wwPDB EM Validation Summary Report (i)

Nov 8, 2022 – 05:11 AM EST

PDB ID	:	6D73
EMDB ID	:	EMD-7822
Title	:	Cryo-EM structure of the zebrafish TRPM2 channel in the presence of Ca2+
Authors	:	Yin, Y.; Wu, M.; Borschel, W.F.; Lander, G.C.; Lee, S.-Y.
Deposited on	:	2018-04-23
Resolution	:	3.80 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

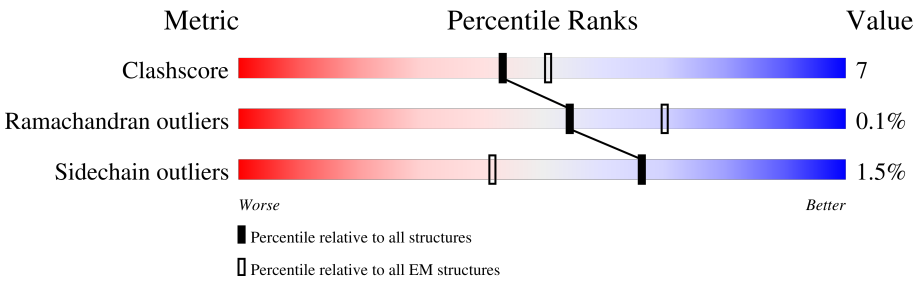
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	1466	31% 72% 11% 16%
1	B	1466	27% 73% 13% 14%
1	C	1466	32% 72% 11% 16%
1	D	1466	27% 73% 13% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 35340 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 Transient receptor potential cation channel, subfamily M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	1256	8892	5756	1567	1534	35	0	0
1	A	1227	8776	5690	1524	1523	39	0	0
1	C	1227	8776	5690	1524	1523	39	0	0
1	D	1256	8892	5756	1567	1534	35	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

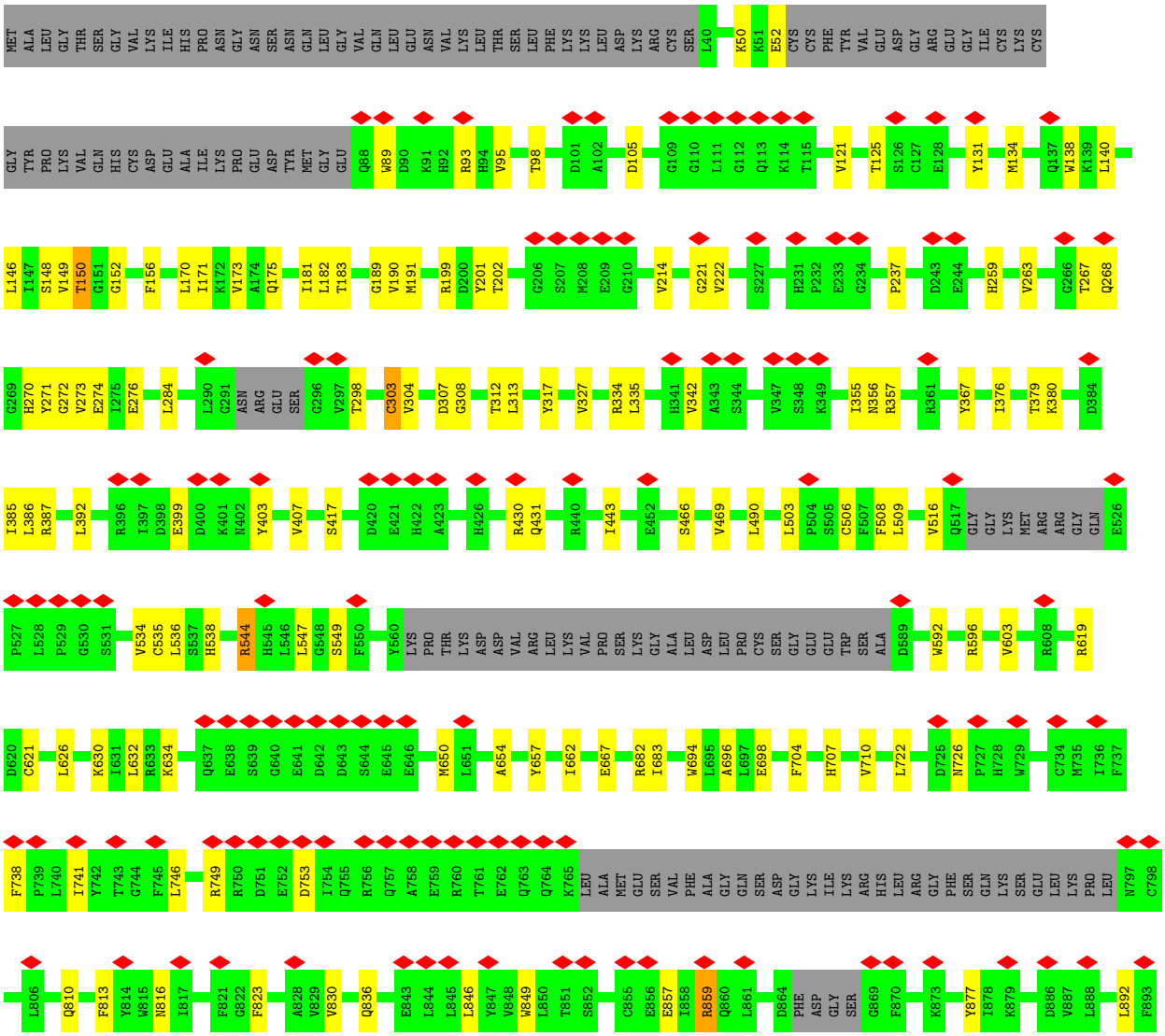
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
2	B	1	1	1	0
2	A	1	1	1	0
2	C	1	1	1	0
2	D	1	1	1	0

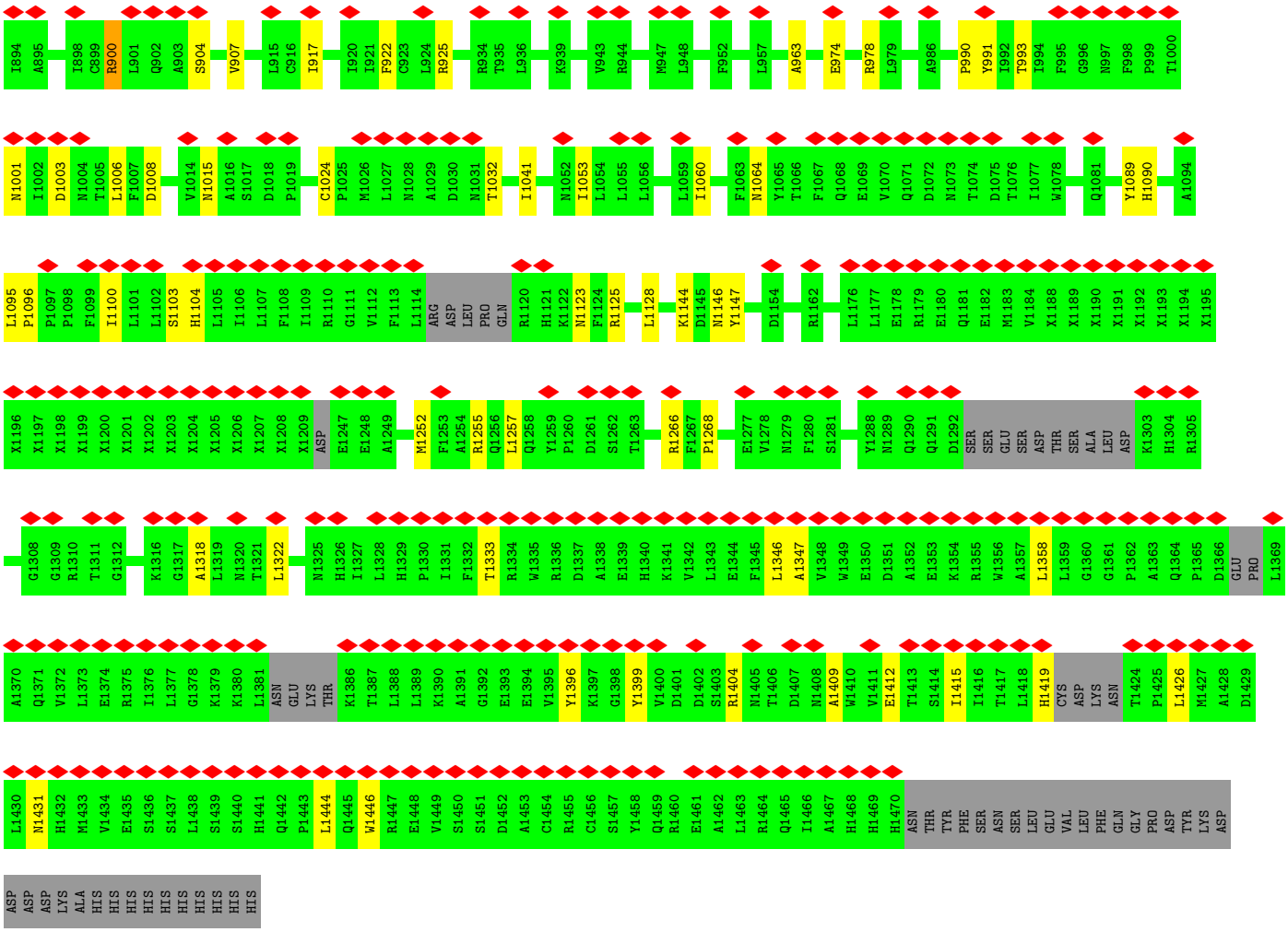
3 Residue-property plots (i)

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: Transient receptor potential cation channel, subfamily M

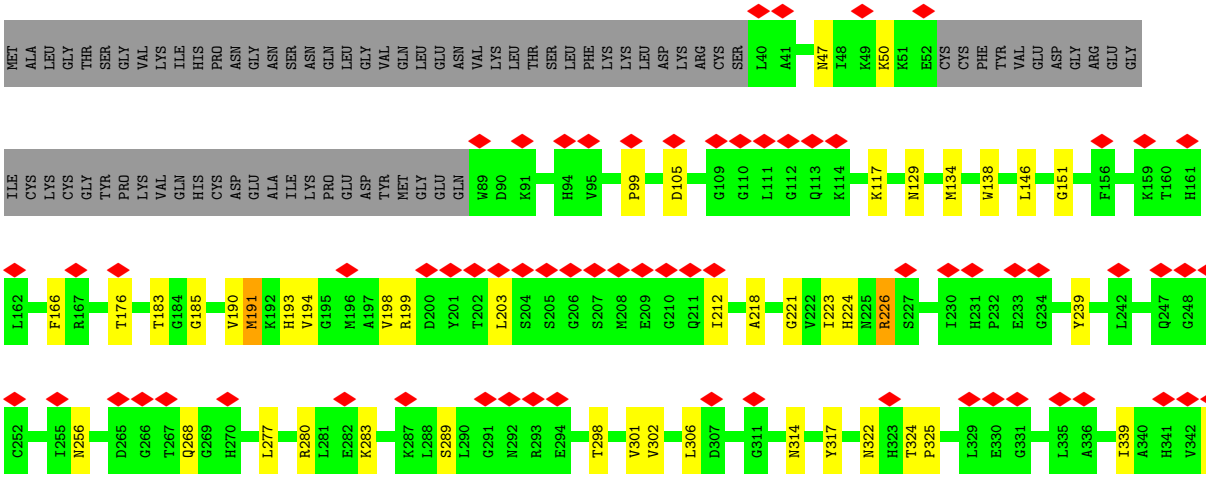
Chain B: 27% 73% 13% 14%

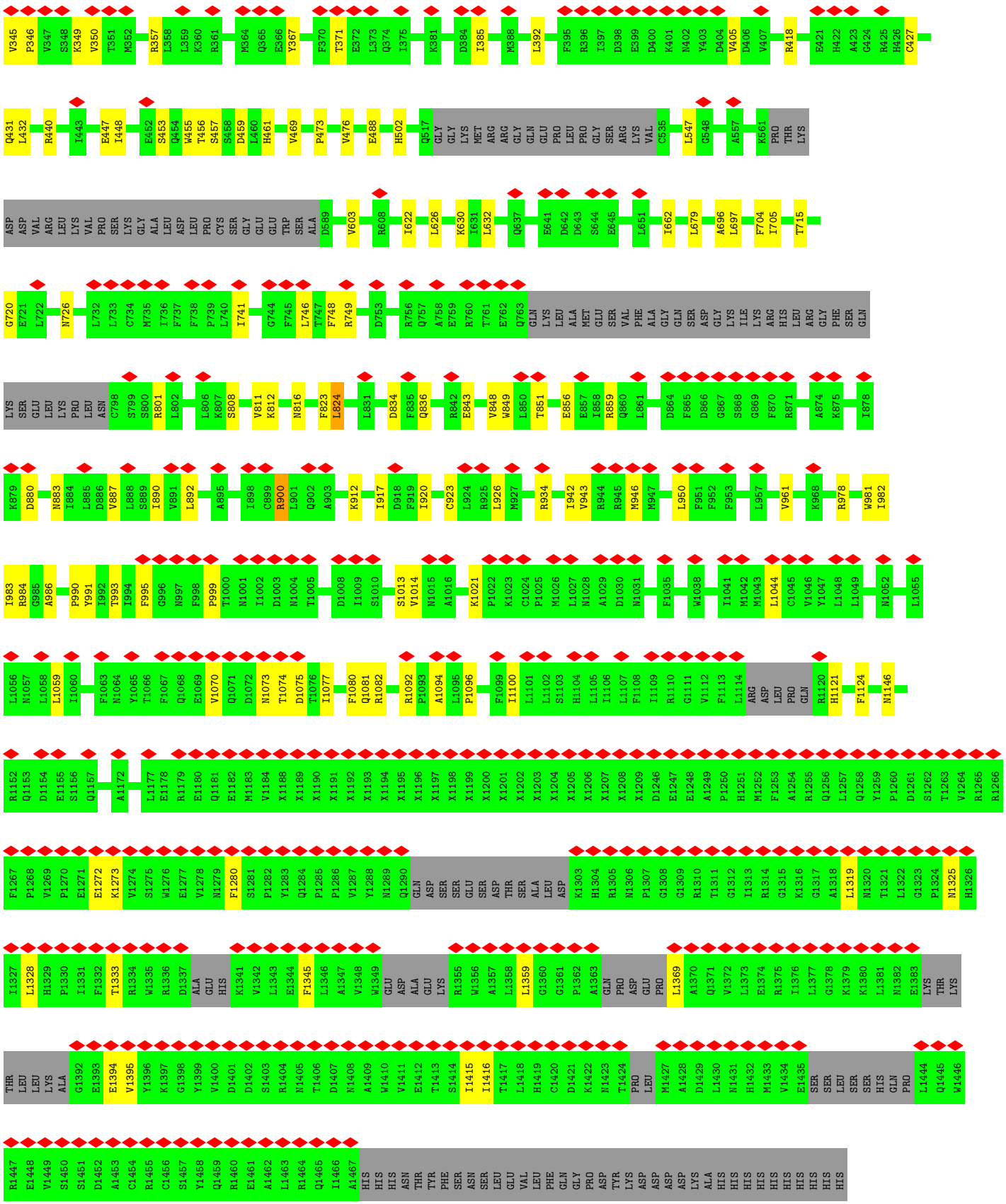




- Molecule 1: Transient receptor potential cation channel, subfamily M

Chain A:

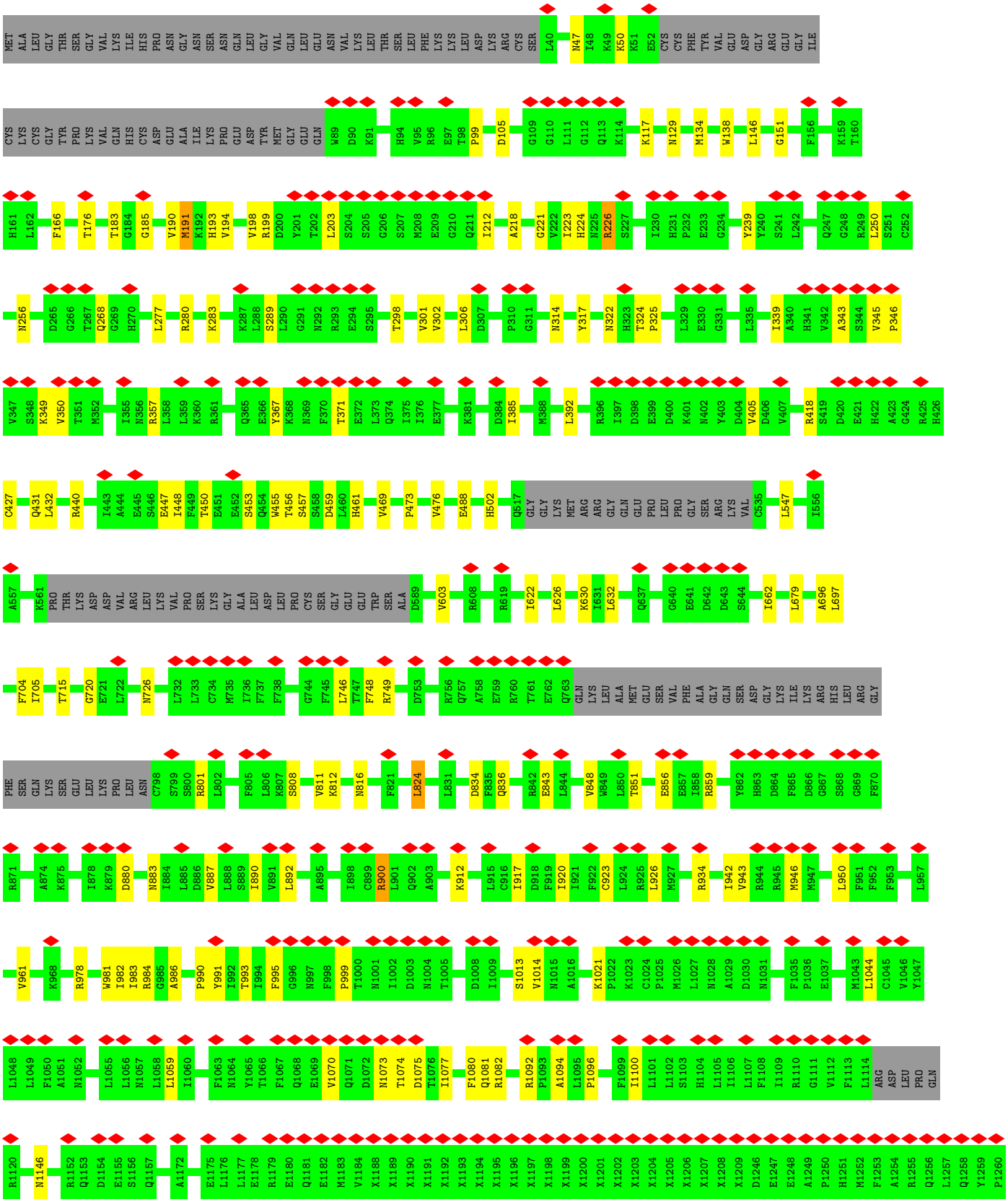


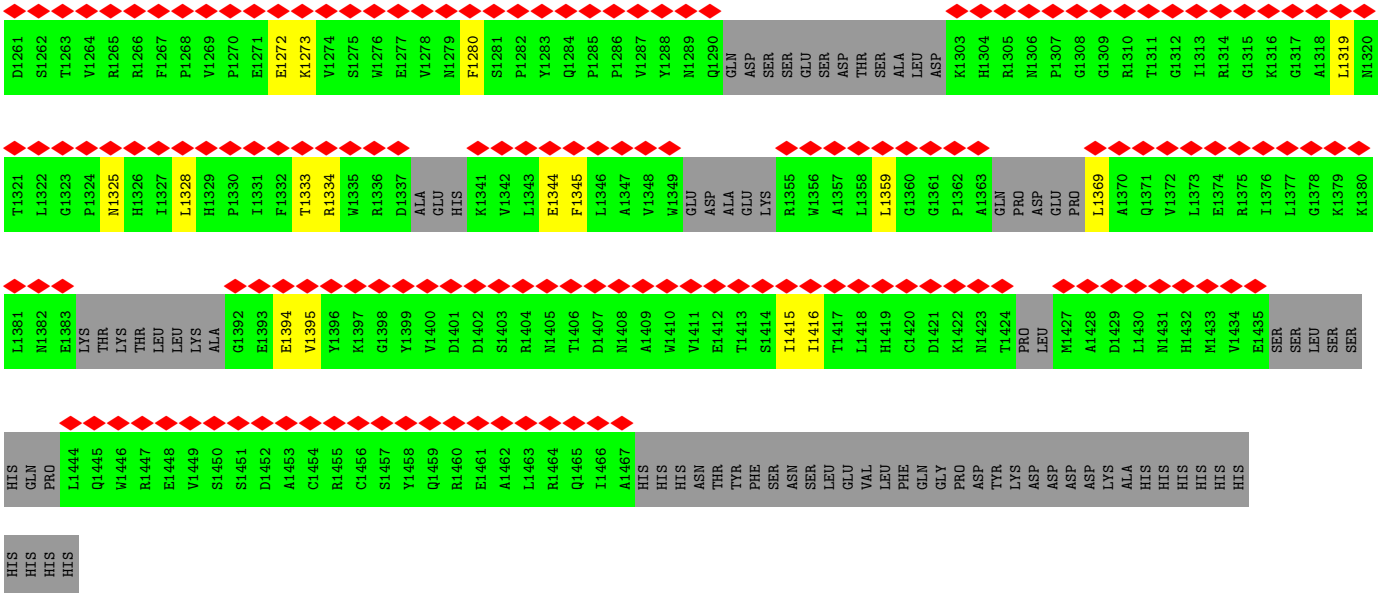


- Molecule 1: Transient receptor potential cation channel, subfamily M

Chain C:

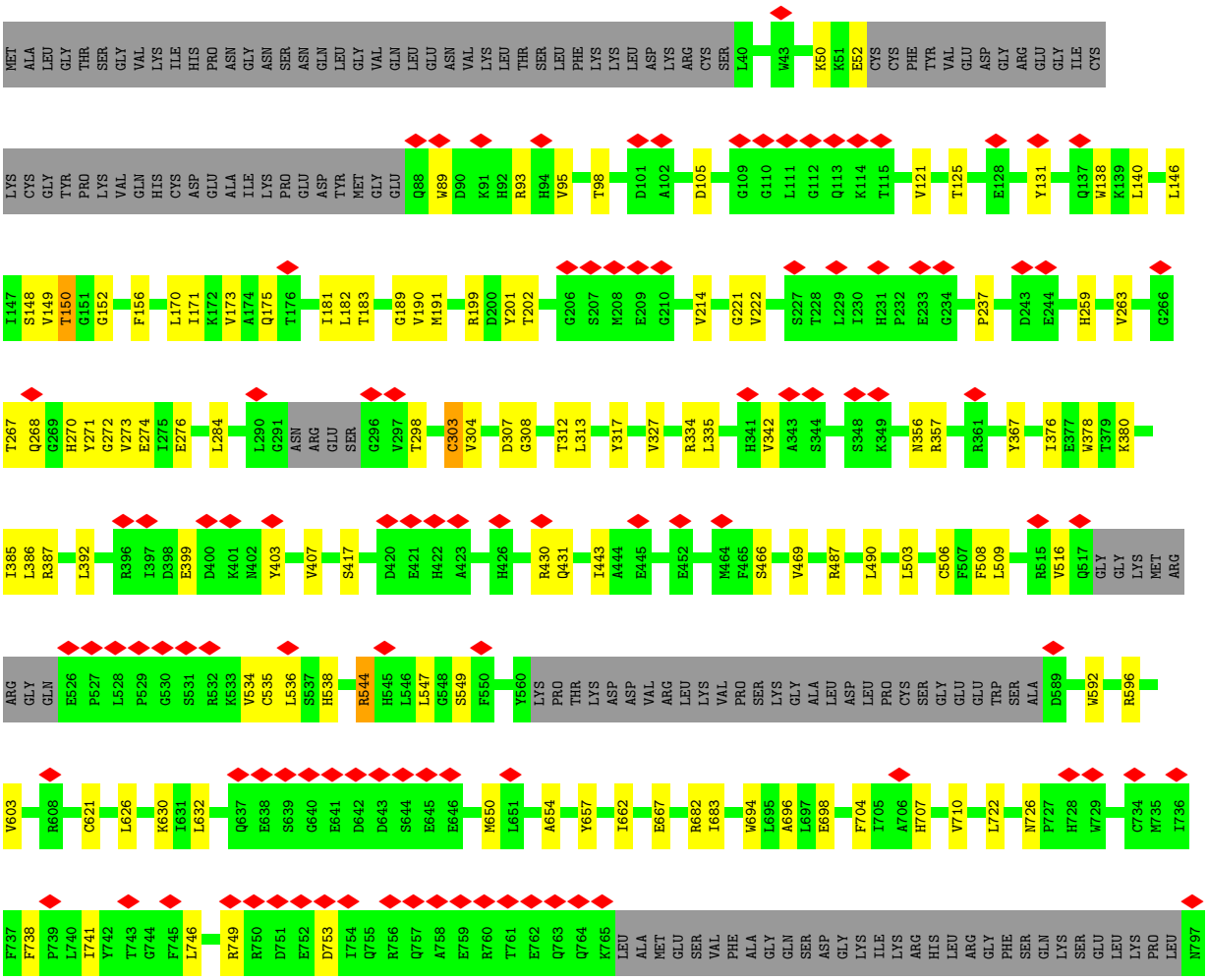
32%
72%
11%
16%

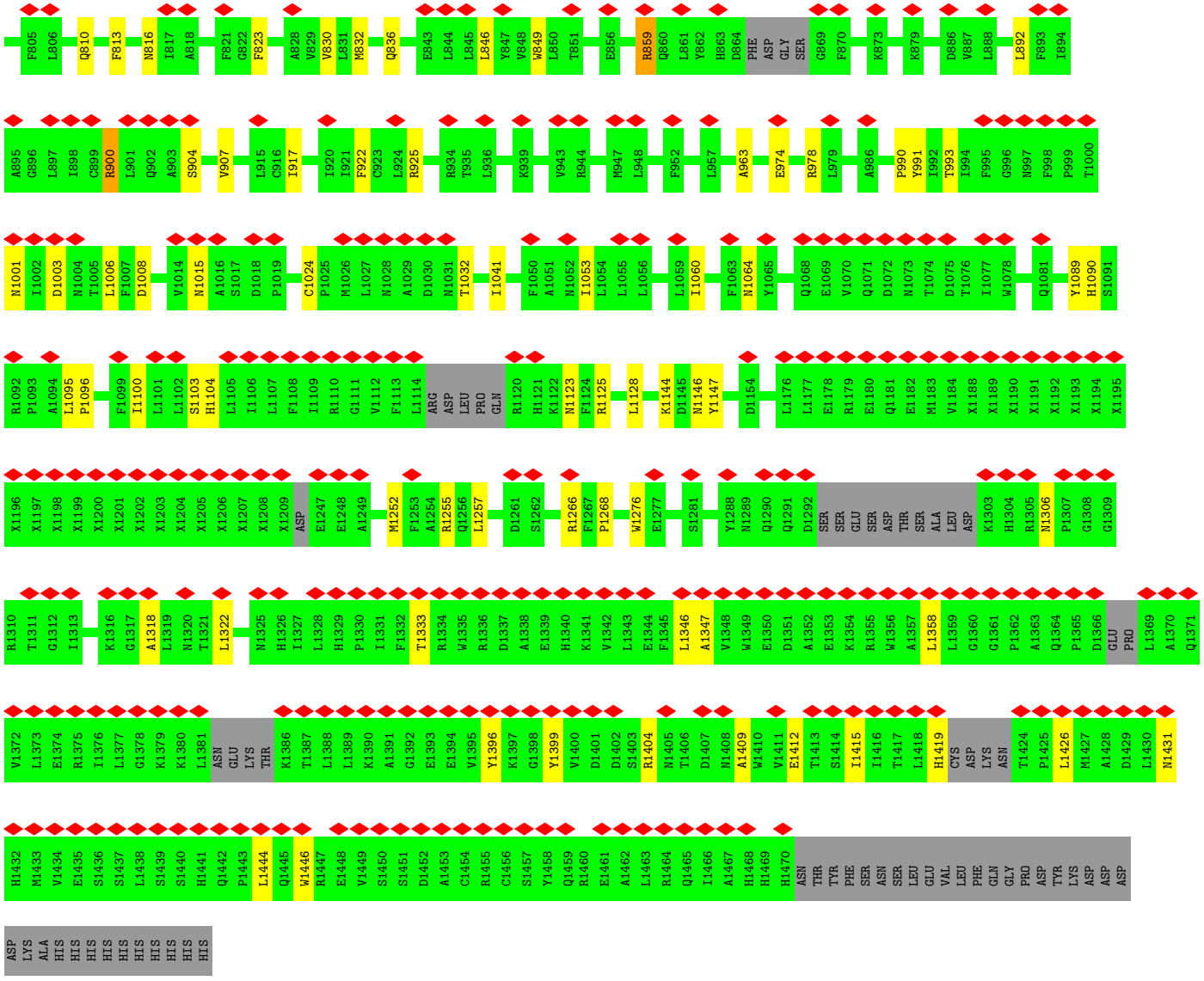

MET ALA LEU GLY THR SER GLY VAL LYS ILE HIS PRO ASN GLY ASN SER ASN GLN LEU GLY VAL GLN LEU GLU ASN VAL LYS LEU THR SER LEU PHE LYS LYS LEU ASP LYS ARG CYS SER L40 N47 I48 K49 K50 K51 E52 CYS CYS PHE TYR VAL GLU ASP GLY ARG GLU GLY ILE
CYS LYS CYS GLY TYR PRO LYS VAL GLN HIS CYS ASP GLU ALA ILE LYS PRO GLU ASP TYR MET GLY GLU GLN W89 D90 K91 H94 V95 R96 E97 T98 P99 D105 G109 G110 L111 G112 Q113 K114 K117 N129 M134 W138 L146 G151 F156 K159 T160
H161 L162 F166 T176 T183 G184 G185 V190 M191 K192 H193 V194 V198 R199 D200 Y201 T202 L203 S204 S205 S206 S207 M208 E209 G210 Q211 I212 A218 G221 V222 I223 H224 N225 R226 S227 I230 H231 P232 E233 G234 Y239 Y240 S241 L242 Q247 G248 R249 L250 S251 C252
N256 D265 G266 T267 Q268 G269 H270 L277 R280 K283 K287 L288 S289 L290 G291 N292 R293 E294 S295 T298 V301 V302 L306 D307 P310 G311 N314 Y317 N322 H323 T324 P325 L329 E330 G331 L335 I339 A340 H341 V342 A343 S344 V345 P346
V347 S348 K349 V350 T351 M352 I355 N356 R357 L358 L359 K360 R361 Q365 E366 Y367 K368 N369 F370 T371 E372 L373 Q374 I375 I376 E377 K381 D384 I385 H388 L392 R396 I397 D398 E399 D400 K401 N402 Y403 D404 Y405 D406 Y407 R418 S419 D420 E421 H422 A423 G424 R425 H426
C427 Q431 L432 R440 I443 A444 E445 S446 E447 I448 F449 T450 E451 E452 S453 Q454 W455 T456 S457 S458 D459 L460 H461 V469 P473 V476 E488 H502 Q517 GLY GLY LYS MET ARG ARG GLY GLN GLU PRO LEU PRO GLY SER ARG LYS VAL C535 L547 I556
A557 K561 PRO THR LYS ASP ASP VAL ARG LEU LYS VAL PRO SER LYS GLY ALA LEU ASP LEU PRO CYS SER GLY GLU GLU TRP SER ALA D589 V603 R608 R619 I622 L626 K630 I631 L632 Q637 G640 E641 D642 D643 S644 I662 L679 A696 L697
F704 I705 T715 G720 E721 L722 N726 L732 L733 C734 M735 I736 F737 F738 G744 F745 L746 T747 F748 R749 D753 R756 Q757 A758 E759 R760 T761 E762 Q763 GLN LYS LEU ALA MET GLU SER VAL PHE ALA GLY GLN SER ASP GLY LYS ILE LYS ARG HIS LEU ARG GLY
PHE SER GLN LYS SER GLU LEU LYS PRO LEU ASN C798 S799 S800 R801 L802 F805 L806 K807 S808 V811 K812 N816 F821 L824 L831 D834 E835 Q836 R842 E843 L844 V848 W849 L850 T851 E856 E857 I858 R859 Y862 H863 D864 F865 D866 G867 S868 G869 F870
R871 A874 K875 I878 K879 D880 N883 I884 L885 D886 V887 L888 S889 I890 V891 L892 A895 I898 C899 R900 L901 Q902 A903 K912 L915 C916 I917 D918 F919 I920 I921 F922 C923 L924 R925 L926 M927 R934 I942 V943 R944 R945 M946 M947 L950 F951 F952 F953 L957
V961 K968 R978 W981 I982 I983 R984 G985 A986 P990 Y991 I992 T993 I994 F995 G996 N997 F998 P999 T1000 N1001 I1002 D1003 N1004 T1005 D1008 I1009 S1013 V1014 N1015 A1016 K1021 P1022 K1023 C1024 P1025 M1026 L1027 N1028 A1029 D1030 N1031 F1035 P1036 E1037 M1043 L1044 C1045 V1046 Y1047
L1048 L1049 F1050 A1051 N1052 L1055 L1056 N1057 L1058 L1059 I1060 F1063 N1064 Y1065 T1066 F1067 Q1068 E1069 V1070 Q1071 D1072 N1073 T1074 D1075 T1076 I1077 F1080 Q1081 R1082 R1092 P1093 A1094 L1095 P1096 F1099 I1100 L1101 L1102 S1103 H1104 L1105 I1106 L1107 F1108 I1109 R1110 G1111 V1112 F1113 L1114 ARG ASP LEU PRO GLN
R1120 N1146 R1152 Q1153 D1154 E1155 S1156 Q1157 A1172 E1175 L1176 L1177 E1178 R1179 E1180 Q1181 E1182 M1183 V1184 X1188 X1189 X1190 X1191 X1192 X1193 X1194 X1195 X1196 X1197 X1198 X1199 X1200 X1201 X1202 X1203 X1204 X1205 X1206 X1207 X1208 X1209 D1246 E1247 E1248 A1249 P1250 H1251 M1252 F1253 A1254 R1255 Q1256 L1257 Q1258 Y1259 P1260



- Molecule 1: Transient receptor potential cation channel, subfamily M

Chain D:




F805 L806 Q810 F813 N816 I817 A818 F821 G822 F823 A828 V829 V830 L831 M832 Q836 E843 L844 L845 L846 Y847 Y848 W849 L850 T851 E856 R859 Q860 L861 Y862 H863 D864 PHE ASP GLY SER G869 F870 K873 K879 D886 V887 L888 L892 F893 I894
A895 G896 L897 I898 C899 R900 L901 Q902 A903 S904 V907 L915 C916 I917 I920 I921 F922 C923 L924 R925 R934 T935 L936 K939 V943 R944 M947 L948 F952 L957 A963 E974 R978 L979 A986 P990 Y991 I992 T993 I994 F995 G996 N997 F998 P999 T1000
N1001 I1002 D1003 N1004 T1005 L1006 F1007 D1008 V1014 N1015 A1016 S1017 D1018 P1019 C1024 P1025 M1026 L1027 N1028 A1029 D1030 N1031 T1032 I1041 F1050 A1051 N1052 I1053 L1054 L1055 L1056 L1059 I1060 F1063 N1064 Y1065 Q1068 E1069 V1070 Q1071 D1072 N1073 T1074 D1075 T1076 I1077 W1078 Q1081 Y1089 H1090 S1091
R1092 P1093 A1094 L1095 P1096 F1099 I1100 L1101 L1102 S1103 H1104 L1105 I1106 L1107 F1108 I1109 R1110 G1111 V1112 F1113 L1114 ARG ASP LEU PRO GLN R1120 H1121 K1122 N1123 F1124 R1125 L1128 K1144 D1145 N1146 Y1147 D1154 L1176 L1177 E1178 R1179 E1180 Q1181 E1182 M1183 V1184 X1188 X1189 X1190 X1191 X1192 X1193 X1194 X1195
X1196 X1197 X1198 X1199 X1200 X1201 X1202 X1203 X1204 X1205 X1206 X1207 X1208 X1209 ASP E1247 E1248 A1249 M1252 F1253 A1254 R1255 Q1256 L1257 D1261 S1262 R1266 F1267 P1268 W1276 E1277 S1281 Y1288 N1289 Q1290 Q1291 D1292 SER SER GLU SER ASP THR SER ALA LEU ASP K1303 H1304 R1305 N1306 P1307 G1308 G1309
R1310 T1311 G1312 I1313 K1316 G1317 A1318 L1319 N1320 T1321 L1322 N1325 H1326 I1327 L1328 H1329 P1330 I1331 F1332 T1333 R1334 W1335 R1336 D1337 A1338 E1339 H1340 K1341 V1342 L1343 E1344 F1345 L1346 A1347 V1348 W1349 E1350 D1351 A1352 E1353 K1354 R1355 W1356 A1357 L1358 L1359 G1360 G1361 P1362 A1363 Q1364 P1365 D1366 GLU PRO L1369 A1370 Q1371
V1372 L1373 E1374 R1375 I1376 L1377 G1378 K1379 K1380 L1381 ASN GLU LYS THR K1386 T1387 L1388 L1389 K1390 A1391 G1392 E1393 E1394 V1395 Y1396 K1397 G1398 Y1399 V1400 D1401 D1402 S1403 R1404 N1405 T1406 D1407 N1408 A1409 W1410 V1411 E1412 T1413 S1414 I1415 I1416 T1417 L1418 H1419 CYS ASP LYS ASN T1424 P1425 L1426 M1427 A1428 D1429 L1430 N1431
H1432 M1433 V1434 E1435 S1436 S1437 L1438 S1439 S1440 H1441 Q1442 P1443 L1444 Q1445 W1446 R1447 E1448 V1449 S1450 S1451 D1452 A1453 C1454 R1455 C1456 S1457 Y1458 Q1459 R1460 E1461 A1462 L1463 R1464 Q1465 I1466 A1467 H1468 H1469 H1470 ASN THR TYR PHE SER ASN SER LEU GLU VAL LEU PHE GLN GLY PRO ASP TYR LYS ASP ASP ASP
ASP LYS ALA HIS HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	93573	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	63	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	368.0, 368.0, 368.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.36	0/8871	0.59	5/12138 (0.0%)
1	B	0.35	0/8995	0.59	4/12326 (0.0%)
1	C	0.36	0/8871	0.59	5/12138 (0.0%)
1	D	0.36	0/8995	0.59	4/12326 (0.0%)
All	All	0.36	0/35732	0.59	18/48928 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	203	LEU	CA-CB-CG	6.77	130.88	115.30
1	A	203	LEU	CA-CB-CG	6.76	130.84	115.30
1	D	272	GLY	N-CA-C	6.55	129.49	113.10
1	B	272	GLY	N-CA-C	6.53	129.42	113.10
1	C	1075	ASP	CB-CG-OD1	6.00	123.70	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1013	SER	Peptide
1	A	1021	LYS	Peptide
1	C	1013	SER	Peptide
1	C	1021	LYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8776	0	7824	109	0
1	B	8892	0	7798	136	0
1	C	8776	0	7824	105	0
1	D	8892	0	7798	133	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	35340	0	31244	468	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 7.

The worst 5 of 468 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:C:346:PRO:HB2	1:C:349:LYS:CB	1.43	1.44
1:A:346:PRO:HB2	1:A:349:LYS:CB	1.43	1.44
1:C:367:TYR:O	1:C:371:THR:HG23	1.40	1.20
1:D:156:PHE:HE1	1:D:189:GLY:C	1.46	1.19
1:B:156:PHE:HE1	1:B:189:GLY:CA	1.57	1.18

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	1177/1466 (80%)	1102 (94%)	74 (6%)	1 (0%)	51	83
1	B	1208/1466 (82%)	1127 (93%)	80 (7%)	1 (0%)	51	83
1	C	1177/1466 (80%)	1103 (94%)	73 (6%)	1 (0%)	51	83
1	D	1208/1466 (82%)	1128 (93%)	79 (6%)	1 (0%)	51	83
All	All	4770/5864 (81%)	4460 (94%)	306 (6%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1014	VAL
1	C	1014	VAL
1	B	1024	CYS
1	D	1024	CYS

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	760/1277 (60%)	751 (99%)	9 (1%)	71	84
1	B	743/1277 (58%)	730 (98%)	13 (2%)	60	78
1	C	760/1277 (60%)	751 (99%)	9 (1%)	71	84
1	D	743/1277 (58%)	730 (98%)	13 (2%)	60	78
All	All	3006/5108 (59%)	2962 (98%)	44 (2%)	66	81

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	934	ARG
1	D	544	ARG
1	C	1073	ASN
1	D	303	CYS
1	D	900	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1146	ASN
1	D	1405	ASN
1	C	314	ASN
1	D	1329	HIS
1	D	1064	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 4 ligands modelled in this entry, 4 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	C	2
1	B	1
1	D	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1209:UNK	C	1246:ASP	N	42.80
1	C	1209:UNK	C	1246:ASP	N	42.80
1	B	1184:VAL	C	1188:UNK	N	10.31
1	D	1184:VAL	C	1188:UNK	N	10.31
1	A	1184:VAL	C	1188:UNK	N	9.14

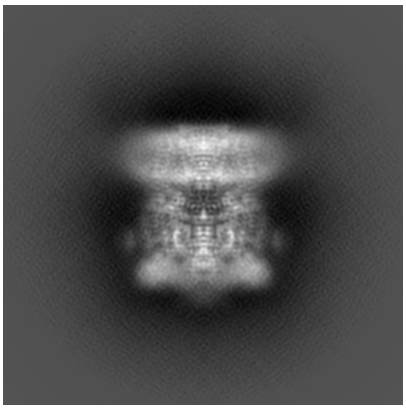
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7822. These allow visual inspection of the internal detail of the map and identification of artifacts.

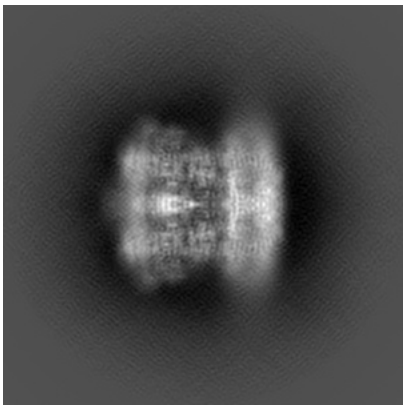
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

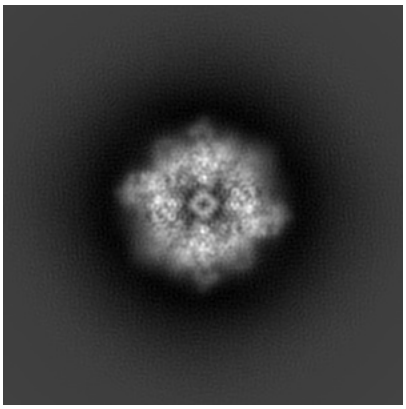
6.1.1 Primary map



X

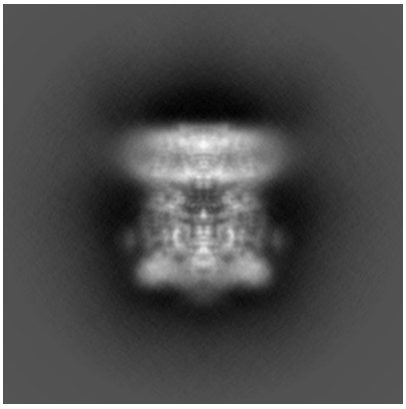


Y

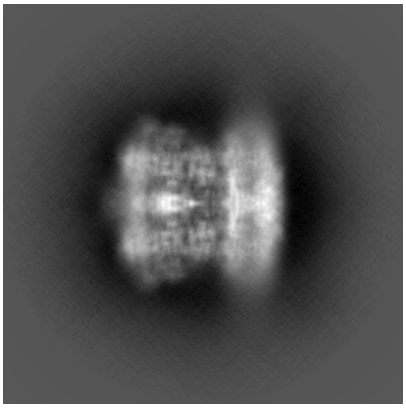


Z

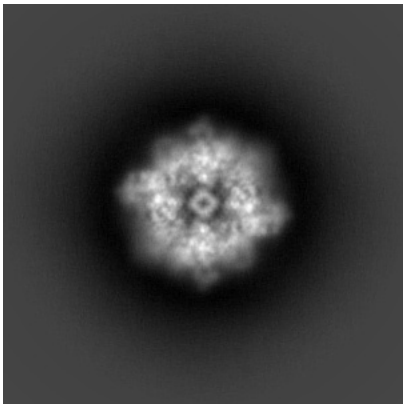
6.1.2 Raw map



X



Y

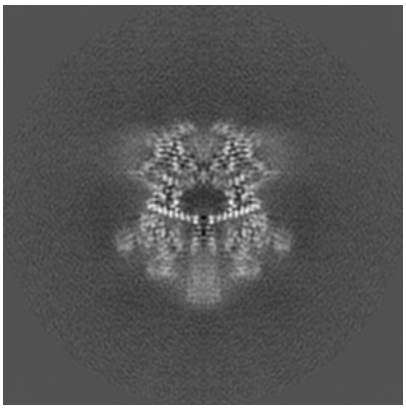


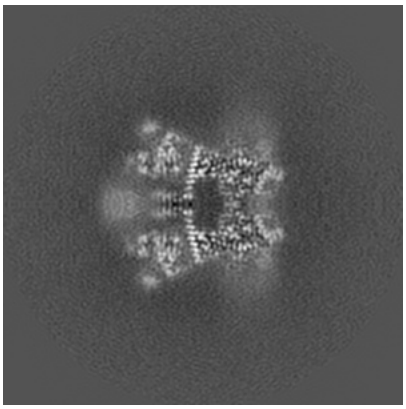
Z

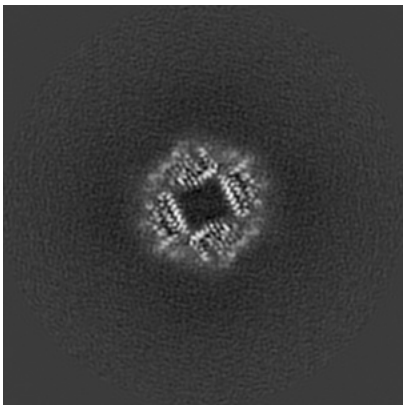
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

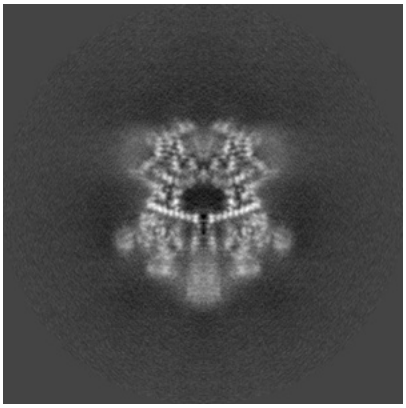
6.2.1 Primary map

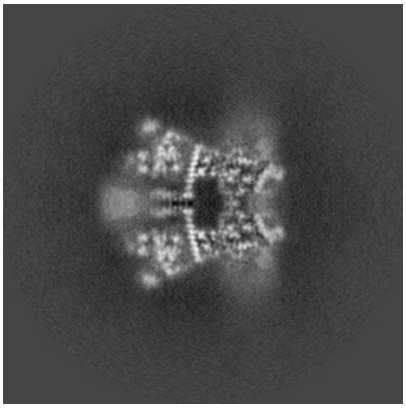

X Index: 160

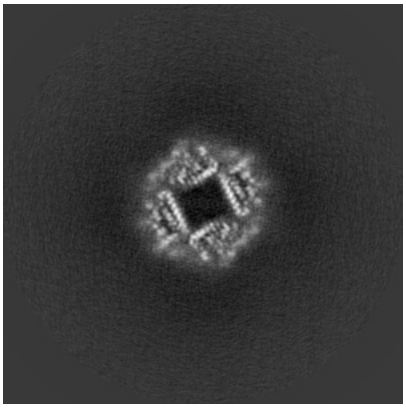

Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160

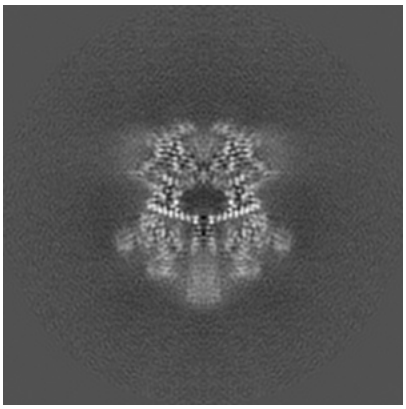

Y Index: 160

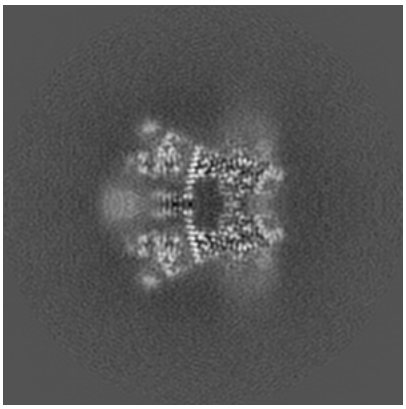

Z Index: 160

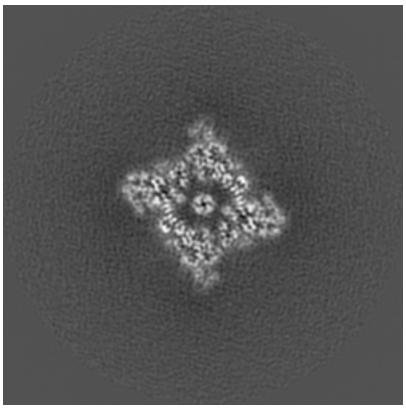
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

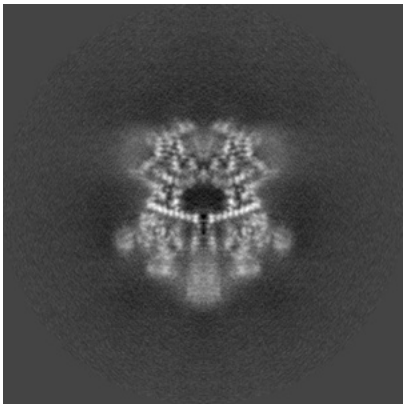
6.3.1 Primary map

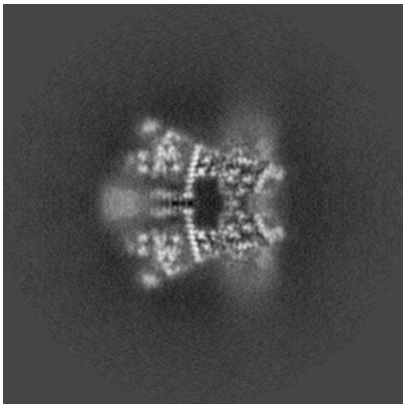

X Index: 160

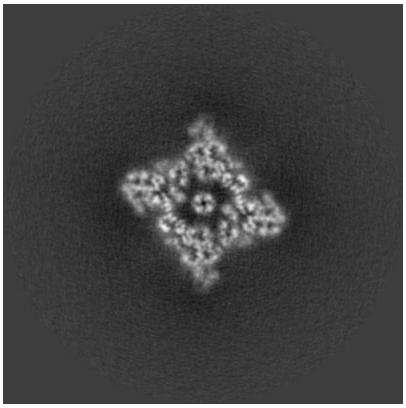

Y Index: 160


Z Index: 137

6.3.2 Raw map


X Index: 160

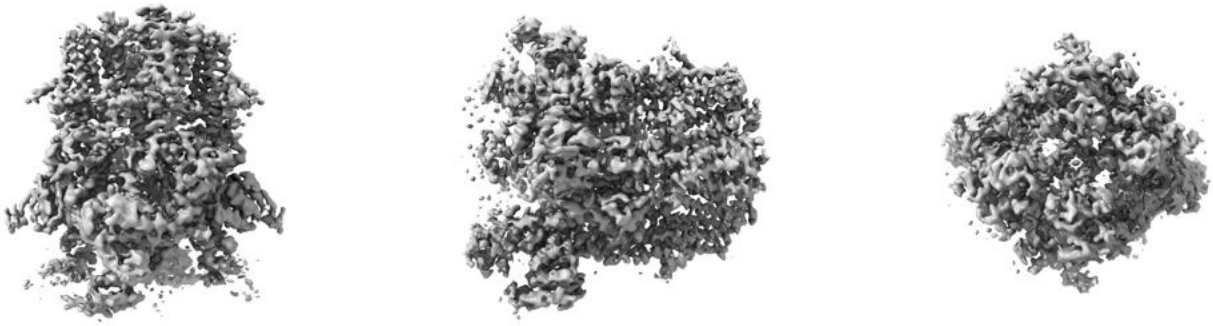

Y Index: 160


Z Index: 137

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

6.4 Orthogonal surface views (i)

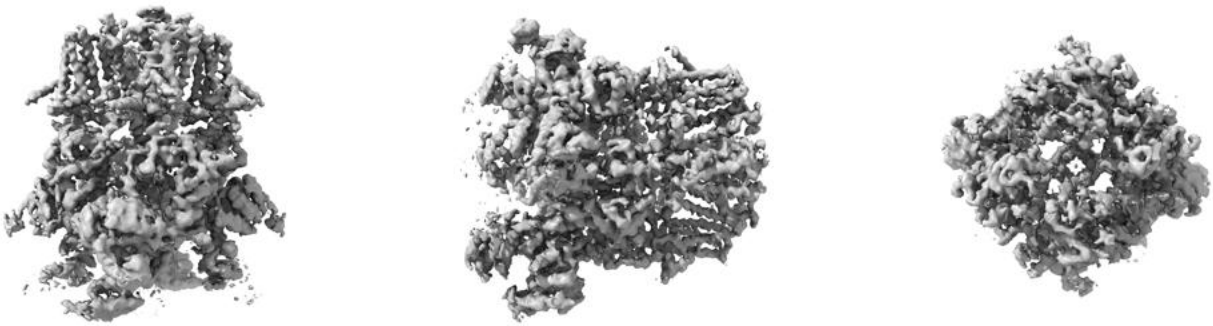
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

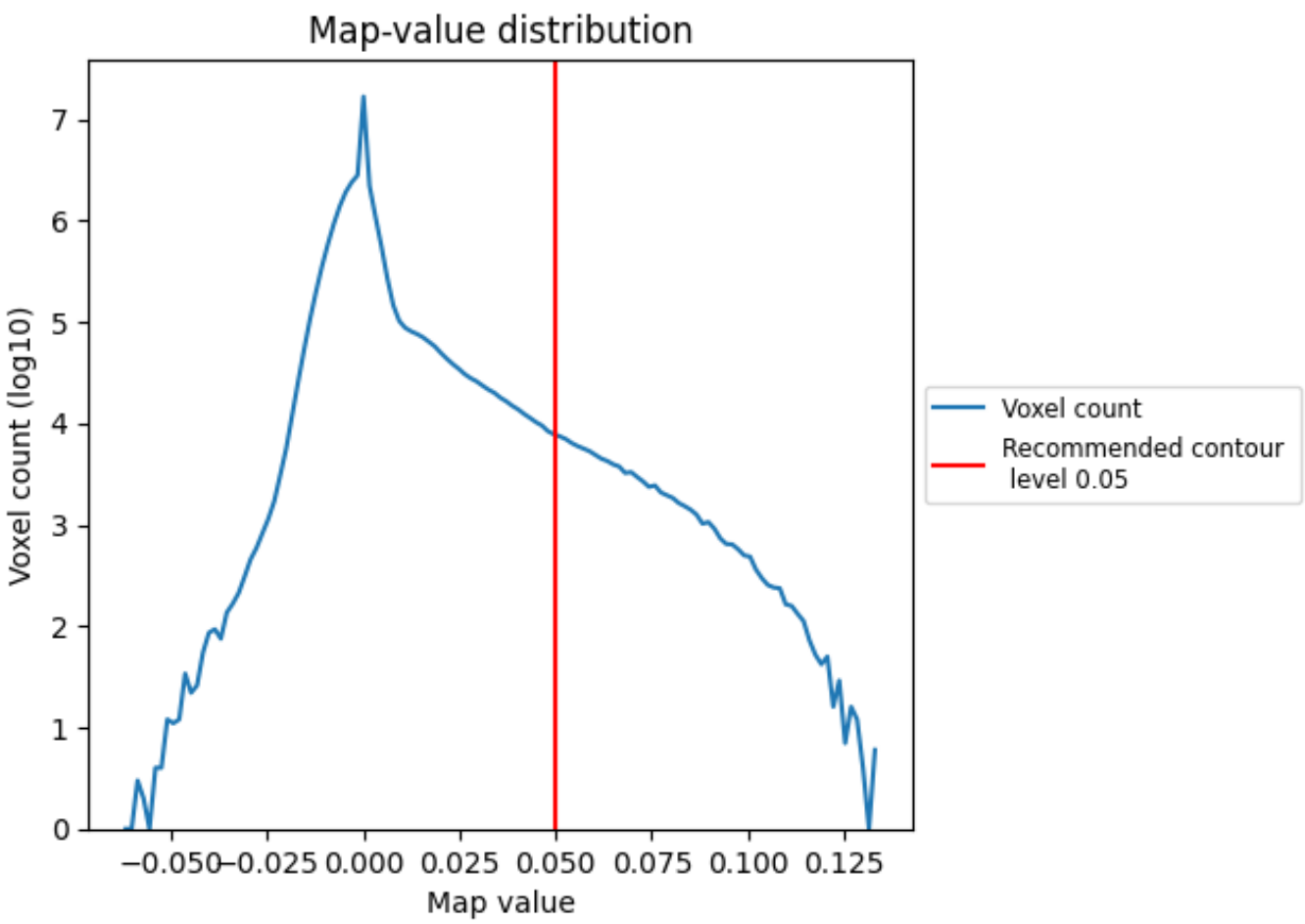
6.5 Mask visualisation (i)

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

7 Map analysis (i)

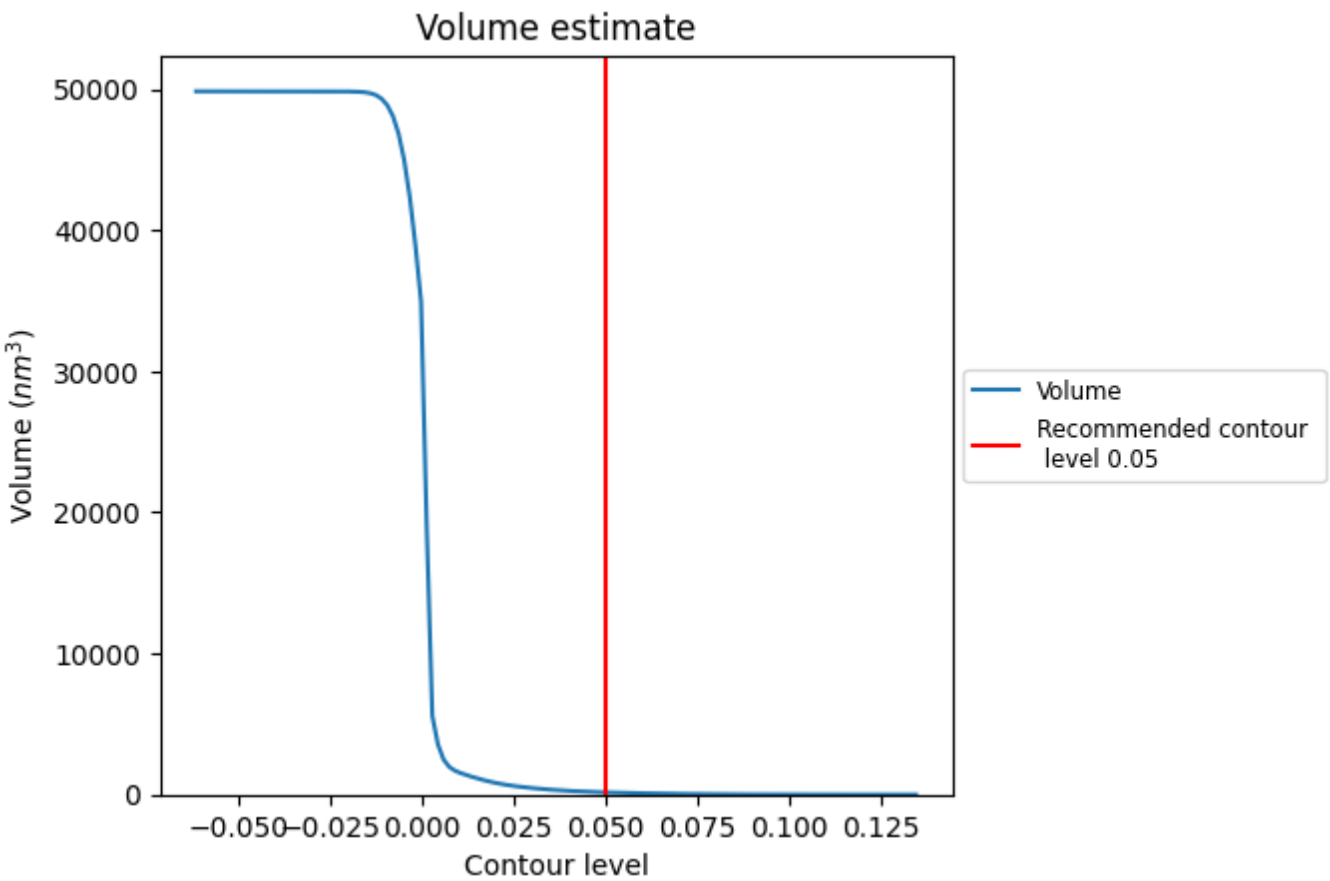
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

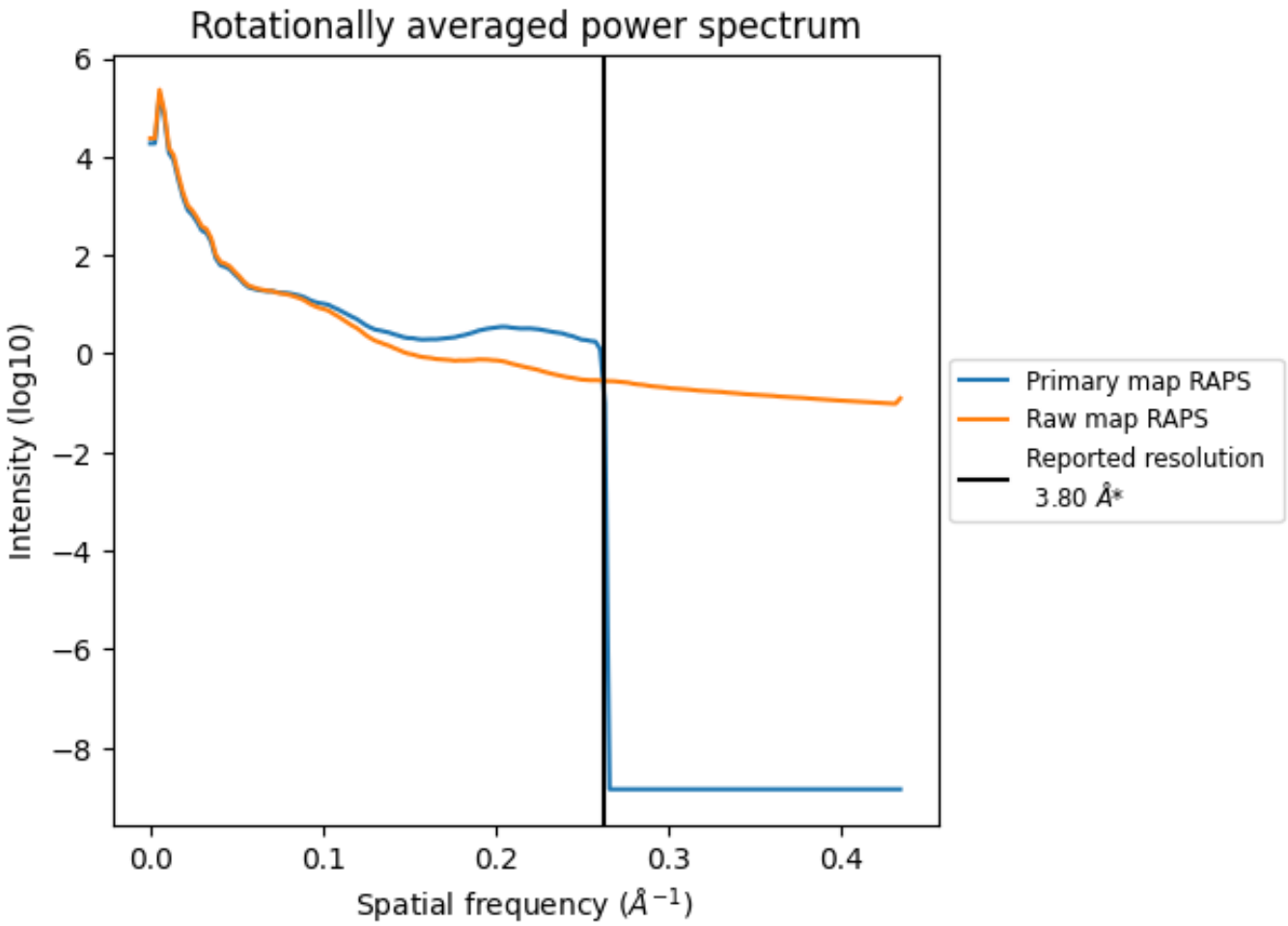
7.2 Volume estimate (i)



The volume at the recommended contour level is 155 nm^3; this corresponds to an approximate mass of 140 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)

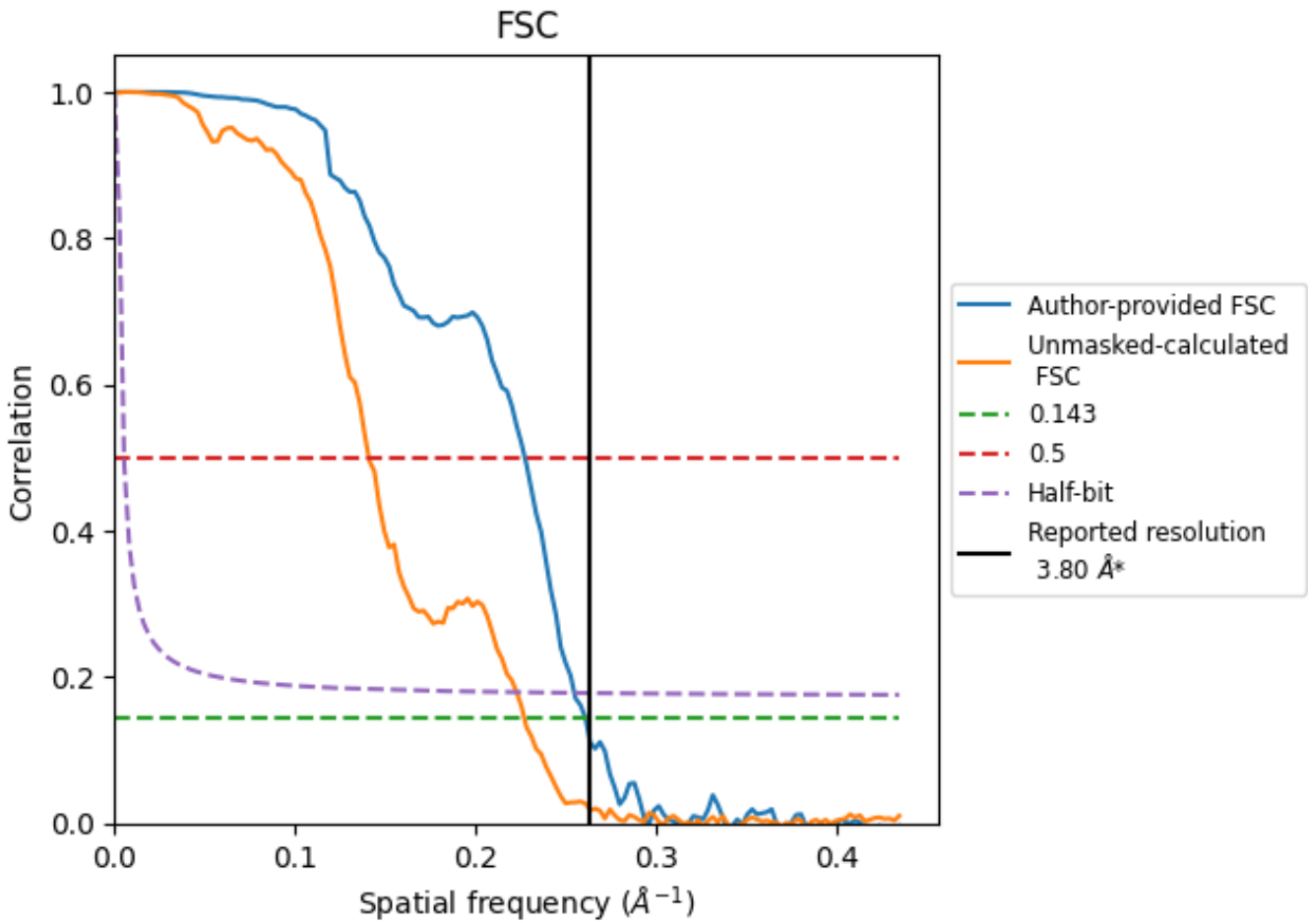


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



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

8.2 Resolution estimates (i)

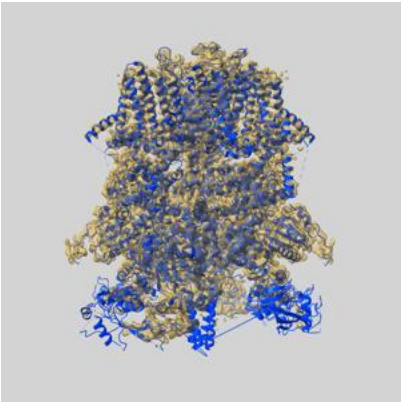
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.83	4.40	3.92
Unmasked-calculated*	4.40	7.10	4.49

*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 4.40 differs from the reported value 3.8 by more than 10 %

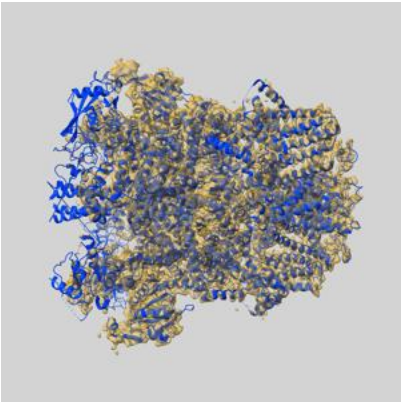
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7822 and PDB model 6D73. Per-residue inclusion information can be found in section 3 on page 4.

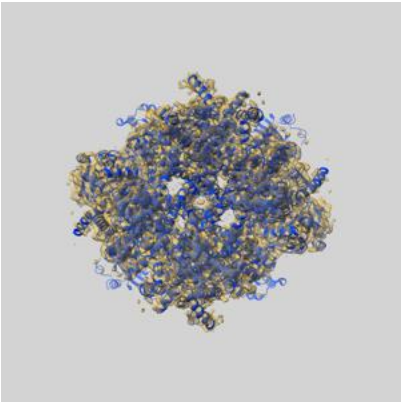
9.1 Map-model overlay (i)



X



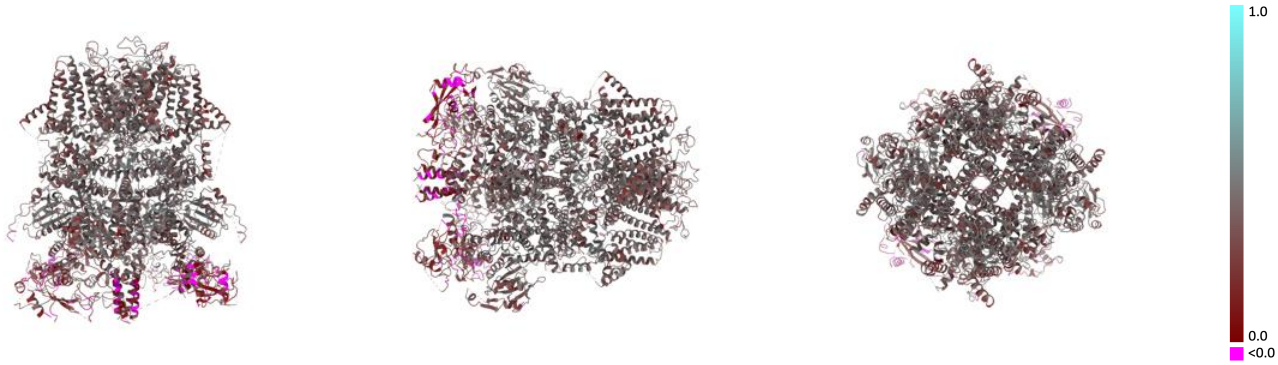
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

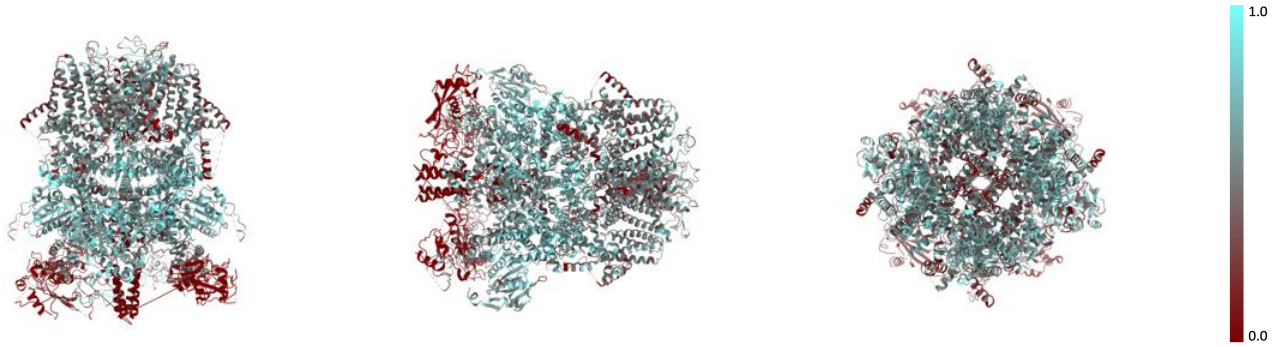
9.2 Q-score mapped to coordinate model (i)



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.

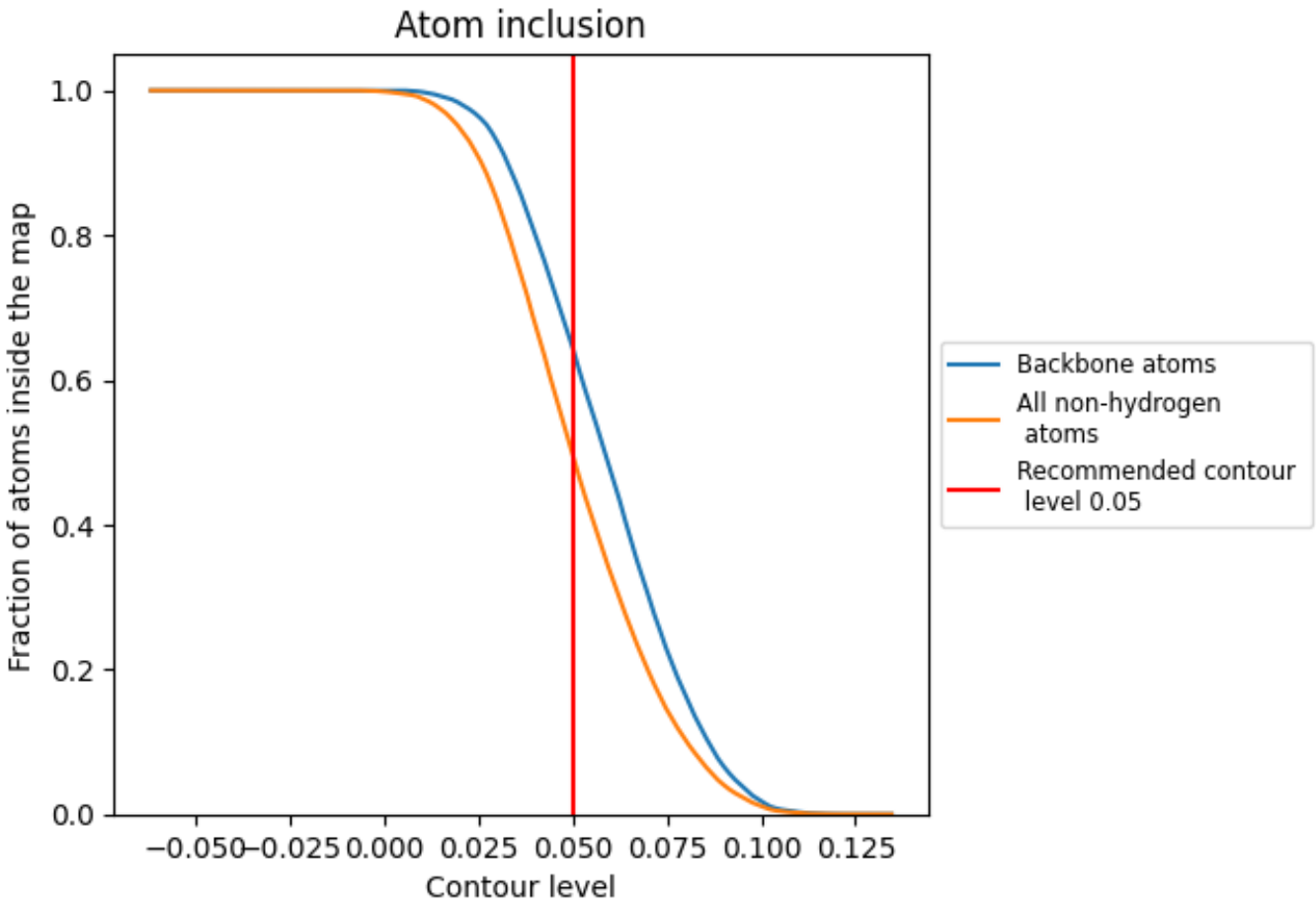
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4969	0.3650
A	0.4774	0.3590
B	0.5163	0.3710
C	0.4769	0.3580
D	0.5164	0.3710