Full wwPDB EM Validation Report ⓘ

Nov 10, 2026 – 03:28 pm GMT

PDB ID	:	9TV4 / pdb_00009tv4
EMDB ID	:	EMD-56299
Title	:	Cryo-EM structure of human UGGT1 complexed with UDP
Authors	:	Aparicio, D.; Guerin, E.M.
Deposited on	:	2026-01-11
Resolution	:	3.80 Å(reported)

This is a Full wwPDB EM Validation 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:

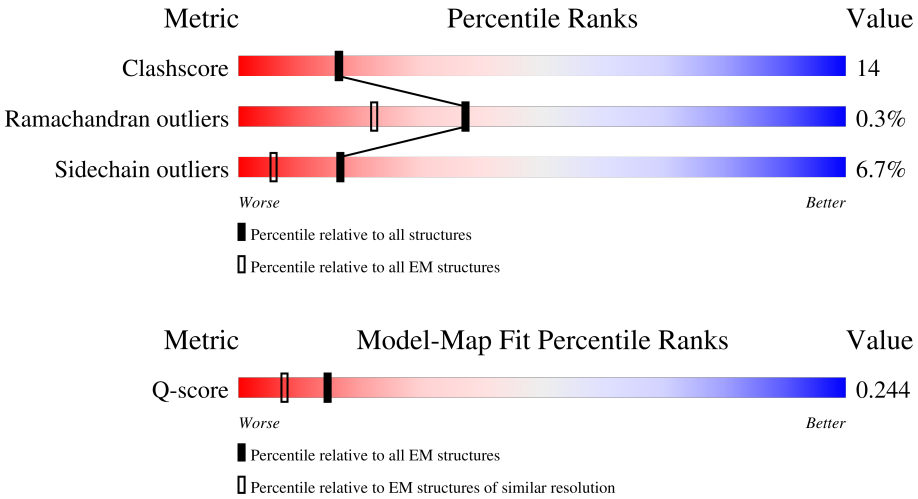
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.51

1 Overall quality at a glance

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	A	1509	8% 55% 18% · 26%

2 Entry composition

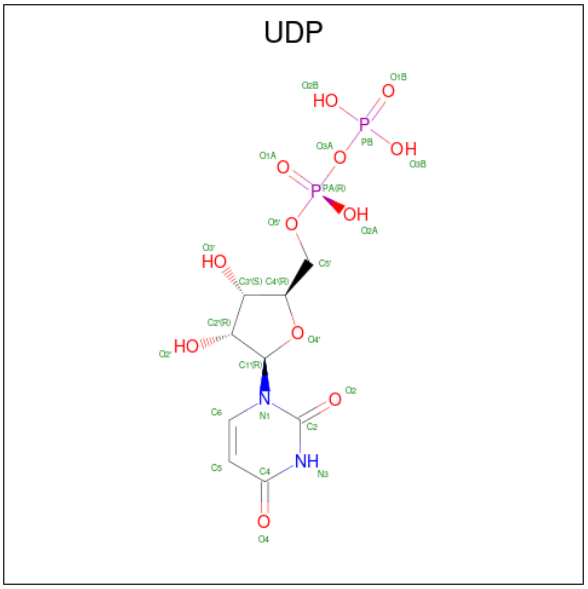
There are 3 unique types of molecules in this entry. The entry contains 7661 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-glucose:glycoprotein glucosyltransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1117	7635	4911	1333	1372	19	0	0

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	25	9	2	12	2	0

- Molecule 3 is water.

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

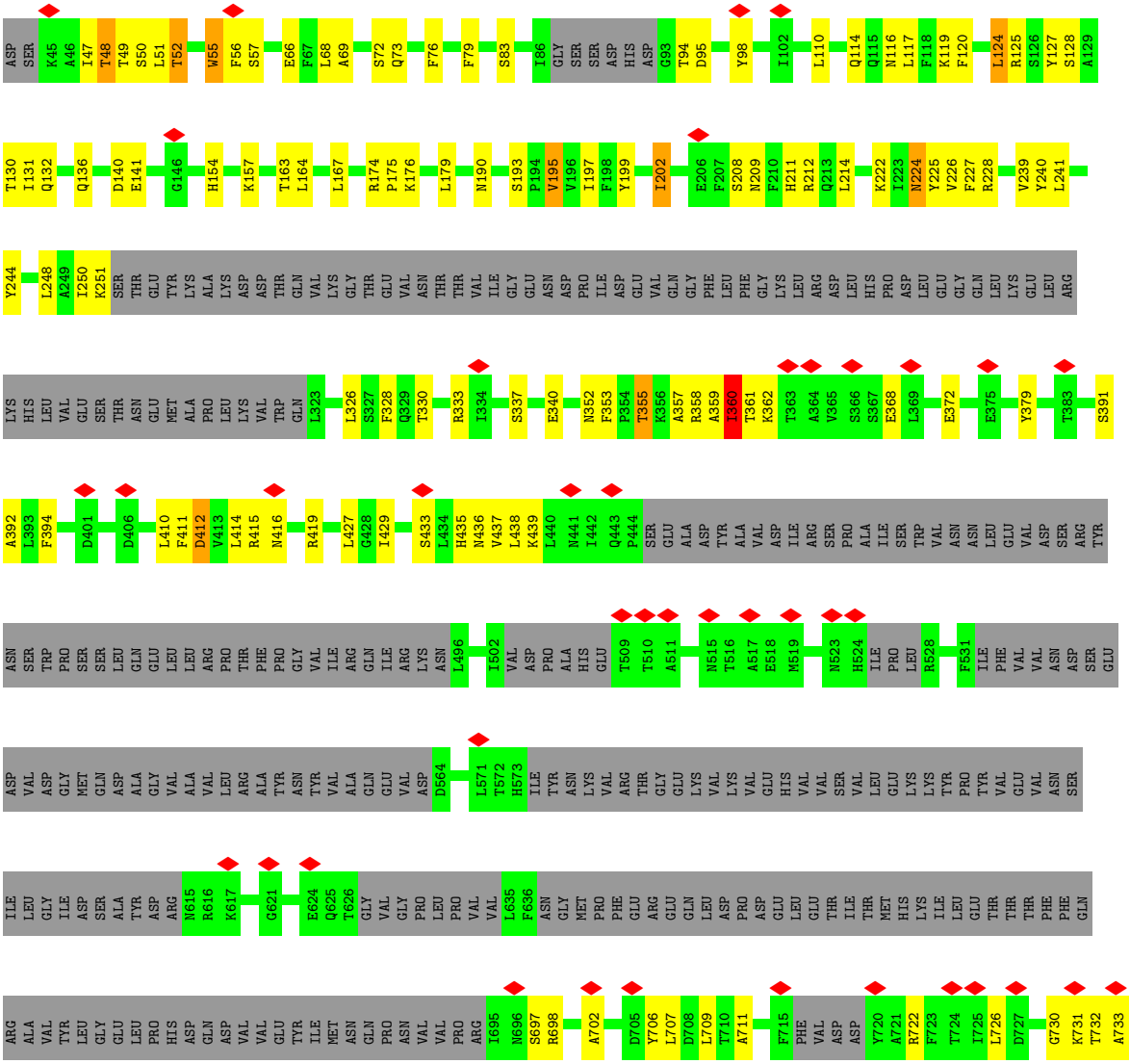
3 Residue-property plots (i)

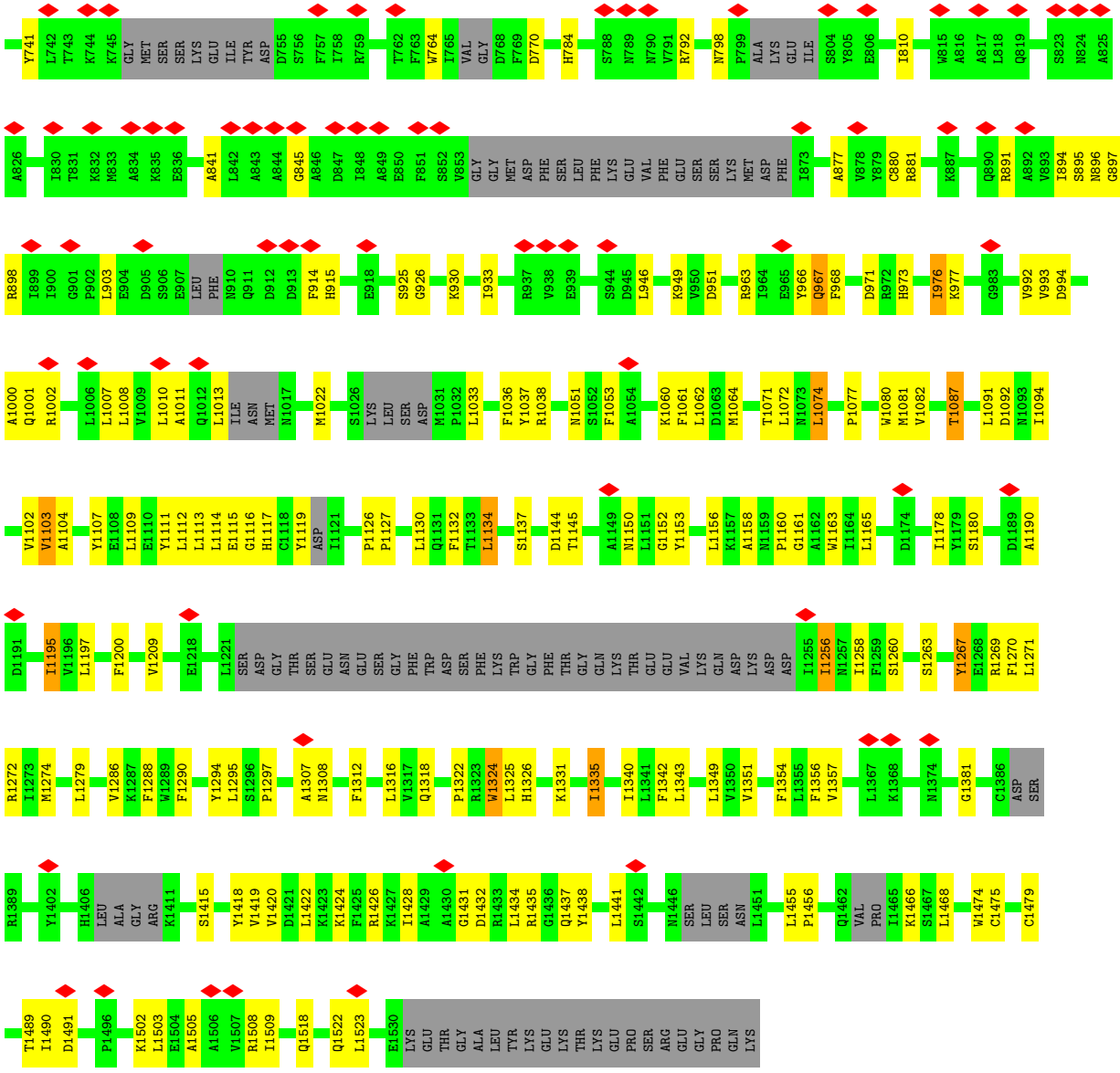
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: UDP-glucose:glycoprotein glucosyltransferase 1

Chain A:






Y741 L742 T743 K744 K745 GLY MET SER SER LYS GLU ILE TYR ASP D755 S756 F757 I758 R759 T762 F763 W764 I765 VAL GLY D768 F769 D770 H784 S788 N789 N790 V791 R792 N798 P799 ALA LYS GLU ILE S804 Y805 E806 I810 W815 A816 A817 L818 Q819 S823 N824 A825
A826 I830 T831 K832 M833 A834 K835 E836 A841 L842 A843 A844 G845 A846 D847 I848 A849 E850 F851 S852 V853 GLY GLY MET ASP PHE SER LEU PHE LYS GLU VAL PHE GLU SER SER LYS MET ASP PHE I873 A877 V878 Y879 C880 R881 K887 Q890 R891 A892 V893 I894 S895 N896 G897
R898 I899 I900 G901 P902 L903 E904 D905 S906 E907 LEU PHE N910 Q911 D912 D913 F914 H915 E918 S925 G926 K930 I933 R937 V938 E939 S944 D945 L946 K949 V950 D951 R963 I964 E965 Y966 Q967 F968 D971 R972 H973 I976 K977 G983 V992 V993 D994
A1000 Q1001 R1002 L1006 L1007 L1008 V1009 L1010 A1011 Q1012 L1013 ILE ASN MET N1017 M1022 S1026 LYS LEU SER ASP M1031 P1032 L1033 F1036 Y1037 R1038 N1051 S1052 F1053 A1054 K1060 F1061 L1062 D1063 M1064 T1071 L1072 N1073 L1074 P1077 W1080 M1081 V1082 T1087 L1091 D1092 N1093 I1094
V1102 V1103 A1104 Y1107 E1108 L1109 E1110 Y1111 L1112 L1113 L1114 E1115 G1116 H1117 C1118 Y1119 ASP I1121 P1126 P1127 L1130 Q1131 F1132 T1133 L1134 S1137 D1144 T1145 A1149 N1150 L1151 G1152 Y1153 L1156 K1157 A1158 N1159 P1160 G1161 A1162 W1163 T1164 L1165 D1174 I1178 Y1179 S1180 D1189 A1190
D1191 I1195 V1196 L1197 F1200 V1209 E1218 L1221 SER ASP GLY THR SER GLU ASN GLU SER GLY PHE TRP ASP SER PHE LYS TRP GLY PHE THR GLY GLN LYS THR GLU GLU VAL LYS GLN ASP LYS ASP ASP I1255 I1256 N1257 I1258 F1259 S1260 S1263 Y1267 E1268 R1269 F1270 L1271
R1272 I1273 M1274 L1279 V1286 K1287 F1288 W1289 F1290 Y1294 L1295 S1296 P1297 A1307 N1308 F1312 L1316 V1317 Q1318 P1322 R1323 W1324 L1325 H1326 K1331 I1335 I1340 L1341 F1342 L1343 L1349 V1350 V1351 F1354 L1355 F1356 V1357 L1367 K1368 N1374 G1381 C1386 ASP SER
R1389 Y1402 H1406 LEU ALA GLY ARG K1411 S1415 Y1418 V1419 V1420 D1421 L1422 K1423 K1424 F1425 R1426 K1427 I1428 A1429 A1430 G1431 D1432 R1433 L1434 R1435 G1436 Q1437 Y1438 L1441 S1442 N1446 SER LEU SER ASN L1451 L1455 P1456 Q1462 VAL PRO I1465 K1466 S1467 L1468 W1474 C1475 C1479
T1489 I1490 D1491 P1496 K1502 L1503 E1504 A1505 A1506 V1507 R1508 I1509 Q1518 Q1522 L1523 E1530 LYS GLU THR GLY ALA LEU TYR LYS GLU LYS THR LYS GLU PRO SER ARG GLU GLY PRO GLN LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT	Depositor
Number of particles used	56235, 56235, 56235, 56235	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	2.058	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.078	Depositor
Map size (Å)	253.44, 253.44, 253.44	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.66, 0.66, 0.66	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.17	0/7790	0.39	0/10671

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	7635	0	6429	198	0
2	A	25	0	11	5	0
3	A	1	0	0	0	0
All	All	7661	0	6440	199	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.

All (199) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1145:THR:HG23	1:A:1156:LEU:HD12	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:VAL:HG23	1:A:224:ASN:HB2	1.67	0.76
1:A:1518:GLN:O	1:A:1522:GLN:NE2	2.20	0.75
1:A:427:LEU:HD21	1:A:949:LYS:HD3	1.71	0.73
1:A:1260:SER:HA	1:A:1356:PHE:HE1	1.54	0.72
1:A:1263:SER:N	2:A:1601:UDP:O2	2.23	0.71
1:A:117:LEU:HD22	1:A:411:PHE:HE1	1.56	0.70
1:A:358:ARG:C	1:A:360:ILE:H	1.99	0.70
1:A:372:GLU:HG2	1:A:973:HIS:HB3	1.72	0.70
1:A:877:ALA:O	1:A:881:ARG:N	2.25	0.69
1:A:1178:ILE:H	1:A:1190:ALA:HB1	1.58	0.68
1:A:1117:HIS:ND1	1:A:1152:GLY:O	2.28	0.67
1:A:154:HIS:ND1	1:A:175:PRO:O	2.27	0.67
1:A:353:PHE:O	1:A:357:ALA:HB2	1.95	0.67
1:A:1505:ALA:HA	1:A:1508:ARG:HH12	1.58	0.67
1:A:1115:GLU:HB3	1:A:1153:TYR:HE1	1.60	0.66
1:A:435:HIS:O	1:A:439:LYS:N	2.28	0.64
1:A:1474:TRP:HB3	1:A:1490:ILE:HA	1.78	0.64
1:A:1007:LEU:O	1:A:1011:ALA:N	2.30	0.64
1:A:1150:ASN:OD1	1:A:1324:TRP:NE1	2.28	0.64
1:A:770:ASP:HA	1:A:810:ILE:HD13	1.80	0.63
1:A:176:LYS:NZ	1:A:193:SER:O	2.31	0.63
1:A:412:ASP:OD1	1:A:415:ARG:NH2	2.30	0.62
1:A:1343:LEU:HB3	1:A:1354:PHE:HE2	1.65	0.61
1:A:1002:ARG:NH2	1:A:1037:TYR:OH	2.33	0.61
1:A:51:LEU:HG	1:A:241:LEU:HD11	1.82	0.61
1:A:1134:LEU:HB3	1:A:1156:LEU:HD21	1.83	0.60
1:A:1081:MET:HG3	1:A:1113:LEU:HD21	1.82	0.60
1:A:125:ARG:HG3	1:A:128:SER:HB3	1.82	0.60
1:A:140:ASP:OD2	1:A:1137:SER:OG	2.20	0.60
1:A:416:ASN:OD1	1:A:419:ARG:NH2	2.34	0.60
1:A:1274:MET:HE2	1:A:1357:VAL:HG13	1.85	0.59
1:A:202:ILE:HD12	1:A:202:ILE:H	1.67	0.59
1:A:971:ASP:O	1:A:977:LYS:NZ	2.28	0.58
1:A:1294:TYR:HD2	1:A:1335:ILE:HD11	1.68	0.58
1:A:894:ILE:HG23	1:A:897:GLY:H	1.69	0.57
1:A:1115:GLU:HB3	1:A:1153:TYR:CE1	2.38	0.57
1:A:1165:LEU:HD22	1:A:1195:ILE:HD11	1.86	0.57
1:A:244:TYR:HB2	1:A:1074:LEU:HD21	1.87	0.56
1:A:784:HIS:CD2	1:A:914:PHE:HB3	2.41	0.56
1:A:1415:SER:O	1:A:1415:SER:OG	2.20	0.56
1:A:50:SER:HB2	1:A:240:TYR:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1091:LEU:HD23	1:A:1094:ILE:HD11	1.88	0.56
1:A:1144:ASP:OD1	1:A:1144:ASP:N	2.36	0.56
1:A:1116:GLY:O	1:A:1153:TYR:HA	2.06	0.56
1:A:1326:HIS:O	1:A:1438:TYR:OH	2.23	0.56
1:A:1267:TYR:HE2	2:A:1601:UDP:C5	2.24	0.56
1:A:190:ASN:OD1	1:A:193:SER:N	2.40	0.55
1:A:697:SER:O	1:A:698:ARG:HG2	2.06	0.55
1:A:57:SER:HA	1:A:239:VAL:HG13	1.87	0.55
1:A:358:ARG:C	1:A:360:ILE:N	2.61	0.55
1:A:891:ARG:O	1:A:903:LEU:N	2.30	0.55
1:A:1290:PHE:HB2	1:A:1316:LEU:HD22	1.88	0.55
1:A:433:SER:O	1:A:436:ASN:HB2	2.06	0.55
1:A:1356:PHE:HD2	1:A:1418:TYR:CZ	2.26	0.54
1:A:1474:TRP:O	1:A:1491:ASP:N	2.34	0.54
1:A:179:LEU:HD21	1:A:226:VAL:HG21	1.89	0.54
1:A:1114:LEU:HB2	1:A:1197:LEU:HD11	1.90	0.54
1:A:1431:GLY:HA2	1:A:1434:LEU:HD12	1.89	0.54
1:A:967:GLN:OE1	1:A:968:PHE:N	2.41	0.53
1:A:1279:LEU:HD21	1:A:1312:PHE:HB3	1.90	0.53
1:A:1260:SER:HA	1:A:1356:PHE:CE1	2.40	0.53
1:A:368:GLU:O	1:A:973:HIS:NE2	2.42	0.53
1:A:1119:TYR:HA	1:A:1126:PRO:HA	1.91	0.53
1:A:1502:LYS:O	1:A:1505:ALA:N	2.42	0.53
1:A:66:GLU:HG2	1:A:130:THR:HG21	1.90	0.53
1:A:127:TYR:O	1:A:130:THR:HG22	2.09	0.52
1:A:358:ARG:O	1:A:360:ILE:N	2.38	0.52
1:A:1340:ILE:HA	1:A:1343:LEU:HD11	1.91	0.52
1:A:1158:ALA:HB1	1:A:1163:TRP:CE2	2.44	0.52
1:A:392:ALA:HB1	1:A:394:PHE:CE1	2.45	0.51
1:A:1130:LEU:HG	1:A:1132:PHE:HE1	1.75	0.51
1:A:120:PHE:CE2	1:A:124:LEU:HD11	2.46	0.51
1:A:209:ASN:N	1:A:209:ASN:OD1	2.42	0.51
1:A:976:ILE:H	1:A:1022:MET:HB3	1.74	0.51
1:A:1508:ARG:HB3	1:A:1508:ARG:NH1	2.26	0.50
1:A:1505:ALA:O	1:A:1509:ILE:HG12	2.11	0.50
1:A:764:TRP:HB2	1:A:894:ILE:HB	1.92	0.50
1:A:352:ASN:OD1	1:A:1038:ARG:NH1	2.43	0.50
1:A:1081:MET:HE1	1:A:1318:GLN:HB2	1.94	0.50
1:A:1502:LYS:O	1:A:1503:LEU:C	2.55	0.50
1:A:51:LEU:HD13	1:A:1107:TYR:HB3	1.93	0.49
1:A:1422:LEU:HD13	1:A:1426:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:HD22	1:A:114:GLN:HB3	1.93	0.49
1:A:933:ILE:HG23	1:A:946:LEU:HD22	1.94	0.49
1:A:711:ALA:HB3	1:A:733:ALA:HB2	1.93	0.49
1:A:722:ARG:O	1:A:726:LEU:HG	2.13	0.49
1:A:1475:CYS:O	1:A:1479:CYS:N	2.45	0.49
1:A:333:ARG:O	1:A:337:SER:OG	2.26	0.48
1:A:128:SER:HA	1:A:131:ILE:HD12	1.95	0.48
1:A:798:ASN:HA	1:A:877:ALA:HB1	1.95	0.48
1:A:1112:LEU:HD12	1:A:1160:PRO:HG3	1.95	0.48
1:A:211:HIS:HD1	1:A:225:TYR:HH	1.61	0.48
1:A:1381:GLY:HA2	1:A:1466:LYS:O	2.14	0.48
1:A:877:ALA:HA	1:A:880:CYS:HB2	1.95	0.48
1:A:1114:LEU:HD11	1:A:1195:ILE:HG21	1.96	0.48
1:A:1424:LYS:O	1:A:1428:ILE:HG22	2.13	0.48
1:A:706:TYR:HD1	1:A:897:GLY:HA3	1.79	0.47
1:A:841:ALA:O	1:A:845:GLY:N	2.47	0.47
1:A:1505:ALA:HA	1:A:1508:ARG:NH1	2.28	0.47
1:A:926:GLY:O	1:A:930:LYS:N	2.45	0.47
1:A:95:ASP:HB2	1:A:1053:PHE:HB2	1.96	0.47
1:A:193:SER:OG	1:A:222:LYS:O	2.33	0.47
1:A:895:SER:O	1:A:895:SER:OG	2.25	0.47
1:A:1082:VAL:HG12	1:A:1109:LEU:HA	1.97	0.47
1:A:208:SER:O	1:A:212:ARG:HD3	2.14	0.47
1:A:167:LEU:O	1:A:174:ARG:NH2	2.48	0.47
1:A:1127:PRO:HG3	1:A:1209:VAL:HG11	1.97	0.47
1:A:784:HIS:CE1	1:A:915:HIS:HA	2.50	0.46
1:A:1340:ILE:HD12	1:A:1456:PRO:HD3	1.97	0.46
1:A:1381:GLY:O	1:A:1418:TYR:HA	2.15	0.46
1:A:1437:GLN:O	1:A:1441:LEU:HG	2.15	0.46
1:A:326:LEU:HD23	1:A:360:ILE:HG22	1.97	0.46
1:A:1267:TYR:CE2	2:A:1601:UDP:C6	3.04	0.46
1:A:1270:PHE:HZ	1:A:1503:LEU:HG	1.80	0.46
2:A:1601:UDP:H6	2:A:1601:UDP:C5'	2.27	0.46
1:A:1038:ARG:HB2	1:A:1061:PHE:CZ	2.50	0.46
1:A:68:LEU:HD12	1:A:79:PHE:CD2	2.50	0.46
1:A:117:LEU:HD11	1:A:414:LEU:HG	1.96	0.46
1:A:360:ILE:H	1:A:360:ILE:HG12	1.62	0.46
1:A:1010:LEU:O	1:A:1013:LEU:HG	2.16	0.46
1:A:1422:LEU:HD23	1:A:1422:LEU:HA	1.78	0.46
1:A:116:ASN:O	1:A:119:LYS:HG2	2.15	0.46
1:A:741:TYR:HB3	1:A:792:ARG:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ARG:O	1:A:360:ILE:HG12	2.14	0.45
1:A:726:LEU:HD22	1:A:730:GLY:HA3	1.98	0.45
1:A:1474:TRP:N	1:A:1489:THR:O	2.49	0.45
1:A:1153:TYR:CE2	1:A:1322:PRO:HB3	2.51	0.45
1:A:1071:THR:OG1	1:A:1092:ASP:O	2.20	0.45
1:A:1134:LEU:HD21	1:A:1163:TRP:HB3	1.97	0.45
1:A:214:LEU:HB3	1:A:225:TYR:CE2	2.52	0.45
1:A:810:ILE:HD12	1:A:810:ILE:H	1.80	0.45
1:A:702:ALA:O	1:A:898:ARG:NH2	2.50	0.45
1:A:1518:GLN:C	1:A:1522:GLN:HE21	2.23	0.45
1:A:179:LEU:HD23	1:A:179:LEU:HA	1.81	0.45
1:A:1087:THR:HG23	1:A:1297:PRO:HG2	1.98	0.45
1:A:1130:LEU:HG	1:A:1132:PHE:CE1	2.51	0.45
1:A:1322:PRO:HD2	1:A:1325:LEU:HD12	1.98	0.45
1:A:47:ILE:HD12	1:A:248:LEU:HD21	1.99	0.45
1:A:1144:ASP:HB2	1:A:1349:LEU:HD23	1.99	0.44
1:A:1256:ILE:HD11	1:A:1258:ILE:HD11	1.97	0.44
1:A:248:LEU:O	1:A:1036:PHE:N	2.49	0.44
1:A:429:ILE:HG21	1:A:437:VAL:HG21	1.98	0.44
1:A:1267:TYR:CE2	2:A:1601:UDP:C5	3.03	0.44
1:A:1271:LEU:HD11	1:A:1290:PHE:CE1	2.53	0.44
1:A:1422:LEU:HD13	1:A:1426:ARG:CZ	2.48	0.44
1:A:48:THR:HG23	1:A:1104:ALA:HA	2.00	0.44
1:A:1258:ILE:HB	1:A:1288:PHE:CD1	2.51	0.44
1:A:1269:ARG:HA	1:A:1272:ARG:CZ	2.48	0.44
1:A:49:THR:OG1	1:A:1072:LEU:HD11	2.18	0.44
1:A:52:THR:HG22	1:A:240:TYR:CE1	2.52	0.44
1:A:438:LEU:HB3	1:A:963:ARG:HH21	1.82	0.44
1:A:726:LEU:HB3	1:A:731:LYS:N	2.33	0.44
1:A:1468:LEU:HD12	1:A:1468:LEU:HA	1.85	0.43
1:A:925:SER:OG	1:A:926:GLY:N	2.49	0.43
1:A:1307:ALA:HA	1:A:1312:PHE:CE1	2.53	0.43
1:A:391:SER:HA	1:A:992:VAL:O	2.18	0.43
1:A:410:LEU:O	1:A:410:LEU:HD12	2.19	0.43
1:A:709:LEU:O	1:A:949:LYS:NZ	2.38	0.43
1:A:50:SER:HB2	1:A:240:TYR:HE1	1.83	0.43
1:A:1094:ILE:HD13	1:A:1103:VAL:HG21	2.00	0.43
1:A:154:HIS:CE1	1:A:176:LYS:HD3	2.53	0.43
1:A:1288:PHE:CD2	1:A:1312:PHE:HE2	2.37	0.43
1:A:72:SER:OG	1:A:73:GLN:N	2.52	0.43
1:A:136:GLN:NE2	1:A:1161:GLY:HA3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:TYR:OH	1:A:228:ARG:NH1	2.48	0.43
1:A:379:TYR:O	1:A:379:TYR:HD1	2.01	0.43
1:A:435:HIS:HA	1:A:438:LEU:HB2	2.00	0.43
1:A:994:ASP:O	1:A:1000:ALA:HB2	2.19	0.43
1:A:1008:LEU:HD23	1:A:1008:LEU:HA	1.83	0.43
1:A:55:TRP:HB3	1:A:132:GLN:CD	2.44	0.42
1:A:197:ILE:HA	1:A:226:VAL:O	2.19	0.42
1:A:1308:ASN:OD1	1:A:1308:ASN:C	2.62	0.42
1:A:427:LEU:HD23	1:A:427:LEU:HA	1.78	0.42
1:A:1060:LYS:HE3	1:A:1062:LEU:HD11	2.01	0.42
1:A:1294:TYR:CG	1:A:1331:LYS:HE3	2.54	0.42
1:A:120:PHE:CZ	1:A:124:LEU:HD21	2.55	0.42
1:A:326:LEU:H	1:A:326:LEU:HD12	1.84	0.42
1:A:707:LEU:HD11	1:A:732:THR:HG22	2.02	0.42
1:A:69:ALA:HA	1:A:76:PHE:HB2	2.02	0.42
1:A:76:PHE:HZ	1:A:227:PHE:HE2	1.68	0.42
1:A:1270:PHE:CZ	1:A:1503:LEU:HG	2.55	0.42
1:A:1432:ASP:OD1	1:A:1435:ARG:NH2	2.53	0.42
1:A:117:LEU:HD23	1:A:117:LEU:HA	1.79	0.41
1:A:1064:MET:HE3	1:A:1064:MET:HB3	1.82	0.41
1:A:1343:LEU:HD22	1:A:1420:VAL:HG21	2.02	0.41
1:A:1351:VAL:HG13	1:A:1422:LEU:HD12	2.02	0.41
1:A:976:ILE:HD13	1:A:976:ILE:HA	1.85	0.41
1:A:340:GLU:N	1:A:340:GLU:OE2	2.53	0.41
1:A:1523:LEU:HD12	1:A:1523:LEU:HA	1.80	0.41
1:A:94:THR:HB	1:A:1051:ASN:O	2.21	0.41
1:A:250:ILE:O	1:A:251:LYS:HG3	2.21	0.41
1:A:925:SER:OG	1:A:951:ASP:OD2	2.32	0.41
1:A:154:HIS:CE1	1:A:176:LYS:HA	2.56	0.41
1:A:1077:PRO:HD2	1:A:1080:TRP:CE3	2.56	0.40
1:A:361:THR:O	1:A:362:LYS:C	2.63	0.40
1:A:141:GLU:HG3	1:A:157:LYS:HE2	2.04	0.40
1:A:1256:ILE:HG23	1:A:1286:VAL:HG12	2.03	0.40
1:A:1081:MET:HB2	1:A:1111:TYR:HB2	2.04	0.40

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	1069/1509 (71%)	973 (91%)	93 (9%)	3 (0%)	36 67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	ILE
1	A	359	ALA
1	A	355	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	597/1343 (44%)	557 (93%)	40 (7%)	15 41

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	THR
1	A	52	THR
1	A	55	TRP
1	A	56	PHE
1	A	83	SER
1	A	98	TYR
1	A	124	LEU
1	A	163	THR

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Mol	Chain	Res	Type
1	A	164	LEU
1	A	195	VAL
1	A	202	ILE
1	A	224	ASN
1	A	328	PHE
1	A	330	THR
1	A	355	THR
1	A	360	ILE
1	A	412	ASP
1	A	896	ASN
1	A	966	TYR
1	A	967	GLN
1	A	976	ILE
1	A	993	VAL
1	A	1001	GLN
1	A	1033	LEU
1	A	1074	LEU
1	A	1087	THR
1	A	1102	VAL
1	A	1103	VAL
1	A	1134	LEU
1	A	1180	SER
1	A	1195	ILE
1	A	1200	PHE
1	A	1256	ILE
1	A	1267	TYR
1	A	1295	LEU
1	A	1324	TRP
1	A	1335	ILE
1	A	1342	PHE
1	A	1419	VAL
1	A	1455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	1439	GLN
1	A	1470	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)

1 ligand is modelled in this entry.

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	UDP	A	1601	-	24,26,26	0.66	0	37,40,40	0.73	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
2	UDP	A	1601	-	-	6/16/32/32	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1601	UDP	O3'-C3'-C4'	-2.25	104.55	111.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1601	UDP	O4'-C4'-C5'-O5'
2	A	1601	UDP	C5'-O5'-PA-O3A
2	A	1601	UDP	C3'-C4'-C5'-O5'
2	A	1601	UDP	PB-O3A-PA-O1A
2	A	1601	UDP	C5'-O5'-PA-O1A
2	A	1601	UDP	PB-O3A-PA-O2A

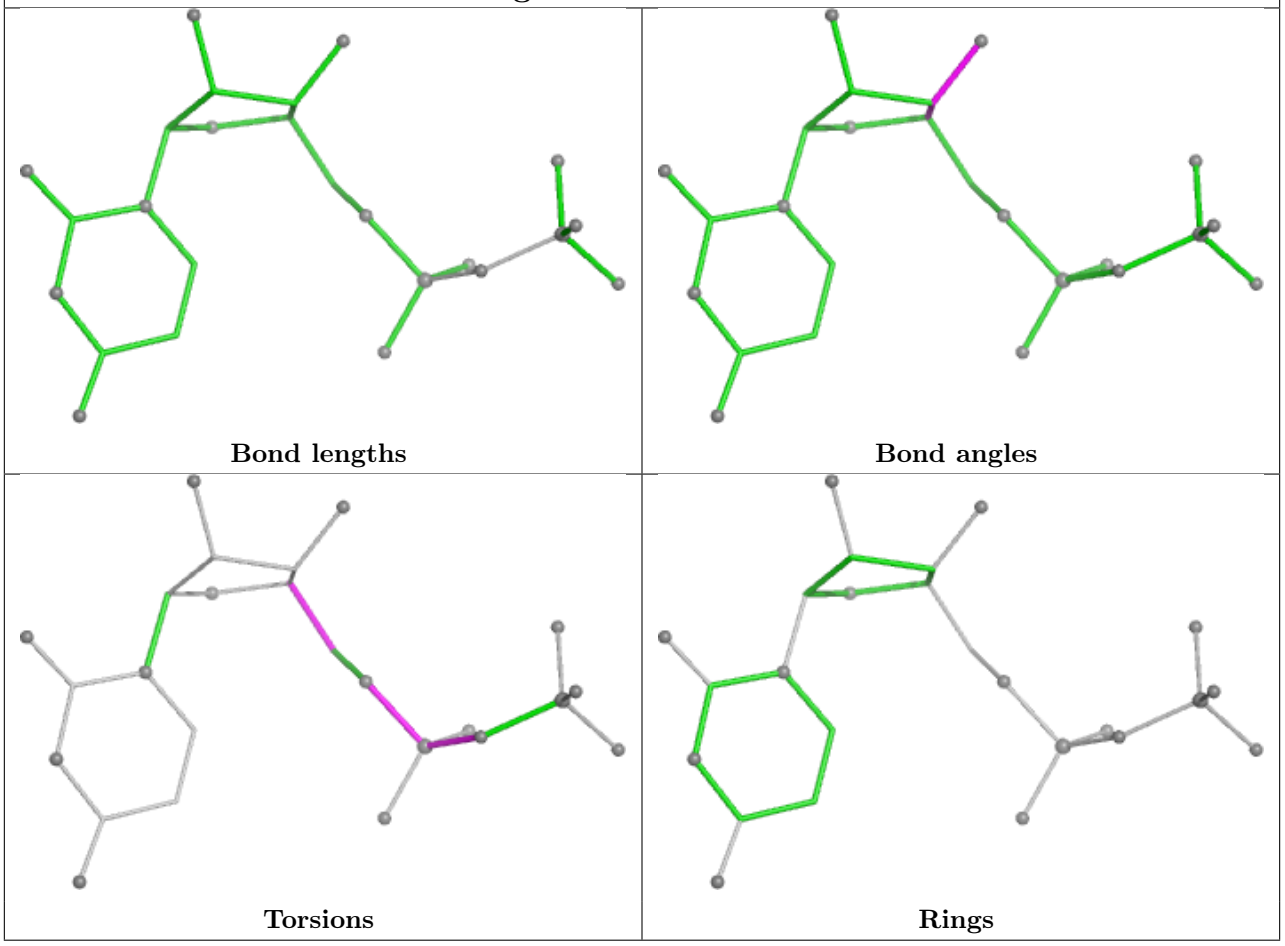
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1601	UDP	5	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 UDP A 1601



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.

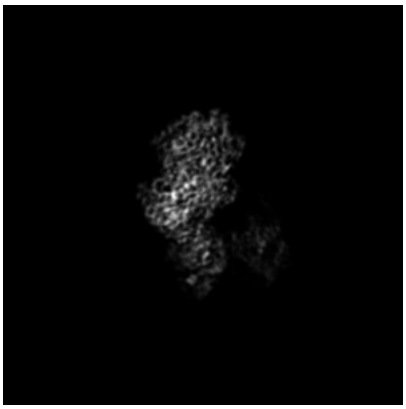
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-56299. These allow visual inspection of the internal detail of the map and identification of artifacts.

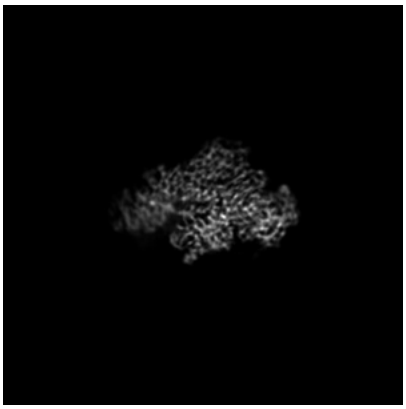
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

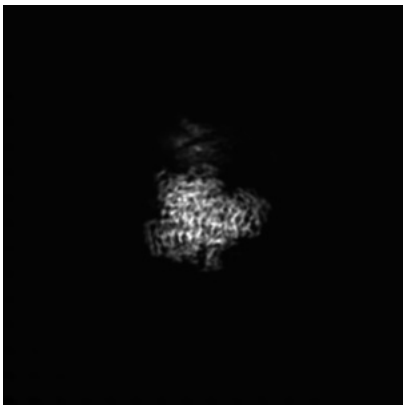
6.1.1 Primary map



X

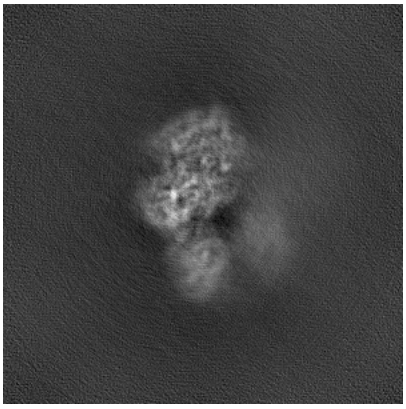


Y

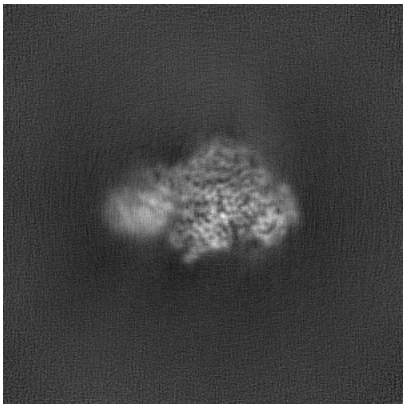


Z

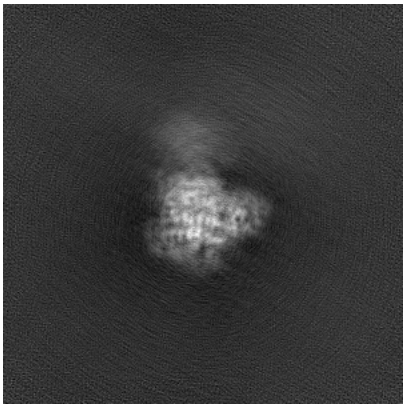
6.1.2 Raw map



X



Y



Z

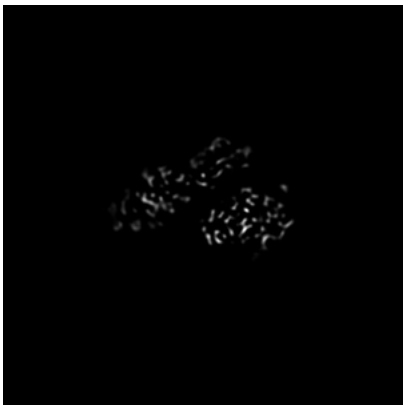
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 192

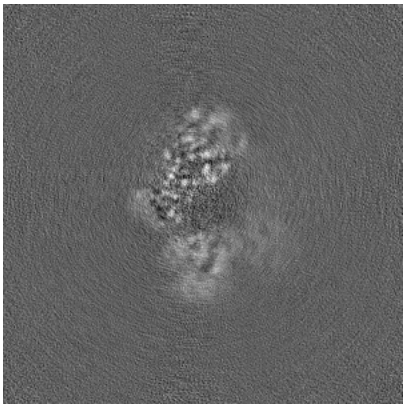


Y Index: 192

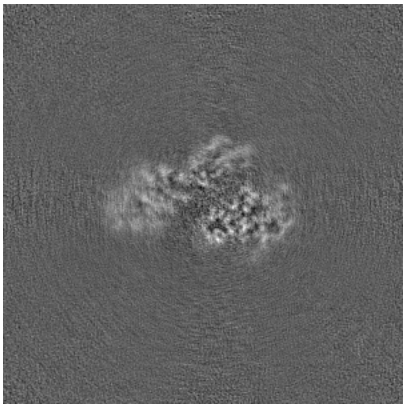


Z Index: 192

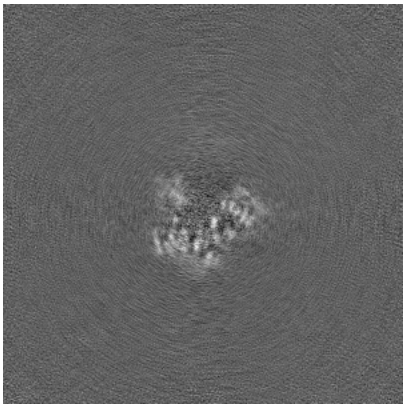
6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

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

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 180

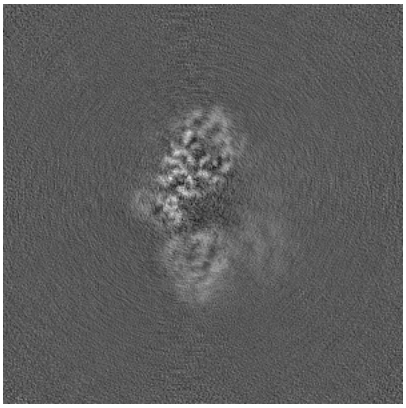


Y Index: 174

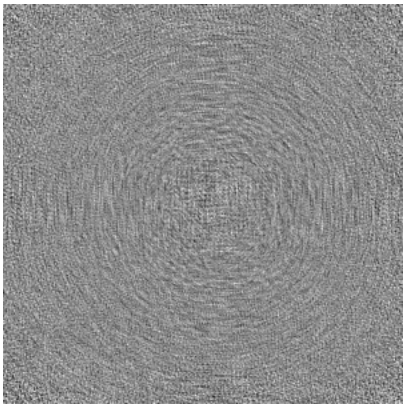


Z Index: 203

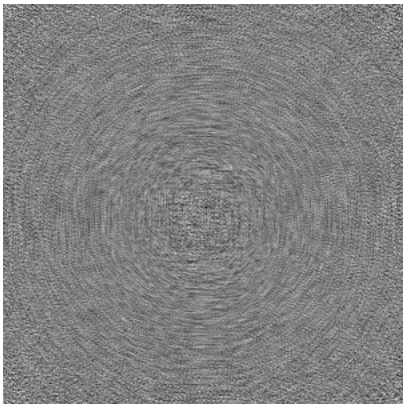
6.3.2 Raw map



X Index: 188



Y Index: 0

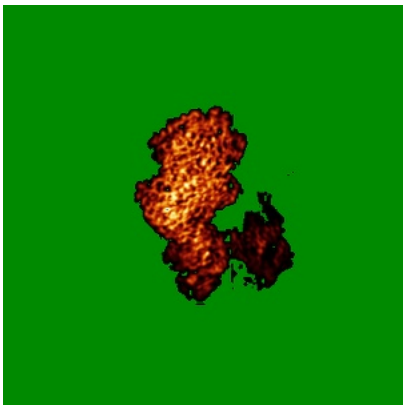


Z Index: 0

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

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

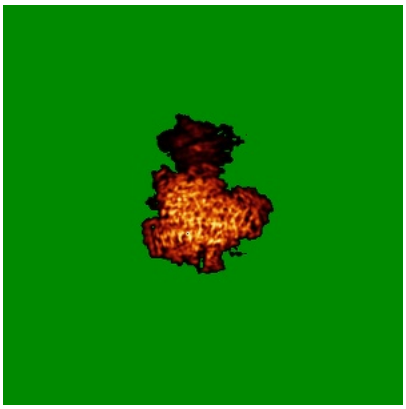
6.4.1 Primary map



X

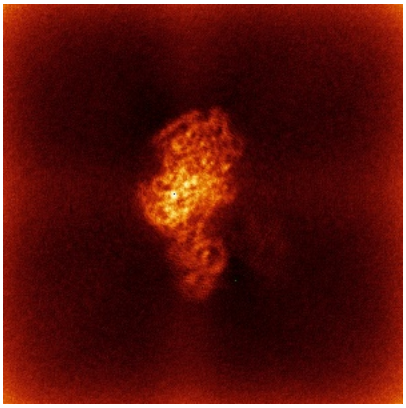


Y

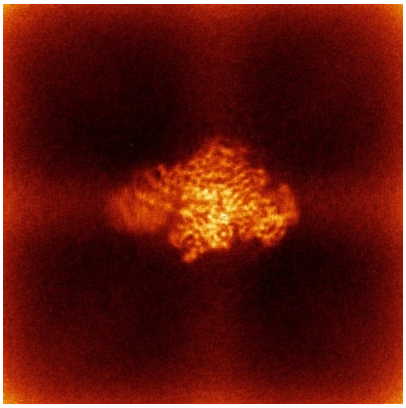


Z

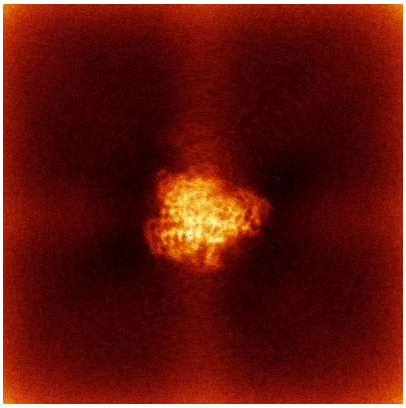
6.4.2 Raw map



X



Y

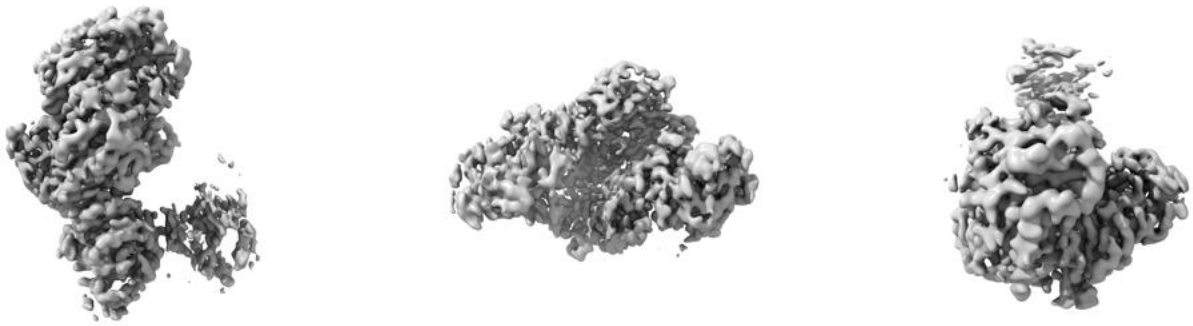


Z

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 0.078. 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.

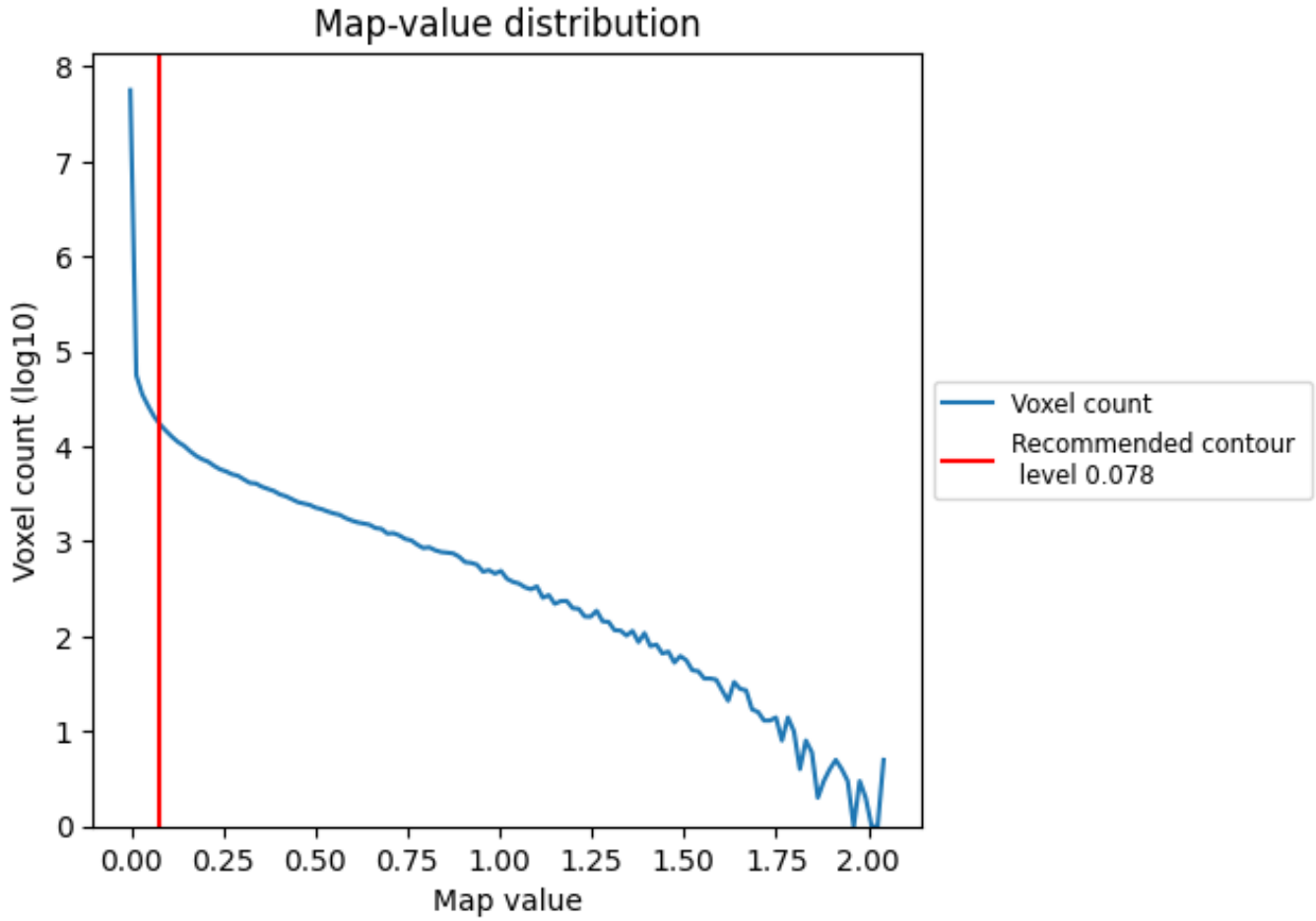
6.6 Mask visualisation (i)

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

7 Map analysis

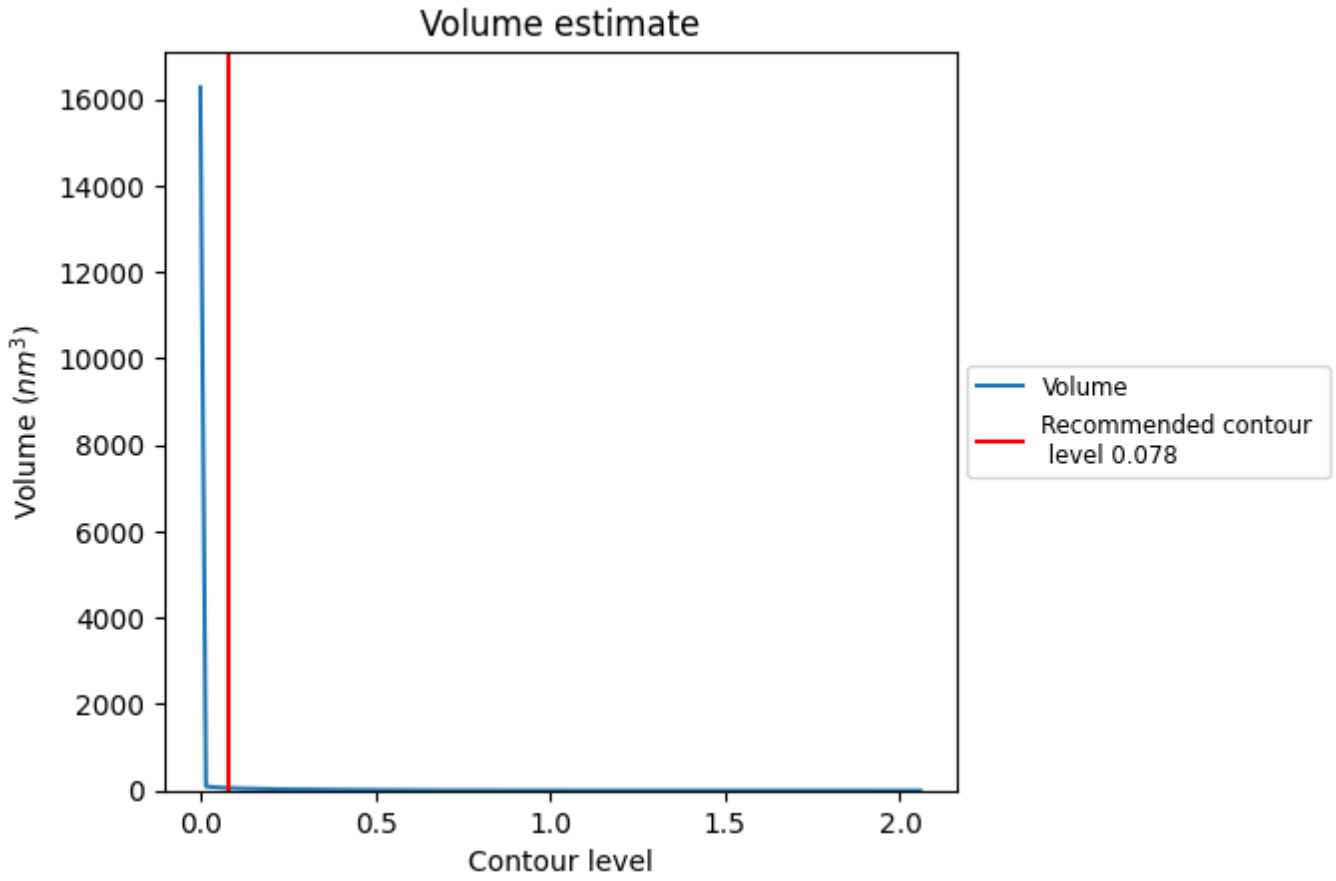
This section contains the results of statistical analysis of the map.

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.

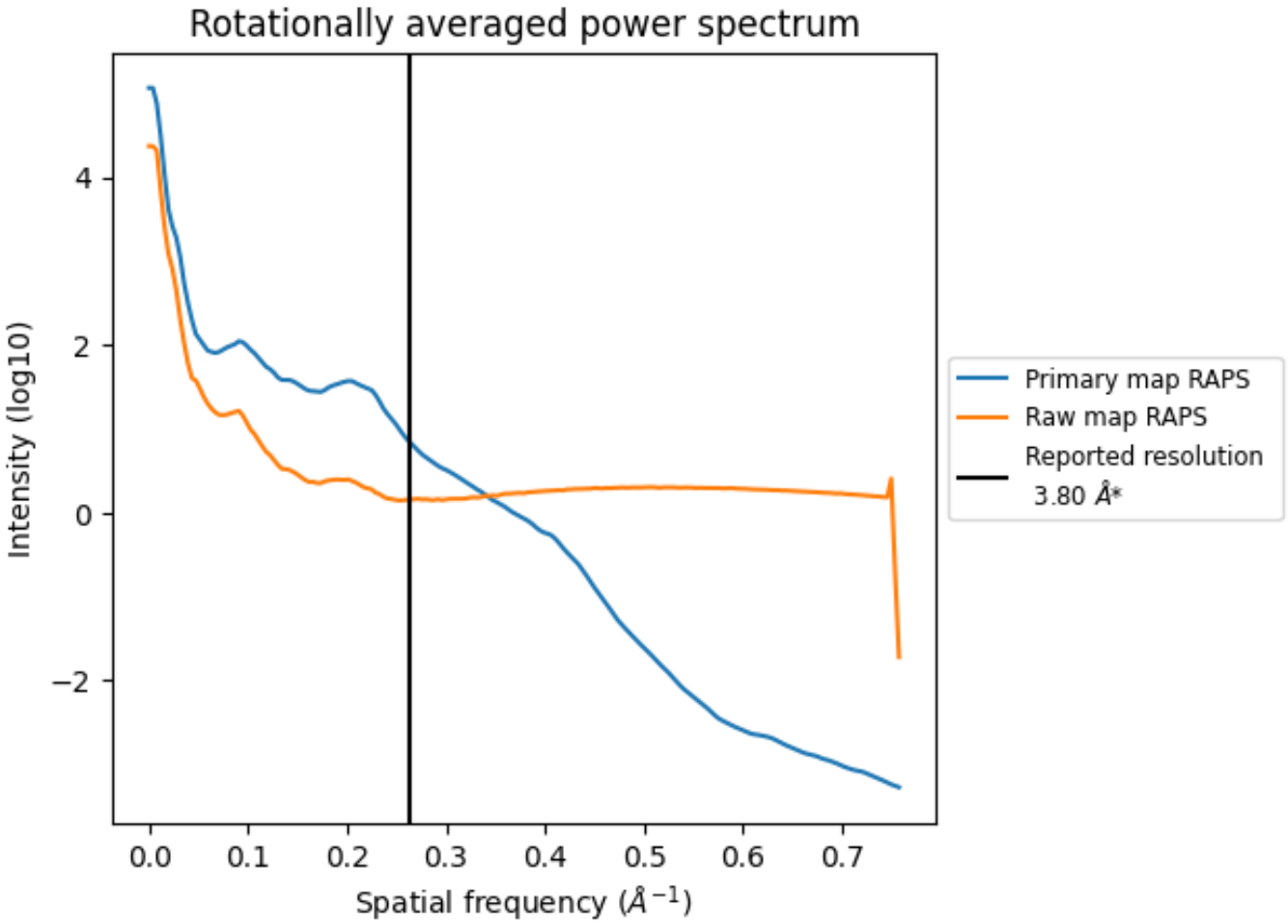
7.2 Volume estimate



The volume at the recommended contour level is 60 nm^3; this corresponds to an approximate mass of 54 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)

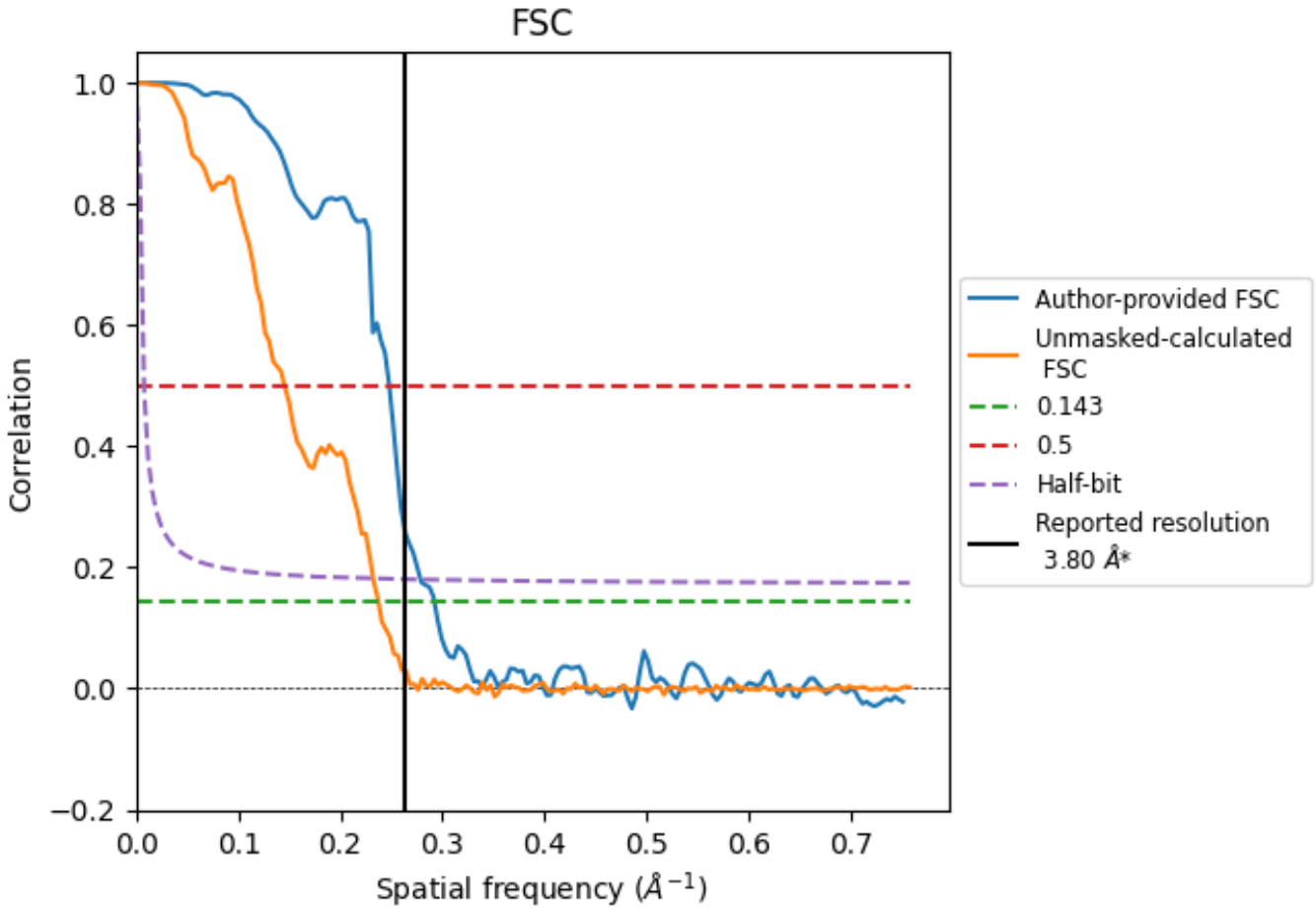


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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)

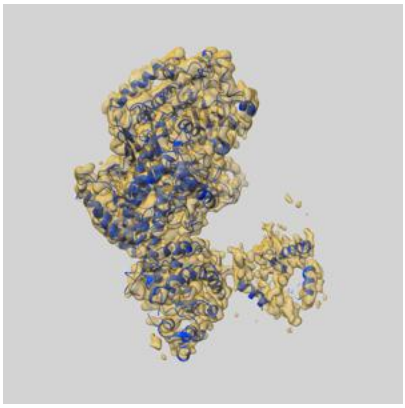
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	3.42	4.03	3.59
Unmasked-calculated*	4.21	6.88	4.31

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

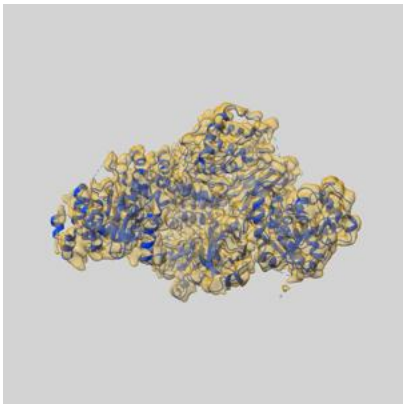
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-56299 and PDB model 9TV4. Per-residue inclusion information can be found in section 3 on page 4.

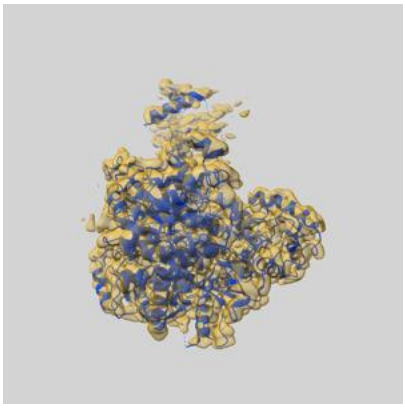
9.1 Map-model overlay



X



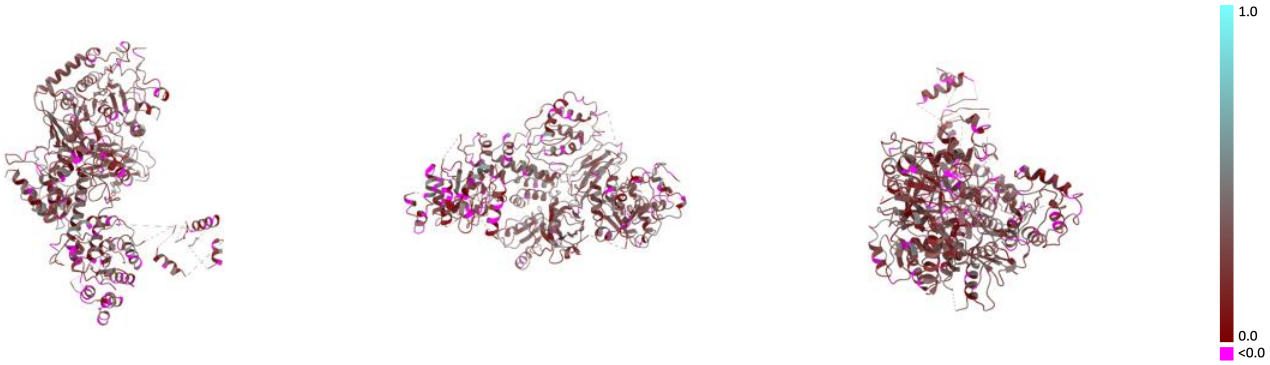
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.078 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.

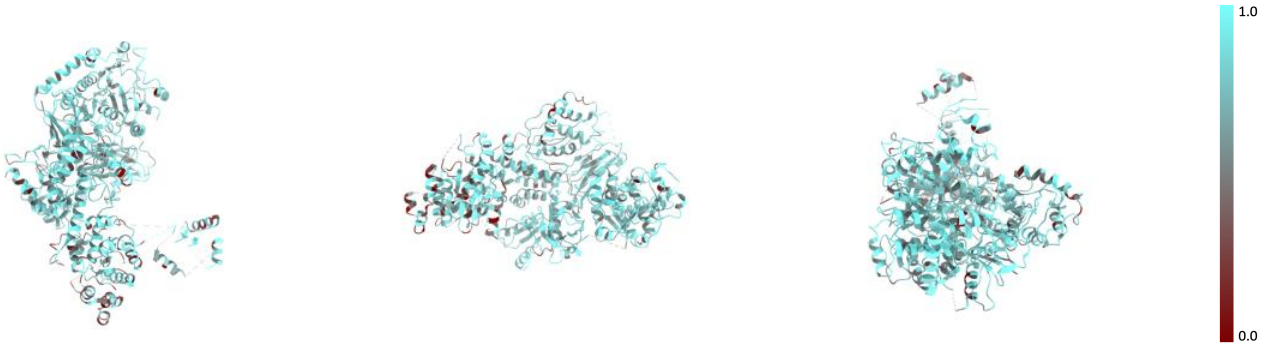
9.2 Q-score mapped to coordinate model (i)



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.

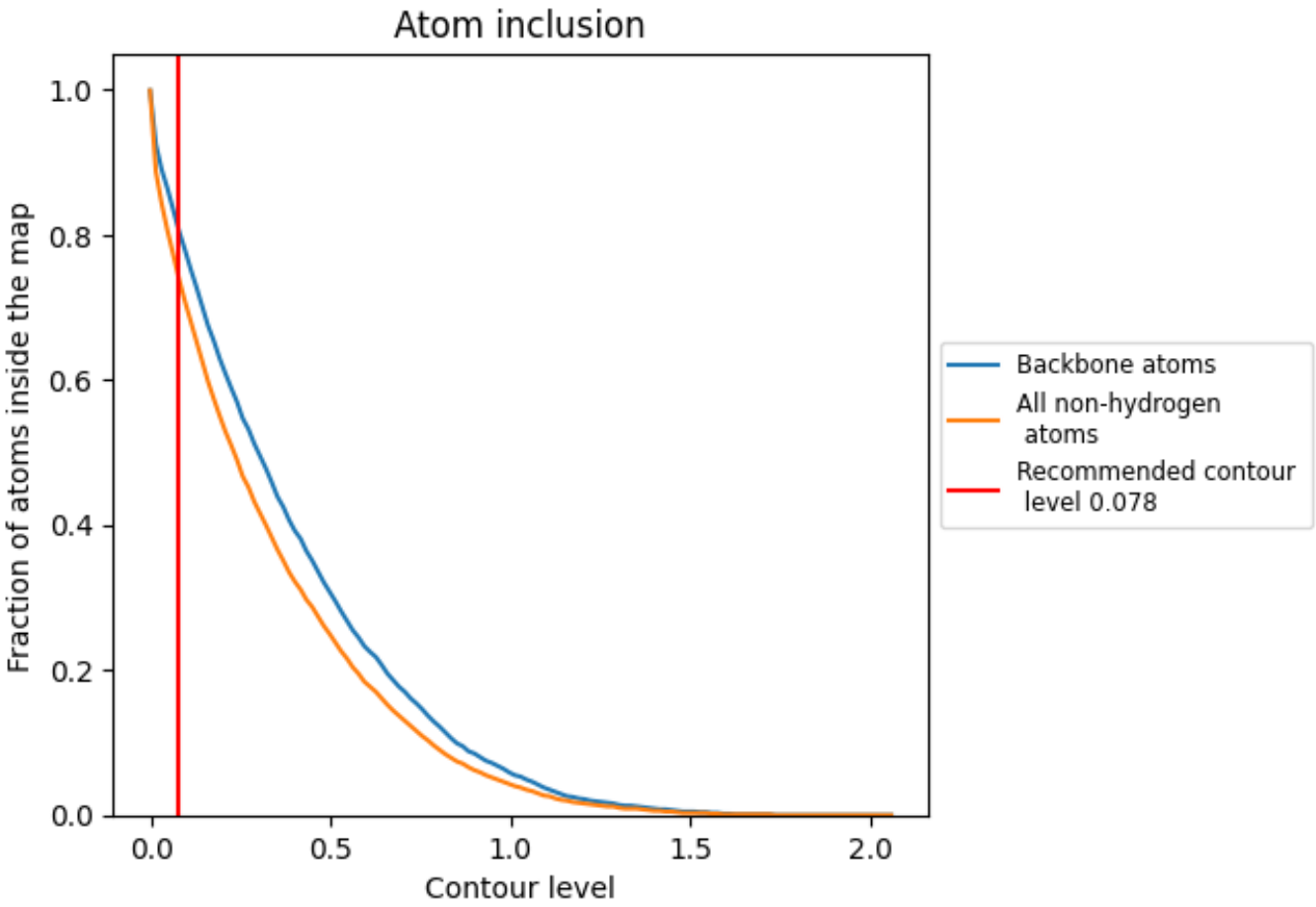
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.078).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 74% 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 (0.078) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7410	0.2440
A	0.7410	0.2440