wwPDB EM Validation Summary Report (i)

Mar 9, 2026 – 02:52 AM UTC

PDB ID	:	8E6Q / pdb_00008e6q
EMDB ID	:	EMD-27922
Title	:	Human TRPM2 ion channel in 1 mM ADPR
Authors	:	Wang, L.; Fu, T.M.; Xia, S.; Wu, H.
Deposited on	:	2022-08-23
Resolution	:	3.40 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:

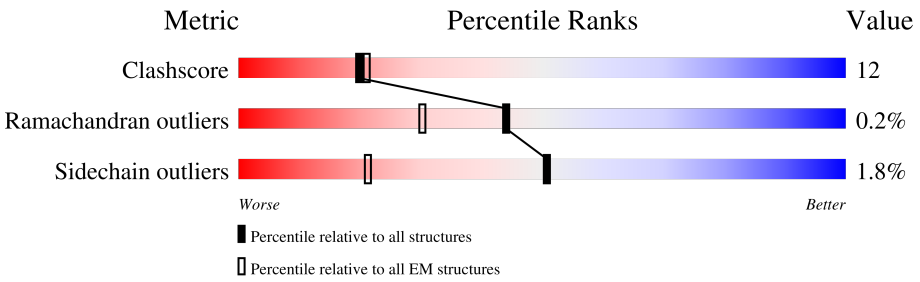
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

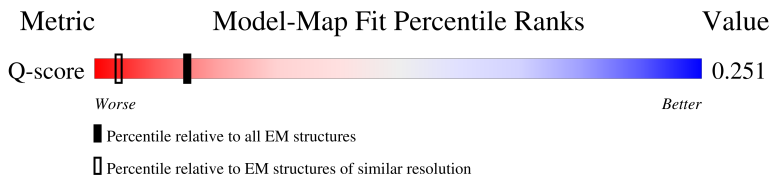
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	1503	27% 66% 22% • 10%
1	B	1503	28% 67% 22% • 10%
1	C	1503	28% 66% 23% • 10%
1	D	1503	27% 66% 23% • 10%

2 Entry composition (i)

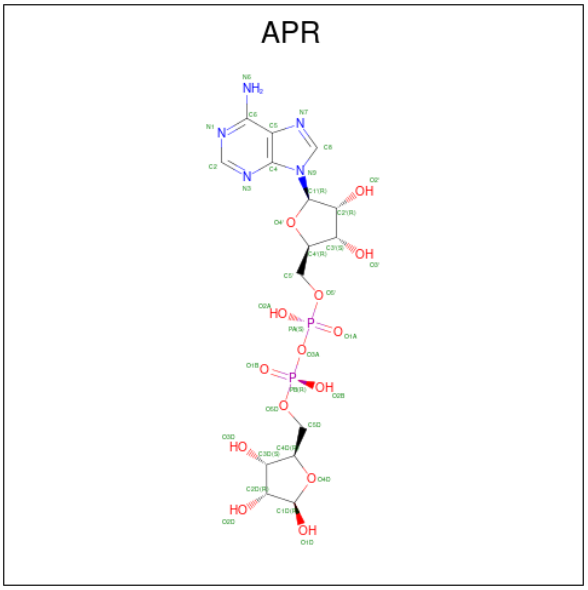
There are 2 unique types of molecules in this entry. The entry contains 40888 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1348	10150	6560	1776	1772	42	0	0
1	B	1348	10150	6560	1776	1772	42	0	0
1	C	1348	10150	6560	1776	1772	42	0	0
1	D	1348	10150	6560	1776	1772	42	0	0

- Molecule 2 is ADENOSINE-5-DIPHOSPHORIBOSE (CCD ID: APR) (formula: $C_{15}H_{23}N_5O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	36	15	5	14	2	0
2	A	1	36	15	5	14	2	0

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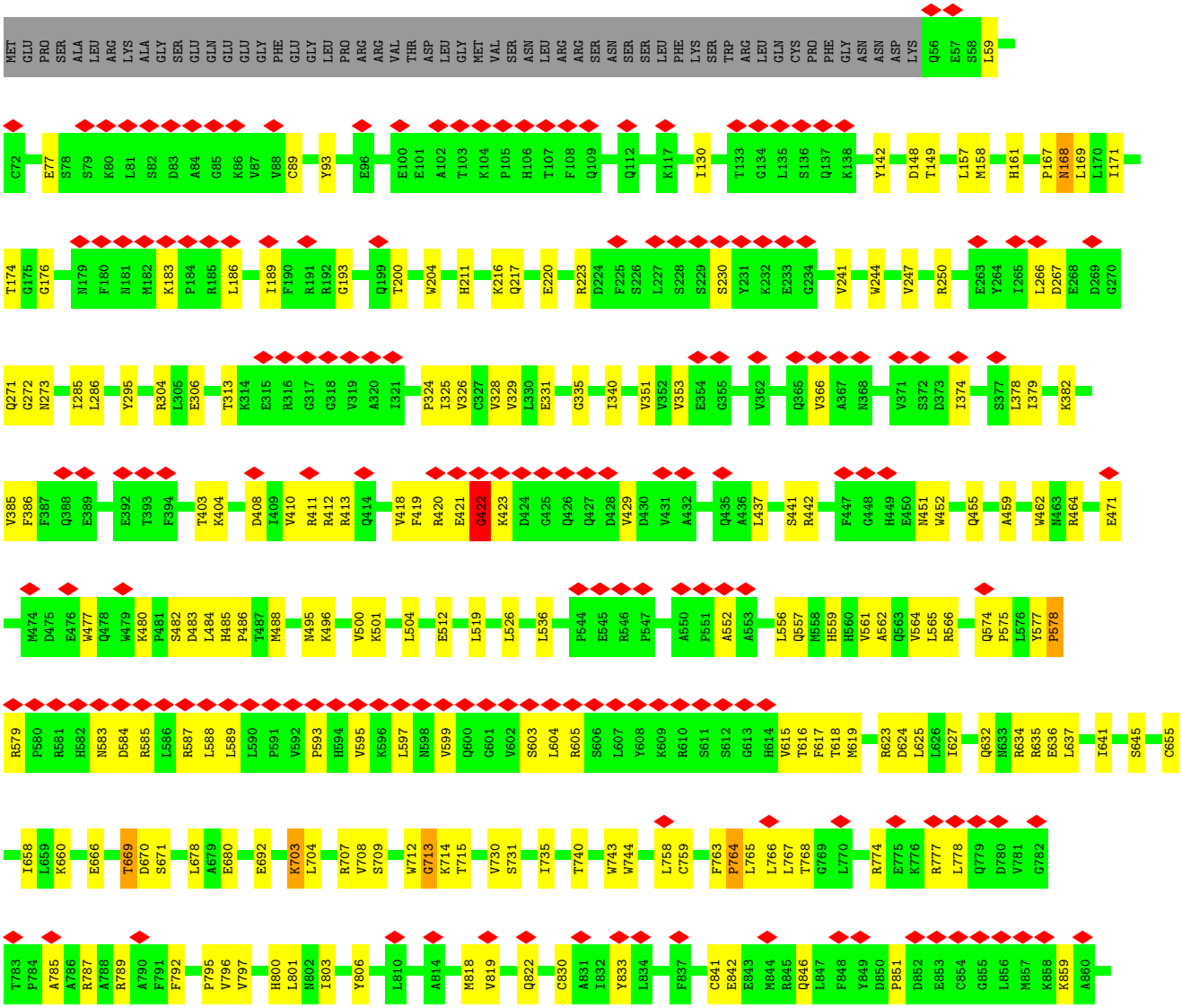
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	B	1	36	15	5	14	2	0
			Total	C	N	O	P	
2	B	1	36	15	5	14	2	0
			Total	C	N	O	P	
2	C	1	36	15	5	14	2	0
			Total	C	N	O	P	
2	C	1	36	15	5	14	2	0
			Total	C	N	O	P	
2	D	1	36	15	5	14	2	0
			Total	C	N	O	P	
2	D	1	36	15	5	14	2	0

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 member 2

Chain A:



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F935 F936 F937 L938 F939 L940 L941 A942 V943 W944 V945 V946 S947 F948 G949 V950 A951 K952 Q953 A954 I955 L956 I957 H958 N959 E960 R961 R962 V963 D964 W965 L966 F967 R968 G969 A970 V971 Y972 H973 S974 Y975 L976 T977 I978 F979 G980 Q981 I982 P983 G984 Y985 I986 D987 G988 VAL ASN PHE ASN PRO GLU

HIS CYS SER PRO ASN GLY THR ASP PRO TYR LYS PRO LYS CYS PRO GLU SER ASP ALA THR GLN GLN GLN ARG PRO ALA F1020 P1021 E1022 W1023 L1024 T1025 V1026 L1027 L1028 L1029 C1030 L1031 Y1032 L1033 L1034 F1035 T1036 N1037 I1038 L1039 L1040 L1041 N1042 L1043 L1044 I1045 A1046 M1047 F1048 N1049 Y1050 T1051 F1052 Q1053 Q1054

V1055 Q1056 E1057 H1058 T1059 D1060 K1064 R1067 E1073 A1079 A1080 P1081 F1084 I1085 H1089 L1090 Q1091 L1092 F1093 I1094 K1095 R1096 V1097 V1098 L1099 K1100 T1101 P1102 A1103 K1104 R1105 H1106 K1112 K1115 K1129 E1130 N1131 Y1132 L1133 Q1134 N1135 R1136 Q1137 F1138 Q1139 Q1140 K1141 Q1142 R1143 P1144 E1145

I1148 E1149 D1150 K1154 D1160 D1163 L1164 D1165 PRO LEU LYS ARG SER GLY SER MET GLU GLN ARG LEU ALA SER LEU GLU GLU GLN VAL ALA GLN THR ALA GLN ALA LEU HIS TRP ILE VAL ARG THR LEU ARG ALA SER GLY PHE SER SER GLU ALA ASP VAL PRO THR LEU ALA

SER GLN LYS ALA ALA GLU GLU PRO ASP ALA GLU PRO GLY GLY ARG LYS LYS THR GLU GLU PRO G1235 D1236 S1237 V1240 N1241 A1242 R1243 H1244 L1245 L1246 N1249 R1254 F1255 P1256 V1257 P1258 K1261 V1262 P1263 W1264 E1265 T1266 E1267 F1268 L1269 I1270 Y1271 D1272 P1273 E1279 R1280 K1281 D1282 A1283

A1284 A1285 M1286 D1287 P1288 M1289 G1290 D1291 T1292 L1293 E1294 P1295 L1296 S1297 T1298 I1299 Q1300 V1303 V1304 D1305 G1306 L1307 R1308 D1309 R1310 R1311 S1312 F1313 H1314 G1315 P1316 V1319 Q1320 A1321 G1322 L1323 P1324 L1325 N1326 R1330 F1342 G1343 P1344 N1345 H1346 T1347 L1348 Y1349 P1350 M1351 Y1352 T1353 R1356 R1357 N1358

E1359 D1360 G1361 A1362 R1365 K1366 S1367 I1368 K1369 K1370 M1371 L1372 E1373 K1378 L1379 P1380 L1381 S1382 W1385 G1389 G1390 E1393 P1394 G1395 E1396 M1397 L1398 P1399 R1400 R1404 I1405 L1406 H1410 M1422 E1423 K1426 G1427 Y1428 M1429 W1439 I1440 E1441 T1442 V1443 A1444 V1445 S1446 V1447 D1451

Q1452 N1453 D1454 V1455 E1456 S1462 A1466 C1467 D1468 S1469 G1470 A1471 S1472 I1473 R1474 V1477 V1478 D1479 L1484 L1491 K1494 A1495 E1498 H1502 Y1503

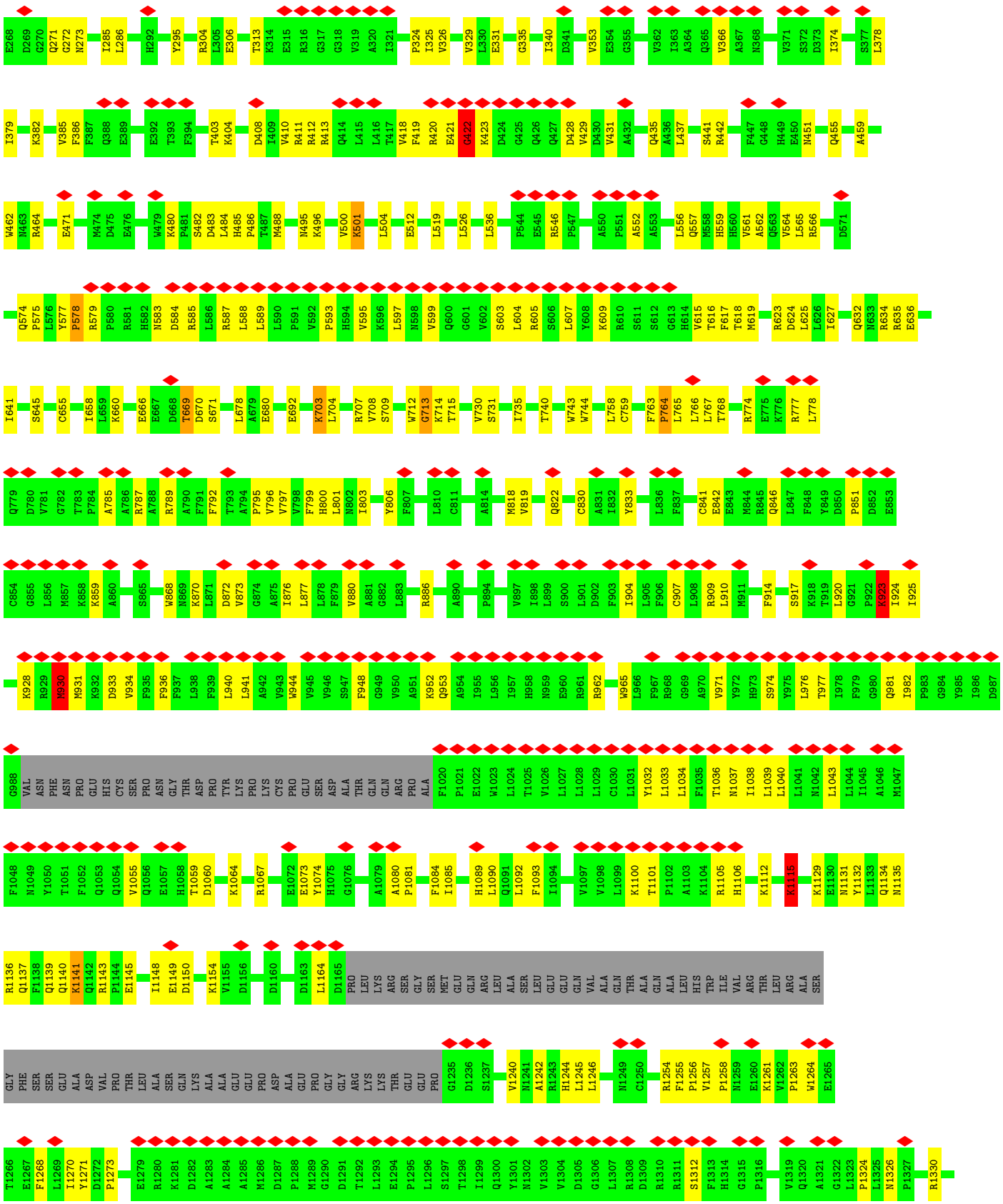
- Molecule 1: Transient receptor potential cation channel subfamily M member 2

Chain B:

MET GLU PRO SER ALA LEU ARG LYS ALA GLY SER GLU GLN GLU GLU GLY PHE GLU GLY LEU PRO ARG ARG VAL THR ASP LEU GLY MET VAL SER ASN LEU ARG ARG SER ASN SER SER LEU PHE LYS SER TRP ARG LEU GLN CYS PRO PHE GLY ASN ASN ASP LYS Q56 E57 S58 L59

C72 E77 S78 S79 K80 L81 S82 D83 A84 G85 K86 V87 V88 C89 Y93 E96 E100 E101 A102 T103 K104 P105 H106 T107 F108 Q109 Q112 K117 I130 T133 G134 L135 S136 Q137 K138 Y142 S146 Q147 D148 T149 L157 M158 H161 P167 N168 L169 L170

I171 T174 G175 G176 N179 F180 N181 M182 K183 P184 R185 L186 I189 F190 R191 R192 G193 Q199 T200 W204 H211 K216 Q217 E220 R223 D224 F225 S226 L227 S228 S229 S230 Y231 K232 E233 G234 V241 W244 V247 H248 R249 R250 E263 Y264 I265 L266 D267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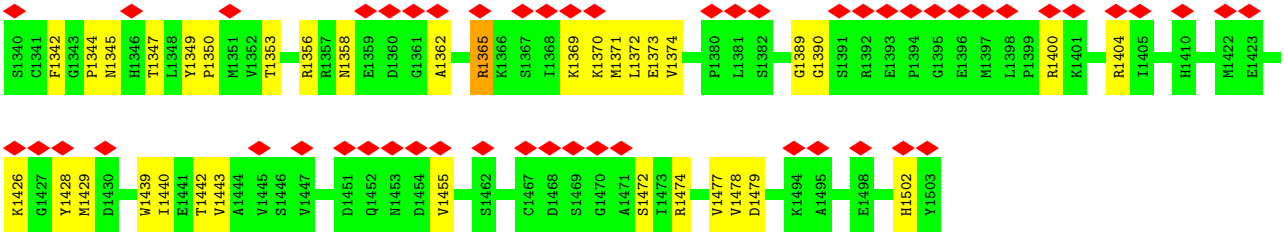
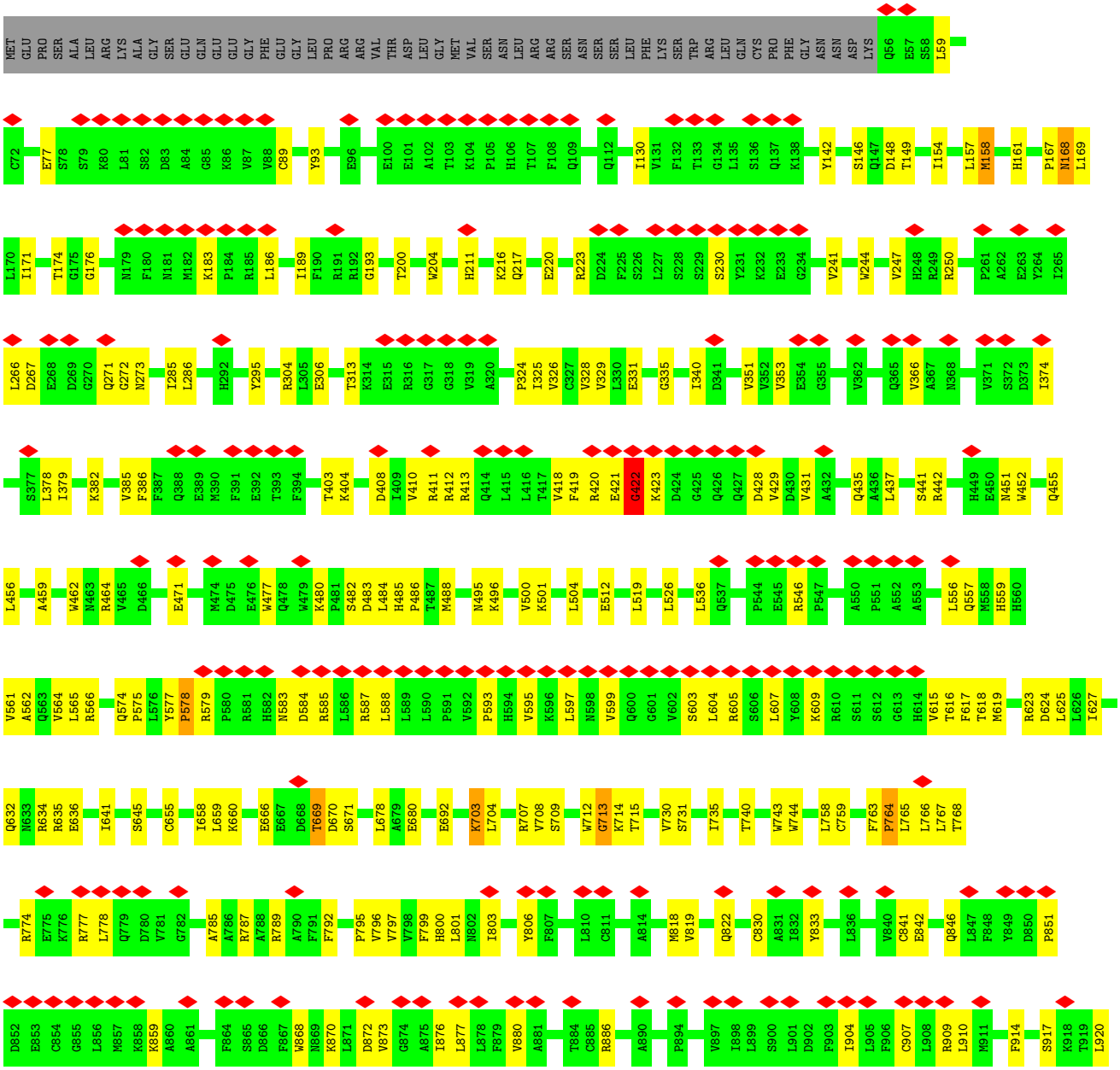
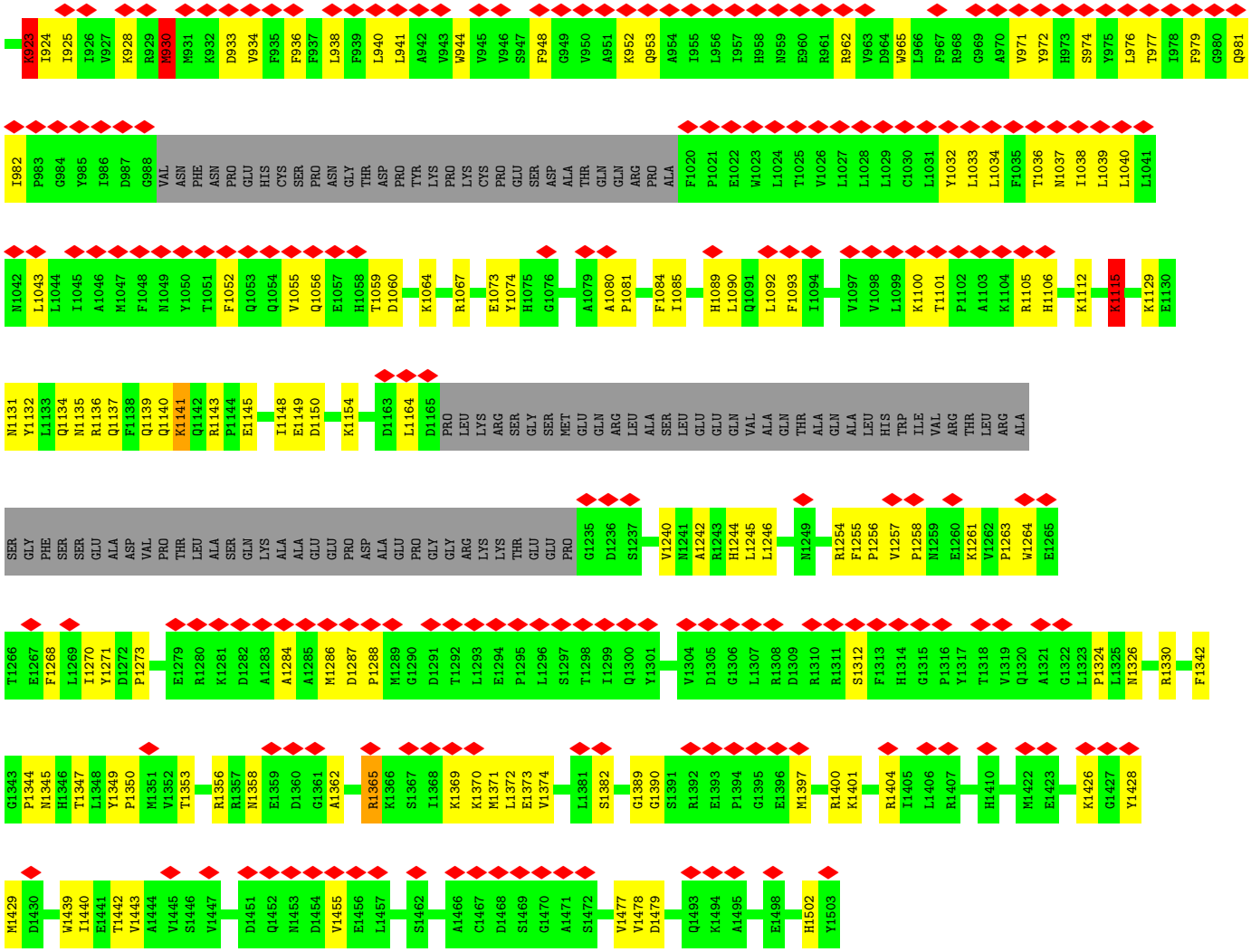
I379 K382 V385 F386 F387 Q388 E389 E392 T393 F394 T403 K404 D408 I409 V410 R411 R412 R413 Q414 L415 L416 T417 V418 F419 R420 E421 G422 K423 D424 G425 Q426 Q427 D428 V429 D430 V431 A432 Q435 A436 L437 S441 R442 F447 G448 H449 E450 M451 Q455 A459
W462 M463 R464 E471 M474 D475 E476 W479 K480 P481 S482 D483 L484 H485 P486 T487 M488 N495 K496 V500 K501 L504 E512 L519 L526 L536 P544 E545 R546 P547 A550 P551 A552 A553 L556 Q557 M558 H559 H560 V561 A562 Q563 V564 L565 R566 D571
Q574 P575 L576 Y577 P578 R579 P580 R581 H582 N583 D584 R585 L586 R587 L588 L589 L590 P591 V592 P593 H594 V595 K596 L597 N598 V599 Q600 G601 V602 S603 L604 R605 S606 L607 Y608 K609 R610 S611 S612 G613 H614 V615 T616 F617 T618 M619 R623 D624 L625 L626 I627 Q632 N633 R634 R635 E636
I641 S645 C655 I658 L659 K660 E666 E667 D668 T669 D670 S671 L678 A679 E680 E692 K703 L704 R707 V708 S709 W712 G713 K714 T715 V730 S731 I735 T740 W743 W744 L758 C759 F763 P764 L765 L766 L767 T768 R774 E775 K776 R777 L778
Q779 D780 V781 G782 T783 P784 A785 A786 R787 A788 R789 A790 F791 F792 T793 A794 P795 V796 V797 V798 F799 H800 L801 N802 I803 Y806 F807 L810 C811 A814 M818 V819 Q822 C830 A831 I832 Y833 L836 F837 C841 E842 E843 M844 R845 Q846 L847 F848 Y849 D850 P851 D852 E853
C854 G855 L856 M857 K858 K859 A860 S865 W868 N869 K870 L871 D872 V873 G874 A875 I876 L877 L878 F879 V880 A881 G882 L883 R886 A890 P894 V897 I898 L899 S900 L901 D902 F903 I904 L905 F906 C907 L908 R909 L910 M911 F914 S917 K918 T919 L920 G921 P922 K923 I924 I925
K928 R929 M930 M931 K932 D933 V934 F935 F936 F937 L938 F939 L940 L941 A942 V943 W944 V945 V946 S947 F948 G949 V950 A951 K952 Q953 A954 I955 L956 I957 H958 N959 E960 R961 R962 W965 L966 F967 R968 G969 A970 V971 Y972 H973 S974 Y975 L976 T977 I978 F979 G980 Q981 I982 P983 G984 Y985 I986 D987
G988 VAL ASN PHE ASN PRO GLU HIS CYS SER PRO ASN GLY THR ASP PRO TYR LYS PRO LYS CYS PRO GLU SER ASP ALA THR GLN GLN ARG PRO ALA F1020 P1021 E1022 W1023 L1024 T1025 V1026 L1027 L1028 L1029 C1030 L1031 Y1032 L1033 L1034 F1035 T1036 N1037 I1038 L1039 L1040 L1041 N1042 L1043 L1044 I1045 A1046 M1047
F1048 N1049 Y1050 T1051 F1052 Q1053 Q1054 V1055 Q1056 E1057 H1058 T1059 D1060 K1064 R1067 E1072 E1073 Y1074 H1075 G1076 A1079 A1080 P1081 F1084 I1085 H1089 L1090 Q1091 L1092 F1093 I1094 V1097 V1098 L1099 K1100 T1101 P1102 A1103 K1104 R1105 H1106 K1112 K1115 K1129 E1130 N1131 Y1132 L1133 Q1134 N1135
R1136 Q1137 F1138 Q1139 Q1140 K1141 Q1142 R1143 P1144 E1145 I1148 E1149 D1150 K1154 V1155 D1156 D1160 D1163 L1164 D1165 PRO LEU LYS ARG SER GLY SER MET GLU GLN ARG LEU ALA SER LEU GLU GLU GLN VAL ALA GLN THR ALA GLN ALA LEU HIS TRP ILE VAL ARG THR LEU ARG ALA SER
GLY PHE SER SER GLU ALA ASP VAL PRO THR LEU ALA SER GLN LYS ALA ALA GLU GLU PRO ASP ALA GLU PRO GLY GLY ARG LYS LYS THR GLU GLU PRO G1235 D1236 S1237 V1240 N1241 A1242 R1243 H1244 L1245 L1246 N1249 C1250 R1254 F1255 P1256 V1257 P1258 N1259 E1260 K1261 V1262 P1263 W1264 E1265
T1266 E1267 F1268 L1269 I1270 Y1271 D1272 P1273 E1279 R1280 K1281 D1282 A1283 A1284 A1285 M1286 D1287 P1288 M1289 G1290 D1291 T1292 L1293 E1294 P1295 L1296 S1297 T1298 I1299 Q1300 Y1301 N1302 V1303 V1304 D1305 G1306 L1307 R1308 D1309 R1310 R1311 S1312 F1313 H1314 G1315 P1316 V1319 Q1320 A1321 G1322 L1323 P1324 L1325 N1326 P1327 R1330



- Molecule 1: Transient receptor potential cation channel subfamily M member 2

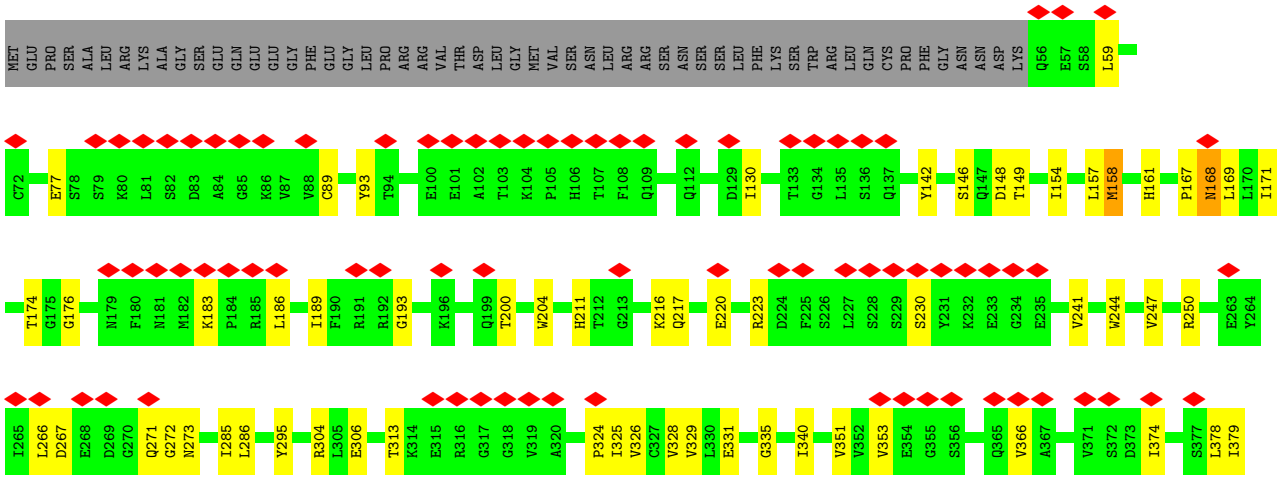
Chain C:

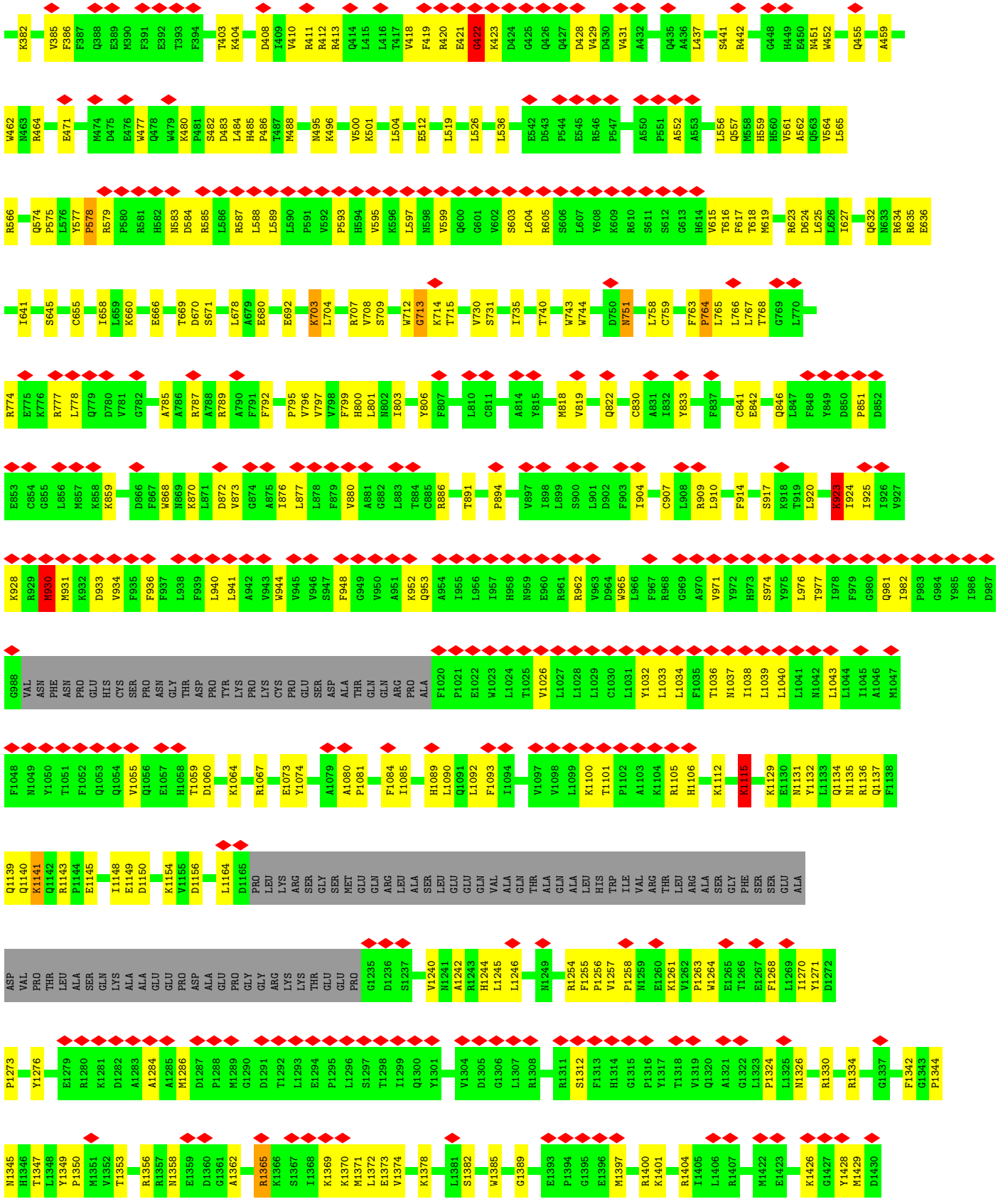




• Molecule 1: Transient receptor potential cation channel subfamily M member 2

Chain D:

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W462 N463 R464 E471 M474 D475 E476 W477 Q478 W479 K480 P481 S482 D483 L484 H485 P486 T487 M488 N495 K496 V500 K501 L504 E512 L519 L526 L536 E542 D543 P544 E545 R546 P547 A550 P551 A552 A553 L556 Q557 M558 H559 H560 V561 A562 Q563 V564 L565
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R774 E775 K776 R777 L778 Q779 D780 V781 G782 A785 A786 R787 A788 R789 A790 F791 F792 P795 V796 V797 V798 F799 H800 L801 N802 I803 Y806 F807 L810 C811 A814 Y815 M818 V819 Q822 C830 A831 I832 Y833 F837 C841 E842 Q846 L847 F848 Y849 D850 P851 D852
E853 C854 G855 L856 M857 K858 K859 D866 F867 W868 N869 K870 L871 D872 V873 G874 A875 I876 L877 L878 F879 V880 A881 G882 L883 T884 C885 R886 T891 P894 V897 I898 L899 S900 L901 D902 F903 I904 C907 L908 R909 L910 F914 S917 K918 T919 L920 K923 I924 I925 I926 V927
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G988 VAL ASN PHE ASN PRO GLU HIS CYS SER PRO ASN GLY THR ASP PRO TYR LYS PRO LYS CYS PRO GLU SER ASP ALA THR GLN GLN ARG PRO ALA F1020 P1021 E1022 W1023 L1024 T1025 V1026 L1027 L1028 L1029 C1030 L1031 Y1032 L1033 L1034 F1035 T1036 N1037 I1038 L1039 L1040 L1041 N1042 L1043 L1044 I1045 A1046 M1047
F1048 N1049 Y1050 T1051 F1052 Q1053 Q1054 V1055 Q1056 E1057 H1058 T1059 D1060 K1064 R1067 E1073 Y1074 A1079 A1080 P1081 F1084 I1085 H1089 L1090 Q1091 L1092 F1093 I1094 V1097 V1098 L1099 K1100 T1101 P1102 A1103 K1104 R1105 H1106 K1112 K1115 K1129 E1130 N1131 Y1132 L1133 Q1134 N1135 R1136 Q1137 F1138
Q1139 Q1140 K1141 Q1142 R1143 P1144 E1145 I1148 E1149 D1150 K1154 V1155 D1156 L1164 D1165 PRO LEU LYS ARG SER GLY SER MET GLU GLN ARG LEU ALA SER LEU GLU GLU GLN VAL ALA GLN THR ALA GLN ALA LEU HIS TRP ILE VAL ARG THR LEU ARG ALA SER GLY PHE SER SER GLU ALA
ASP VAL PRO THR LEU ALA SER GLN LYS ALA ALA GLU GLU PRO ASP ALA GLU PRO GLY GLY ARG LYS LYS THR GLU GLU PRO G1235 D1236 S1237 V1240 N1241 A1242 R1243 H1244 L1245 L1246 M1249 R1254 F1255 P1256 V1257 P1258 N1259 E1260 K1261 V1262 P1263 W1264 E1265 T1266 E1267 F1268 L1269 I1270 Y1271 D1272
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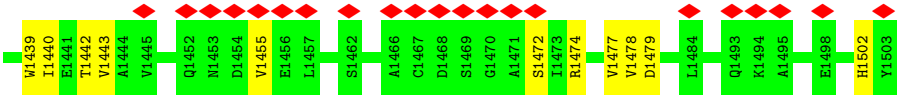
N1345 H1346 T1347 L1348 Y1349 P1350 M1351 Y1352 T1353 R1356 R1357 N1358 E1359 D1360 G1361 A1362 R1365 K1366 S1367 I1368 K1369 K1370 M1371 L1372 E1373 V1374 K1378 L1381 S1382 W1385 G1389 E1393 P1394 G1395 E1396 M1397 R1400 K1401 R1404 I1405 L1406 R1407 M1422 E1423 K1426 G1427 Y1428 M1429 D1430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A1444
V1445
Q1452
N1453
D1454
V1455
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A1466
C1467
D1468
S1469
G1470
A1471
S1472
I1473
R1474
V1477
V1478
D1479
L1484
Q1493
K1494
A1495
E1498
H1502
Y1503

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135036	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 ($e^-/Å^2$)	49	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.187	Depositor
Minimum map value	-1.194	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.246	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: APR

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	0.16	0/10402	0.47	6/14191 (0.0%)
1	B	0.16	0/10402	0.47	6/14191 (0.0%)
1	C	0.16	0/10402	0.47	6/14191 (0.0%)
1	D	0.16	0/10402	0.47	6/14191 (0.0%)
All	All	0.16	0/41608	0.47	24/56764 (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	5
1	B	0	5
1	C	0	5
1	D	0	4
All	All	0	19

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1115	LYS	CB-CG-CD	6.90	127.17	111.30
1	A	1115	LYS	CB-CG-CD	6.88	127.12	111.30
1	B	1115	LYS	CB-CG-CD	6.88	127.12	111.30
1	C	1115	LYS	CB-CG-CD	6.88	127.12	111.30
1	B	930	MET	CB-CG-SD	6.78	133.03	112.70

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	421	GLU	Peptide
1	A	422	GLY	Peptide
1	A	666	GLU	Peptide
1	A	669	THR	Peptide
1	A	713	GLY	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	10150	0	9654	247	0
1	B	10150	0	9654	249	0
1	C	10150	0	9654	257	0
1	D	10150	0	9654	255	0
2	A	72	0	42	2	0
2	B	72	0	42	2	0
2	C	72	0	42	3	0
2	D	72	0	42	3	0
All	All	40888	0	38784	989	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 12.

The worst 5 of 989 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:930:MET:HG2	1:B:1039:LEU:HD11	1.43	0.98
1:A:1039:LEU:HD11	1:D:930:MET:HG2	1.48	0.96
1:B:930:MET:HG2	1:C:1039:LEU:HD11	1.53	0.88
1:C:930:MET:HG2	1:D:1039:LEU:HD11	1.60	0.84
1:C:1356:ARG:NH2	1:C:1371:MET:SD	2.54	0.81

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	1342/1503 (89%)	1232 (92%)	107 (8%)	3 (0%)	43	71
1	B	1342/1503 (89%)	1231 (92%)	108 (8%)	3 (0%)	43	71
1	C	1342/1503 (89%)	1233 (92%)	106 (8%)	3 (0%)	43	71
1	D	1342/1503 (89%)	1231 (92%)	108 (8%)	3 (0%)	43	71
All	All	5368/6012 (89%)	4927 (92%)	429 (8%)	12 (0%)	44	71

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1455	VAL
1	B	1455	VAL
1	C	1455	VAL
1	D	1455	VAL
1	A	670	ASP

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	981/1318 (74%)	964 (98%)	17 (2%)	53	67
1	B	981/1318 (74%)	964 (98%)	17 (2%)	53	67
1	C	981/1318 (74%)	964 (98%)	17 (2%)	53	67
1	D	981/1318 (74%)	963 (98%)	18 (2%)	51	67
All	All	3924/5272 (74%)	3855 (98%)	69 (2%)	51	67

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	731	SER
1	D	758	LEU
1	D	1145	GLU
1	B	758	LEU
1	B	731	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	161	HIS
1	C	953	GLN
1	D	958	HIS
1	C	271	GLN
1	C	557	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	APR	A	1601	-	39,39,39	0.54	0	56,60,60	0.63	0
2	APR	D	1601	-	39,39,39	0.53	0	56,60,60	0.64	0
2	APR	D	1602	-	39,39,39	0.55	0	56,60,60	0.65	0
2	APR	C	1602	-	39,39,39	0.54	0	56,60,60	0.65	0
2	APR	A	1602	-	39,39,39	0.54	0	56,60,60	0.65	0
2	APR	C	1601	-	39,39,39	0.53	0	56,60,60	0.63	0
2	APR	B	1601	-	39,39,39	0.54	0	56,60,60	0.63	0
2	APR	B	1602	-	39,39,39	0.54	0	56,60,60	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	APR	A	1601	-	-	2/22/54/54	0/4/4/4
2	APR	D	1601	-	-	2/22/54/54	0/4/4/4
2	APR	D	1602	-	-	3/22/54/54	0/4/4/4
2	APR	C	1602	-	-	3/22/54/54	0/4/4/4
2	APR	A	1602	-	-	3/22/54/54	0/4/4/4
2	APR	C	1601	-	-	2/22/54/54	0/4/4/4
2	APR	B	1601	-	-	2/22/54/54	0/4/4/4
2	APR	B	1602	-	-	3/22/54/54	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1602	APR	C5'-O5'-PA-O2A
2	A	1602	APR	C5'-O5'-PA-O3A
2	B	1602	APR	C5'-O5'-PA-O2A
2	B	1602	APR	C5'-O5'-PA-O3A
2	C	1602	APR	C5'-O5'-PA-O2A

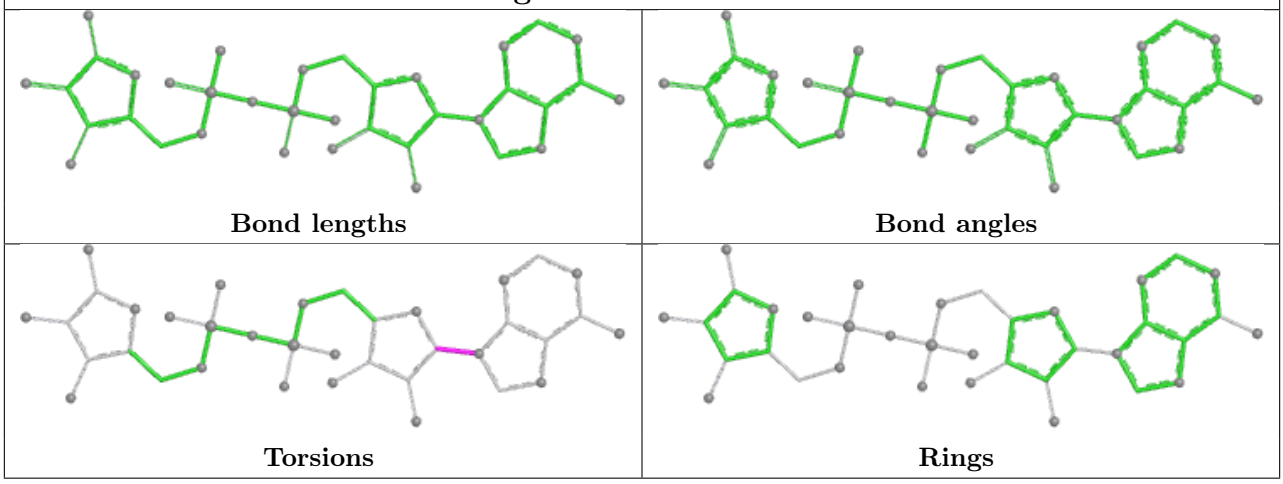
There are no ring outliers.

6 monomers are involved in 10 short contacts:

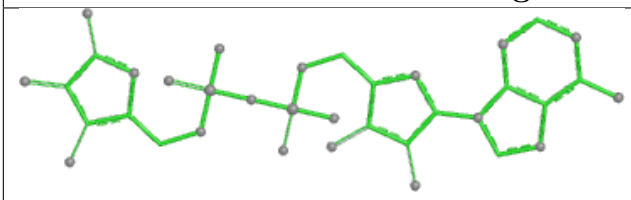
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1601	APR	2	0
2	D	1601	APR	2	0
2	D	1602	APR	1	0
2	C	1602	APR	1	0
2	C	1601	APR	2	0
2	B	1601	APR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand APR A 1601



Ligand APR D 1601



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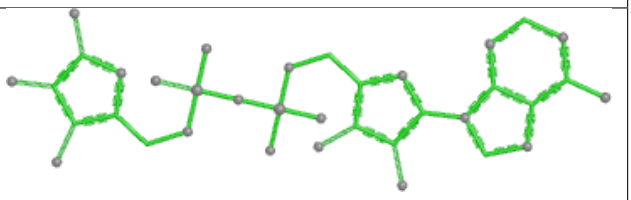
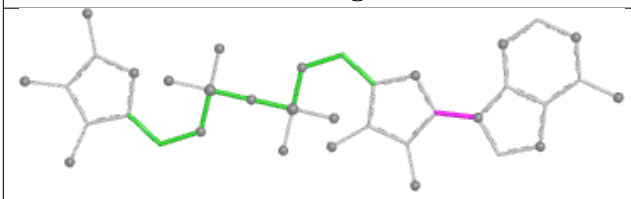
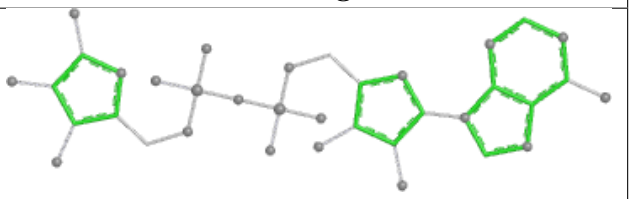


Bond angles

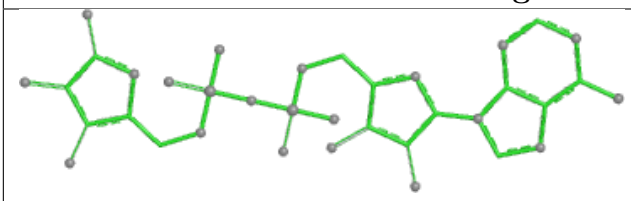


Torsions



Rings

Ligand APR D 1602



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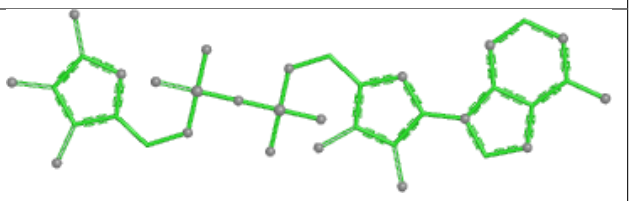

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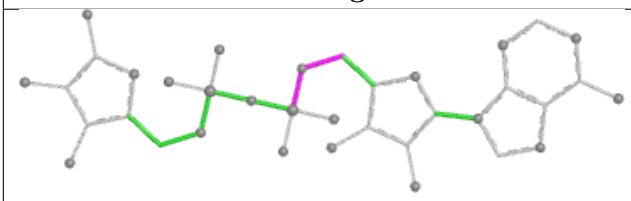

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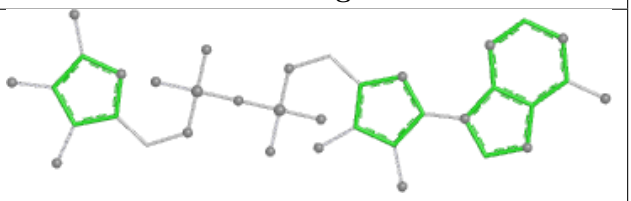

Rings

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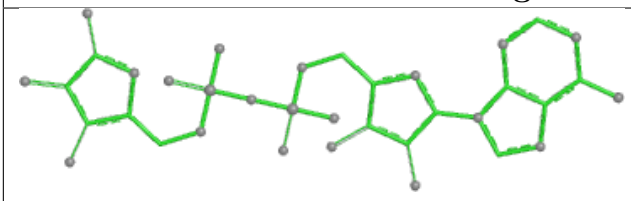

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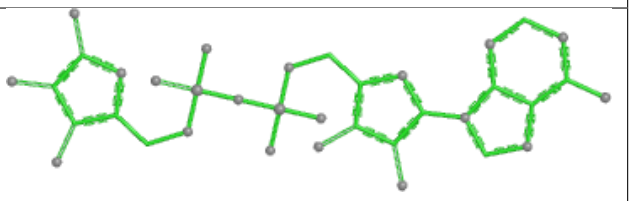

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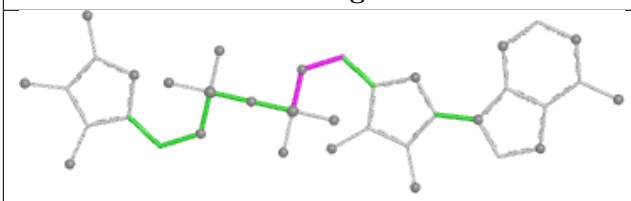

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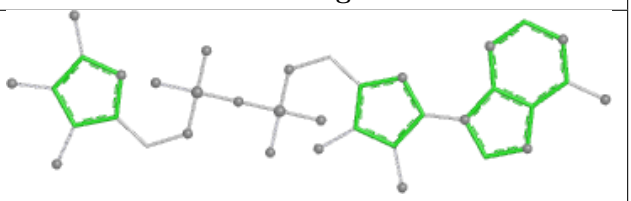

Rings

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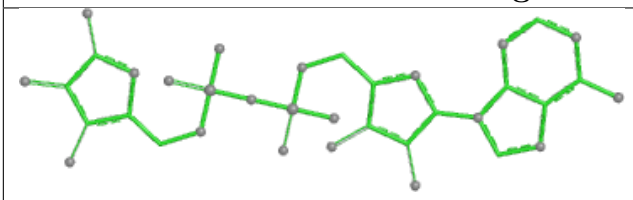

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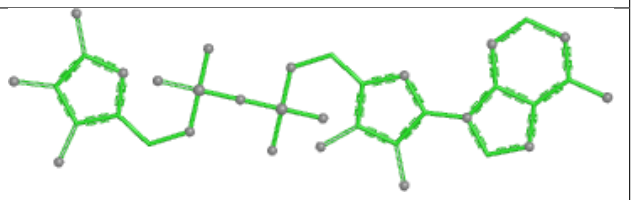
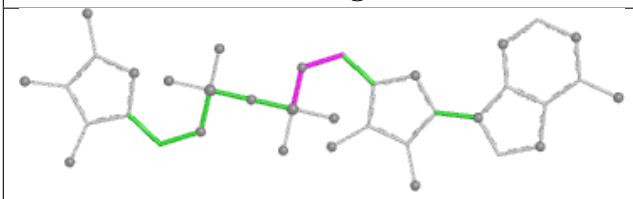


Bond angles



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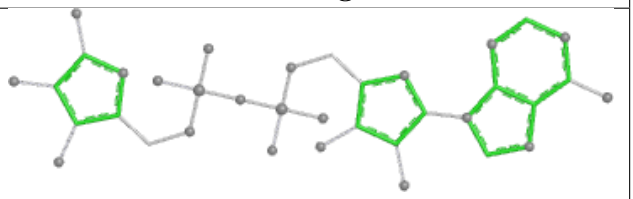
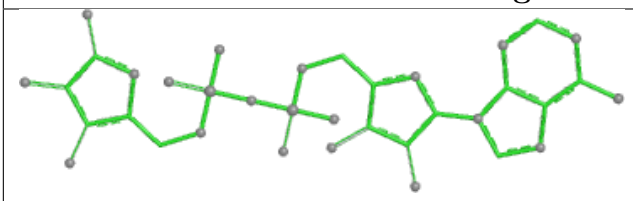


Rings

Ligand APR C 1601



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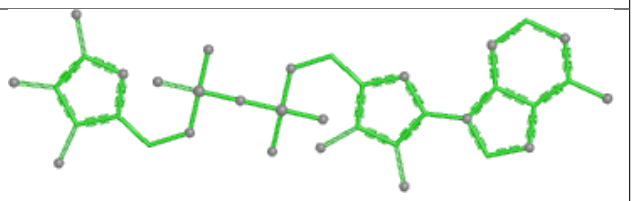

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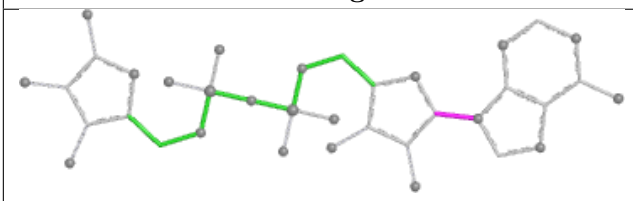

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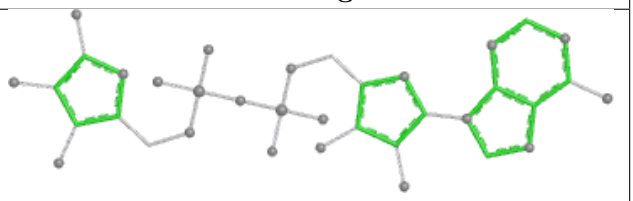
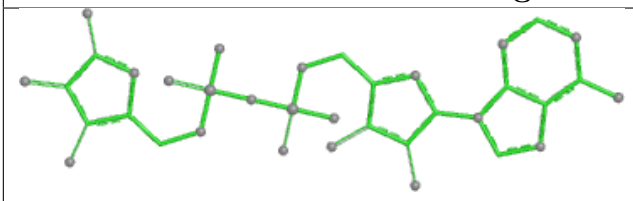
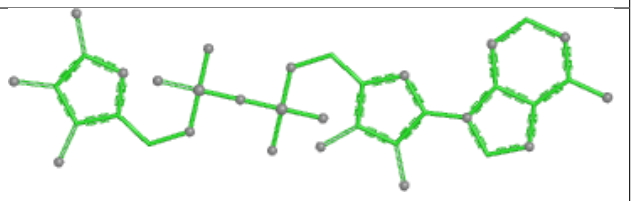


Rings

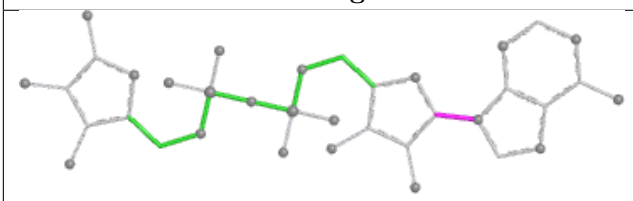
Ligand APR B 1601



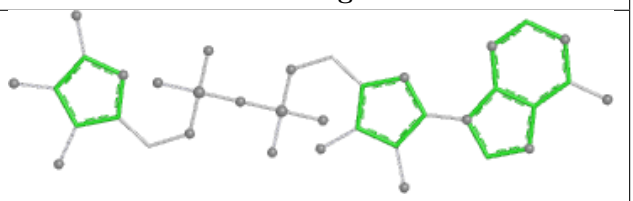
Bond lengths



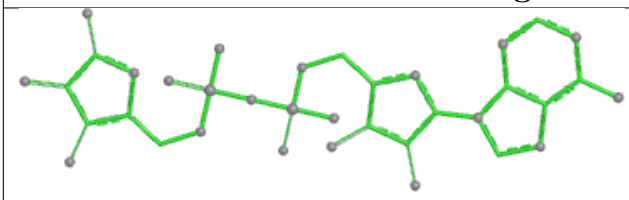
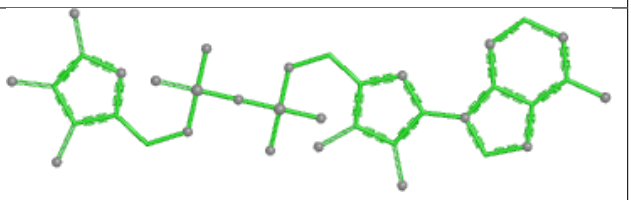
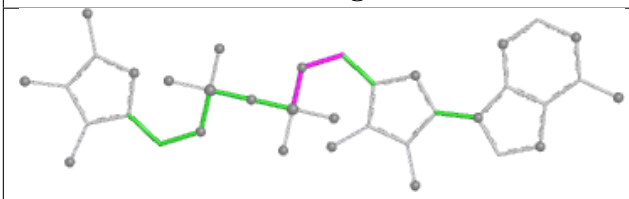
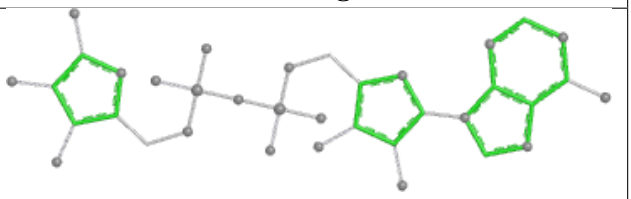
Bond angles



Torsions



Rings

Ligand APR B 1602	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

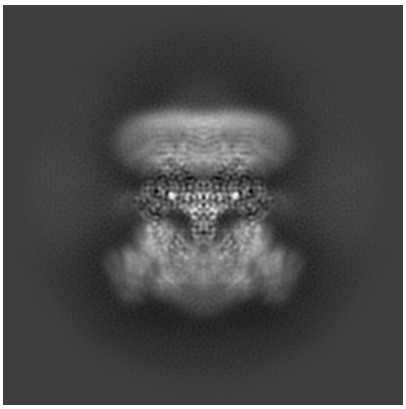
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-27922. These allow visual inspection of the internal detail of the map and identification of artifacts.

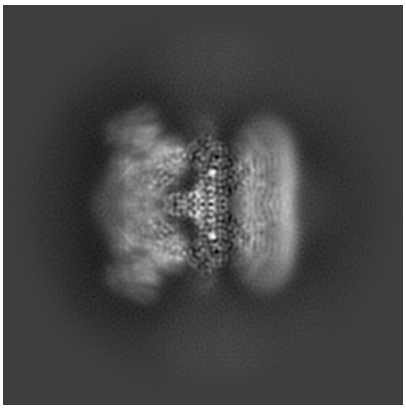
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

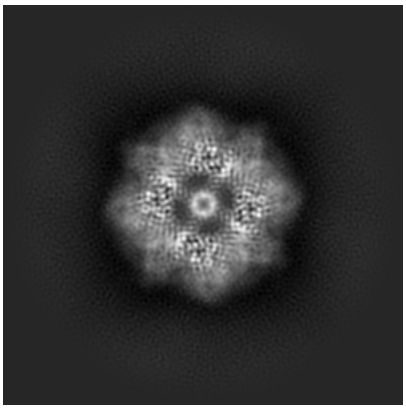
6.1.1 Primary map



X

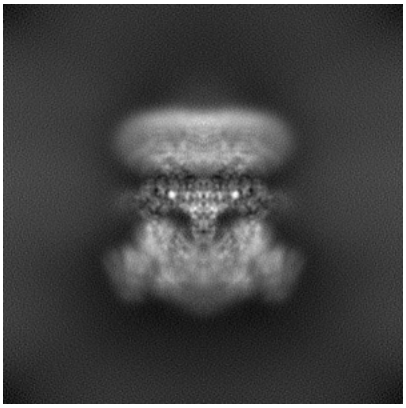


Y

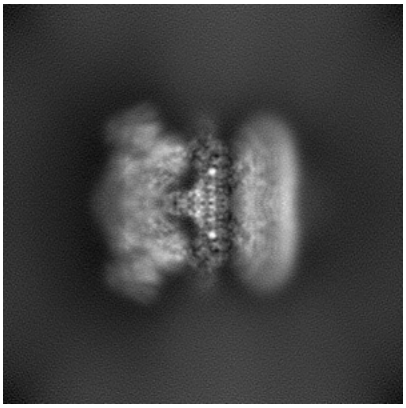


Z

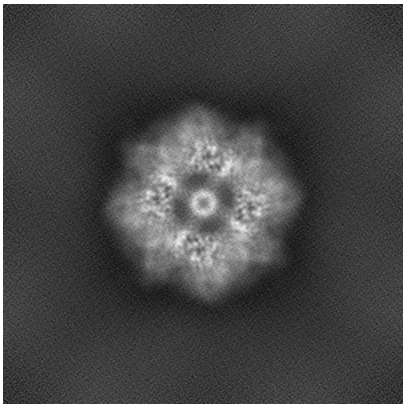
6.1.2 Raw map



X



Y

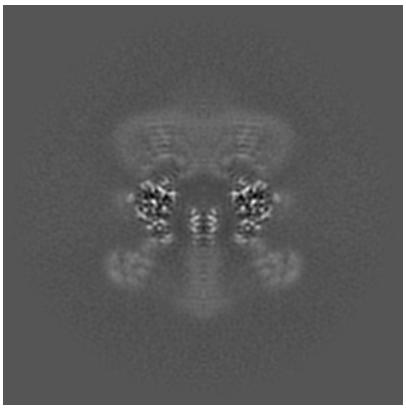


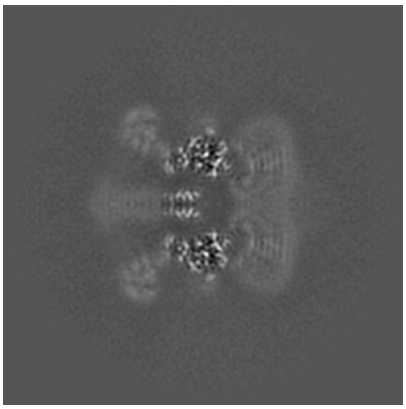
Z

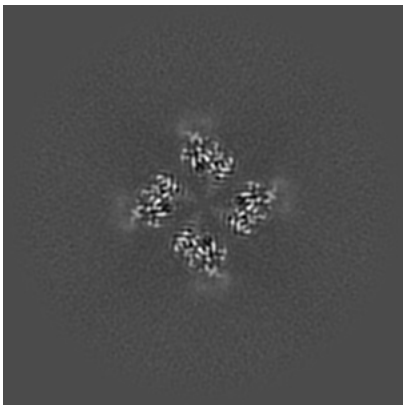
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

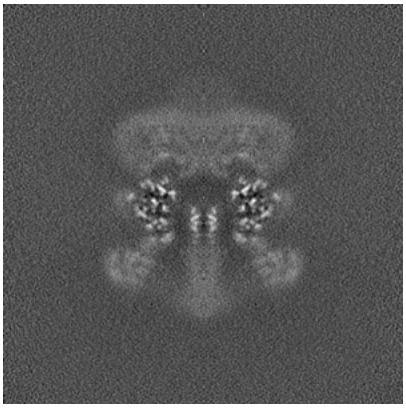
6.2.1 Primary map

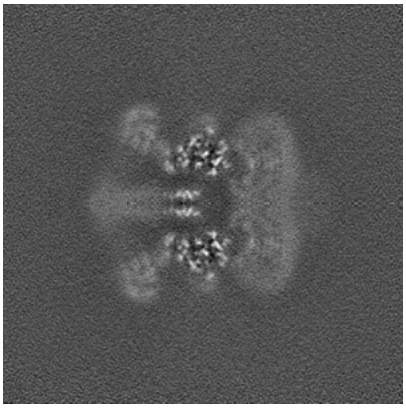

X Index: 150

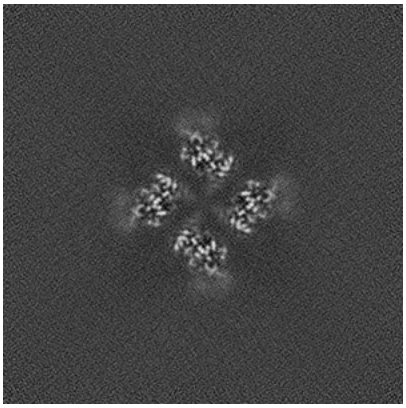

Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150

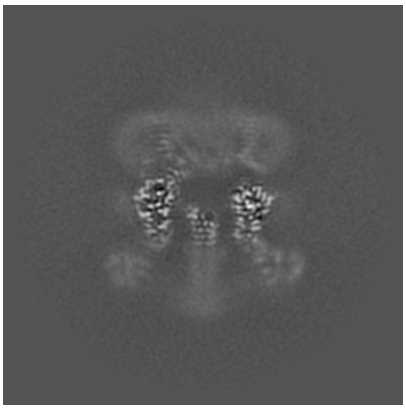

Y Index: 150

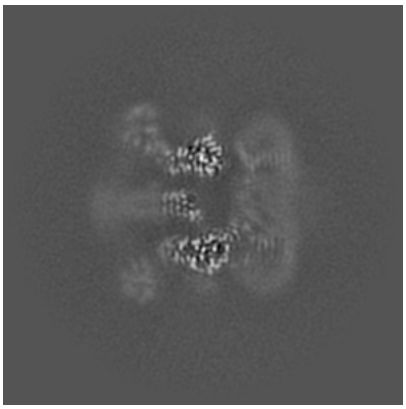

Z Index: 150

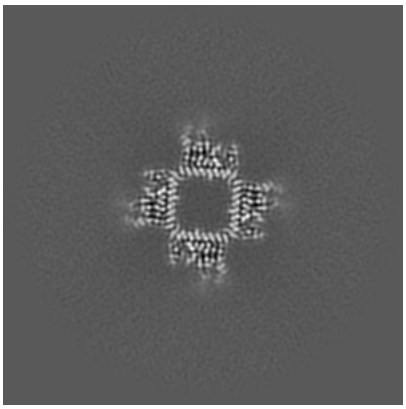
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

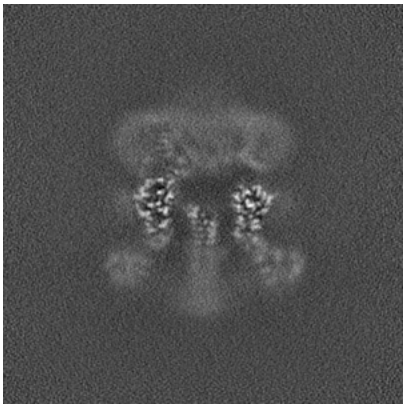
6.3.1 Primary map

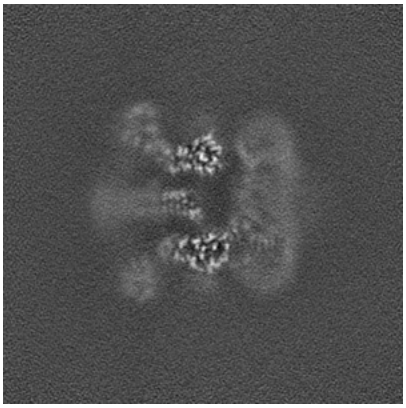

X Index: 147

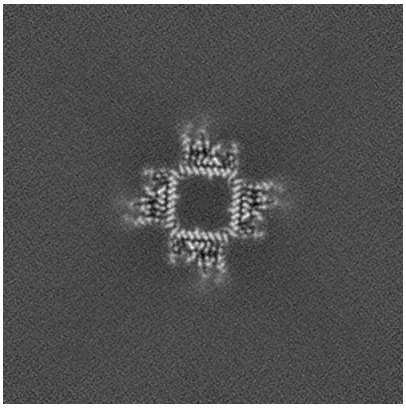

Y Index: 153


Z Index: 157

6.3.2 Raw map


X Index: 147

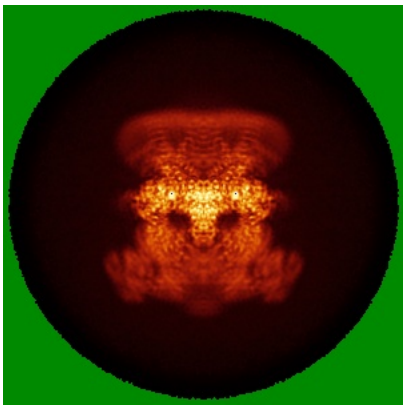

Y Index: 153

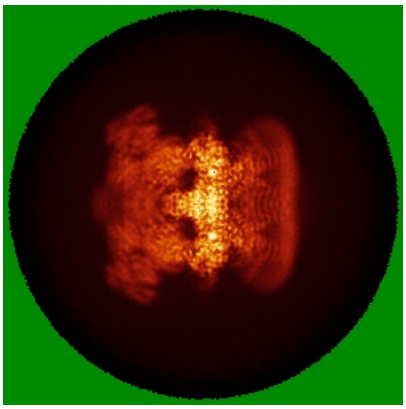

Z Index: 157

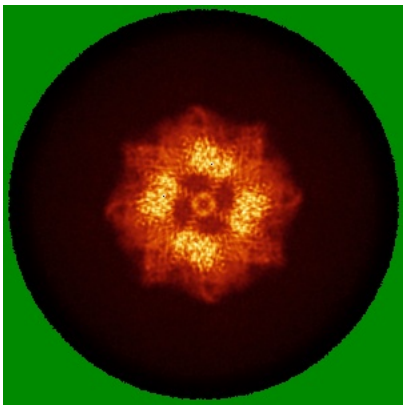
The images above show the largest variance slices of the map in three orthogonal directions.

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

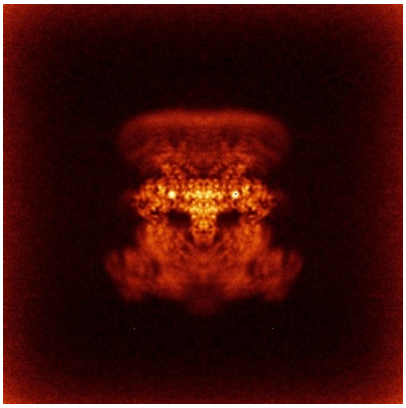
6.4.1 Primary map

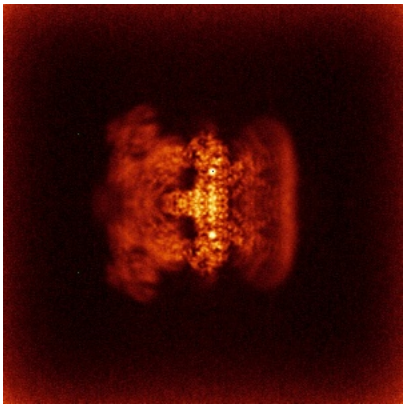

X

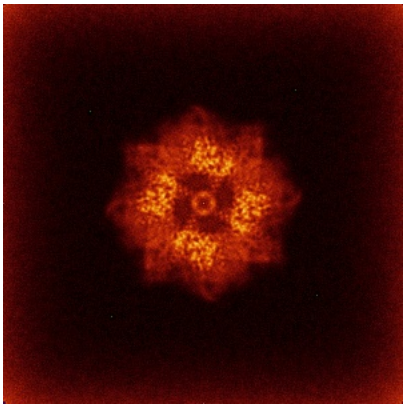

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.246. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

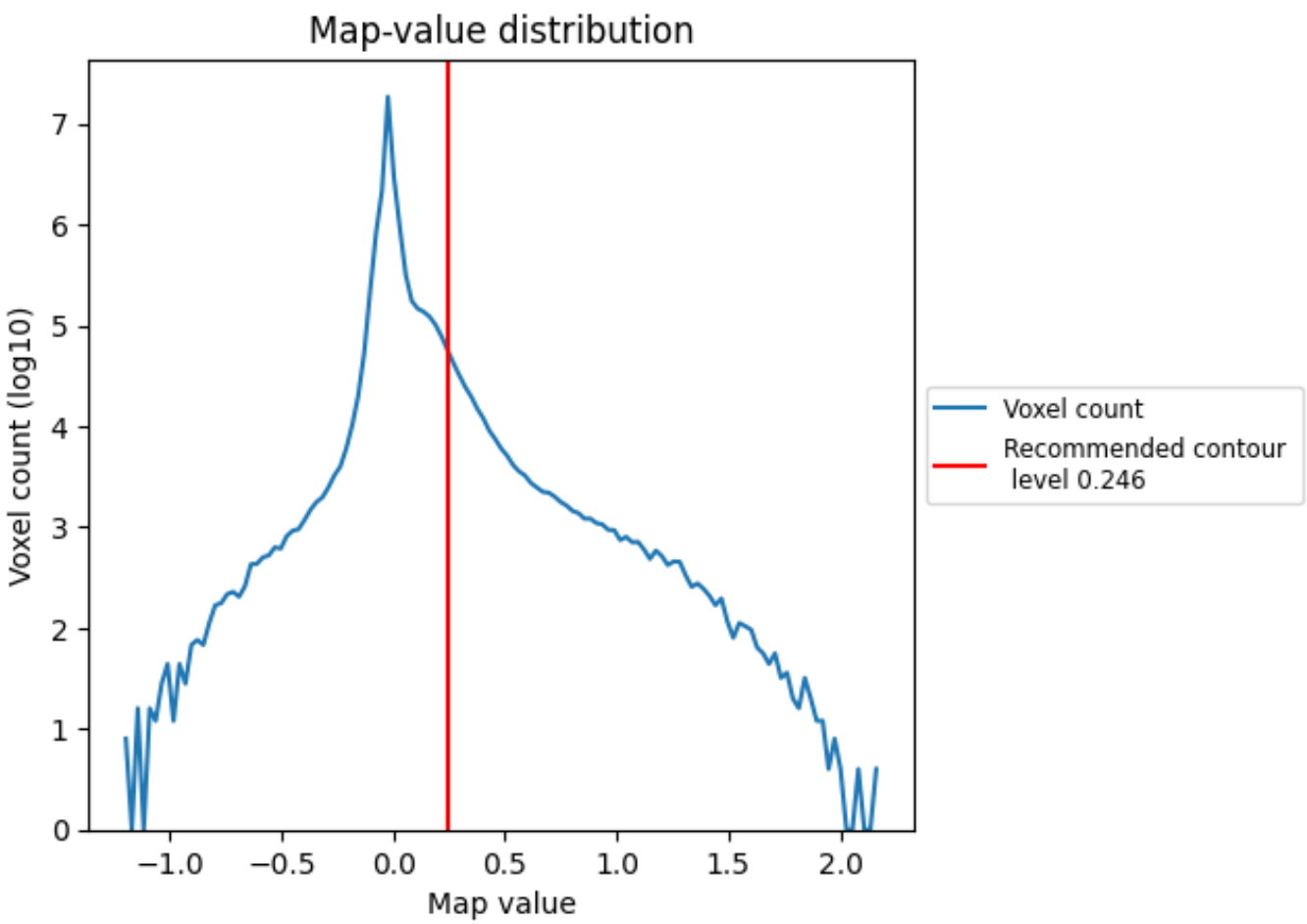
6.6 Mask visualisation (i)

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

7 Map analysis (i)

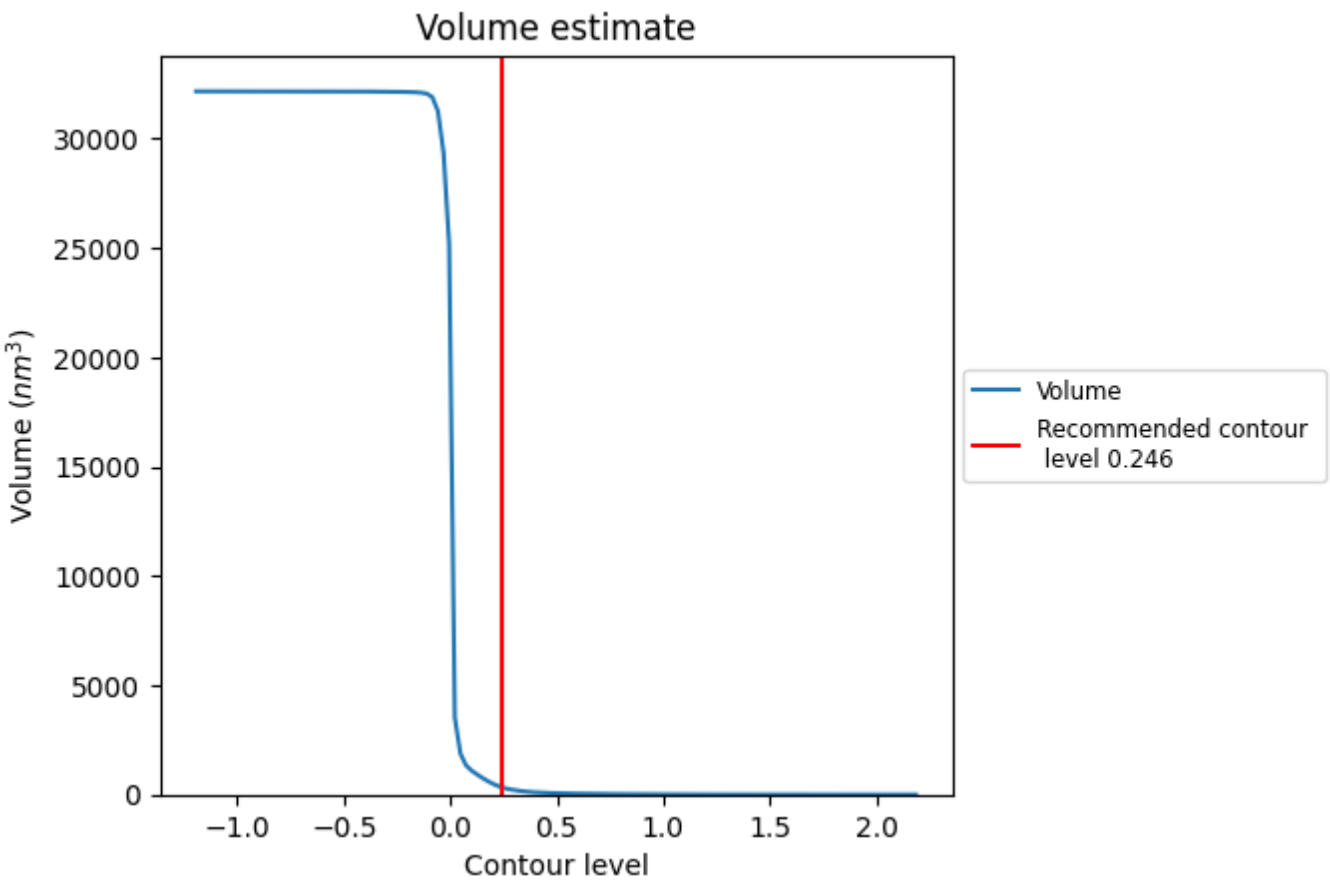
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

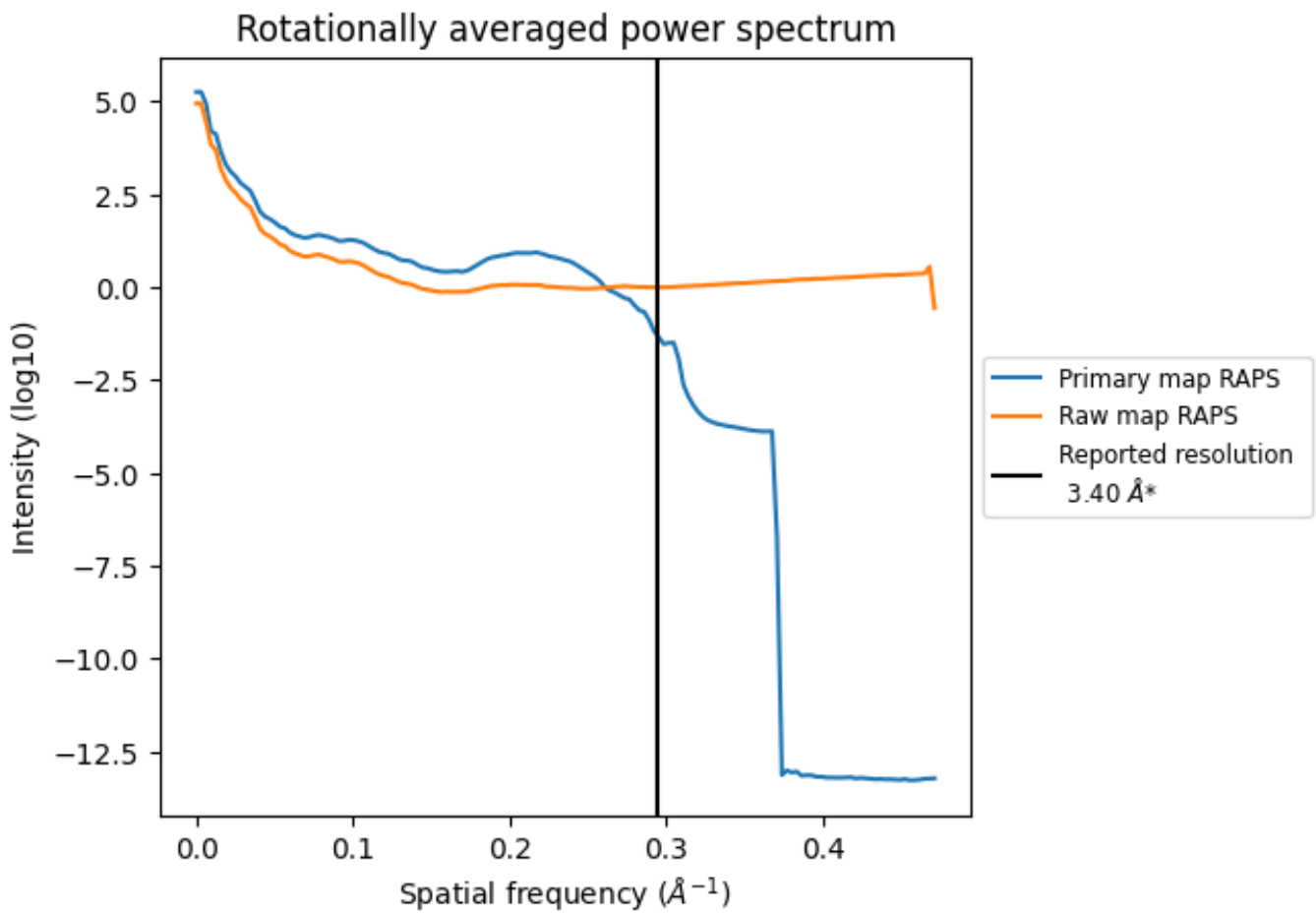
7.2 Volume estimate (i)



The volume at the recommended contour level is 322 nm^3; this corresponds to an approximate mass of 291 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)

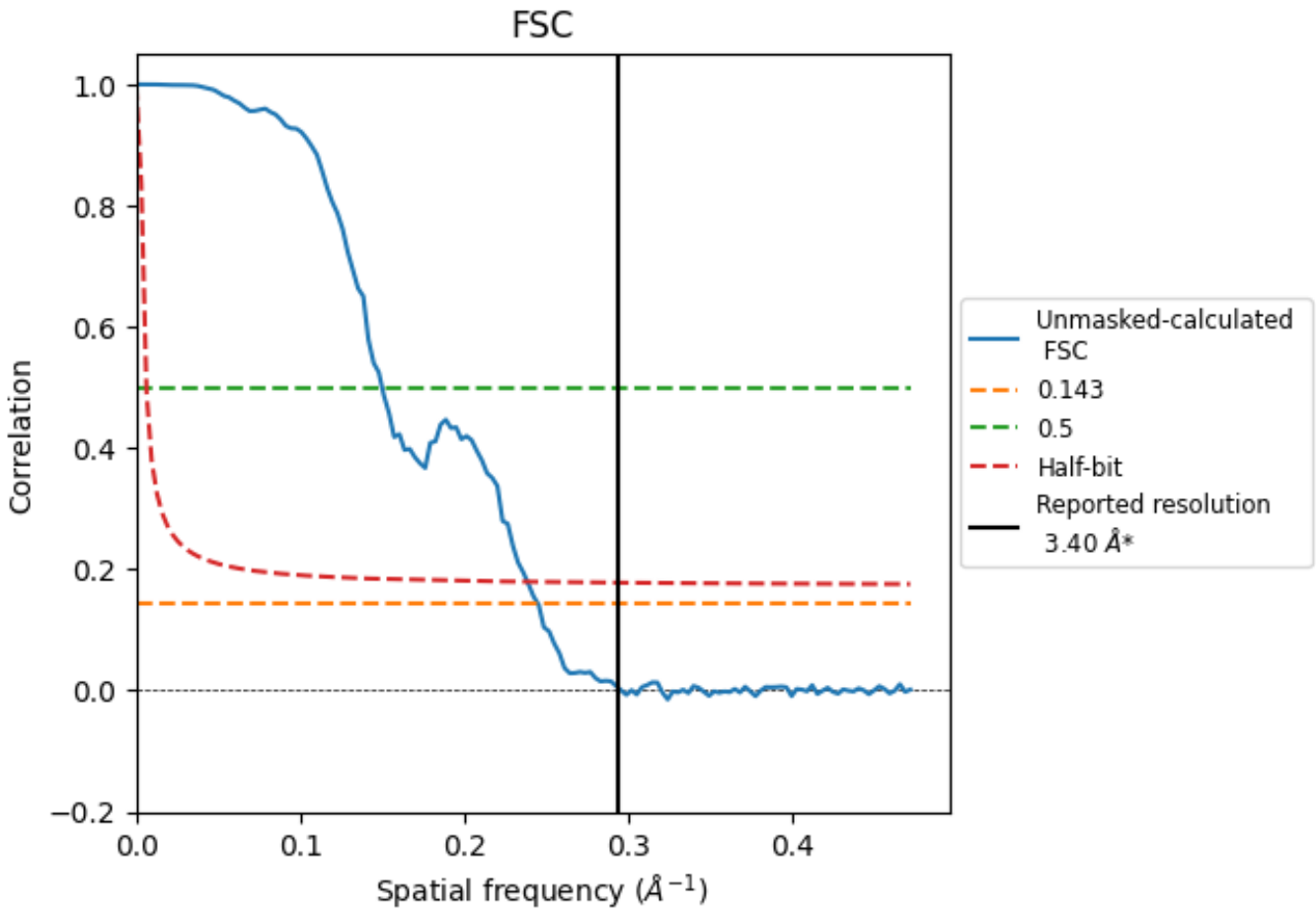


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

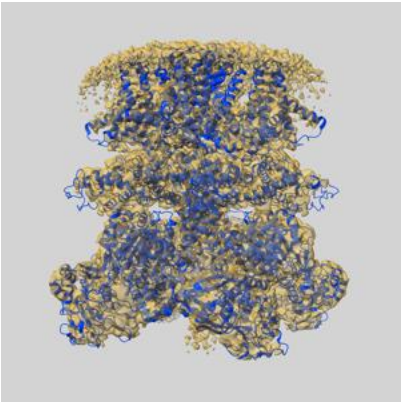
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.08	6.67	4.19

*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 4.08 differs from the reported value 3.4 by more than 10 %

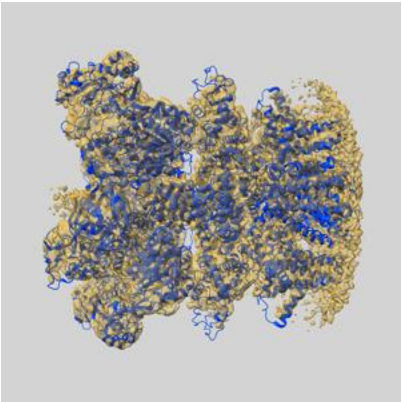
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-27922 and PDB model 8E6Q. Per-residue inclusion information can be found in section 3 on page 5.

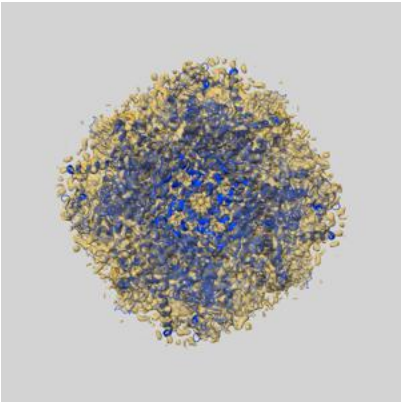
9.1 Map-model overlay (i)



X



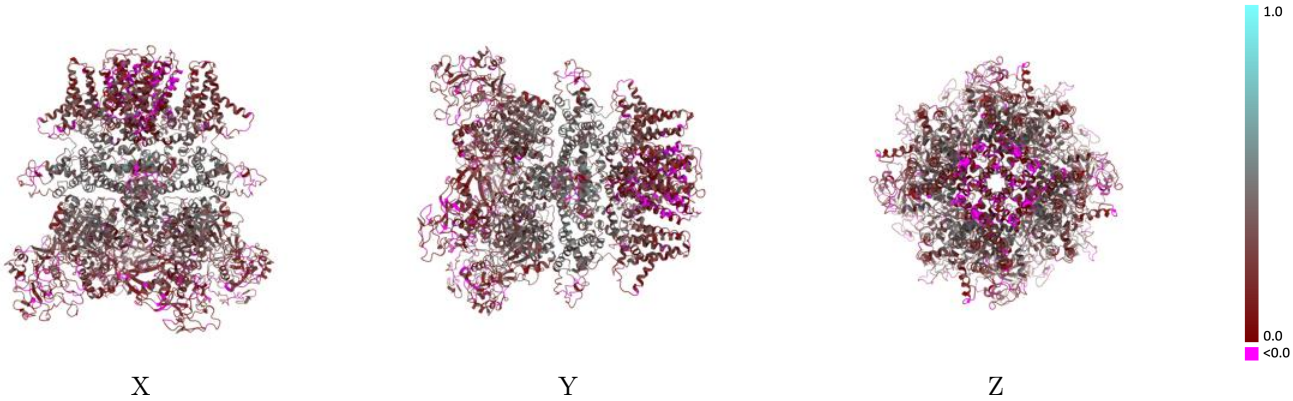
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.246 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)

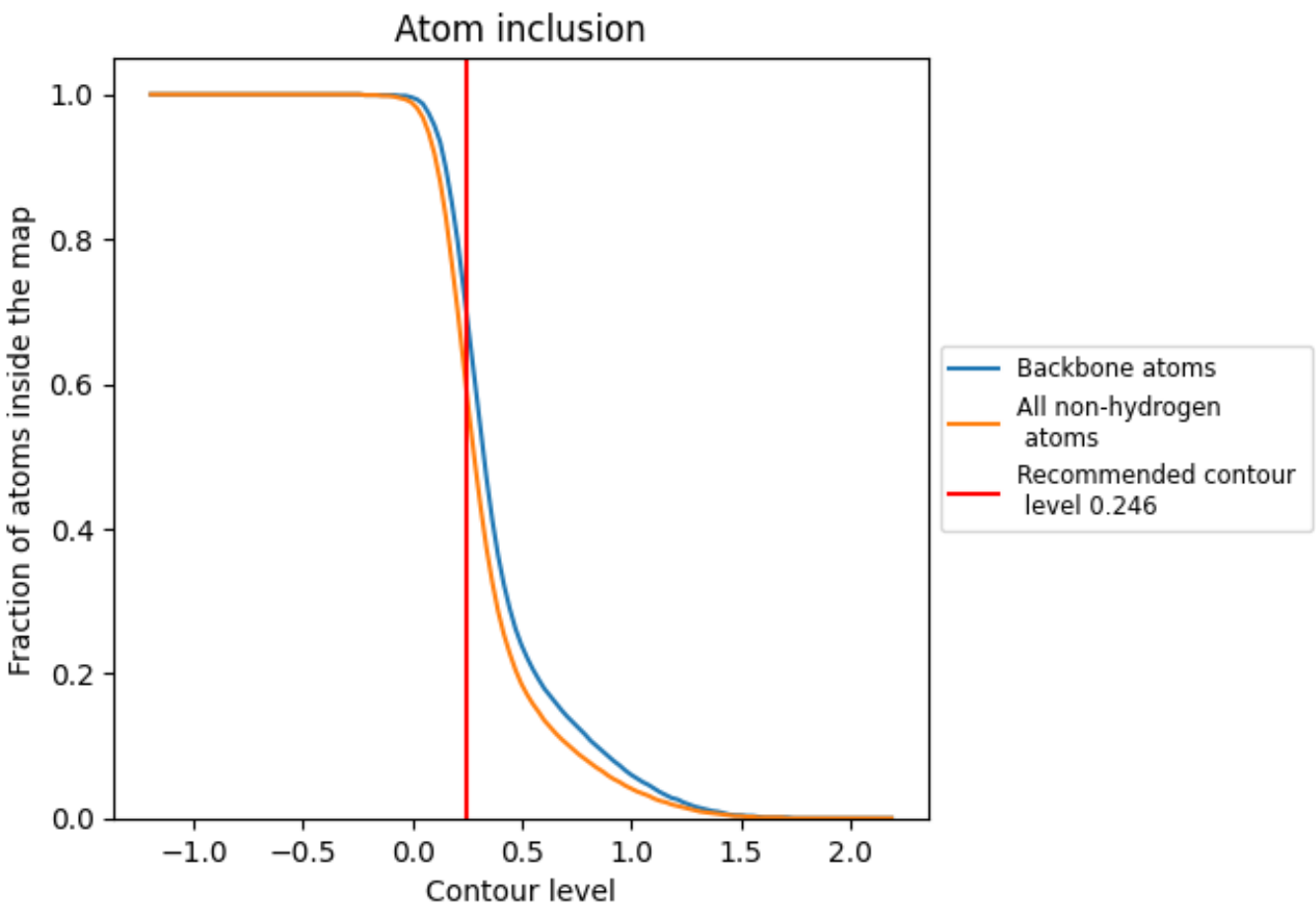


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 59% 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 (0.246) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5930	0.2510
A	0.6030	0.2580
B	0.5890	0.2480
C	0.5910	0.2470
D	0.5900	0.2520