wwPDB EM Validation Summary Report

Sep 23, 2026 – 07:23 am BST

PDB ID	:	9TUB / pdb_00009tub
EMDB ID	:	EMD-56255
Title	:	CryoEM structure of DruE:ATPgammaS:DNA from Druantia type III - dimer 4
Authors	:	Grass, L.M.; Himpich, S.; Hilal, T.; Loll, B.; Wahl, M.C.
Deposited on	:	2026-01-08
Resolution	:	3.80 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 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:

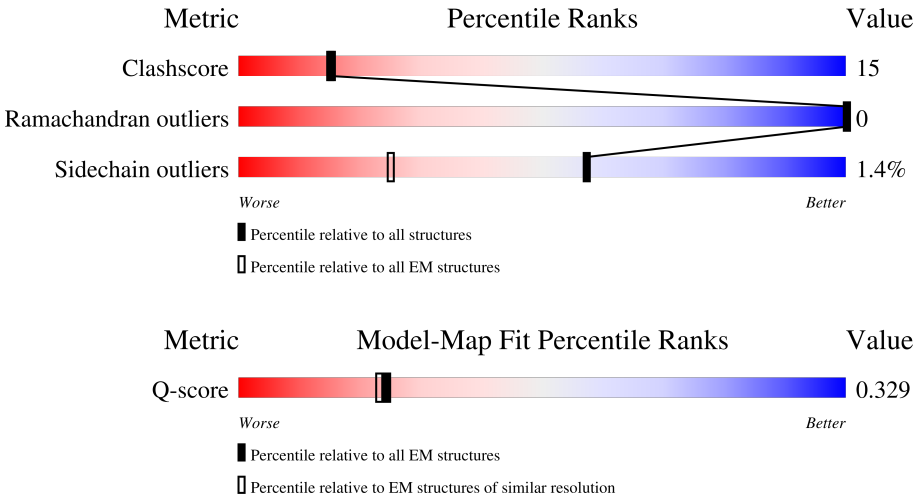
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 (i)

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	G	30	33% 30% 10% 60%
1	i	30	17% 83%
2	Y	2108	5% 60% 27% 13%
2	y	2108	5% 63% 34%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	30	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 31776 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 DNA chain called DNA (5'-D(P*GP*AP*AP*GP*AP*GP*AP*CP*TP*AP*TP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
1	i	5	Total	C	N	O	P	0	0
			102	49	20	28	5		
1	G	12	Total	C	N	O	P	0	0
			249	118	50	69	12		

- Molecule 2 is a protein called DEAD/DEAH box helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	y	2048	Total	C	N	O	S	0	0
			16264	10264	2906	3022	72		
2	Y	1843	Total	C	N	O	S	0	0
			14619	9219	2618	2715	67		

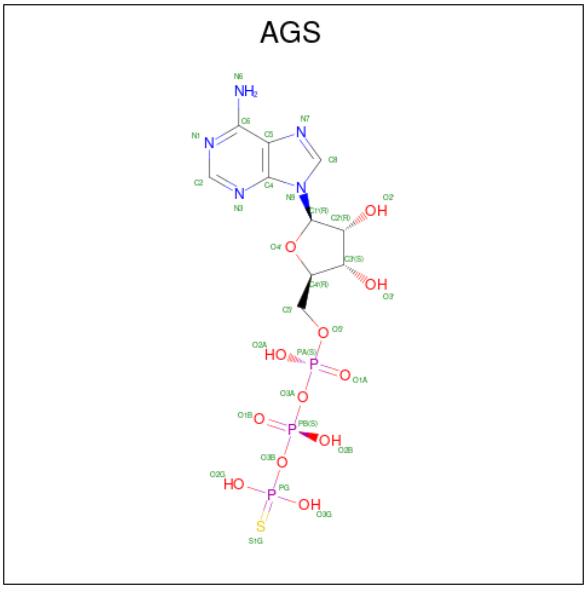
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	-3	GLY	-	expression tag	UNP A0A4P8BDA5
y	-2	ALA	-	expression tag	UNP A0A4P8BDA5
y	-1	GLU	-	expression tag	UNP A0A4P8BDA5
y	0	PHE	-	expression tag	UNP A0A4P8BDA5
Y	-3	GLY	-	expression tag	UNP A0A4P8BDA5
Y	-2	ALA	-	expression tag	UNP A0A4P8BDA5
Y	-1	GLU	-	expression tag	UNP A0A4P8BDA5
Y	0	PHE	-	expression tag	UNP A0A4P8BDA5

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*AP*TP*AP*GP*TP*CP*TP*CP*TP*AP*GP*GP*CP*TP*GP*CP*CP*AP*GP*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	23	Total	C	N	O	P	0	0
			470	223	86	138	23		

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
4	y	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	Y	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

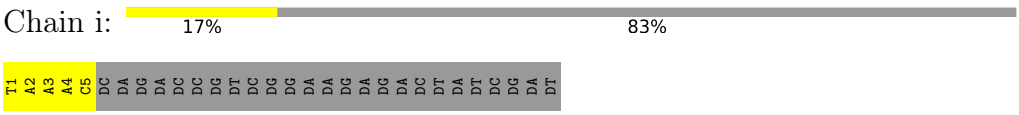
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	y	5	Total	Zn	0
			5	5	
5	Y	5	Total	Zn	0
			5	5	

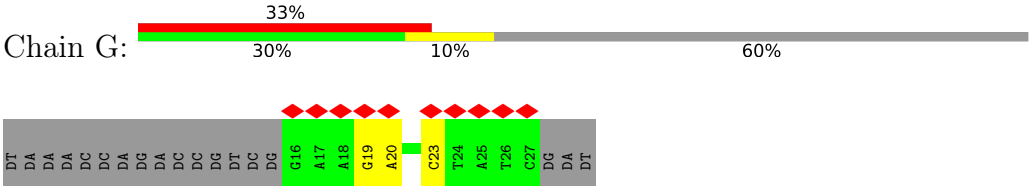
3 Residue-property plots (i)

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.

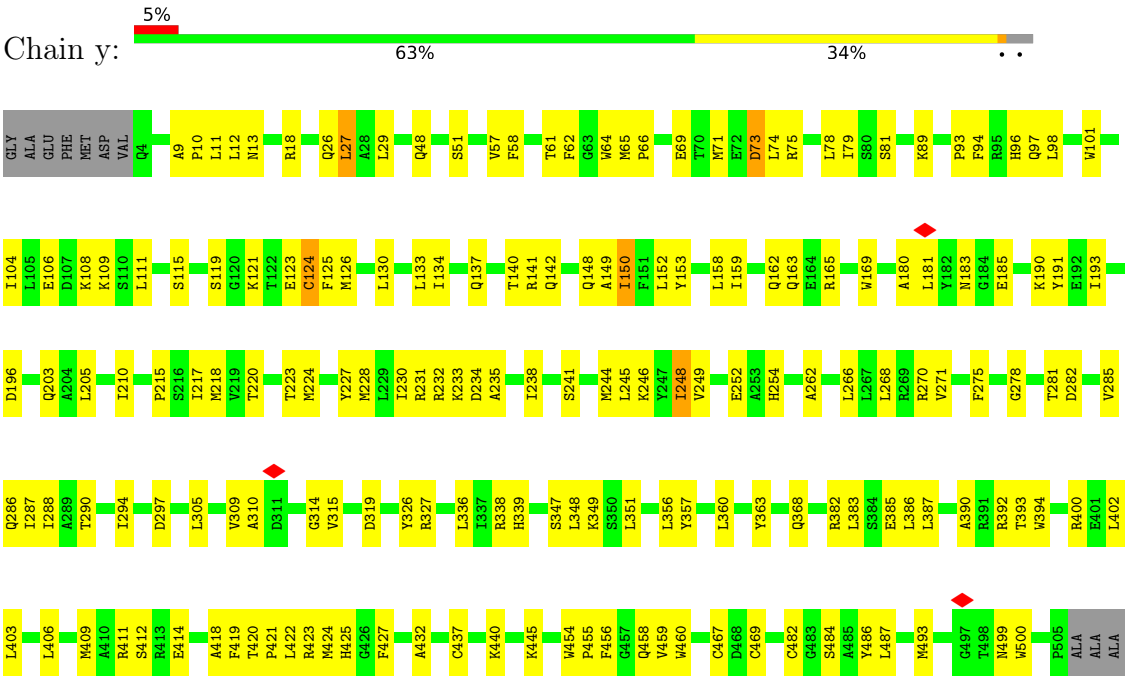
• Molecule 1: DNA (5'-D(P*GP*AP*AP*GP*AP*GP*AP*CP*TP*AP*TP*C)-3')

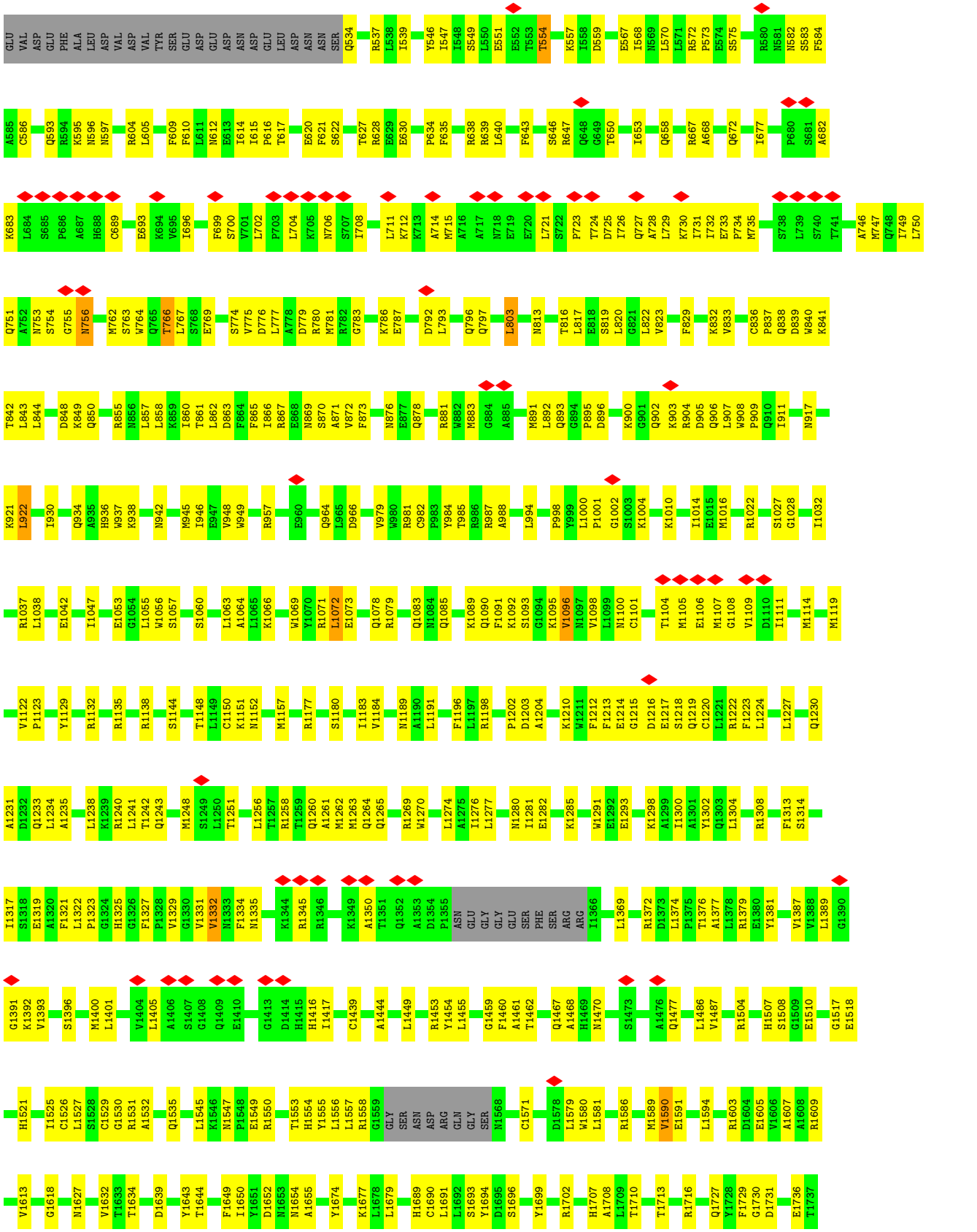


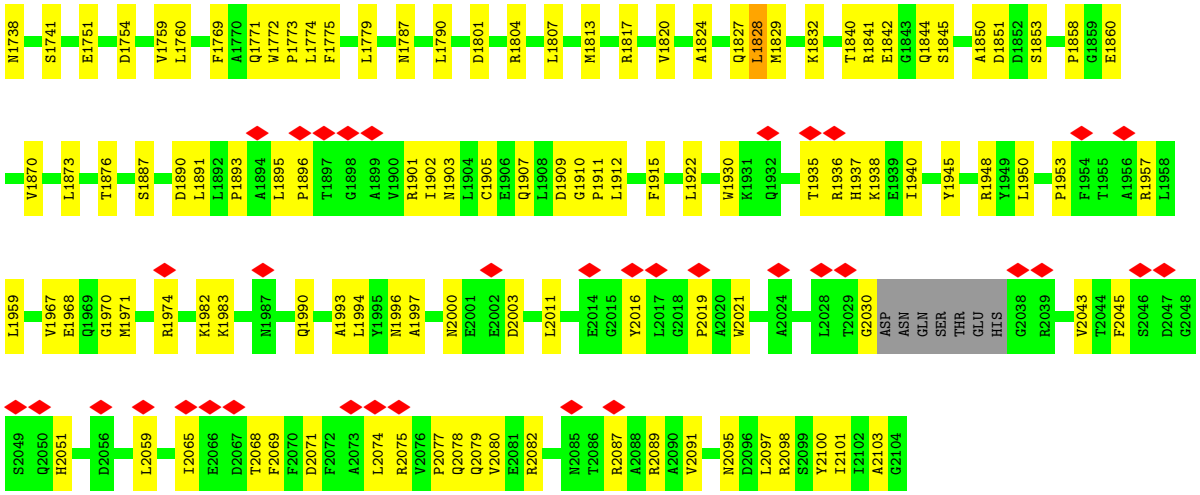
• Molecule 1: DNA (5'-D(P*GP*AP*AP*GP*AP*GP*AP*CP*TP*AP*TP*C)-3')



• Molecule 2: DEAD/DEAH box helicase

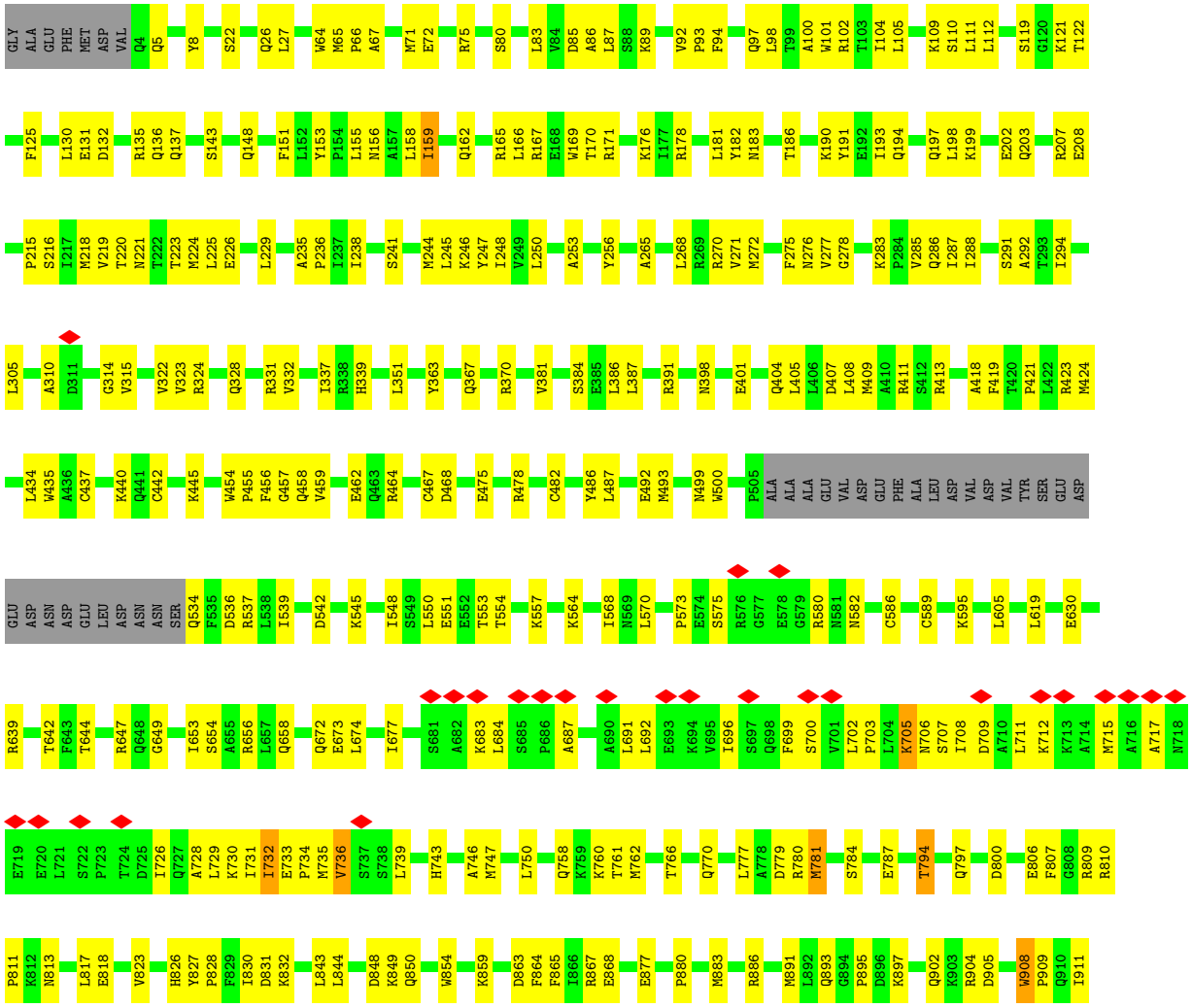


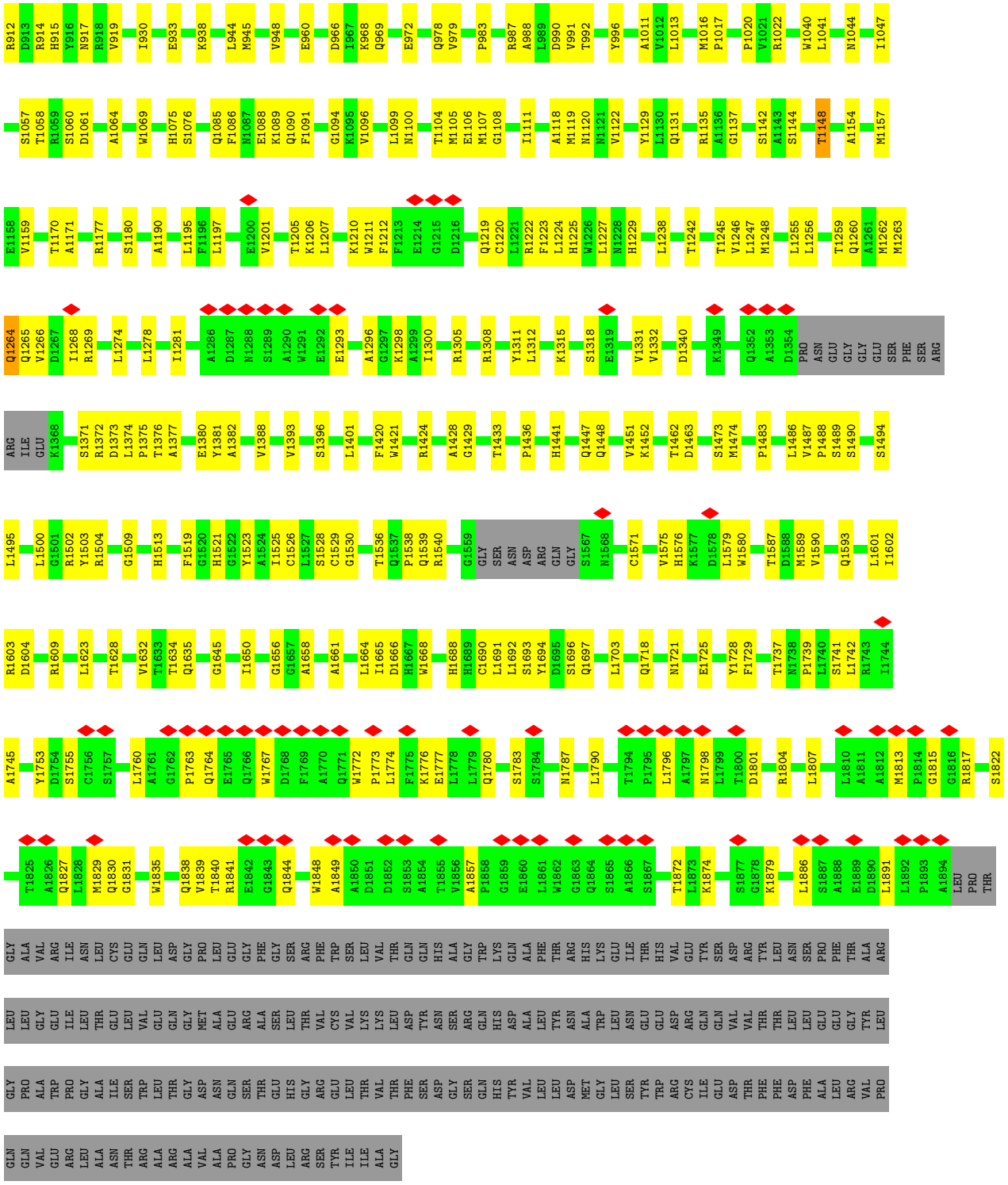

GLU VAL ASP GLU PHE ALA LEU ASP VAL ASP VAL TYR SER GLU ASP GLU ASP ASN ASP GLU LEU ASP ASN ASN SER Q534 R537 L538 I539 Y546 I547 I548 S549 L550 E551 E552 T553 T554 K557 I558 D559 E567 I568 N569 L570 L571 R572 P573 E574 S575 R580 N581 N582 S583 F584
A585 C586 Q593 R594 K595 N596 N597 R604 L605 F609 F610 L611 N612 E613 I614 I615 P616 T617 E620 F621 S622 T627 R628 E629 E630 P634 F635 R638 R639 L640 F643 S646 R647 Q648 G649 T650 I653 Q658 R667 A668 Q672 I677 P680 S681 A682
K683 L684 S685 P686 A687 H688 C689 E693 K694 V695 I696 F699 S700 V701 L702 P703 L704 K705 N706 S707 I708 L711 K712 K713 A714 M715 A716 A717 N718 E719 E720 L721 S722 P723 T724 D725 I726 Q727 A728 L729 K730 I731 I732 E733 P734 M735 S738 L739 S740 T741 A746 M747 Q748 I749 L750
Q751 A752 N753 S754 G755 N756 M762 S763 W764 Q765 T766 L767 S768 E769 S774 V775 D776 L777 A778 D779 R780 M781 R782 G783 K786 E787 D792 L793 Q796 Q797 L803 N813 T816 L817 E818 S819 L820 G821 L822 V823 F829 K832 V833 C836 P837 Q838 D839 W840 K841
T842 L843 L844 D848 K849 Q850 R855 N856 L857 L858 K859 I860 T861 L862 D863 F864 F865 I866 R867 E868 N869 S870 A871 V872 F873 N876 E877 Q878 R881 W882 M883 G884 A885 M891 L892 Q893 G894 P895 D896 K900 G901 Q902 K903 R904 D905 Q906 L907 W908 P909 Q910 I911 N917
K921 L922 I930 Q934 A935 H936 W937 K938 N942 M945 I946 E947 V948 W949 R957 E960 Q964 L965 D966 V979 W980 R981 C982 P983 Y984 T985 R986 R987 A988 L994 P998 Y999 L1000 P1001 G1002 S1003 K1004 K1010 I1014 E1015 M1016 R1022 S1027 G1028 I1032
R1037 L1038 E1042 I1047 E1053 G1064 L1055 W1056 S1057 S1060 L1063 A1064 L1065 K1066 W1069 Y1070 R1071 L1072 E1073 Q1078 R1079 Q1083 N1084 Q1085 K1089 Q1090 F1091 K1092 S1093 G1094 K1095 V1096 N1097 V1098 L1099 N1100 C1101 T1104 M1105 E1106 M1107 G1108 V1109 D1110 I1111 M1114 M1119
V1122 P1123 Y1129 R1132 R1135 R1138 S1144 T1148 L1149 C1150 K1151 N1152 M1157 R1177 S1180 I1183 V1184 N1189 A1190 L1191 F1196 L1197 R1198 P1202 D1203 A1204 K1210 W1211 F1212 F1213 E1214 G1215 D1216 E1217 S1218 Q1219 C1220 L1221 R1222 F1223 L1224 L1227 Q1230
A1231 D1232 Q1233 L1234 A1235 L1238 K1239 R1240 L1241 T1242 Q1243 M1248 S1249 L1250 T1251 L1256 T1257 R1258 T1259 Q1260 A1261 M1262 M1263 Q1264 Q1265 R1269 W1270 L1274 A1275 I1276 L1277 N1280 I1281 E1282 K1285 W1291 E1292 E1293 K1298 A1299 I1300 A1301 Y1302 Q1303 L1304 R1308 F1313 S1314
I1317 S1318 E1319 A1320 F1321 L1322 P1323 G1324 H1325 G1326 F1327 P1328 V1329 G1330 V1331 V1332 N1333 F1334 N1335 K1344 R1345 R1346 K1349 A1350 T1351 Q1352 A1353 D1354 P1355 ASN GLU GLY GLY GLU SER PHE SER ARG ARG I1366 L1369 R1372 D1373 L1374 P1375 T1376 A1377 L1378 R1379 E1380 Y1381 V1387 V1388 L1389 G1390
G1391 K1392 V1393 S1396 M1400 L1401 V1404 L1405 A1406 S1407 G1408 Q1409 E1410 G1413 D1414 H1415 H1416 I1417 C1439 A1444 L1449 R1453 Y1454 L1455 G1459 F1460 A1461 T1462 Q1467 A1468 H1469 N1470 S1473 A1476 Q1477 L1486 V1487 R1504 H1507 S1508 G1509 E1510 G1517 E1518
H1521 I1525 C1526 L1527 S1528 C1529 G1530 R1531 A1532 Q1535 L1545 K1546 N1547 P1548 E1549 R1550 T1553 H1554 Y1555 L1556 L1557 R1558 G1559 GLY SER ASN ASP ARG GLN GLY SER N1568 C1571 D1578 L1579 W1580 L1581 R1586 M1589 V1590 E1591 L1594 R1603 D1604 E1605 V1606 A1607 A1608 R1609
V1613 G1618 N1627 V1632 T1633 T1634 D1639 Y1643 T1644 F1649 I1650 Y1651 D1652 N1653 N1654 A1655 Y1674 K1677 L1678 L1679 H1689 C1690 L1691 L1692 S1693 Y1694 D1695 S1696 Y1699 R1702 H1707 A1708 L1709 T1710 T1713 R1716 Q1727 Y1728 F1729 G1730 D1731 E1736 T1737



• Molecule 2: DEAD/DEAH box helicase



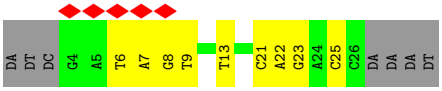




• Molecule 3: DNA (5'-D(P*GP*AP*TP*AP*GP*TP*CP*TP*CP*TP*AP*GP*GP*CP*TP*GP*CP*CP*AP*GP*AP*CP*C)-3')

Chain I:




DA
DT
DC
G4
A5
T6
A7
G8
T9
T13
C21
A22
G23
A24
C25
C26
DA
DA
DT

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21652	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 ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.350	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	319.488, 319.488, 319.488	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1093334, 1.1093334, 1.1093334	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	G	0.16	0/280	0.30	0/430
1	i	0.17	0/114	0.36	0/173
2	Y	0.11	0/14945	0.30	0/20251
2	y	0.11	0/16630	0.31	0/22543
3	I	0.22	0/526	0.40	0/809
All	All	0.12	0/32495	0.31	0/44206

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	G	249	0	135	4	0
1	i	102	0	57	9	0
2	Y	14619	0	14480	400	0
2	y	16264	0	16076	527	0
3	I	470	0	259	9	0
4	Y	31	0	12	3	0
4	y	31	0	12	1	0
5	Y	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	y	5	0	0	0	0
All	All	31776	0	31031	928	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 15.

The worst 5 of 928 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:Y:863:ASP:O	2:Y:867:ARG:HB2	1.77	0.84
2:y:12:LEU:HD21	2:y:403:LEU:HD21	1.62	0.81
2:y:1317:ILE:HG22	2:y:1322:LEU:HB2	1.64	0.80
2:Y:826:HIS:O	2:Y:972:GLU:HB2	1.83	0.79
2:y:779:ASP:OD1	2:y:780:ARG:N	2.15	0.79

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	
2	Y	1835/2108 (87%)	1755 (96%)	80 (4%)	0	100	100
2	y	2038/2108 (97%)	1946 (96%)	92 (4%)	0	100	100
All	All	3873/4216 (92%)	3701 (96%)	172 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	Y	1572/1795 (88%)	1556 (99%)	16 (1%)	68	74
2	y	1745/1795 (97%)	1715 (98%)	30 (2%)	53	67
All	All	3317/3590 (92%)	3271 (99%)	46 (1%)	57	70

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	y	1828	LEU
2	Y	736	VAL
2	y	2016	TYR
2	Y	619	LEU
2	Y	794	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
2	Y	1078	GLN
2	Y	1087	ASN
2	Y	1513	HIS
2	y	893	GLN
2	y	876	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 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	AGS	Y	2206	-	29,33,33	0.47	1 (3%)	39,52,52	0.65	1 (2%)
4	AGS	y	2201	-	29,33,33	0.47	1 (3%)	39,52,52	0.67	1 (2%)

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
4	AGS	Y	2206	-	-	2/21/38/38	0/3/3/3
4	AGS	y	2201	-	-	9/21/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	2206	AGS	PG-S1G	2.16	1.95	1.90
4	y	2201	AGS	PG-S1G	2.14	1.95	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	y	2201	AGS	PA-O3A-PB	-3.40	121.17	132.83
4	Y	2206	AGS	PA-O3A-PB	-3.23	121.75	132.83

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	y	2201	AGS	PB-O3B-PG-O2G

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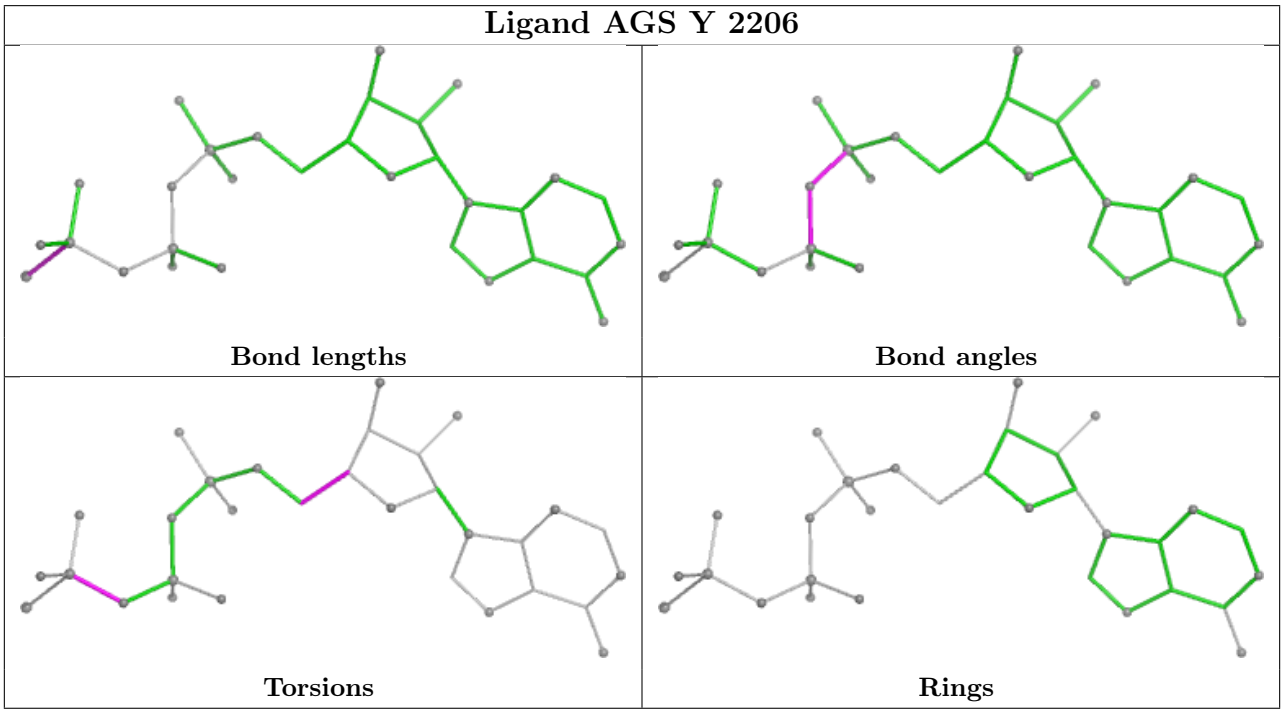
Mol	Chain	Res	Type	Atoms
4	y	2201	AGS	PB-O3B-PG-O3G
4	y	2201	AGS	C5'-O5'-PA-O1A
4	y	2201	AGS	O4'-C4'-C5'-O5'
4	y	2201	AGS	C2'-C1'-N9-C8

There are no ring outliers.

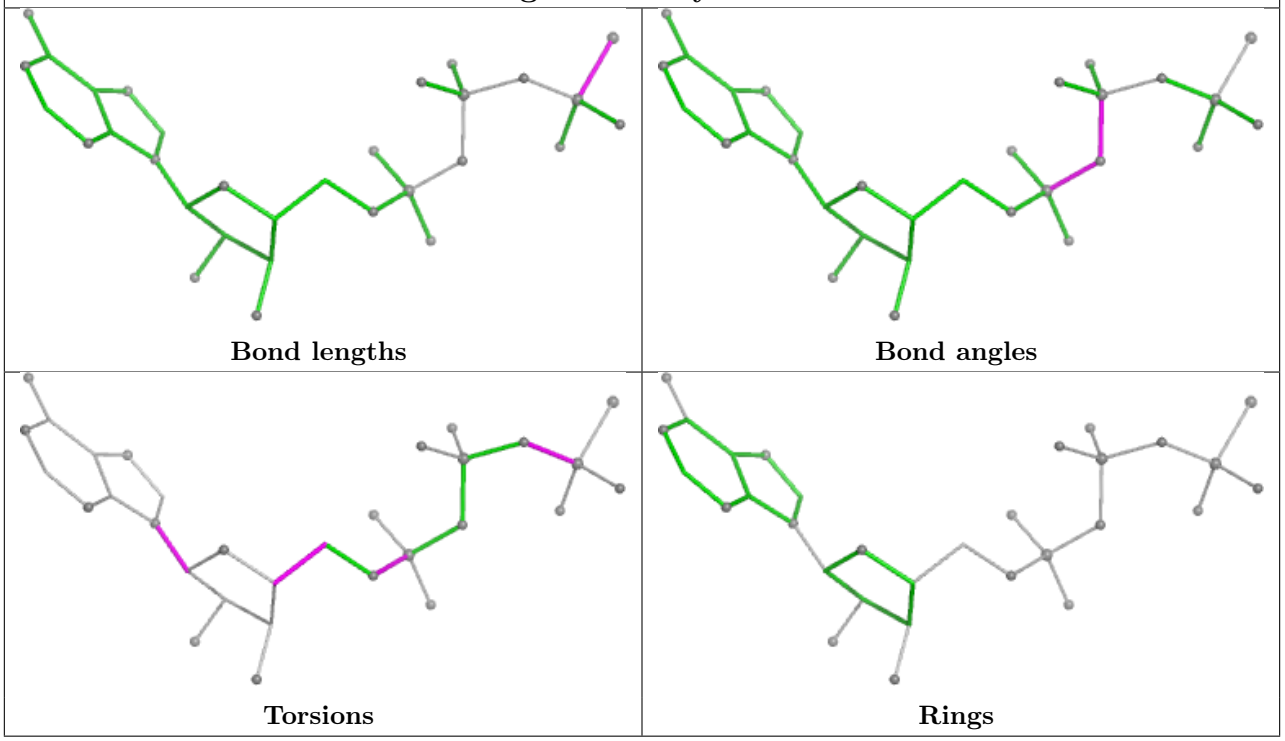
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Y	2206	AGS	3	0
4	y	2201	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.



Ligand AGS y 2201



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.

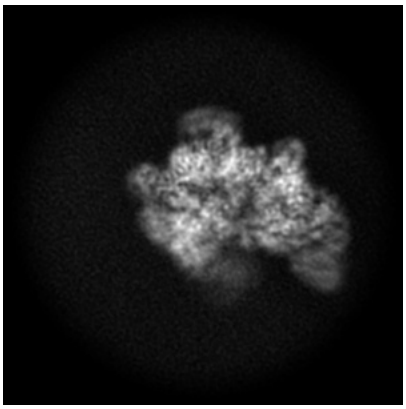
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-56255. These allow visual inspection of the internal detail of the map and identification of artifacts.

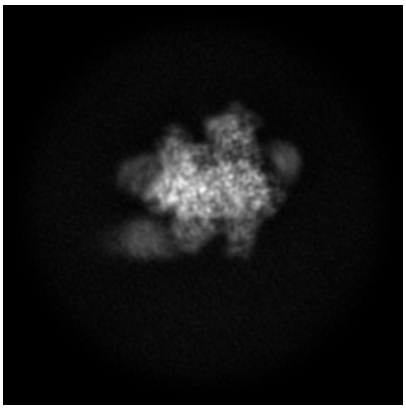
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

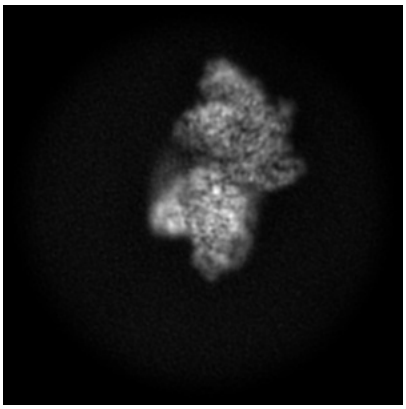
6.1.1 Primary map



X

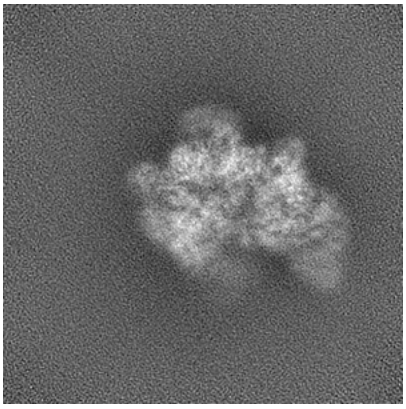


Y

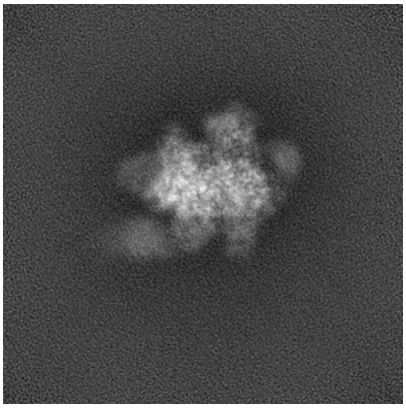


Z

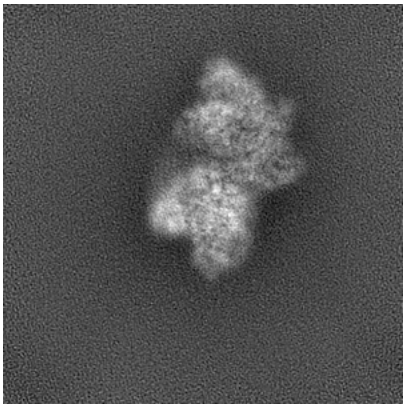
6.1.2 Raw map



X



Y

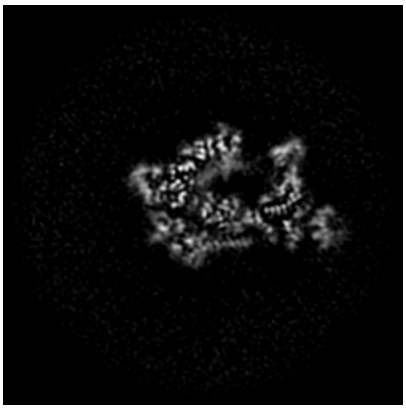


Z

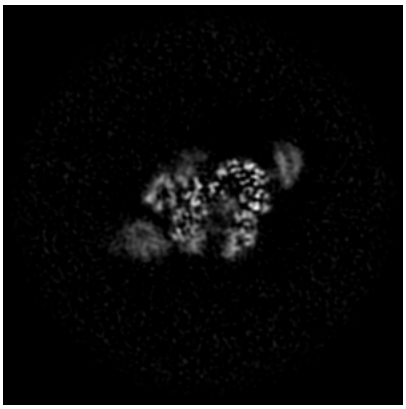
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

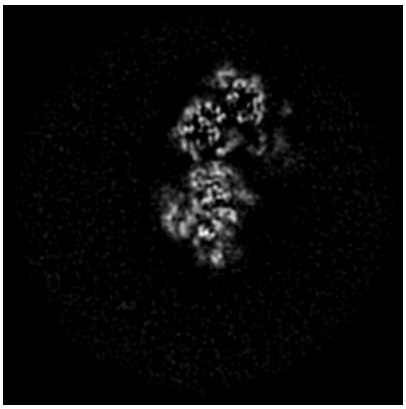
6.2.1 Primary map



X Index: 144

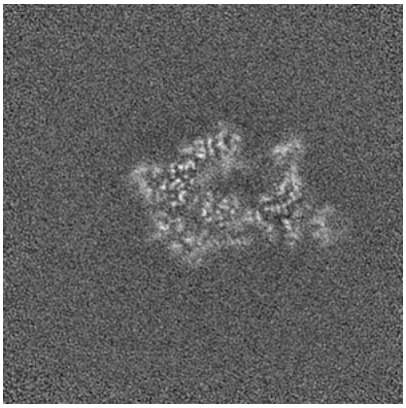


Y Index: 144

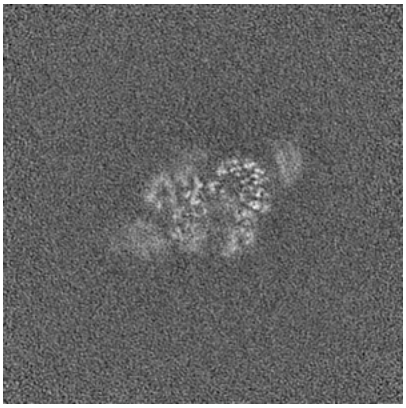


Z Index: 144

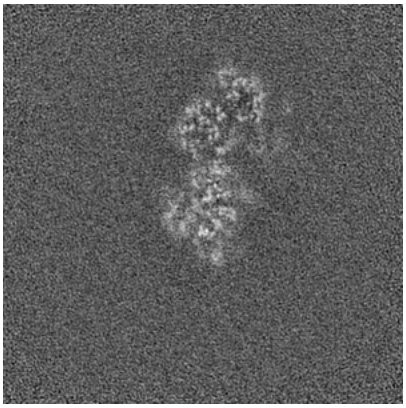
6.2.2 Raw map



X Index: 144



Y Index: 144

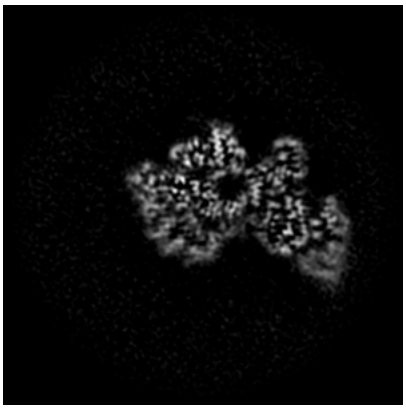


Z Index: 144

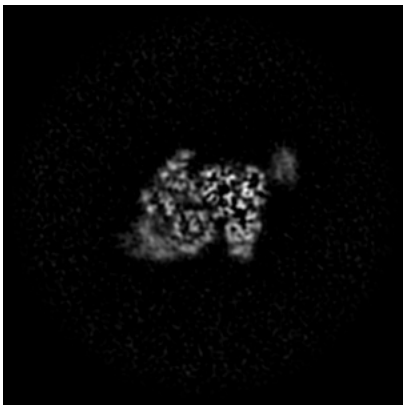
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

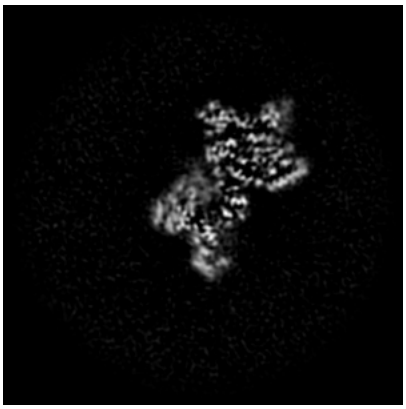
6.3.1 Primary map



X Index: 154

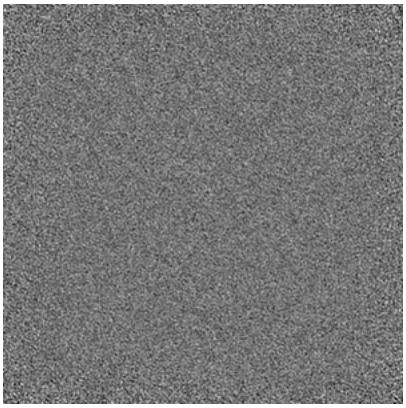


Y Index: 132

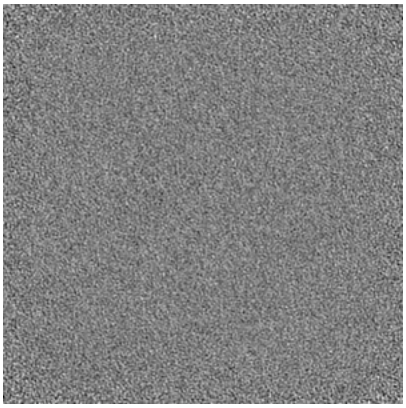


Z Index: 168

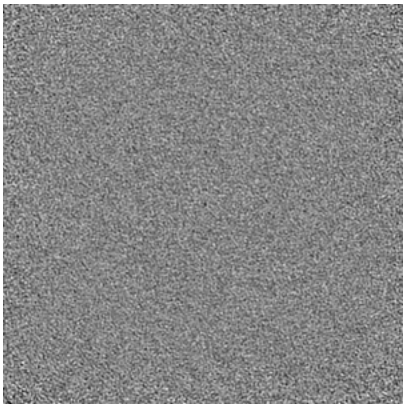
6.3.2 Raw map



X Index: 0



Y Index: 0

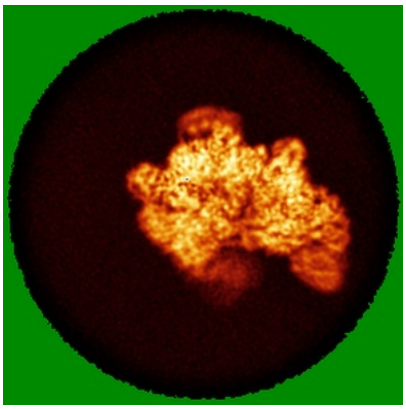


Z Index: 0

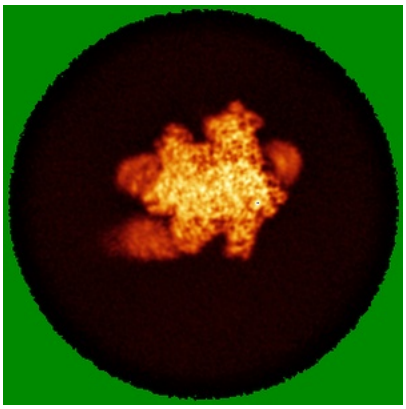
The images above show the largest variance slices of the map in three orthogonal directions.

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

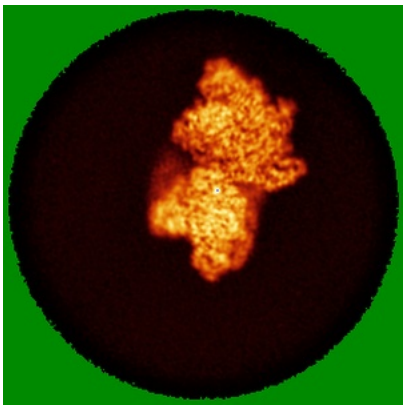
6.4.1 Primary map



X

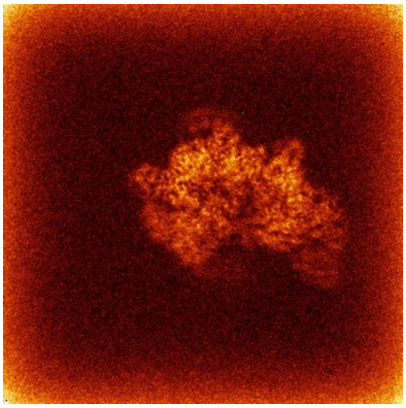


Y

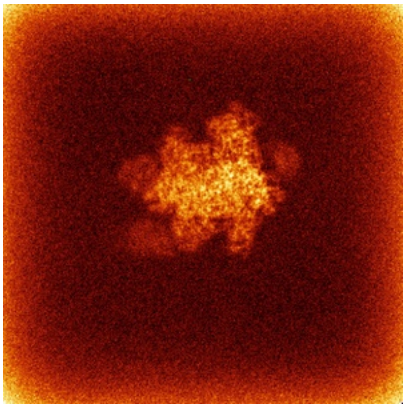


Z

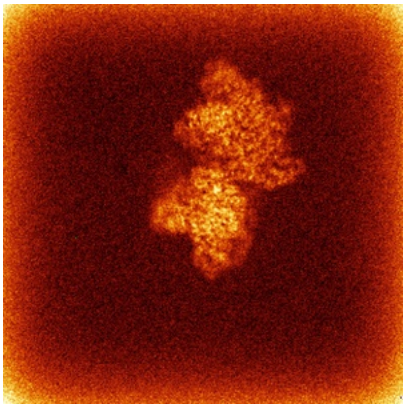
6.4.2 Raw map



X



Y

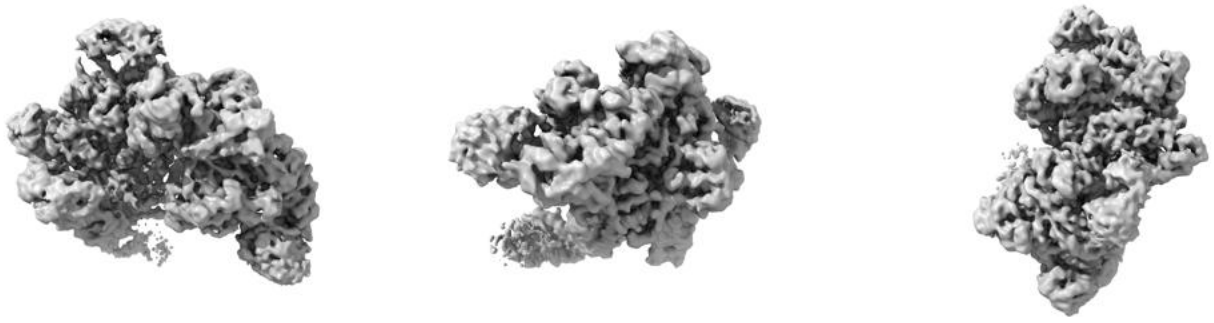


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

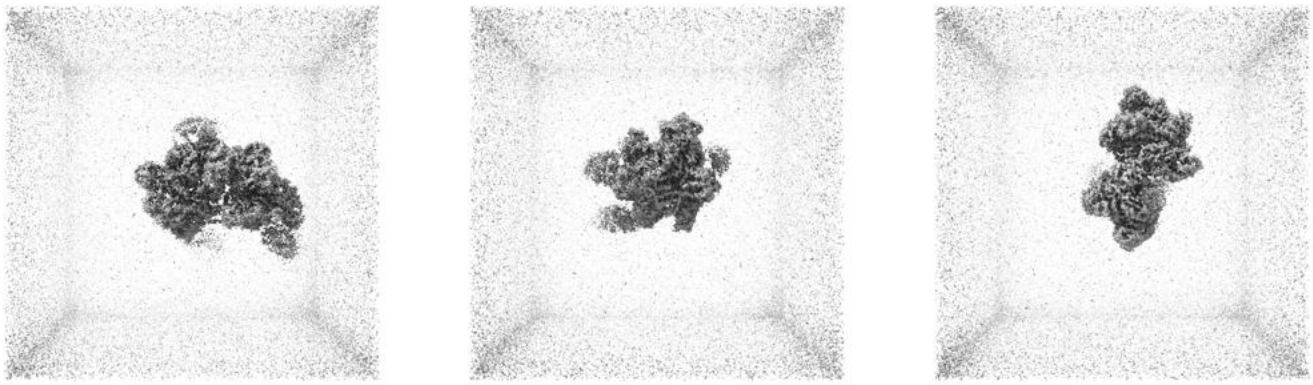
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

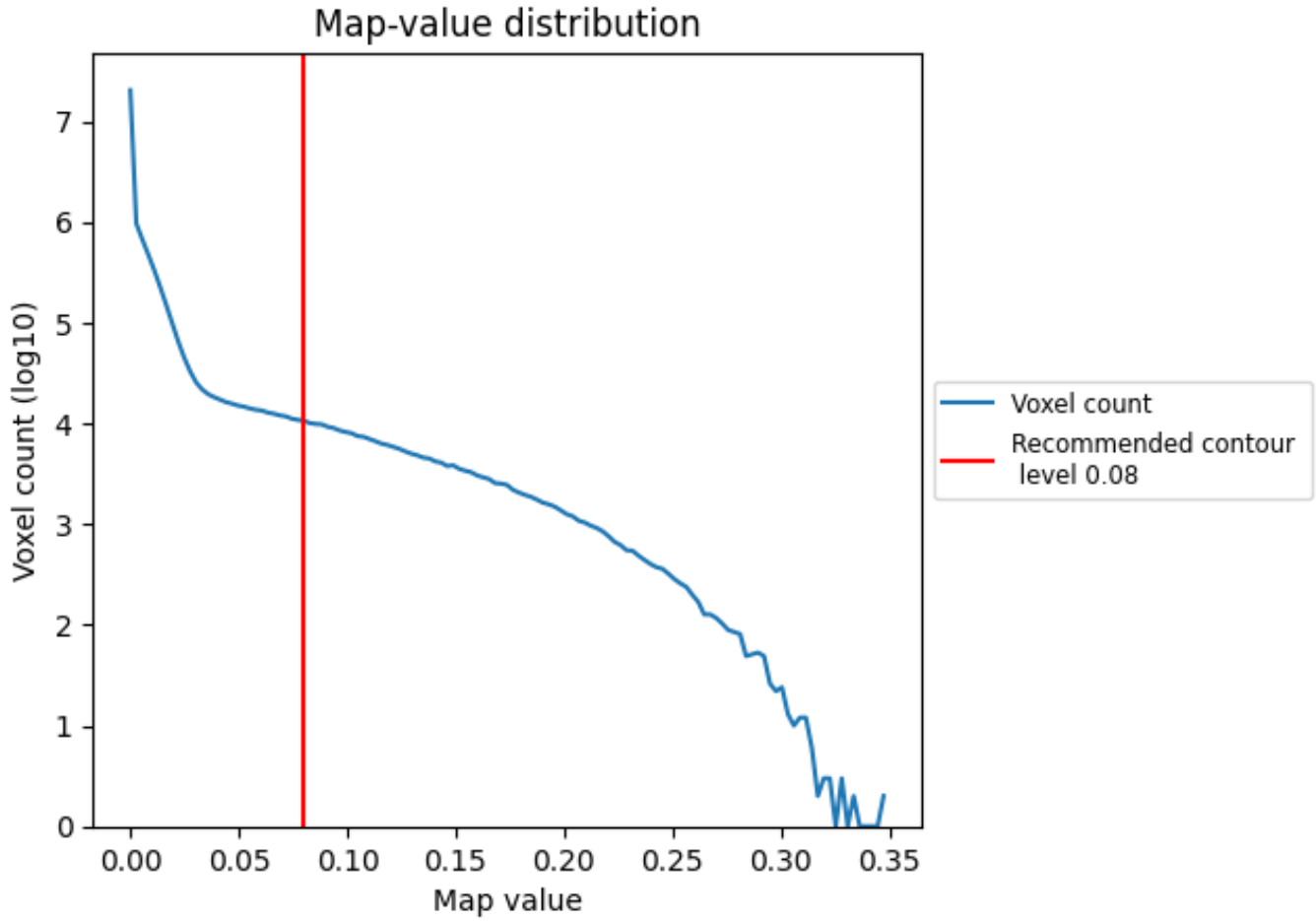
6.6 Mask visualisation (i)

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

7 Map analysis

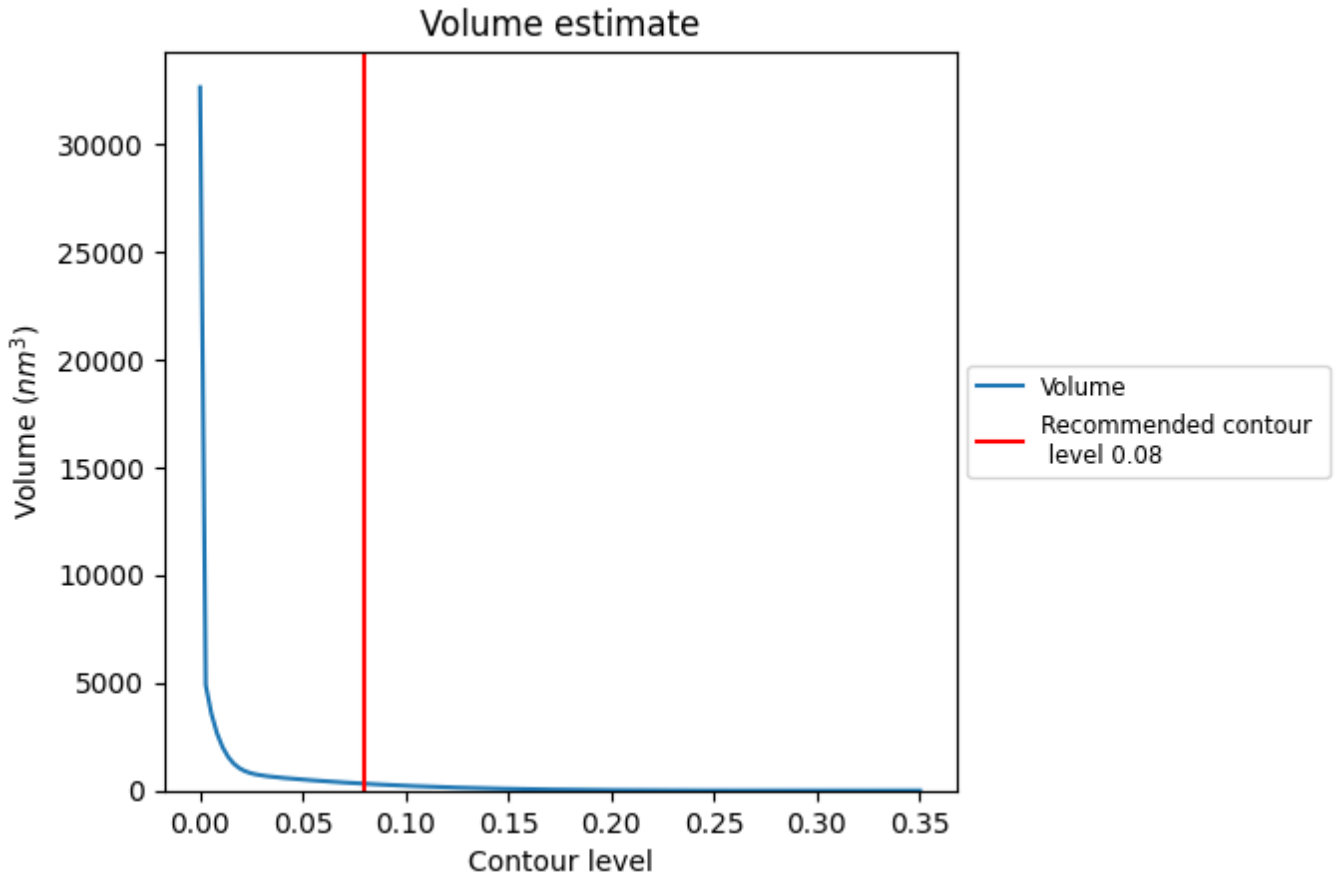
This section contains the results of statistical analysis of the map.

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.

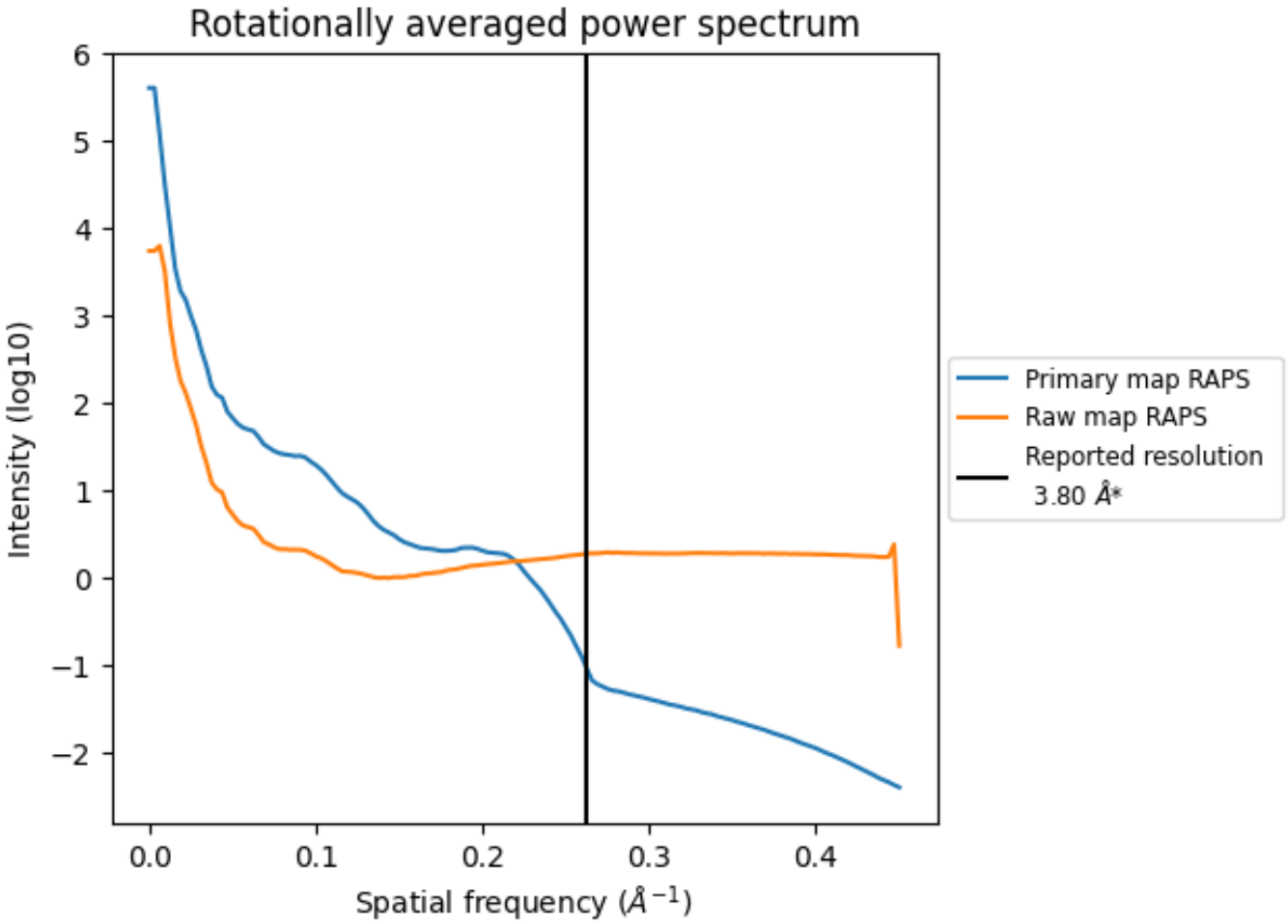
7.2 Volume estimate (i)



The volume at the recommended contour level is 318 nm^3; this corresponds to an approximate mass of 287 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)

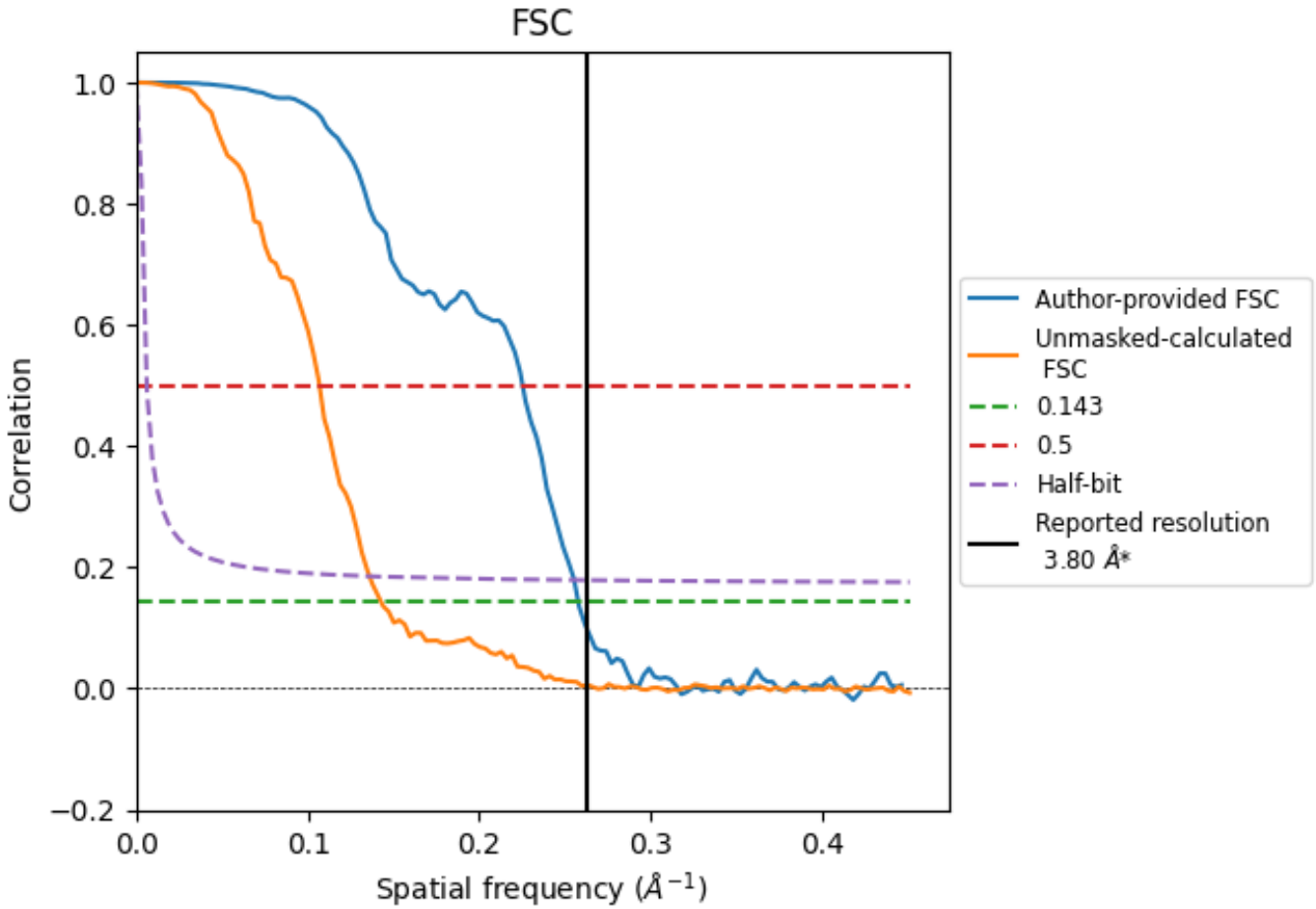


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

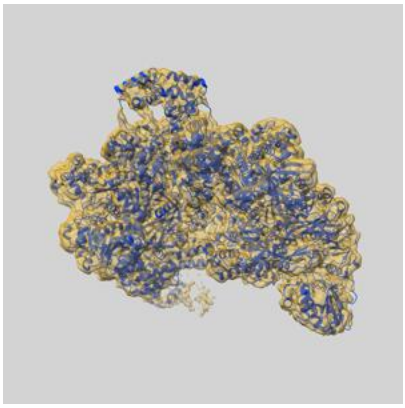
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.88	4.44	3.92
Unmasked-calculated*	7.01	9.35	7.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.01 differs from the reported value 3.8 by more than 10 %

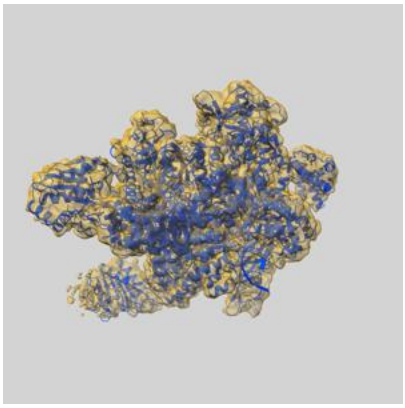
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-56255 and PDB model 9TUB. Per-residue inclusion information can be found in section 3 on page 6.

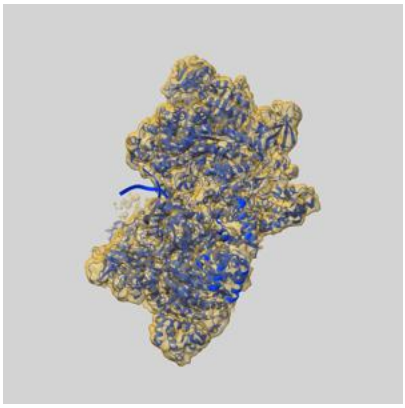
9.1 Map-model overlay



X



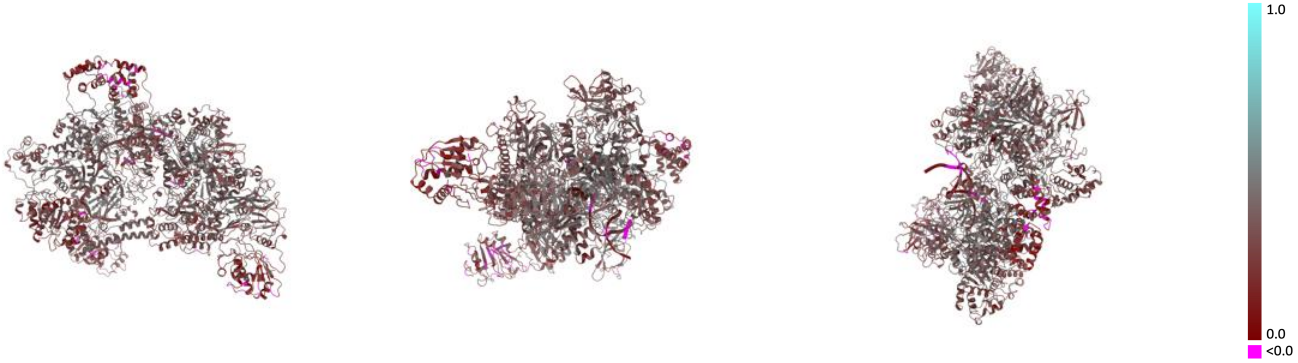
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

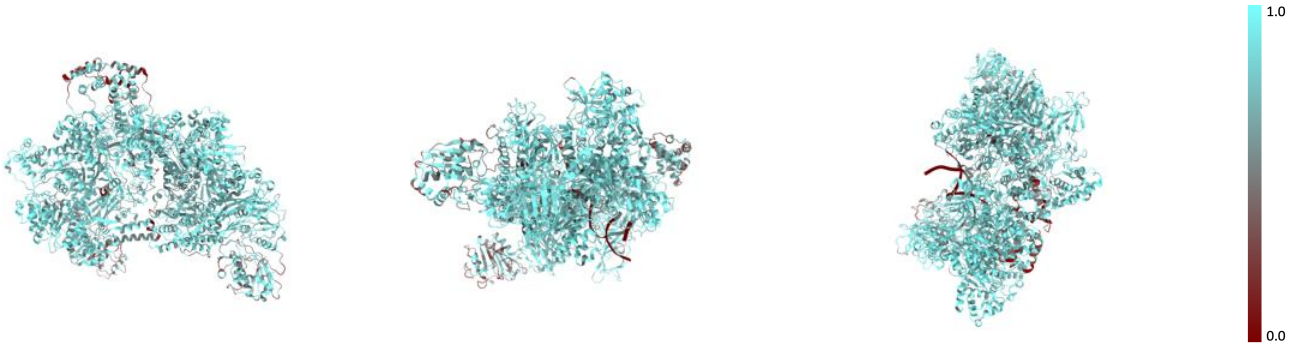
9.2 Q-score mapped to coordinate model



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.

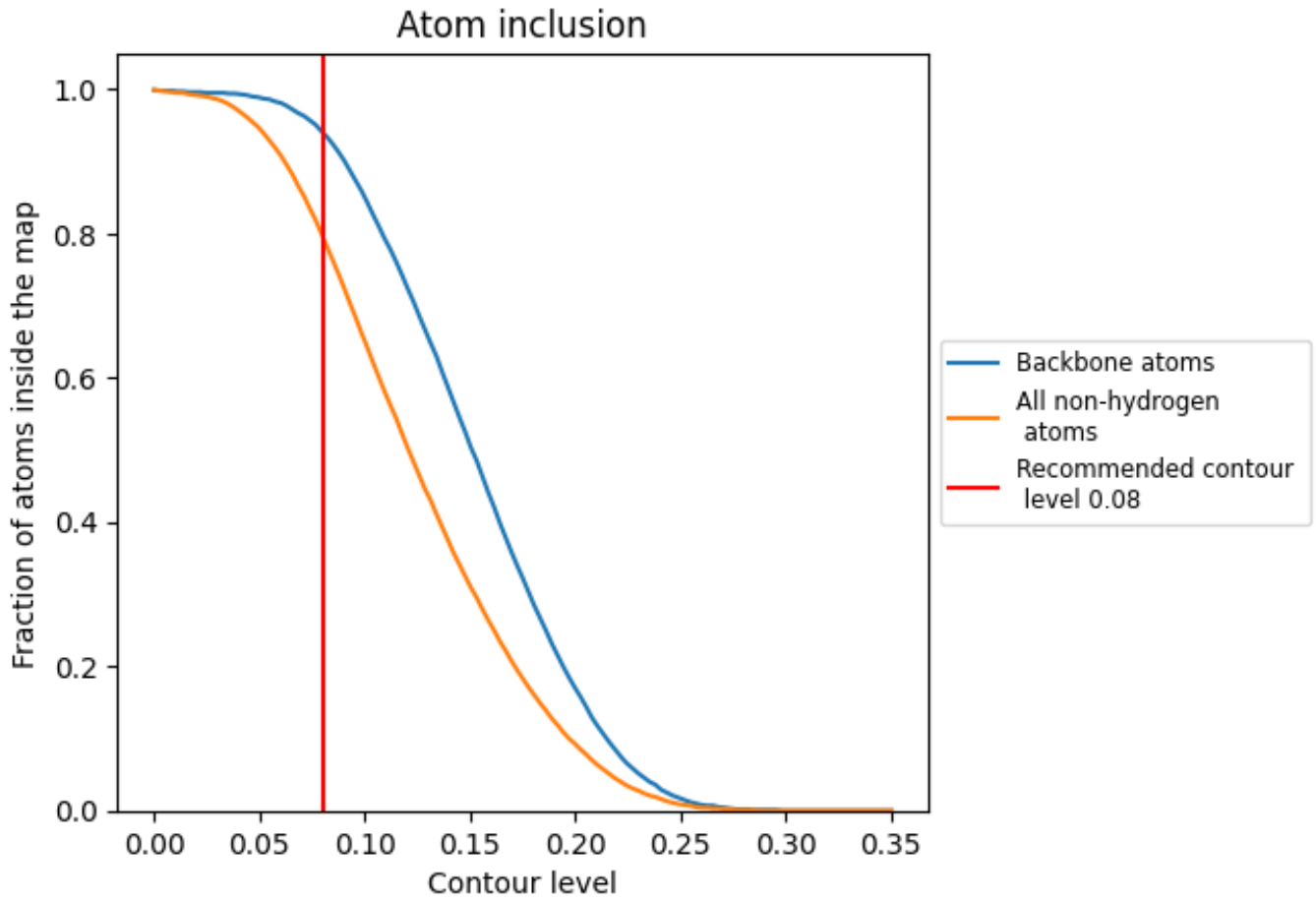
9.3 Atom inclusion mapped to coordinate model



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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 80% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7960	0.3290
G	0.1570	0.0490
I	0.6170	0.2430
Y	0.8230	0.3280
i	0.8330	0.3070
y	0.7860	0.3360

