wwPDB EM Validation Summary Report (i)

Sep 23, 2026 – 07:26 am BST

PDB ID	:	9TU8 / pdb_00009tu8
EMDB ID	:	EMD-56252
Title	:	CryoEM structure of DruE:ATPgammaS:DNA from Druantia type III - dimer 1
Authors	:	Grass, L.M.; Himpich, S.; Hilal, T.; Loll, B.; Wahl, M.C.
Deposited on	:	2026-01-08
Resolution	:	3.90 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:

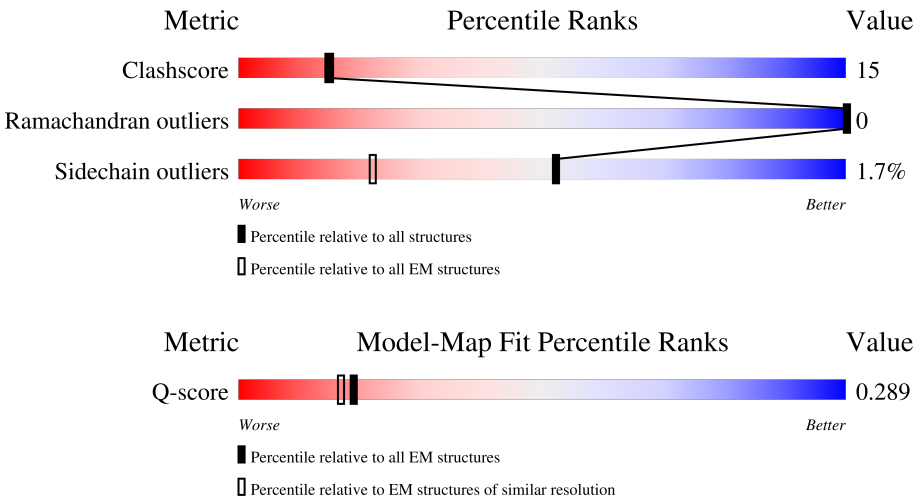
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.90 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	8855 (3.40 - 4.40)

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	Y	2108	69% 29%
1	y	2108	58% 38%
2	I	30	33% 57% 10%
2	i	30	20% 77%

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Mol	Chain	Length	Quality of chain
3	G	30	50% 40% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 34015 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 DEAD/DEAH box helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Y	2068	16419	10354	2932	3061	72	0	0
1	y	2050	16275	10265	2912	3026	72	0	0

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 2 is a DNA chain called DNA (5'-D(P*AP*CP*CP*AP*AP*AP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	i	7	142	68	28	39	7	0	0
2	I	27	551	262	101	161	27	0	0

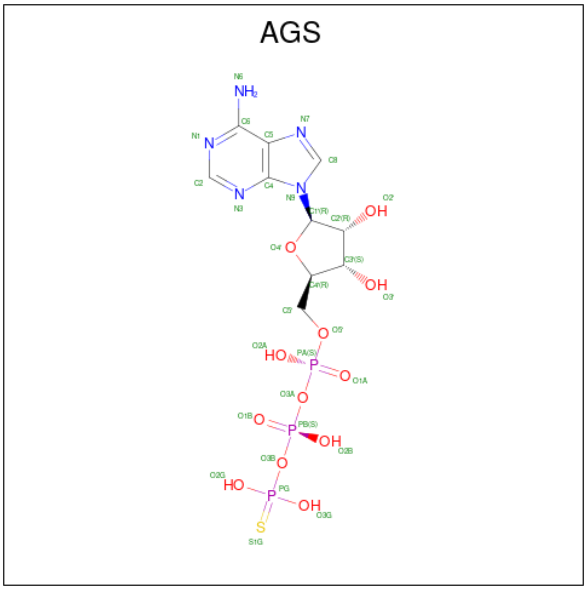
- Molecule 3 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	G	27	556	263	109	157	27	0	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



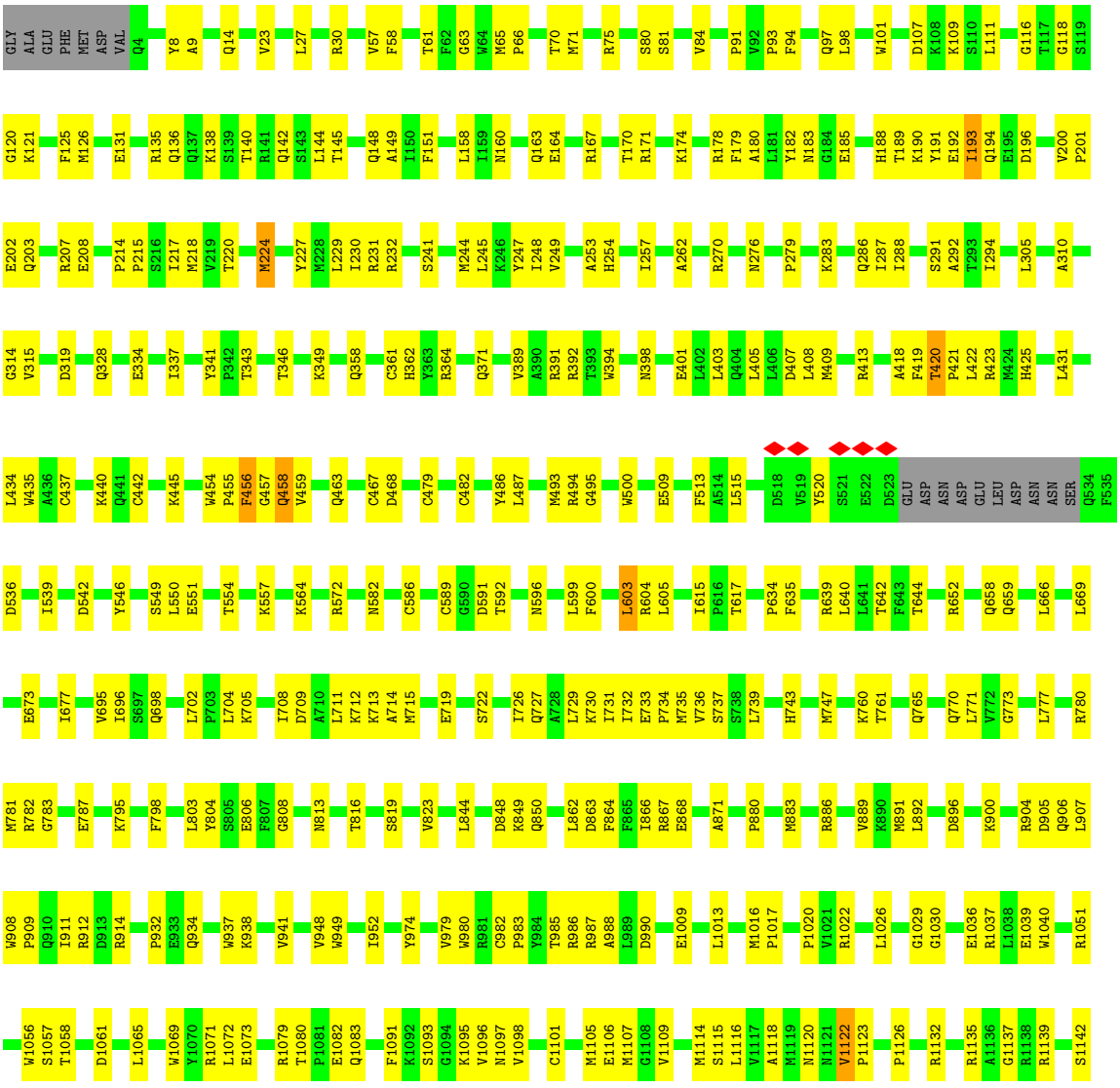
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
5	Y	1	31	10	5	12	3	1	0
			Total	C	N	O	P	S	
5	y	1	31	10	5	12	3	1	0

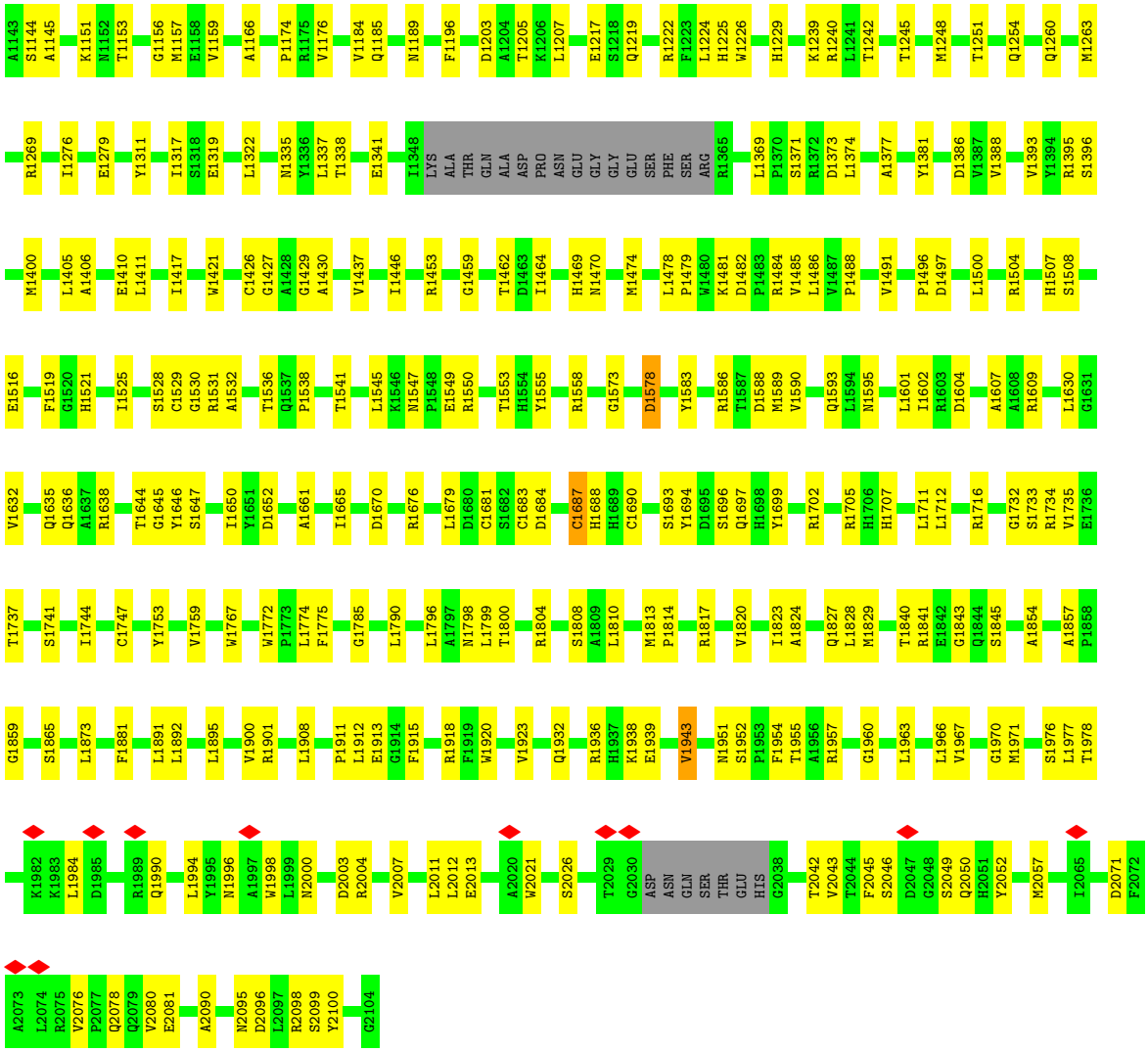
3 Residue-property plots (i)

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: DEAD/DEAH box helicase

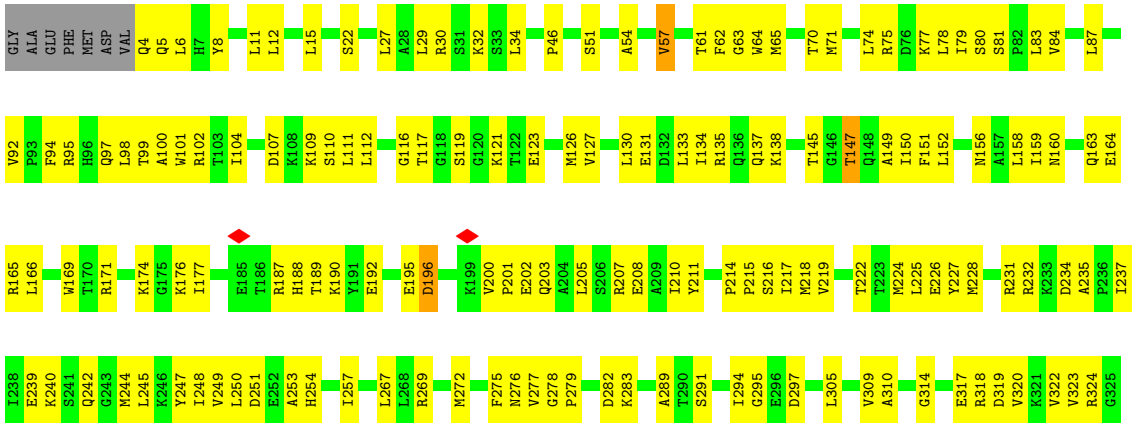
Chain Y:

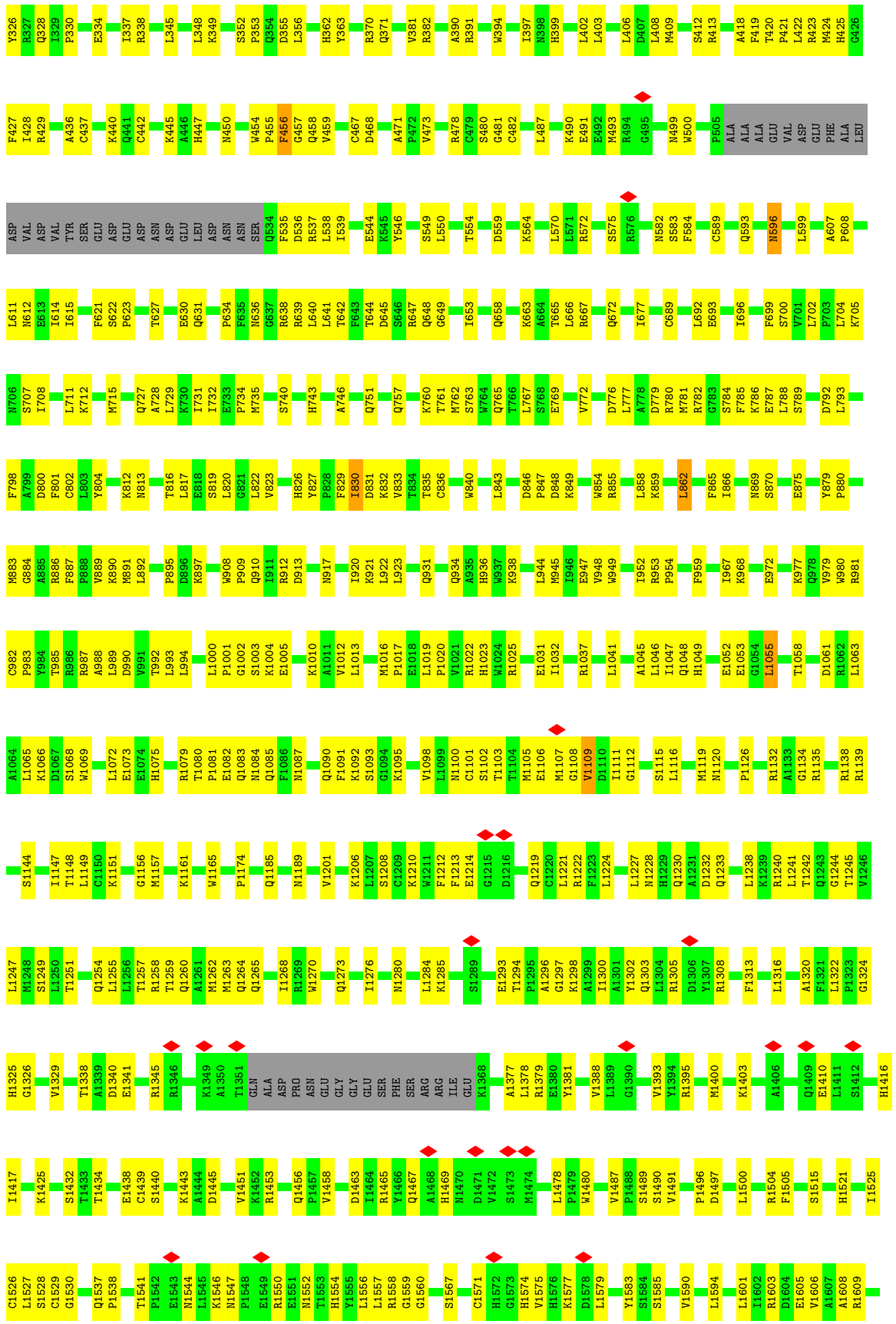


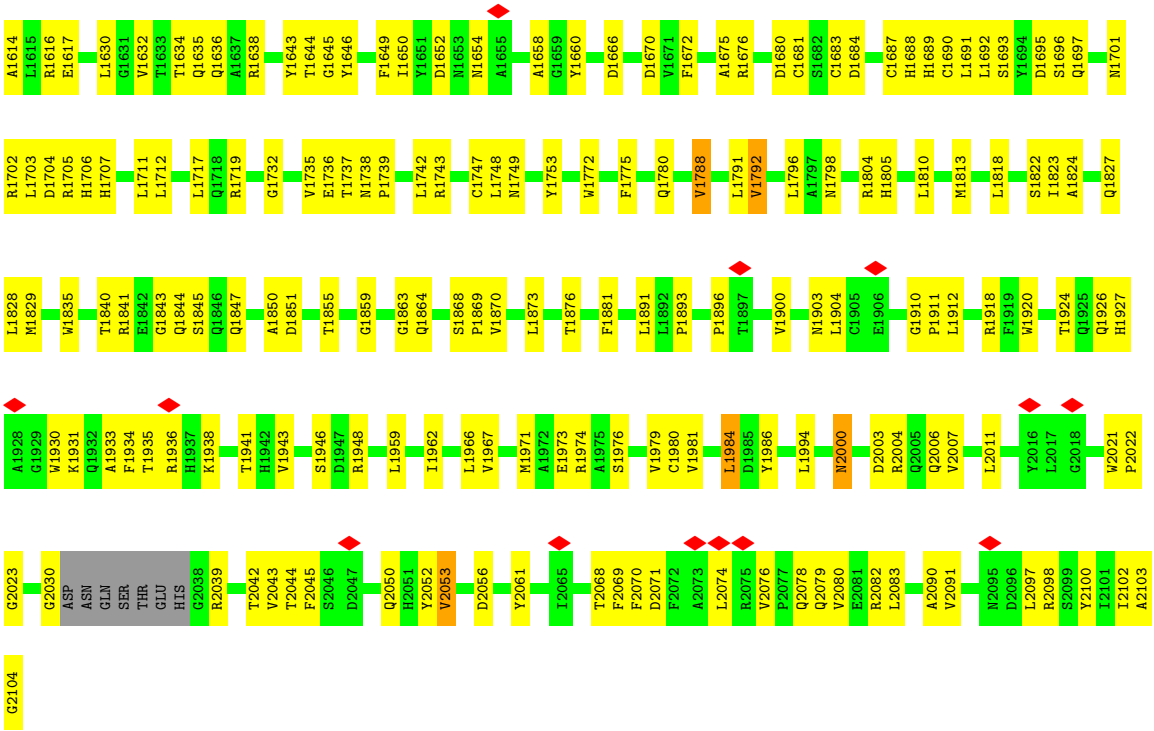


- Molecule 1: DEAD/DEAH box helicase

Chain y:

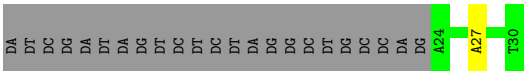



Y326 R327 Q328 I329 P330 E334 I337 R338 L345 L348 K349 S352 P353 Q354 D355 L356 H362 Y363 R370 Q371 V381 R382 A390 R391 W394 I397 N398 H399 L402 L403 L406 D407 L408 M409 S412 R413 A418 F419 T420 P421 L422 R423 M424 H425 G426
F427 I428 R429 A436 C437 K440 Q441 C442 K445 A446 H447 N450 W454 P455 F456 G457 Q458 V459 C467 D468 A471 P472 V473 R478 C479 S480 G481 C482 L487 K490 E491 E492 M493 R494 G495 N499 W500 P505 ALA ALA ALA 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 F535 D536 R537 L538 I539 E544 K545 Y546 S549 L550 T554 D559 K564 L570 L571 R572 S575 R576 N582 S583 F584 C589 Q593 N596 L599 A607 P608
L611 N612 E613 I614 I615 F621 S622 P623 T627 E630 Q631 P634 F635 N636 G637 R638 R639 L640 L641 T642 F643 T644 D645 S646 R647 Q648 G649 I653 Q658 K663 A664 T665 L666 R667 Q672 I677 C689 L692 E693 I696 F699 S700 V701 L702 P703 L704 K705
N706 S707 I708 L711 K712 M715 Q727 A728 L729 K730 I731 I732 E733 P734 M735 S740 H743 A746 Q751 Q757 K760 T761 M762 S763 W764 Q765 T766 L767 S768 E769 V772 D776 L777 A778 D779 R780 M781 R782 G783 S784 F785 K786 E787 L788 S789 D792 L793
F798 A799 D800 F801 C802 L803 Y804 K812 N813 T816 L817 E818 S819 L820 G821 L822 V823 H826 Y827 P828 F829 I830 D831 K832 V833 T834 T835 C836 W840 L843 D846 P847 D848 K849 W854 R855 L858 K859 L862 F865 I866 N869 S870 E875 Y879 P880
N883 G884 A885 R886 F887 P888 V889 K890 M891 L892 P895 D896 K897 W908 P909 Q910 I911 R912 D913 N917 I920 K921 L922 L923 Q931 Q934 A935 H936 W937 K938 L944 M945 I946 E947 V948 W949 I952 R953 P954 F959 I967 K968 E972 K977 Q978 V979 W980 R981
C982 P983 Y984 T985 R986 R987 A988 L989 D990 V991 T992 L993 L994 L1000 P1001 G1002 S1003 K1004 E1005 K1010 A1011 V1012 L1013 M1016 P1017 E1018 L1019 P1020 V1021 R1022 H1023 W1024 R1025 E1031 I1032 R1037 L1041 A1045 L1046 I1047 Q1048 H1049 E1052 E1053 G1054 L1055 T1058 D1061 R1062 L1063
A1064 L1065 K1066 D1067 S1068 W1069 L1072 E1073 E1074 H1075 R1079 T1080 P1081 E1082 Q1083 N1084 Q1085 F1086 N1087 Q1090 F1091 K1092 S1093 G1094 K1095 V1098 L1099 N1100 C1101 S1102 T1103 T1104 M1105 E1106 M1107 G1108 V1109 D1110 I1111 G1112 S1115 L1116 M1119 N1120 P1126 R1132 A1133 G1134 R1135 R1138 R1139
S1144 I1147 T1148 L1149 C1150 K1151 G1156 M1157 K1161 W1165 P1174 Q1185 N1189 V1201 K1206 L1207 S1208 C1209 K1210 W1211 F1212 F1213 E1214 G1215 D1216 Q1219 C1220 L1221 R1222 F1223 L1224 L1227 N1228 H1229 Q1230 A1231 D1232 Q1233 L1238 K1239 R1240 L1241 T1242 Q1243 G1244 T1245 V1246
L1247 M1248 S1249 L1250 T1251 Q1254 L1255 L1256 T1257 R1258 T1259 Q1260 A1261 M1262 M1263 Q1264 Q1265 I1268 R1269 W1270 Q1273 I1276 N1280 L1284 K1285 S1289 E1293 T1294 P1295 A1296 G1297 K1298 A1299 I1300 A1301 Y1302 Q1303 L1304 R1305 D1306 Y1307 R1308 F1313 L1316 A1320 F1321 L1322 P1323 G1324
H1325 G1326 V1329 T1338 A1339 D1340 E1341 R1345 R1346 K1349 A1350 T1351 GLN ALA ASP PRO ASN GLU GLY GLY GLU SER PHE SER ARG ARG ILE GLU K1368 A1377 L1378 R1379 E1380 Y1381 V1388 L1389 G1390 V1393 Y1394 R1395 M1400 K1403 A1406 Q1409 E1410 L1411 S1412 H1416
I1417 K1425 S1432 T1433 T1434 E1438 C1439 S1440 K1443 A1444 D1445 V1451 K1452 R1453 Q1456 P1457 V1458 D1463 I1464 R1465 Y1466 Q1467 A1468 H1469 N1470 D1471 V1472 S1473 M1474 L1478 P1479 W1480 V1487 P1488 S1489 S1490 V1491 P1496 D1497 L1500 R1504 F1505 S1515 H1521 I1525
C1526 L1527 S1528 C1529 G1530 Q1537 P1538 T1541 P1542 E1543 N1544 L1545 K1546 N1547 P1548 E1549 R1550 E1551 N1552 T1553 H1554 Y1555 L1556 L1557 R1558 G1559 G1560 S1567 C1571 H1572 G1573 H1574 V1575 H1576 K1577 D1578 L1579 Y1583 S1584 S1585 V1590 L1594 L1601 I1602 R1603 D1604 E1605 V1606 A1607 A1608 R1609



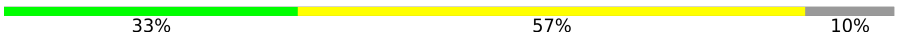
- Molecule 2: DNA (5'-D(P*AP*CP*CP*AP*AP*AP*T)-3')

Chain i:



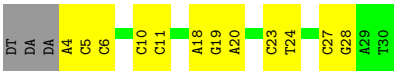
- Molecule 2: DNA (5'-D(P*AP*CP*CP*AP*AP*AP*T)-3')

Chain I:



- Molecule 3: DNA (27-MER)

Chain G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20914	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	0.260	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.04	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 (i)

5.1 Standard geometry (i)

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	Y	0.11	0/16787	0.27	0/22755
1	y	0.10	0/16641	0.30	1/22555 (0.0%)
2	I	0.20	0/617	0.39	0/949
2	i	0.10	0/159	0.25	0/242
3	G	0.16	0/625	0.30	0/962
All	All	0.11	0/34829	0.29	1/47463 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	y	1643	TYR	CB-CA-C	-5.36	110.38	116.54

There are no chirality outliers.

There are no planarity outliers.

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	Y	16419	0	16203	409	0
1	y	16275	0	16083	584	0
2	I	551	0	304	16	0
2	i	142	0	79	2	0
3	G	556	0	302	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Y	5	0	0	0	0
4	y	5	0	0	0	0
5	Y	31	0	12	4	0
5	y	31	0	12	4	0
All	All	34015	0	32995	1004	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 1004 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:y:1529:CYS:SG	1:y:1554:HIS:CD2	2.58	0.96
1:y:1119:MET:HE1	1:y:1132:ARG:HG2	1.63	0.81
1:y:2074:LEU:HD13	1:y:2078:GLN:HB3	1.65	0.79
1:Y:1753:TYR:HA	1:Y:1841:ARG:HG3	1.66	0.76
1:Y:1967:VAL:HB	1:Y:2021:TRP:HE1	1.51	0.76

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	Y	2060/2108 (98%)	1956 (95%)	104 (5%)	0	100	100
1	y	2042/2108 (97%)	1956 (96%)	86 (4%)	0	100	100
All	All	4102/4216 (97%)	3912 (95%)	190 (5%)	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	
1	Y	1761/1795 (98%)	1733 (98%)	28 (2%)	55	69
1	y	1746/1795 (97%)	1713 (98%)	33 (2%)	50	66
All	All	3507/3590 (98%)	3446 (98%)	61 (2%)	52	68

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	y	57	VAL
1	y	1788	VAL
1	y	305	LEU
1	y	1735	VAL
1	y	2000	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	1727	GLN
1	y	1636	GLN
1	y	13	ASN
1	y	1273	GLN
1	Y	1990	GLN

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	$\#\|Z\| > 2$
5	AGS	y	2206	-	29,33,33	0.46	1 (3%)	39,52,52	0.75	1 (2%)
5	AGS	Y	2206	-	29,33,33	0.47	1 (3%)	39,52,52	0.66	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
5	AGS	y	2206	-	-	6/21/38/38	0/3/3/3
5	AGS	Y	2206	-	-	4/21/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	y	2206	AGS	PG-S1G	2.15	1.95	1.90
5	Y	2206	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})
5	y	2206	AGS	PA-O3A-PB	-3.97	119.20	132.83
5	Y	2206	AGS	PA-O3A-PB	-3.31	121.48	132.83

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	y	2206	AGS	PB-O3A-PA-O5'
5	y	2206	AGS	C5'-O5'-PA-O3A
5	y	2206	AGS	O4'-C4'-C5'-O5'
5	y	2206	AGS	C3'-C4'-C5'-O5'
5	y	2206	AGS	C4'-C5'-O5'-PA

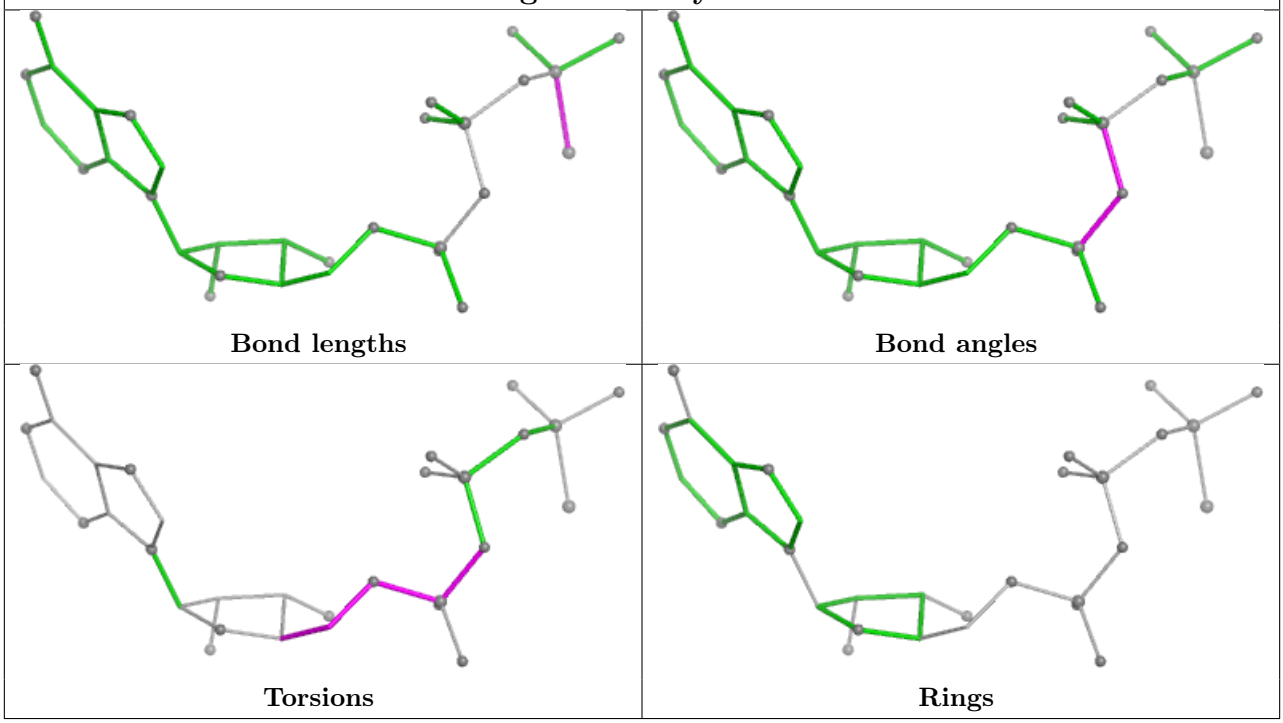
There are no ring outliers.

2 monomers are involved in 8 short contacts:

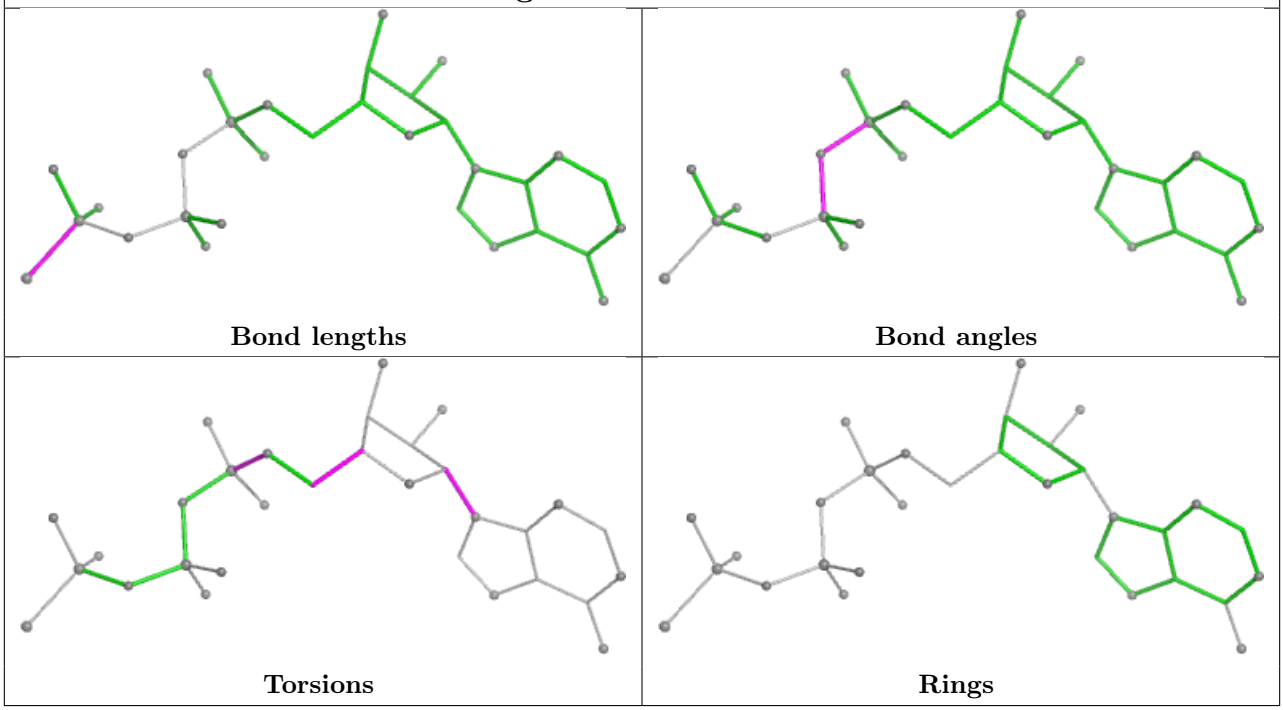
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	y	2206	AGS	4	0
5	Y	2206	AGS	4	0

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 2206



Ligand AGS Y 2206



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.

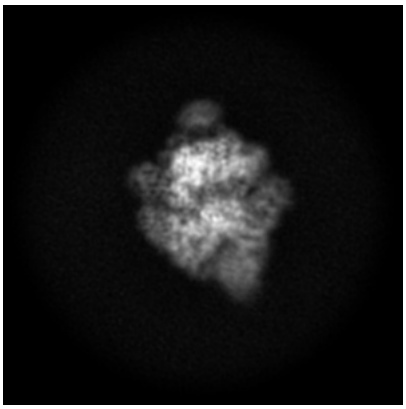
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-56252. These allow visual inspection of the internal detail of the map and identification of artifacts.

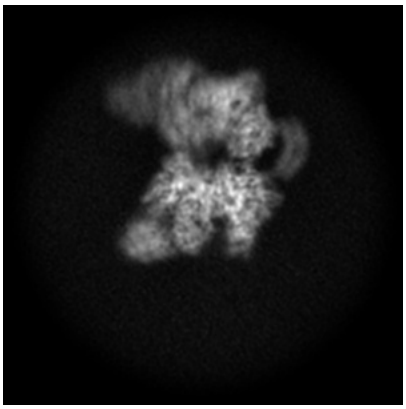
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

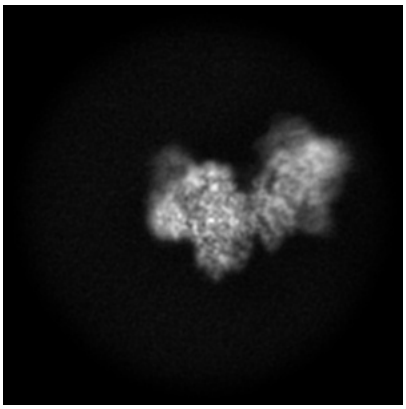
6.1.1 Primary map



X

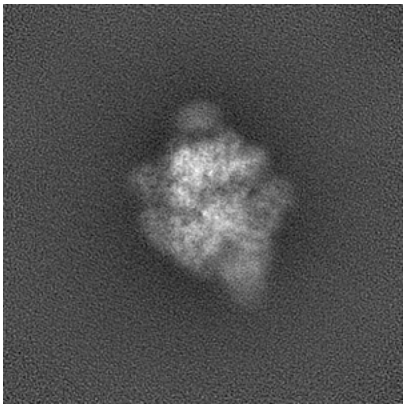


Y

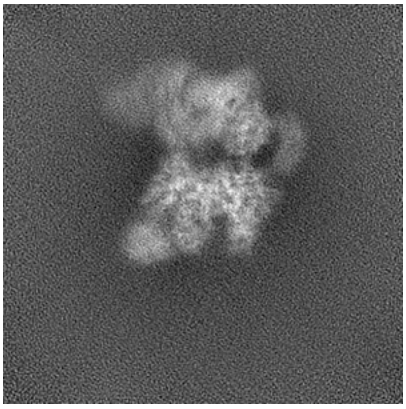


Z

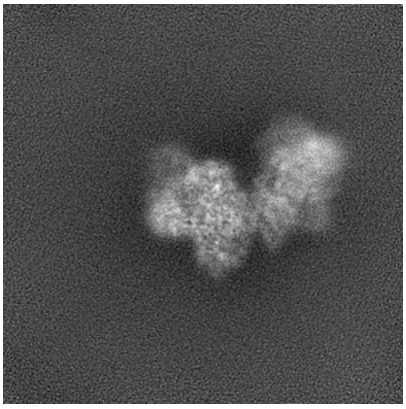
6.1.2 Raw map



X



Y

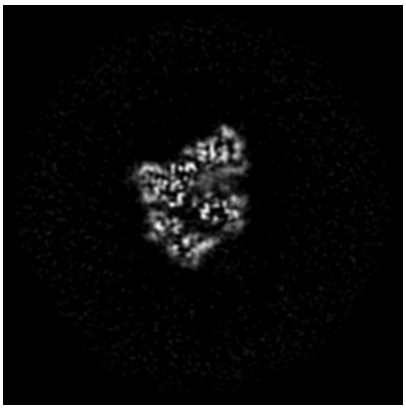


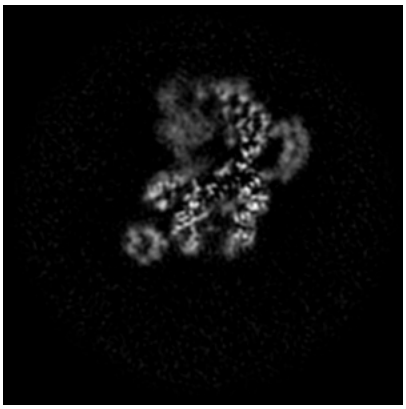
Z

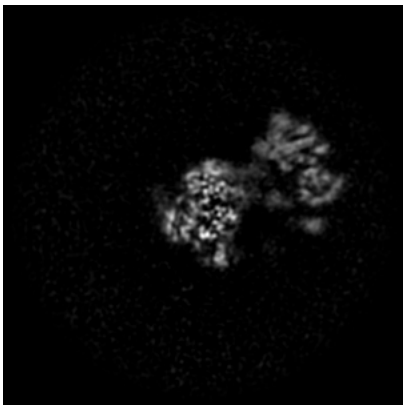
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

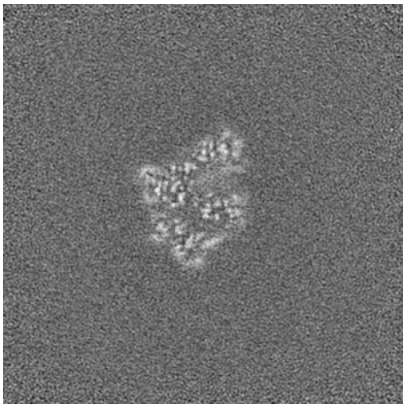
6.2.1 Primary map

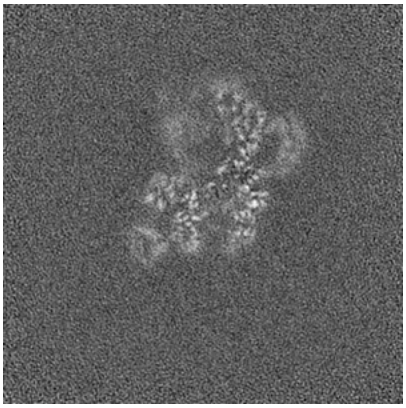

X Index: 144

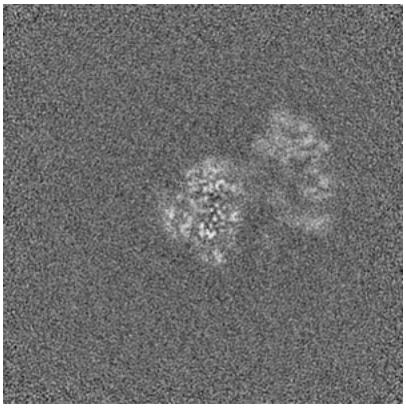

Y Index: 144


Z Index: 144

6.2.2 Raw map


X Index: 144

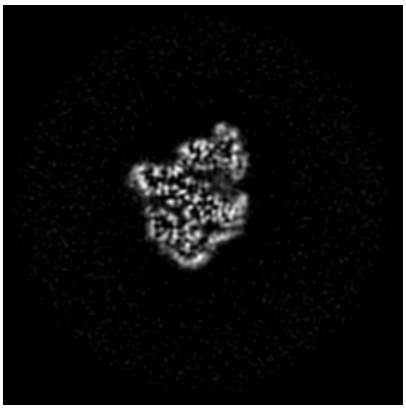

Y Index: 144


Z Index: 144

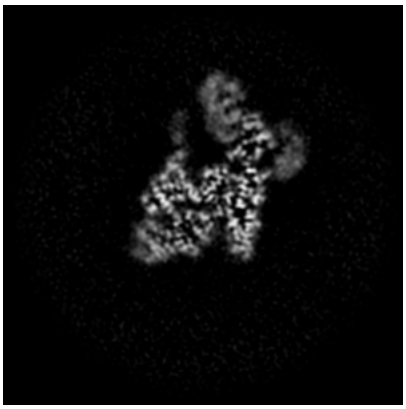
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

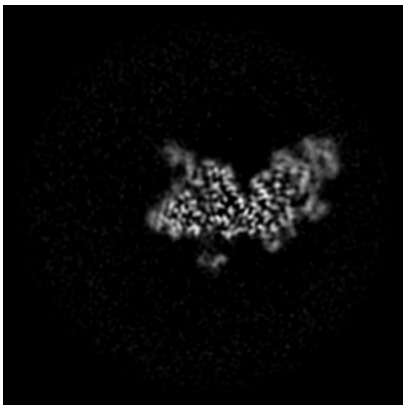
6.3.1 Primary map



X Index: 149

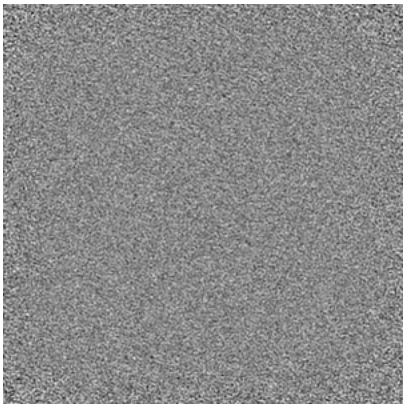


Y Index: 132

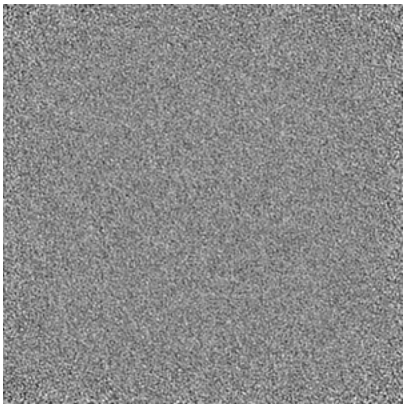


Z Index: 174

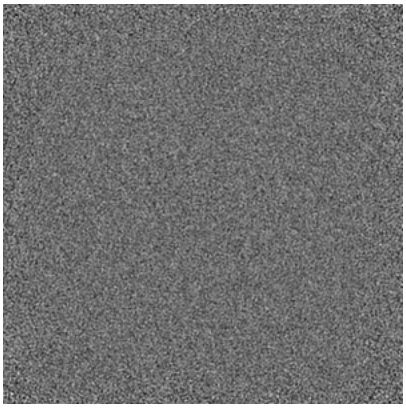
6.3.2 Raw map



X Index: 0



Y Index: 0

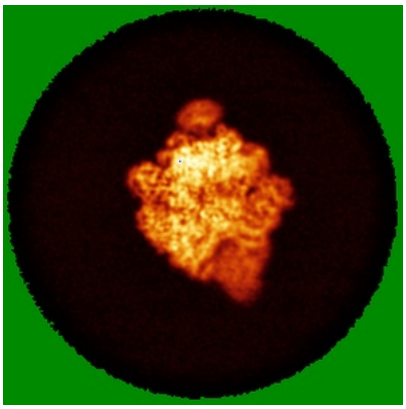


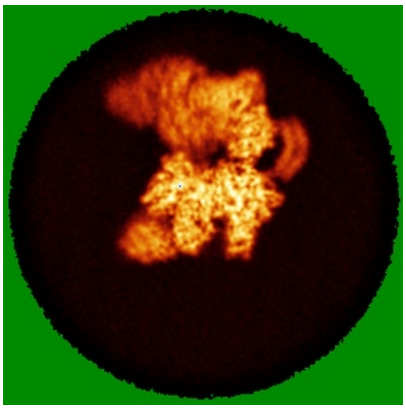
Z Index: 0

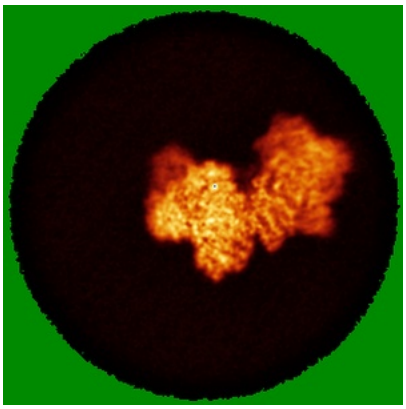
The images above show the largest variance slices of the map in three orthogonal directions.

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

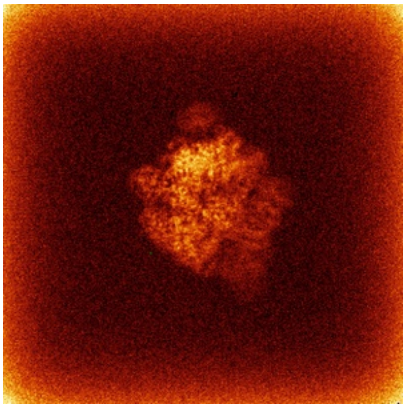
6.4.1 Primary map

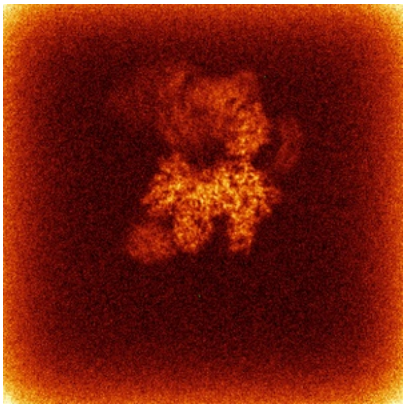

X

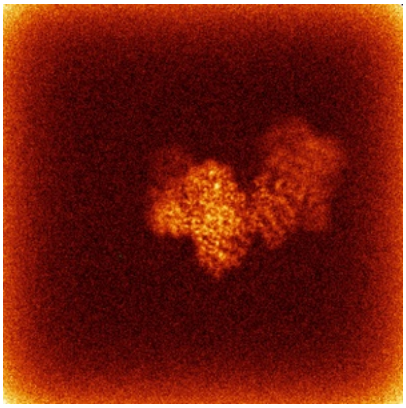

Y


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.

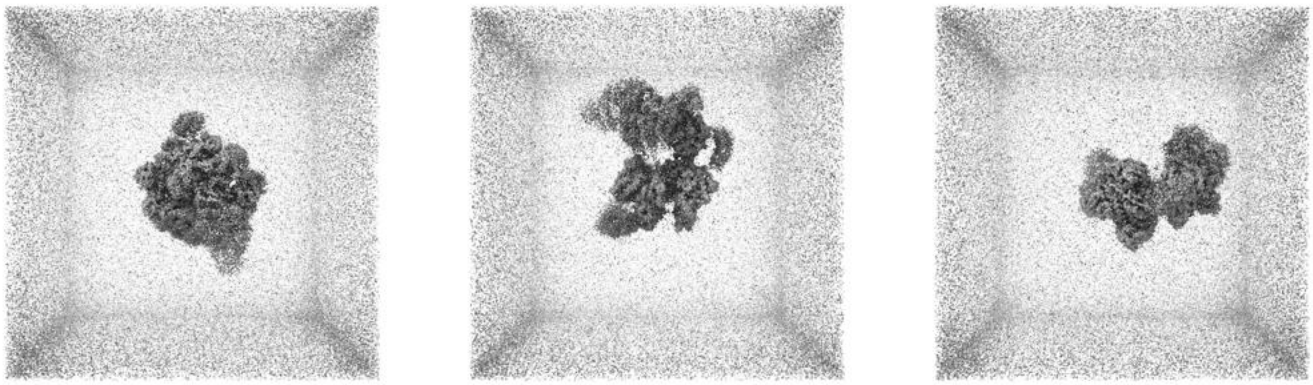
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

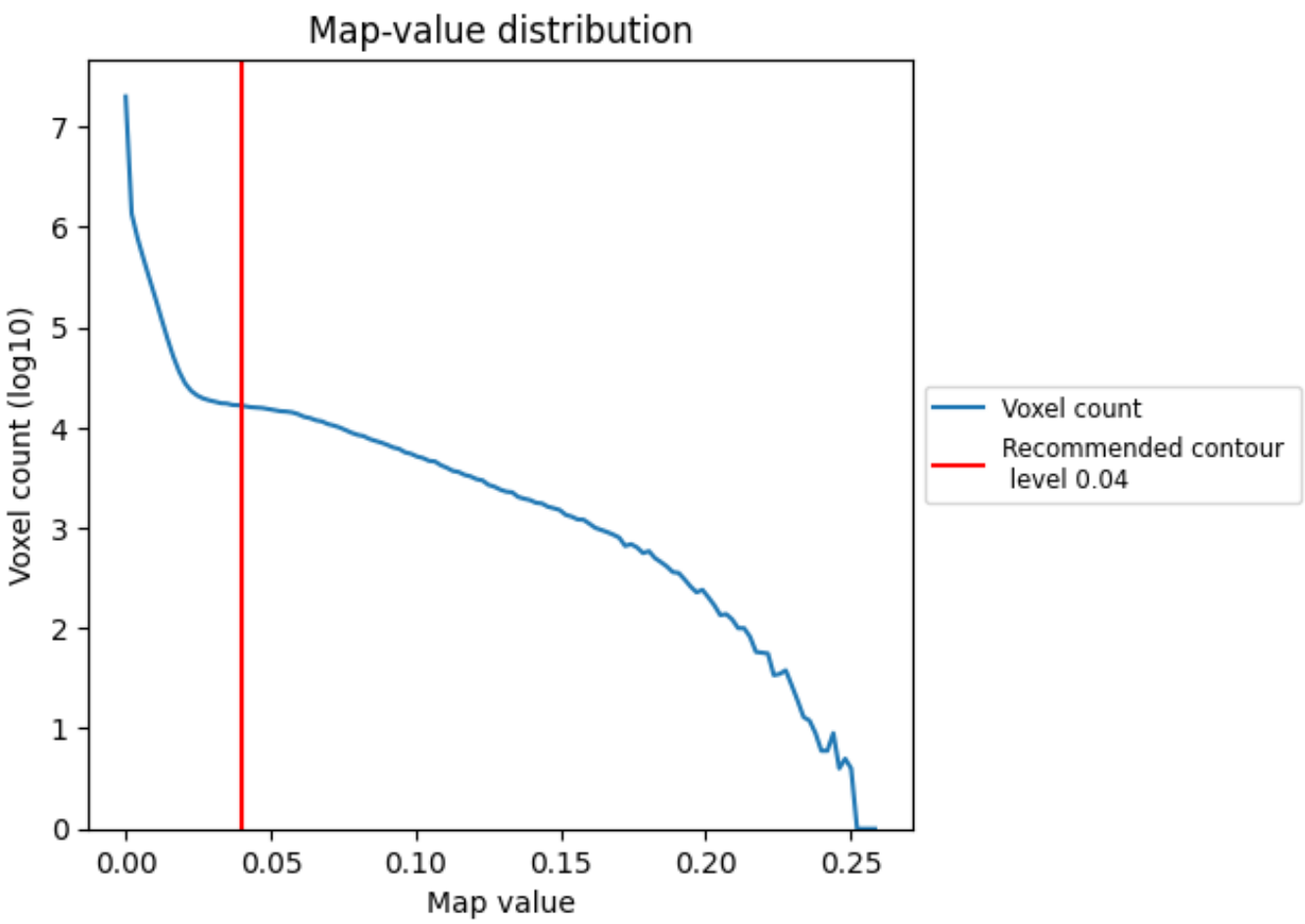
6.6 Mask visualisation (i)

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

7 Map analysis (i)

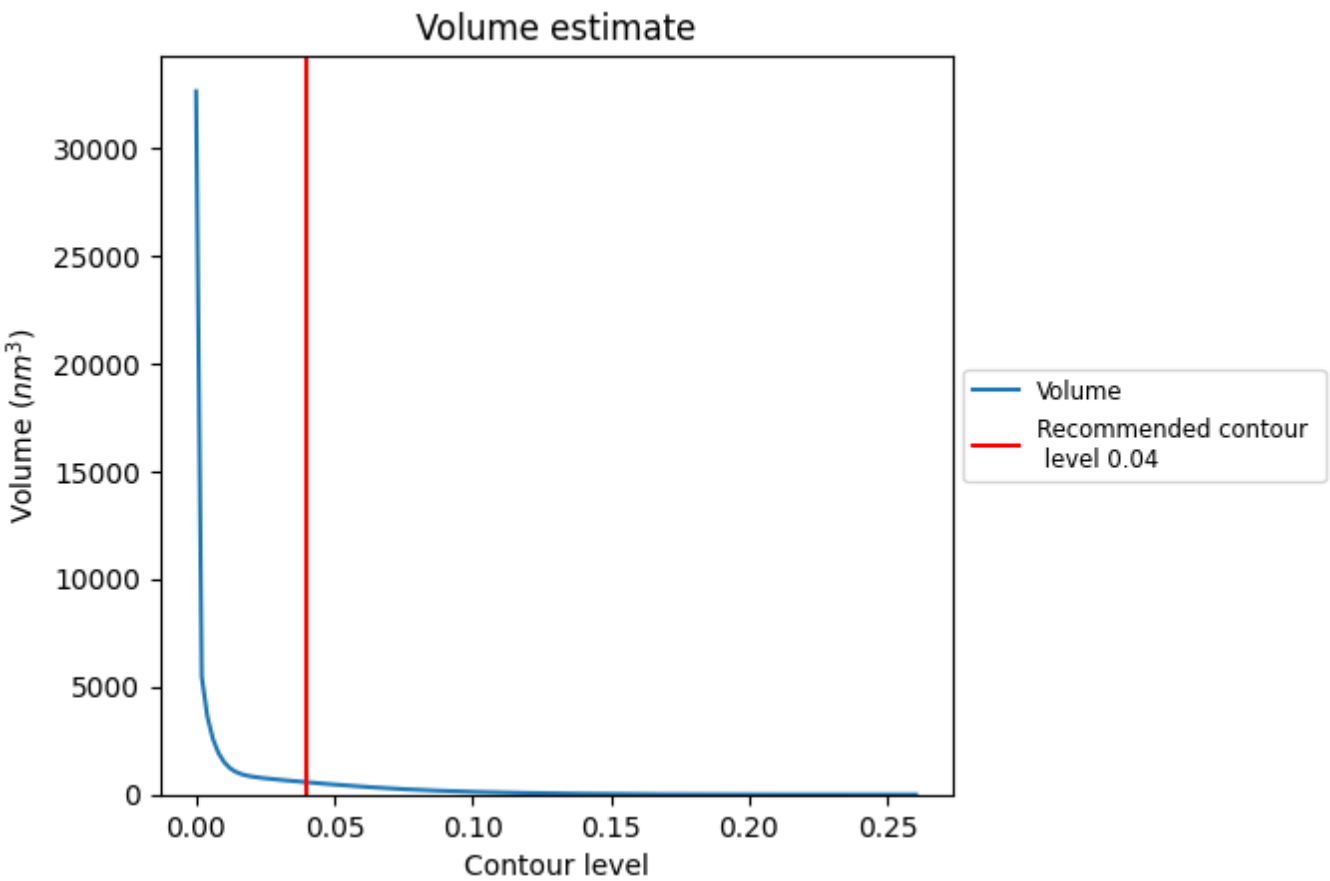
This section contains the results of statistical analysis of the map.

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.

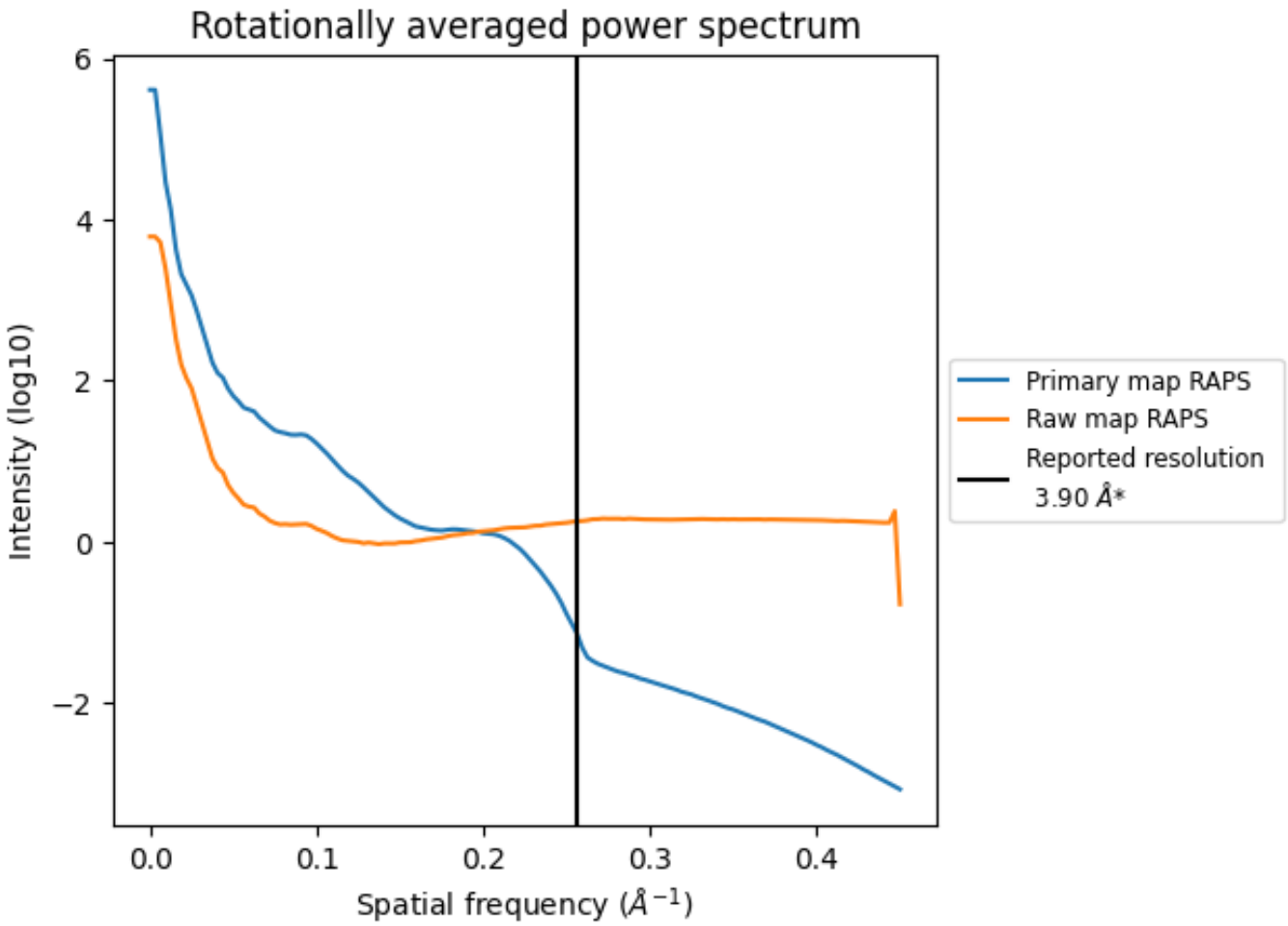
7.2 Volume estimate (i)



The volume at the recommended contour level is 571 nm^3; this corresponds to an approximate mass of 516 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)

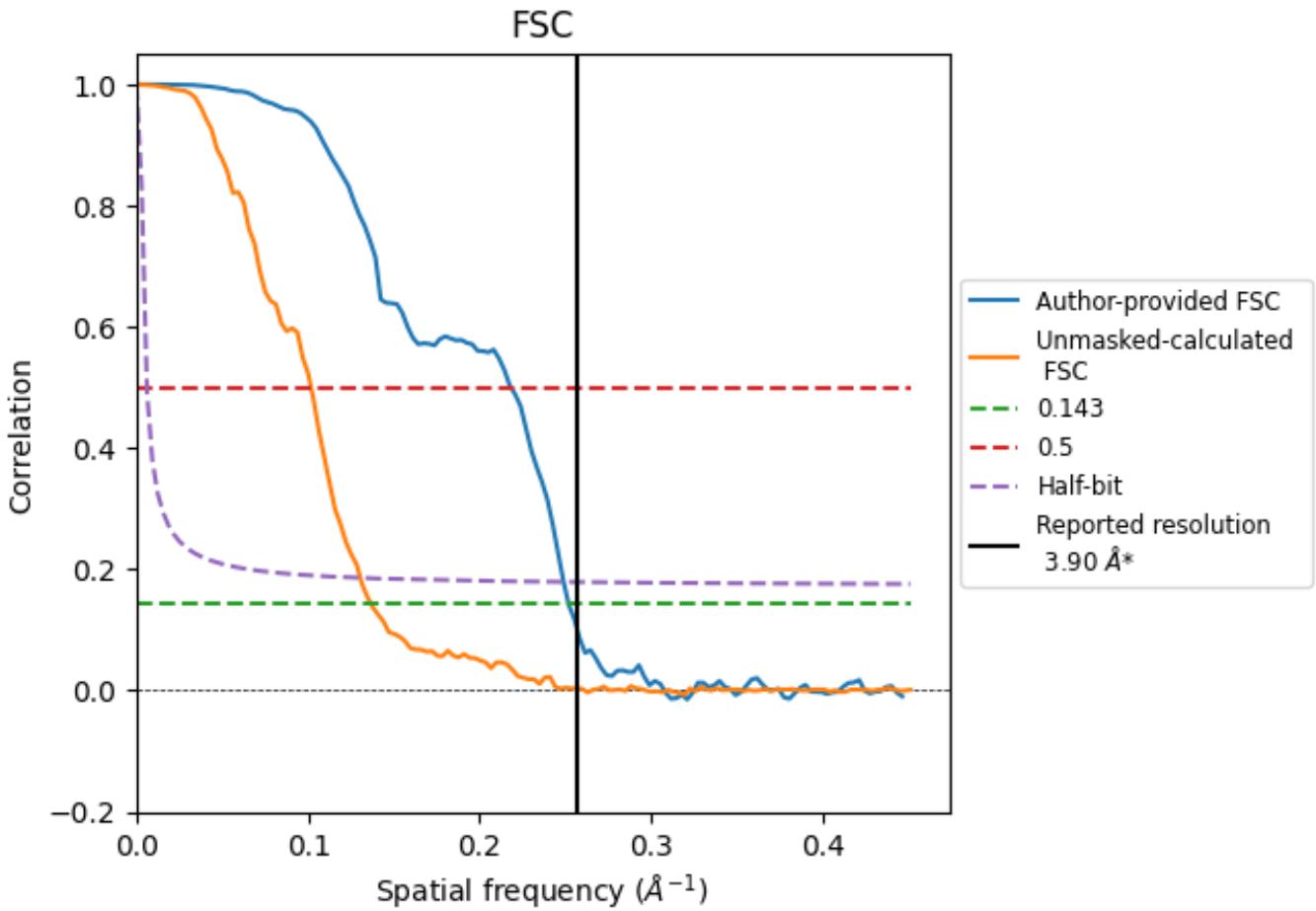


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

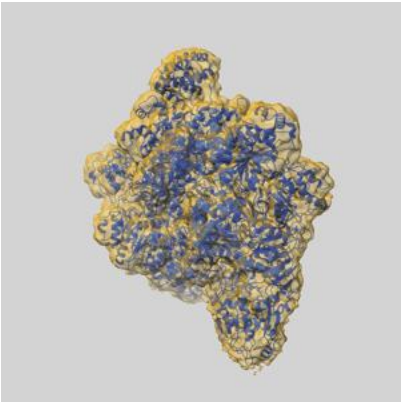
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.97	4.58	4.02
Unmasked-calculated*	7.32	9.82	7.66

*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 7.32 differs from the reported value 3.9 by more than 10 %

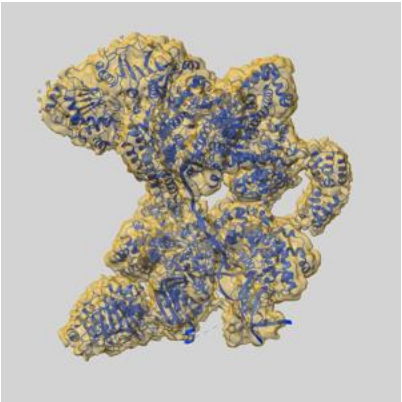
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-56252 and PDB model 9TU8. Per-residue inclusion information can be found in section 3 on page 6.

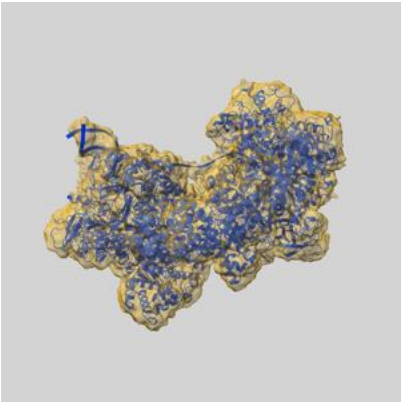
9.1 Map-model overlay (i)



X



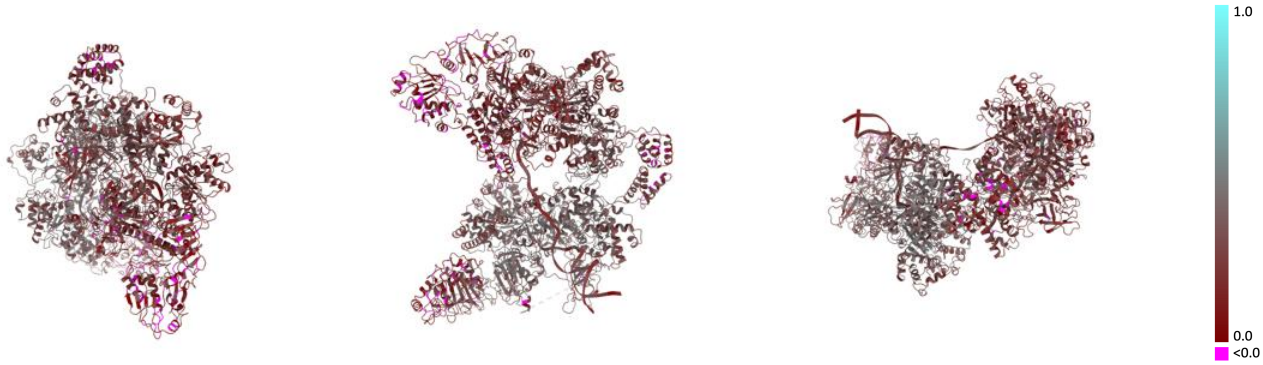
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

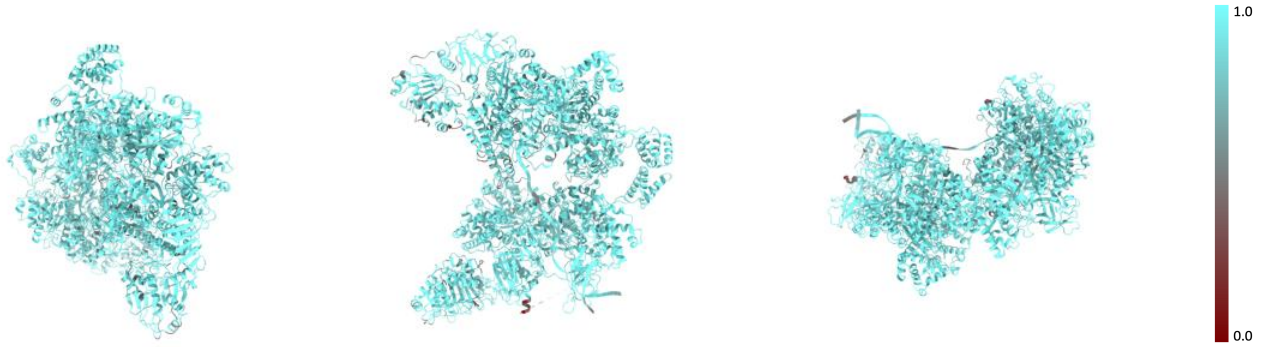
9.2 Q-score mapped to coordinate model (i)



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.

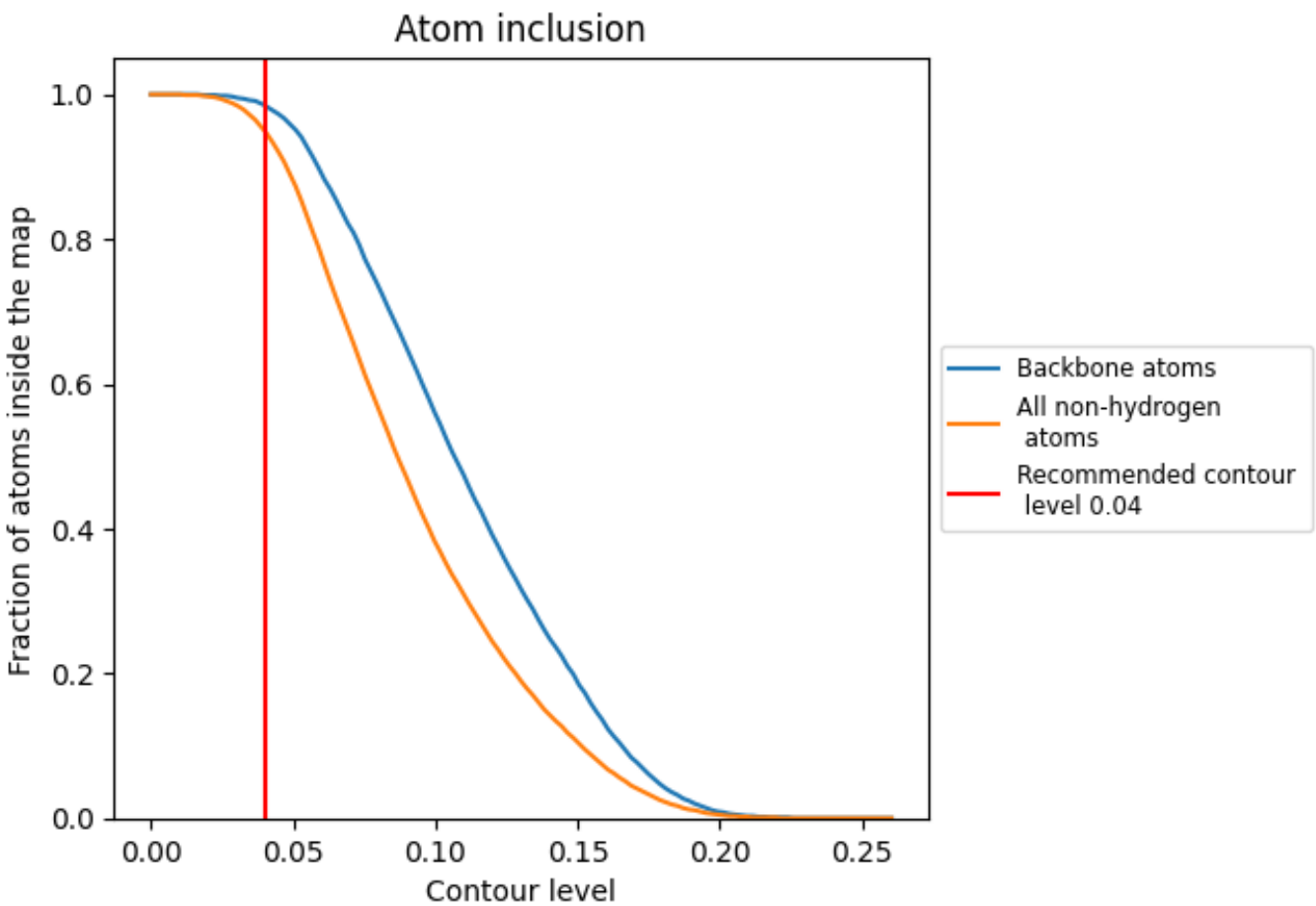
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 95% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9490	0.2890
G	0.8580	0.2390
I	0.9440	0.2980
Y	0.9680	0.3400
i	0.9300	0.3080
y	0.9340	0.2390