Full wwPDB EM Validation Report ⓘ

Jan 5, 2023 – 02:39 PM JST

PDB ID	:	8HGH
EMDB ID	:	EMD-34739
Title	:	Structure of 2:2 PAPP-A.STC2 complex
Authors	:	Zhong, Q.H.; Chu, H.L.; Wang, G.P.; Zhang, C.; Wei, Y.; Qiao, J.; Hang, J.
Deposited on	:	2022-11-14
Resolution	:	4.16 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:

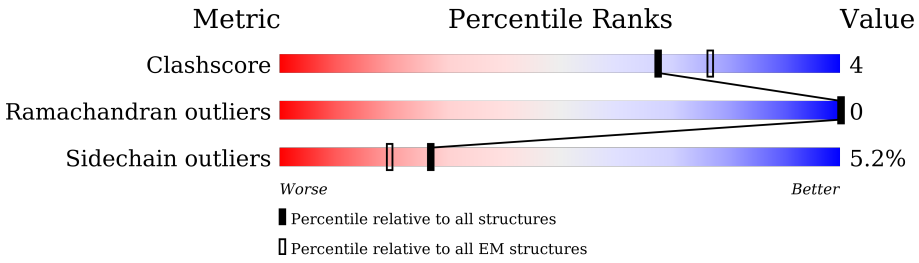
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.16 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	1944	46% 65% 9% 25%
1	B	1944	44% 65% 10% 25%
2	C	302	25% 46% 10% • 43%
2	G	302	30% 48% 7% • 43%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25512 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 Maltose/maltodextrin-binding periplasmic protein,Pappalysin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1462	Total	C	N	O	S	0	0
			11420	7150	1974	2199	97		
1	B	1462	Total	C	N	O	S	0	0
			11420	7150	1974	2199	97		

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-396	ALA	-	expression tag	UNP P0AEX9
A	-395	ALA	-	expression tag	UNP P0AEX9
A	-394	SER	-	expression tag	UNP P0AEX9
A	-393	HIS	-	expression tag	UNP P0AEX9
A	-392	HIS	-	expression tag	UNP P0AEX9
A	-391	HIS	-	expression tag	UNP P0AEX9
A	-390	HIS	-	expression tag	UNP P0AEX9
A	-389	HIS	-	expression tag	UNP P0AEX9
A	-388	HIS	-	expression tag	UNP P0AEX9
A	-387	HIS	-	expression tag	UNP P0AEX9
A	-386	HIS	-	expression tag	UNP P0AEX9
A	-385	HIS	-	expression tag	UNP P0AEX9
A	-384	HIS	-	expression tag	UNP P0AEX9
A	-383	SER	-	expression tag	UNP P0AEX9
A	-382	GLY	-	expression tag	UNP P0AEX9
A	-15	ASP	-	linker	UNP P0AEX9
A	-14	TYR	-	linker	UNP P0AEX9
A	-13	ASP	-	linker	UNP P0AEX9
A	-12	ILE	-	linker	UNP P0AEX9
A	-11	PRO	-	linker	UNP P0AEX9
A	-10	THR	-	linker	UNP P0AEX9
A	-9	THR	-	linker	UNP P0AEX9
A	-8	GLU	-	linker	UNP P0AEX9
A	-7	ASN	-	linker	UNP P0AEX9
A	-6	LEU	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	TYR	-	linker	UNP P0AEX9
A	-4	PHE	-	linker	UNP P0AEX9
A	-3	GLN	-	linker	UNP P0AEX9
A	-2	GLY	-	linker	UNP P0AEX9
A	-1	GLU	-	linker	UNP P0AEX9
A	0	PHE	-	linker	UNP P0AEX9
B	-396	ALA	-	expression tag	UNP P0AEX9
B	-395	ALA	-	expression tag	UNP P0AEX9
B	-394	SER	-	expression tag	UNP P0AEX9
B	-393	HIS	-	expression tag	UNP P0AEX9
B	-392	HIS	-	expression tag	UNP P0AEX9
B	-391	HIS	-	expression tag	UNP P0AEX9
B	-390	HIS	-	expression tag	UNP P0AEX9
B	-389	HIS	-	expression tag	UNP P0AEX9
B	-388	HIS	-	expression tag	UNP P0AEX9
B	-387	HIS	-	expression tag	UNP P0AEX9
B	-386	HIS	-	expression tag	UNP P0AEX9
B	-385	HIS	-	expression tag	UNP P0AEX9
B	-384	HIS	-	expression tag	UNP P0AEX9
B	-383	SER	-	expression tag	UNP P0AEX9
B	-382	GLY	-	expression tag	UNP P0AEX9
B	-15	ASP	-	linker	UNP P0AEX9
B	-14	TYR	-	linker	UNP P0AEX9
B	-13	ASP	-	linker	UNP P0AEX9
B	-12	ILE	-	linker	UNP P0AEX9
B	-11	PRO	-	linker	UNP P0AEX9
B	-10	THR	-	linker	UNP P0AEX9
B	-9	THR	-	linker	UNP P0AEX9
B	-8	GLU	-	linker	UNP P0AEX9
B	-7	ASN	-	linker	UNP P0AEX9
B	-6	LEU	-	linker	UNP P0AEX9
B	-5	TYR	-	linker	UNP P0AEX9
B	-4	PHE	-	linker	UNP P0AEX9
B	-3	GLN	-	linker	UNP P0AEX9
B	-2	GLY	-	linker	UNP P0AEX9
B	-1	GLU	-	linker	UNP P0AEX9
B	0	PHE	-	linker	UNP P0AEX9

- Molecule 2 is a protein called Stanniocalcin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	171	Total	C	N	O	S	0	0
			1335	834	241	243	17		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	171	Total	C	N	O	S	0	0
			1335	834	241	243	17		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

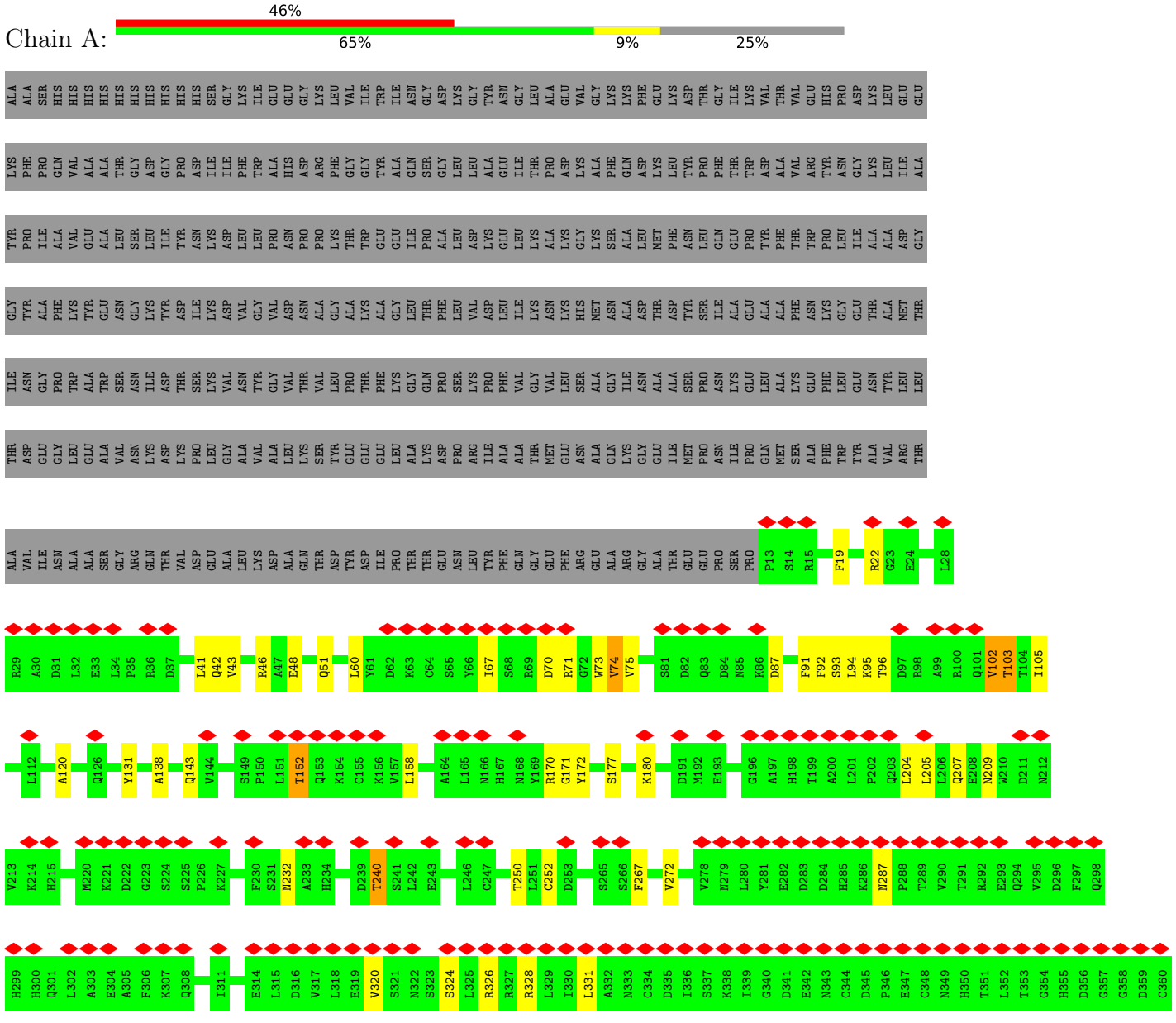
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	

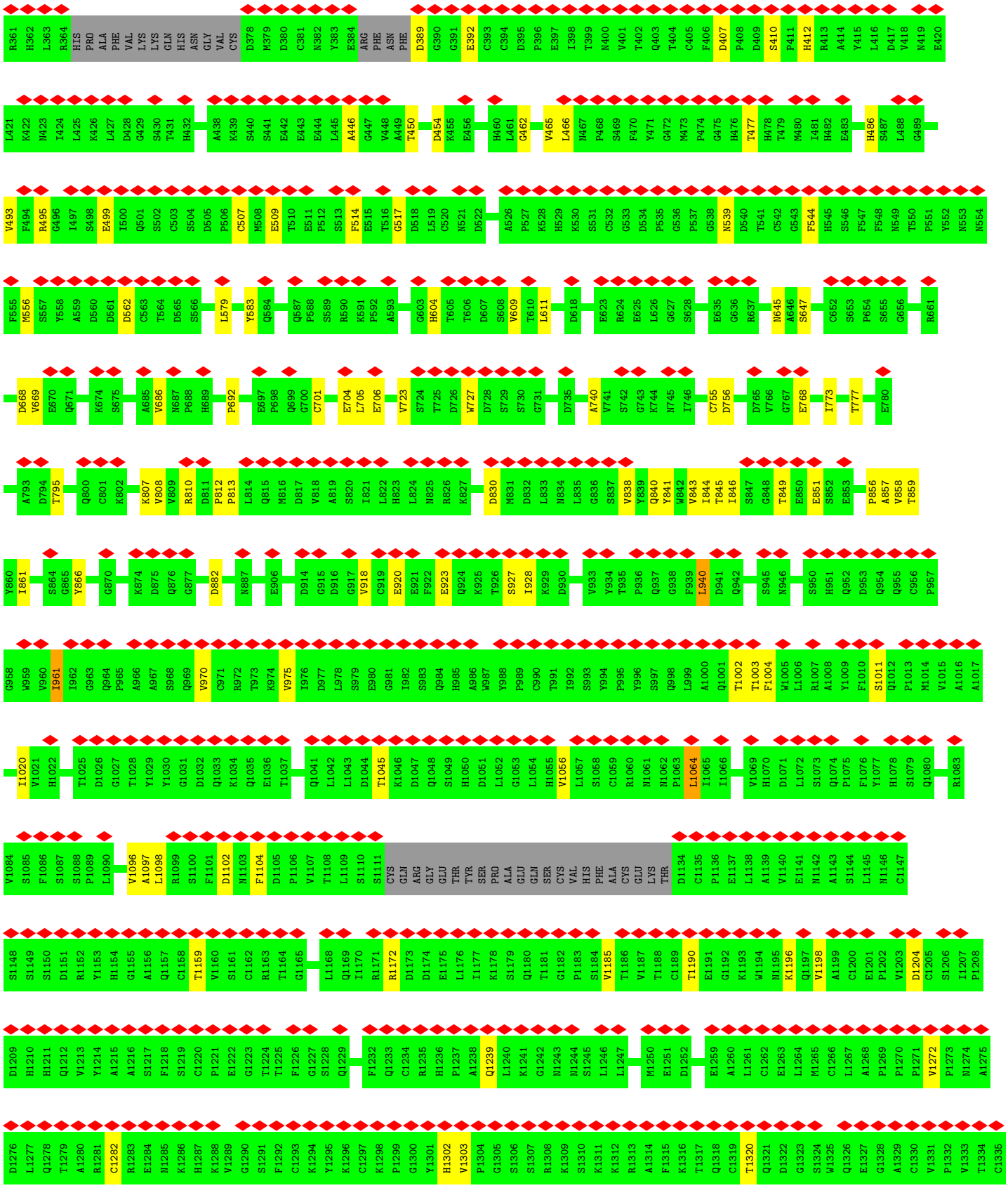
3 Residue-property plots (i)

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: Maltose/maltodextrin-binding periplasmic protein,Pappalysin-1

Chain A:

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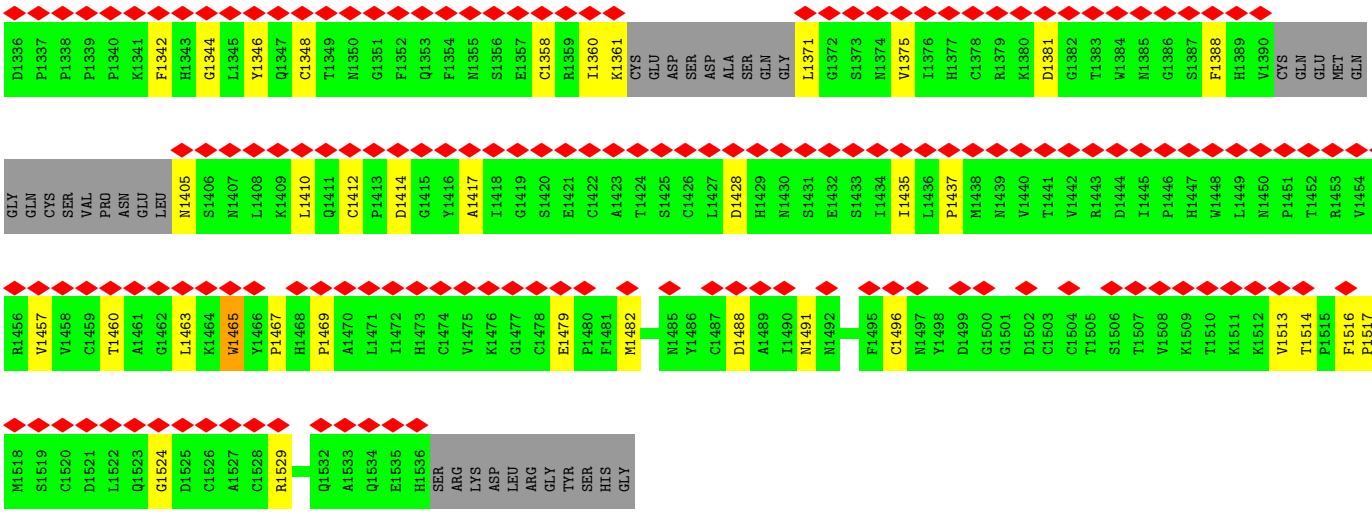
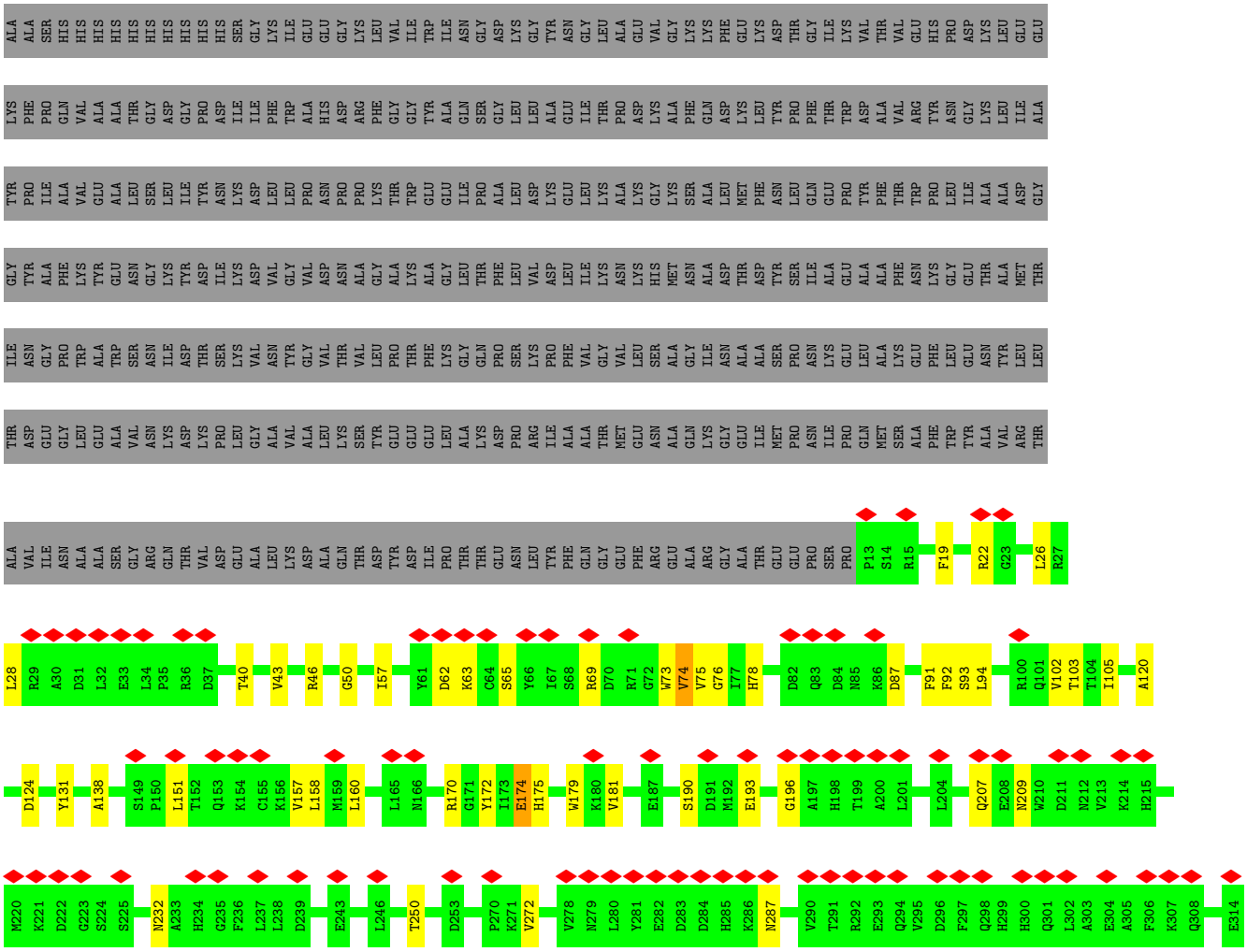
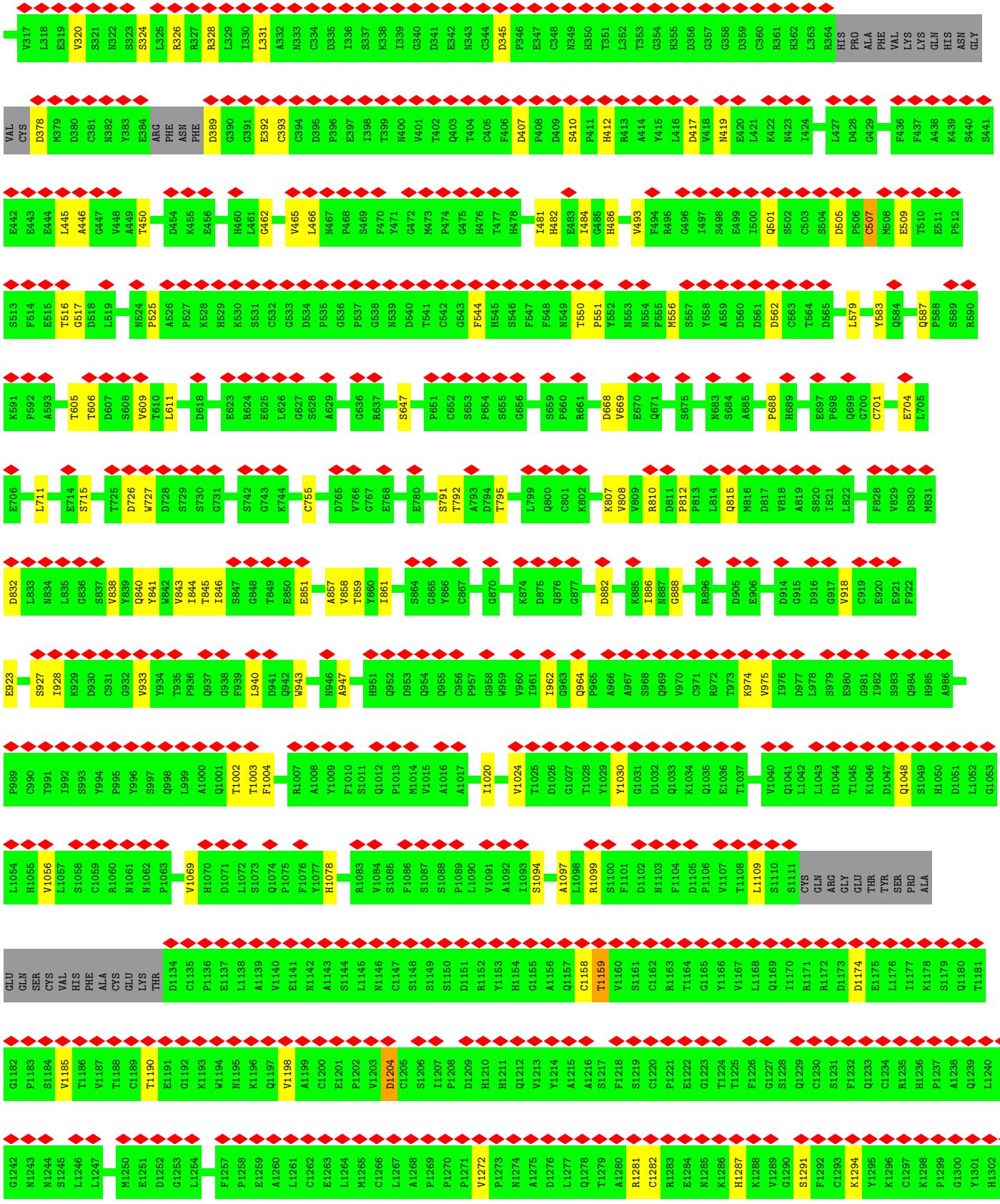
L421 K422 N423 I424 L425 K426 L427 D428 G429 S430 T431 H432 A438 K439 S440 S441 E442 E443 E444 L445 A446 G447 V448 A449 T450 D454 K455 E456 H460 L461 G462 V465 L466 N467 P468 S469 F470 Y471 G472 M473 P474 G475 H476 T477 H478 T479 M480 I481 H482 E483 H486 S487 L488 G489
V493 F494 R495 G496 I497 S498 E499 I500 Q501 S502 C503 S504 D505 P506 C507 M508 E509 T510 E511 P512 S513 F514 E515 T516 G517 D518 L519 C520 N521 D522 A526 P527 K528 H529 K530 S531 C532 G533 D534 P535 G536 P537 G538 N539 D540 T541 C542 G543 F544 H545 S546 F547 F548 N549 T550 P551 Y552 N553 N554
F555 M556 S557 Y558 A559 D560 D561 D562 C563 T564 D565 S566 L579 Y583 Q584 Q587 P588 S589 R590 K591 P592 A593 G603 H604 T605 T606 D607 S608 V609 T610 L611 D618 E623 R624 E625 L626 G627 S628 E635 G636 R637 N645 A646 S647 C652 S653 P654 S655 G656 R661
D668 V669 E670 Q671 K674 S675 A685 V686 N687 P688 H689 P692 E697 P698 Q699 G700 C701 E704 L705 E706 V723 S724 T725 D726 W727 D728 S729 S730 G731 D735 A740 V741 S742 G743 K744 N745 I746 C755 D756 D765 V766 G767 E768 I773 T777 E780
A793 D794 T795 Q800 C801 K802 K807 V808 V809 R810 D811 P812 P813 L814 Q815 M816 D817 V818 A819 S820 I821 L822 H823 L824 N825 R826 K827 D830 M831 D832 L833 N834 L835 G836 S837 V838 Y839 Q840 Y841 W842 V843 I844 T845 I846 S847 G848 T849 E850 E851 S852 E853 P856 A857 V858 T859
Y860 I861 S864 G865 Y866 G870 K874 D875 Q876 G877 D882 N887 E906 D914 G915 D916 G917 V918 C919 E920 E921 F922 E923 Q924 K925 T926 S927 I928 K929 D930 V933 Y934 T935 P936 Q937 G938 F939 L940 D941 Q942 S945 N946 S950 H951 Q952 D953 Q954 Q955 C956 P957
G958 W959 V960 I961 I962 G963 Q964 P965 A966 A967 S968 Q969 V970 C971 R972 T973 K974 V975 I976 D977 L978 S979 E980 G981 I982 S983 Q984 H985 A986 W987 Y988 P989 C990 T991 I992 S993 Y994 P995 Y996 S997 Q998 L999 A1000 Q1001 T1002 T1003 F1004 W1005 L1006 R1007 A1008 Y1009 F1010 S1011 Q1012 P1013 M1014 V1015 A1016 A1017
I1020 V1021 H1022 T1025 D1026 G1027 T1028 Y1029 Y1030 G1031 D1032 Q1033 K1034 Q1035 E1036 T1037 Q1041 L1042 L1043 D1044 T1045 K1046 D1047 Q1048 S1049 H1050 D1051 L1052 G1053 L1054 H1055 V1056 L1057 S1058 C1059 R1060 N1061 N1062 P1063 L1064 I1065 I1066 V1069 H1070 D1071 L1072 S1073 Q1074 P1075 F1076 Y1077 H1078 S1079 Q1080 R1083
V1084 S1085 F1086 S1087 S1088 P1089 L1090 V1096 A1097 L1098 R1099 S1100 F1101 D1102 N1103 F1104 D1105 P1106 V1107 T1108 L1109 S1110 S1111 CYS GLN ARG GLY GLU THR TYR SER PRO ALA GLU GLN SER CYS VAL HIS PHE ALA CYS GLU LYS THR D1134 C1135 P1136 E1137 L1138 A1139 V1140 E1141 N1142 A1143 S1144 L1145 N1146 C1147
S1148 S1149 S1150 D1151 R1152 Y1153 H1154 G1155 A1156 Q1157 C1158 T1159 V1160 S1161 C1162 R1163 T1164 G1165 L1168 Q1169 I1170 R1171 R1172 D1173 D1174 E1175 L1176 I1177 K1178 S1179 Q1180 T1181 G1182 P1183 S1184 V1185 T1186 V1187 T1188 C1189 T1190 E1191 G1192 K1193 W1194 N1195 K1196 Q1197 V1198 A1199 C1200 E1201 P1202 V1203 D1204 C1205 S1206 I1207 P1208
D1209 H1210 H1211 Q1212 V1213 Y1214 A1215 A1216 S1217 F1218 S1219 C1220 P1221 E1222 G1223 T1224 T1225 F1226 G1227 S1228 Q1229 F1232 Q1233 C1234 R1235 H1236 P1237 A1238 Q1239 L1240 K1241 G1242 N1243 N1244 S1245 L1246 L1247 M1250 E1251 D1252 E1259 A1260 L1261 C1262 E1263 L1264 M1265 C1266 L1267 A1268 P1269 P1270 P1271 V1272 P1273 N1274 A1275
D1276 L1277 Q1278 T1279 A1280 R1281 C1282 R1283 E1284 N1285 K1286 H1287 K1288 V1289 G1290 S1291 F1292 C1293 K1294 Y1295 K1296 C1297 K1298 P1299 G1300 Y1301 H1302 V1303 P1304 G1305 S1306 S1307 R1308 K1309 S1310 K1311 K1312 R1313 A1314 F1315 K1316 T1317 Q1318 C1319 T1320 Q1321 D1322 C1323 S1324 W1325 Q1326 E1327 G1328 A1329 C1330 V1331 P1332 V1333 T1334 C1335



• Molecule 1: Maltose/maltodextrin-binding periplasmic protein,Pappalysin-1

Chain B:

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VAL CYS D378 M379 D380 C381 N382 Y383 E384 ARG PHE ASN PHE D389 G390 G391 E392 C393 C394 D395 P396 E397 I398 T399 N400 V401 T402 Q403 T404 C405 F406 D407 P408 D409 S410 P411 H412 R413 A414 Y415 L416 D417 Y418 N419 E420 L421 K422 N423 I424 L427 D428 G429 F436 F437 A438 K439 S440 S441
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E706 L711 E714 S715 T725 D726 W727 D728 S729 S730 G731 S742 G743 K744 C755 D765 V766 G767 E768 E780 S791 T792 A793 D794 T795 L799 Q800 C801 K802 K807 V808 V809 R810 D811 P812 P813 L814 Q815 M816 D817 V818 A819 S820 I821 L822 F828 V829 D830 M831
D832 L833 N834 L835 G836 S837 V838 Y839 Q840 Y841 W842 V843 I844 T845 I846 S847 G848 T849 E850 E851 A857 V858 T859 Y860 I861 S864 G865 Y866 C867 G870 K874 D875 Q876 G877 D882 K885 I886 N887 G888 R896 D905 E906 D914 G915 D916 G917 V918 C919 E920 E921 F922
E923 S927 I928 K929 D930 C931 G932 V933 Y934 T935 P936 Q937 G938 F939 L940 D941 Q942 W943 N946 A947 H951 Q952 D953 Q954 Q955 C956 P957 G958 W959 V960 I961 I962 G963 Q964 P965 A966 A967 S968 Q969 V970 C971 R972 T973 K974 V975 I976 D977 L978 S979 E980 G981 I982 S983 Q984 H985 A986
P989 C990 T991 I992 S993 Y994 P995 Y996 S997 Q998 L999 A1000 Q1001 T1002 T1003 F1004 R1007 A1008 Y1009 F1010 S1011 Q1012 P1013 M1014 V1015 A1016 A1017 I1020 V1024 T1025 D1026 G1027 T1028 Y1029 Y1030 G1031 D1032 Q1033 K1034 Q1035 E1036 T1037 V1040 Q1041 L1042 L1043 D1044 T1045 K1046 D1047 Q1048 S1049 H1050 D1051 L1052 G1053
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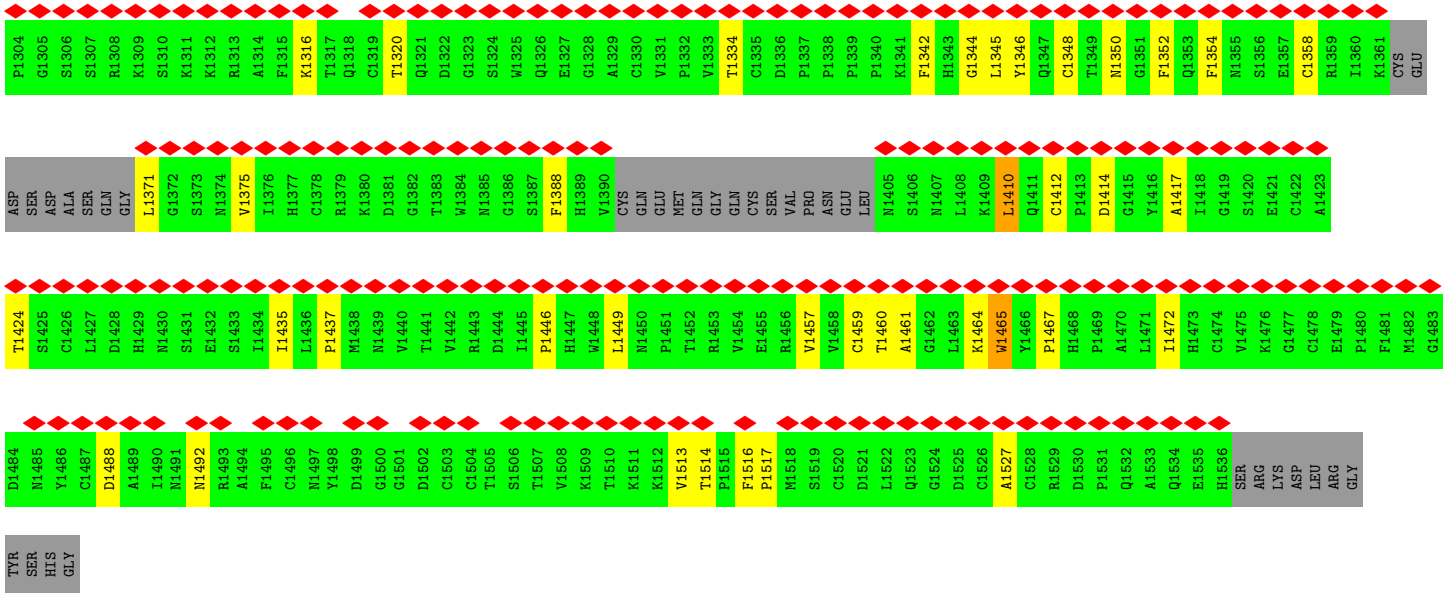
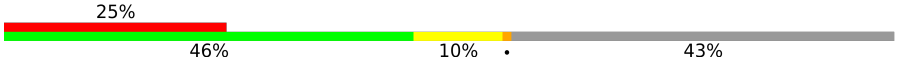
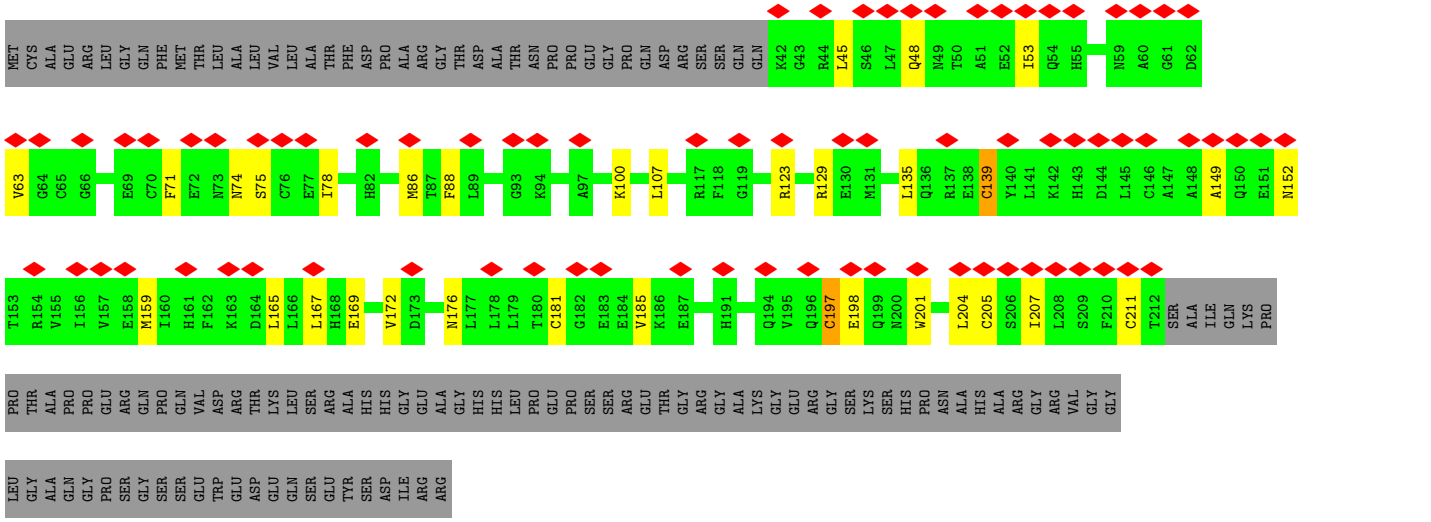
GLU GLN SER CYS VAL HIS PHE ALA CYS GLU LYS THR D1134 C1135 P1136 E1137 L1138 A1139 V1140 E1141 N1142 A1143 S1144 L1145 N1146 C1147 S1148 S1149 S1150 D1151 R1152 Y1153 H1154 G1155 A1156 Q1157 C1158 T1159 V1160 S1161 C1162 R1163 T1164 G1165 Y1166 V1167 L1168 Q1169 I1170 R1171 R1172 D1173 D1174 E1175 L1176 I1177 K1178 S1179 Q1180 T1181
G1182 P1183 S1184 V1185 T1186 V1187 T1188 C1189 T1190 E1191 G1192 K1193 W1194 N1195 K1196 Q1197 V1198 A1199 C1200 E1201 P1202 V1203 D1204 C1205 S1206 I1207 P1208 D1209 H1210 H1211 Q1212 V1213 Y1214 A1215 A1216 S1217 F1218 S1219 C1220 P1221 E1222 G1223 T1224 T1225 F1226 G1227 S1228 Q1229 C1230 S1231 F1232 Q1233 C1234 R1235 H1236 P1237 A1238 Q1239 L1240 K1241
G1242 N1243 N1244 S1245 L1246 L1247 M1250 E1251 D1252 G1253 L1254 F1257 P1258 E1259 A1260 L1261 C1262 E1263 L1264 M1265 C1266 L1267 A1268 P1269 P1270 P1271 V1272 P1273 N1274 A1275 D1276 L1277 Q1278 T1279 A1280 R1281 C1282 R1283 E1284 N1285 K1286 H1287 K1288 V1289 G1290 S1291 F1292 C1293 K1294 Y1295 K1296 C1297 K1298 P1299 G1300 Y1301 H1302 V1303



• Molecule 2: Stanniocalcin-2

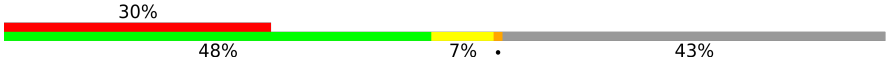
Chain C:

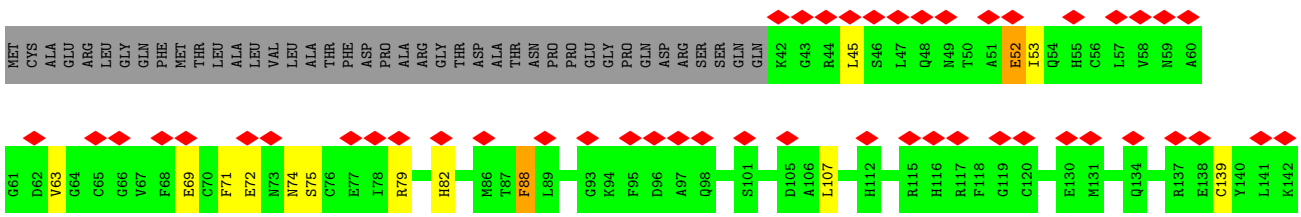


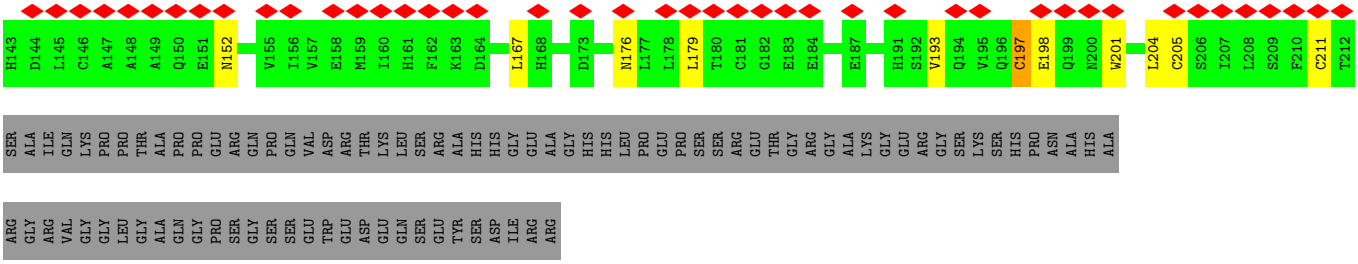


• Molecule 2: Stanniocalcin-2

Chain G:






H143 D144 L145 C146 A147 A148 A149 Q150 E151 N152 V155 I156 V157 E158 M159 I160 H161 F162 K163 D164 L167 H168 D173 N176 L177 L178 L179 T180 C181 G182 E183 E184 E187 H191 S192 V193 Q194 V195 Q196 C197 E198 Q199 N200 W201 L204 C205 S206 I207 L208 S209 F210 C211 T212
SER ALA ILE GLN LYS PRO PRO THR ALA PRO PRO GLU ARG GLN PRO GLN VAL ASP ARG THR LYS LEU SER ARG ALA HIS HIS GLY GLU ALA GLY HIS HIS LEU PRO GLU PRO SER SER ARG GLU THR GLY ARG GLY ALA LYS GLY GLU ARG GLY SER LYS SER HIS PRO ASN ALA HIS ALA
ARG GLY ARG VAL GLY GLY LEU GLY ALA GLN GLY PRO SER GLY SER SER GLU TRP GLU ASP GLU GLN SER GLU TYR SER ASP ILE ARG ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	253671	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 ($e^-/Å^2$)	59.8	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0217	Depositor
Map size (Å)	270.08, 270.08, 270.08	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.27	0/11725	0.50	0/15963
1	B	0.27	0/11725	0.50	0/15963
2	C	0.28	0/1357	0.52	0/1825
2	G	0.28	0/1357	0.52	0/1825
All	All	0.27	0/26164	0.50	0/35576

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	11420	0	10786	83	0
1	B	11420	0	10786	92	0
2	C	1335	0	1313	14	0
2	G	1335	0	1313	13	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	25512	0	24198	195	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 (195) 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:1405:ASN:HB2	1:A:1469:PRO:HB2	1.76	0.68
1:B:482:HIS:NE2	1:B:486:HIS:CE1	2.70	0.60
1:A:509:GLU:HB2	1:A:517:GLY:HA3	1.84	0.59
1:B:1020:ILE:HB	1:B:1097:ALA:HB3	1.85	0.58
1:A:1185:VAL:HG11	1:A:1198:VAL:HG11	1.85	0.58
1:B:1414:ASP:HB3	1:B:1417:ALA:HB3	1.85	0.58
1:B:19:PHE:O	1:B:170:ARG:HA	2.04	0.57
1:B:1281:ARG:HH12	1:B:1291:SER:HB3	1.69	0.57
2:C:211:CYS:N	2:G:211:CYS:SG	2.78	0.56
1:B:174:GLU:OE1	1:B:175:HIS:ND1	2.38	0.56
1:B:287:ASN:OD1	1:B:326:ARG:NH2	2.39	0.55
2:C:211:CYS:SG	2:G:211:CYS:N	2.80	0.55
1:A:209:ASN:OD1	1:A:209:ASN:N	2.40	0.55
1:A:1414:ASP:HB3	1:A:1417:ALA:HB3	1.90	0.54
1:A:46:ARG:HB3	1:A:172:TYR:HB2	1.90	0.54
1:A:1020:ILE:HB	1:A:1097:ALA:HB3	1.89	0.54
1:B:63:LYS:HA	1:B:69:ARG:HH22	1.72	0.54
1:B:509:GLU:HG2	1:B:525:PRO:HG3	1.90	0.53
2:C:207:ILE:HG21	2:G:193:VAL:HG21	1.91	0.53
1:B:65:SER:O	1:B:69:ARG:NH1	2.41	0.53
1:B:1204:ASP:OD1	1:B:1204:ASP:N	2.41	0.53
1:A:645:ASN:HB3	1:A:706:GLU:HB3	1.90	0.53
1:A:87:ASP:OD1	1:A:87:ASP:N	2.40	0.53
1:B:46:ARG:HB3	1:B:172:TYR:HB2	1.91	0.53
1:A:204:LEU:HD11	1:A:207:GLN:HB2	1.90	0.53
1:A:846:ILE:HG22	1:A:851:GLU:HA	1.91	0.53
1:A:1204:ASP:OD1	1:A:1204:ASP:N	2.41	0.53
1:B:50:GLY:O	1:B:170:ARG:NH1	2.42	0.53
1:B:1020:ILE:HD11	1:B:1099:ARG:HH21	1.74	0.53
1:A:668:ASP:N	1:A:668:ASP:OD1	2.42	0.52
1:A:1457:VAL:HG13	1:A:1467:PRO:HB2	1.89	0.52
1:B:668:ASP:OD1	1:B:668:ASP:N	2.43	0.52
1:B:815:GLN:NE2	1:B:832:ASP:OD2	2.42	0.52
1:B:1342:PHE:HD2	1:B:1388:PHE:HB3	1.74	0.52
1:A:73:TRP:HB3	1:A:94:LEU:HD13	1.91	0.52
1:A:19:PHE:O	1:A:170:ARG:HA	2.09	0.52
1:B:886:ILE:HG22	1:B:888:GLY:H	1.74	0.52
1:A:41:LEU:O	1:A:120:ALA:HA	2.11	0.51
1:B:1435:ILE:HG12	1:B:1472:ILE:HG12	1.92	0.51
1:B:1459:CYS:HA	1:B:1464:LYS:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ILE:HG23	1:A:138:ALA:HB3	1.93	0.51
2:G:45:LEU:HD11	2:G:74:ASN:HB2	1.92	0.51
1:B:838:VAL:HG12	1:B:861:ILE:HG12	1.91	0.51
1:A:71:ARG:NH1	1:A:96:THR:O	2.43	0.51
1:B:509:GLU:HB2	1:B:517:GLY:HA3	1.93	0.50
1:A:1516:PHE:HB2	2:C:100:LYS:HE2	1.92	0.50
2:C:45:LEU:HD11	2:C:74:ASN:HB2	1.93	0.50
1:A:51:GLN:NE2	1:A:170:ARG:O	2.44	0.50
1:B:1435:ILE:HG22	1:B:1437:PRO:HD3	1.93	0.50
1:A:120:ALA:HB3	1:A:131:TYR:HB2	1.94	0.50
1:A:882:ASP:OD1	1:A:882:ASP:N	2.44	0.50
1:A:287:ASN:OD1	1:A:326:ARG:NH2	2.44	0.50
1:B:882:ASP:OD1	1:B:882:ASP:N	2.43	0.49
1:B:807:LYS:HE2	1:B:844:ILE:HD11	1.94	0.49
1:A:1524:GLY:O	1:A:1529:ARG:NH2	2.46	0.49
1:B:579:LEU:HA	1:B:583:TYR:HB2	1.93	0.49
2:C:45:LEU:HA	2:C:75:SER:HB3	1.95	0.49
1:B:1350:ASN:ND2	1:B:1354:PHE:O	2.41	0.49
1:B:1460:THR:OG1	1:B:1461:ALA:N	2.45	0.49
2:C:53:ILE:HD11	2:C:71:PHE:HA	1.95	0.49
1:B:324:SER:O	1:B:328:ARG:NH1	2.46	0.49
1:A:42:GLN:HB2	1:A:177:SER:HB3	1.95	0.49
1:B:87:ASP:OD1	1:B:87:ASP:N	2.43	0.49
1:A:539:ASN:HA	1:B:1048:GLN:HE22	1.78	0.48
1:B:105:ILE:HG23	1:B:138:ALA:HB3	1.95	0.48
1:A:1002:THR:OG1	1:A:1003:THR:N	2.45	0.48
1:B:73:TRP:HB3	1:B:94:LEU:HD13	1.95	0.48
1:A:1348:CYS:HA	1:A:1358:CYS:HA	1.95	0.48
1:B:791:SER:OG	1:B:792:THR:N	2.47	0.48
2:G:72:GLU:OE1	2:G:79:ARG:NH2	2.46	0.48
1:A:807:LYS:HE2	1:A:844:ILE:HD11	1.95	0.48
1:B:501:GLN:NE2	1:B:505:ASP:OD1	2.47	0.48
1:A:180:LYS:HE2	1:A:205:LEU:HD13	1.94	0.48
1:A:562:ASP:OD1	1:A:562:ASP:N	2.43	0.48
1:B:196:GLY:O	1:B:207:GLN:NE2	2.47	0.47
2:C:172:VAL:O	2:C:176:ASN:ND2	2.47	0.47
1:B:62:ASP:O	1:B:69:ARG:NH2	2.47	0.47
1:A:940:LEU:HB2	1:A:1102:ASP:HB3	1.95	0.47
1:B:1185:VAL:HG11	1:B:1198:VAL:HG11	1.96	0.47
1:A:75:VAL:HG22	1:A:92:PHE:HD1	1.79	0.47
1:A:579:LEU:HA	1:A:583:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:810:ARG:HG2	1:B:812:PRO:HD2	1.97	0.47
2:C:149:ALA:HB1	2:C:185:VAL:HG21	1.96	0.47
2:G:74:ASN:N	2:G:74:ASN:OD1	2.46	0.47
1:A:1342:PHE:HD2	1:A:1388:PHE:HB3	1.79	0.47
1:B:1410:LEU:HB3	1:B:1424:THR:HG22	1.96	0.47
1:A:48:GLU:HG2	1:A:171:GLY:HA2	1.97	0.47
2:G:53:ILE:HD11	2:G:71:PHE:HA	1.96	0.47
1:A:1346:TYR:HA	1:A:1360:ILE:HG22	1.97	0.46
1:A:1435:ILE:HG22	1:A:1437:PRO:HD3	1.97	0.46
1:B:407:ASP:HB2	1:B:410:SER:HB2	1.97	0.46
1:A:152:THR:O	1:A:152:THR:OG1	2.34	0.46
1:B:209:ASN:OD1	1:B:209:ASN:N	2.49	0.46
1:B:345:ASP:N	1:B:345:ASP:OD1	2.48	0.46
1:B:120:ALA:HB3	1:B:131:TYR:HB2	1.97	0.46
1:A:232:ASN:OD1	1:A:232:ASN:N	2.49	0.46
1:B:378:ASP:N	1:B:393:CYS:HG	2.13	0.46
1:B:840:GLN:HG2	1:B:859:THR:HG22	1.97	0.46
1:A:838:VAL:HG12	1:A:861:ILE:HG12	1.98	0.45
1:B:1281:ARG:O	1:B:1287:HIS:NE2	2.49	0.45
2:G:45:LEU:HA	2:G:75:SER:HB3	1.98	0.45
1:A:407:ASP:HB2	1:A:410:SER:HB2	1.98	0.45
1:A:1361:LYS:HE2	1:A:1361:LYS:HB2	1.86	0.45
2:G:107:LEU:HD13	2:G:107:LEU:HA	1.83	0.45
1:B:688:PRO:O	2:C:123:ARG:NH2	2.49	0.45
1:A:450:THR:HG21	1:A:462:GLY:HA2	1.99	0.45
1:A:647:SER:OG	1:A:704:GLU:OE1	2.31	0.45
1:A:1011:SER:HB3	1:B:1174:ASP:HA	1.98	0.45
1:B:57:ILE:HG13	1:B:76:GLY:HA2	1.99	0.45
1:B:1516:PHE:CG	1:B:1517:PRO:HD3	2.52	0.45
1:A:740:ALA:HB1	1:A:768:GLU:HG2	1.99	0.45
1:A:920:GLU:HB2	1:A:923:GLU:HB2	1.99	0.45
1:A:1064:LEU:HA	1:A:1064:LEU:HD13	1.85	0.45
2:C:197:CYS:SG	2:C:198:GLU:N	2.89	0.45
1:A:324:SER:O	1:A:328:ARG:NH1	2.50	0.45
1:B:190:SER:HA	1:B:193:GLU:HG2	1.97	0.45
1:B:40:THR:HB	1:B:179:TRP:HB2	1.98	0.44
1:B:1158:CYS:SG	1:B:1159:THR:N	2.90	0.44
1:A:1344:GLY:H	1:A:1346:TYR:HD1	1.64	0.44
1:A:1381:ASP:N	1:A:1381:ASP:OD1	2.49	0.44
1:B:841:TYR:O	1:B:857:ALA:HA	2.18	0.44
1:A:841:TYR:O	1:A:857:ALA:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:GLN:H	1:B:587:GLN:HG2	1.66	0.44
2:C:152:ASN:OD1	2:C:152:ASN:N	2.50	0.44
1:A:830:ASP:OD1	1:A:830:ASP:N	2.50	0.44
1:A:961:ILE:H	1:A:961:ILE:HG12	1.64	0.44
1:B:75:VAL:HG22	1:B:92:PHE:HD1	1.82	0.44
1:B:923:GLU:HG2	1:B:927:SER:HB3	2.00	0.44
2:G:197:CYS:SG	2:G:198:GLU:N	2.91	0.44
2:C:129:ARG:NH1	2:C:169:GLU:OE1	2.43	0.44
1:B:647:SER:OG	1:B:704:GLU:OE1	2.30	0.43
1:B:1492:ASN:ND2	1:B:1527:ALA:O	2.47	0.43
1:B:1294:LYS:HD3	1:B:1316:LYS:HZ1	1.82	0.43
1:B:1446:PRO:HG2	1:B:1449:LEU:HB2	2.00	0.43
1:A:95:LYS:HB2	1:A:102:VAL:HB	2.01	0.43
1:A:1479:GLU:H	1:A:1491:ASN:HD21	1.66	0.43
1:B:562:ASP:OD1	1:B:562:ASP:N	2.41	0.43
1:B:974:LYS:HB3	1:B:1030:TYR:HA	2.00	0.43
2:C:135:LEU:O	2:C:139:CYS:HB2	2.17	0.43
1:A:495:ARG:HA	1:A:499:GLU:HB2	2.01	0.43
1:A:1482:MET:HE1	1:A:1496:CYS:HB3	1.99	0.43
1:B:389:ASP:HB2	1:B:392:GLU:HB2	1.99	0.43
1:B:417:ASP:OD2	1:B:419:ASN:ND2	2.42	0.43
1:B:1348:CYS:HA	1:B:1358:CYS:HA	1.99	0.43
1:A:389:ASP:HB2	1:A:392:GLU:HB2	2.01	0.43
1:A:446:ALA:HB1	1:A:466:LEU:HA	2.01	0.43
1:B:846:ILE:HG22	1:B:851:GLU:HA	2.00	0.43
1:A:1172:ARG:HG3	1:A:1196:LYS:HG2	2.01	0.43
1:B:933:VAL:HG11	1:B:1020:ILE:HD13	2.01	0.43
1:B:1334:THR:HG23	1:B:1352:PHE:HB3	2.01	0.42
1:B:1457:VAL:HG13	1:B:1467:PRO:HG2	2.00	0.42
1:A:923:GLU:HG2	1:A:927:SER:HB3	2.00	0.42
1:B:726:ASP:N	1:B:726:ASP:OD1	2.51	0.42
1:B:1002:THR:OG1	1:B:1003:THR:N	2.52	0.42
1:A:103:THR:HG22	1:A:143:GLN:HE21	1.84	0.42
1:A:810:ARG:HG2	1:A:812:PRO:HD2	2.00	0.42
1:A:91:PHE:HA	1:A:105:ILE:O	2.19	0.42
1:A:1516:PHE:CD2	1:A:1517:PRO:HD3	2.54	0.42
1:B:74:VAL:HG13	1:B:93:SER:HB2	2.00	0.42
1:B:550:THR:HA	1:B:551:PRO:HD3	1.95	0.42
1:A:705:LEU:HD12	1:A:773:ILE:HD11	2.02	0.42
1:B:28:LEU:HD22	1:B:158:LEU:HD22	2.02	0.42
1:A:604:HIS:ND1	1:A:866:TYR:OH	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1463:LEU:HG	1:A:1465:TRP:H	1.85	0.42
1:A:686:VAL:HG11	1:A:692:PRO:HA	2.01	0.42
2:G:69:GLU:OE1	2:G:82:HIS:NE2	2.53	0.42
1:B:1344:GLY:H	1:B:1346:TYR:HD1	1.68	0.42
1:A:812:PRO:HA	1:A:813:PRO:HD3	1.92	0.41
1:B:26:LEU:HD12	1:B:160:LEU:HD23	2.01	0.41
1:A:1488:ASP:HA	1:A:1516:PHE:HD2	1.85	0.41
1:B:1345:LEU:HG	1:B:1465:TRP:CH2	2.54	0.41
1:A:74:VAL:HG13	1:A:93:SER:HB2	2.02	0.41
1:B:91:PHE:HA	1:B:105:ILE:O	2.21	0.41
1:B:493:VAL:HG13	1:B:556:MET:HB2	2.01	0.41
1:A:70:ASP:OD1	1:A:70:ASP:N	2.47	0.41
1:A:840:GLN:HG2	1:A:859:THR:HG22	2.02	0.41
1:B:1024:VAL:HG13	1:B:1094:SER:HB2	2.01	0.41
1:B:605:THR:OG1	1:B:606:THR:N	2.52	0.41
1:B:947:ALA:H	1:B:962:ILE:HD11	1.85	0.41
1:A:1428:ASP:OD1	1:A:1428:ASP:N	2.51	0.41
1:B:943:TRP:CD1	1:B:964:GLN:HG2	2.56	0.41
1:A:493:VAL:HG13	1:A:556:MET:HB2	2.01	0.41
1:A:830:ASP:OD2	1:A:841:TYR:OH	2.36	0.41
1:B:507:CYS:HB2	1:B:516:THR:HG23	2.03	0.41
1:B:1457:VAL:HG22	1:B:1467:PRO:HB2	2.02	0.41
1:A:240:THR:O	1:A:240:THR:OG1	2.39	0.41
1:A:267:PHE:HZ	1:A:856:PRO:HD3	1.86	0.40
1:A:1302:HIS:ND1	1:A:1303:VAL:O	2.53	0.40
1:B:450:THR:HG21	1:B:462:GLY:HA2	2.02	0.40
2:G:88:PHE:HD1	2:G:88:PHE:HA	1.71	0.40
1:B:446:ALA:HB1	1:B:466:LEU:HA	2.03	0.40
1:B:1294:LYS:HB2	1:B:1316:LYS:HZ3	1.86	0.40
1:B:481:ILE:O	1:B:484:ILE:HB	2.21	0.40
1:B:151:LEU:HD13	1:B:151:LEU:HA	1.98	0.40
2:G:52:GLU:H	2:G:52:GLU:HG3	1.76	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	1450/1944 (75%)	1405 (97%)	45 (3%)	0	100	100
1	B	1450/1944 (75%)	1399 (96%)	51 (4%)	0	100	100
2	C	169/302 (56%)	162 (96%)	7 (4%)	0	100	100
2	G	169/302 (56%)	163 (96%)	6 (4%)	0	100	100
All	All	3238/4492 (72%)	3129 (97%)	109 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	1284/1676 (77%)	1219 (95%)	65 (5%)	24	51
1	B	1284/1676 (77%)	1228 (96%)	56 (4%)	28	54
2	C	148/251 (59%)	133 (90%)	15 (10%)	7	28
2	G	148/251 (59%)	136 (92%)	12 (8%)	11	37
All	All	2864/3854 (74%)	2716 (95%)	148 (5%)	27	50

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	43	VAL
1	A	60	LEU
1	A	67	ILE
1	A	74	VAL
1	A	102	VAL
1	A	103	THR
1	A	152	THR

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Mol	Chain	Res	Type
1	A	158	LEU
1	A	240	THR
1	A	250	THR
1	A	252	CYS
1	A	272	VAL
1	A	320	VAL
1	A	331	LEU
1	A	412	HIS
1	A	454	ASP
1	A	465	VAL
1	A	477	THR
1	A	486	HIS
1	A	507	CYS
1	A	514	PHE
1	A	544	PHE
1	A	609	VAL
1	A	611	LEU
1	A	669	VAL
1	A	701	CYS
1	A	723	VAL
1	A	727	TRP
1	A	755	CYS
1	A	756	ASP
1	A	777	THR
1	A	795	THR
1	A	808	VAL
1	A	843	VAL
1	A	845	THR
1	A	849	THR
1	A	858	VAL
1	A	918	VAL
1	A	928	ILE
1	A	940	LEU
1	A	961	ILE
1	A	970	VAL
1	A	975	VAL
1	A	1004	PHE
1	A	1045	THR
1	A	1056	VAL
1	A	1064	LEU
1	A	1096	VAL
1	A	1098	LEU

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Mol	Chain	Res	Type
1	A	1104	PHE
1	A	1159	THR
1	A	1190	THR
1	A	1239	GLN
1	A	1272	VAL
1	A	1282	CYS
1	A	1320	THR
1	A	1371	LEU
1	A	1375	VAL
1	A	1410	LEU
1	A	1412	CYS
1	A	1460	THR
1	A	1465	TRP
1	A	1513	VAL
1	A	1514	THR
1	B	22	ARG
1	B	43	VAL
1	B	74	VAL
1	B	78	HIS
1	B	102	VAL
1	B	103	THR
1	B	124	ASP
1	B	157	VAL
1	B	174	GLU
1	B	181	VAL
1	B	232	ASN
1	B	250	THR
1	B	272	VAL
1	B	320	VAL
1	B	331	LEU
1	B	412	HIS
1	B	445	LEU
1	B	465	VAL
1	B	507	CYS
1	B	544	PHE
1	B	609	VAL
1	B	611	LEU
1	B	669	VAL
1	B	701	CYS
1	B	711	LEU
1	B	715	SER
1	B	727	TRP

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Mol	Chain	Res	Type
1	B	755	CYS
1	B	795	THR
1	B	808	VAL
1	B	843	VAL
1	B	845	THR
1	B	858	VAL
1	B	918	VAL
1	B	928	ILE
1	B	940	LEU
1	B	975	VAL
1	B	1004	PHE
1	B	1056	VAL
1	B	1069	VAL
1	B	1078	HIS
1	B	1109	LEU
1	B	1159	THR
1	B	1190	THR
1	B	1204	ASP
1	B	1272	VAL
1	B	1282	CYS
1	B	1320	THR
1	B	1371	LEU
1	B	1375	VAL
1	B	1410	LEU
1	B	1412	CYS
1	B	1465	TRP
1	B	1488	ASP
1	B	1513	VAL
1	B	1514	THR
2	C	48	GLN
2	C	63	VAL
2	C	78	ILE
2	C	86	MET
2	C	88	PHE
2	C	107	LEU
2	C	139	CYS
2	C	159	MET
2	C	165	LEU
2	C	167	LEU
2	C	181	CYS
2	C	197	CYS
2	C	201	TRP

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Mol	Chain	Res	Type
2	C	204	LEU
2	C	205	CYS
2	G	52	GLU
2	G	63	VAL
2	G	88	PHE
2	G	139	CYS
2	G	152	ASN
2	G	167	LEU
2	G	176	ASN
2	G	179	LEU
2	G	197	CYS
2	G	201	TRP
2	G	204	LEU
2	G	205	CYS

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	1239	GLN
1	A	1491	ASN
2	C	176	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

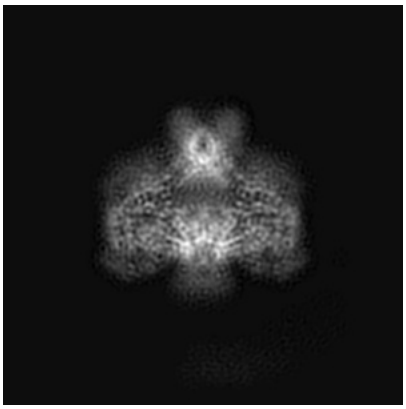
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34739. These allow visual inspection of the internal detail of the map and identification of artifacts.

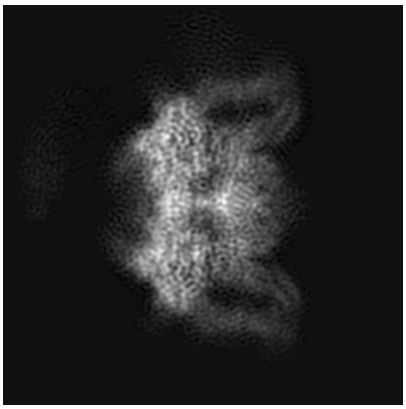
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

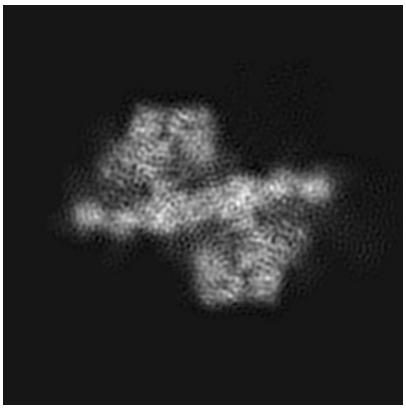
6.1.1 Primary map



X

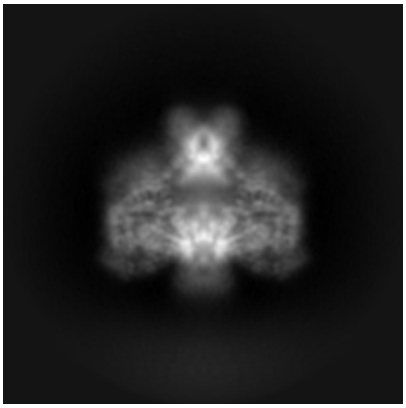


Y

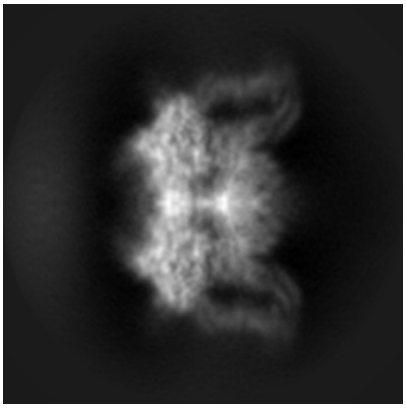


Z

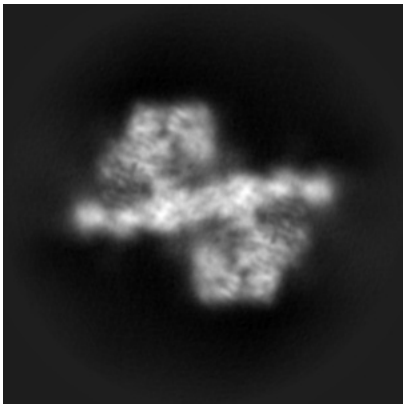
6.1.2 Raw map



X



Y

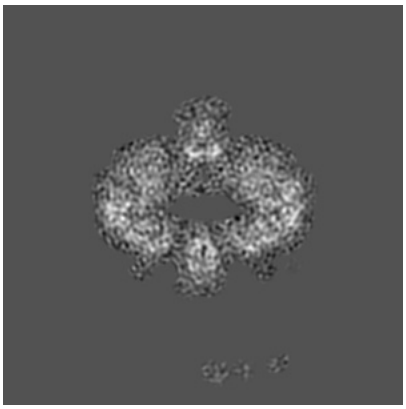


Z

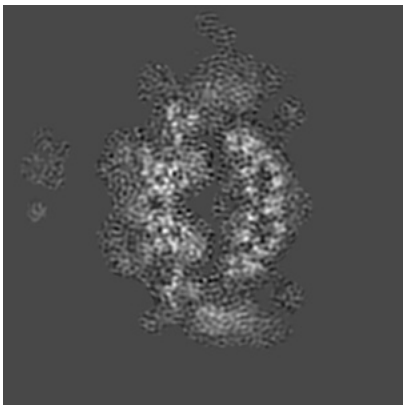
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

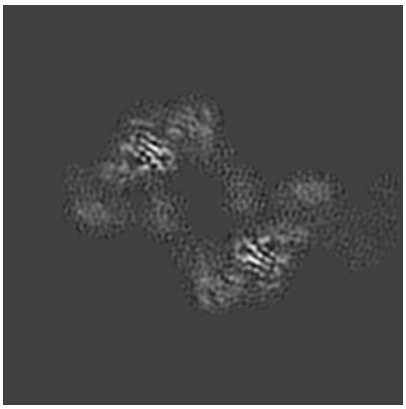
6.2.1 Primary map



X Index: 128

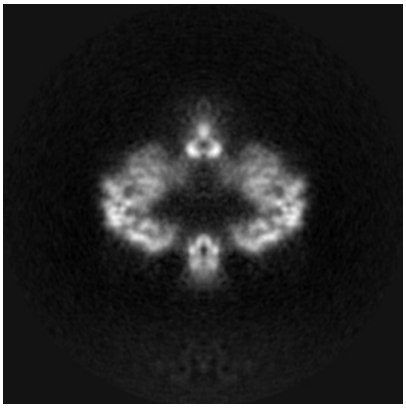


Y Index: 128

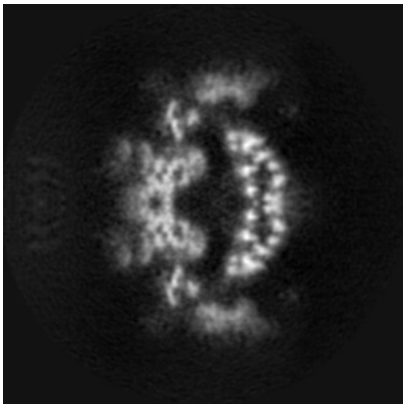


Z Index: 128

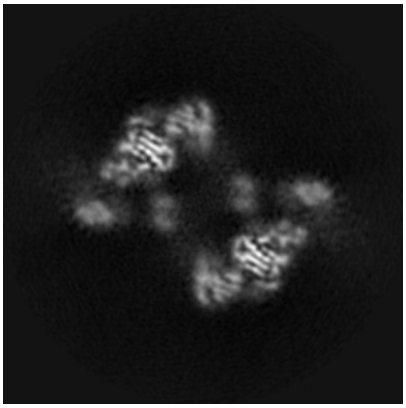
6.2.2 Raw map



X Index: 128



Y Index: 128

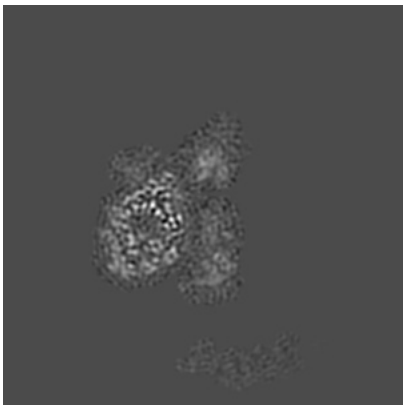


Z Index: 128

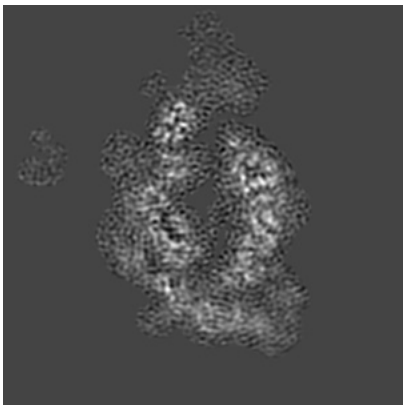
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

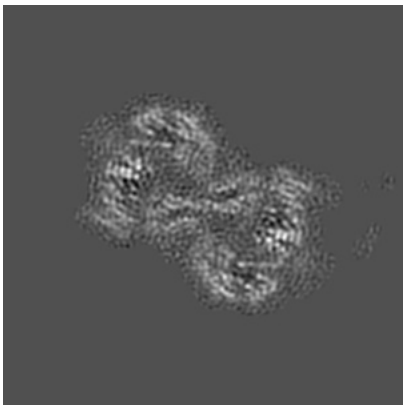
6.3.1 Primary map



X Index: 164

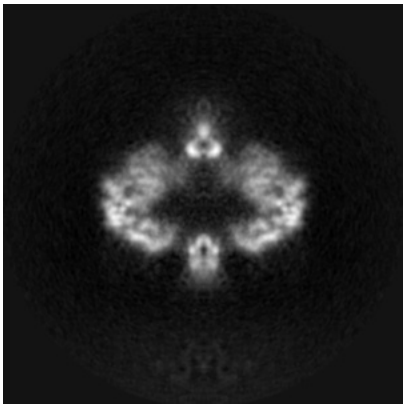


Y Index: 123

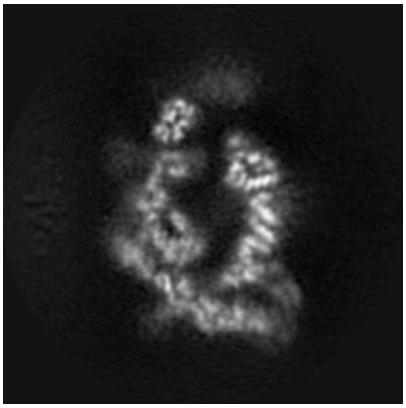


Z Index: 106

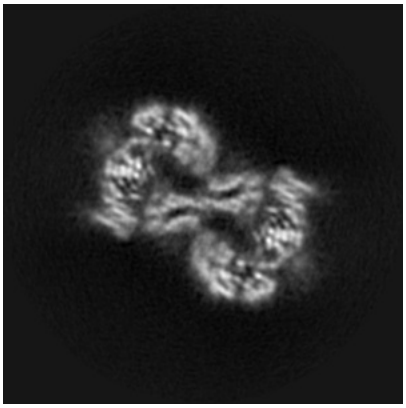
6.3.2 Raw map



X Index: 128



Y Index: 122



Z Index: 106

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 0.0217. 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.

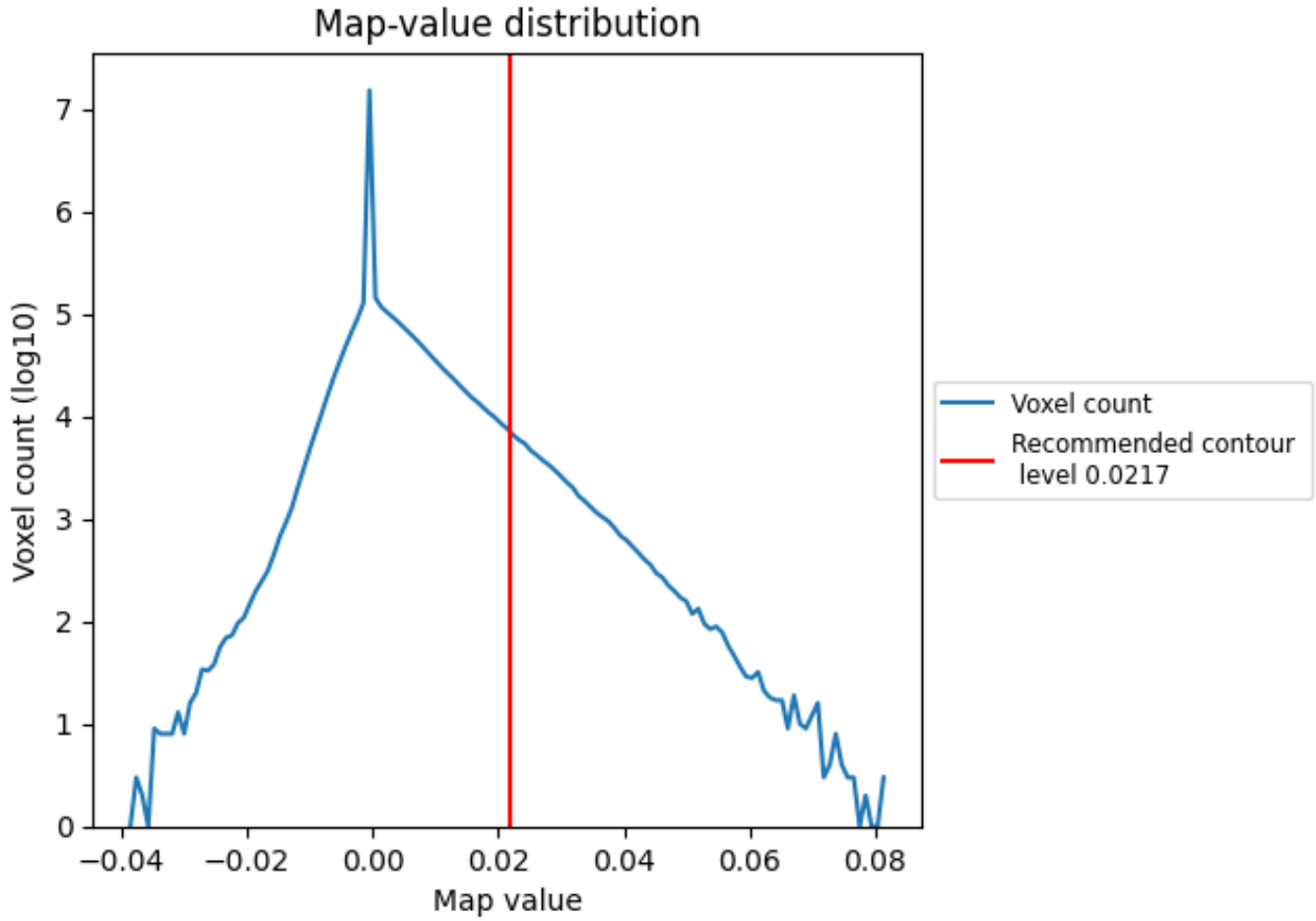
6.5 Mask visualisation (i)

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

7 Map analysis

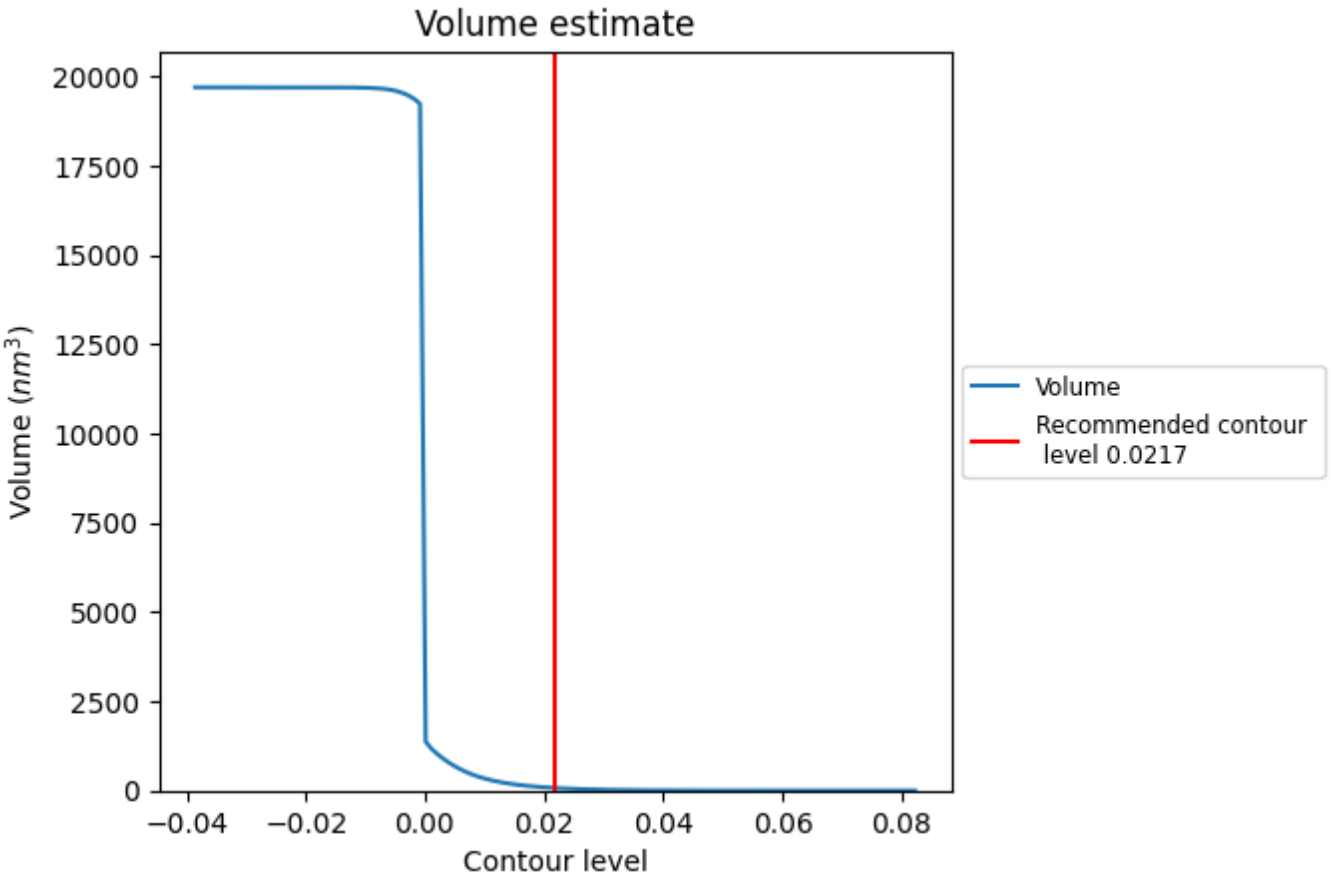
This section contains the results of statistical analysis of the map.

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.

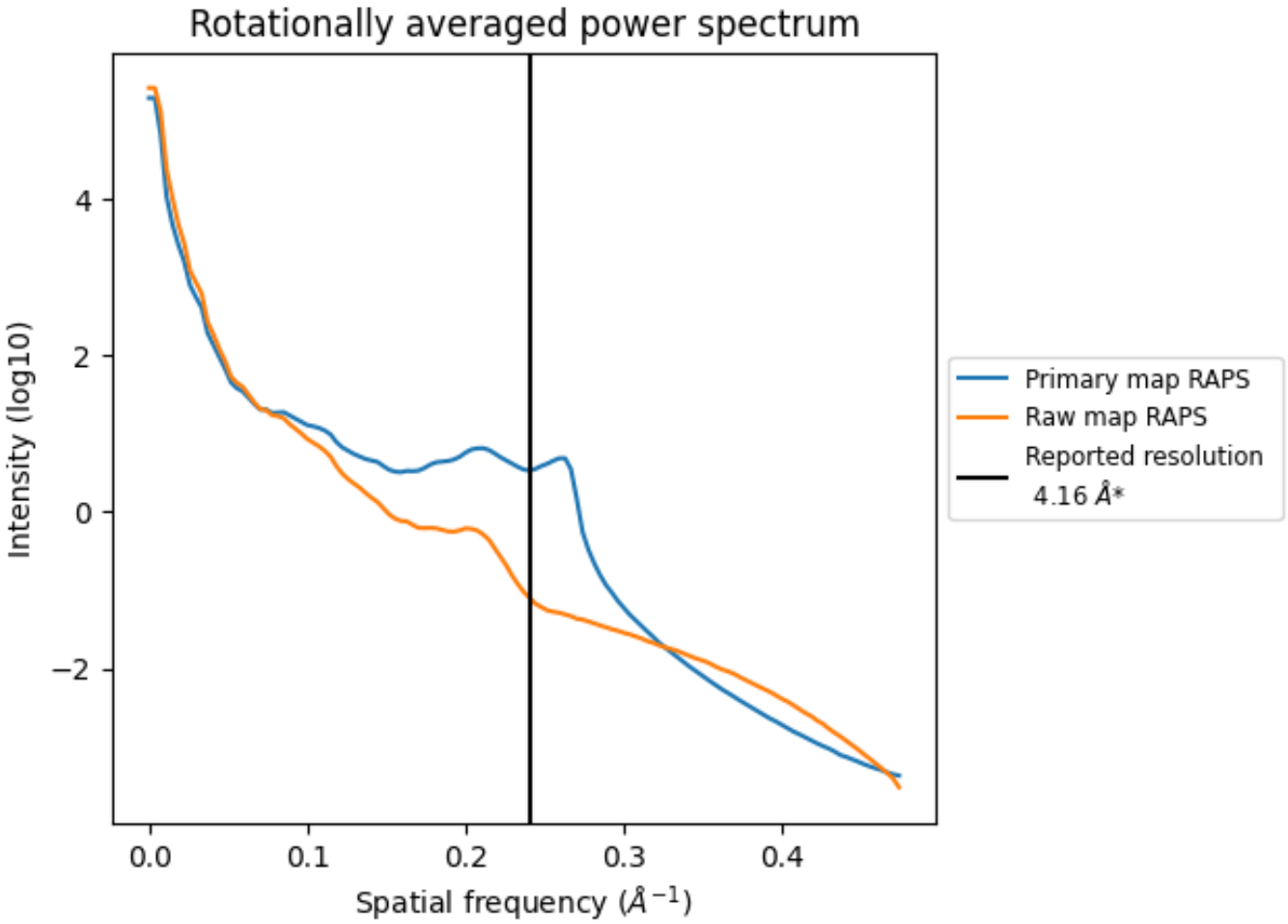
7.2 Volume estimate



The volume at the recommended contour level is 73 nm^3; this corresponds to an approximate mass of 66 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)

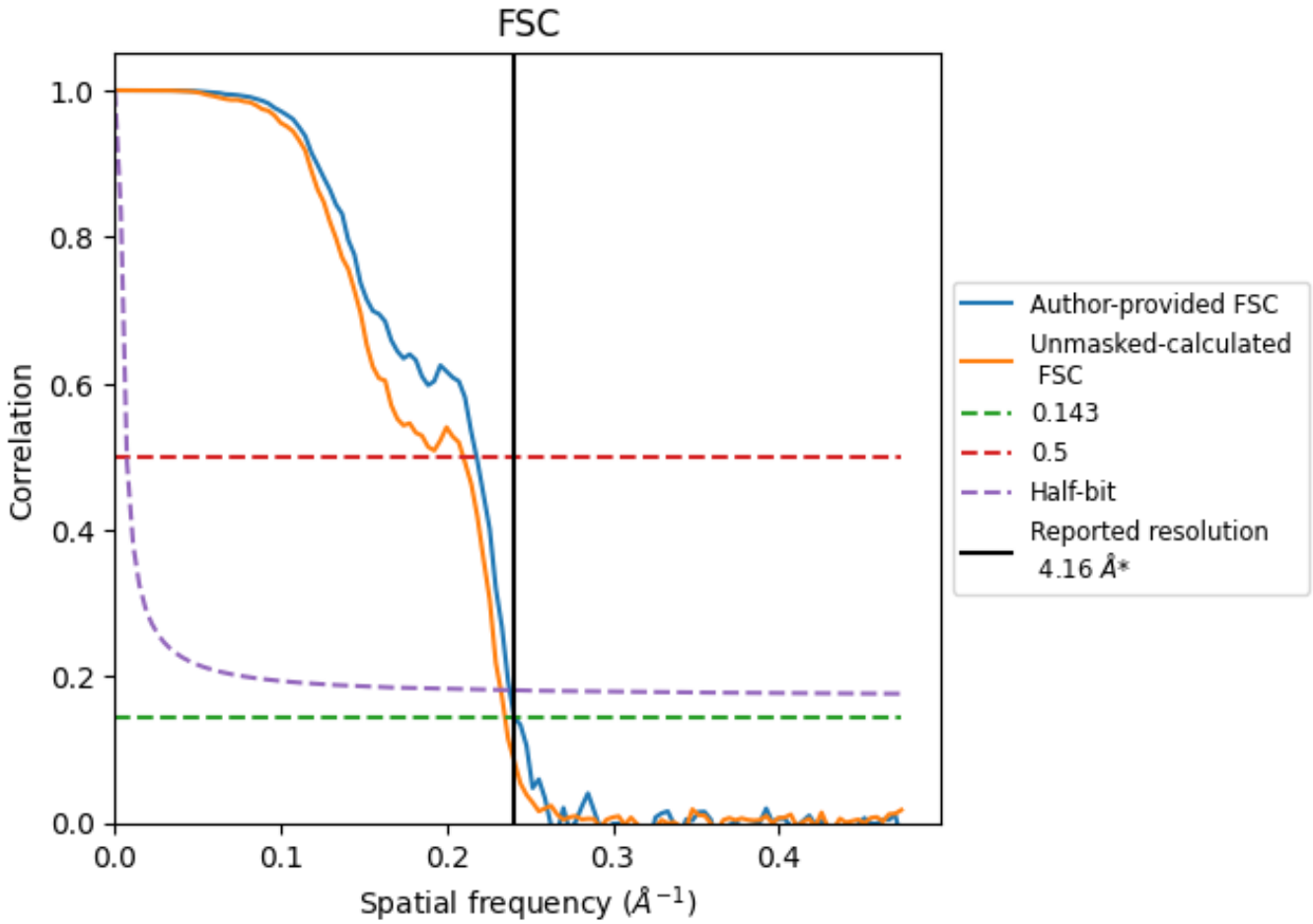


*Reported resolution corresponds to spatial frequency of 0.240 $Å^{-1}$

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 0.240 Å^{-1}

8.2 Resolution estimates (i)

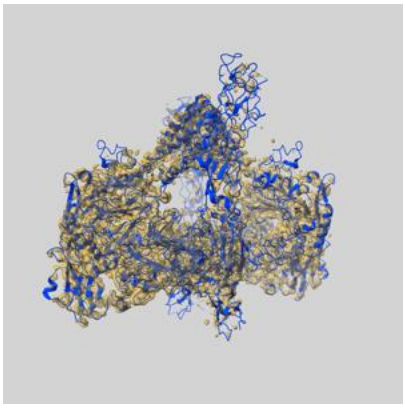
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.16	-	-
Author-provided FSC curve	4.15	4.59	4.20
Unmasked-calculated*	4.25	4.76	4.30

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

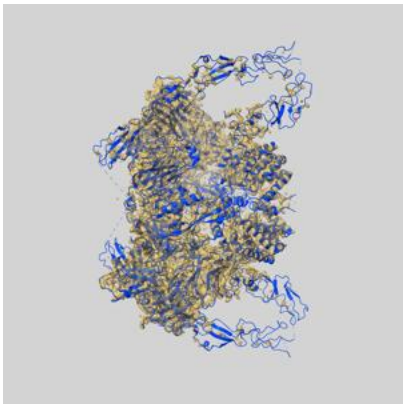
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34739 and PDB model 8HGH. Per-residue inclusion information can be found in section 3 on page 6.

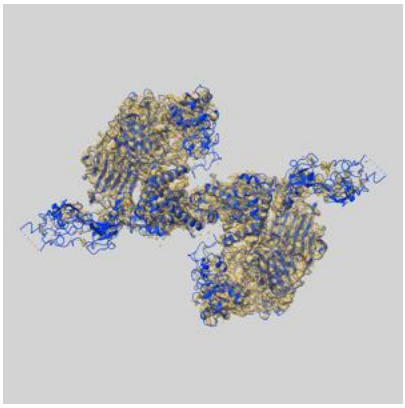
9.1 Map-model overlay



X



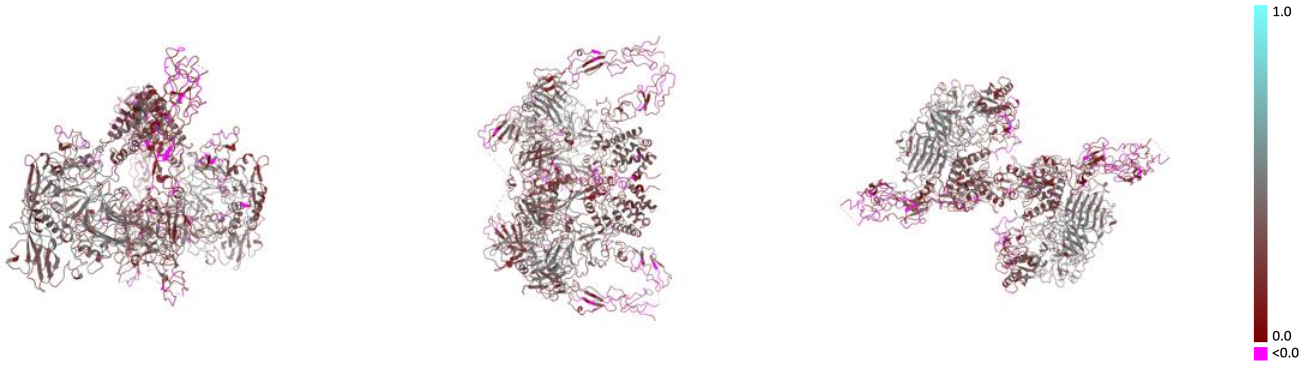
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0217 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.

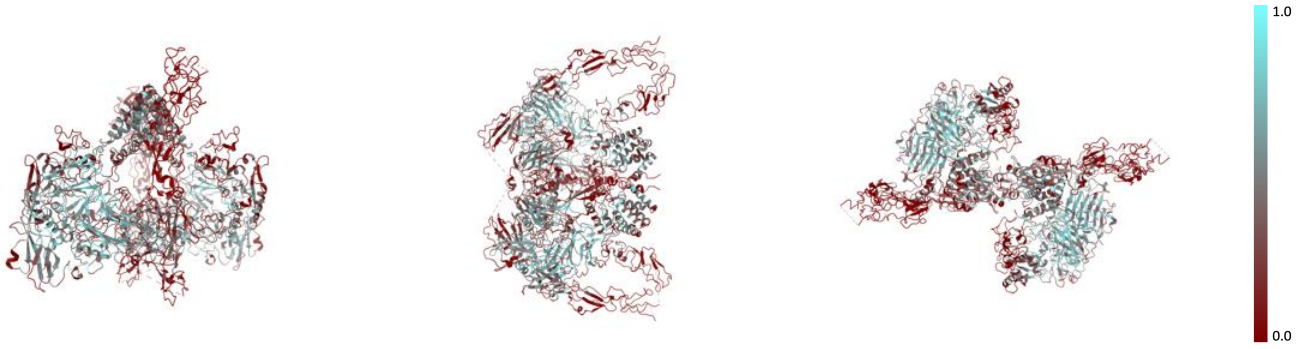
9.2 Q-score mapped to coordinate model (i)



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.

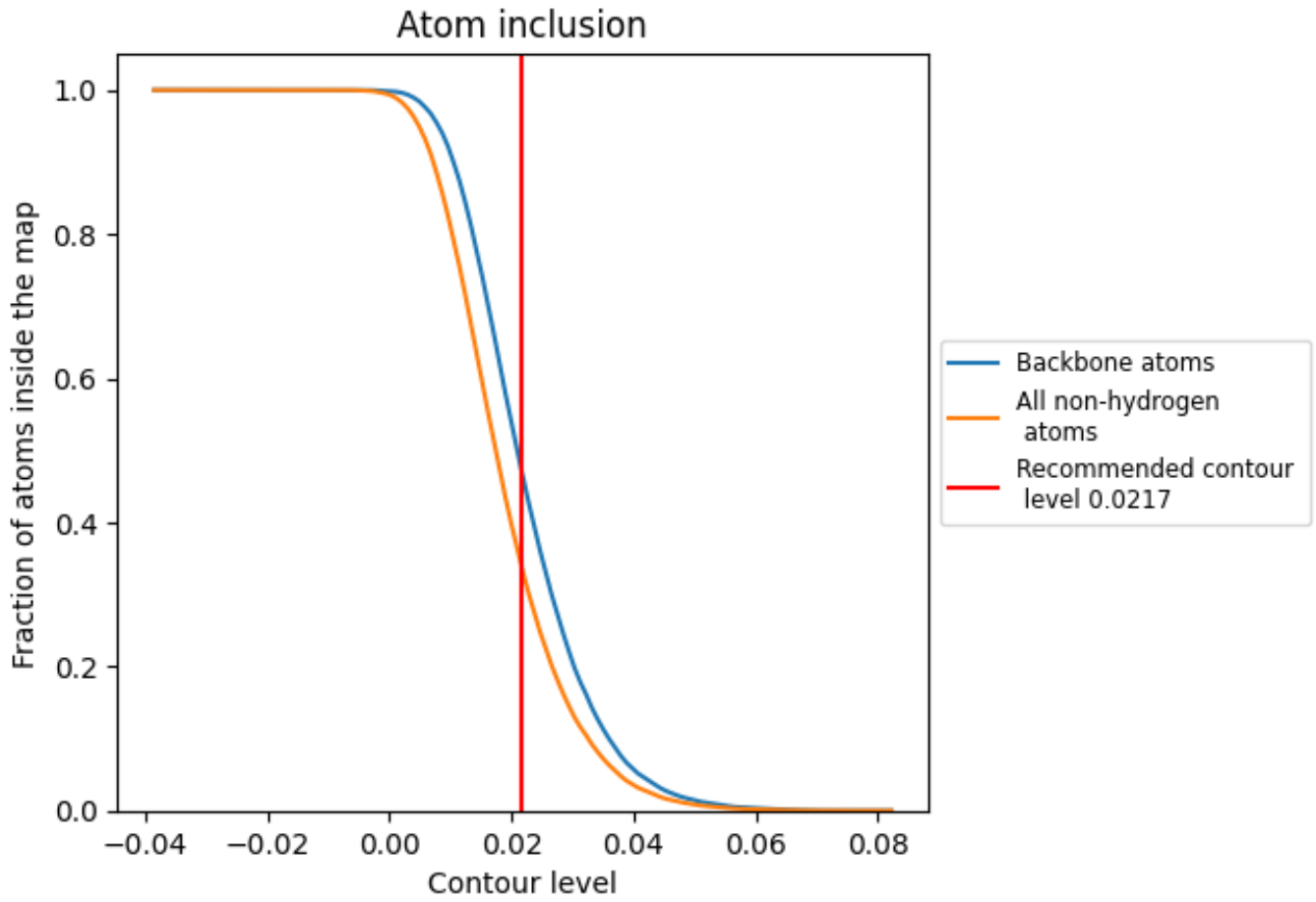
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0217).

9.4 Atom inclusion (i)



At the recommended contour level, 47% of all backbone atoms, 34% 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 (0.0217) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3361	0.2950
A	0.3265	0.2920
B	0.3324	0.2970
C	0.4088	0.3080
G	0.3761	0.2910