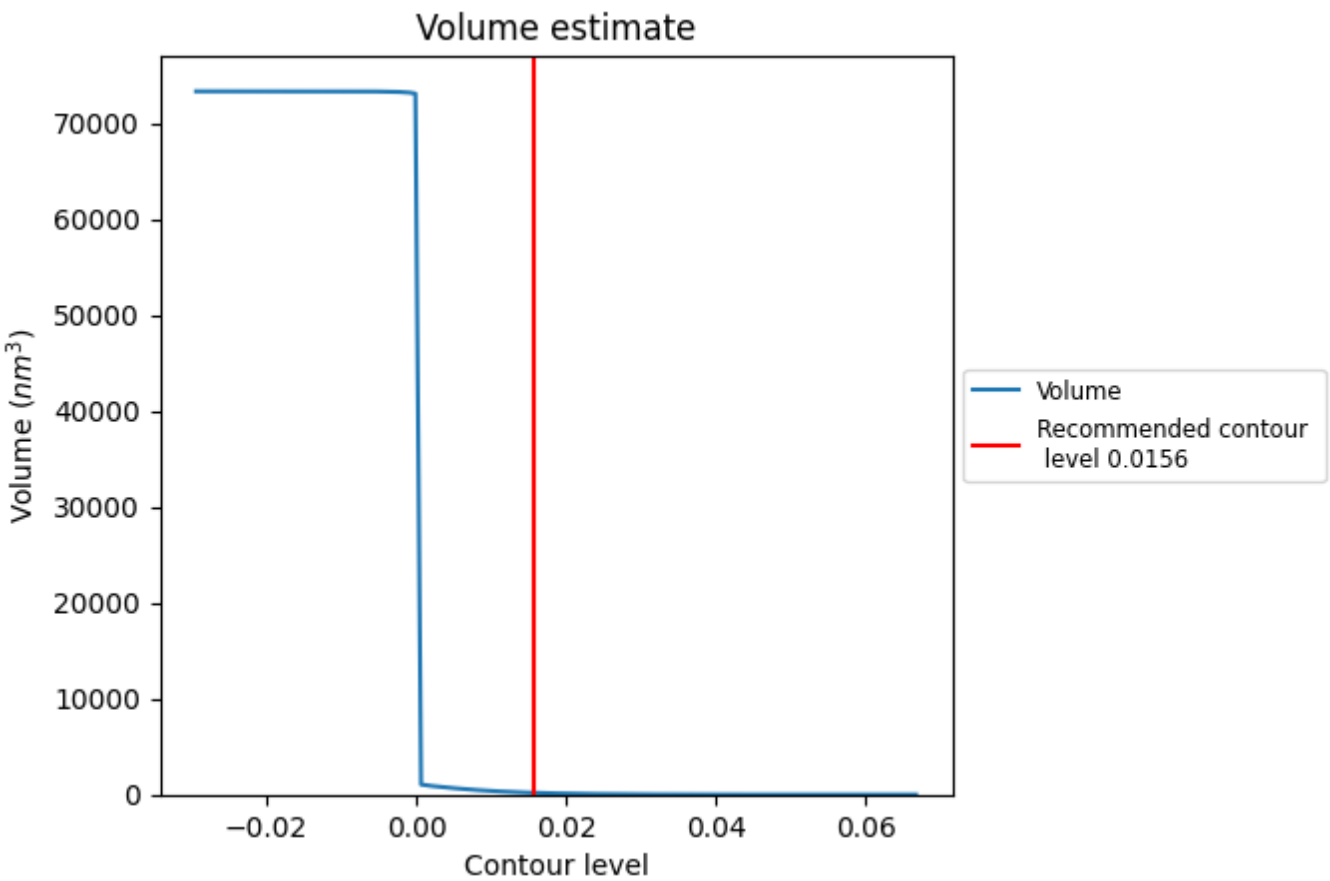
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

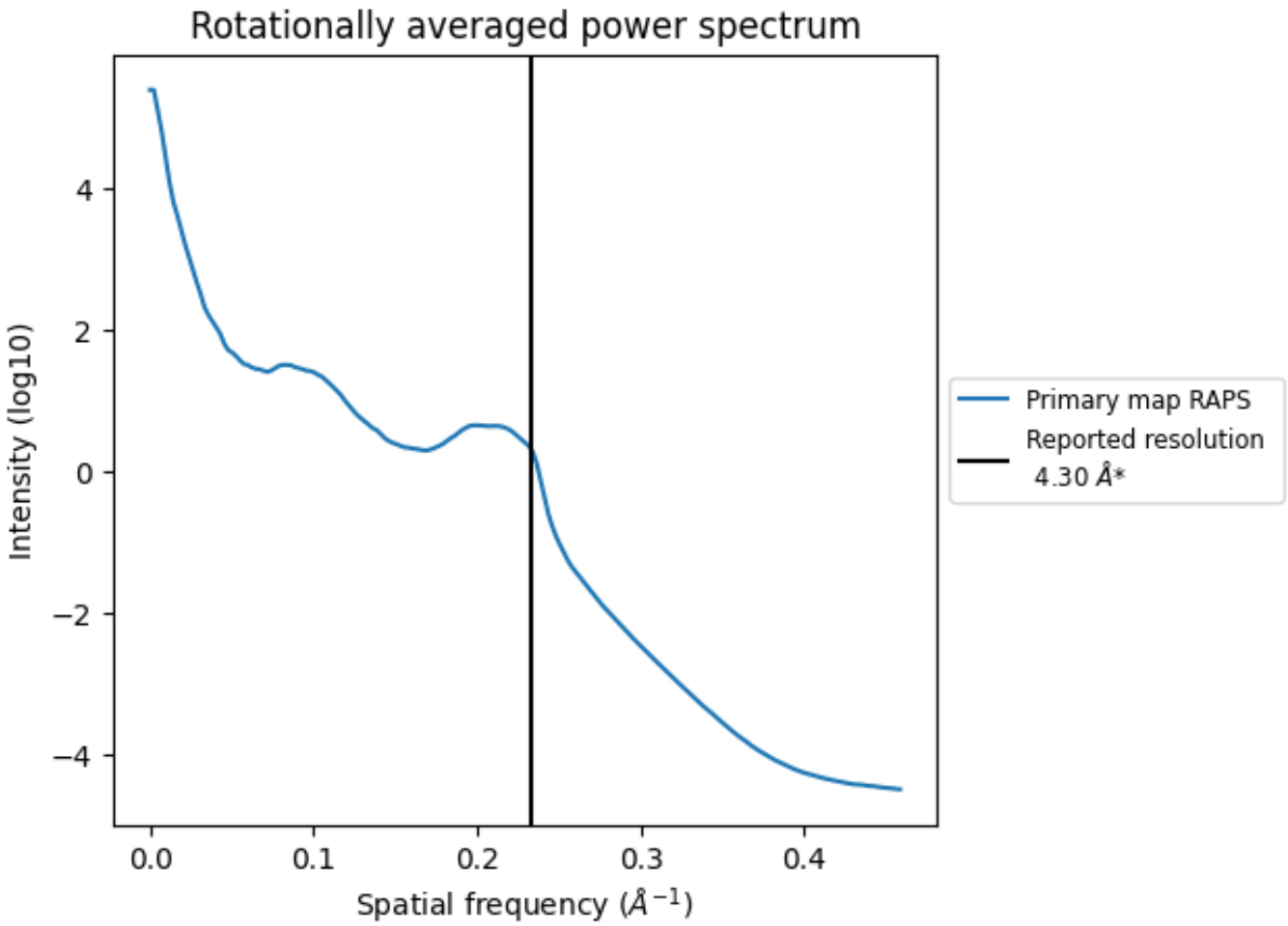
7.2 Volume estimate (i)



The volume at the recommended contour level is 185 nm^3; this corresponds to an approximate mass of 167 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)

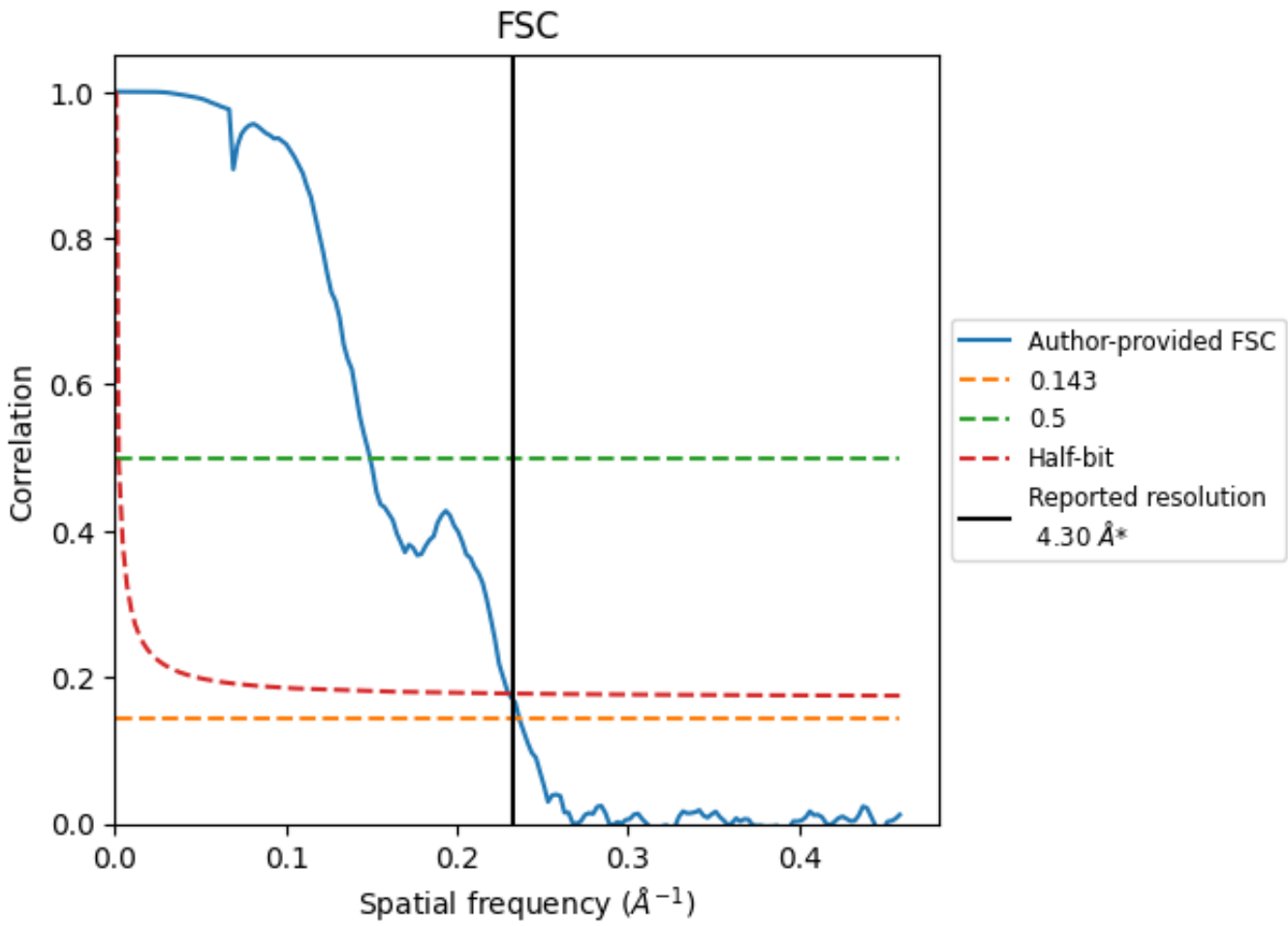


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

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 0.233 Å^{-1}

8.2 Resolution estimates (i)

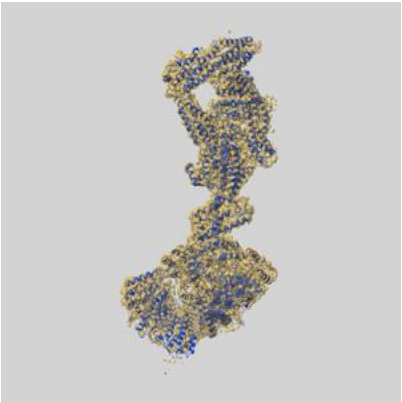
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.23	6.71	4.34
Unmasked-calculated*	-	-	-

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

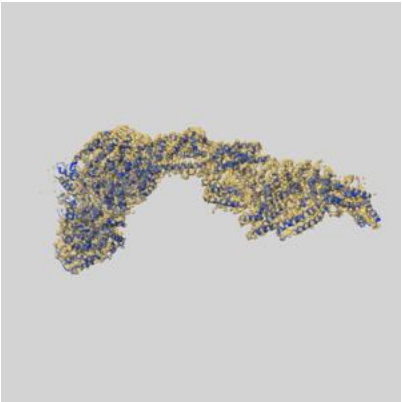
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0328 and PDB model 6I26. Per-residue inclusion information can be found in section 3 on page 4.

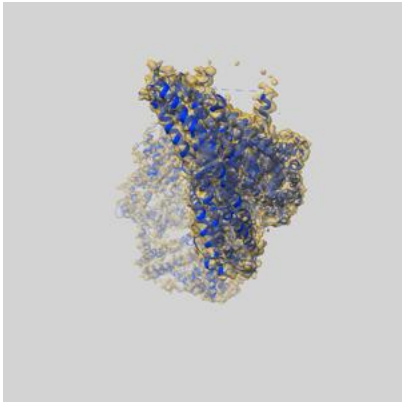
9.1 Map-model overlay (i)



X



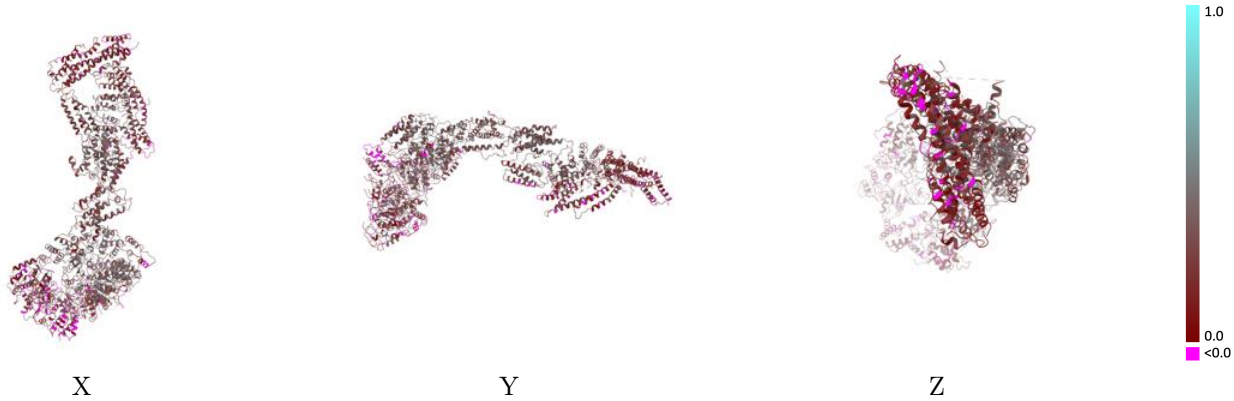
Y



Z

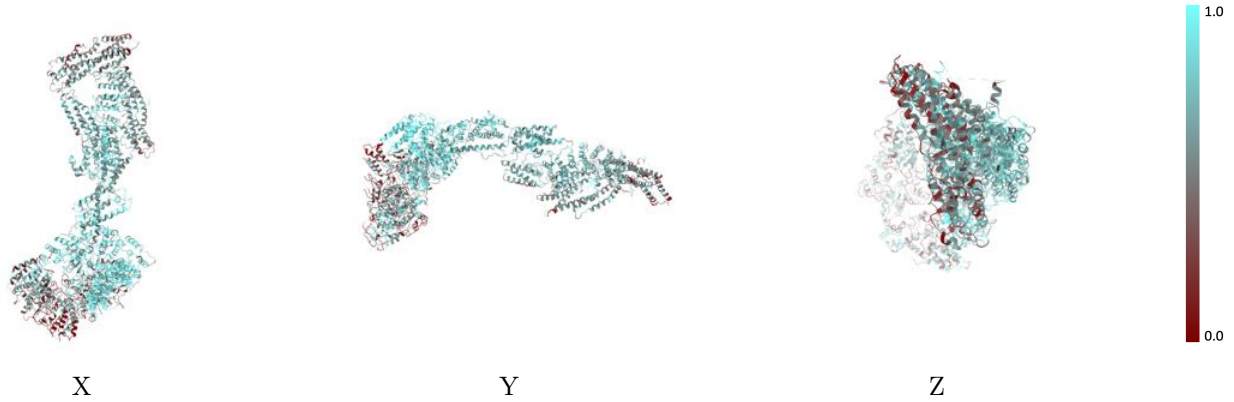
The images above show the 3D surface view of the map at the recommended contour level 0.0156 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



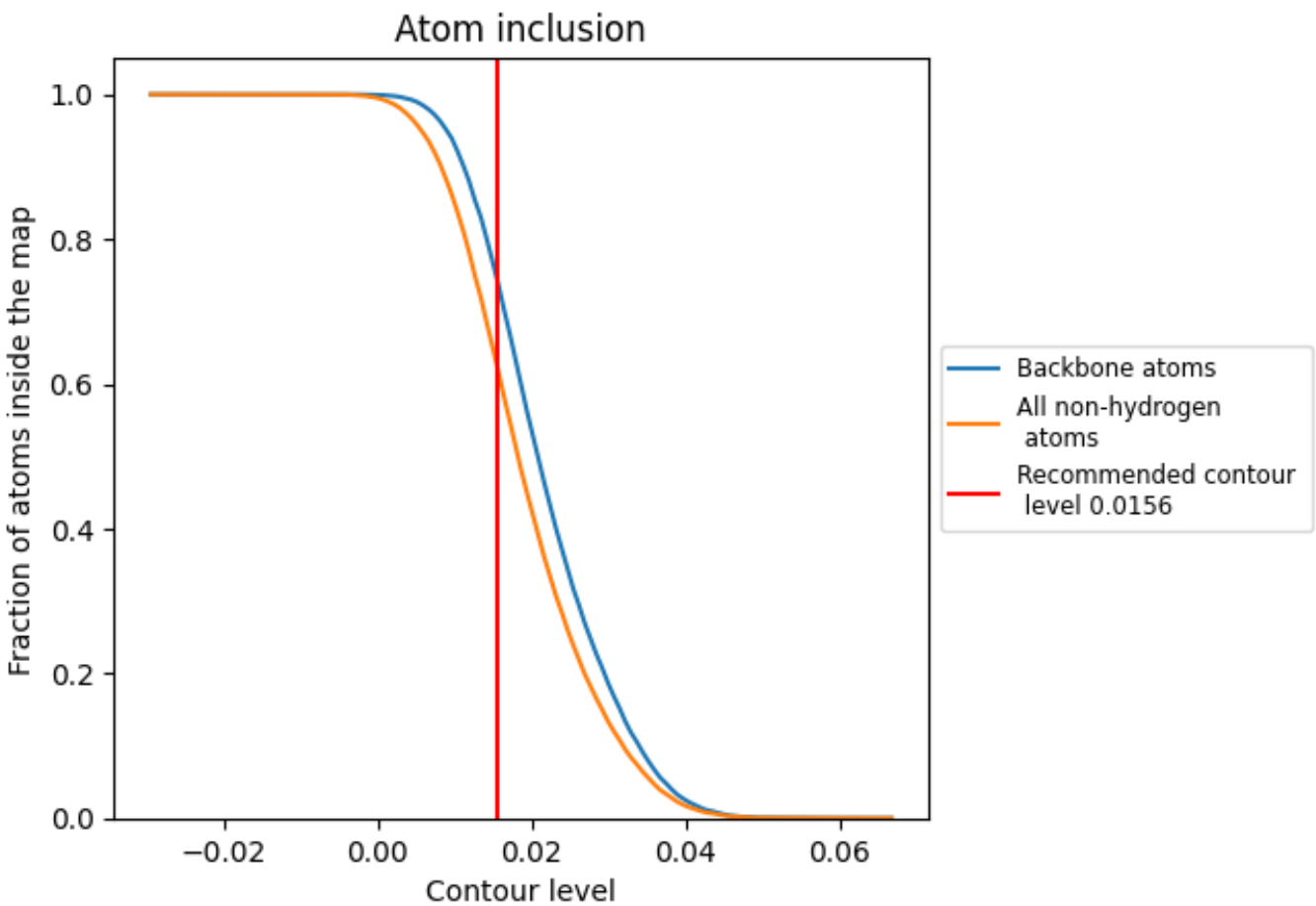
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.0156).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0156) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6214	0.2710
A	0.6214	0.2710