wwPDB EM Validation Summary Report

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PDB ID	:	6SKZ
EMDB ID	:	EMD-10232
Title	:	Structure of the closed conformation of CtTel1
Authors	:	Jansma, M.; Eustermann, S.E.; Kostrewa, D.; Lammens, K.; Hopfner, K.P.
Deposited on	:	2019-08-16
Resolution	:	3.40 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*
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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:

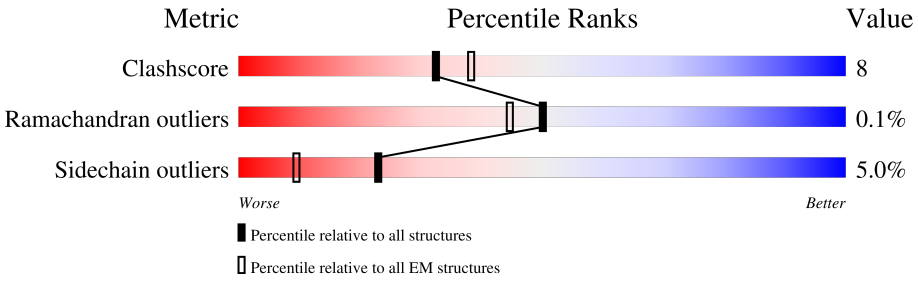
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

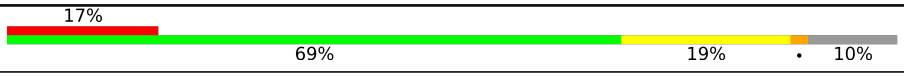
The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2944	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20930 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.

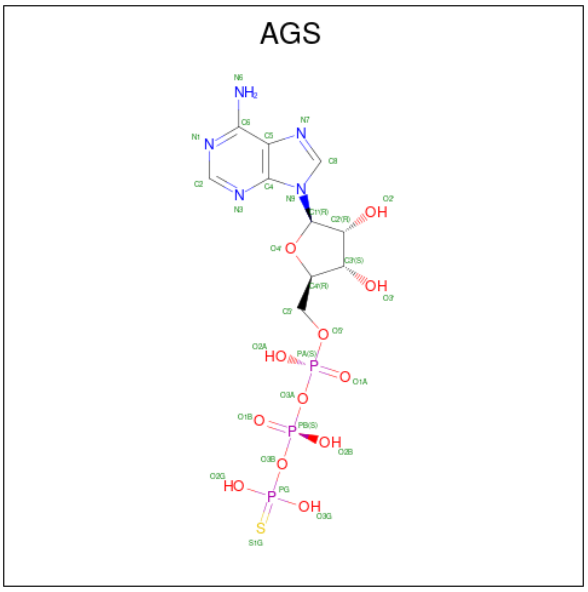
- Molecule 1 is a protein called Serine/threonine-protein kinase Tel1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2638	20898	13292	3638	3874	94	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2847	LEU	PHE	conflict	UNP G0S4S9
A	2848	TYR	-	insertion	UNP G0S4S9
A	2849	GLN	-	insertion	UNP G0S4S9
A	2850	TRP	-	insertion	UNP G0S4S9
A	2851	SER	-	insertion	UNP G0S4S9
A	2852	ILE	-	insertion	UNP G0S4S9
A	2853	SER	-	insertion	UNP G0S4S9
A	2854	PRO	-	insertion	UNP G0S4S9
A	2855	VAL	-	insertion	UNP G0S4S9
A	2856	ARG	-	insertion	UNP G0S4S9
A	2857	MET	-	insertion	UNP G0S4S9
A	2858	ALA	-	insertion	UNP G0S4S9
A	2859	LYS	-	insertion	UNP G0S4S9
A	2860	LEU	-	insertion	UNP G0S4S9
A	2861	GLN	-	insertion	UNP G0S4S9
A	2862	ASN	-	insertion	UNP G0S4S9
A	2863	ALA	-	insertion	UNP G0S4S9
A	2864	ARG	-	insertion	UNP G0S4S9
A	2865	GLU	-	insertion	UNP G0S4S9
A	2866	VAL	-	insertion	UNP G0S4S9

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

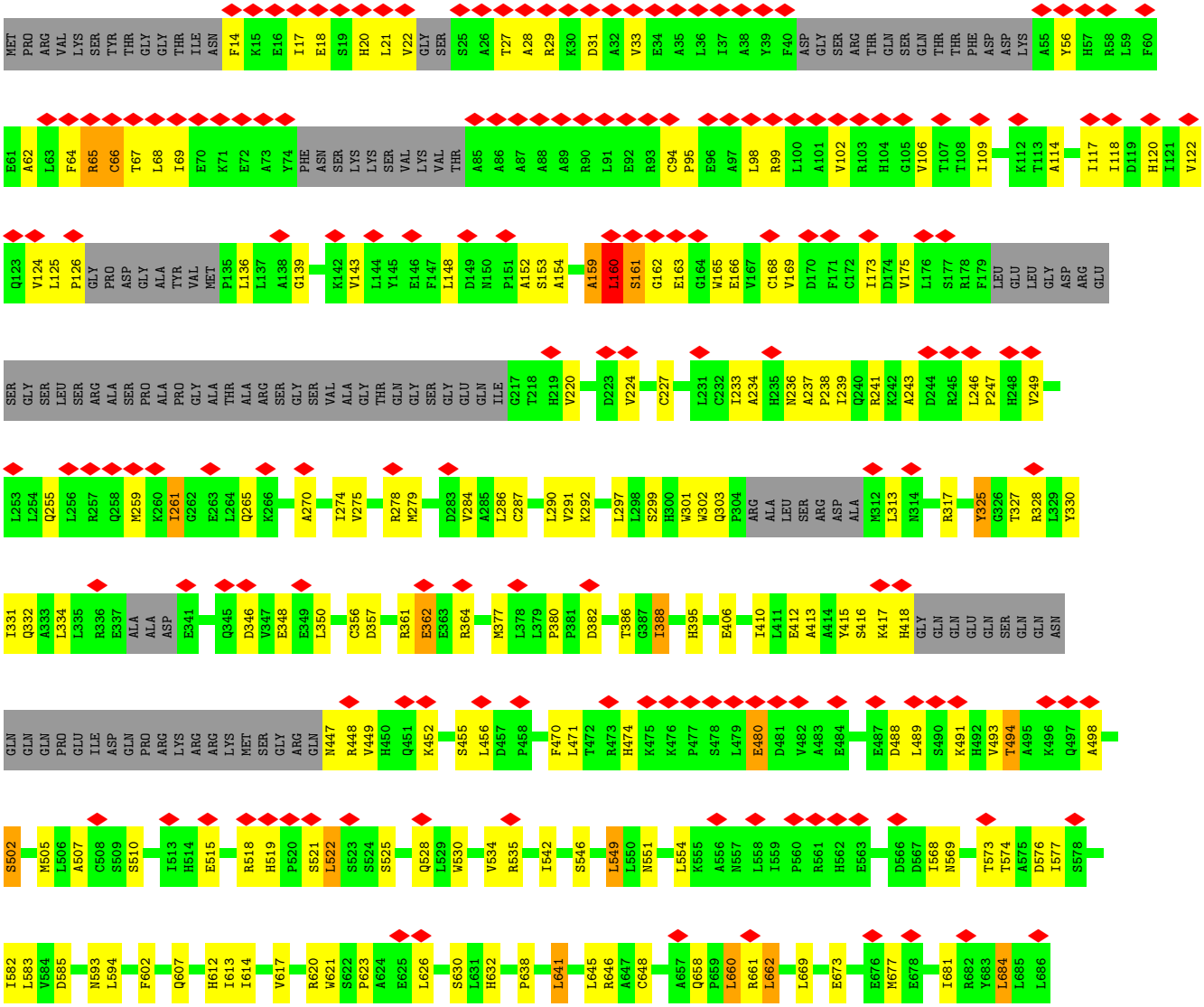
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	

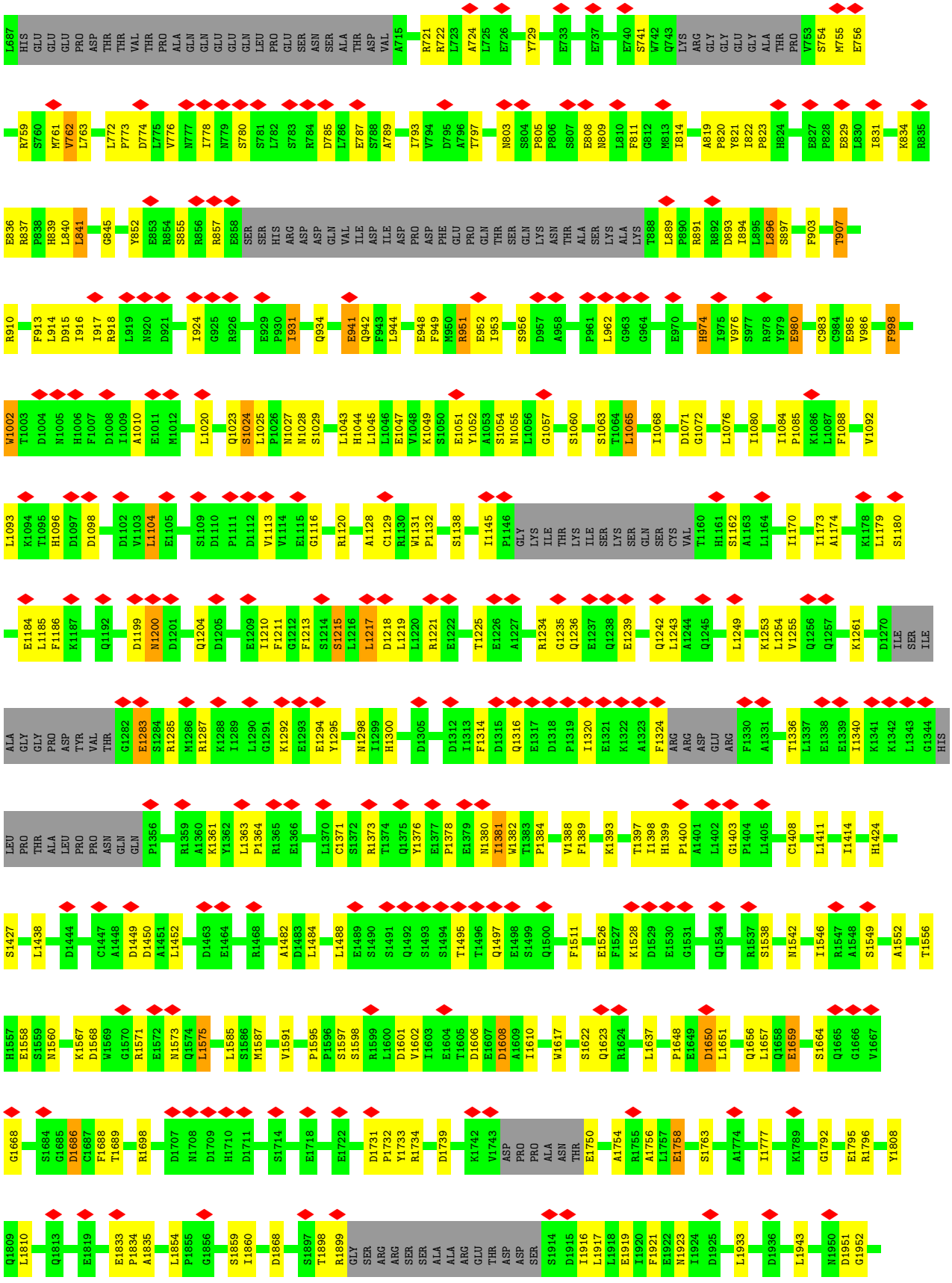
3 Residue-property plots (i)

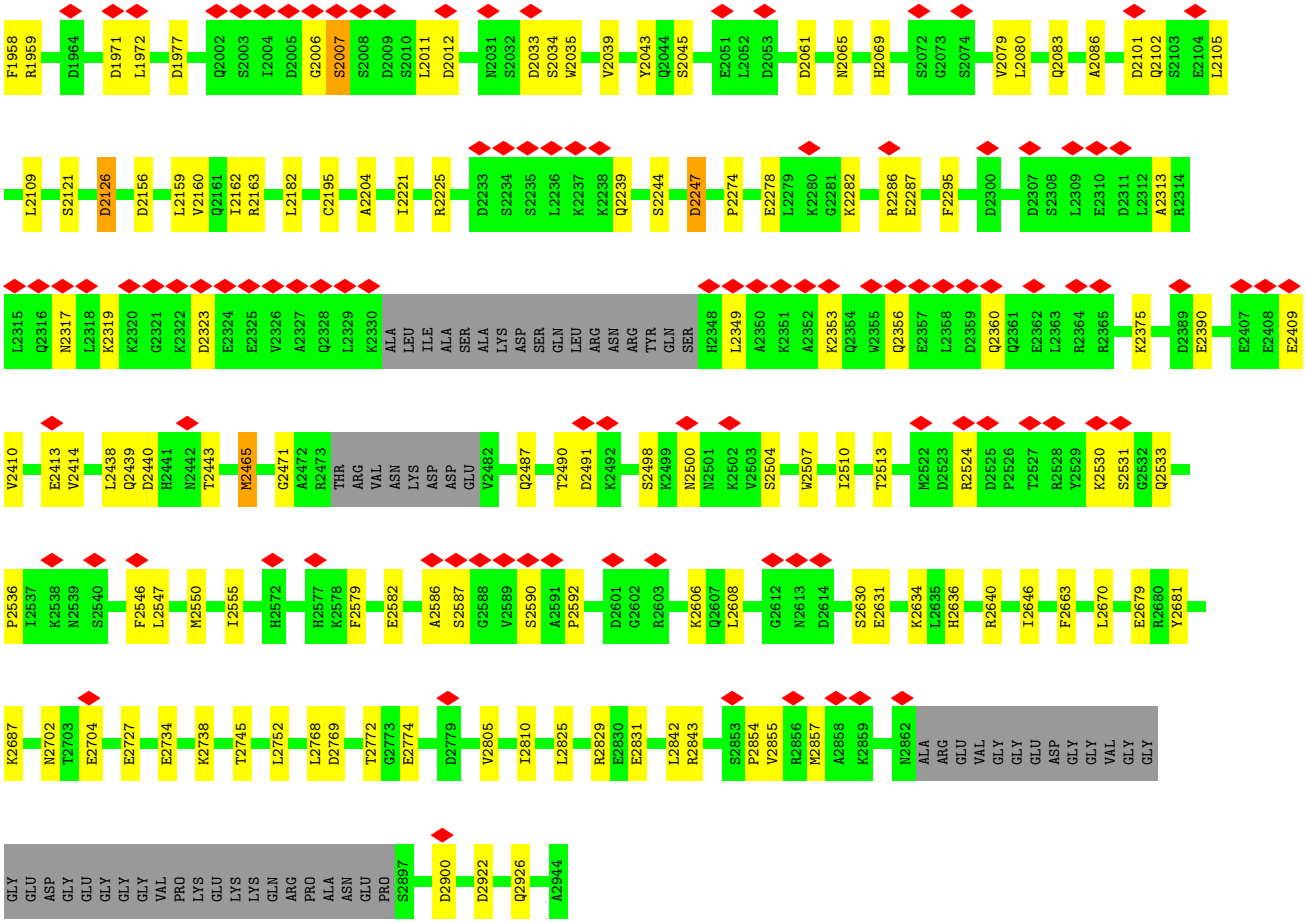
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Serine/threonine-protein kinase Tel1

Chain A:




L687 HIS GLU GLU GLU PRO ASP THR THR VAL THR PRO ALA GLN GLN GLU GLU GLN LEU PRO GLU SER ASN SER ALA THR ASP VAL A715
R721 R722 L723 A724 L725 E726 Y729 E733 E737 E740 S741 W742 Q743 LYS ARG GLY GLY GLU GLY ALA THR PRO V753 S754 M755 E756
R759 S760 M761 V762 L763
L772 P773 D774 L775 V776 N777 T778 W779 S780 S781 L782 S783 R784 D785 L786 E787 S788 A789
T793 V794 D795 A796 T797
N803 S804 P805 P806 S807 E808 N809 L810 F811 Q812 M813 I814
A819 P820 Y821 I822 P823 H824
E827 P828 E829 L830 I831
K834 R835
E836 R837 P838 H839 L840 L841
G845
Y852 E853 R854 S855 R856 R857 E858 SER SER HIS ARG ASP ASP GLN VAL ILE ASP ILE ASP PRO ASP PHE GLU PRO GLN THR SER GLN LYS ASN THR ALA SER LYS ALA LYS T888 L889 P890 R891 R892 D893 I894 L895 L896 S897
F903
T907
R910
F913 L914 D915 I916 I917 R918 L919 N920 D921
I924 G925 R926
E929 P930 I931
Q934
E941 Q942 F943 L944
E948 F949 M950 R951 E952 I953
S956 D957 A958
P961 L962 G963 G964
E970
H974 I975 V976 S977 R978 Y979 E980
C983 C984 E985 V986
F998
W1002 T1003 D1004 N1005 H1006 F1007 D1008 I1009 A1010 E1011 M1012
L1020
Q1023 S1024 L1025 P1026 N1027 N1028 S1029
L1043 H1044 L1045 L1046 E1047 V1048 K1049 S1050
E1051 Y1052 A1053 S1054 N1055 L1056 G1057
S1060
S1063 T1064 L1065
I1068
D1071 G1072
L1076
I1080
I1084 P1085
K1086 L1087 F1088
V1092
L1093 K1094 T1095 H1096 D1097 D1098
D1102 V1103 L1104 E1105
S1109 D1110 P1111 D1112 V1113 V1114 E1115 G1116
R1120
A1128
C1129 R1130 W1131 P1132
S1138
I1145 P1146 GLY LYS ILE THR LYS ILE SER LYS SER GLN SER CYS VAL T1160 H1161 S1162 A1163 L1164
I1170
I1173 A1174
K1178 L1179 S1180
E1184 L1185 F1186 K1187
Q1192
D1199 N1200 D1201
Q1204 D1205
E1209 I1210 F1211 G1212 F1213
S1214 S1215 L1216 L1217 D1218 L1219 L1220
R1221 E1222
T1225 E1226 A1227
R1234 G1235 Q1236 E1237 Q1238 E1239
Q1242 L1243 A1244 Q1245
L1249
K1253 L1254 V1255 Q1256 Q1257
K1261
D1270 ILE SER ILE
ALA GLY GLY PRO ASP TYR VAL THR G1282 E1283 S1284 R1285 M1286 R1287 K1288 I1289 L1290 G1291 K1292 E1293 E1294 Y1295
N1298 I1299 H1300
D1305
D1312 I1313 F1314 D1315 Q1316 E1317 D1318 P1319 I1320 E1321 K1322 A1323 F1324 ARG ARG ASP GLU ARG F1330 A1331
T1336 L1337 E1338 E1339 I1340 K1341 K1342 L1343 G1344 HIS
LEU PRO THR ALA LEU PRO PRO ASN GLN GLN P1356
R1359 A1360 K1361 Y1362 L1363 P1364 R1365 E1366
L1370 C1371 S1372 R1373 T1374 Q1375 Y1376 E1377 P1378 E1379 N1380 I1381 W1382 T1383 P1384
V1388 F1389
K1393
T1397 I1398 H1399 P1400 A1401 L1402 G1403 P1404 L1405
C1408
L1411
I1414
H1424
S1427
L1438
D1444
C1447 A1448 D1449 D1450
A1451 L1452
D1463 E1464
R1468
A1482 D1483 L1484
L1488
E1489 S1490 S1491 Q1492 S1493 S1494 T1495 T1496 Q1497 E1498 S1499 Q1500
F1511
E1526 F1527 K1528 D1529 E1530 G1531
Q1534
R1537 S1538
N1542
I1546 R1547 A1548 S1549
A1552
T1556
H1557 E1558 S1559 N1560
K1567 D1568 W1569 G1570 R1571 E1572 N1573 Q1574 L1575
L1585 S1586 M1587
V1591
P1595 P1596 S1597 S1598
R1599 L1600 D1601 V1602 I1603 E1604 T1605 D1606 E1607 D1608 A1609 I1610
W1617
S1622 Q1623 R1624
L1637
P1648 E1649 D1650 L1651
Q1656 L1657 Q1658 E1659
S1664 Q1665 G1666 V1667
G1668
S1684 G1685 D1686 C1687 F1688 T1689
R1698
D1707 N1708 D1709 H1710 D1711
S1714
E1718
E1722
D1731 P1732 Y1733 R1734
D1739
K1742 V1743 ASP PRO PRO ALA ASN THR E1750
A1754
R1755 A1756 L1757 E1758
S1763
A1774
I1777
K1789
G1792
E1795 R1796
Y1808
Q1809 L1810
Q1813
E1819
E1833 P1834 A1835
L1854 P1855 G1856
S1859 I1860
D1868
S1897 T1898 R1899 GLY SER ARG ARG SER SER ALA ALA ARG GLU THR ASP ASP SER S1914 D1915 I1916 L1917 L1918 E1919 I1920 F1921 E1922 N1923 I1924 D1925
L1933
D1936
L1943
N1950 D1951 G1952


F1958 R1959 D1964 D1971 L1972 D1977 Q2002 S2003 I2004 D2005 G2006 S2007 S2008 D2009 S2010 L2011 D2012 N2031 S2032 D2033 S2034 W2035 V2039 Y2043 Q2044 S2045 E2051 L2052 D2053 D2061 N2065 H2069 S2072 G2073 S2074 V2079 L2080 Q2083 A2086 D2101 Q2102 S2103 E2104 L2105
L2109 S2121 D2126 D2156 L2159 V2160 Q2161 I2162 R2163 L2182 C2195 A2204 I2221 R2225 D2233 S2234 S2235 L2236 K2237 K2238 Q2239 S2244 D2247 P2274 E2278 L2279 K2280 G2281 K2282 R2286 E2287 F2295 D2300 D2307 S2308 L2309 E2310 D2311 L2312 A2313 R2314
L2315 Q2316 N2317 L2318 K2319 K2320 G2321 K2322 D2323 E2324 E2325 V2326 A2327 Q2328 L2329 K2330 ALA LEU ILE ALA SER ALA LYS ASP SER GLN LEU ARG ASN ARG TYR GLN SER H2348 L2349 A2350 K2351 A2352 K2353 Q2354 W2355 Q2356 E2357 L2358 D2359 Q2360 Q2361 E2362 L2363 R2364 R2365 K2375 D2389 E2390 E2407 E2408 E2409
V2410 E2413 V2414 L2438 Q2439 D2440 H2441 N2442 T2443 M2465 G2471 A2472 R2473 THR ARG VAL ASN LYS ASP ASP GLU V2482 Q2487 T2490 D2491 K2492 S2498 K2499 N2500 K2501 K2502 V2503 S2504 W2507 I2510 T2513 M2522 D2523 R2524 D2525 P2526 T2527 R2528 Y2529 K2530 S2531 G2532 Q2533
P2536 I2537 K2538 N2539 S2540 F2546 L2547 M2550 I2555 H2572 H2577 K2578 F2579 E2582 A2586 S2587 G2588 V2589 S2590 A2591 P2592 D2601 G2602 R2603 K2606 Q2607 L2608 G2612 N2613 D2614 S2630 E2631 K2634 L2635 H2636 R2640 I2646 F2663 L2670 E2679 R2680 Y2681
K2687 N2702 T2703 E2704 E2727 E2734 K2738 T2745 L2752 L2768 D2769 T2772 G2773 E2774 D2779 V2805 I2810 L2825 R2829 E2830 E2831 L2842 R2843 S2853 P2854 V2855 R2856 M2857 A2858 K2859 N2862 ALA ARG GLU VAL GLY GLY GLU ASP GLY GLY VAL GLY GLY
GLY GLU ASP GLY GLU GLY GLY GLY VAL PRO LYS GLU LYS LYS GLN ARG PRO ALA ASN GLU PRO S2897 D2900 D2922 Q2926 A2944

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	132127	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 ($e^-/Å^2$)	55.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0126	Depositor
Map size (Å)	372.768, 372.768, 372.768	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.49	0/21306	0.51	2/28856 (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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2007	SER	N-CA-CB	-7.69	98.97	110.50
1	A	1758	GLU	C-N-CA	-5.79	107.21	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	ALA	Peptide
1	A	2006	GLY	Peptide
1	A	259	MET	Peptide
1	A	361	ARG	Peptide

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	20898	0	21075	346	0
2	A	31	0	12	1	0
3	A	1	0	0	0	0
All	All	20930	0	21087	347	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.

The worst 5 of 347 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:1528:LYS:NZ	1:A:1573:ASN:OD1	1.96	0.97
1:A:1917:LEU:HD21	1:A:2810:ILE:HD13	1.48	0.93
1:A:2702:ASN:ND2	1:A:2704:GLU:OE1	2.00	0.93
1:A:2012:ASP:OD1	1:A:2034:SER:OG	1.87	0.92
1:A:721:ARG:HB3	1:A:778:ILE:HD11	1.63	0.80

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	2596/2944 (88%)	2401 (92%)	193 (7%)	2 (0%)	48 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2007	SER
1	A	160	LEU

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	2281/2529 (90%)	2166 (95%)	115 (5%)	20 46

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	983	CYS
1	A	2491	ASP
1	A	1217	LEU
1	A	2487	GLN
1	A	1810	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2360	GLN
1	A	2770	HIS
1	A	2446	GLN
1	A	2624	GLN
1	A	2925	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AGS	A	3001	3	26,33,33	0.81	1 (3%)	26,52,52	1.16	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGS	A	3001	3	-	10/17/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	AGS	PG-S1G	2.09	1.95	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3001	AGS	PA-O3A-PB	-4.13	118.65	132.83
2	A	3001	AGS	C5-C6-N6	2.22	123.73	120.35

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

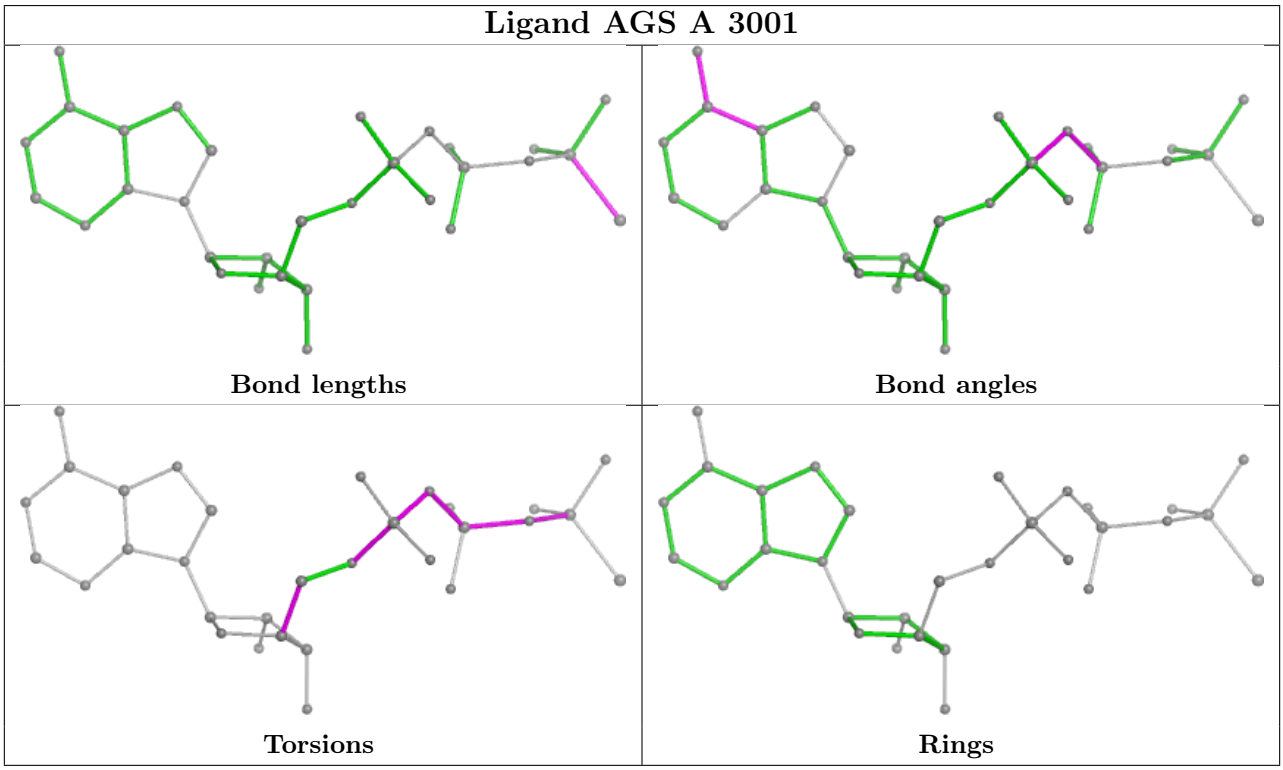
Mol	Chain	Res	Type	Atoms
2	A	3001	AGS	PB-O3B-PG-O2G
2	A	3001	AGS	PB-O3B-PG-O3G
2	A	3001	AGS	C5'-O5'-PA-O1A
2	A	3001	AGS	C5'-O5'-PA-O3A
2	A	3001	AGS	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	AGS	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

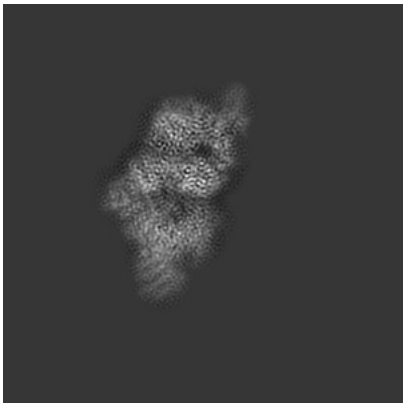
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10232. These allow visual inspection of the internal detail of the map and identification of artifacts.

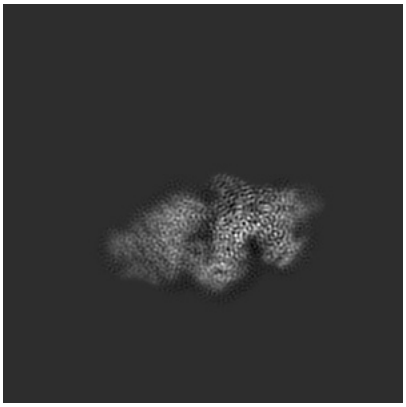
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

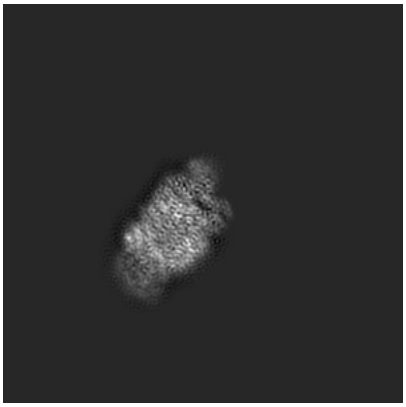
6.1.1 Primary map



X



Y



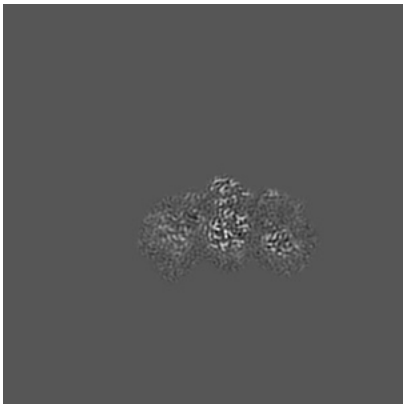
Z

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

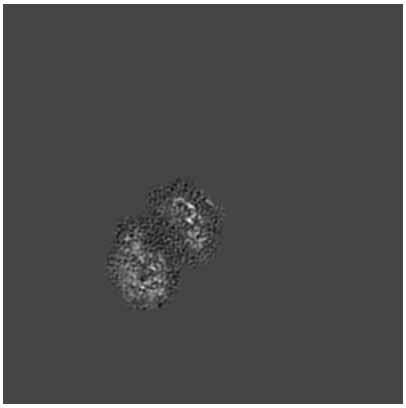
6.2 Central slices

6.2.1 Primary map

X Index: 176



Y Index: 176

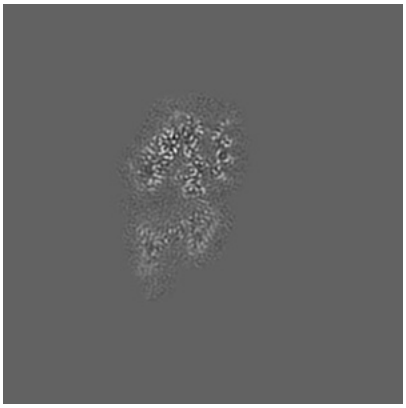


Z Index: 176

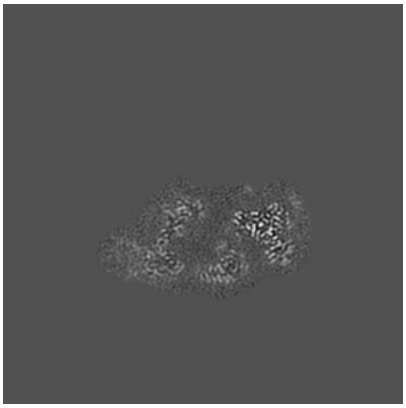
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

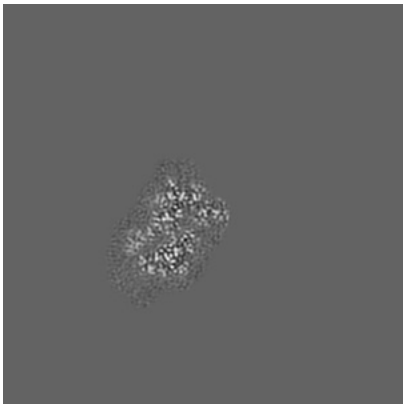
6.3.1 Primary map



X Index: 154



Y Index: 147

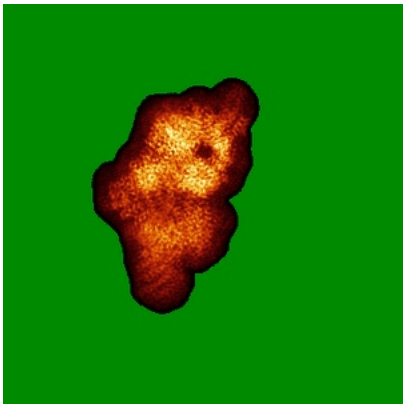


Z Index: 205

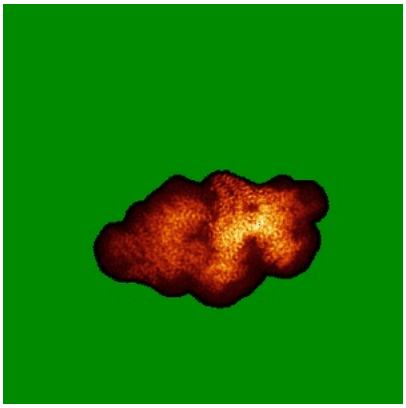
The images above show the largest variance slices of the map in three orthogonal directions.

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

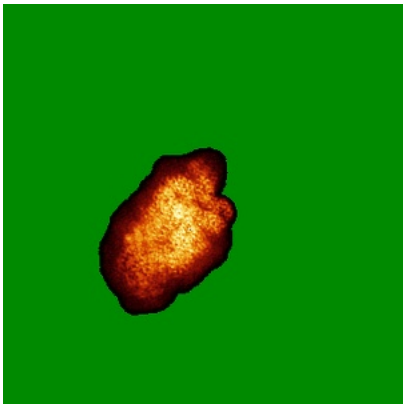
6.4.1 Primary map



X



Y



Z

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 0.0126. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

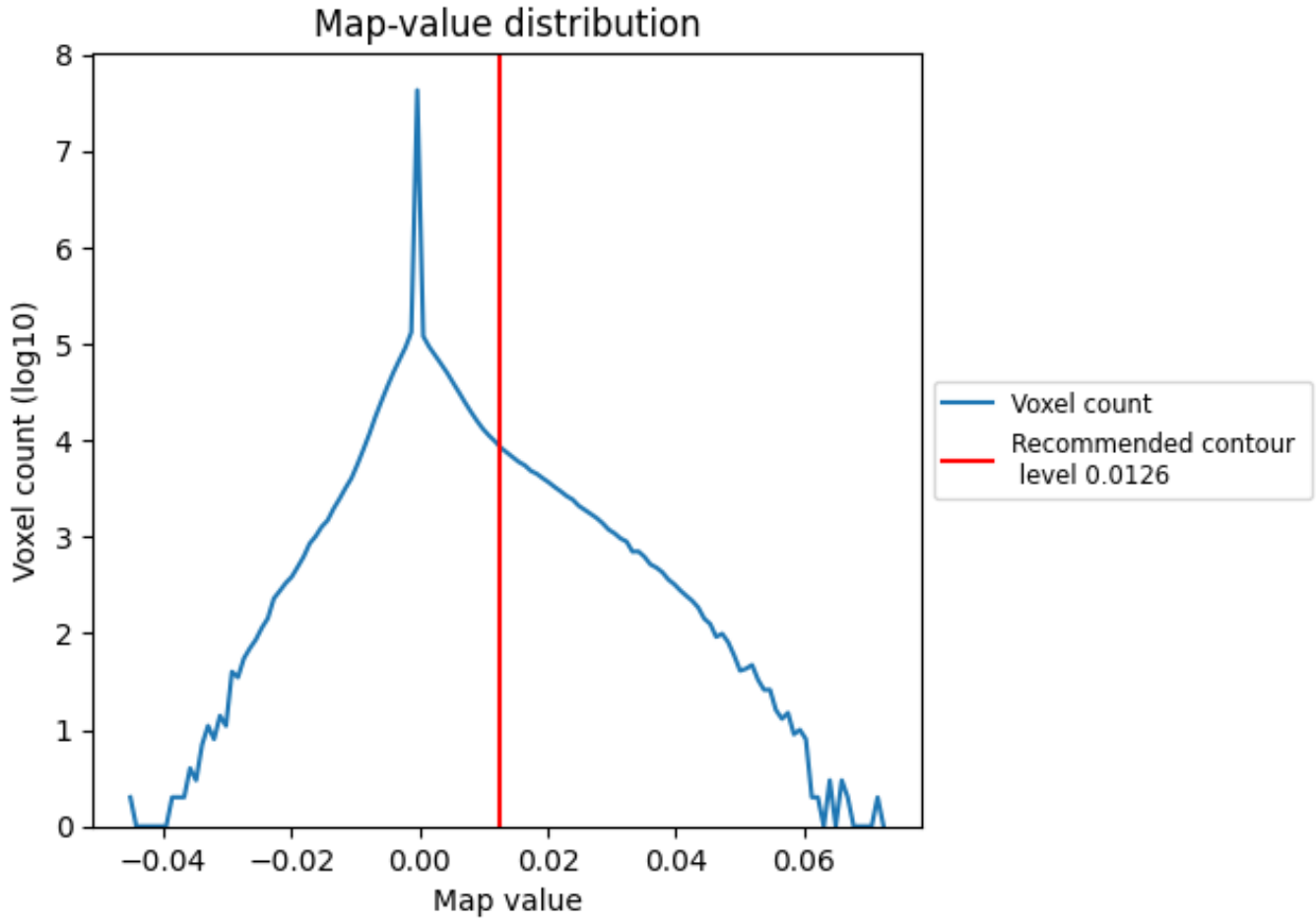
6.6 Mask visualisation (i)

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

7 Map analysis

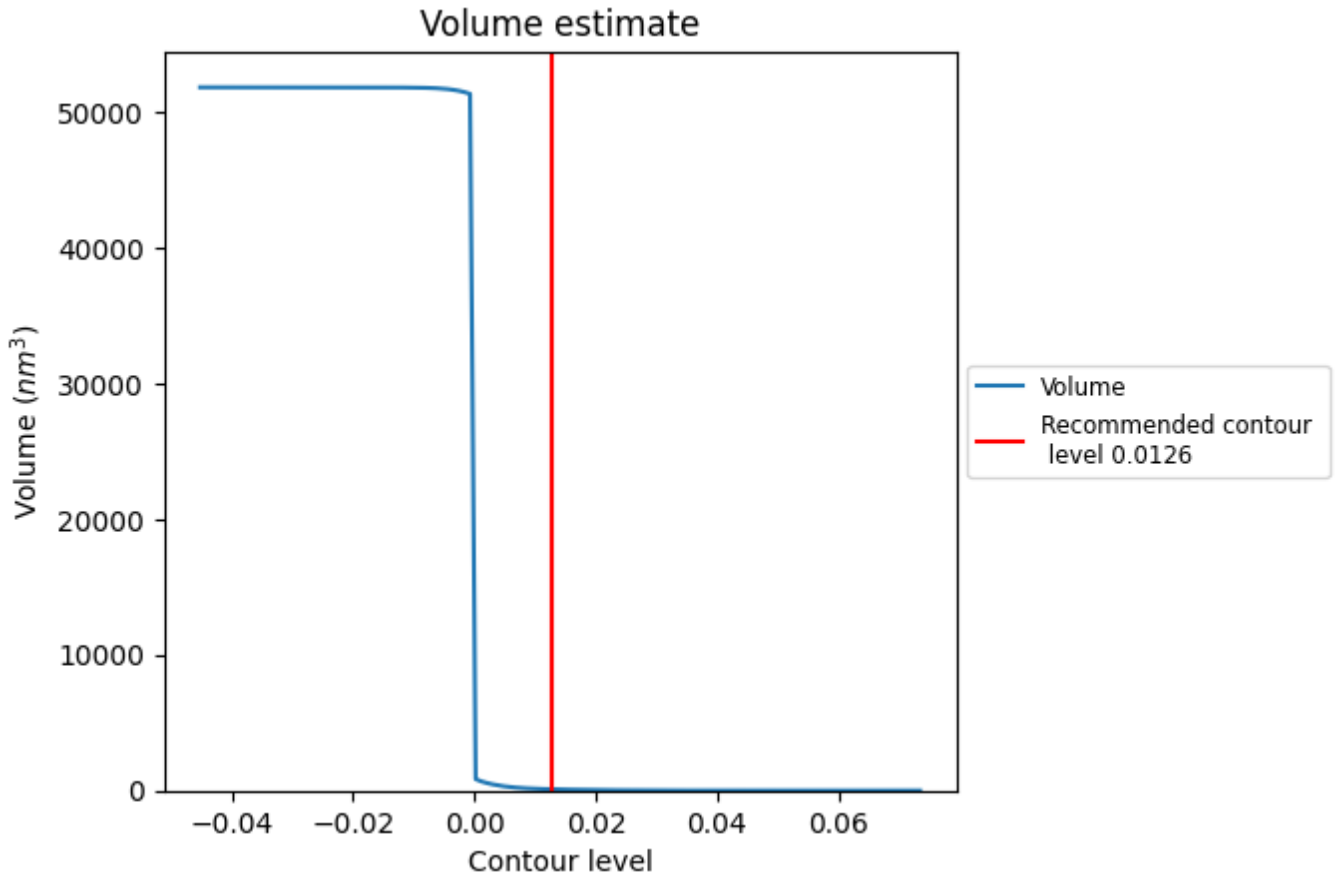
This section contains the results of statistical analysis of the map.

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.

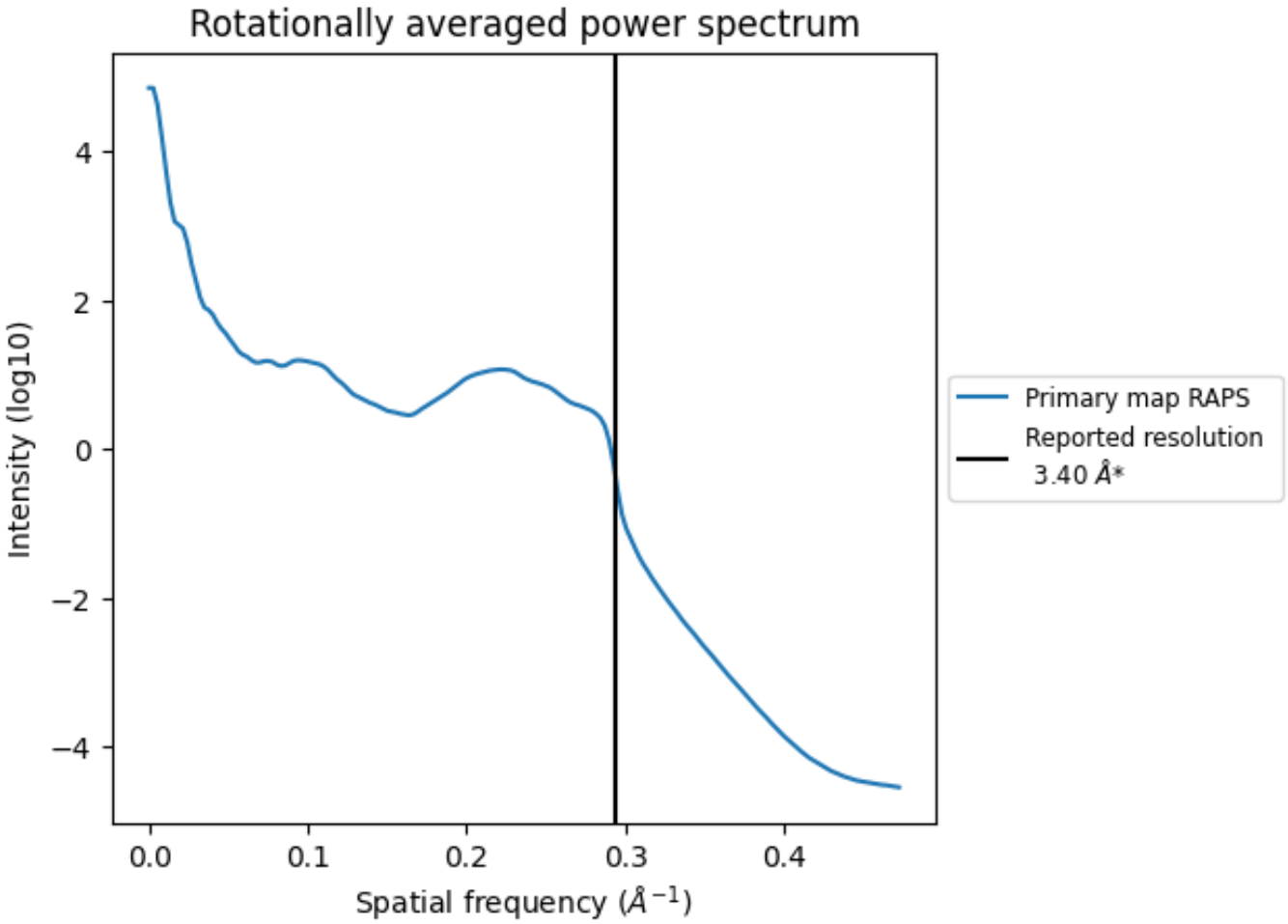
7.2 Volume estimate (i)



The volume at the recommended contour level is 98 nm^3; this corresponds to an approximate mass of 88 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)

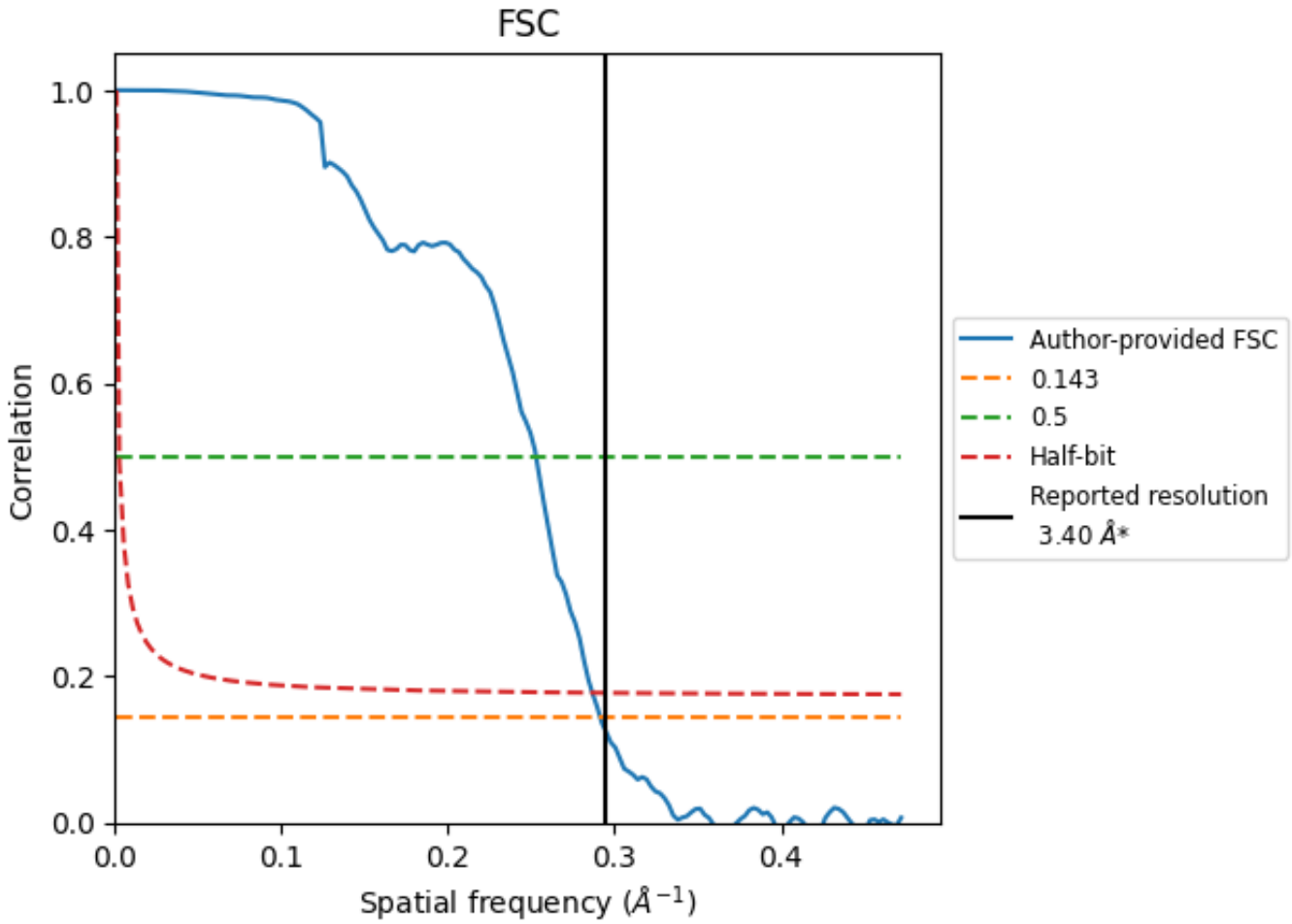


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

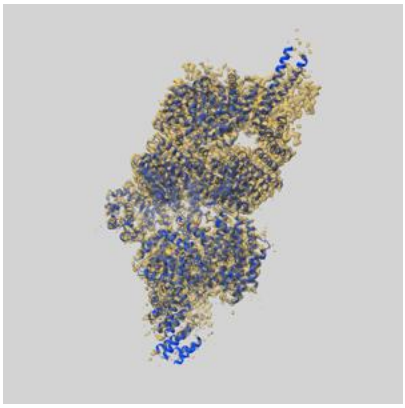
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	3.96	3.49
Unmasked-calculated*	-	-	-

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

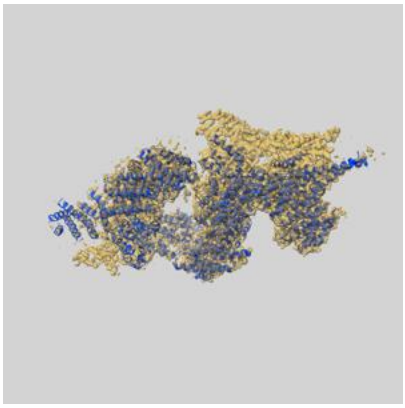
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10232 and PDB model 6SKZ. Per-residue inclusion information can be found in section 3 on page 5.

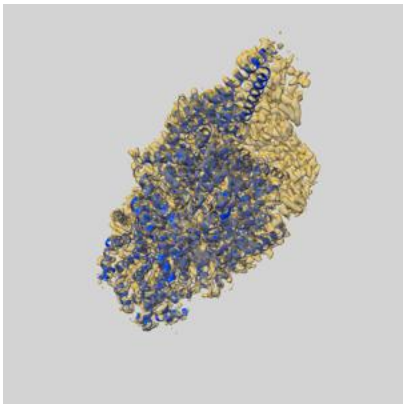
9.1 Map-model overlay



X



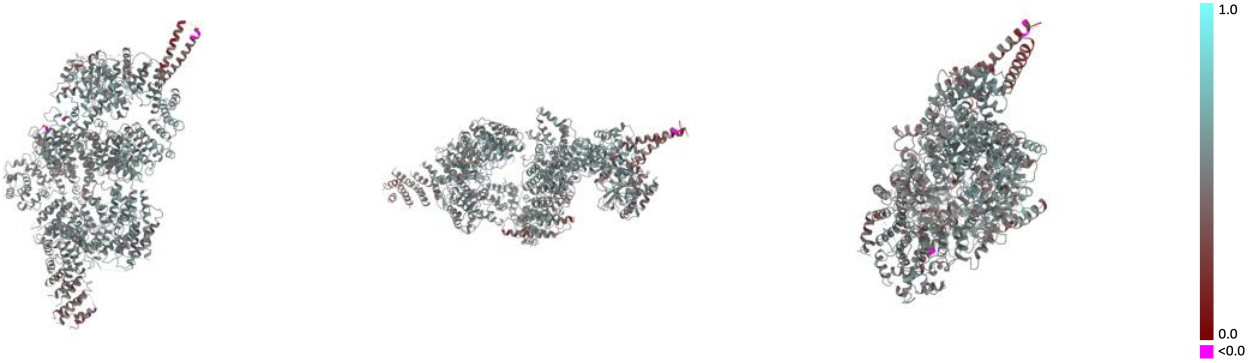
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0126 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.

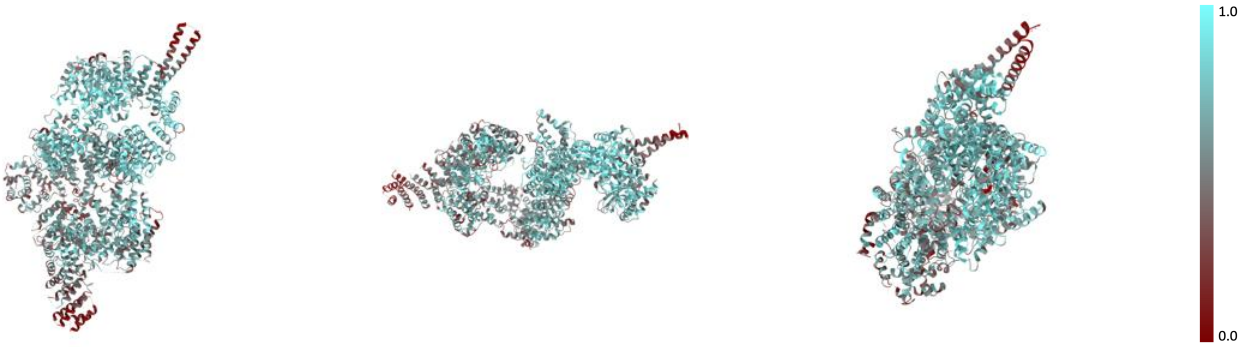
9.2 Q-score mapped to coordinate model (i)



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.

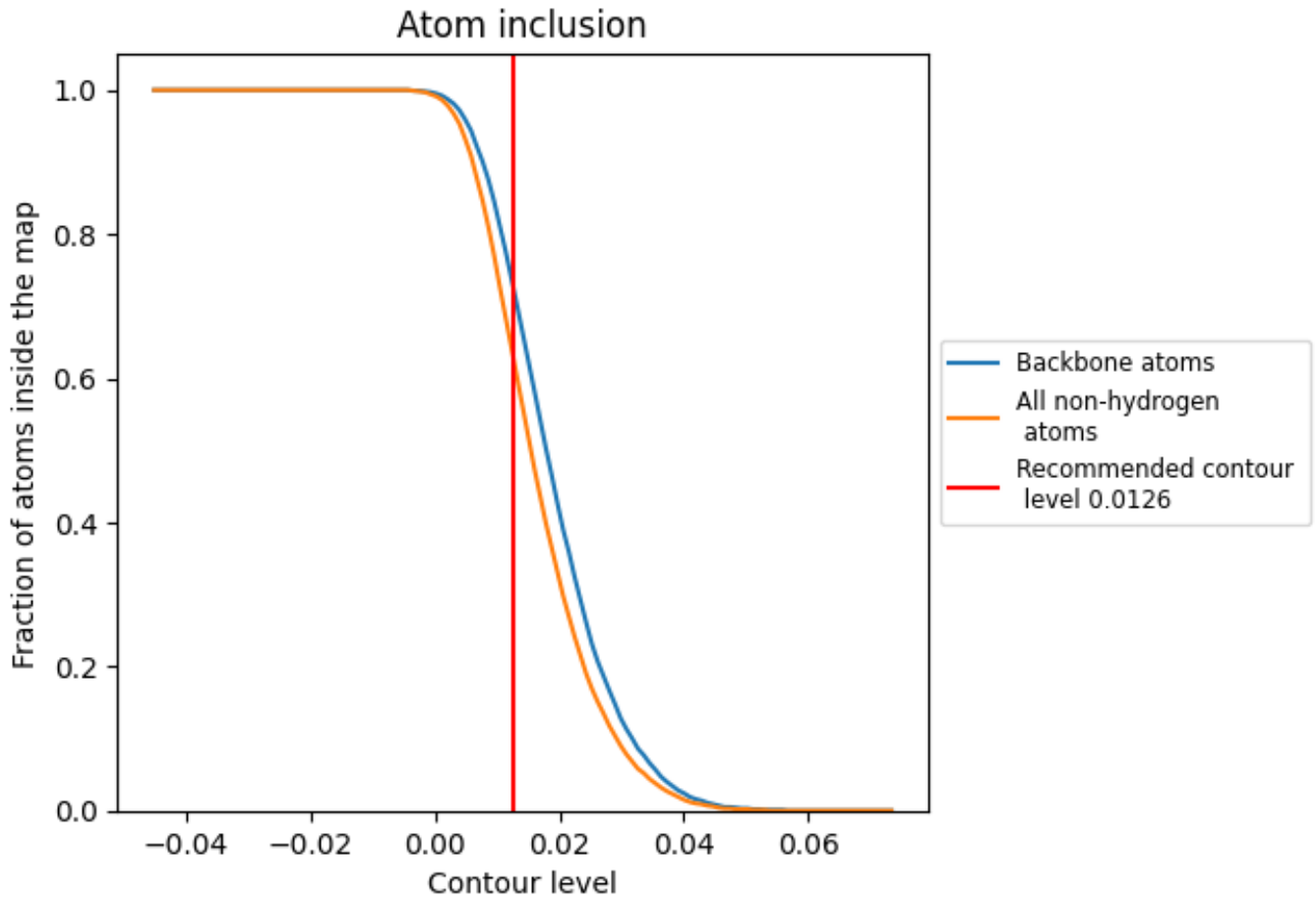
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0126).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 63% 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 (0.0126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6270	0.4990
A	0.6270	0.4990