Full wwPDB EM Validation Report

Jan 27, 2022 – 03:35 am GMT

PDB ID	:	7Q97
EMDB ID	:	EMD-13867
Title	:	Structure of the bacterial type VI secretion system effector RhsA.
Authors	:	Guenther, P.; Quentin, D.; Ahmad, S.; Sachar, K.; Gatsogiannis, C.; Whitney, J.C.; Raunser, S.
Deposited on	:	2021-11-12
Resolution	:	3.30 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 following versions of software and data (see references ⓘ) were used in the production of this report:

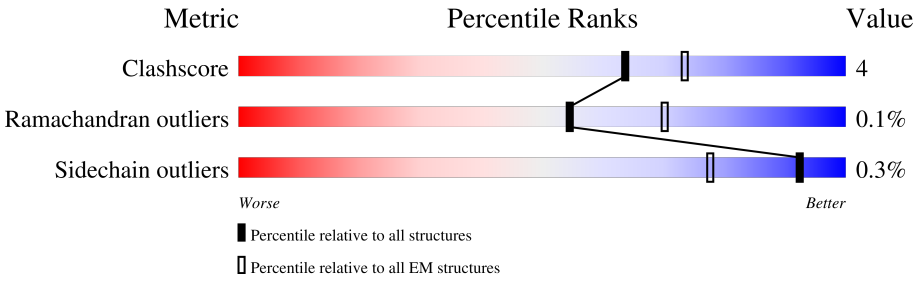
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1426	43% 65% 8% 27%
1	B	1426	43% 65% 8% 27%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 32806 atoms, of which 15752 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 Rhs family protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1047	Total	C	H	N	O	S	2	0
			16403	5311	7876	1575	1629	12		
1	B	1047	Total	C	H	N	O	S	2	0
			16403	5311	7876	1575	1629	12		

There are 148 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	MET	deletion	UNP Q4K3M9
A	?	-	SER	deletion	UNP Q4K3M9
A	?	-	ASP	deletion	UNP Q4K3M9
A	?	-	ALA	deletion	UNP Q4K3M9
A	?	-	LEU	deletion	UNP Q4K3M9
A	?	-	TRP	deletion	UNP Q4K3M9
A	?	-	ALA	deletion	UNP Q4K3M9
A	?	-	ALA	deletion	UNP Q4K3M9
A	?	-	ARG	deletion	UNP Q4K3M9
A	?	-	LEU	deletion	UNP Q4K3M9
A	?	-	GLY	deletion	UNP Q4K3M9
A	?	-	ASP	deletion	UNP Q4K3M9
A	?	-	GLY	deletion	UNP Q4K3M9
A	?	-	LEU	deletion	UNP Q4K3M9
A	?	-	GLU	deletion	UNP Q4K3M9
A	?	-	HIS	deletion	UNP Q4K3M9
A	?	-	THR	deletion	UNP Q4K3M9
A	?	-	SER	deletion	UNP Q4K3M9
A	?	-	MET	deletion	UNP Q4K3M9
A	?	-	MET	deletion	UNP Q4K3M9
A	?	-	ALA	deletion	UNP Q4K3M9
A	?	-	ASP	deletion	UNP Q4K3M9
A	?	-	ILE	deletion	UNP Q4K3M9
A	?	-	LEU	deletion	UNP Q4K3M9
A	?	-	GLY	deletion	UNP Q4K3M9
A	?	-	GLY	deletion	UNP Q4K3M9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP Q4K3M9
A	?	-	LEU	deletion	UNP Q4K3M9
A	?	-	GLU	deletion	UNP Q4K3M9
A	?	-	VAL	deletion	UNP Q4K3M9
A	?	-	ALA	deletion	UNP Q4K3M9
A	?	-	ALA	deletion	UNP Q4K3M9
A	?	-	ASN	deletion	UNP Q4K3M9
A	?	-	VAL	deletion	UNP Q4K3M9
A	?	-	ALA	deletion	UNP Q4K3M9
A	?	-	ILE	deletion	UNP Q4K3M9
A	?	-	GLY	deletion	UNP Q4K3M9
A	?	-	ALA	deletion	UNP Q4K3M9
A	?	-	LEU	deletion	UNP Q4K3M9
A	?	-	ALA	deletion	UNP Q4K3M9
A	?	-	THR	deletion	UNP Q4K3M9
A	?	-	MET	deletion	UNP Q4K3M9
A	?	-	ALA	deletion	UNP Q4K3M9
A	?	-	VAL	deletion	UNP Q4K3M9
A	?	-	ALA	deletion	UNP Q4K3M9
A	?	-	ALA	deletion	UNP Q4K3M9
A	?	-	ALA	deletion	UNP Q4K3M9
A	?	-	ALA	deletion	UNP Q4K3M9
A	?	-	GLY	deletion	UNP Q4K3M9
A	?	-	ILE	deletion	UNP Q4K3M9
A	?	-	THR	deletion	UNP Q4K3M9
A	?	-	VAL	deletion	UNP Q4K3M9
A	?	-	ALA	deletion	UNP Q4K3M9
A	?	-	THR	deletion	UNP Q4K3M9
A	?	-	GLY	deletion	UNP Q4K3M9
A	?	-	GLY	deletion	UNP Q4K3M9
A	?	-	LEU	deletion	UNP Q4K3M9
A	?	-	GLY	deletion	UNP Q4K3M9
A	?	-	ALA	deletion	UNP Q4K3M9
A	?	-	CYS	deletion	UNP Q4K3M9
A	?	-	VAL	deletion	UNP Q4K3M9
A	61	MET	LEU	conflict	UNP Q4K3M9
A	63	SER	-	insertion	UNP Q4K3M9
A	64	SER	LEU	conflict	UNP Q4K3M9
A	65	HIS	VAL	conflict	UNP Q4K3M9
A	66	HIS	VAL	conflict	UNP Q4K3M9
A	67	HIS	GLY	conflict	UNP Q4K3M9
A	68	HIS	VAL	conflict	UNP Q4K3M9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	69	HIS	VAL	conflict	UNP Q4K3M9
A	70	HIS	VAL	conflict	UNP Q4K3M9
A	71	SER	GLY	conflict	UNP Q4K3M9
A	72	GLN	VAL	conflict	UNP Q4K3M9
A	73	ASP	VAL	conflict	UNP Q4K3M9
A	74	PRO	MET	conflict	UNP Q4K3M9
B	?	-	MET	deletion	UNP Q4K3M9
B	?	-	SER	deletion	UNP Q4K3M9
B	?	-	ASP	deletion	UNP Q4K3M9
B	?	-	ALA	deletion	UNP Q4K3M9
B	?	-	LEU	deletion	UNP Q4K3M9
B	?	-	TRP	deletion	UNP Q4K3M9
B	?	-	ALA	deletion	UNP Q4K3M9
B	?	-	ALA	deletion	UNP Q4K3M9
B	?	-	ARG	deletion	UNP Q4K3M9
B	?	-	LEU	deletion	UNP Q4K3M9
B	?	-	GLY	deletion	UNP Q4K3M9
B	?	-	ASP	deletion	UNP Q4K3M9
B	?	-	GLY	deletion	UNP Q4K3M9
B	?	-	LEU	deletion	UNP Q4K3M9
B	?	-	GLU	deletion	UNP Q4K3M9
B	?	-	HIS	deletion	UNP Q4K3M9
B	?	-	THR	deletion	UNP Q4K3M9
B	?	-	SER	deletion	UNP Q4K3M9
B	?	-	MET	deletion	UNP Q4K3M9
B	?	-	MET	deletion	UNP Q4K3M9
B	?	-	ALA	deletion	UNP Q4K3M9
B	?	-	ASP	deletion	UNP Q4K3M9
B	?	-	ILE	deletion	UNP Q4K3M9
B	?	-	LEU	deletion	UNP Q4K3M9
B	?	-	GLY	deletion	UNP Q4K3M9
B	?	-	GLY	deletion	UNP Q4K3M9
B	?	-	VAL	deletion	UNP Q4K3M9
B	?	-	LEU	deletion	UNP Q4K3M9
B	?	-	GLU	deletion	UNP Q4K3M9
B	?	-	VAL	deletion	UNP Q4K3M9
B	?	-	ALA	deletion	UNP Q4K3M9
B	?	-	ALA	deletion	UNP Q4K3M9
B	?	-	ASN	deletion	UNP Q4K3M9
B	?	-	VAL	deletion	UNP Q4K3M9
B	?	-	ALA	deletion	UNP Q4K3M9
B	?	-	ILE	deletion	UNP Q4K3M9

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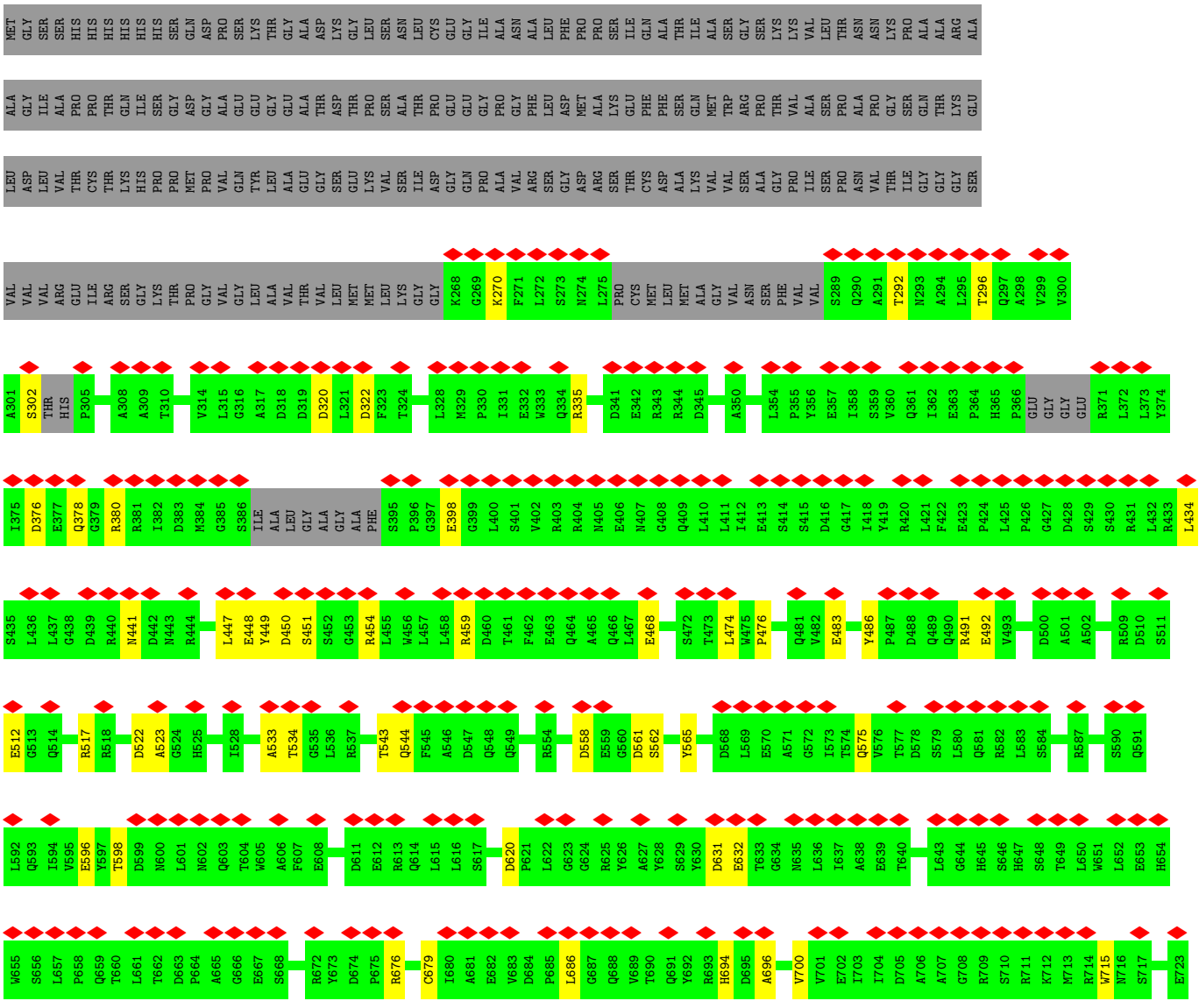
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP Q4K3M9
B	?	-	ALA	deletion	UNP Q4K3M9
B	?	-	LEU	deletion	UNP Q4K3M9
B	?	-	ALA	deletion	UNP Q4K3M9
B	?	-	THR	deletion	UNP Q4K3M9
B	?	-	MET	deletion	UNP Q4K3M9
B	?	-	ALA	deletion	UNP Q4K3M9
B	?	-	VAL	deletion	UNP Q4K3M9
B	?	-	ALA	deletion	UNP Q4K3M9
B	?	-	ALA	deletion	UNP Q4K3M9
B	?	-	ALA	deletion	UNP Q4K3M9
B	?	-	ALA	deletion	UNP Q4K3M9
B	?	-	GLY	deletion	UNP Q4K3M9
B	?	-	ILE	deletion	UNP Q4K3M9
B	?	-	THR	deletion	UNP Q4K3M9
B	?	-	VAL	deletion	UNP Q4K3M9
B	?	-	ALA	deletion	UNP Q4K3M9
B	?	-	THR	deletion	UNP Q4K3M9
B	?	-	GLY	deletion	UNP Q4K3M9
B	?	-	GLY	deletion	UNP Q4K3M9
B	?	-	LEU	deletion	UNP Q4K3M9
B	?	-	GLY	deletion	UNP Q4K3M9
B	?	-	ALA	deletion	UNP Q4K3M9
B	?	-	CYS	deletion	UNP Q4K3M9
B	?	-	VAL	deletion	UNP Q4K3M9
B	61	MET	LEU	conflict	UNP Q4K3M9
B	63	SER	-	insertion	UNP Q4K3M9
B	64	SER	LEU	conflict	UNP Q4K3M9
B	65	HIS	VAL	conflict	UNP Q4K3M9
B	66	HIS	VAL	conflict	UNP Q4K3M9
B	67	HIS	GLY	conflict	UNP Q4K3M9
B	68	HIS	VAL	conflict	UNP Q4K3M9
B	69	HIS	VAL	conflict	UNP Q4K3M9
B	70	HIS	VAL	conflict	UNP Q4K3M9
B	71	SER	GLY	conflict	UNP Q4K3M9
B	72	GLN	VAL	conflict	UNP Q4K3M9
B	73	ASP	VAL	conflict	UNP Q4K3M9
B	74	PRO	MET	conflict	UNP Q4K3M9

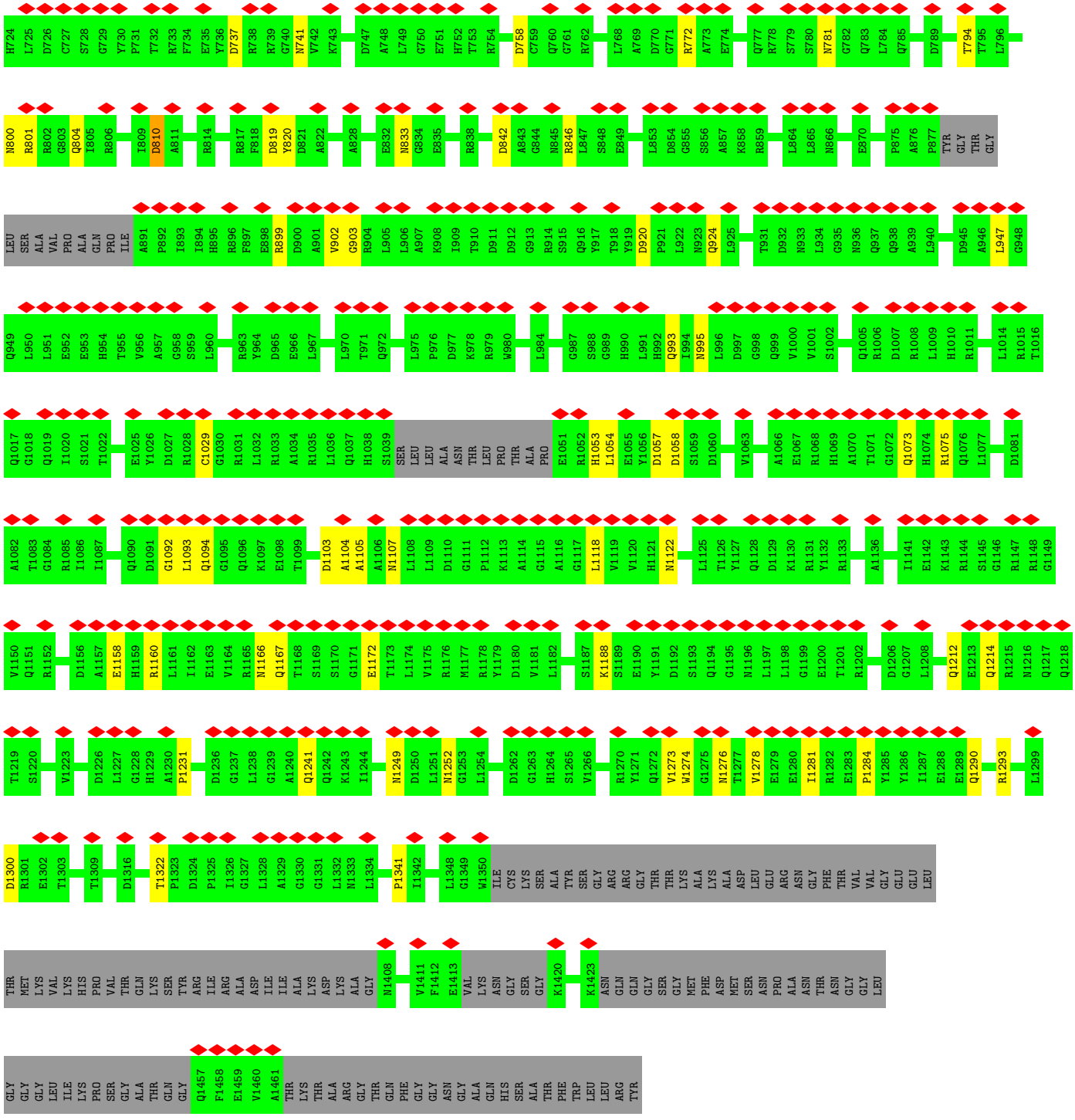
3 Residue-property plots (i)

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: Rhs family protein

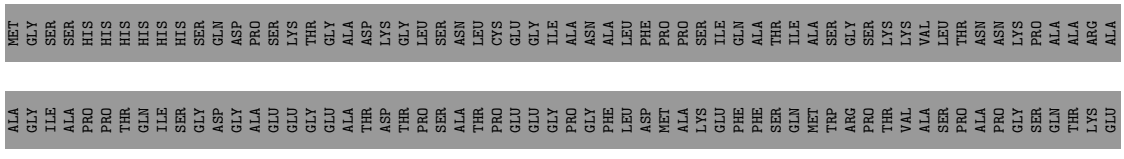
Chain A:

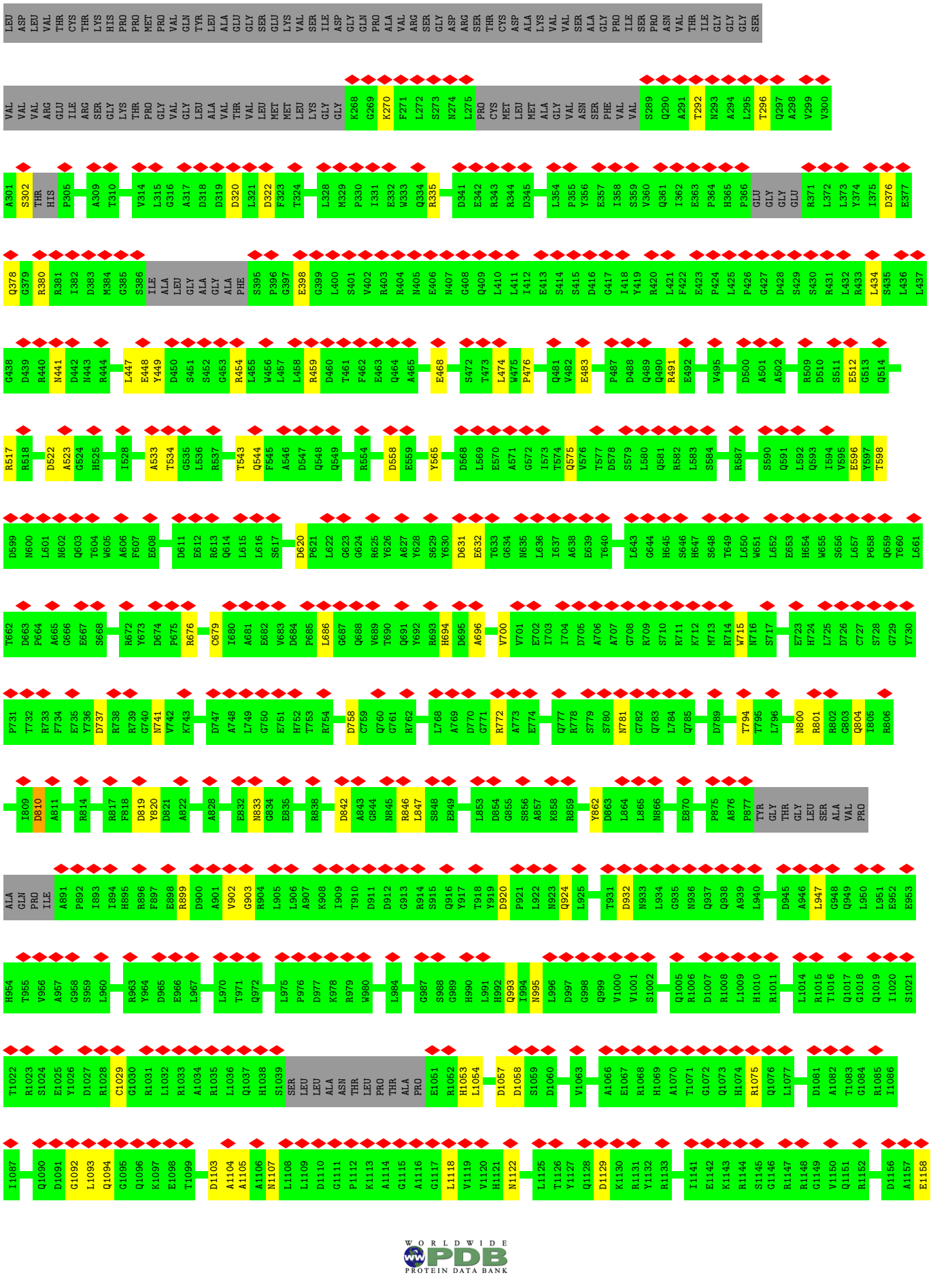


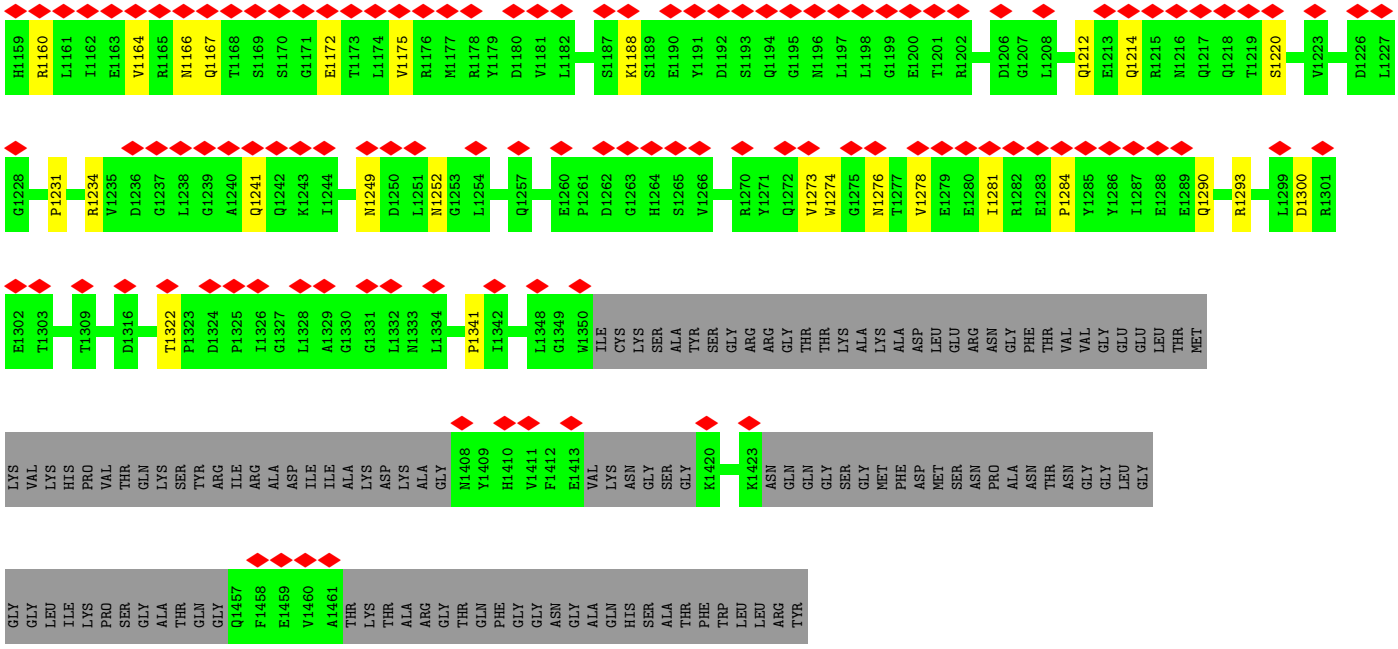


• Molecule 1: Rhs family protein

Chain B:




LEU ASP LEU VAL THR CYS THR LYS HIS PRO PRO MET PRO VAL GLN TYR LEU ALA GLU GLY SER GLU LYS VAL SER ILE ASP GLY GLN PRO ALA VAL ARG SER GLY ASP ARG SER THR CYS ASP ALA LYS VAL VAL SER ALA GLY PRO ILE SER PRO ASN VAL THR ILE GLY GLY GLY SER
VAL VAL VAL ARG GLU ILE ARG SER GLY LYS THR PRO GLY VAL GLY LEU ALA VAL THR VAL LEU MET MET LEU LYS GLY GLY K268 G269 K270 F271 L272 S273 N274 L275 PRO CYS MET LEU MET ALA GLY VAL ASN SER PHE VAL VAL S289 Q290 A291 T292 N293 A294 L295 T296 Q297 A298 V299 V300
A301 S302 THR HIS P305 A309 T310 V314 L315 G316 A317 D318 D319 D320 L321 D322 F323 T324 L328 M329 P330 I331 E332 W333 Q334 R335 D341 E342 R343 R344 D345 L354 P355 Y356 E357 I358 S359 V360 Q361 I362 E363 P364 H365 P366 GLU GLY GLY GLU R371 L372 L373 Y374 I375 D376 E377
Q378 G379 R380 R381 I382 D383 M384 G385 S386 ILE ALA LEU GLY ALA GLY ALA PHE S395 P396 G397 E398 G399 L400 S401 V402 R403 R404 N405 E406 N407 G408 Q409 L410 L411 I412 E413 S414 S415 D416 G417 I418 Y419 R420 L421 F422 E423 P424 L425 P426 G427 D428 S429 S430 R431 L432 R433 L434 S435 L436 L437
G438 D439 R440 N441 D442 N443 R444 L447 E448 Y449 D450 S451 S452 G453 R454 L455 W456 L457 L458 R459 D460 T461 F462 E463 Q464 A465 E468 S472 T473 L474 W475 P476 Q481 V482 E483 P487 D488 Q489 Q490 R491 E492 V495 D500 A501 A502 R509 D510 S511 E512 G513 Q514
R517 R518 D522 A523 G524 H525 I528 A533 T534 G535 L536 R537 T543 Q544 F545 A546 D547 Q548 Q549 R554 D558 E559 Y565 D568 L569 E570 A571 G572 I573 T574 Q575 V576 T577 D578 S579 L580 Q581 R582 L583 S584 R587 S590 Q591 L592 Q593 I594 V595 E596 Y597 T598
D599 N600 L601 N602 Q603 T604 W605 A606 F607 E608 D611 E612 R613 Q614 L615 L616 S617 D620 P621 L622 G623 G624 R625 Y626 A627 Y628 S629 Y630 D631 E632 T633 G634 N635 L636 I637 A638 E639 T640 L643 G644 H645 S646 H647 S648 T649 L650 W651 L652 E653 H654 W655 S656 L657 P658 Q659 T660 L661
T662 D663 P664 A665 G666 E667 S668 R672 Y673 D674 P675 R676 C679 I680 A681 E682 V683 D684 P685 L686 G687 Q688 V689 T690 Q691 Y692 R693 H694 D695 A696 V700 V701 E702 I703 I704 D705 A706 A707 G708 R709 S710 R711 K712 M713 R714 W715 N716 S717 E723 H724 L725 D726 C727 S728 G729 Y730
P731 T732 R733 F734 E735 Y736 D737 R738 R739 G740 N741 V742 K743 D747 A748 L749 G750 E751 H752 T753 R754 D758 C759 Q760 G761 R762 L768 A769 D770 G771 R772 A773 E774 Q777 R778 S779 S780 N781 G782 Q783 L784 Q785 D789 T794 T795 L796 N800 R801 R802 G803 Q804 I805 R806
I809 D810 A811 R814 R817 F818 D819 Y820 D821 A822 A828 E832 N833 G834 E835 R838 D842 A843 G844 N845 R846 L847 S848 E849 L853 D854 G855 S856 A857 K858 R859 Y862 D863 L864 L865 N866 E870 P875 A876 P877 TYR GLY THR GLY LEU SER ALA VAL PRO
ALA GLN PRO ILE A891 P892 I893 I894 H895 R896 F897 E898 R899 D900 A901 V902 G903 R904 L905 L906 A907 K908 I909 T910 D911 D912 G913 R914 S915 Q916 Y917 T918 Y919 D920 P921 L922 N923 Q924 L925 T931 D932 N933 L934 G935 N936 Q937 Q938 A939 L940 D945 A946 L947 G948 Q949 L950 L951 E952 E953
H954 T955 V956 A957 G958 S959 L960 R963 Y964 D965 E966 L967 L970 T971 Q972 L975 P976 D977 K978 R979 W980 L984 G987 S988 G989 H990 L991 H992 Q993 I994 N995 L996 D997 G998 Q999 V1000 V1001 S1002 Q1005 R1006 D1007 R1008 L1009 H1010 R1011 L1014 R1015 T1016 Q1017 G1018 Q1019 I1020 S1021
T1022 R1023 S1024 E1025 Y1026 D1027 R1028 C1029 G1030 R1031 L1032 R1033 A1034 R1035 L1036 Q1037 H1038 S1039 SER LEU LEU ALA ASN THR LEU PRO THR ALA PRO E1051 R1052 H1053 L1054 D1057 D1058 S1059 D1060 V1063 A1066 E1067 R1068 H1069 A1070 T1071 G1072 Q1073 H1074 R1075 Q1076 L1077 D1081 A1082 T1083 G1084 R1085 I1086
I1087 Q1090 D1091 G1092 L1093 Q1094 G1095 Q1096 K1097 E1098 T1099 D1103 A1104 A1105 A1106 N1107 L1108 L1109 D1110 G1111 P1112 K1113 A1114 G1115 A1116 G1117 L1118 V1119 V1120 H1121 N1122 L1125 T1126 Y1127 Q1128 D1129 K1130 R1131 Y1132 R1133 I1141 E1142 K1143 R1144 S1145 G1146 R1147 R1148 G1149 V1150 Q1151 R1152 D1156 A1157 E1158


H1159 R1160 L1161 I1162 E1163 V1164 R1165 N1166 Q1167 T1168 S1169 S1170 G1171 E1172 T1173 L1174 V1175 R1176 M1177 R1178 Y1179 D1180 V1181 L1182
S1187 K1188 S1189 E1190 Y1191 D1192 S1193 Q1194 G1195 N1196 L1197 L1198 G1199 E1200 T1201 R1202
D1206 G1207 L1208
Q1212 E1213 Q1214 R1215 N1216 Q1217 Q1218 T1219 S1220
V1223
D1226 L1227
G1228 P1231 R1234 V1235 D1236 G1237 L1238 G1239 A1240 Q1241 Q1242 K1243 L1244 N1249 D1250 L1251 N1252 G1253 L1254 Q1257 E1260 P1261 D1262 G1263 H1264 S1265 V1266 R1270 Y1271 Q1272 V1273 W1274 G1275 N1276 T1277 V1278 E1279 E1280 I1281 R1282 E1283 P1284 Y1285 Y1286 I1287 E1288 E1289 Q1290 R1293 L1299 D1300 R1301
E1302 T1303 T1309 D1316 T1322 P1323 D1324 P1325 I1326 G1327 L1328 A1329 G1330 G1331 L1332 N1333 L1334 P1341 I1342 L1348 G1349 W1350
ILE CYS LYS SER ALA TYR SER GLY ARG ARG GLY THR THR LYS ALA LYS ALA ASP LEU GLU ARG ASN GLY PHE THR VAL VAL GLY GLU GLU LEU THR MET
LYS VAL LYS HIS PRO VAL THR GLN LYS SER TYR ARG ILE ARG ALA ASP ILE ILE ALA LYS ASP LYS ALA GLY
N1408 Y1409 H1410 V1411 F1412 E1413
VAL LYS ASN GLY SER GLY
K1420 K1423
ASN GLN GLN GLY SER GLY MET PHE ASP MET SER ASN PRO ALA ASN THR ASN GLY GLY LEU GLY
GLY GLY LEU ILE LYS PRO SER GLY ALA THR GLN GLY
Q1457 F1458 E1459 V1460 A1461
THR LYS THR ALA ARG GLY THR GLN PHE GLY GLY ASN GLY ALA GLN HIS SER ALA THR PHE TRP LEU LEU ARG TYR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	454740	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	61	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	105000	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.166	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0331	Depositor
Map size (Å)	262.08002, 262.08002, 262.08002	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9100001, 0.9100001, 0.9100001	Depositor

5 Model quality

5.1 Standard geometry

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	0.46	0/8737	0.59	0/11828
1	B	0.46	0/8737	0.59	0/11828
All	All	0.46	0/17474	0.59	0/23656

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	8527	7876	8060	71	0
1	B	8527	7876	8060	73	0
All	All	17054	15752	16120	142	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 4.

All (142) 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:302:SER:OG	1:A:565:TYR:OH	1.94	0.86
1:B:302:SER:OG	1:B:565:TYR:OH	1.94	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1290:GLN:OE1	1:B:1293:ARG:NH1	2.11	0.84
1:A:1290:GLN:OE1	1:A:1293:ARG:NH1	2.11	0.82
1:A:441:ASN:OD1	1:A:676:ARG:NH2	2.17	0.77
1:B:441:ASN:OD1	1:B:676:ARG:NH2	2.17	0.77
1:A:398:GLU:OE1	1:A:398:GLU:N	2.20	0.74
1:A:902:VAL:HG12	1:A:903:GLY:H	1.53	0.74
1:B:1278:VAL:HG11	1:B:1281:ILE:HD11	1.70	0.74
1:B:398:GLU:N	1:B:398:GLU:OE1	2.20	0.73
1:B:902:VAL:HG12	1:B:903:GLY:H	1.53	0.73
1:A:1278:VAL:HG11	1:A:1281:ILE:HD11	1.69	0.73
1:B:483:GLU:OE1	1:B:491:ARG:NH1	2.24	0.71
1:A:993:GLN:OE1	1:A:995:ASN:ND2	2.24	0.71
1:B:575:GLN:N	1:B:575:GLN:OE1	2.24	0.71
1:A:483:GLU:OE1	1:A:491:ARG:NH1	2.24	0.70
1:A:575:GLN:N	1:A:575:GLN:OE1	2.24	0.70
1:B:993:GLN:OE1	1:B:995:ASN:ND2	2.24	0.70
1:B:899:ARG:NH1	1:B:903:GLY:O	2.24	0.70
1:A:899:ARG:NH1	1:A:903:GLY:O	2.24	0.69
1:B:1252:ASN:ND2	1:B:1341:PRO:O	2.25	0.69
1:A:1252:ASN:ND2	1:A:1341:PRO:O	2.25	0.69
1:A:558:ASP:OD2	1:A:801:ARG:NH2	2.31	0.64
1:A:596:GLU:OE2	1:A:598:THR:OG1	2.15	0.64
1:B:596:GLU:OE2	1:B:598:THR:OG1	2.15	0.64
1:A:1188:LYS:NZ	1:A:1300:ASP:OD2	2.31	0.64
1:B:833:ASN:CG	1:B:1118:LEU:HD13	2.19	0.63
1:B:1188:LYS:NZ	1:B:1300:ASP:OD2	2.31	0.63
1:A:737:ASP:OD1	1:A:741:ASN:N	2.32	0.62
1:B:737:ASP:OD1	1:B:741:ASN:N	2.32	0.62
1:A:833:ASN:CG	1:A:1118:LEU:HD13	2.19	0.62
1:B:558:ASP:OD2	1:B:801:ARG:NH2	2.31	0.62
1:A:448:GLU:OE2	1:A:459:ARG:NE	2.31	0.61
1:A:902:VAL:HG12	1:A:903:GLY:N	2.15	0.61
1:B:448:GLU:OE2	1:B:459:ARG:NE	2.31	0.61
1:A:534:THR:OG1	1:A:801:ARG:O	2.11	0.61
1:B:902:VAL:HG12	1:B:903:GLY:N	2.15	0.61
1:B:534:THR:OG1	1:B:801:ARG:O	2.11	0.60
1:B:1241:GLN:N	1:B:1241:GLN:OE1	2.36	0.59
1:A:1241:GLN:N	1:A:1241:GLN:OE1	2.36	0.59
1:A:794:THR:OG1	1:B:512:GLU:OE2	2.18	0.58
1:A:1103:ASP:OD1	1:A:1104:ALA:N	2.36	0.58
1:B:1092:GLY:O	1:B:1094:GLN:NE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1103:ASP:OD1	1:B:1104:ALA:N	2.36	0.58
1:B:378:GLN:N	1:B:378:GLN:OE1	2.38	0.57
1:A:378:GLN:OE1	1:A:378:GLN:N	2.38	0.57
1:A:1092:GLY:O	1:A:1094:GLN:NE2	2.36	0.57
1:A:842:ASP:OD1	1:A:846:ARG:N	2.36	0.57
1:A:522:ASP:OD1	1:A:523:ALA:N	2.36	0.56
1:A:833:ASN:OD1	1:A:1118:LEU:HD13	2.05	0.56
1:B:833:ASN:OD1	1:B:1118:LEU:HD13	2.05	0.56
1:B:533:ALA:O	1:B:781:ASN:ND2	2.39	0.56
1:A:902:VAL:CG1	1:A:903:GLY:H	2.19	0.56
1:A:631:ASP:OD1	1:A:632:GLU:N	2.36	0.56
1:A:533:ALA:O	1:A:781:ASN:ND2	2.39	0.55
1:B:322:ASP:OD1	1:B:335:ARG:NH1	2.40	0.55
1:B:902:VAL:CG1	1:B:903:GLY:H	2.19	0.55
1:A:322:ASP:OD1	1:A:335:ARG:NH1	2.40	0.54
1:A:512:GLU:OE2	1:B:794:THR:OG1	2.17	0.54
1:B:631:ASP:OD1	1:B:632:GLU:N	2.36	0.54
1:A:454:ARG:NH1	1:A:476:PRO:O	2.42	0.53
1:B:454:ARG:NH1	1:B:476:PRO:O	2.42	0.53
1:A:1075:ARG:O	1:A:1092:GLY:N	2.42	0.52
1:B:842:ASP:OD1	1:B:846:ARG:N	2.36	0.51
1:B:522:ASP:OD1	1:B:523:ALA:N	2.36	0.51
1:A:434:LEU:O	1:A:449:TYR:OH	2.19	0.50
1:A:1158:GLU:OE1	1:A:1160:ARG:NH2	2.45	0.50
1:B:1158:GLU:OE1	1:B:1160:ARG:NH2	2.45	0.50
1:B:1220:SER:HG	1:B:1234:ARG:HE	1.58	0.49
1:B:1167:GLN:OE1	1:B:1172:GLU:HG2	2.12	0.49
1:A:1167:GLN:OE1	1:A:1172:GLU:HG2	2.12	0.49
1:A:270:LYS:HB3	1:A:270:LYS:NZ	2.28	0.49
1:B:1075:ARG:O	1:B:1092:GLY:N	2.42	0.49
1:B:434:LEU:O	1:B:449:TYR:OH	2.19	0.48
1:B:270:LYS:NZ	1:B:270:LYS:HB3	2.28	0.48
1:A:320:ASP:OD1	1:A:517:ARG:NH1	2.47	0.48
1:B:1057:ASP:OD1	1:B:1058:ASP:N	2.41	0.48
1:B:819:ASP:OD1	1:B:820:TYR:N	2.47	0.48
1:B:772:ARG:NH2	1:B:1029:CYS:SG	2.87	0.48
1:A:772:ARG:NH2	1:A:1029:CYS:SG	2.87	0.47
1:B:1107:ASN:ND2	1:B:1122:ASN:OD1	2.40	0.47
1:A:1053:HIS:C	1:A:1054:LEU:HD12	2.34	0.47
1:A:819:ASP:OD1	1:A:820:TYR:N	2.47	0.47
1:A:1104:ALA:O	1:A:1105:ALA:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1231:PRO:O	1:B:1249:ASN:ND2	2.48	0.47
1:B:1053:HIS:C	1:B:1054:LEU:HD12	2.34	0.47
1:A:543:THR:HG22	1:A:544:GLN:N	2.31	0.46
1:B:800:ASN:OD1	1:B:804:GLN:N	2.48	0.46
1:B:679:CYS:O	1:B:694:HIS:NE2	2.48	0.46
1:A:800:ASN:OD1	1:A:804:GLN:N	2.48	0.46
1:A:676:ARG:NH2	1:A:696:ALA:O	2.44	0.46
1:A:679:CYS:O	1:A:694:HIS:NE2	2.48	0.46
1:B:543:THR:HG22	1:B:544:GLN:N	2.30	0.46
1:A:1231:PRO:O	1:A:1249:ASN:ND2	2.48	0.46
1:B:320:ASP:OD1	1:B:517:ARG:NH1	2.47	0.46
1:A:376:ASP:OD1	1:A:380:ARG:N	2.48	0.46
1:A:1057:ASP:OD1	1:A:1058:ASP:N	2.41	0.46
1:A:1166:ASN:OD1	1:A:1167:GLN:N	2.49	0.46
1:B:376:ASP:OD1	1:B:380:ARG:N	2.48	0.46
1:B:1104:ALA:O	1:B:1105:ALA:HB3	2.14	0.46
1:A:810:ASP:OD1	1:A:810:ASP:N	2.48	0.45
1:B:700:VAL:O	1:B:715:TRP:NE1	2.45	0.45
1:B:1166:ASN:OD1	1:B:1167:GLN:N	2.49	0.45
1:B:810:ASP:N	1:B:810:ASP:OD1	2.48	0.45
1:A:620:ASP:N	1:A:620:ASP:OD1	2.48	0.45
1:B:620:ASP:N	1:B:620:ASP:OD1	2.48	0.45
1:A:468:GLU:OE1	1:A:491:ARG:NH2	2.44	0.45
1:A:700:VAL:O	1:A:715:TRP:NE1	2.45	0.44
1:B:902:VAL:CG1	1:B:903:GLY:N	2.79	0.44
1:B:1093:LEU:HD12	1:B:1093:LEU:N	2.32	0.44
1:A:292:THR:O	1:A:296:THR:HG23	2.18	0.44
1:A:1093:LEU:HD12	1:A:1093:LEU:N	2.33	0.44
1:B:292:THR:O	1:B:296:THR:HG23	2.18	0.44
1:A:686:LEU:HD11	1:A:947:LEU:HD13	2.00	0.43
1:B:474:LEU:H	1:B:474:LEU:HD12	1.83	0.43
1:A:474:LEU:H	1:A:474:LEU:HD12	1.83	0.43
1:A:947:LEU:HD12	1:A:947:LEU:N	2.33	0.43
1:B:676:ARG:NH2	1:B:696:ALA:O	2.44	0.43
1:B:1212:GLN:OE1	1:B:1214:GLN:NE2	2.52	0.43
1:B:447:LEU:HD12	1:B:447:LEU:N	2.34	0.43
1:A:447:LEU:HD12	1:A:447:LEU:N	2.34	0.42
1:A:1273:VAL:HG23	1:A:1274:TRP:N	2.34	0.42
1:B:947:LEU:N	1:B:947:LEU:HD12	2.33	0.42
1:A:902:VAL:CG1	1:A:903:GLY:N	2.79	0.42
1:A:1212:GLN:OE1	1:A:1214:GLN:NE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1273:VAL:HG23	1:B:1274:TRP:N	2.34	0.42
1:A:1073:GLN:OE1	1:A:1073:GLN:N	2.38	0.42
1:B:1129:ASP:OD1	1:B:1129:ASP:N	2.50	0.42
1:B:468:GLU:OE1	1:B:491:ARG:NH2	2.44	0.41
1:B:932:ASP:N	1:B:932:ASP:OD1	2.53	0.41
1:B:686:LEU:HD11	1:B:947:LEU:HD13	2.00	0.41
1:A:920:ASP:HB2	1:A:924:GLN:HG2	2.01	0.41
1:B:847:LEU:O	1:B:862:TYR:OH	2.32	0.41
1:B:1276:ASN:ND2	1:B:1293:ARG:HB3	2.35	0.41
1:A:1276:ASN:ND2	1:A:1293:ARG:HB3	2.34	0.41
1:B:920:ASP:HB2	1:B:924:GLN:HG2	2.01	0.41
1:A:561:ASP:OD1	1:A:562:SER:N	2.54	0.40
1:A:486:TYR:OH	1:A:492:GLU:OE1	2.25	0.40
1:A:1107:ASN:ND2	1:A:1122:ASN:OD1	2.40	0.40
1:A:450:ASP:OD1	1:A:451:SER:N	2.53	0.40
1:B:1054:LEU:HD12	1:B:1054:LEU:N	2.36	0.40
1:B:1164:VAL:HB	1:B:1175:VAL:CG2	2.52	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	1029/1426 (72%)	992 (96%)	36 (4%)	1 (0%)	51	81
1	B	1029/1426 (72%)	992 (96%)	36 (4%)	1 (0%)	51	81
All	All	2058/2852 (72%)	1984 (96%)	72 (4%)	2 (0%)	54	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1284	PRO

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Mol	Chain	Res	Type
1	B	1284	PRO

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	890/1178 (76%)	887 (100%)	3 (0%)	92 96
1	B	890/1178 (76%)	887 (100%)	3 (0%)	92 96
All	All	1780/2356 (76%)	1774 (100%)	6 (0%)	92 96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	758	ASP
1	A	810	ASP
1	A	1322	THR
1	B	758	ASP
1	B	810	ASP
1	B	1322	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1010	HIS
1	A	1196	ASN
1	A	1214	GLN
1	A	1276	ASN
1	B	1010	HIS
1	B	1196	ASN
1	B	1214	GLN
1	B	1276	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

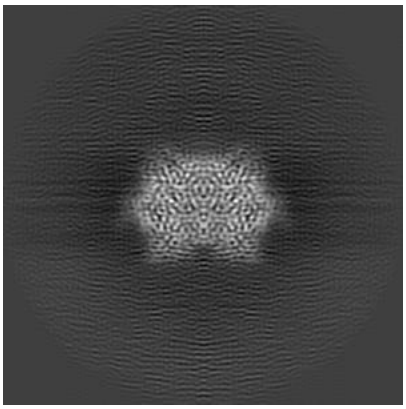
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13867. These allow visual inspection of the internal detail of the map and identification of artifacts.

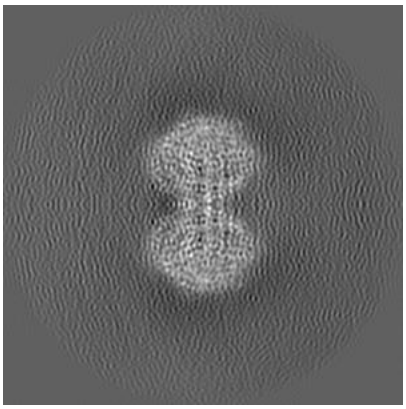
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

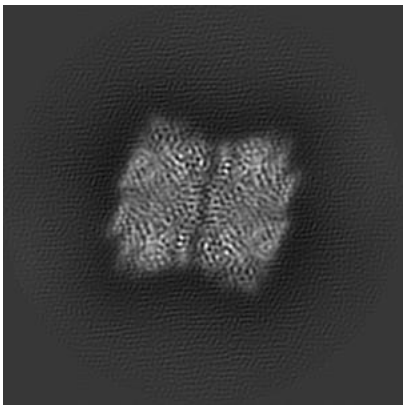
6.1.1 Primary map



X

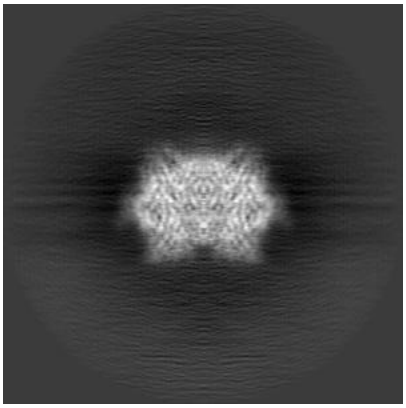


Y

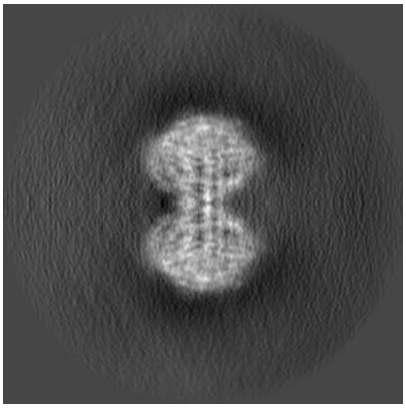


Z

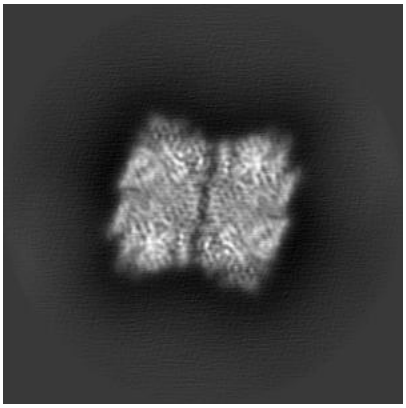
6.1.2 Raw map



X



Y



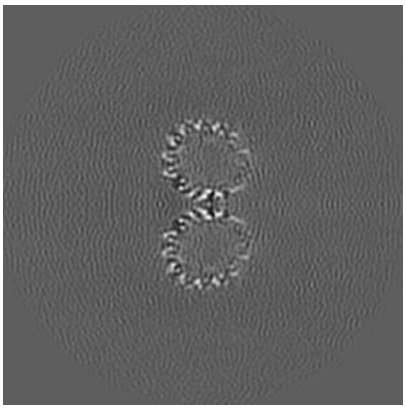
Z

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

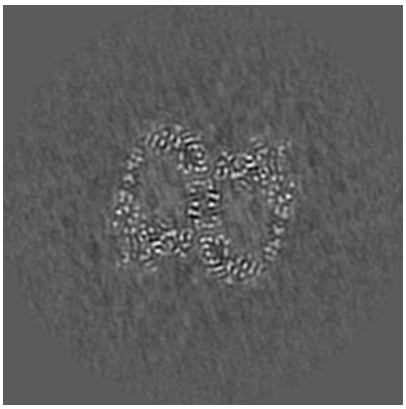
6.2 Central slices (i)

6.2.1 Primary map

X Index: 144

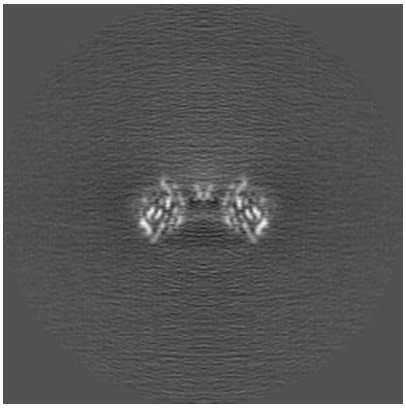


Y Index: 144

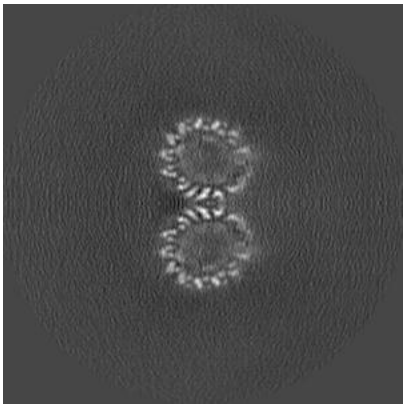


Z Index: 144

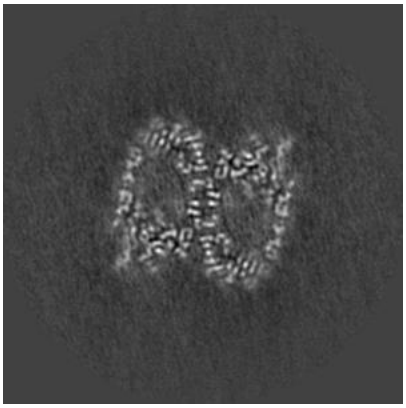
6.2.2 Raw map



X Index: 144



Y Index: 144

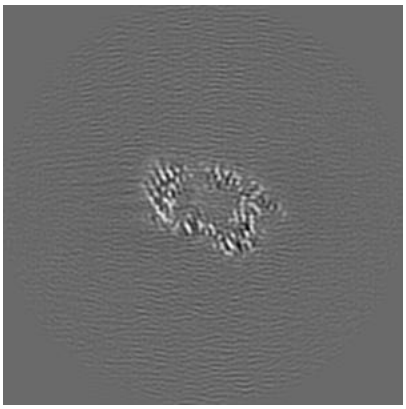


Z Index: 144

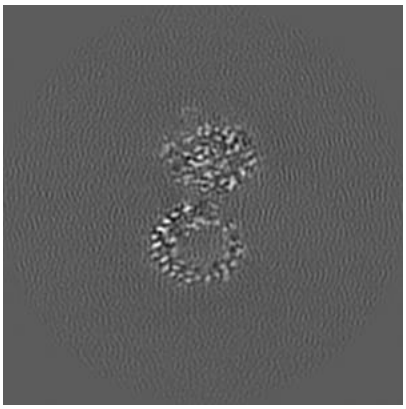
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

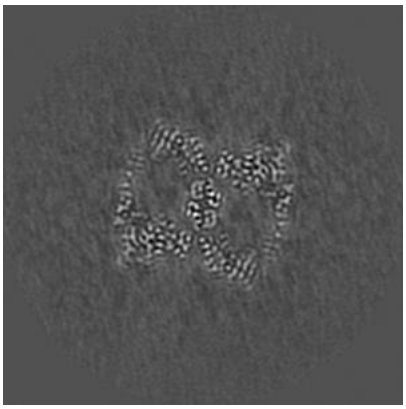
6.3.1 Primary map



X Index: 128

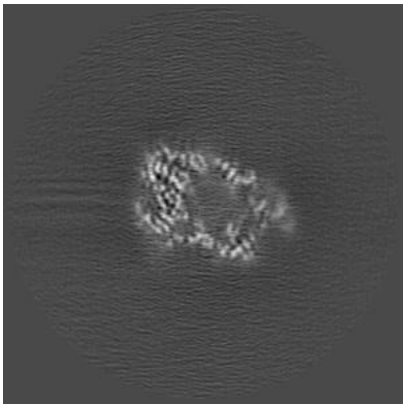


Y Index: 167

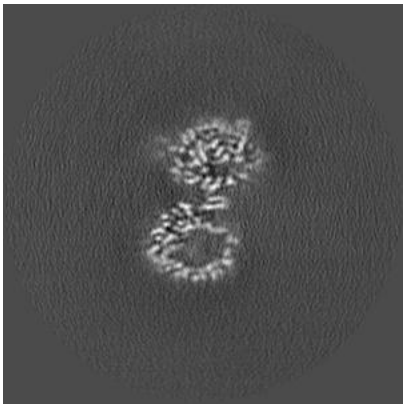


Z Index: 146

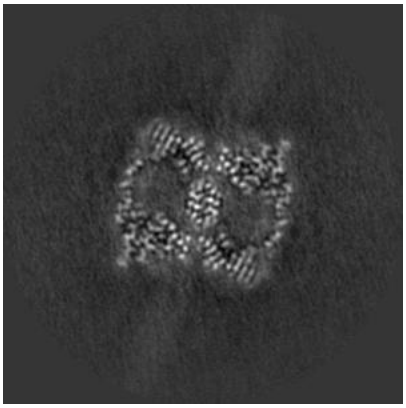
6.3.2 Raw map



X Index: 107



Y Index: 173

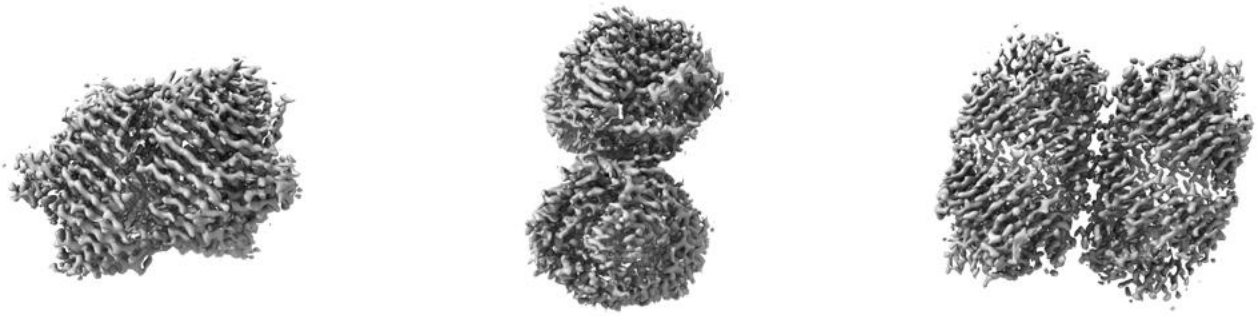


Z Index: 147

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0331. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

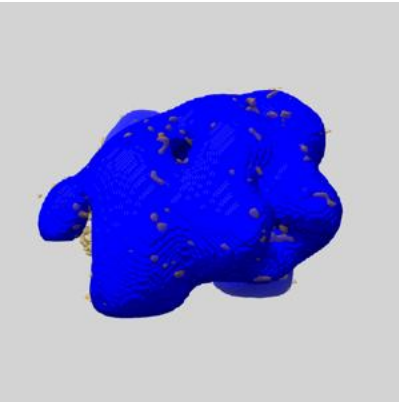
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

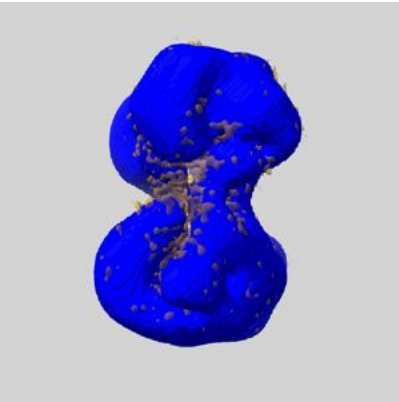
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

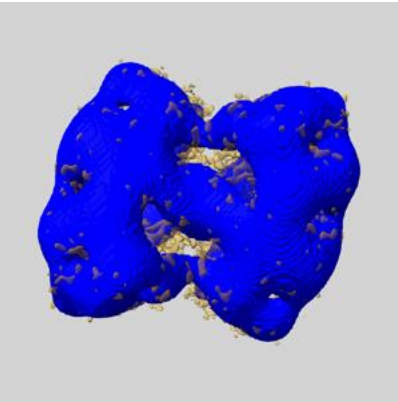
6.5.1 emd_13867_msk_1.map (i)



X



Y

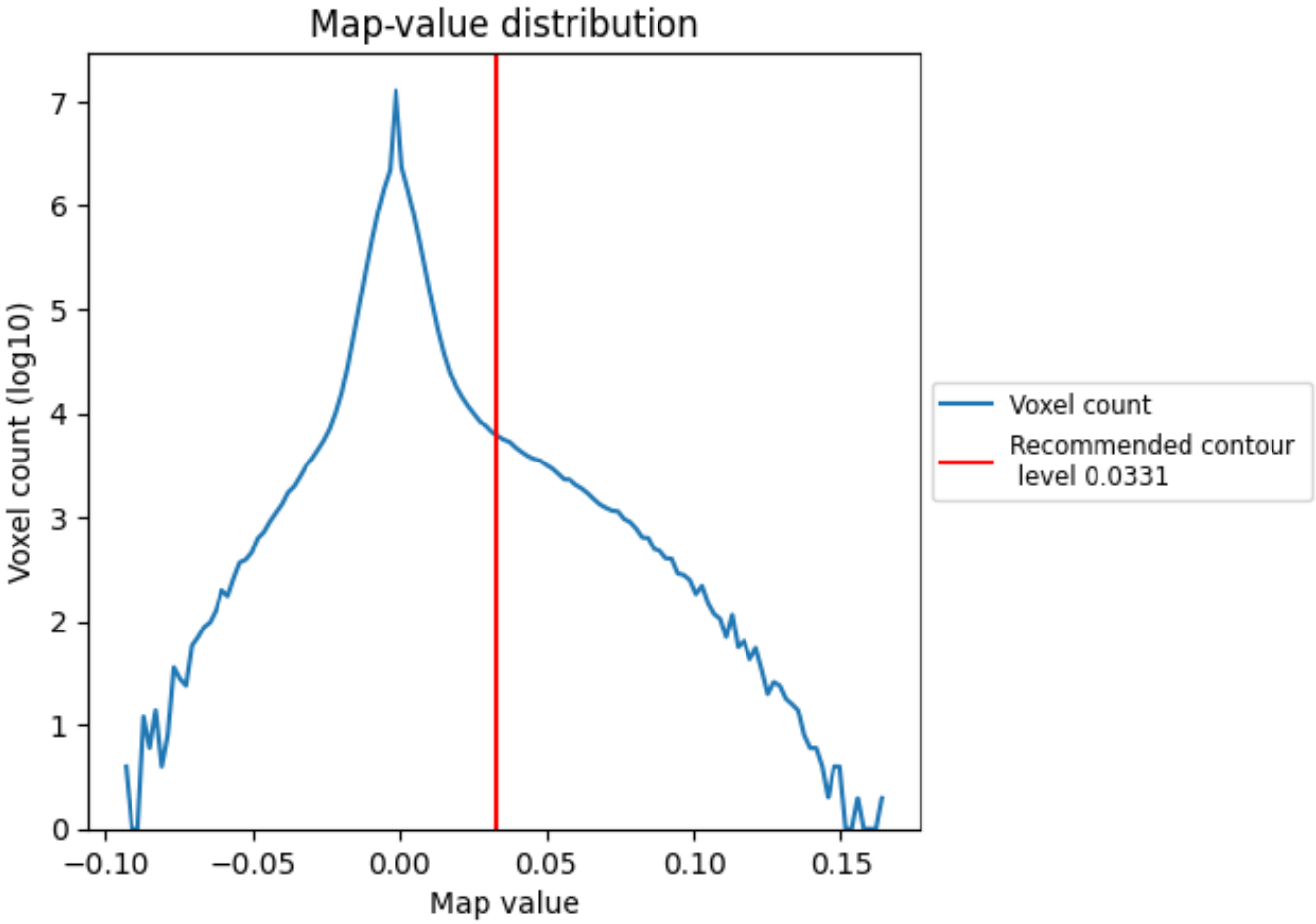


Z

7 Map analysis

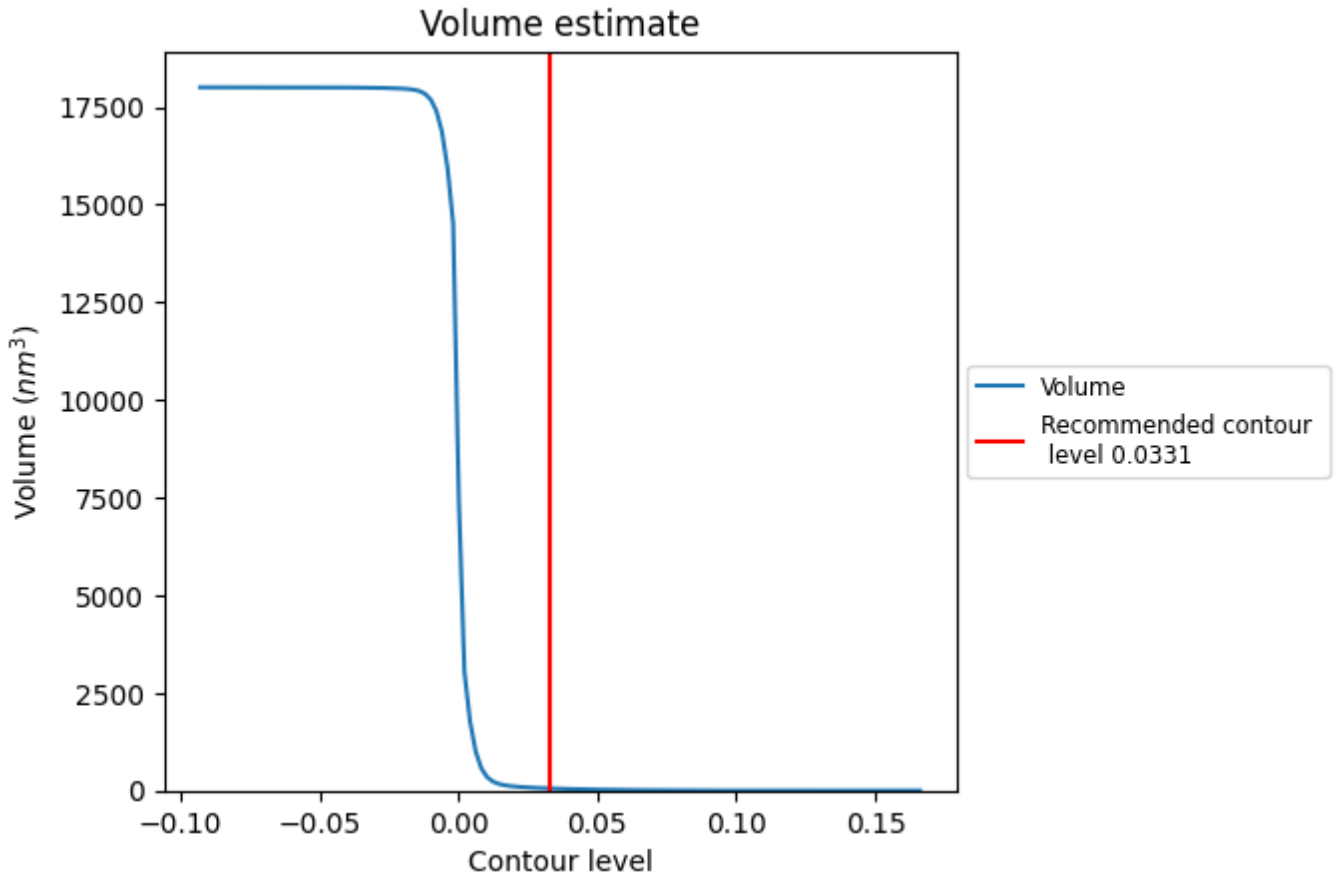
This section contains the results of statistical analysis of the map.

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.

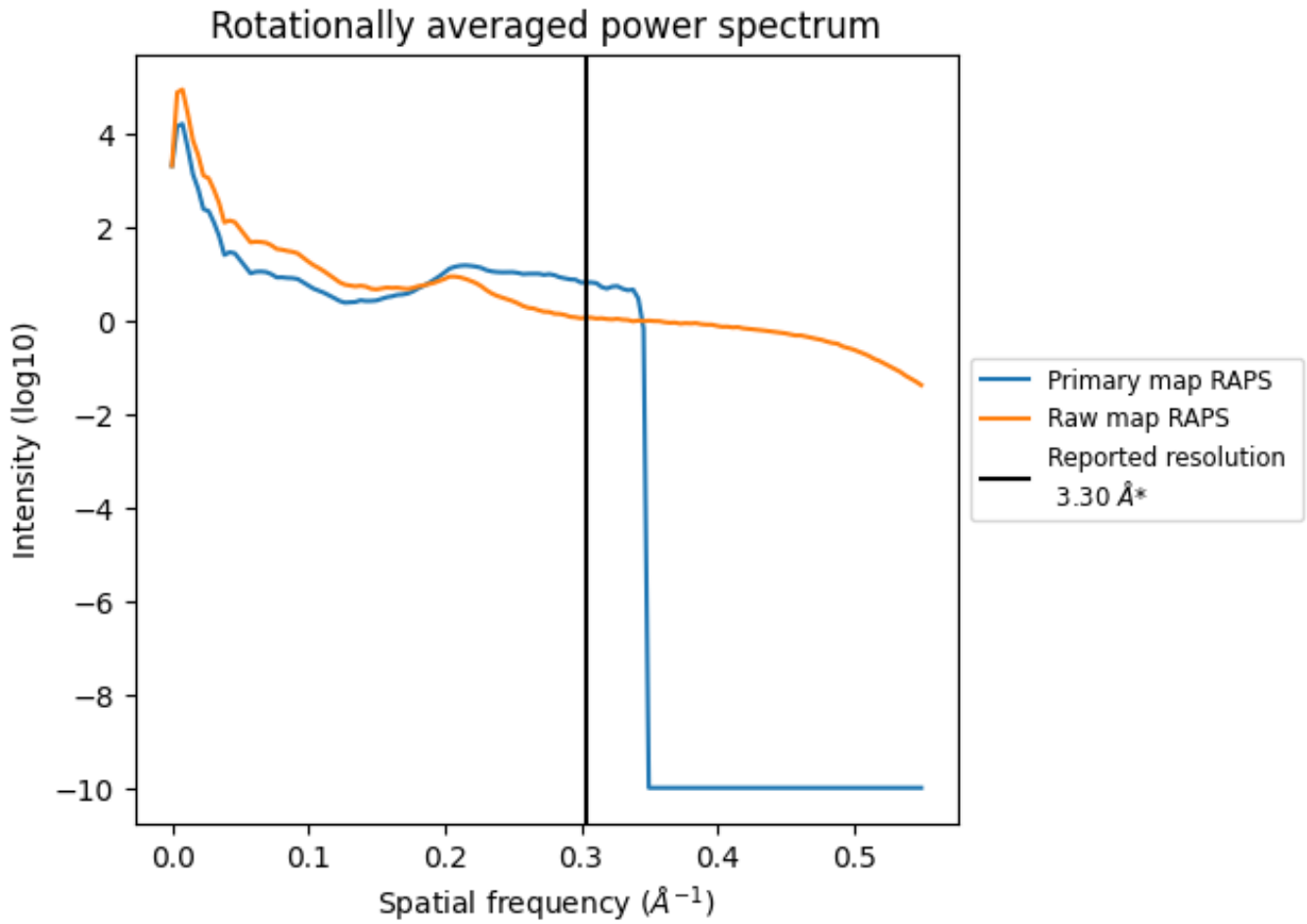
7.2 Volume estimate



The volume at the recommended contour level is 54 nm^3; this corresponds to an approximate mass of 49 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)

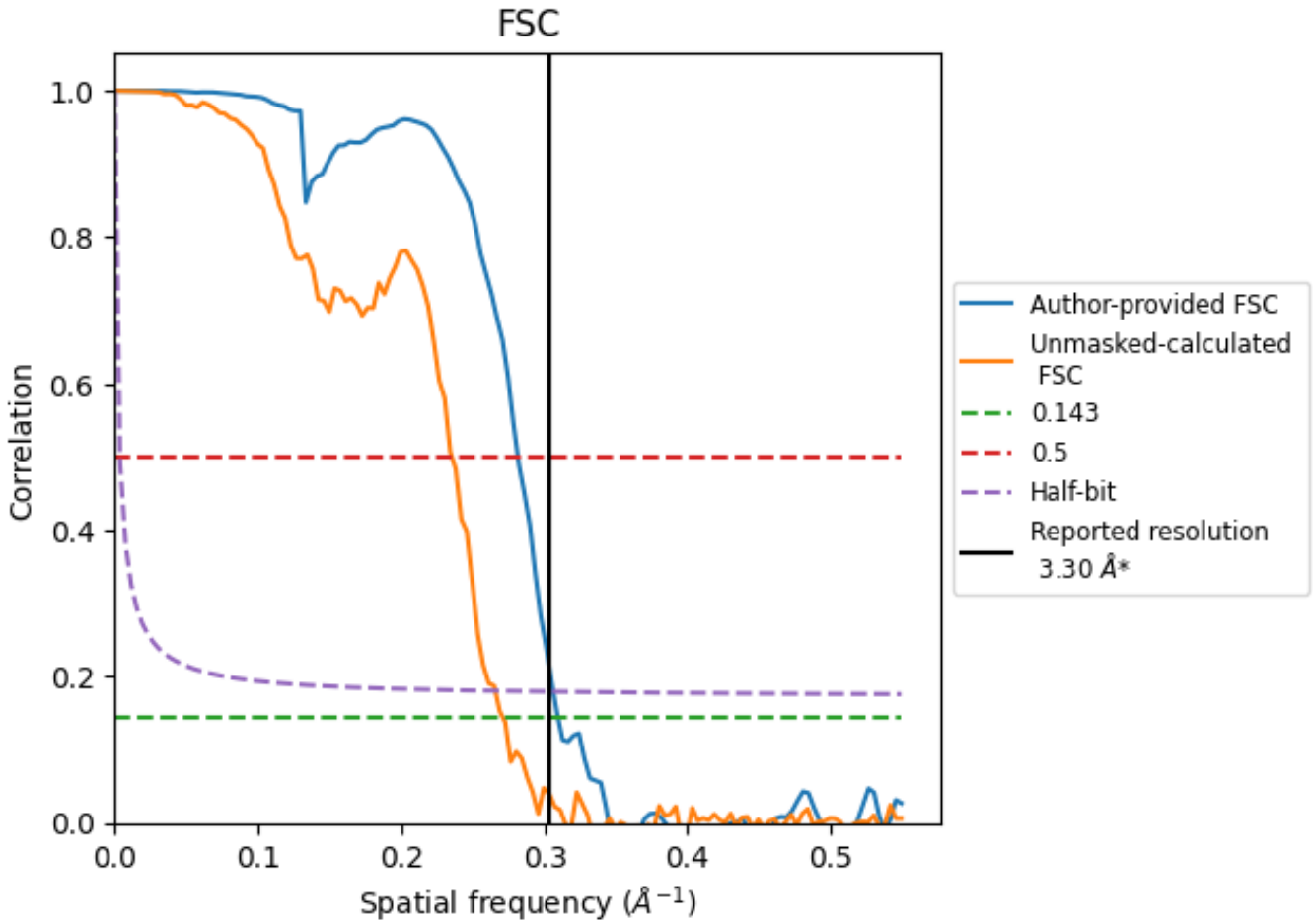


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 $Å^{-1}$

8.2 Resolution estimates (i)

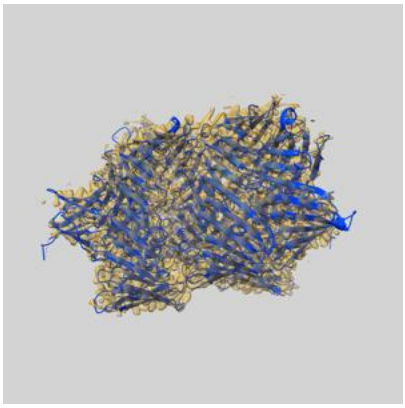
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.23	3.55	3.26
Unmasked-calculated*	3.69	4.25	3.76

*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 3.69 differs from the reported value 3.3 by more than 10 %

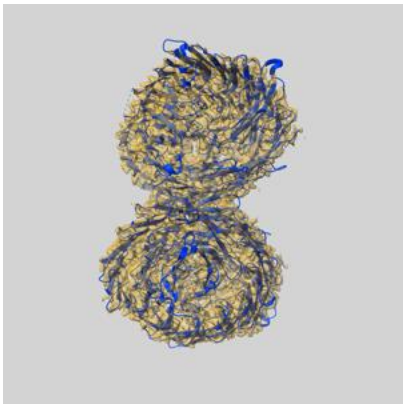
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13867 and PDB model 7Q97. Per-residue inclusion information can be found in section 3 on page 7.

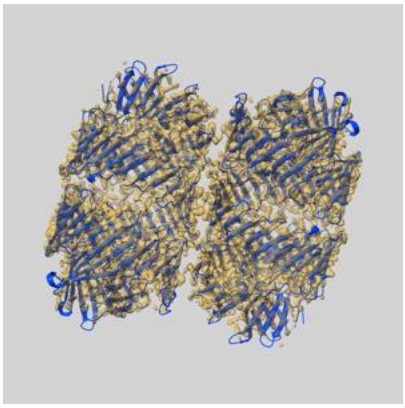
9.1 Map-model overlay



X



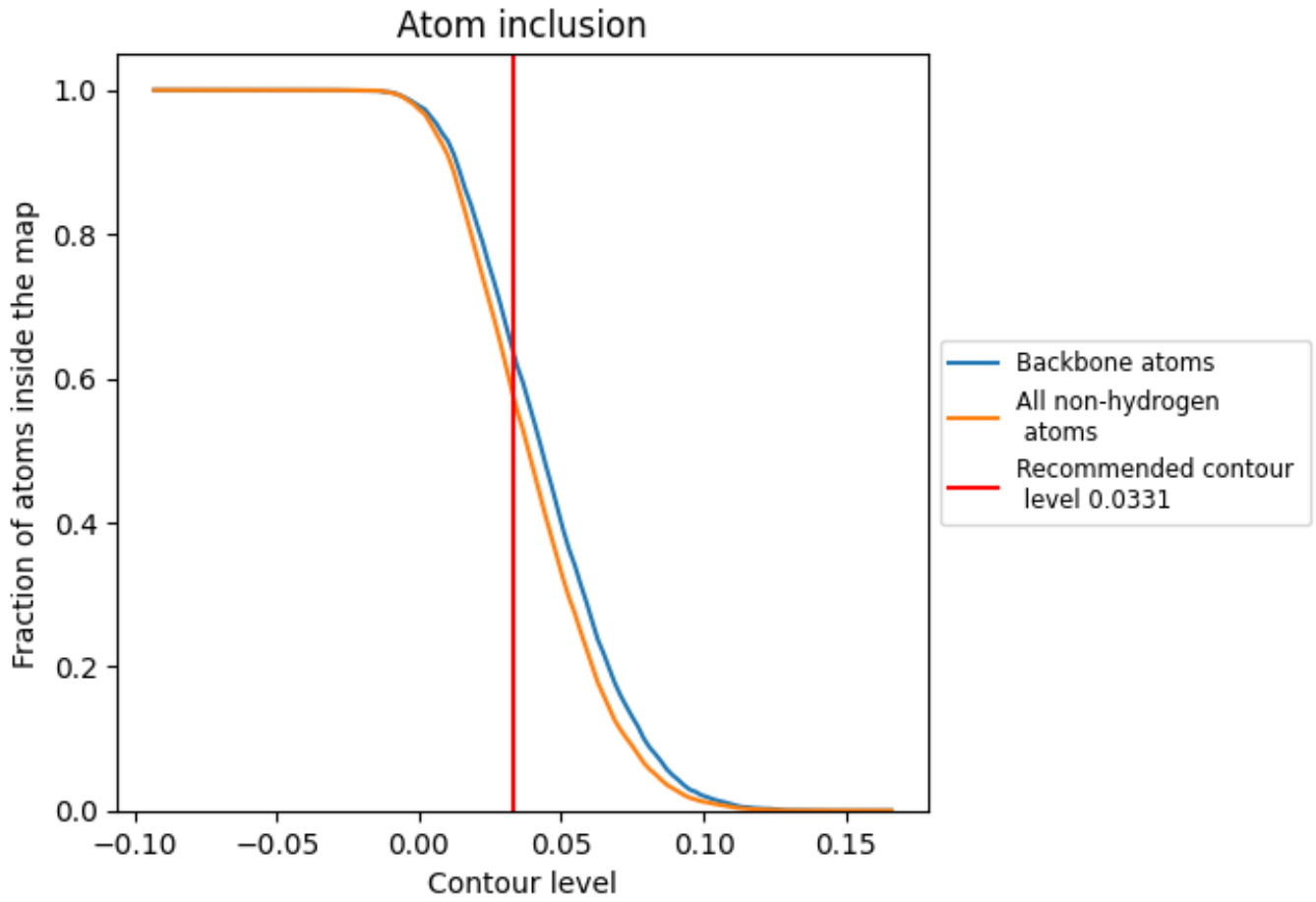
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0331 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.