wwPDB EM Validation Summary Report

Jan 22, 2022 – 06:03 am GMT

PDB ID	:	7O4H
EMDB ID	:	EMD-12718
Title	:	The structure of the native CNGA1/CNGB1 CNG channel from retinal rods
Authors	:	Barret, D.C.A.; Marino, J.
Deposited on	:	2021-04-06
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 following versions of software and data (see references (1)) were used in the production of this report:

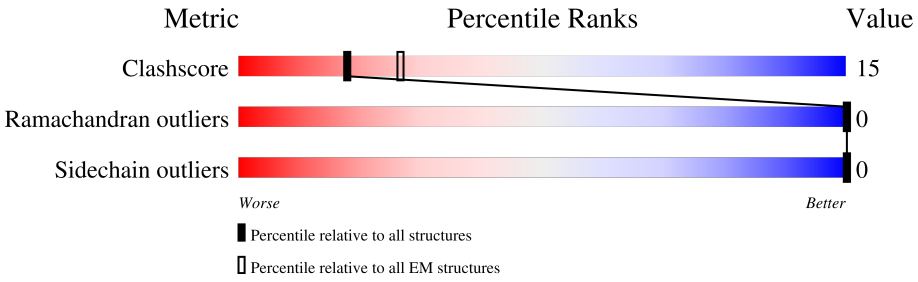
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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)
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	690	10% 47% 20% 33%
1	B	690	46% 22% 32%
1	C	690	48% 19% 33%
2	D	1394	11% 17% 11% 73%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14195 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 cGMP-gated cation channel alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	465	Total	C	N	O	S	0	0
			3705	2416	592	679	18		
1	B	468	Total	C	N	O	S	0	0
			3765	2453	607	689	16		
1	C	464	Total	C	N	O	S	0	0
			3748	2445	608	678	17		

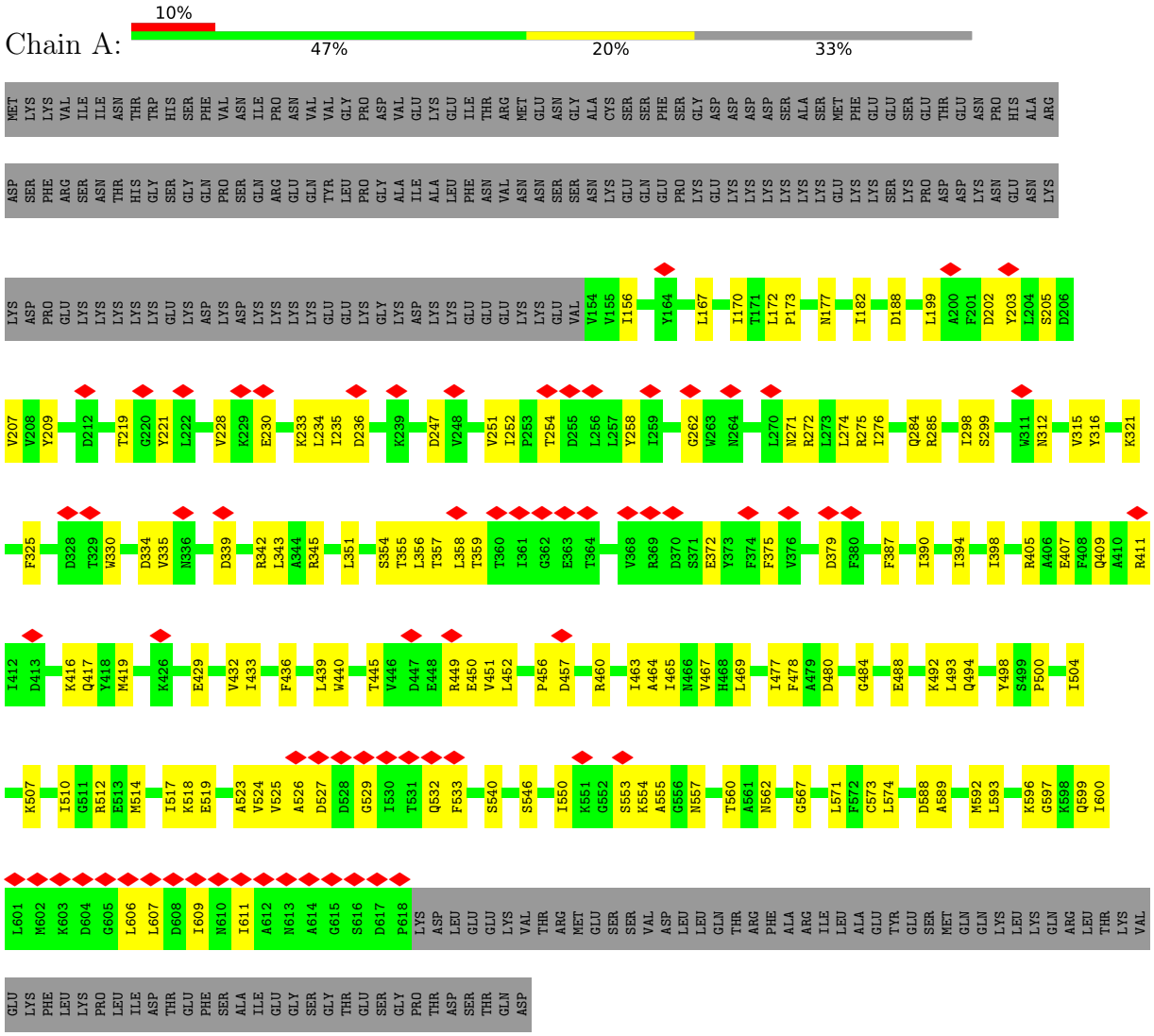
- Molecule 2 is a protein called Cyclic nucleotide-gated cation channel beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	383	Total	C	N	O	S	0	0
			2977	1932	506	526	13		

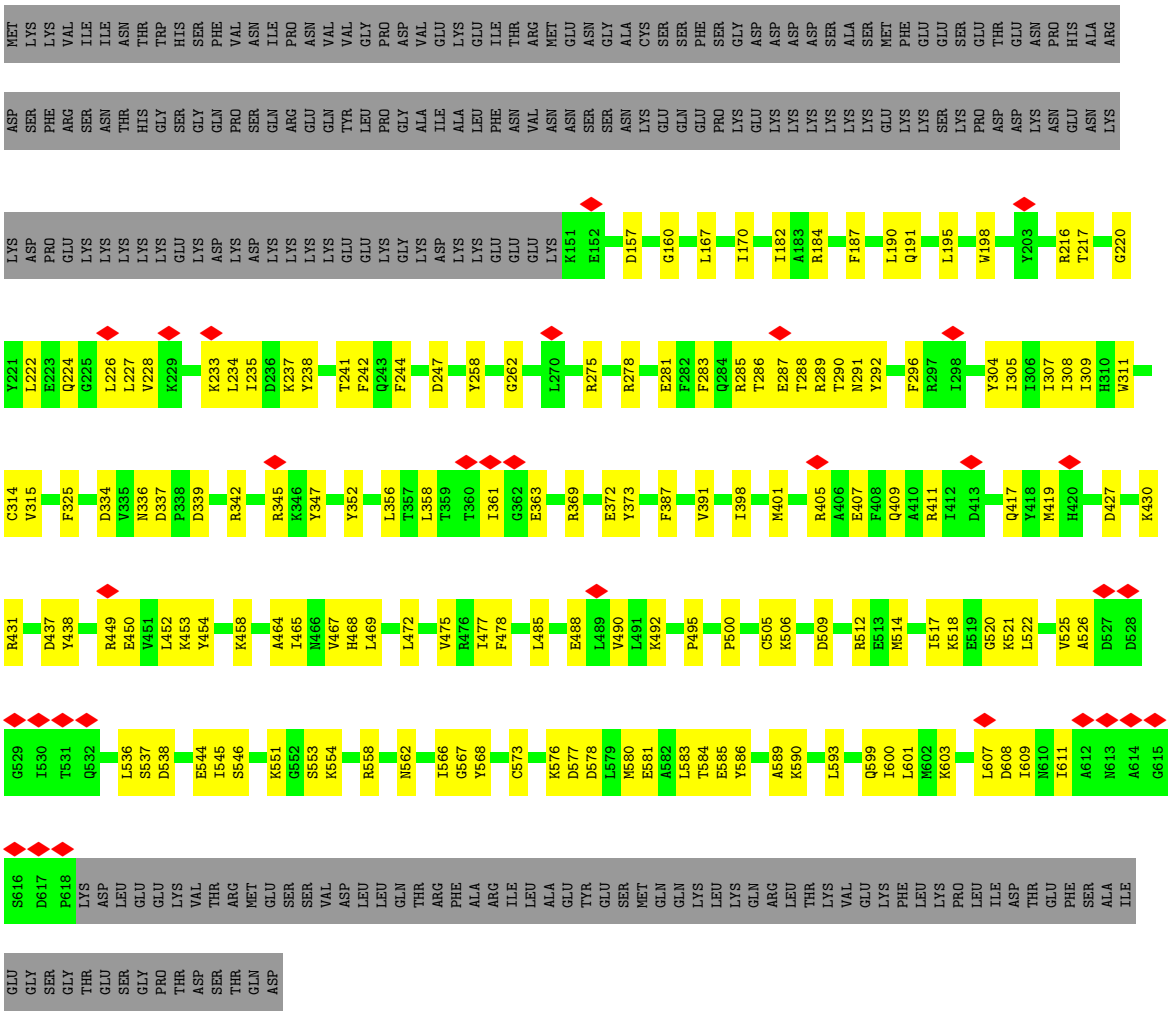
3 Residue-property plots (i)

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: cGMP-gated cation channel alpha-1

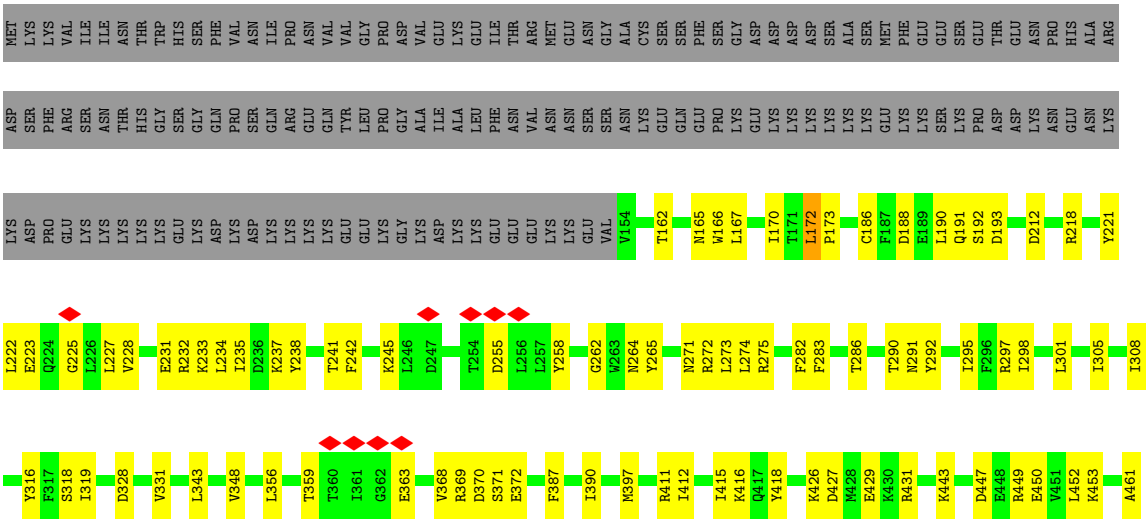


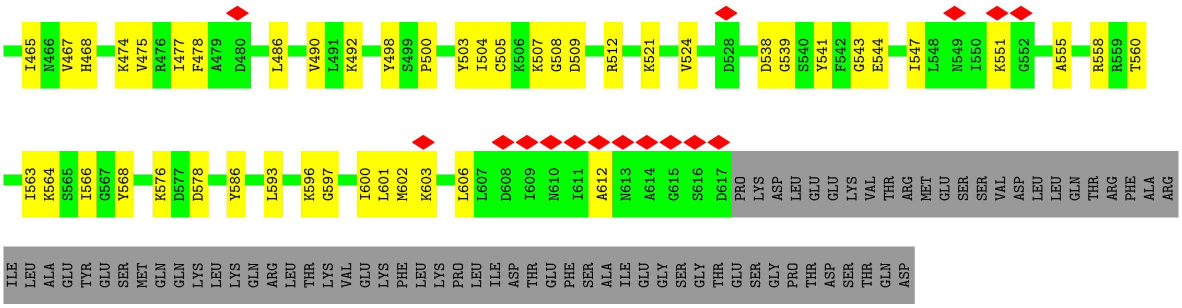
• Molecule 1: cGMP-gated cation channel alpha-1



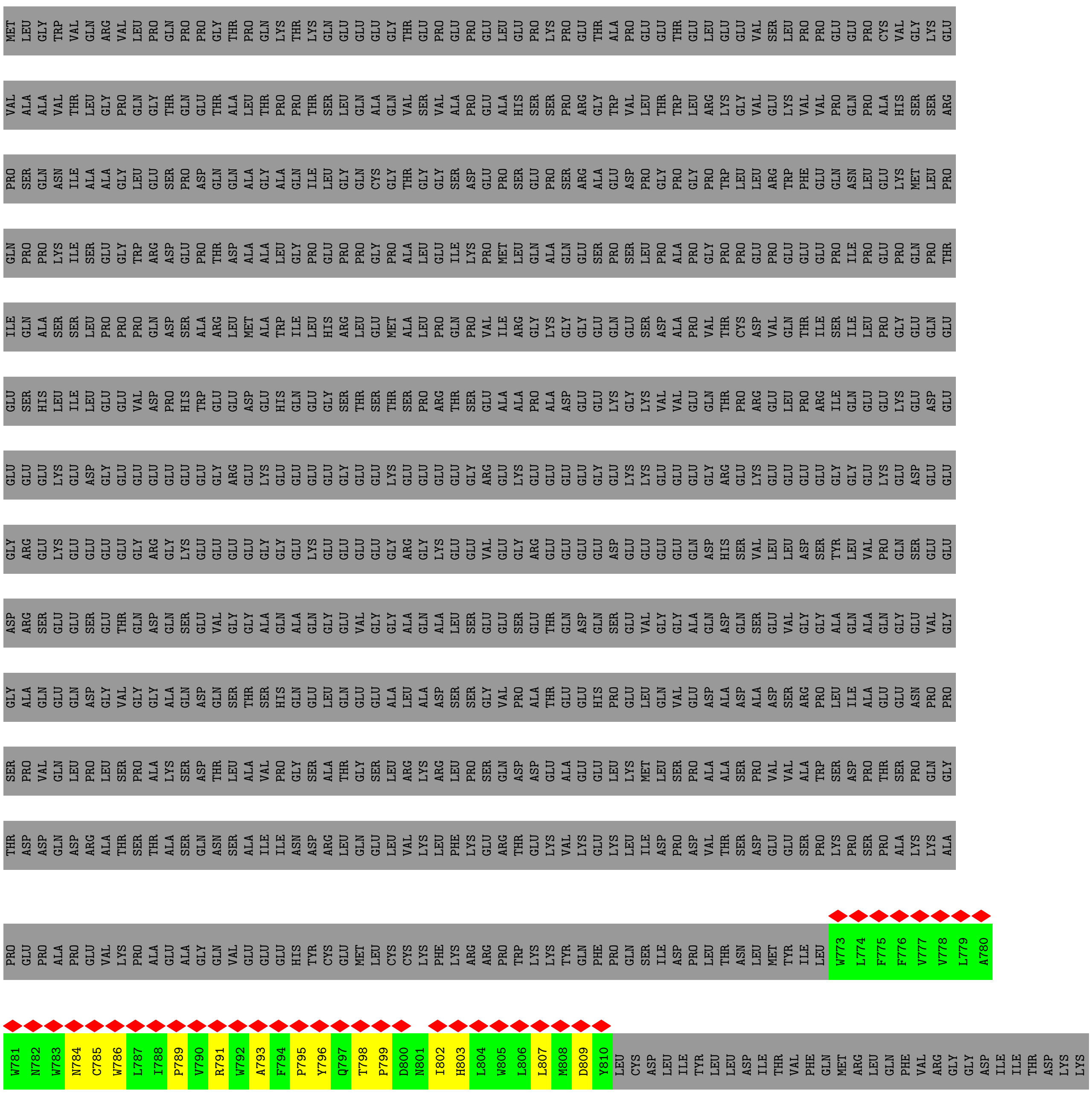
• Molecule 1: cGMP-gated cation channel alpha-1

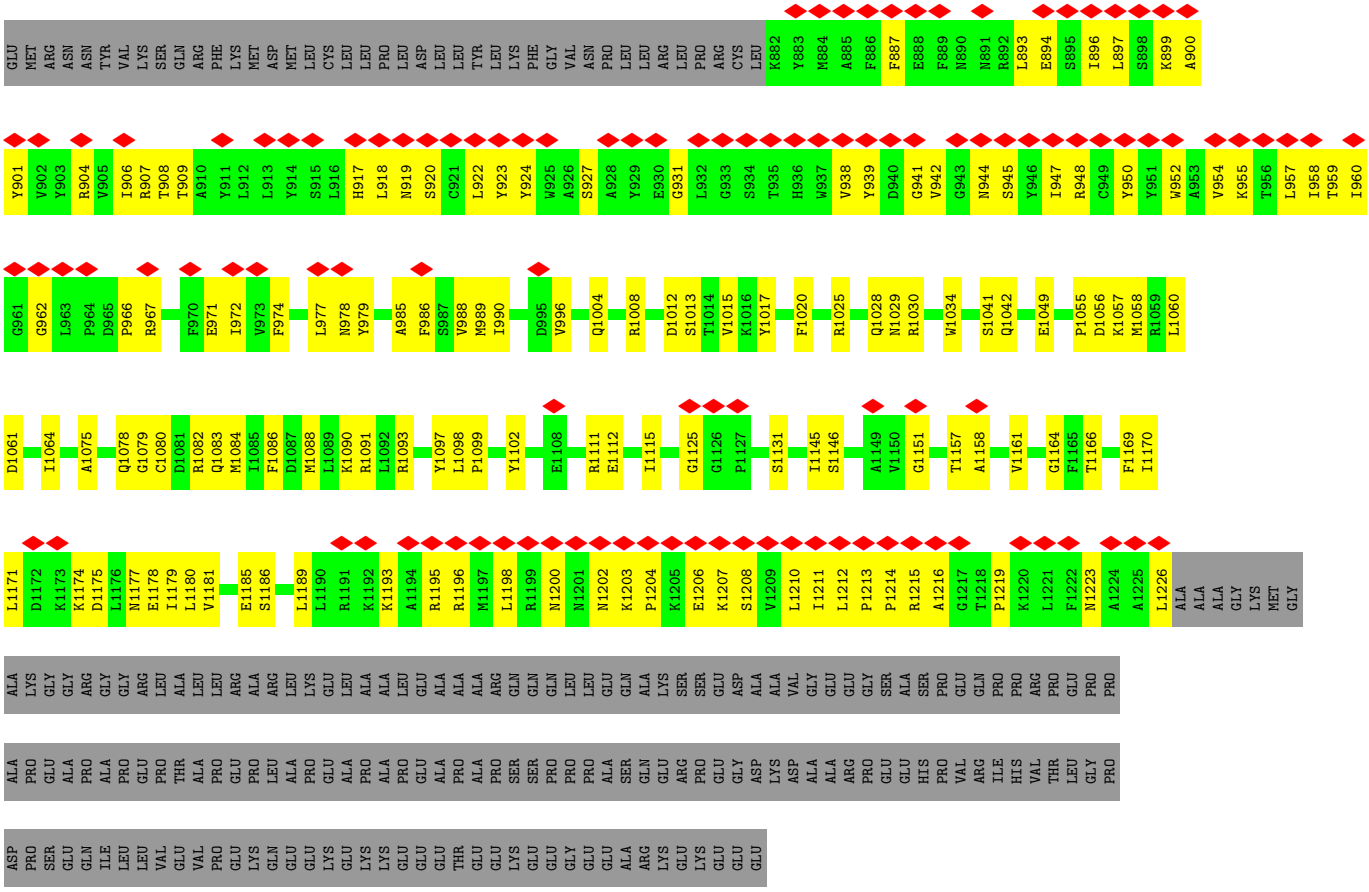
Chain C:





• Molecule 2: Cyclic nucleotide-gated cation channel beta-1




GLU MET ARG ASN ASN TYR VAL LYS SER GLN ARG PHE LYS MET ASP MET LEU CYS LEU LEU LEU PRO LEU ASP LEU LEU TYR LEU LYS PHE GLY VAL ASN PRO LEU LEU ARG LEU PRO ARG CYS LEU
K882 Y883 M884 A885 F886 F887 E888 F889 N890 N891 R892 L893 E894 S895 I896 L897 S898 K899 A900
Y901 V902 Y903 R904 V905 I906 R907 T908 T909 A910 Y911 L912 L913 Y914 S915 L916 H917 L918 N919 S920 C921 L922 Y923 Y924 W925 A926 S927 A928 Y929 E930 G931 L932 G933 S934 T935 H936 W937 V938 Y939 D940 G941 V942 G943 N944 S945 Y946 I947 R948 C949 Y950 Y951 W952 A953 V954 K955 T956 L957 I958 T959 I960
G961 G962 L963 P964 D965 P966 R967 F970 E971 I972 V973 F974 L977 N978 Y979 A985 F986 S987 V988 M989 I990 D995 V996 Q1004 R1008 D1012 S1013 T1014 V1015 K1016 Y1017 F1020 R1025 Q1028 N1029 R1030 W1034 S1041 Q1042 E1049 P1055 D1056 K1057 M1058 R1059 L1060
D1061 I1064 A1075 Q1078 G1079 C1080 D1081 R1082 Q1083 M1084 I1085 F1086 D1087 M1088 L1089 K1090 R1091 L1092 R1093 Y1097 L1098 P1099 Y1102 E1108 R1111 E1112 I1115 G1125 G1126 P1127 S1131 I1145 S1146 A1149 V1150 G1151 T1157 A1158 V1161 G1164 F1165 T1166 F1169 I1170
L1171 D1172 K1173 K1174 D1175 L1176 N1177 E1178 I1179 L1180 V1181 E1185 S1186 L1189 L1190 R1191 K1192 K1193 A1194 R1195 R1196 M1197 L1198 R1199 N1200 N1201 N1202 K1203 P1204 K1205 E1206 K1207 S1208 V1209 L1210 I1211 L1212 P1213 P1214 R1215 A1216 G1217 T1218 P1219 K1220 L1221 F1222 N1223 A1224 A1225 L1226
ALA ALA ALA GLY LYS MET GLY
ALA LYS GLY GLY ARG GLY GLY ARG LEU ALA LEU LEU ARG ALA ARG LEU LYS GLU LEU ALA ALA LEU GLU GLU ALA ALA ALA ARG GLN GLN GLN LEU LEU GLU GLN ALA LYS SER SER GLU ASP ALA ALA VAL GLY GLU GLU GLY SER ALA SER PRO GLU GLN PRO PRO ARG PRO GLU PRO PRO
ALA PRO GLU ALA PRO ALA PRO GLU PRO THR ALA PRO GLU PRO LEU ALA PRO GLU ALA PRO ALA PRO SER SER PRO PRO PRO ALA SER GLN GLU ARG PRO GLU GLY ASP LYS ASP ALA ALA ARG PRO GLU GLU HIS PRO VAL ARG ILE HIS VAL THR LEU GLY PRO
ASP PRO SER GLU GLN ILE LEU LEU VAL GLU VAL PRO GLU LYS GLN GLU GLU LYS GLU LYS LYS GLU GLU GLU THR GLU GLU LYS GLU GLU GLY GLU GLU ALA ARG LYS GLU LYS GLU GLU GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118084	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 ($e^-/Å^2$)	1.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.242	Depositor
Minimum map value	-0.122	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.051	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.33	0/3790	0.53	0/5152
1	B	0.35	0/3850	0.51	0/5222
1	C	0.36	0/3834	0.52	1/5197 (0.0%)
2	D	0.31	0/3052	0.51	0/4158
All	All	0.34	0/14526	0.52	1/19729 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	172	LEU	CA-CB-CG	5.25	127.37	115.30

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	3705	0	3648	99	0
1	B	3765	0	3751	119	0
1	C	3748	0	3752	98	0
2	D	2977	0	2872	119	0
All	All	14195	0	14023	420	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 15.

The worst 5 of 420 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)
2:D:1004:GLN:HB3	2:D:1008:ARG:HH12	1.41	0.83
1:C:512:ARG:HH12	1:C:576:LYS:H	1.27	0.82
1:B:554:LYS:HG3	1:B:607:LEU:HG	1.63	0.79
1:C:368:VAL:N	1:C:372:GLU:OE2	2.16	0.78
1:A:512:ARG:NH2	1:A:546:SER:O	2.17	0.78

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	463/690 (67%)	393 (85%)	70 (15%)	0	100	100
1	B	466/690 (68%)	410 (88%)	56 (12%)	0	100	100
1	C	462/690 (67%)	403 (87%)	59 (13%)	0	100	100
2	D	379/1394 (27%)	311 (82%)	68 (18%)	0	100	100
All	All	1770/3464 (51%)	1517 (86%)	253 (14%)	0	100	100

There are no Ramachandran outliers to report.

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	393/621 (63%)	393 (100%)	0	100	100
1	B	404/621 (65%)	404 (100%)	0	100	100
1	C	403/621 (65%)	403 (100%)	0	100	100
2	D	299/1185 (25%)	299 (100%)	0	100	100
All	All	1499/3048 (49%)	1499 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	417	GLN
1	B	599	GLN
2	D	1200	ASN
1	A	532	GLN
1	A	177	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)

There are no ligands in this entry.

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.

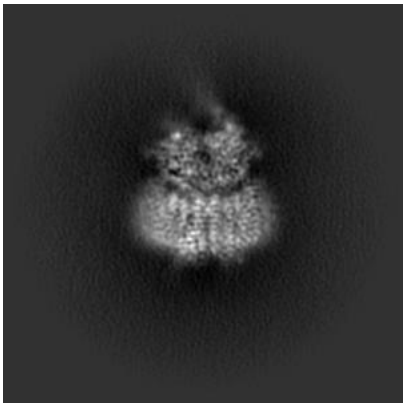
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12718. These allow visual inspection of the internal detail of the map and identification of artifacts.

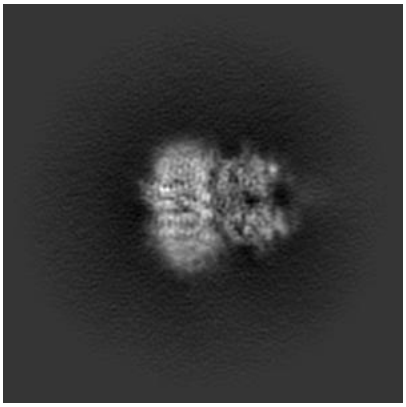
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

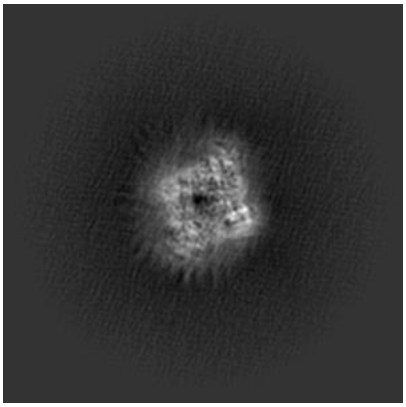
6.1.1 Primary map



X



Y

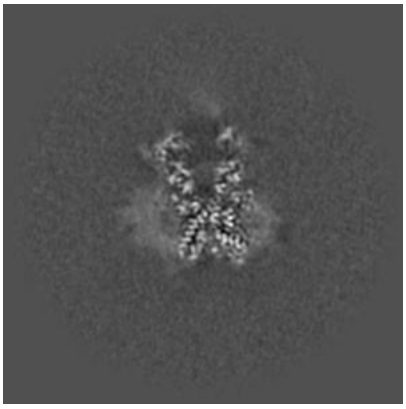


Z

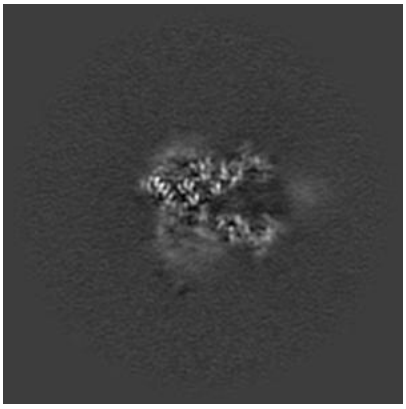
The images above show the map projected in three orthogonal directions.

6.2 Central slices

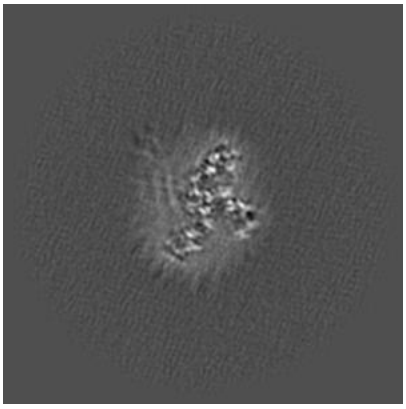
6.2.1 Primary map



X Index: 150



Y Index: 150

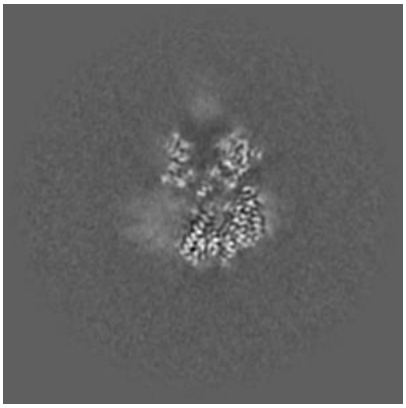


Z Index: 150

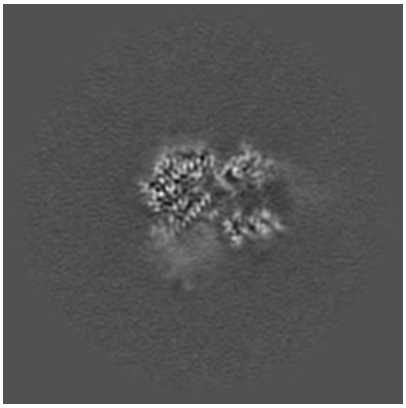
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

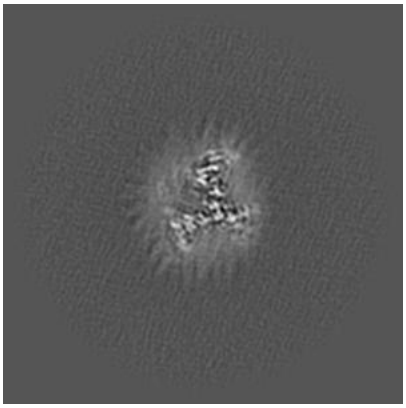
6.3.1 Primary map



X Index: 160



Y Index: 143



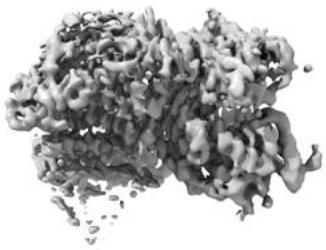
Z Index: 122

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

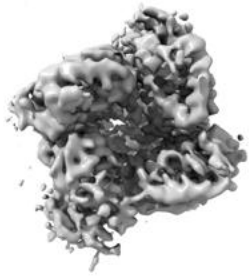
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.051. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

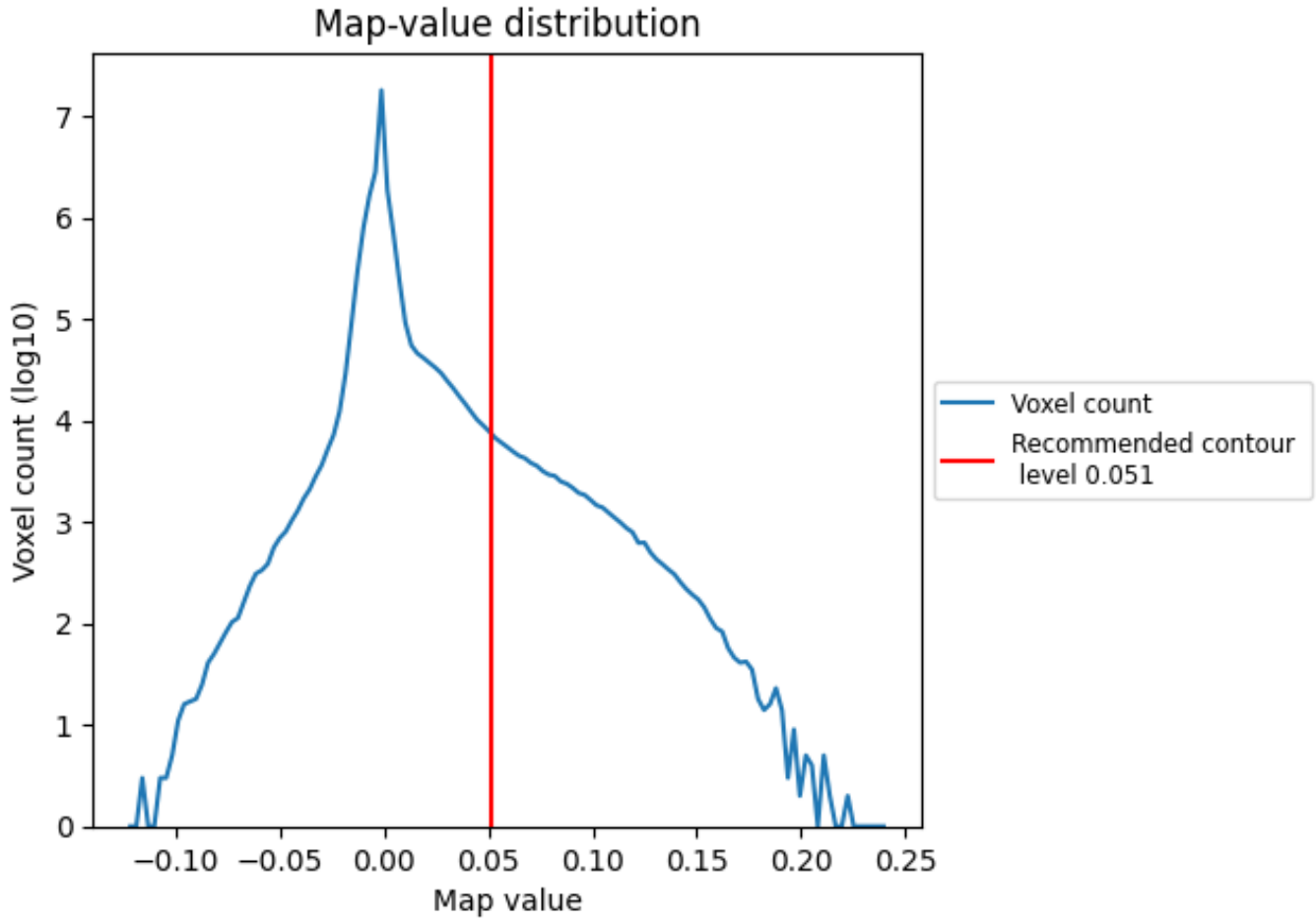
6.5 Mask visualisation (i)

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

7 Map analysis

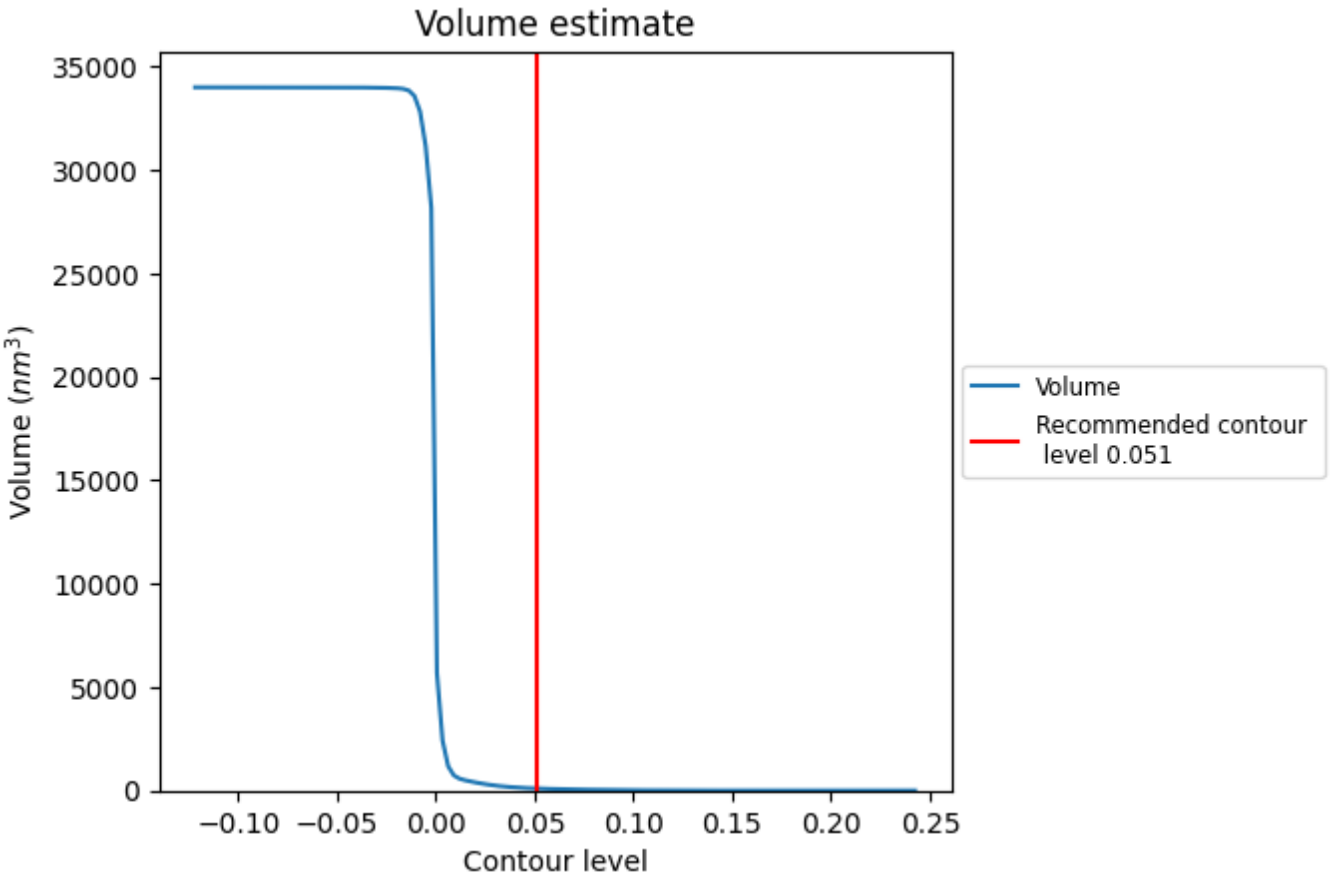
This section contains the results of statistical analysis of the map.

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.

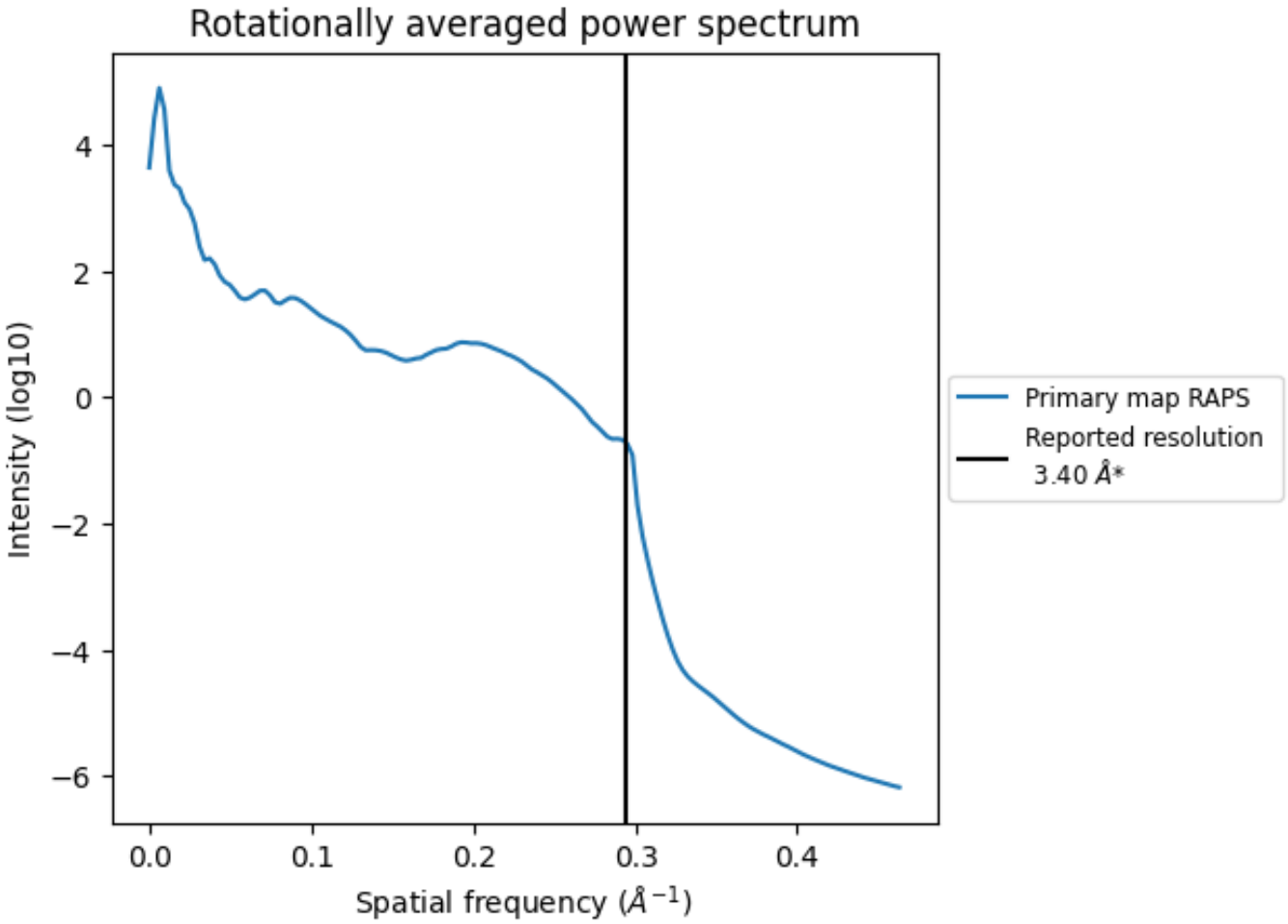
7.2 Volume estimate (i)



The volume at the recommended contour level is 100 nm^3; this corresponds to an approximate mass of 90 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}

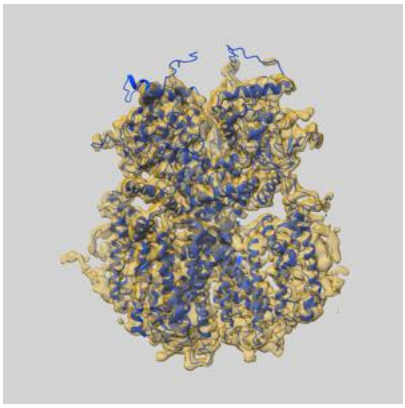
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

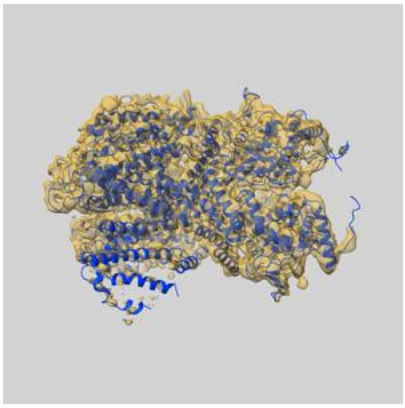
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12718 and PDB model 7O4H. Per-residue inclusion information can be found in section 3 on page 4.

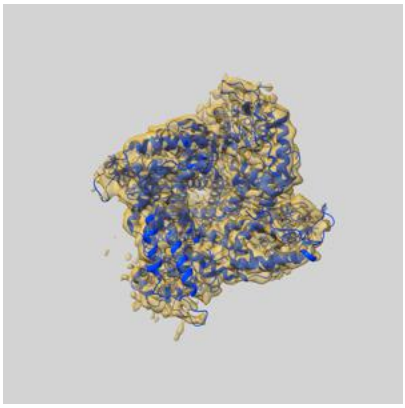
9.1 Map-model overlay



X



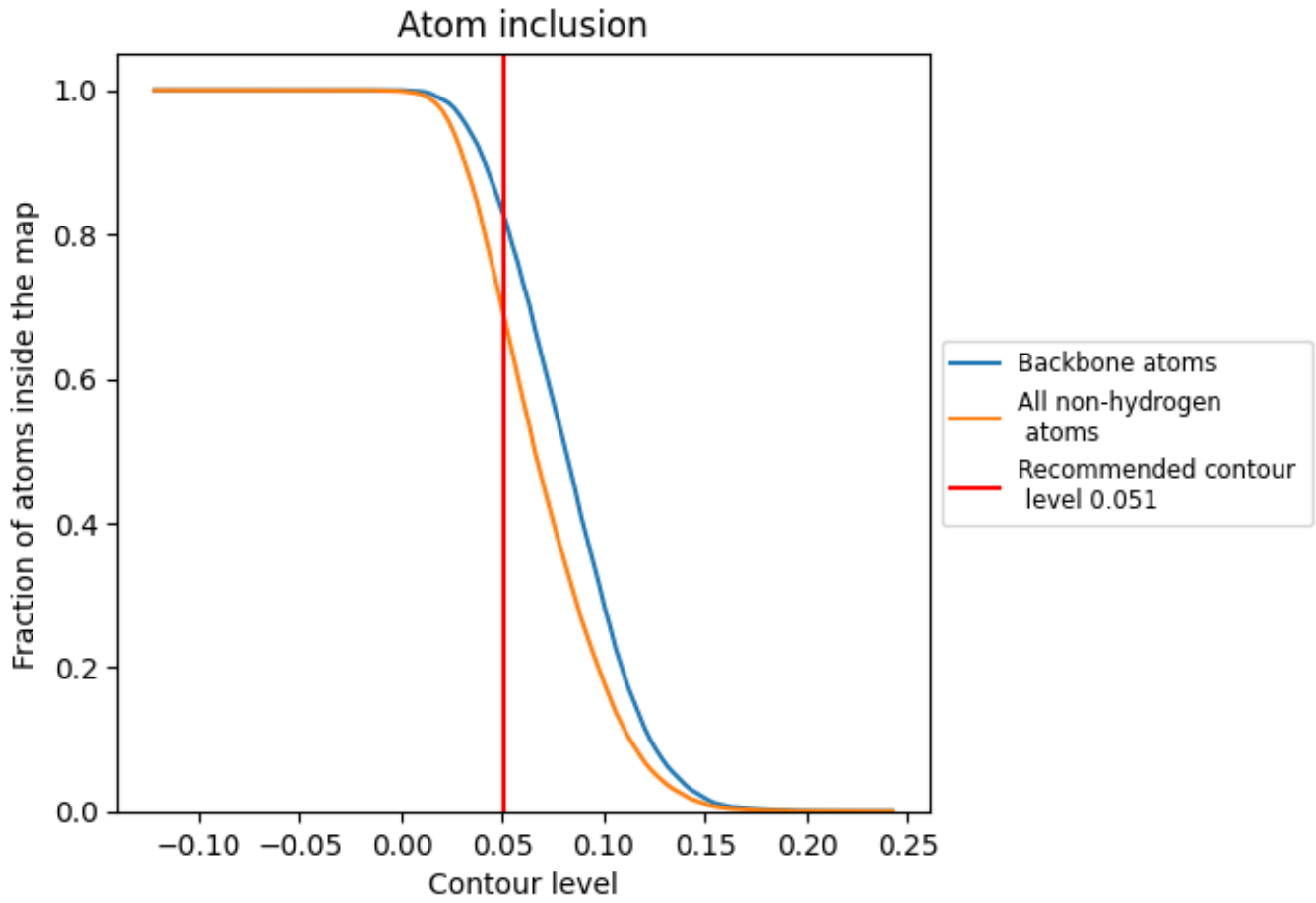
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.051 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.