wwPDB EM Validation Summary Report ⓘ

Jan 29, 2022 – 06:14 am GMT

PDB ID	:	7OTP
EMDB ID	:	EMD-13064
Title	:	DNA-PKcs in complex with ATPgammaS-Mg
Authors	:	Liang, S.; Thomas, S.E.; Blundell, T.L.
Deposited on	:	2021-06-10
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

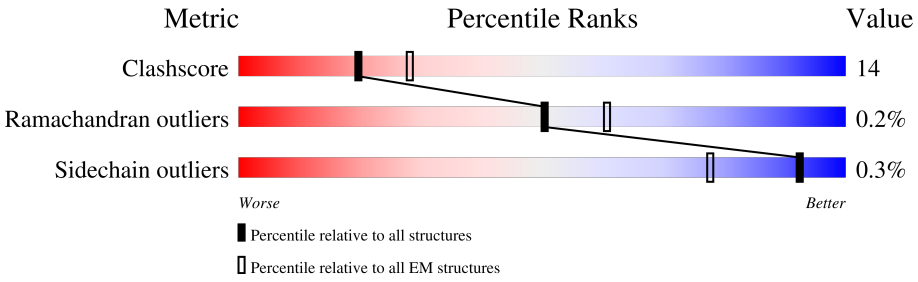
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	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	4148	5% 62% 26% 12%

2 Entry composition (i)

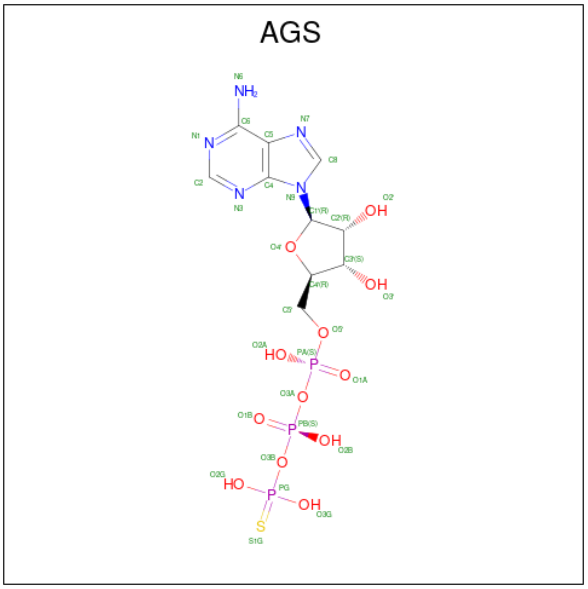
There are 3 unique types of molecules in this entry. The entry contains 29039 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA-dependent protein kinase catalytic subunit,DNA-PKcs.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3656	29006	18606	4902	5307	191	0	0

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

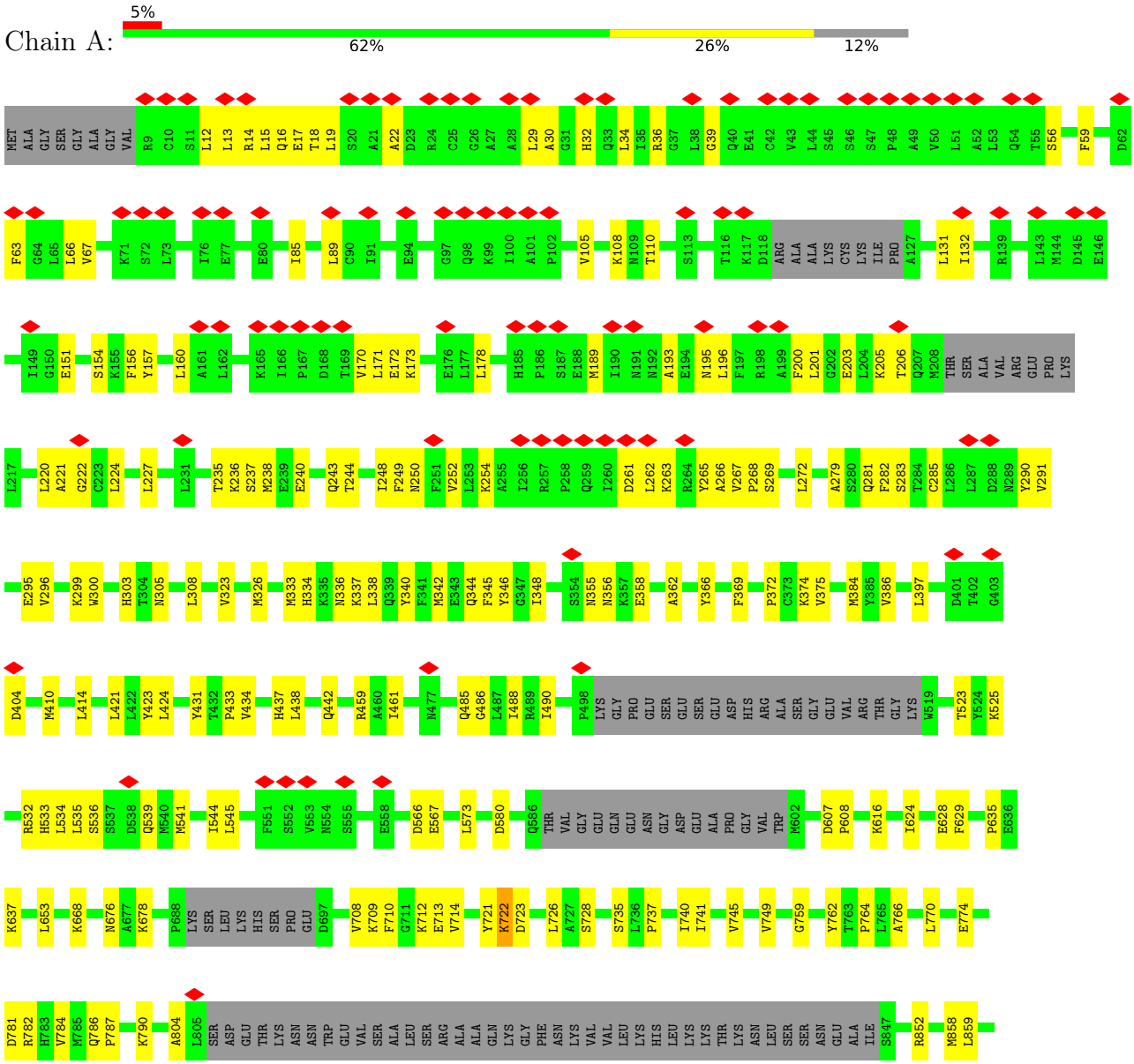
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
3	A	2	2	2	0

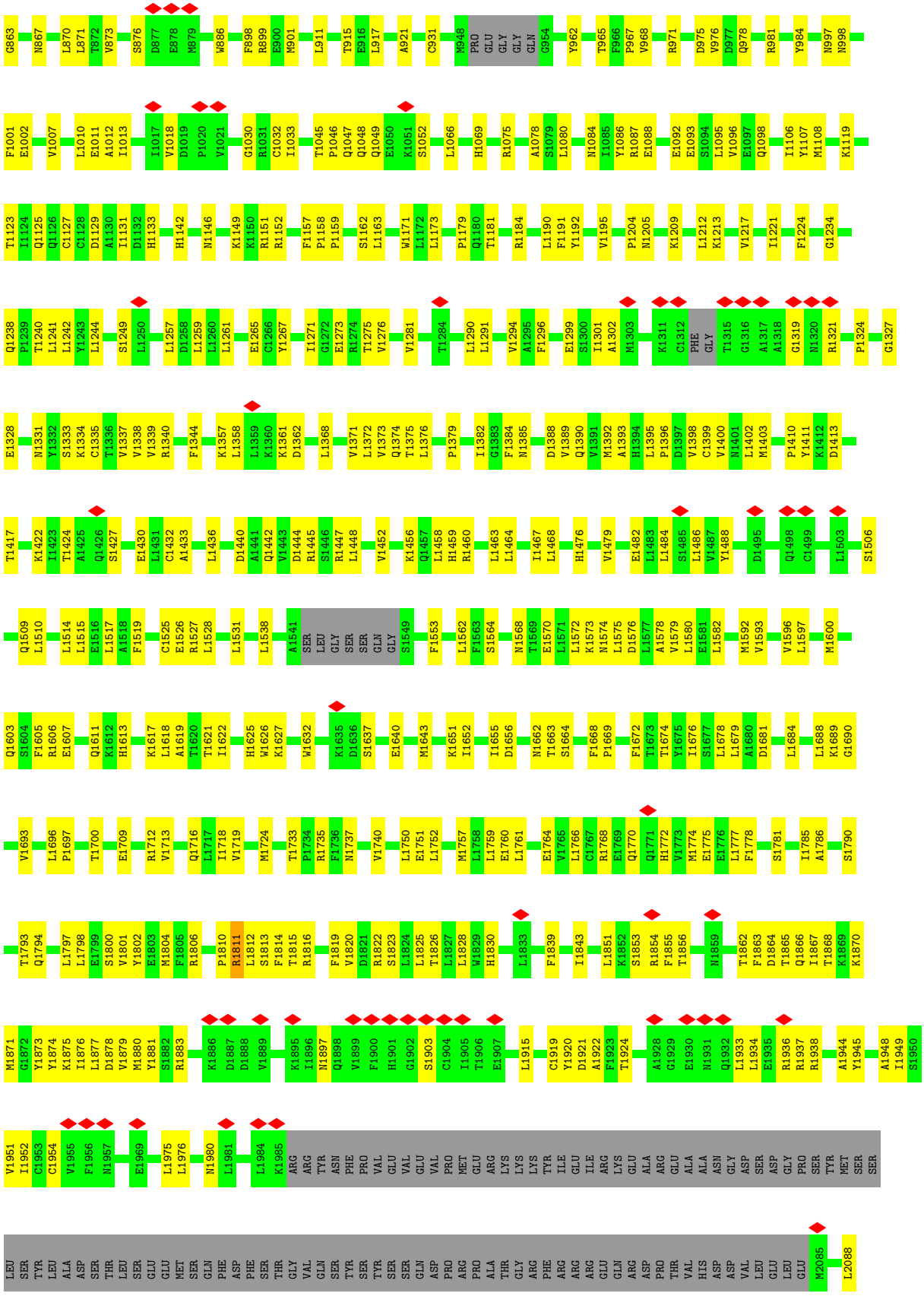
3 Residue-property plots (i)

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: DNA-dependent protein kinase catalytic subunit,DNA-PKcs

Chain A:

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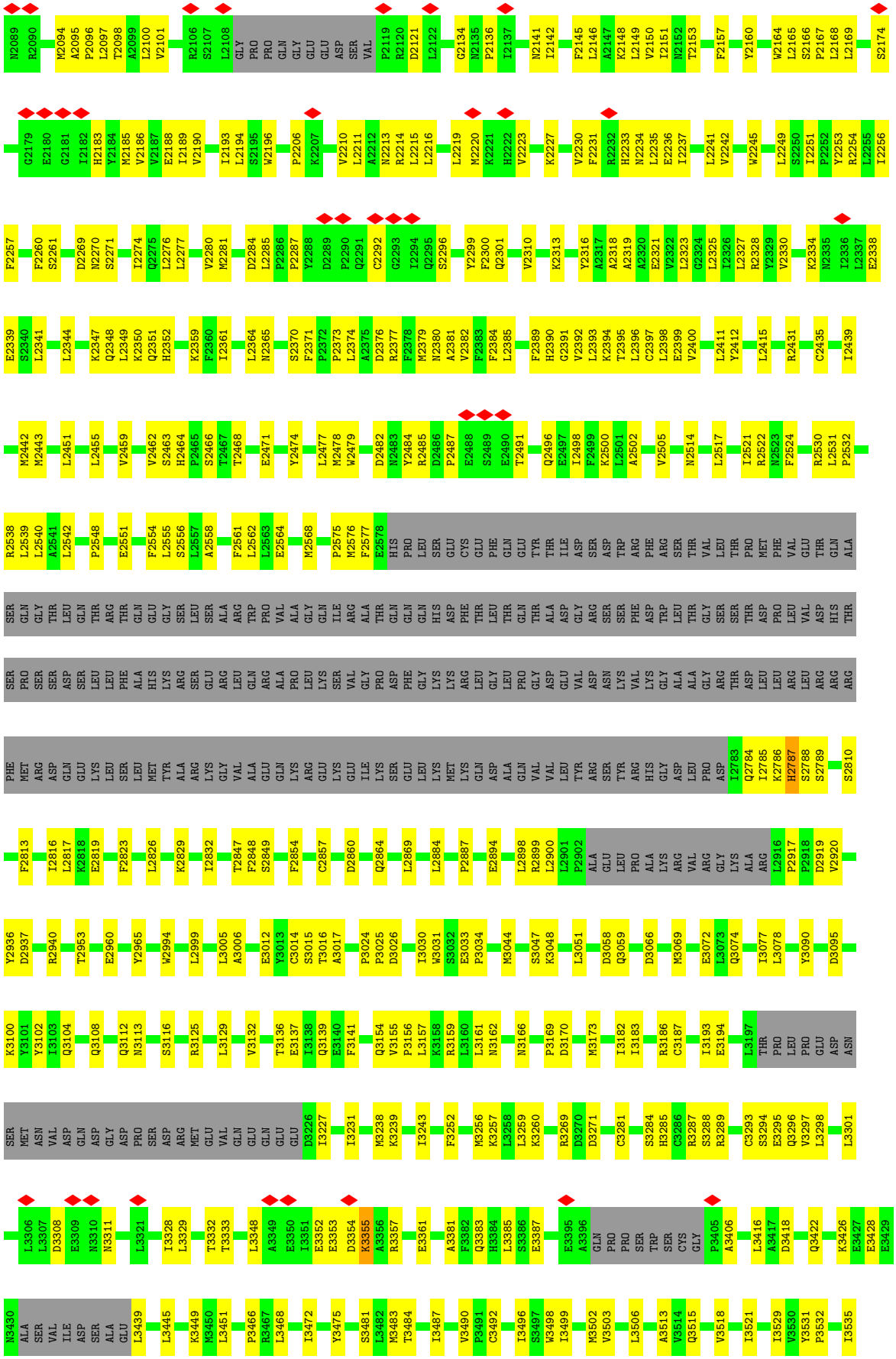
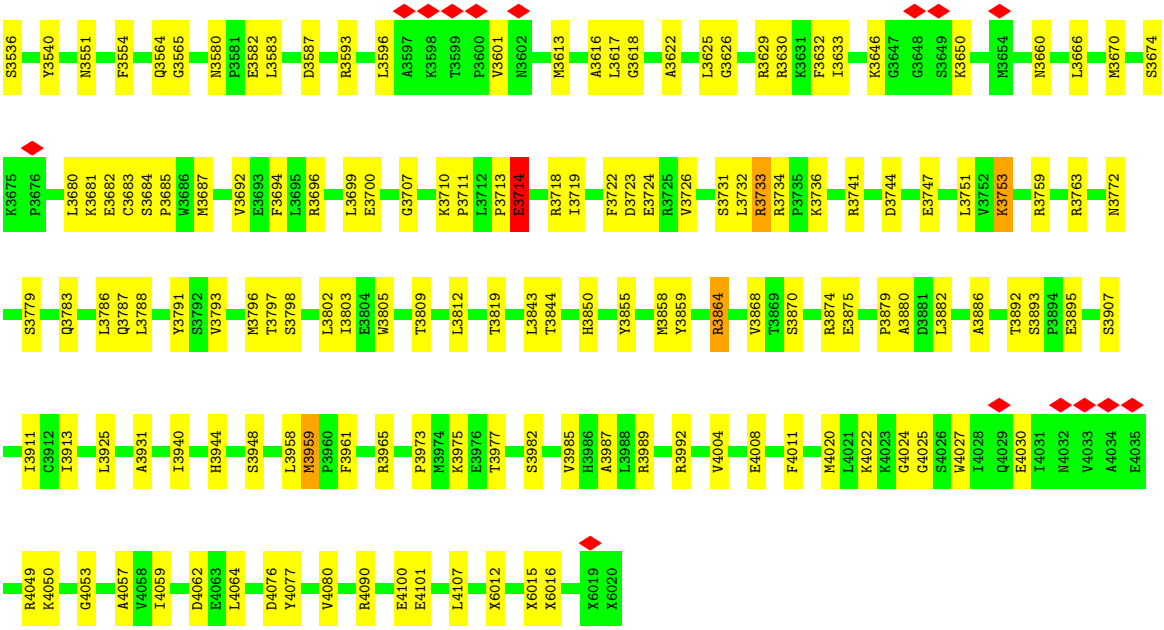
F1001 E1002 V1007 L1010 E1011 A1012 I1013 I1017 V1018 D1019 P1020 V1021 G1030 R1031 C1032 I1033 T1045 P1046 Q1047 Q1048 Q1049 E1050 K1051 S1052 L1066 H1069 R1075 A1078 S1079 L1080 N1084 I1085 Y1086 R1087 E1088 E1092 E1093 S1094 L1095 V1096 E1097 Q1098 I1106 Y1107 M1108 K1119
T1123 I1124 Q1125 Q1126 C1127 C1128 D1129 A1130 I1131 D1132 H1133 H1142 N1146 K1149 K1150 R1151 R1152 F1157 P1158 P1159 S1162 L1163 W1171 L1172 L1173 P1179 Q1180 T1181 R1184 L1190 F1191 Y1192 V1195 P1204 N1205 K1209 L1212 K1213 V1217 I1221 F1224 G1234
Q1238 P1239 T1240 L1241 L1242 Y1243 L1244 S1249 L1250 L1257 D1258 L1259 L1260 L1261 E1265 C1266 Y1267 I1271 C1272 E1273 R1274 T1275 V1276 V1281 T1284 L1290 L1291 V1294 A1295 F1296 E1299 S1300 I1301 A1302 M1303 K1311 C1312 PHE GLY T1315 G1316 A1317 A1318 G1319 N1320 R1321 P1324 G1327
E1328 N1331 Y1332 S1333 K1334 C1335 T1336 V1337 V1338 V1339 R1340 F1344 K1357 L1358 L1359 K1360 K1361 D1362 L1368 V1371 L1372 V1373 Q1374 T1375 L1376 P1379 I1382 G1383 F1384 N1385 D1388 V1389 Q1390 V1391 M1392 A1393 H1394 L1395 P1396 D1397 V1398 C1399 V1400 N1401 L1402 M1403 P1410 Y1411 K1412 D1413
T1417 K1422 I1423 T1424 A1425 Q1426 S1427 E1430 L1431 C1432 A1433 L1436 D1440 A1441 Q1442 V1443 D1444 R1445 S1446 R1447 L1448 V1452 K1456 Q1457 L1458 H1459 R1460 L1463 L1464 I1467 L1468 H1476 V1479 E1482 L1483 L1484 S1485 L1486 V1487 Y1488 D1495 Q1498 C1499 L1503 S1506
Q1509 L1510 L1514 L1515 E1516 L1517 A1518 F1519 C1525 E1526 R1527 L1528 L1531 L1538 A1541 SER LEU GLY SER SER GLN GLY S1549 F1553 L1562 F1563 S1564 N1568 T1569 E1570 L1571 L1572 K1573 N1574 L1575 D1576 L1577 A1578 V1579 L1580 E1581 L1582 M1592 V1593 V1596 L1597 M1600
Q1603 S1604 F1605 R1606 E1607 Q1611 K1612 H1613 K1617 L1618 A1619 T1620 T1621 I1622 H1625 W1626 K1627 W1632 K1635 D1636 S1637 E1640 M1643 K1651 I1652 I1655 D1656 N1662 T1663 S1664 F1668 P1669 F1672 T1673 T1674 Y1675 S1677 L1678 L1679 A1680 D1681 L1684 L1688 K1689 G1690
V1693 L1696 P1697 T1700 E1709 R1712 V1713 Q1716 L1717 I1718 V1719 M1724 T1733 P1734 R1735 F1736 N1737 V1740 L1750 E1751 L1752 M1757 L1758 L1759 E1760 L1761 E1764 V1765 L1766 C1767 R1768 E1769 Q1770 Q1771 H1772 V1773 M1774 E1775 E1776 L1777 F1778 S1781 I1785 A1786 S1790
T1793 Q1794 L1797 L1798 E1799 S1800 V1801 Y1802 E1803 M1804 F1805 R1806 P1810 R1811 L1812 S1813 F1814 T1815 R1816 F1819 V1820 D1821 R1822 S1823 L1824 L1825 T1826 L1827 L1828 W1829 H1830 L1833 F1839 I1843 L1851 K1852 S1853 R1854 F1855 T1856 N1859 T1862 F1863 D1864 T1865 Q1866 I1867 T1868 K1869 K1870
M1871 G1872 Y1873 Y1874 K1875 I1876 L1877 D1878 V1879 M1880 Y1881 S1882 R1883 K1886 D1887 D1888 V1889 K1895 I1896 N1897 Q1898 V1899 F1900 H1901 G1902 S1903 C1904 I1905 T1906 E1907 L1915 C1919 Y1920 D1921 A1922 F1923 T1924 A1928 G1929 E1930 N1931 Q1932 L1933 L1934 E1935 R1936 R1937 R1938 A1944 Y1945 A1948 I1949 S1950
V1951 I1952 C1953 C1954 V1955 F1956 N1957 E1969 L1975 L1976 N1980 L1981 L1984 K1985 ARG ARG TYR ASN PHE PRO VAL GLU VAL GLU VAL PRO MET GLU ARG LYS LYS TYR ILE GLU ILE ARG LYS GLU ALA ARG GLU ALA ALA ASN GLY ASP SER ASP GLY PRO SER TYR MET SER SER
LEU SER TYR LEU ALA ASP SER THR LEU SER GLU GLU MET SER GLN PHE ASP PHE SER THR GLY VAL GLN SER TYR SER TYR SER SER GLN ASP PRO ARG PRO ALA THR GLY ARG PHE ARG ARG ARG GLU GLN ARG ASP PRO THR VAL HIS ASP ASP VAL LEU GLU LEU GLU M2086 L2088

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K3675 P3676 L3680 K3681 E3682 C3683 S3684 P3685 W3686 M3687 V3692 E3693 F3694 L3695 R3696 L3699 E3700 G3707 K3710 P3711 L3712 P3713 E3714 R3718 I3719 F3722 D3723 E3724 R3725 V3726 S3731 L3732 R3733 R3734 P3735 K3736 R3741 D3744 E3747 L3751 V3752 K3753 R3759 R3763 N3772
S3779 Q3783 L3786 Q3787 L3788 Y3791 S3792 V3793 M3796 T3797 S3798 L3802 I3803 E3804 W3805 T3809 L3812 T3819 L3843 T3844 H3850 Y3855 M3858 Y3859 R3864 V3868 T3869 S3870 R3874 E3875 P3879 A3880 D3881 L3882 A3886 T3892 S3893 P3894 E3895 S3907
I3911 C3912 I3913 L3925 A3931 I3940 H3944 S3948 L3958 M3959 P3960 F3961 R3965 P3973 M3974 K3975 E3976 T3977 S3982 V3985 H3986 A3987 L3988 R3989 R3992 V4004 E4008 F4011 M4020 L4021 K4022 K4023 G4024 G4025 S4026 W4027 I4028 Q4029 E4030 I4031 N4032 V4033 A4034 E4035
R4049 K4050 G4053 A4057 V4058 I4059 D4062 E4063 L4064 D4076 Y4077 V4080 R4090 E4100 E4101 L4107 X6012 X6015 X6016 X6019 X6020

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63313	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 ($e^-/Å^2$)	46.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.339	Depositor
Minimum map value	-1.286	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.056	Depositor
Recommended contour level	0.23	Depositor
Map size (Å)	339.04, 339.04, 339.04	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.36	0/29498	0.51	0/39889

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	29006	0	29184	761	0
2	A	31	0	11	3	0
3	A	2	0	0	0	0
All	All	29039	0	29195	764	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 14.

The worst 5 of 764 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)
2:A:6101:AGS:C4'	2:A:6101:AGS:O4'	1.63	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:MET:HG3	1:A:193:ALA:HB2	1.53	0.90
1:A:3618:GLY:H	1:A:3633:ILE:HD12	1.41	0.85
1:A:3670:MET:O	1:A:3674:SER:HB3	1.76	0.84
1:A:1482:GLU:O	1:A:1486:LEU:HB2	1.77	0.83

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	3602/4148 (87%)	3284 (91%)	311 (9%)	7 (0%)	47 78

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3714	GLU
1	A	3354	ASP
1	A	3406	ALA
1	A	723	ASP
1	A	2787	HIS

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	3195/3671 (87%)	3185 (100%)	10 (0%)	92 97

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3753	LYS
1	A	3864	ARG
1	A	3959	MET
1	A	3355	LYS
1	A	3696	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	GLN
1	A	1048	GLN
1	A	1083	ASN
1	A	2496	GLN
1	A	3162	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)

Of 3 ligands modelled in this entry, 2 are 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	6101	3	26,33,33	3.77	8 (30%)	26,52,52	1.62	4 (15%)

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	6101	3	-	3/17/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6101	AGS	PG-S1G	10.31	2.13	1.90
2	A	6101	AGS	O4'-C4'	8.47	1.63	1.45
2	A	6101	AGS	O4'-C1'	-7.98	1.29	1.41
2	A	6101	AGS	C3'-C4'	-7.49	1.33	1.53
2	A	6101	AGS	O2'-C2'	-3.77	1.34	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	6101	AGS	N3-C2-N1	-4.43	121.75	128.68
2	A	6101	AGS	C3'-C2'-C1'	3.49	106.24	100.98
2	A	6101	AGS	PA-O3A-PB	-3.12	122.13	132.83
2	A	6101	AGS	C2'-C3'-C4'	2.57	107.64	102.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	6101	AGS	O4'-C4'-C5'-O5'
2	A	6101	AGS	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	A	6101	AGS	PB-O3A-PA-O1A

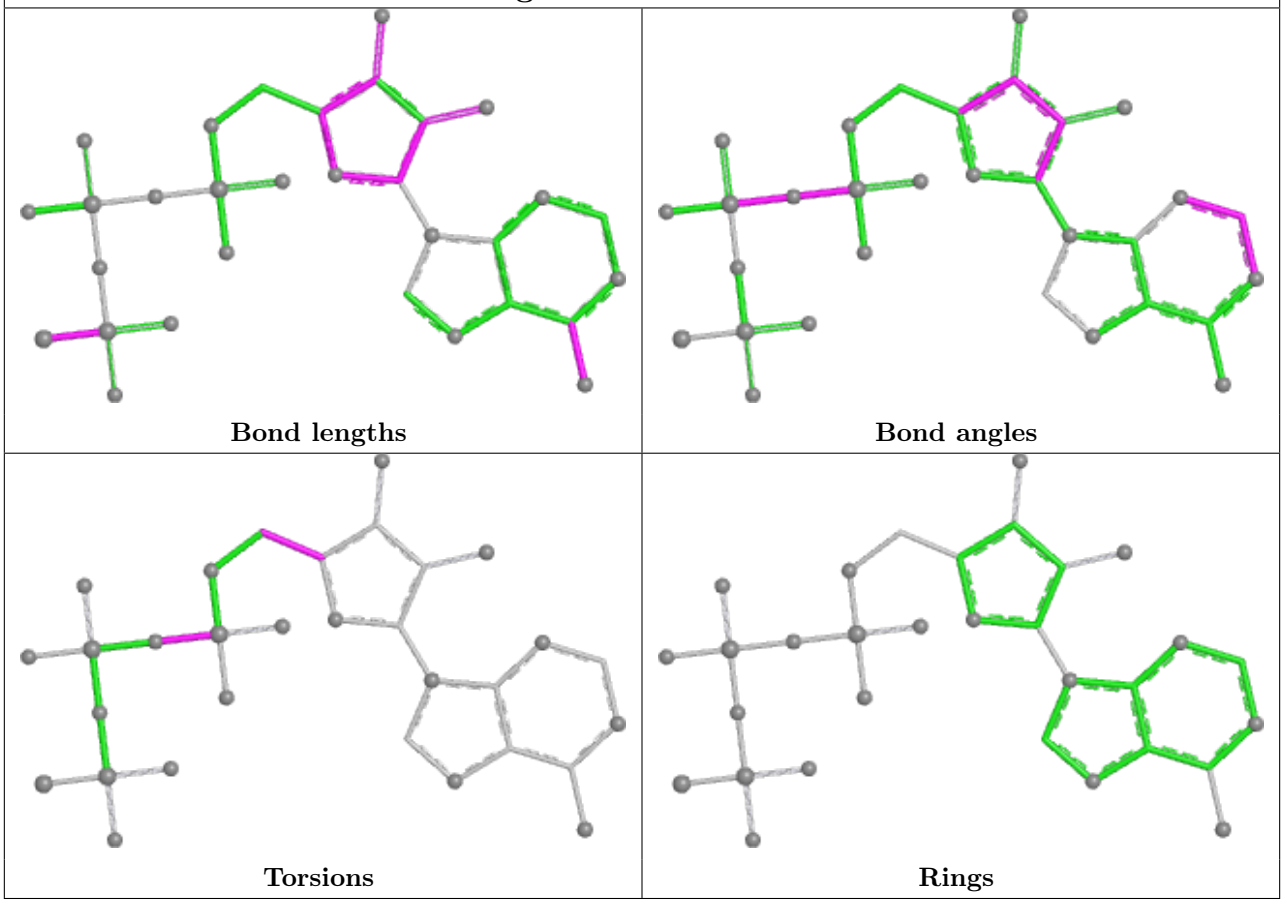
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6101	AGS	3	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.

Ligand AGS A 6101



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	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4128:MET	C	6001:UNK	N	81.75

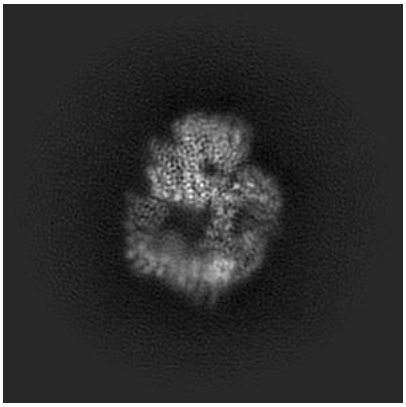
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13064. These allow visual inspection of the internal detail of the map and identification of artifacts.

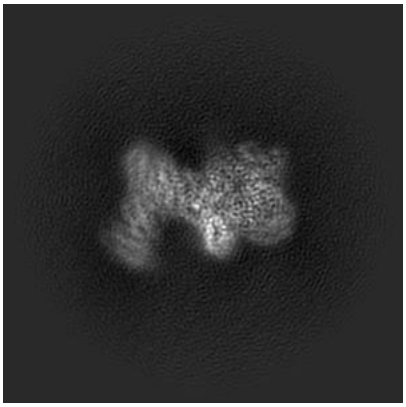
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

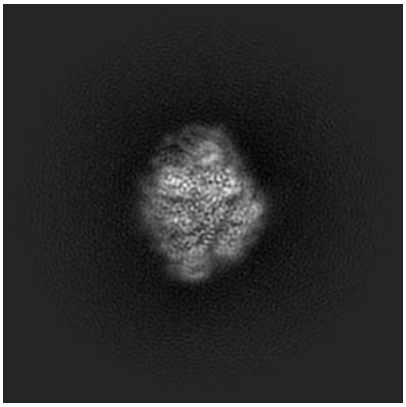
6.1.1 Primary map



X



Y

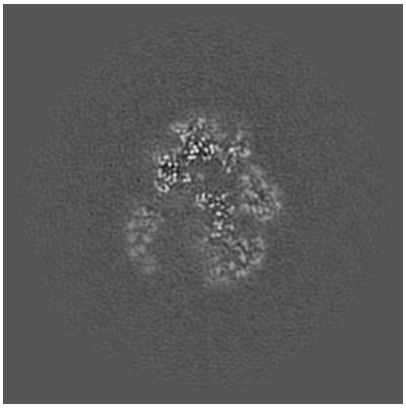


Z

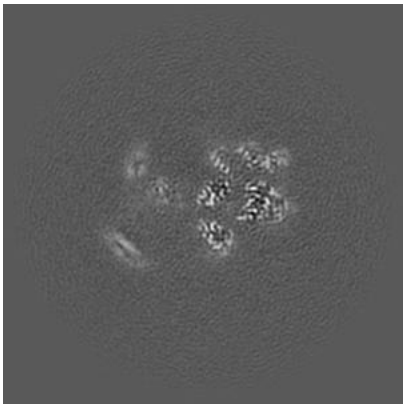
The images above show the map projected in three orthogonal directions.

6.2 Central slices

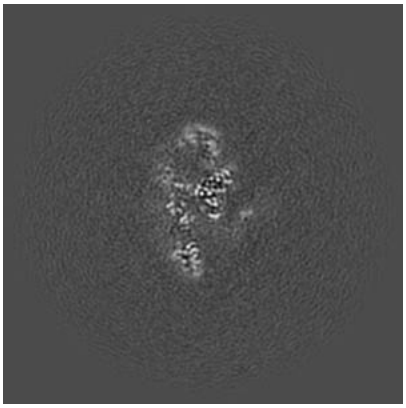
6.2.1 Primary map



X Index: 130



Y Index: 130

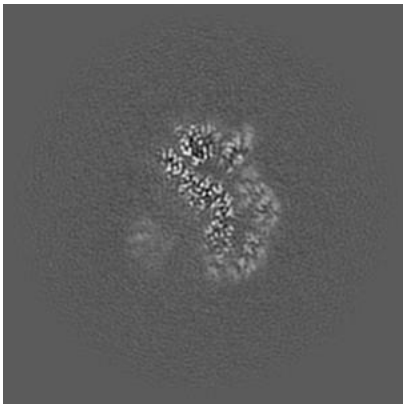


Z Index: 130

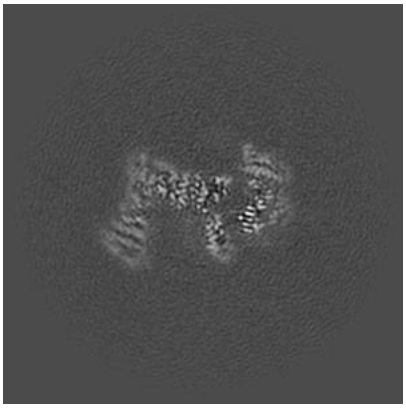
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

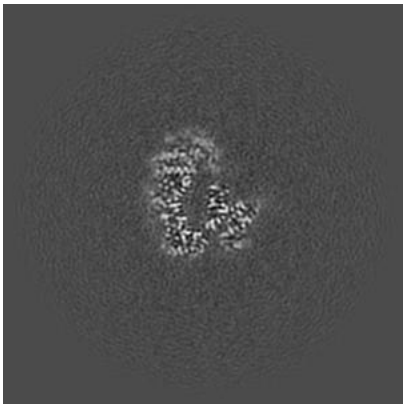
6.3.1 Primary map



X Index: 135



Y Index: 138



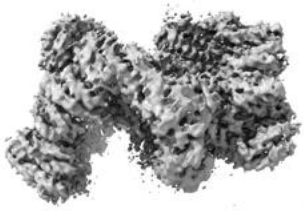
Z Index: 141

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

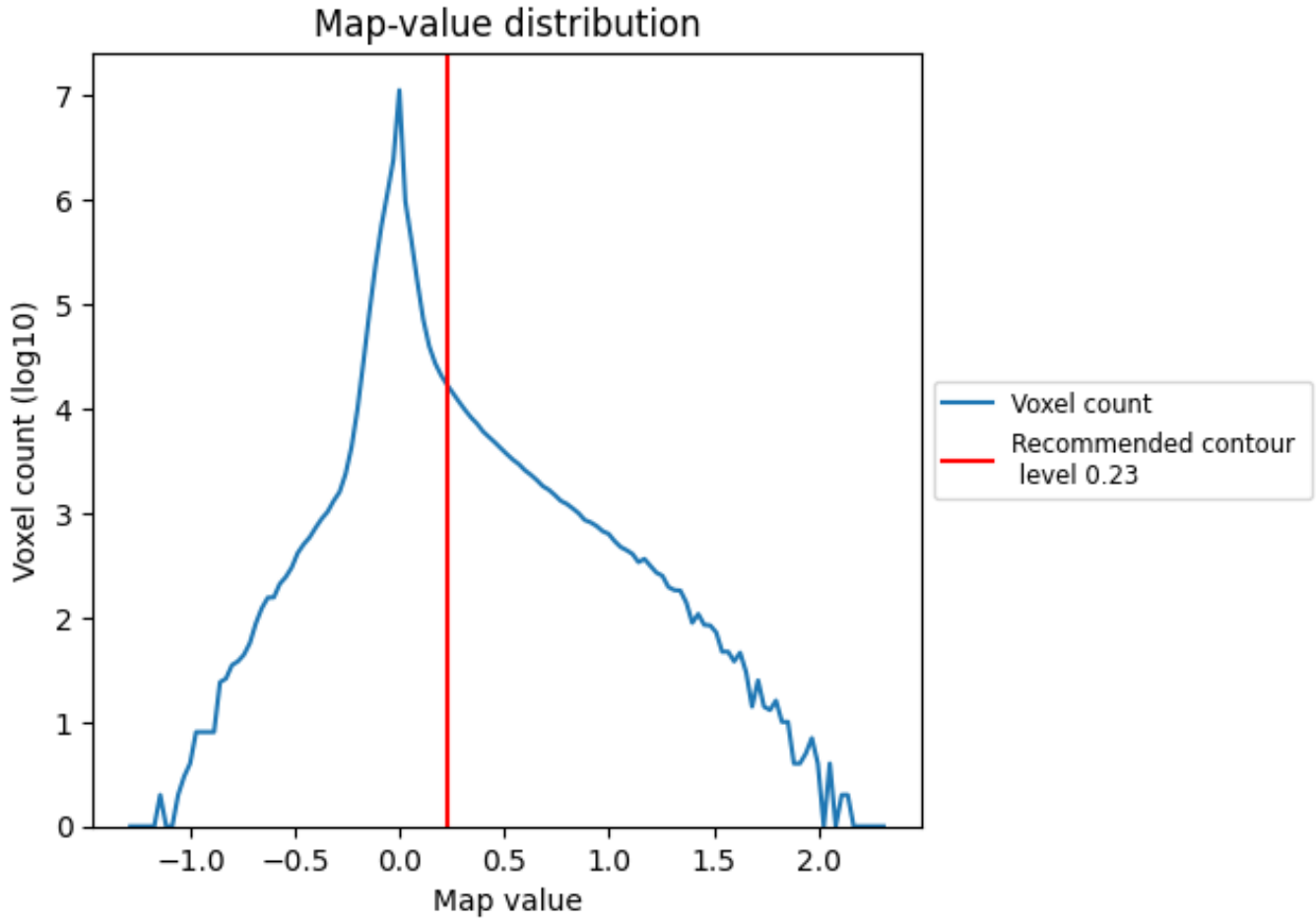
6.5 Mask visualisation (i)

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

7 Map analysis

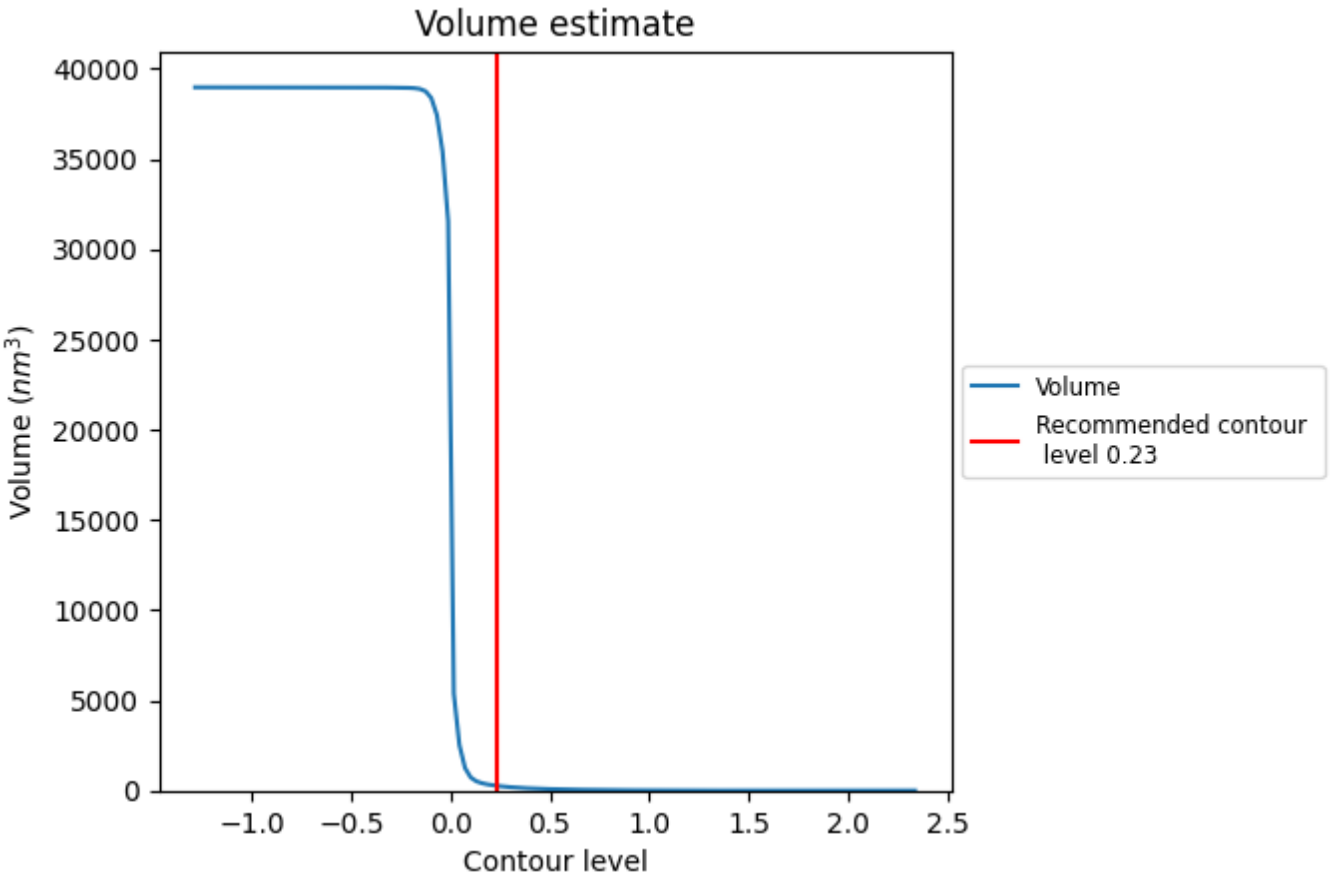
This section contains the results of statistical analysis of the map.

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.

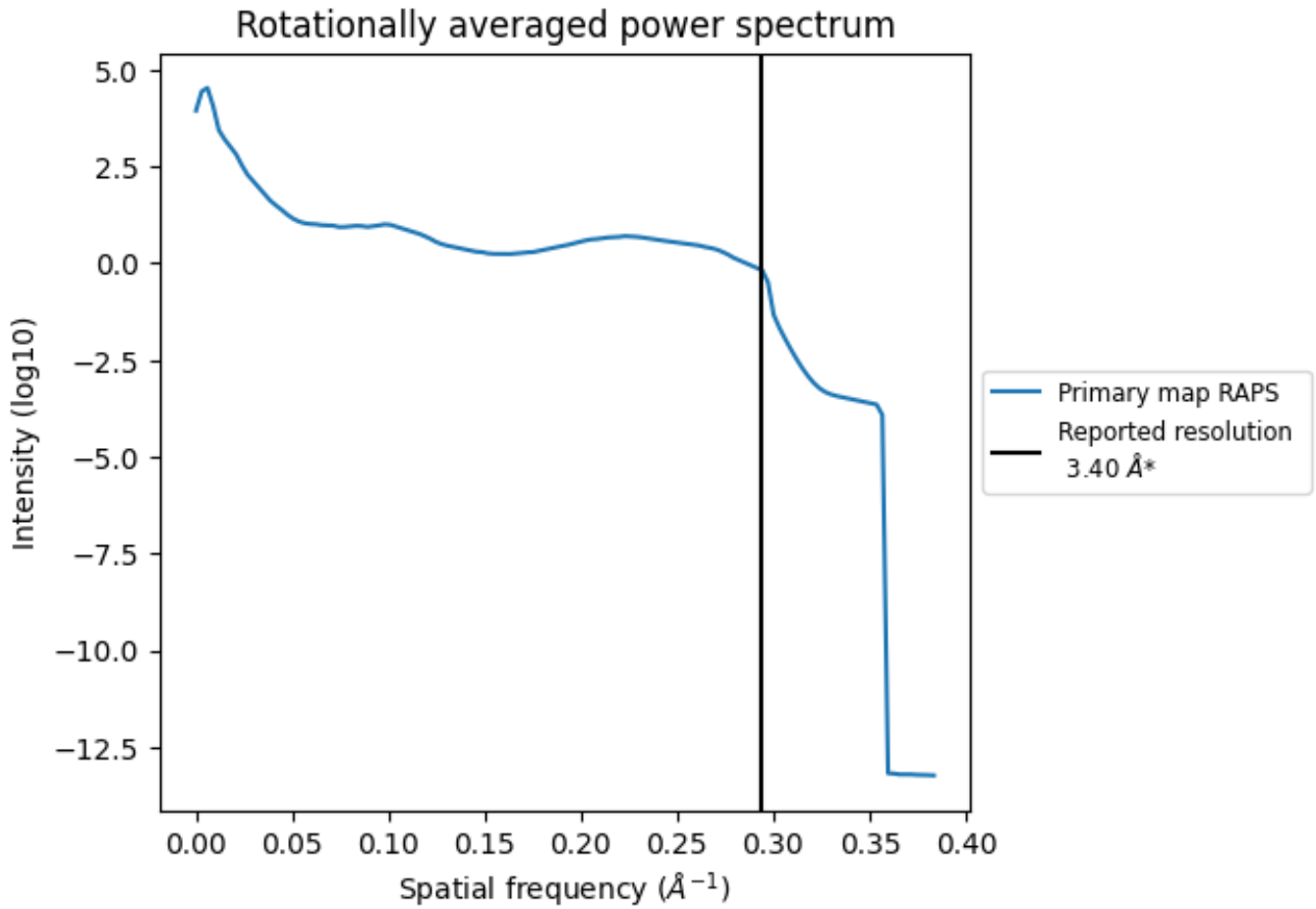
7.2 Volume estimate (i)



The volume at the recommended contour level is 269 nm^3; this corresponds to an approximate mass of 243 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 $Å^{-1}$

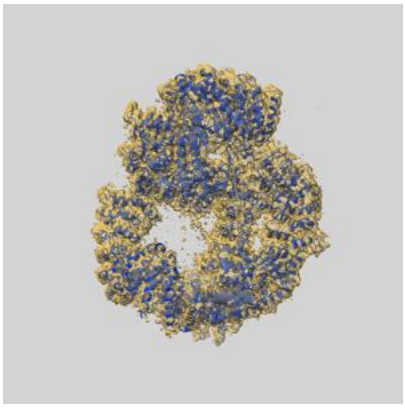
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

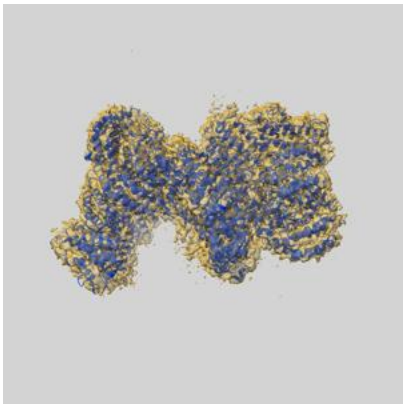
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13064 and PDB model 7OTP. Per-residue inclusion information can be found in section 3 on page 4.

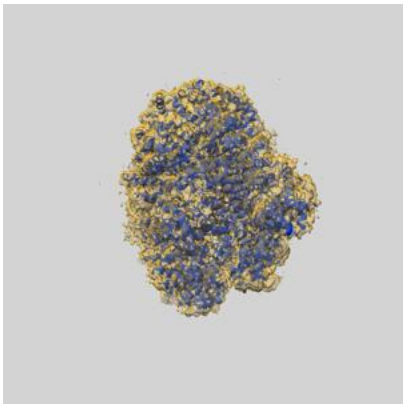
9.1 Map-model overlay



X



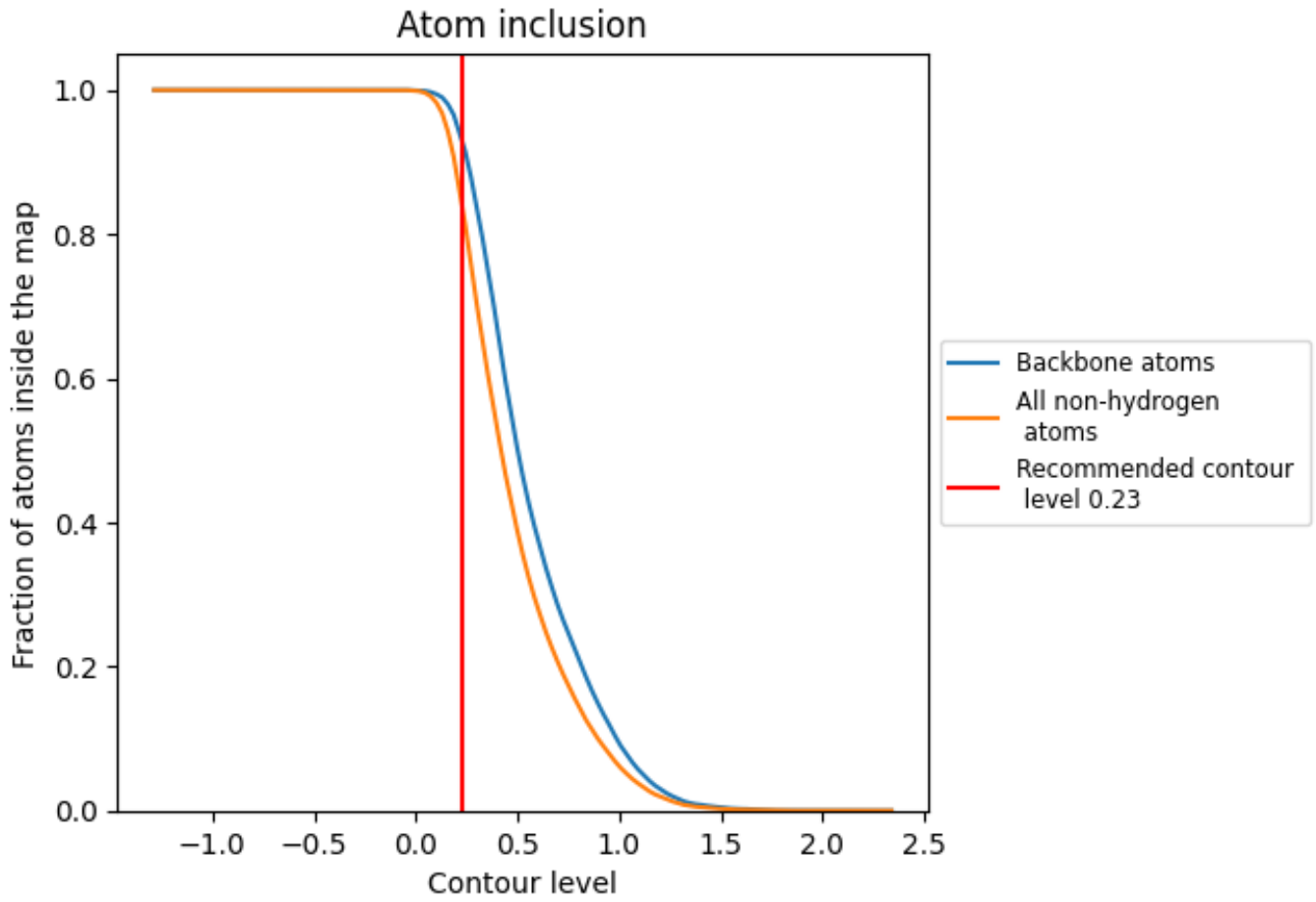
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.23 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 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.