Full wwPDB EM Validation Report

Nov 6, 2022 – 07:30 AM EST

PDB ID	:	6BCL
EMDB ID	:	EMD-7082
Title	:	cryo-EM structure of TRPM4 in apo state with long coiled coil at 3.5 angstrom resolution
Authors	:	Guo, J.; She, J.; Chen, Q.; Bai, X.; Jiang, Y.
Deposited on	:	2017-10-20
Resolution	:	3.54 Å(reported)

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

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

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

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

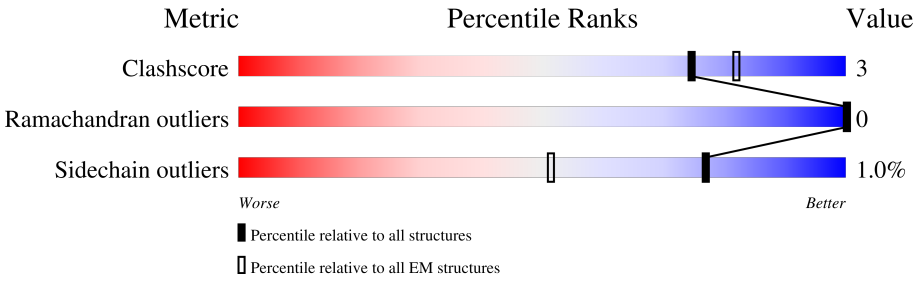
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.54 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	1254	30% 70% 7% 23%
1	B	1254	30% 70% 7% 23%
1	C	1254	30% 70% 7% 23%
1	D	1254	30% 70% 7% 23%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 30474 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 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	967	Total	C	N	O	S	0	0
			7618	4907	1335	1342	34		
1	A	967	Total	C	N	O	S	0	0
			7618	4907	1335	1342	34		
1	C	967	Total	C	N	O	S	0	0
			7618	4907	1335	1342	34		
1	D	967	Total	C	N	O	S	0	0
			7618	4907	1335	1342	34		

There are 164 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1214	ARG	-	expression tag	UNP Q7TN37
B	1215	ASN	-	expression tag	UNP Q7TN37
B	1216	SER	-	expression tag	UNP Q7TN37
B	1217	LYS	-	expression tag	UNP Q7TN37
B	1218	ALA	-	expression tag	UNP Q7TN37
B	1219	TYR	-	expression tag	UNP Q7TN37
B	1220	VAL	-	expression tag	UNP Q7TN37
B	1221	ASP	-	expression tag	UNP Q7TN37
B	1222	GLU	-	expression tag	UNP Q7TN37
B	1223	LEU	-	expression tag	UNP Q7TN37
B	1224	THR	-	expression tag	UNP Q7TN37
B	1225	SER	-	expression tag	UNP Q7TN37
B	1226	ARG	-	expression tag	UNP Q7TN37
B	1227	GLY	-	expression tag	UNP Q7TN37
B	1228	ARG	-	expression tag	UNP Q7TN37
B	1229	LEU	-	expression tag	UNP Q7TN37
B	1230	GLU	-	expression tag	UNP Q7TN37
B	1231	VAL	-	expression tag	UNP Q7TN37
B	1232	LEU	-	expression tag	UNP Q7TN37
B	1233	PHE	-	expression tag	UNP Q7TN37
B	1234	GLN	-	expression tag	UNP Q7TN37

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1235	GLY	-	expression tag	UNP Q7TN37
B	1236	PRO	-	expression tag	UNP Q7TN37
B	1237	ASP	-	expression tag	UNP Q7TN37
B	1238	TYR	-	expression tag	UNP Q7TN37
B	1239	LYS	-	expression tag	UNP Q7TN37
B	1240	ASP	-	expression tag	UNP Q7TN37
B	1241	ASP	-	expression tag	UNP Q7TN37
B	1242	ASP	-	expression tag	UNP Q7TN37
B	1243	ASP	-	expression tag	UNP Q7TN37
B	1244	LYS	-	expression tag	UNP Q7TN37
B	1245	HIS	-	expression tag	UNP Q7TN37
B	1246	HIS	-	expression tag	UNP Q7TN37
B	1247	HIS	-	expression tag	UNP Q7TN37
B	1248	HIS	-	expression tag	UNP Q7TN37
B	1249	HIS	-	expression tag	UNP Q7TN37
B	1250	HIS	-	expression tag	UNP Q7TN37
B	1251	HIS	-	expression tag	UNP Q7TN37
B	1252	HIS	-	expression tag	UNP Q7TN37
B	1253	HIS	-	expression tag	UNP Q7TN37
B	1254	HIS	-	expression tag	UNP Q7TN37
A	1214	ARG	-	expression tag	UNP Q7TN37
A	1215	ASN	-	expression tag	UNP Q7TN37
A	1216	SER	-	expression tag	UNP Q7TN37
A	1217	LYS	-	expression tag	UNP Q7TN37
A	1218	ALA	-	expression tag	UNP Q7TN37
A	1219	TYR	-	expression tag	UNP Q7TN37
A	1220	VAL	-	expression tag	UNP Q7TN37
A	1221	ASP	-	expression tag	UNP Q7TN37
A	1222	GLU	-	expression tag	UNP Q7TN37
A	1223	LEU	-	expression tag	UNP Q7TN37
A	1224	THR	-	expression tag	UNP Q7TN37
A	1225	SER	-	expression tag	UNP Q7TN37
A	1226	ARG	-	expression tag	UNP Q7TN37
A	1227	GLY	-	expression tag	UNP Q7TN37
A	1228	ARG	-	expression tag	UNP Q7TN37
A	1229	LEU	-	expression tag	UNP Q7TN37
A	1230	GLU	-	expression tag	UNP Q7TN37
A	1231	VAL	-	expression tag	UNP Q7TN37
A	1232	LEU	-	expression tag	UNP Q7TN37
A	1233	PHE	-	expression tag	UNP Q7TN37
A	1234	GLN	-	expression tag	UNP Q7TN37
A	1235	GLY	-	expression tag	UNP Q7TN37

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1236	PRO	-	expression tag	UNP Q7TN37
A	1237	ASP	-	expression tag	UNP Q7TN37
A	1238	TYR	-	expression tag	UNP Q7TN37
A	1239	LYS	-	expression tag	UNP Q7TN37
A	1240	ASP	-	expression tag	UNP Q7TN37
A	1241	ASP	-	expression tag	UNP Q7TN37
A	1242	ASP	-	expression tag	UNP Q7TN37
A	1243	ASP	-	expression tag	UNP Q7TN37
A	1244	LYS	-	expression tag	UNP Q7TN37
A	1245	HIS	-	expression tag	UNP Q7TN37
A	1246	HIS	-	expression tag	UNP Q7TN37
A	1247	HIS	-	expression tag	UNP Q7TN37
A	1248	HIS	-	expression tag	UNP Q7TN37
A	1249	HIS	-	expression tag	UNP Q7TN37
A	1250	HIS	-	expression tag	UNP Q7TN37
A	1251	HIS	-	expression tag	UNP Q7TN37
A	1252	HIS	-	expression tag	UNP Q7TN37
A	1253	HIS	-	expression tag	UNP Q7TN37
A	1254	HIS	-	expression tag	UNP Q7TN37
C	1214	ARG	-	expression tag	UNP Q7TN37
C	1215	ASN	-	expression tag	UNP Q7TN37
C	1216	SER	-	expression tag	UNP Q7TN37
C	1217	LYS	-	expression tag	UNP Q7TN37
C	1218	ALA	-	expression tag	UNP Q7TN37
C	1219	TYR	-	expression tag	UNP Q7TN37
C	1220	VAL	-	expression tag	UNP Q7TN37
C	1221	ASP	-	expression tag	UNP Q7TN37
C	1222	GLU	-	expression tag	UNP Q7TN37
C	1223	LEU	-	expression tag	UNP Q7TN37
C	1224	THR	-	expression tag	UNP Q7TN37
C	1225	SER	-	expression tag	UNP Q7TN37
C	1226	ARG	-	expression tag	UNP Q7TN37
C	1227	GLY	-	expression tag	UNP Q7TN37
C	1228	ARG	-	expression tag	UNP Q7TN37
C	1229	LEU	-	expression tag	UNP Q7TN37
C	1230	GLU	-	expression tag	UNP Q7TN37
C	1231	VAL	-	expression tag	UNP Q7TN37
C	1232	LEU	-	expression tag	UNP Q7TN37
C	1233	PHE	-	expression tag	UNP Q7TN37
C	1234	GLN	-	expression tag	UNP Q7TN37
C	1235	GLY	-	expression tag	UNP Q7TN37
C	1236	PRO	-	expression tag	UNP Q7TN37

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1237	ASP	-	expression tag	UNP Q7TN37
C	1238	TYR	-	expression tag	UNP Q7TN37
C	1239	LYS	-	expression tag	UNP Q7TN37
C	1240	ASP	-	expression tag	UNP Q7TN37
C	1241	ASP	-	expression tag	UNP Q7TN37
C	1242	ASP	-	expression tag	UNP Q7TN37
C	1243	ASP	-	expression tag	UNP Q7TN37
C	1244	LYS	-	expression tag	UNP Q7TN37
C	1245	HIS	-	expression tag	UNP Q7TN37
C	1246	HIS	-	expression tag	UNP Q7TN37
C	1247	HIS	-	expression tag	UNP Q7TN37
C	1248	HIS	-	expression tag	UNP Q7TN37
C	1249	HIS	-	expression tag	UNP Q7TN37
C	1250	HIS	-	expression tag	UNP Q7TN37
C	1251	HIS	-	expression tag	UNP Q7TN37
C	1252	HIS	-	expression tag	UNP Q7TN37
C	1253	HIS	-	expression tag	UNP Q7TN37
C	1254	HIS	-	expression tag	UNP Q7TN37
D	1214	ARG	-	expression tag	UNP Q7TN37
D	1215	ASN	-	expression tag	UNP Q7TN37
D	1216	SER	-	expression tag	UNP Q7TN37
D	1217	LYS	-	expression tag	UNP Q7TN37
D	1218	ALA	-	expression tag	UNP Q7TN37
D	1219	TYR	-	expression tag	UNP Q7TN37
D	1220	VAL	-	expression tag	UNP Q7TN37
D	1221	ASP	-	expression tag	UNP Q7TN37
D	1222	GLU	-	expression tag	UNP Q7TN37
D	1223	LEU	-	expression tag	UNP Q7TN37
D	1224	THR	-	expression tag	UNP Q7TN37
D	1225	SER	-	expression tag	UNP Q7TN37
D	1226	ARG	-	expression tag	UNP Q7TN37
D	1227	GLY	-	expression tag	UNP Q7TN37
D	1228	ARG	-	expression tag	UNP Q7TN37
D	1229	LEU	-	expression tag	UNP Q7TN37
D	1230	GLU	-	expression tag	UNP Q7TN37
D	1231	VAL	-	expression tag	UNP Q7TN37
D	1232	LEU	-	expression tag	UNP Q7TN37
D	1233	PHE	-	expression tag	UNP Q7TN37
D	1234	GLN	-	expression tag	UNP Q7TN37
D	1235	GLY	-	expression tag	UNP Q7TN37
D	1236	PRO	-	expression tag	UNP Q7TN37
D	1237	ASP	-	expression tag	UNP Q7TN37

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1238	TYR	-	expression tag	UNP Q7TN37
D	1239	LYS	-	expression tag	UNP Q7TN37
D	1240	ASP	-	expression tag	UNP Q7TN37
D	1241	ASP	-	expression tag	UNP Q7TN37
D	1242	ASP	-	expression tag	UNP Q7TN37
D	1243	ASP	-	expression tag	UNP Q7TN37
D	1244	LYS	-	expression tag	UNP Q7TN37
D	1245	HIS	-	expression tag	UNP Q7TN37
D	1246	HIS	-	expression tag	UNP Q7TN37
D	1247	HIS	-	expression tag	UNP Q7TN37
D	1248	HIS	-	expression tag	UNP Q7TN37
D	1249	HIS	-	expression tag	UNP Q7TN37
D	1250	HIS	-	expression tag	UNP Q7TN37
D	1251	HIS	-	expression tag	UNP Q7TN37
D	1252	HIS	-	expression tag	UNP Q7TN37
D	1253	HIS	-	expression tag	UNP Q7TN37
D	1254	HIS	-	expression tag	UNP Q7TN37

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

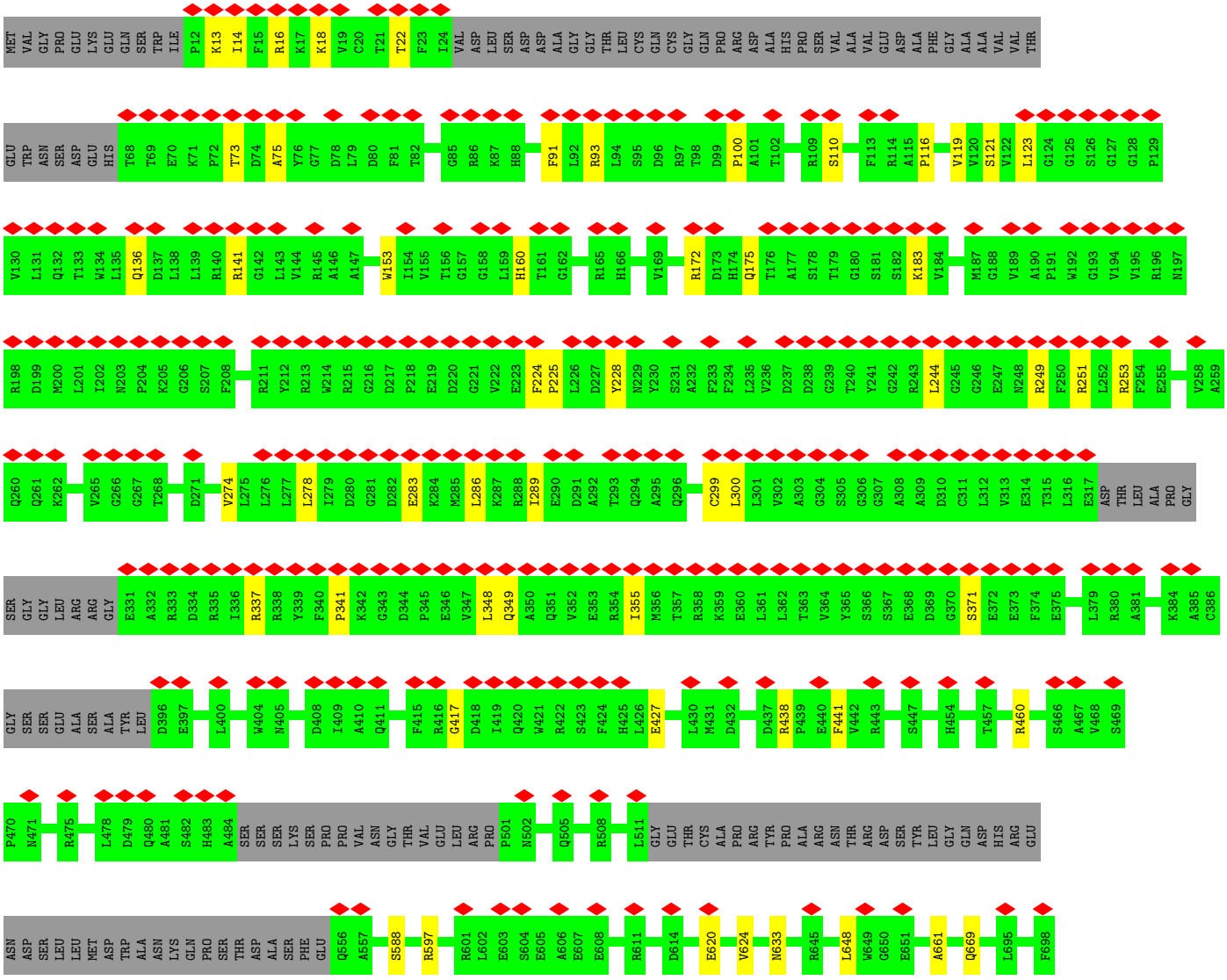
Mol	Chain	Residues	Atoms		AltConf
			Total	Na	
2	A	2	2	2	0

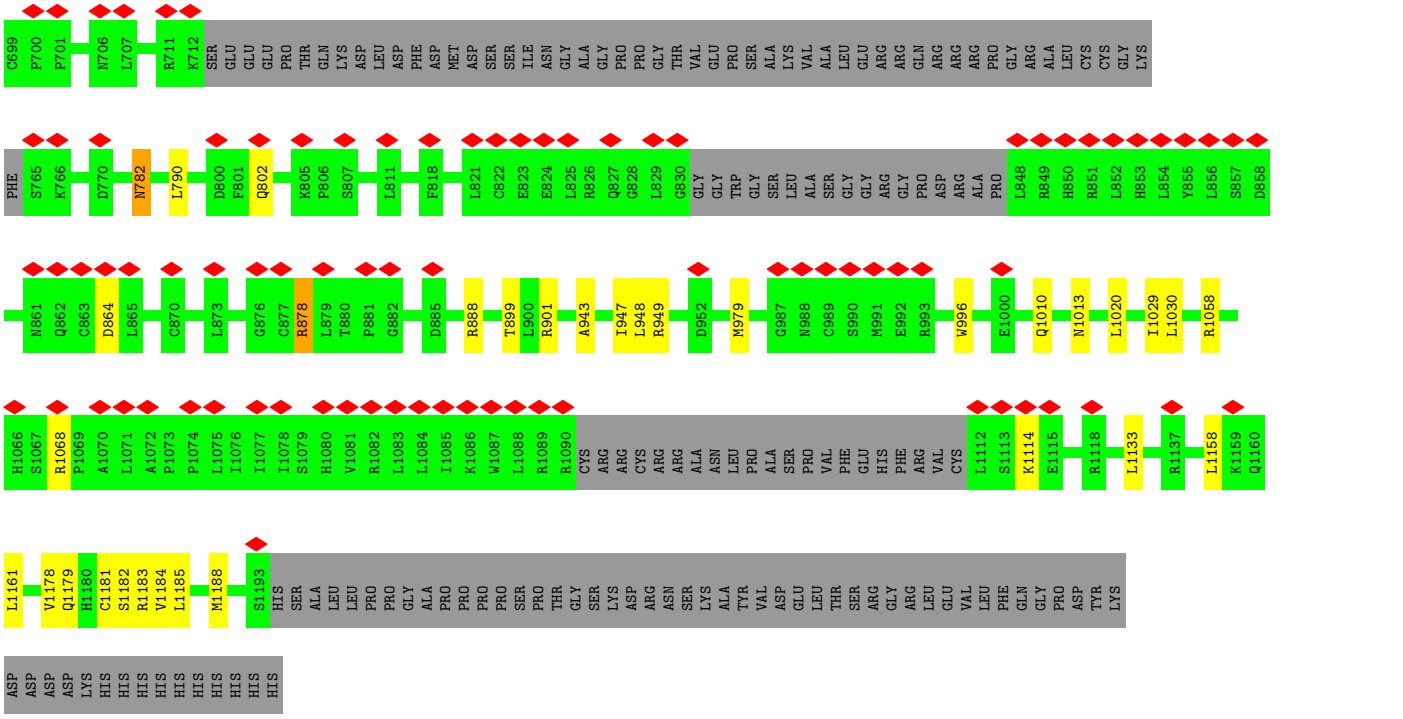
3 Residue-property plots (i)

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 4

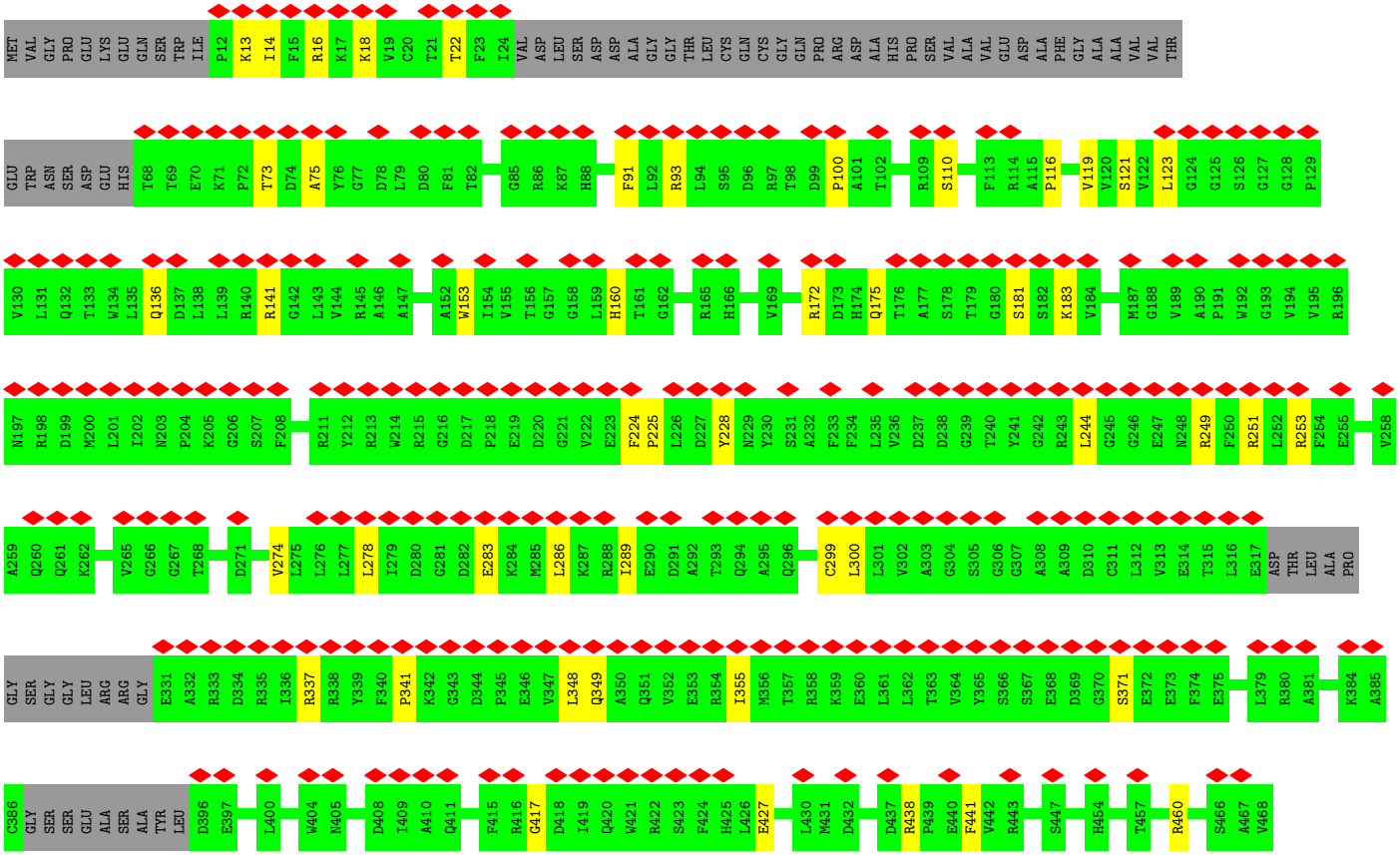
Chain B:

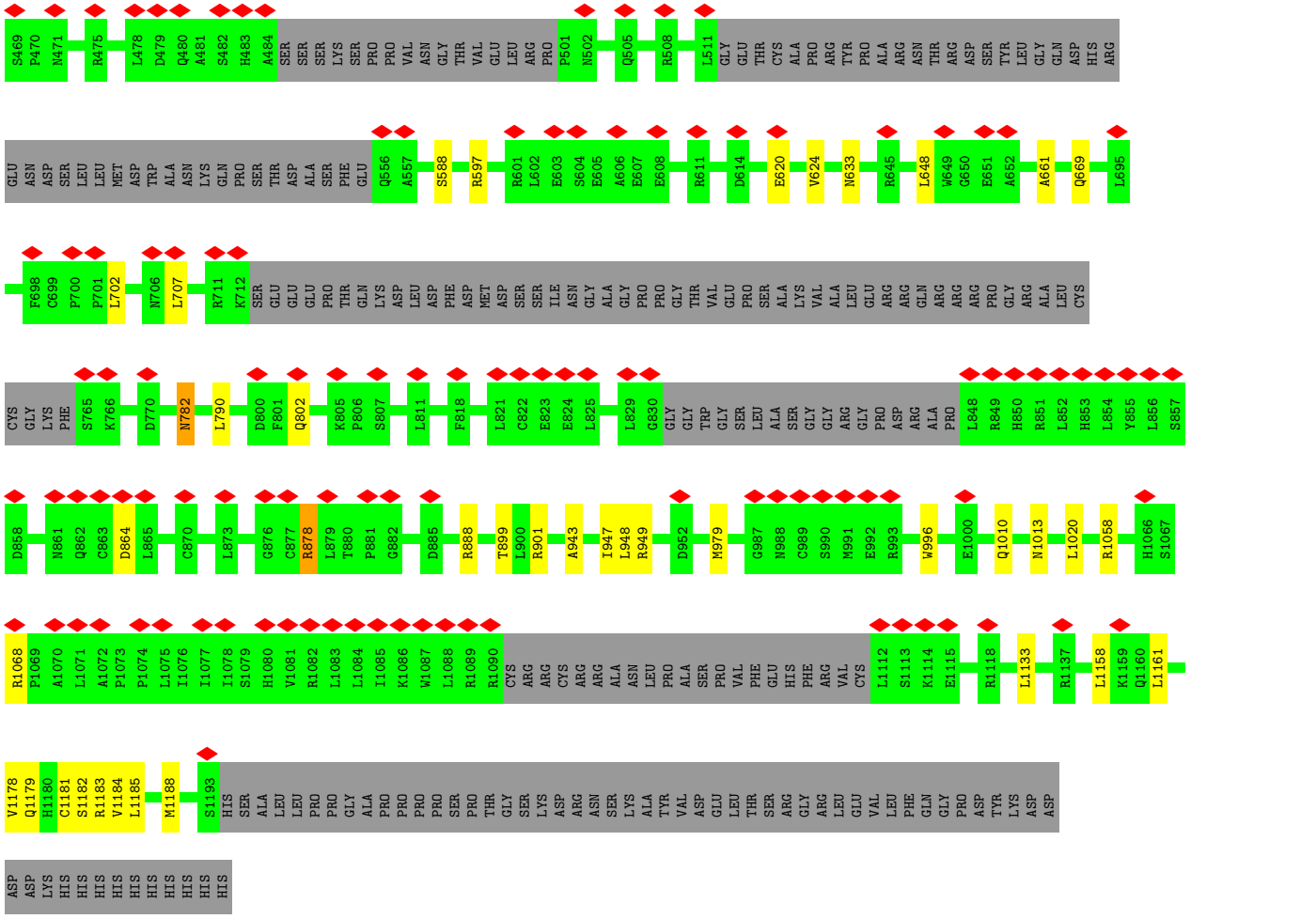




• Molecule 1: Transient receptor potential cation channel subfamily M member 4

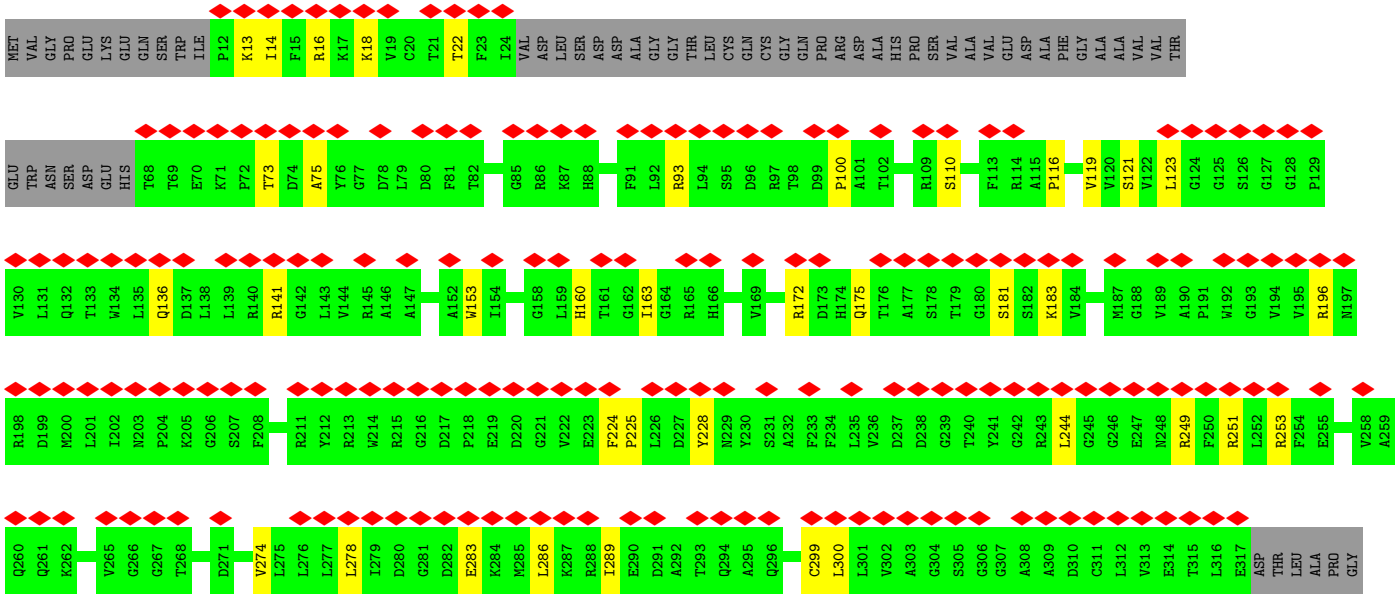
Chain A:

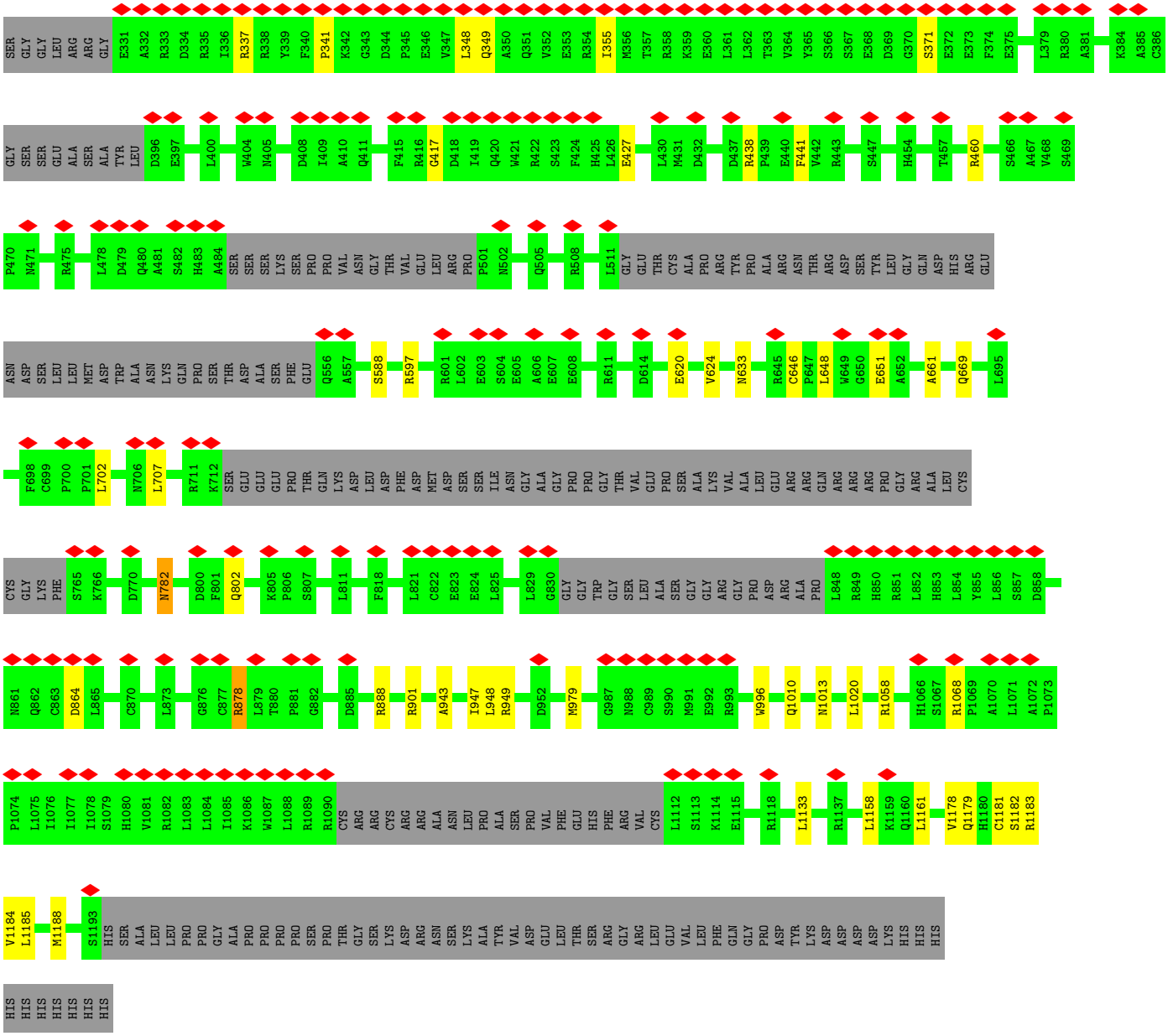




• Molecule 1: Transient receptor potential cation channel subfamily M member 4

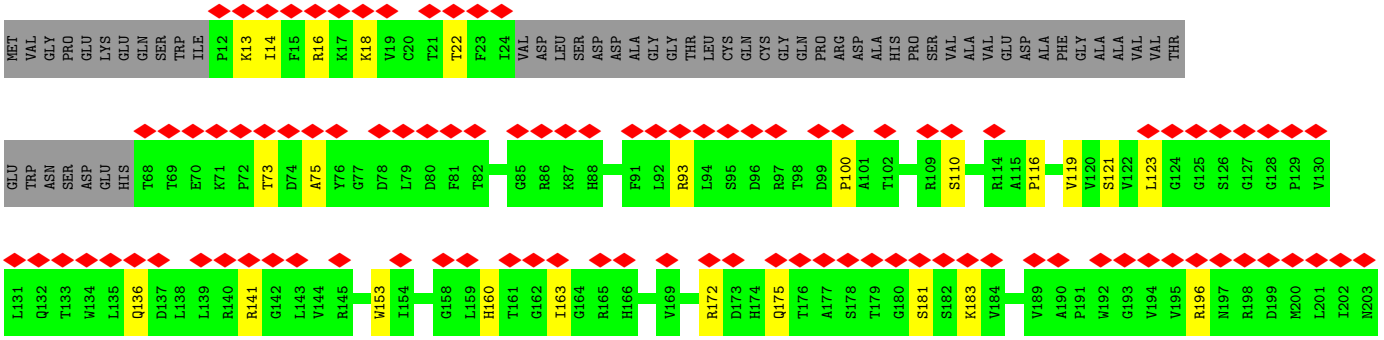
Chain C:

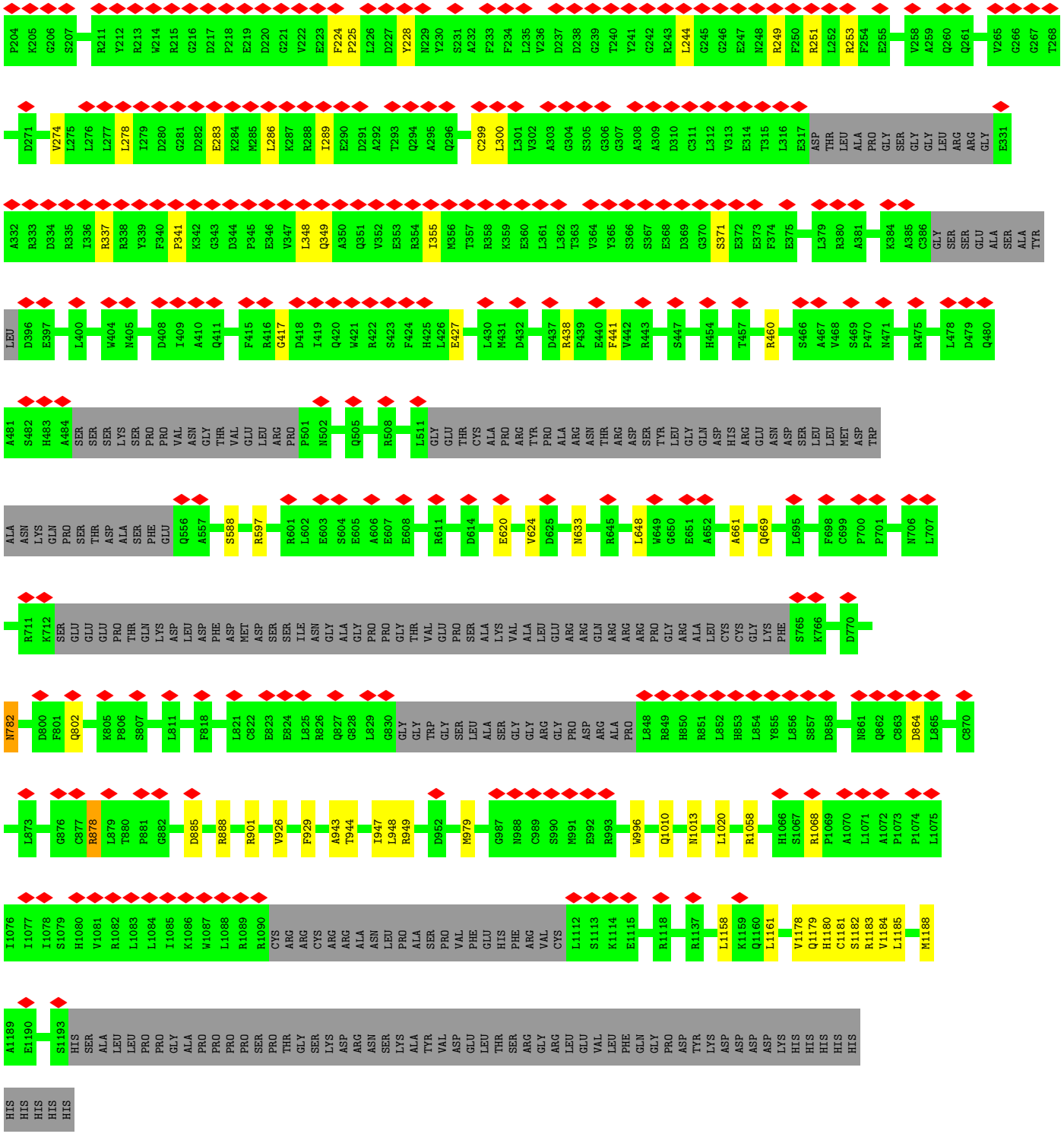




• Molecule 1: Transient receptor potential cation channel subfamily M member 4

Chain D:




P204 K205 G206 S207 R211 Y212 R213 W214 R215 G216 D217 P218 E219 D220 G221 V222 E223 F224 P225 L226 D227 Y228 N229 Y230 S231 A232 F233 F234 L235 V236 D237 D238 G239 T240 Y241 G242 R243 L244 G245 G246 E247 N248 R249 F250 R251 L252 R253 F254 E255 V258 A259 Q260 Q261 V265 G266 G267 T268
D271 V274 L275 L276 L277 L278 I279 D280 G281 D282 E283 K284 M285 L286 K287 R288 I289 E290 D291 A292 T293 Q294 A295 Q296 C299 L300 L301 V302 A303 G304 S305 G306 G307 A308 A309 D310 C311 L312 V313 E314 T315 L316 E317 ASP THR LEU ALA PRO GLY SER GLY GLY LEU ARG ARG GLY E331
A332 R333 D334 R335 I336 R337 R338 Y339 F340 P341 K342 G343 D344 P345 E346 V347 L348 Q349 A350 Q351 V352 E353 R354 I355 M356 T357 R358 K359 E360 L361 L362 T363 V364 Y365 S366 S367 E368 D369 G370 S371 E372 E373 F374 E375 L379 R380 A381 K384 A385 C386 GLY SER SER GLU ALA SER ALA TYR
LEU D396 E397 L400 W404 N405 D408 I409 A410 Q411 F415 R416 G417 D418 I419 Q420 W421 R422 S423 F424 H425 L426 E427 L430 M431 D432 D437 R438 P439 E440 F441 V442 R443 S447 H454 T457 R460 S466 A467 V468 S469 P470 N471 R475 L478 D479 Q480
A481 S482 H483 A484 SER SER SER LYS SER PRO PRO VAL ASN GLY THR VAL GLU LEU ARG PRO P501 N502 Q505 R508 L511 GLY GLU THR CYS ALA PRO ARG TYR PRO ALA ARG ASN THR ARG ASP SER TYR LEU GLY GLN ASP HIS ARG GLU ASN ASP SER LEU LEU MET ASP TRP
ALA ASN LYS GLN PRO SER THR ASP ALA SER PHE GLU Q556 A557 S588 R597 R601 L602 E603 S604 E605 A606 E607 E608 R611 D614 E620 V624 D625 N633 R645 L648 W649 G650 E651 A652 A661 Q669 L695 F698 C699 P700 P701 N706 L707
R711 K712 SER GLU GLU GLU PRO THR GLN LYS ASP LEU ASP PHE ASP MET ASP SER SER ILE ASN GLY ALA GLY PRO PRO PRO GLY THR VAL GLU PRO SER ALA LYS VAL ALA LEU GLU ARG ARG GLN ARG ARG ARG PRO GLY ARG ALA LEU CYS CYS GLY LYS PHE S765 K766 D770
N782 D800 F801 Q802 K805 P806 S807 L811 F818 L821 C822 E823 E824 L825 R826 Q827 G828 L829 G830 GLY GLY TRP GLY SER LEU ALA SER GLY GLY ARG GLY PRO ASP ARG ALA PRO L848 R849 H850 R851 L852 H853 L854 Y855 L856 S857 D858 N861 Q862 C863 D864 L865 C870
L873 G876 C877 R878 L879 T880 P881 G882 D885 R888 R901 V926 F929 A943 T944 I947 L948 R949 D952 M979 G987 N988 C989 S990 M991 E992 R993 W996 Q1010 N1013 L1020 R1058 H1066 S1067 R1068 P1069 A1070 L1071 A1072 P1073 P1074 L1075
I1076 I1077 I1078 S1079 H1080 V1081 R1082 L1083 L1084 I1085 K1086 W1087 L1088 R1089 R1090 CYS ARG ARG CYS ARG ARG ALA ASN LEU PRO ALA SER PRO VAL PHE GLU HIS PHE ARG VAL CYS L1112 S1113 K1114 E1115 R1118 R1137 L1158 K1159 Q1160 L1161 V1178 Q1179 H1180 C1181 S1182 R1183 V1184 L1185 M1188
A1189 E1190 S1193 HIS SER ALA LEU LEU PRO PRO GLY ALA PRO PRO PRO PRO SER PRO THR GLY SER LYS ASP ARG ASN SER LYS ALA TYR VAL ASP GLU LEU THR SER ARG GLY ARG LEU GLU VAL LEU PHE GLN GLY PRO ASP TYR LYS ASP ASP ASP LYS HIS HIS HIS HIS HIS
HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	11545	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The CTF correction was performed during the map refinement in Relion.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	46730	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.168	Depositor
Minimum map value	-0.081	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	276.06003, 276.06003, 276.06003	wwPDB
Map dimensions	258, 258, 258	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.38	0/7786	0.55	0/10558
1	B	0.38	0/7786	0.55	0/10558
1	C	0.38	0/7786	0.55	0/10558
1	D	0.38	0/7786	0.55	0/10558
All	All	0.38	0/31144	0.55	0/42232

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7618	0	7630	51	0
1	B	7618	0	7630	56	0
1	C	7618	0	7630	51	0
1	D	7618	0	7630	57	0
2	A	2	0	0	0	0
All	All	30474	0	30520	192	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 3.

All (192) 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:B:1030:LEU:HD21	1:D:926:VAL:HG21	1.29	1.10
1:D:864:ASP:HB2	1:D:901:ARG:NH1	1.87	0.89
1:B:1030:LEU:CD2	1:D:926:VAL:HG21	2.06	0.86
1:B:949:ARG:NH2	1:D:888:ARG:HG2	1.90	0.86
1:B:888:ARG:HG2	1:A:949:ARG:NH2	1.90	0.85
1:B:949:ARG:HH22	1:D:888:ARG:HG2	1.43	0.83
1:C:864:ASP:HB2	1:C:901:ARG:NH1	1.92	0.83
1:B:888:ARG:HG2	1:A:949:ARG:HH22	1.43	0.82
1:A:864:ASP:HB2	1:A:901:ARG:NH1	1.94	0.81
1:C:888:ARG:HG2	1:D:949:ARG:NH2	1.97	0.80
1:A:888:ARG:HG2	1:C:949:ARG:NH2	1.96	0.79
1:D:948:LEU:O	1:D:948:LEU:HD12	1.84	0.78
1:B:948:LEU:HD12	1:B:948:LEU:O	1.84	0.77
1:C:948:LEU:HD12	1:C:948:LEU:O	1.85	0.76
1:A:948:LEU:HD12	1:A:948:LEU:O	1.85	0.76
1:C:888:ARG:HG2	1:D:949:ARG:HH22	1.49	0.74
1:B:1029:ILE:HD13	1:D:929:PHE:CE2	2.24	0.73
1:A:888:ARG:HG2	1:C:949:ARG:HH22	1.50	0.72
1:B:1029:ILE:CD1	1:D:929:PHE:CE2	2.77	0.68
1:B:136:GLN:HE22	1:D:417:GLY:HA3	1.60	0.66
1:C:417:GLY:HA3	1:D:136:GLN:HE22	1.65	0.62
1:D:864:ASP:HB2	1:D:901:ARG:HH11	1.66	0.60
1:A:802:GLN:O	1:A:878:ARG:NH1	2.35	0.60
1:C:337:ARG:HE	1:C:349:GLN:HA	1.67	0.60
1:B:802:GLN:O	1:B:878:ARG:NH1	2.35	0.59
1:D:337:ARG:HE	1:D:349:GLN:HA	1.67	0.59
1:D:802:GLN:O	1:D:878:ARG:NH1	2.35	0.59
1:C:802:GLN:O	1:C:878:ARG:NH1	2.35	0.59
1:A:337:ARG:HE	1:A:349:GLN:HA	1.67	0.59
1:C:172:ARG:NH2	1:C:228:TYR:OH	2.36	0.59
1:D:172:ARG:NH2	1:D:228:TYR:OH	2.36	0.59
1:D:14:ILE:HG22	1:D:18:LYS:HE3	1.84	0.59
1:C:14:ILE:HG22	1:C:18:LYS:HE3	1.84	0.59
1:B:14:ILE:HG22	1:B:18:LYS:HE3	1.84	0.58
1:B:172:ARG:NH2	1:B:228:TYR:OH	2.36	0.58
1:B:337:ARG:HE	1:B:349:GLN:HA	1.67	0.58
1:A:14:ILE:HG22	1:A:18:LYS:HE3	1.84	0.58
1:A:172:ARG:NH2	1:A:228:TYR:OH	2.36	0.58
1:A:782:ASN:OD1	1:A:1068:ARG:NH1	2.38	0.57
1:C:22:THR:HG23	1:C:73:THR:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:782:ASN:OD1	1:C:1068:ARG:NH1	2.38	0.57
1:D:782:ASN:OD1	1:D:1068:ARG:NH1	2.38	0.57
1:B:782:ASN:OD1	1:B:1068:ARG:NH1	2.38	0.56
1:A:22:THR:HG23	1:A:73:THR:HG22	1.86	0.56
1:B:22:THR:HG23	1:B:73:THR:HG22	1.86	0.56
1:D:22:THR:HG23	1:D:73:THR:HG22	1.86	0.56
1:A:864:ASP:HB2	1:A:901:ARG:HH11	1.71	0.56
1:B:597:ARG:NH1	1:B:661:ALA:O	2.40	0.55
1:D:597:ARG:NH1	1:D:661:ALA:O	2.40	0.55
1:A:597:ARG:NH1	1:A:661:ALA:O	2.40	0.54
1:B:864:ASP:HB2	1:B:901:ARG:NH2	2.22	0.54
1:B:1029:ILE:CD1	1:D:929:PHE:HE2	2.19	0.54
1:C:597:ARG:NH1	1:C:661:ALA:O	2.40	0.54
1:A:417:GLY:HA3	1:C:136:GLN:HE22	1.73	0.54
1:C:75:ALA:HB3	1:C:93:ARG:HB2	1.89	0.54
1:C:996:TRP:O	1:C:1010:GLN:NE2	2.41	0.54
1:A:996:TRP:O	1:A:1010:GLN:NE2	2.41	0.54
1:D:75:ALA:HB3	1:D:93:ARG:HB2	1.89	0.54
1:D:996:TRP:O	1:D:1010:GLN:NE2	2.41	0.54
1:A:75:ALA:HB3	1:A:93:ARG:HB2	1.89	0.53
1:C:864:ASP:HB2	1:C:901:ARG:HH11	1.68	0.53
1:B:75:ALA:HB3	1:B:93:ARG:HB2	1.89	0.53
1:B:996:TRP:O	1:B:1010:GLN:NE2	2.41	0.53
1:B:417:GLY:HA3	1:A:136:GLN:HE22	1.74	0.52
1:D:16:ARG:NH2	1:D:110:SER:OG	2.43	0.52
1:A:16:ARG:NH2	1:A:110:SER:OG	2.43	0.52
1:B:16:ARG:NH2	1:B:110:SER:OG	2.43	0.52
1:A:286:LEU:HD23	1:A:289:ILE:HD12	1.93	0.51
1:C:16:ARG:NH2	1:C:110:SER:OG	2.43	0.51
1:D:123:LEU:HB2	1:D:278:LEU:HD23	1.93	0.51
1:B:119:VAL:HB	1:B:274:VAL:HG22	1.92	0.51
1:C:119:VAL:HB	1:C:274:VAL:HG22	1.92	0.51
1:B:123:LEU:HB2	1:B:278:LEU:HD23	1.93	0.50
1:C:123:LEU:HB2	1:C:278:LEU:HD23	1.93	0.50
1:A:119:VAL:HB	1:A:274:VAL:HG22	1.92	0.50
1:C:141:ARG:HB2	1:C:371:SER:HB2	1.93	0.50
1:D:119:VAL:HB	1:D:274:VAL:HG22	1.92	0.50
1:B:175:GLN:HG3	1:B:183:LYS:HE2	1.94	0.50
1:A:141:ARG:HB2	1:A:371:SER:HB2	1.94	0.50
1:A:175:GLN:HG3	1:A:183:LYS:HE2	1.94	0.50
1:D:175:GLN:HG3	1:D:183:LYS:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LEU:HD23	1:B:289:ILE:HD12	1.93	0.50
1:B:141:ARG:HB2	1:B:371:SER:HB2	1.94	0.50
1:A:123:LEU:HB2	1:A:278:LEU:HD23	1.93	0.50
1:D:286:LEU:HD23	1:D:289:ILE:HD12	1.93	0.50
1:D:299:CYS:SG	1:D:300:LEU:N	2.85	0.50
1:C:175:GLN:HG3	1:C:183:LYS:HE2	1.94	0.49
1:B:299:CYS:SG	1:B:300:LEU:N	2.85	0.49
1:B:1179:GLN:O	1:B:1183:ARG:N	2.42	0.49
1:C:299:CYS:SG	1:C:300:LEU:N	2.85	0.49
1:D:141:ARG:HB2	1:D:371:SER:HB2	1.94	0.49
1:A:299:CYS:SG	1:A:300:LEU:N	2.85	0.49
1:C:286:LEU:HD23	1:C:289:ILE:HD12	1.93	0.49
1:B:1178:VAL:O	1:B:1182:SER:N	2.44	0.48
1:A:1179:GLN:O	1:A:1183:ARG:N	2.42	0.48
1:D:1178:VAL:O	1:D:1182:SER:N	2.44	0.48
1:B:1184:VAL:O	1:B:1188:MET:N	2.44	0.48
1:C:286:LEU:HD12	1:C:348:LEU:HD22	1.97	0.47
1:D:1179:GLN:O	1:D:1183:ARG:N	2.42	0.47
1:B:286:LEU:HD12	1:B:348:LEU:HD22	1.96	0.47
1:B:949:ARG:NH2	1:D:888:ARG:CG	2.72	0.47
1:D:286:LEU:HD12	1:D:348:LEU:HD22	1.97	0.47
1:B:888:ARG:CG	1:A:949:ARG:NH2	2.72	0.47
1:C:1184:VAL:O	1:C:1188:MET:N	2.44	0.47
1:A:286:LEU:HD12	1:A:348:LEU:HD22	1.97	0.46
1:D:1181:CYS:O	1:D:1185:LEU:N	2.44	0.46
1:D:1184:VAL:O	1:D:1188:MET:N	2.44	0.46
1:B:597:ARG:NH2	1:B:620:GLU:OE1	2.49	0.46
1:A:597:ARG:NH2	1:A:620:GLU:OE1	2.49	0.46
1:D:597:ARG:NH2	1:D:620:GLU:OE1	2.49	0.46
1:A:1178:VAL:O	1:A:1182:SER:N	2.44	0.46
1:A:100:PRO:HG3	1:A:253:ARG:HG2	1.98	0.45
1:B:427:GLU:HB3	1:B:460:ARG:HH12	1.82	0.45
1:C:597:ARG:NH2	1:C:620:GLU:OE1	2.49	0.45
1:D:427:GLU:HB3	1:D:460:ARG:HH12	1.81	0.45
1:D:943:ALA:O	1:D:947:ILE:HG13	2.16	0.45
1:B:943:ALA:O	1:B:947:ILE:HG13	2.17	0.45
1:D:100:PRO:HG3	1:D:253:ARG:HG2	1.98	0.45
1:A:1181:CYS:O	1:A:1185:LEU:N	2.44	0.45
1:A:1133:LEU:HD13	1:C:181:SER:HB2	1.99	0.45
1:C:100:PRO:HG3	1:C:253:ARG:HG2	1.98	0.45
1:A:427:GLU:HB3	1:A:460:ARG:HH12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:GLU:HB3	1:C:460:ARG:HH12	1.81	0.45
1:C:1178:VAL:O	1:C:1182:SER:N	2.44	0.45
1:C:1179:GLN:O	1:C:1183:ARG:N	2.42	0.44
1:C:1181:CYS:O	1:C:1185:LEU:N	2.44	0.44
1:B:100:PRO:HG3	1:B:253:ARG:HG2	1.98	0.44
1:A:224:PHE:HE2	1:A:244:LEU:HD11	1.83	0.44
1:A:1184:VAL:O	1:A:1188:MET:N	2.44	0.44
1:C:624:VAL:HG13	1:C:669:GLN:HE21	1.83	0.43
1:B:283:GLU:HG2	1:B:341:PRO:HB3	2.00	0.43
1:C:1133:LEU:HD13	1:D:181:SER:HB2	1.99	0.43
1:C:224:PHE:HE2	1:C:244:LEU:HD11	1.83	0.43
1:A:283:GLU:HG2	1:A:341:PRO:HB3	2.00	0.43
1:B:624:VAL:HG13	1:B:669:GLN:HE21	1.83	0.43
1:D:624:VAL:HG13	1:D:669:GLN:HE21	1.83	0.43
1:D:196:ARG:N	1:D:224:PHE:O	2.52	0.43
1:D:283:GLU:HG2	1:D:341:PRO:HB3	2.00	0.42
1:A:160:HIS:HD2	1:A:225:PRO:HG2	1.85	0.42
1:B:224:PHE:HE2	1:B:244:LEU:HD11	1.83	0.42
1:C:196:ARG:N	1:C:224:PHE:O	2.52	0.42
1:D:163:ILE:H	1:D:163:ILE:HG13	1.59	0.42
1:D:224:PHE:HE2	1:D:244:LEU:HD11	1.83	0.42
1:C:943:ALA:O	1:C:947:ILE:HG13	2.18	0.42
1:B:160:HIS:HD2	1:B:225:PRO:HG2	1.85	0.42
1:B:588:SER:HA	1:B:648:LEU:HD11	2.02	0.42
1:C:283:GLU:HG2	1:C:341:PRO:HB3	2.00	0.42
1:D:588:SER:HA	1:D:648:LEU:HD11	2.02	0.42
1:A:943:ALA:O	1:A:947:ILE:HG13	2.19	0.42
1:C:1158:LEU:HD23	1:C:1161:LEU:HD12	2.02	0.42
1:B:121:SER:HB2	1:B:251:ARG:HH21	1.85	0.42
1:B:948:LEU:HD12	1:B:948:LEU:C	2.39	0.42
1:B:1133:LEU:HD13	1:A:181:SER:HB2	2.00	0.42
1:A:624:VAL:HG13	1:A:669:GLN:HE21	1.84	0.42
1:C:116:PRO:HG3	1:C:153:TRP:CE2	2.55	0.42
1:A:116:PRO:HG3	1:A:153:TRP:CE2	2.55	0.42
1:D:116:PRO:HG3	1:D:153:TRP:CE2	2.55	0.42
1:B:116:PRO:HG3	1:B:153:TRP:CE2	2.55	0.42
1:A:1158:LEU:HD23	1:A:1161:LEU:HD12	2.02	0.42
1:D:121:SER:HB2	1:D:251:ARG:HH21	1.85	0.42
1:D:948:LEU:HD12	1:D:948:LEU:C	2.39	0.42
1:C:163:ILE:H	1:C:163:ILE:HG13	1.59	0.41
1:C:948:LEU:HD12	1:C:948:LEU:C	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1158:LEU:HD23	1:D:1161:LEU:HD12	2.02	0.41
1:C:121:SER:HB2	1:C:251:ARG:HH21	1.85	0.41
1:C:160:HIS:HD2	1:C:225:PRO:HG2	1.85	0.41
1:A:588:SER:HA	1:A:648:LEU:HD11	2.02	0.41
1:C:588:SER:HA	1:C:648:LEU:HD11	2.02	0.41
1:B:1158:LEU:HD23	1:B:1161:LEU:HD12	2.02	0.41
1:D:160:HIS:HD2	1:D:225:PRO:HG2	1.85	0.41
1:B:75:ALA:HB1	1:B:91:PHE:HE2	1.86	0.41
1:B:1181:CYS:O	1:B:1185:LEU:N	2.44	0.41
1:A:121:SER:HB2	1:A:251:ARG:HH21	1.85	0.41
1:A:948:LEU:HD12	1:A:948:LEU:C	2.39	0.41
1:B:949:ARG:NH1	1:D:885:ASP:OD1	2.54	0.41
1:A:438:ARG:HB3	1:A:441:PHE:HD2	1.86	0.41
1:A:979:MET:HE1	1:A:1020:LEU:HD13	2.03	0.41
1:C:438:ARG:HB3	1:C:441:PHE:HD2	1.86	0.41
1:D:979:MET:HE1	1:D:1020:LEU:HD13	2.03	0.41
1:D:1180:HIS:O	1:D:1184:VAL:N	2.49	0.41
1:C:702:LEU:HD21	1:C:707:LEU:HD12	2.03	0.41
1:B:979:MET:HE1	1:B:1020:LEU:HD13	2.03	0.40
1:A:75:ALA:HB1	1:A:91:PHE:HE2	1.85	0.40
1:C:979:MET:HE1	1:C:1020:LEU:HD13	2.03	0.40
1:B:438:ARG:HB3	1:B:441:PHE:HD2	1.86	0.40
1:B:790:LEU:HD13	1:B:899:THR:HG22	2.03	0.40
1:A:702:LEU:HD21	1:A:707:LEU:HD12	2.03	0.40
1:A:790:LEU:HD13	1:A:899:THR:HG22	2.04	0.40
1:D:944:THR:O	1:D:948:LEU:HG	2.21	0.40
1:B:1114:LYS:HA	1:B:1114:LYS:HD2	1.90	0.40
1:C:646:CYS:HB3	1:C:651:GLU:HA	2.04	0.40
1:D:438:ARG:HB3	1:D:441:PHE:HD2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	949/1254 (76%)	894 (94%)	55 (6%)	0	100	100
1	B	949/1254 (76%)	894 (94%)	55 (6%)	0	100	100
1	C	949/1254 (76%)	894 (94%)	55 (6%)	0	100	100
1	D	949/1254 (76%)	894 (94%)	55 (6%)	0	100	100
All	All	3796/5016 (76%)	3576 (94%)	220 (6%)	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	800/1063 (75%)	792 (99%)	8 (1%)	76	89
1	B	800/1063 (75%)	792 (99%)	8 (1%)	76	89
1	C	800/1063 (75%)	792 (99%)	8 (1%)	76	89
1	D	800/1063 (75%)	792 (99%)	8 (1%)	76	89
All	All	3200/4252 (75%)	3168 (99%)	32 (1%)	77	89

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	13	LYS
1	B	249	ARG
1	B	355	ILE
1	B	633	ASN
1	B	782	ASN
1	B	878	ARG
1	B	1013	ASN
1	B	1058	ARG
1	A	13	LYS
1	A	249	ARG
1	A	355	ILE
1	A	633	ASN
1	A	782	ASN

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Mol	Chain	Res	Type
1	A	878	ARG
1	A	1013	ASN
1	A	1058	ARG
1	C	13	LYS
1	C	249	ARG
1	C	355	ILE
1	C	633	ASN
1	C	782	ASN
1	C	878	ARG
1	C	1013	ASN
1	C	1058	ARG
1	D	13	LYS
1	D	249	ARG
1	D	355	ILE
1	D	633	ASN
1	D	782	ASN
1	D	878	ARG
1	D	1013	ASN
1	D	1058	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	136	GLN
1	B	229	ASN
1	B	261	GLN
1	B	436	ASN
1	B	633	ASN
1	A	136	GLN
1	A	229	ASN
1	A	261	GLN
1	A	436	ASN
1	A	633	ASN
1	C	136	GLN
1	C	229	ASN
1	C	261	GLN
1	C	436	ASN
1	C	633	ASN
1	D	136	GLN
1	D	229	ASN
1	D	261	GLN
1	D	436	ASN

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Mol	Chain	Res	Type
1	D	633	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

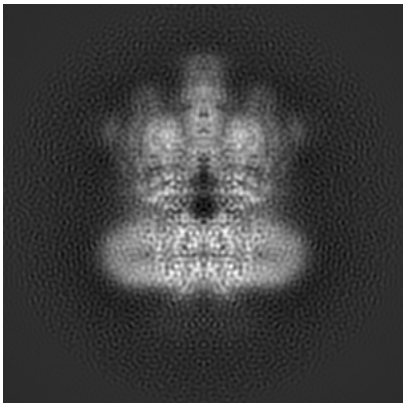
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7082. These allow visual inspection of the internal detail of the map and identification of artifacts.

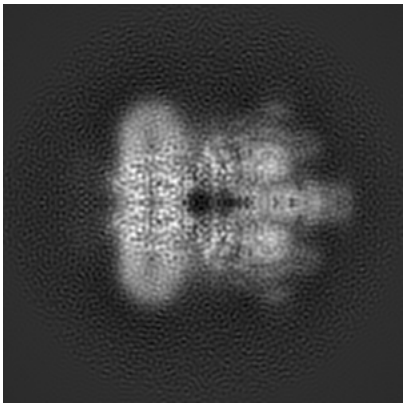
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

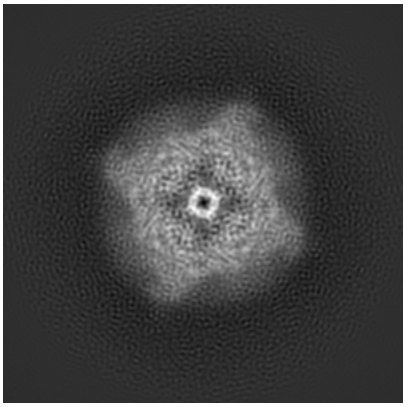
6.1.1 Primary map



X



Y

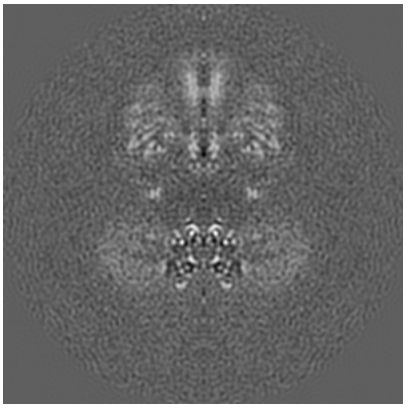


Z

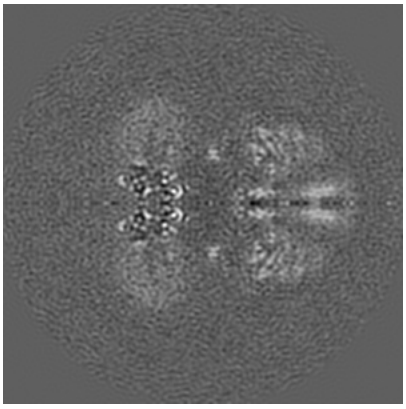
The images above show the map projected in three orthogonal directions.

6.2 Central slices

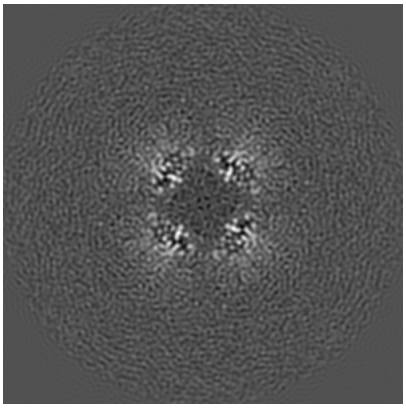
6.2.1 Primary map



X Index: 129



Y Index: 129

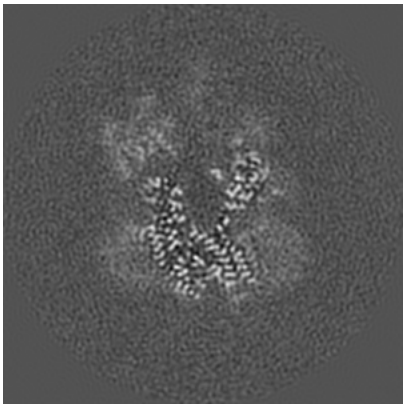


Z Index: 129

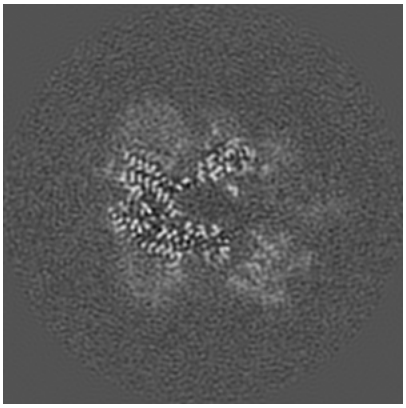
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

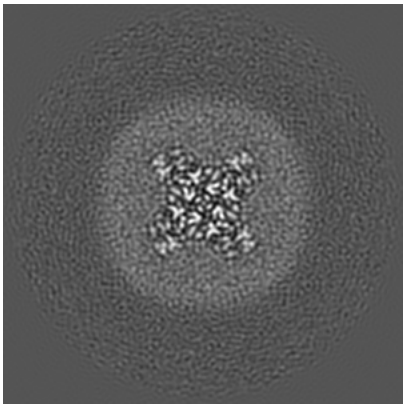
6.3.1 Primary map



X Index: 113



Y Index: 145

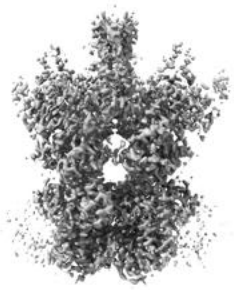


Z Index: 89

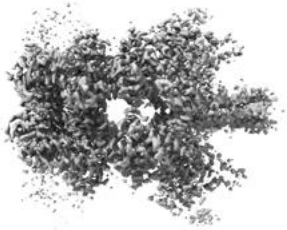
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

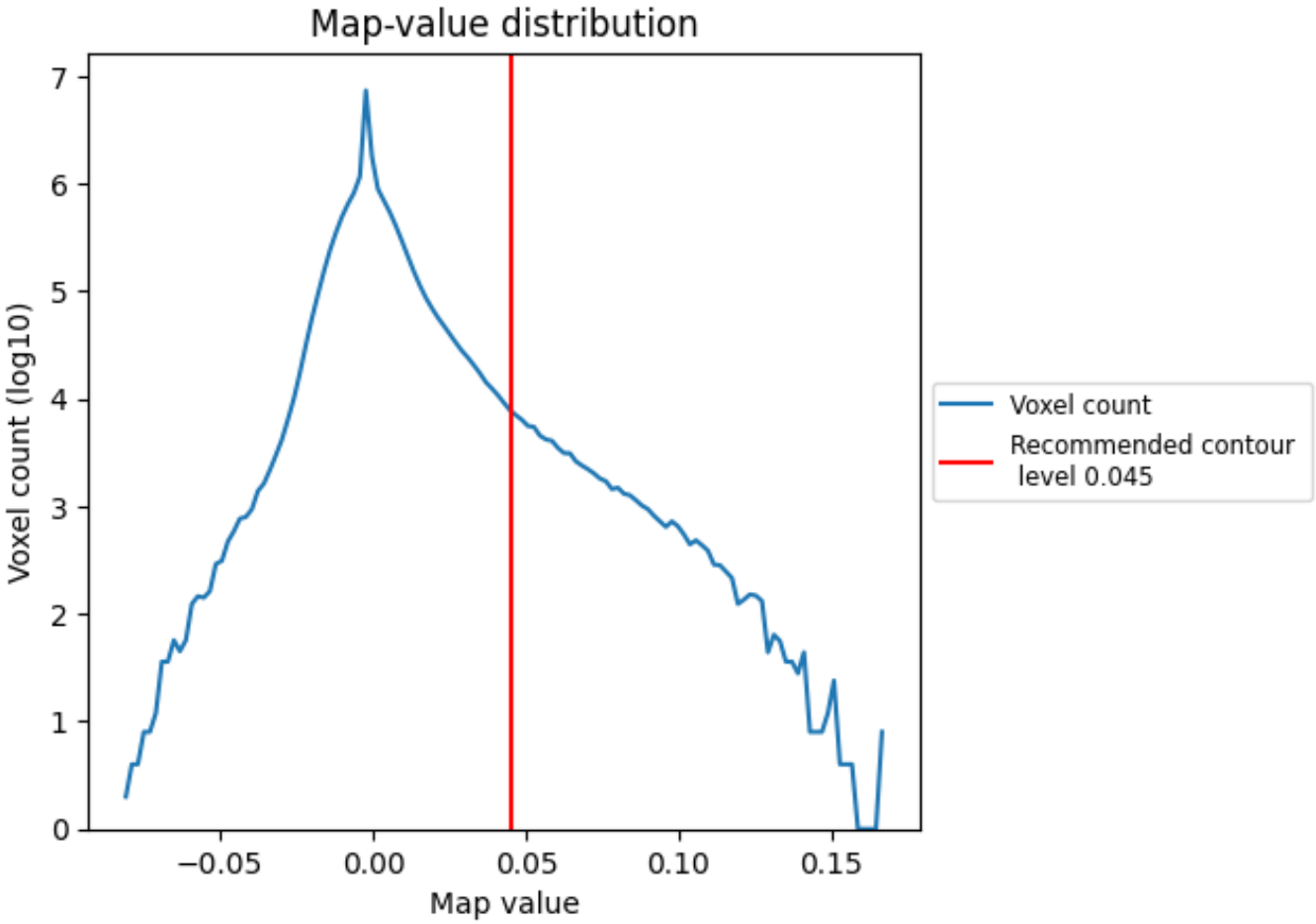
6.5 Mask visualisation (i)

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

7 Map analysis

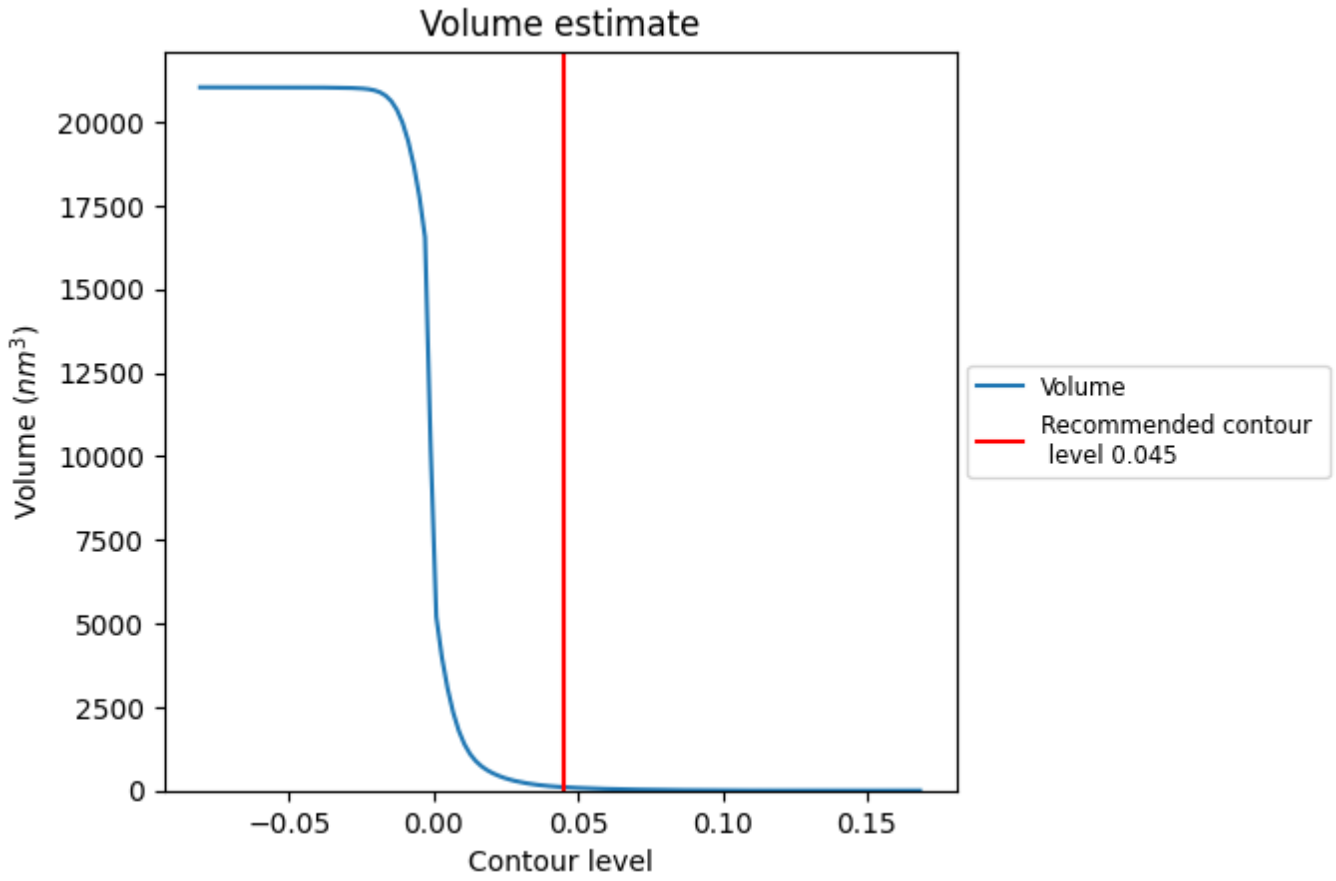
This section contains the results of statistical analysis of the map.

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.

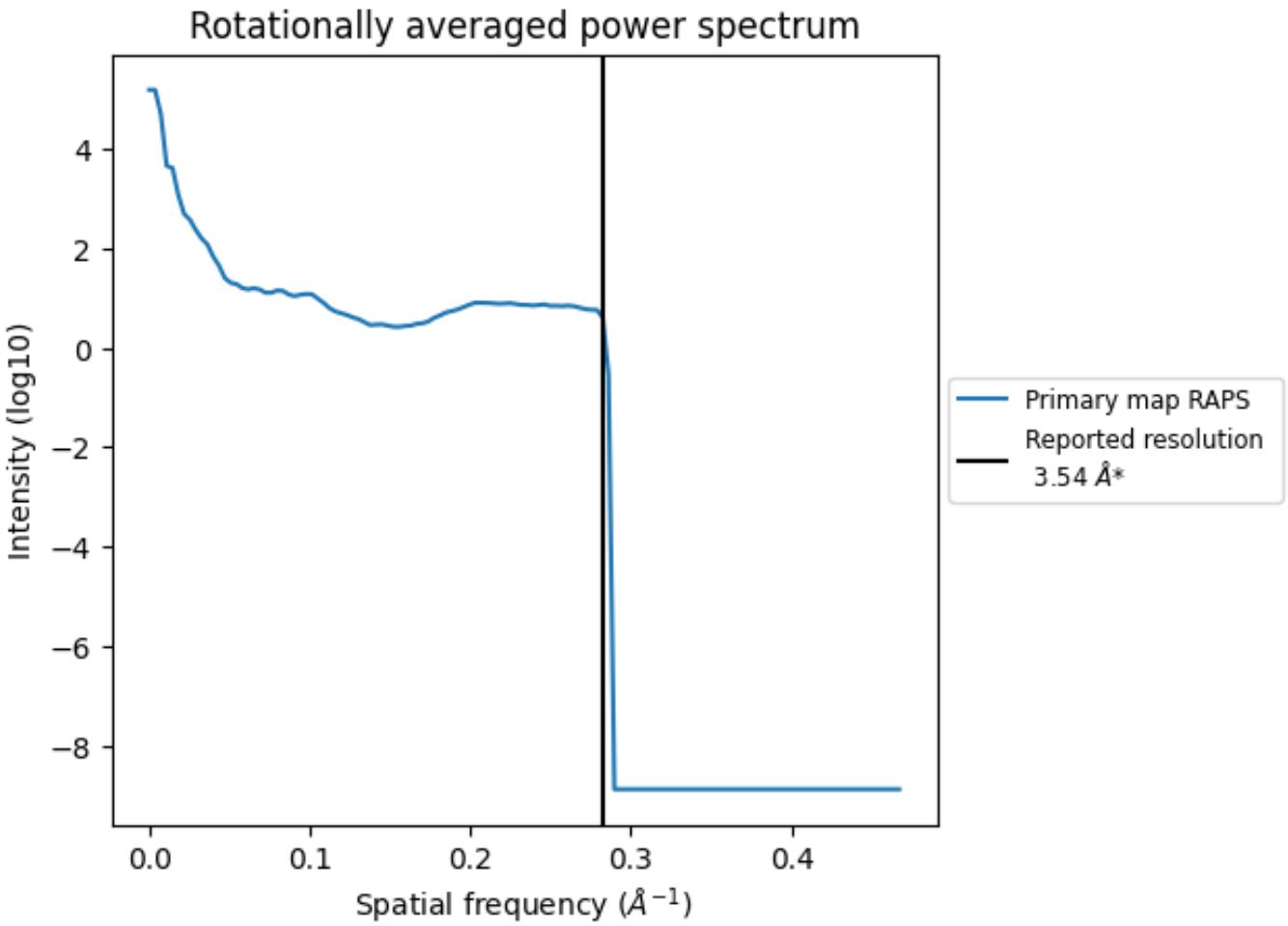
7.2 Volume estimate



The volume at the recommended contour level is 103 nm^3; this corresponds to an approximate mass of 93 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 0.282 Å^{-1}

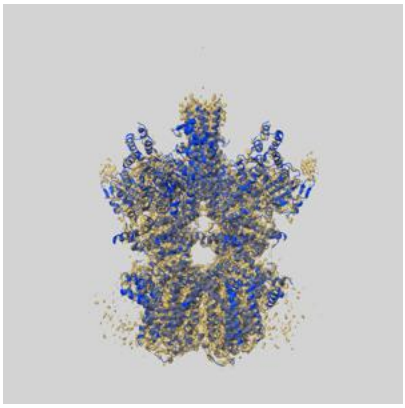
8 Fourier-Shell correlation (i)

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

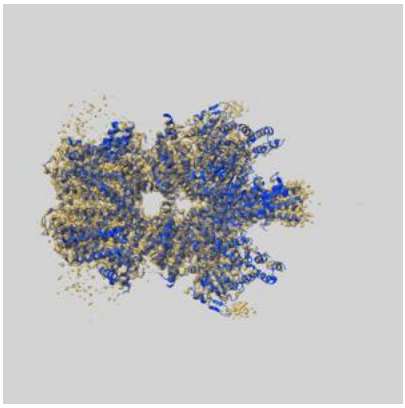
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7082 and PDB model 6BCL. Per-residue inclusion information can be found in section 3 on page 8.

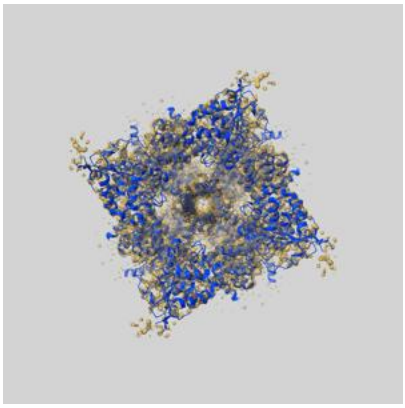
9.1 Map-model overlay



X



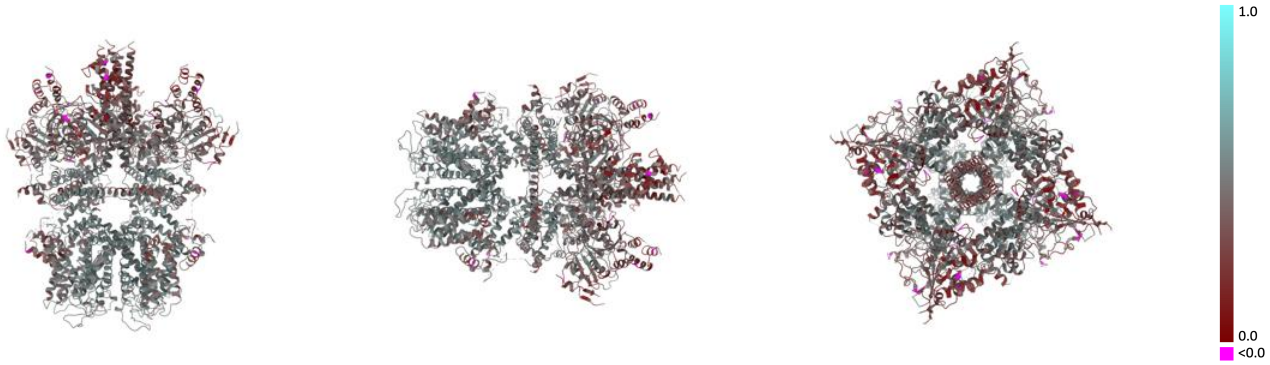
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 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.

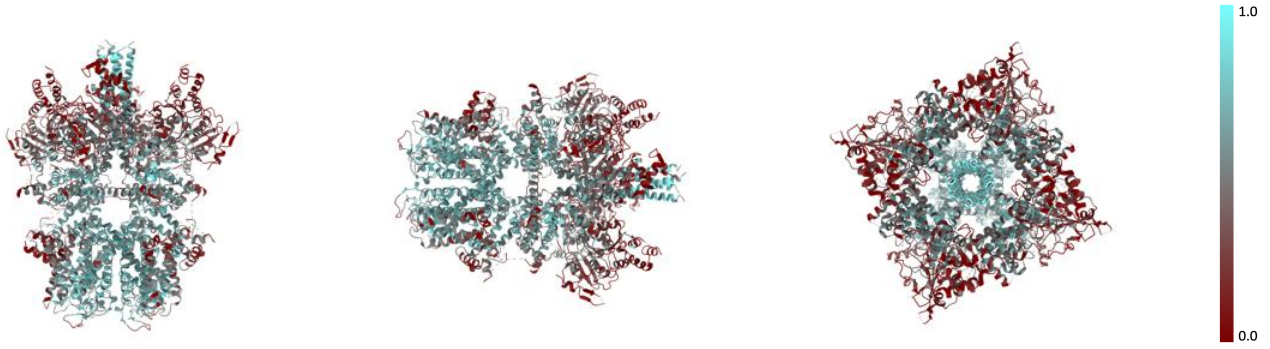
9.2 Q-score mapped to coordinate model (i)



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.

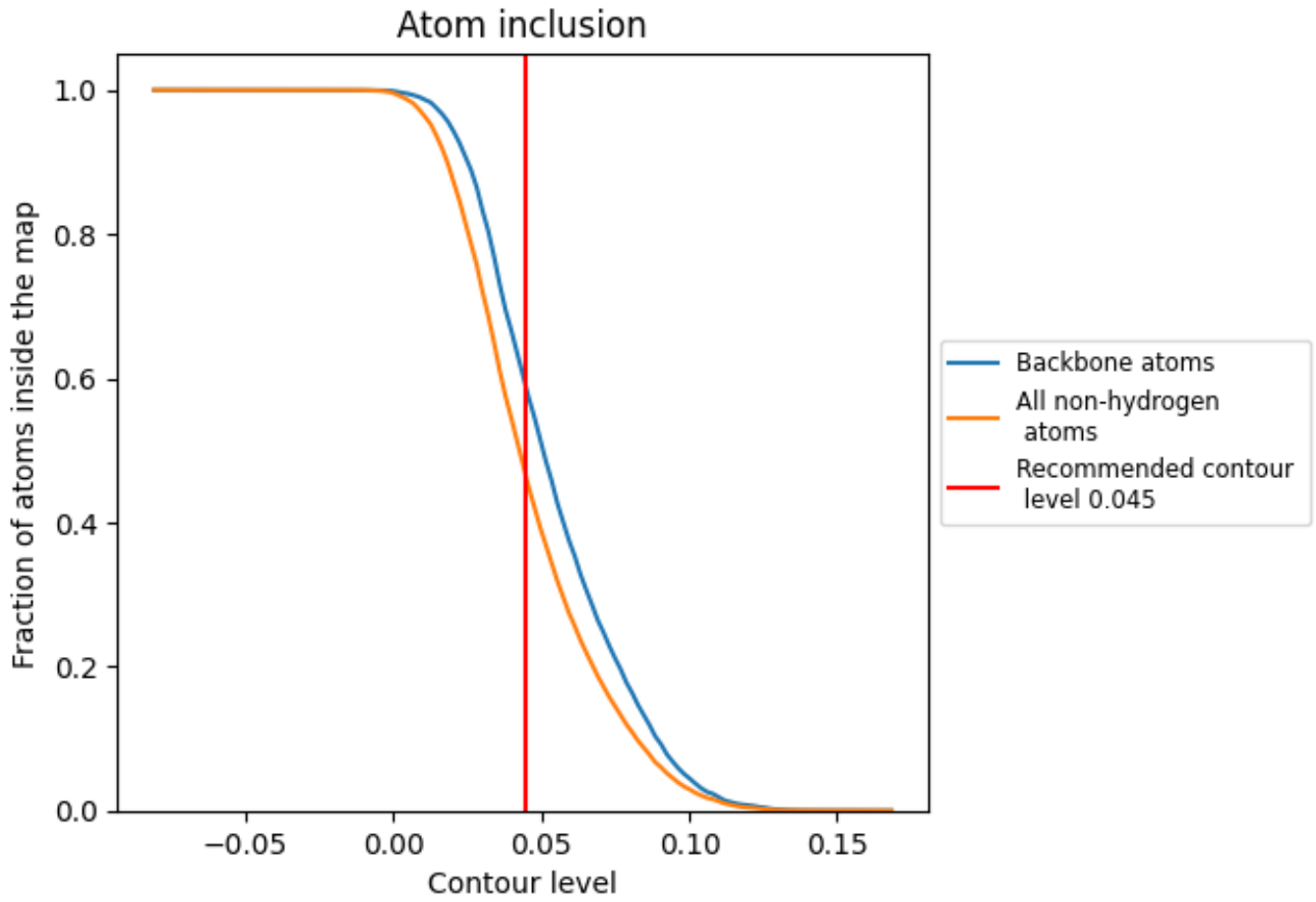
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 46% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4612	0.4300
A	0.4610	0.4300
B	0.4601	0.4300
C	0.4609	0.4300
D	0.4628	0.4290