Full wwPDB EM Validation Report (i)

Nov 6, 2022 – 07:39 AM EST

PDB ID	:	6BCO
EMDB ID	:	EMD-7083
Title	:	cryo-EM structure of TRPM4 in ATP bound state with short coiled coil at 2.9 angstrom resolution
Authors	:	Guo, J.; She, J.; Chen, Q.; Bai, X.; Jiang, Y.
Deposited on	:	2017-10-20
Resolution	:	2.88 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 (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 (1)) were used in the production of this report:

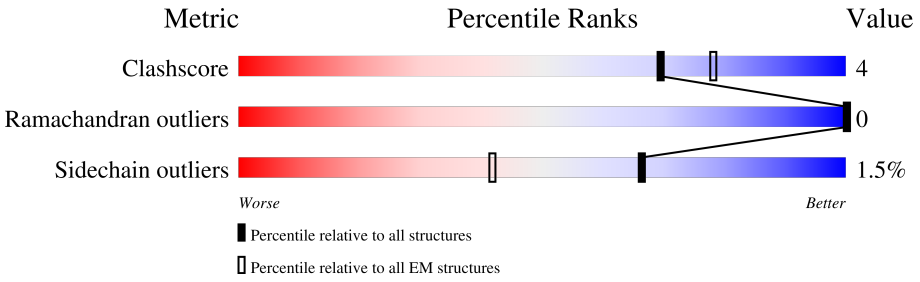
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.88 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	19% 68% 8% 24%
1	B	1254	19% 68% 7% 24%
1	C	1254	19% 68% 8% 24%
1	D	1254	19% 68% 7% 24%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 30432 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
			Total	C	N	O	S		
1	B	952	7577	4884	1322	1336	35	0	0
1	A	952	7577	4884	1322	1336	35	0	0
1	C	952	7577	4884	1322	1336	35	0	0
1	D	952	7577	4884	1322	1336	35	0	0

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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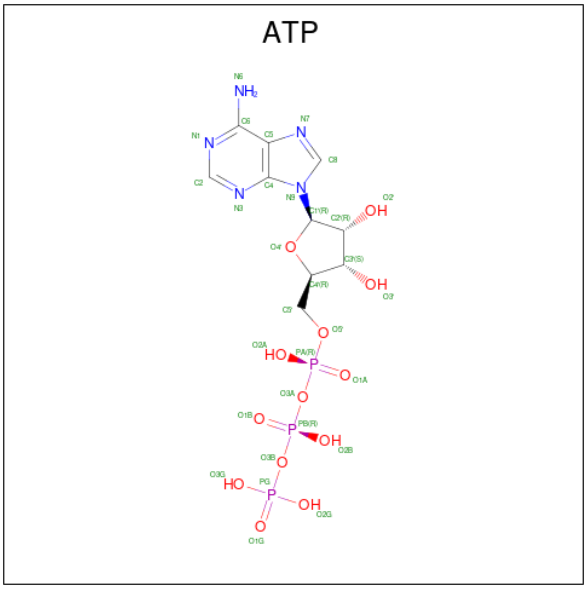
Chain	Residue	Modelled	Actual	Comment	Reference
D	1238	TYR	-	expression tag	UNP Q7TN37
D	1239	LYS	-	expression tag	UNP Q7TN37
D	1240	ASP	-	expression tag	UNP Q7TN37
D	1241	ASP	-	expression tag	UNP Q7TN37
D	1242	ASP	-	expression tag	UNP Q7TN37
D	1243	ASP	-	expression tag	UNP Q7TN37
D	1244	LYS	-	expression 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 ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	B	1	31	10	5	13	3	0
			Total	C	N	O	P	
2	A	1	31	10	5	13	3	0

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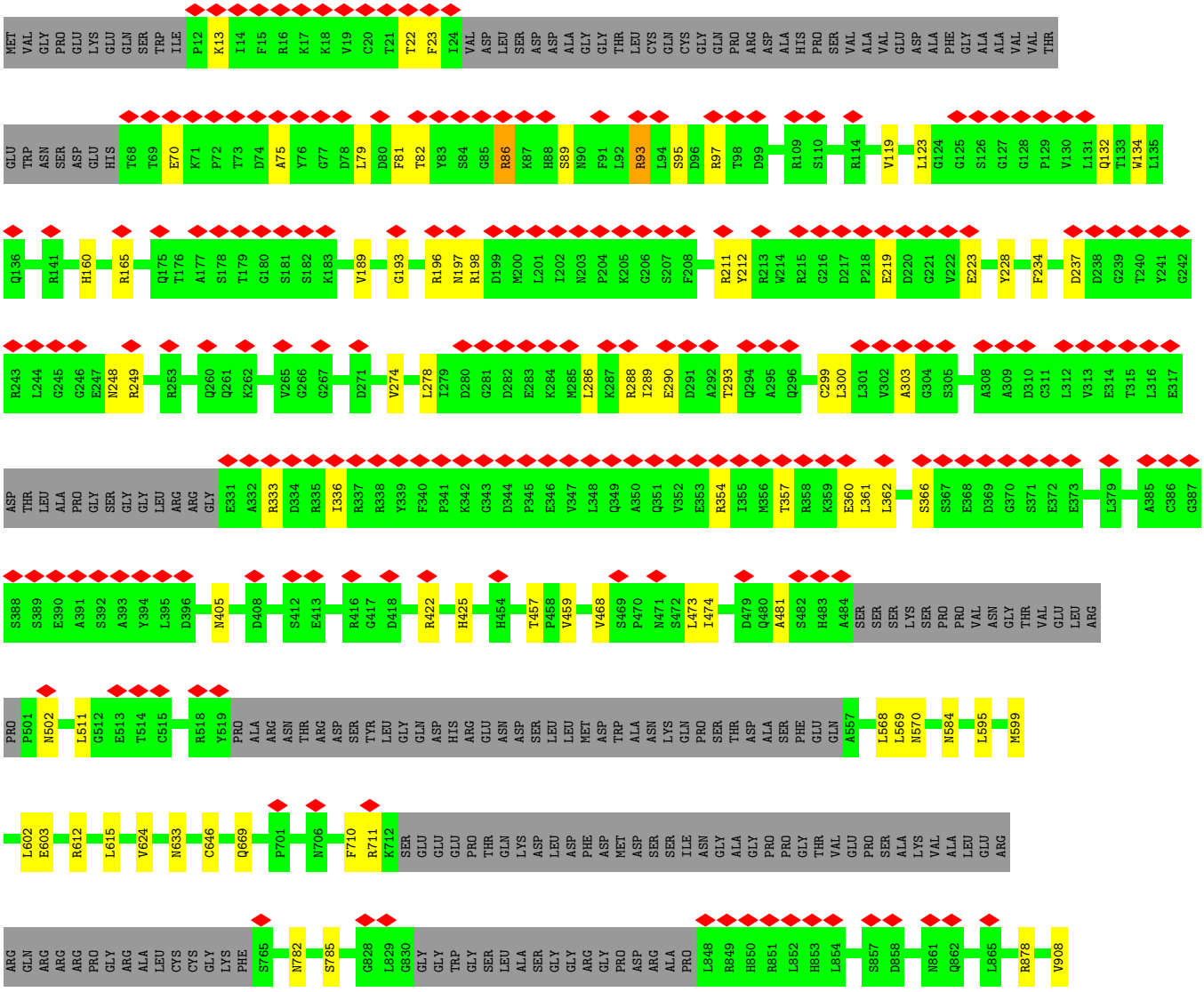
Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

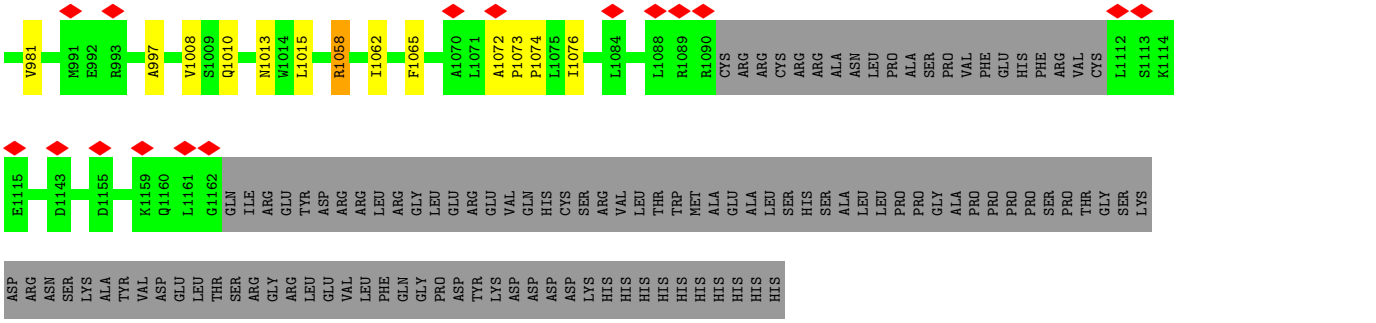
3 Residue-property plots (i)

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

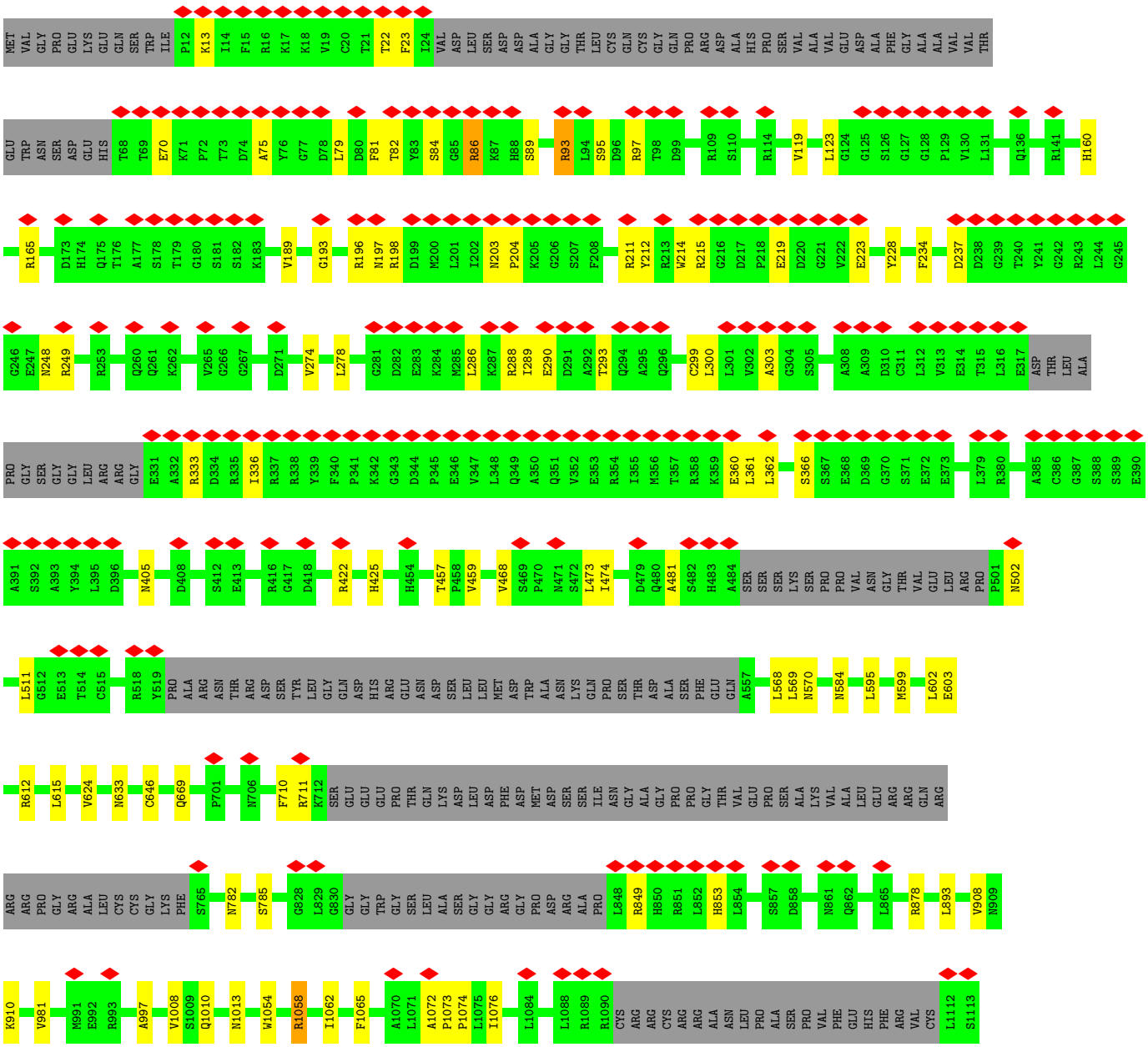
Chain B:

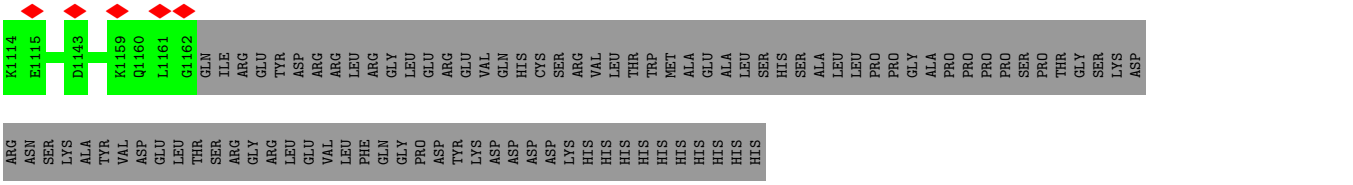




- Molecule 1: Transient receptor potential cation channel subfamily M member 4

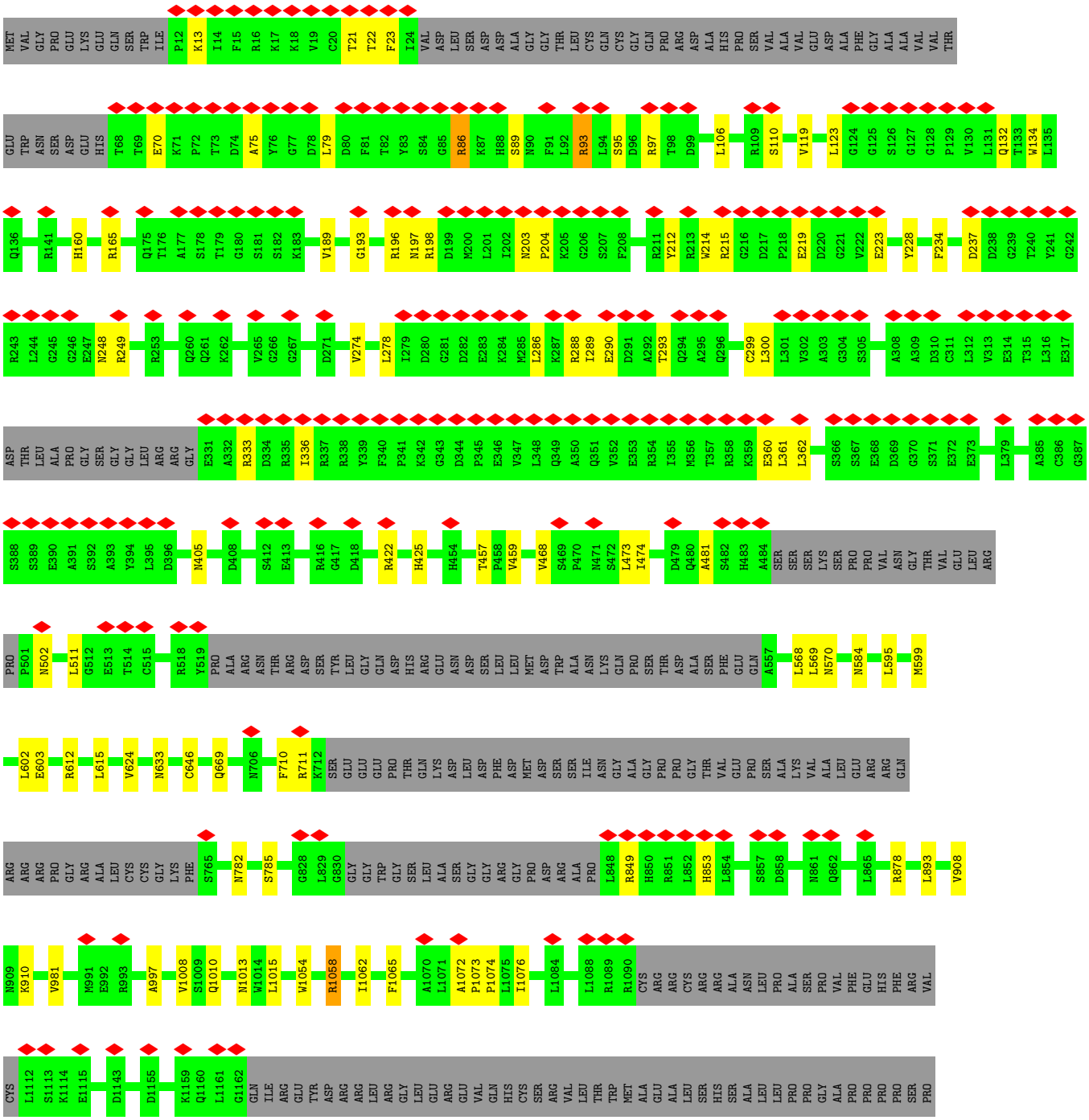
Chain A:

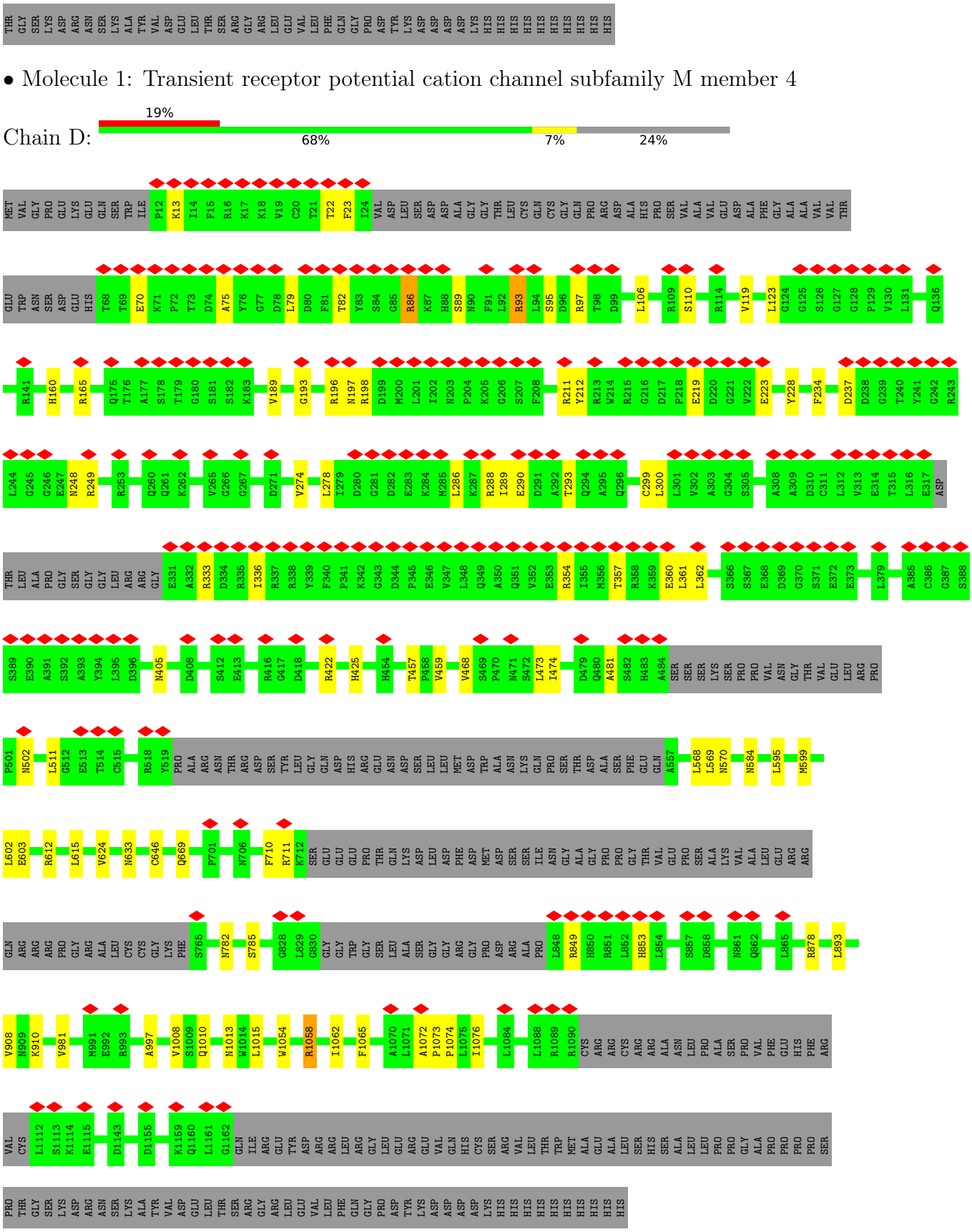




• Molecule 1: Transient receptor potential cation channel subfamily M member 4

Chain C:




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 ASP LYS HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS
• Molecule 1: Transient receptor potential cation channel subfamily M member 4
Chain D:
19%
68%
7%
24%
MET VAL GLY PRO GLU LYS GLU GLN SER TRP ILE P12 K13 I14 F15 R16 K17 K18 V19 C20 T21 T22 F23 I24 VAL ASP LEU SER ASP ASP ALA GLY GLY THR LEU CYS GLN CYS GLY GLN PRO ARG ASP ALA HIS PRO SER VAL ALA VAL GLU ASP ALA PHE GLY ALA ALA VAL VAL THR
GLU TRP ASN SER ASP GLU HIS T68 T69 E70 K71 P72 T73 D74 A75 Y76 G77 D78 L79 D80 F81 T82 Y83 S84 G85 R86 K87 H88 S89 N90 F91 L92 R93 L94 S95 D96 R97 T98 D99 L106 R109 S110 R114 V119 L123 G124 G125 S126 G127 G128 P129 V130 L131 Q136
R141 H160 R165 Q175 T176 A177 S178 T179 G180 S181 S182 K183 V189 G193 R196 N197 R198 D199 M200 L201 I202 N203 P204 K205 G206 S207 F208 R211 Y212 R213 W214 R215 G216 D217 P218 E219 D220 G221 V222 E223 Y228 F234 D237 D238 G239 T240 Y241 G242 R243
L244 G245 G246 E247 N248 R249 R253 Q260 Q261 K262 V265 G266 G267 D271 V274 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 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 S366 S367 E368 D369 G370 S371 E372 E373 L379 A385 C386 G387 S388
S389 E390 A391 S392 A393 Y394 L395 D396 N405 D408 S412 E413 R416 G417 D418 R422 H425 H454 T457 F458 V459 V468 S469 P470 N471 S472 L473 I474 D479 Q480 A481 S482 H483 A484 SER SER SER LYS SER PRO PRO VAL ASN GLY THR VAL GLU LEU ARG PRO
P501 N502 L511 G512 E513 T514 C515 R518 Y519 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 GLN A557 L568 L569 N570 N584 L595 M599
L602 E603 R612 L615 V624 N633 C646 Q669 P701 N706 F710 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 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 N782 S785 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 S857 D858 N861 Q862 L865 R878 L893
V908 N909 K910 V981 M991 E992 R993 A997 V1008 S1009 Q1010 N1013 W1014 L1015 W1054 R1058 I1062 F1065 A1070 L1071 A1072 P1073 P1074 L1075 I1076 L1084 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 D1143 D1155 K1159 Q1160 L1161 G1162 GLN ILE ARG GLU TYR ASP ARG ARG ARG LEU ARG GLY GLY LEU GLU ARG GLU VAL ASP LEU THR TRP MET ALA GLU ALA LEU SER HIS SER ALA LEU LEU PRO PRO PRO VAL PHE GLU HIS PHE ARG
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	196618	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The CTF correction was performed during te 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	0.222	Depositor
Minimum map value	-0.107	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0313	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 (i)

5.1 Standard geometry (i)

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

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	0.35	0/7749	0.54	0/10504
1	B	0.35	0/7749	0.54	0/10504
1	C	0.35	0/7749	0.54	0/10504
1	D	0.35	0/7749	0.54	0/10504
All	All	0.35	0/30996	0.54	0/42016

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 (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	7577	0	7663	59	0
1	B	7577	0	7663	56	0
1	C	7577	0	7663	59	0
1	D	7577	0	7663	56	0
2	A	31	0	12	2	0
2	B	31	0	12	2	0
2	C	31	0	12	2	0
2	D	31	0	12	2	0
All	All	30432	0	30700	227	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (227) 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:1073:PRO:O	1:A:1076:ILE:HG12	1.94	0.68
1:C:1073:PRO:N	1:C:1074:PRO:HD2	2.08	0.68
1:C:1073:PRO:O	1:C:1076:ILE:HG12	1.94	0.68
1:D:1073:PRO:N	1:D:1074:PRO:HD2	2.09	0.68
1:B:1073:PRO:N	1:B:1074:PRO:HD2	2.08	0.67
1:B:1073:PRO:O	1:B:1076:ILE:HG12	1.94	0.67
1:D:1073:PRO:O	1:D:1076:ILE:HG12	1.93	0.67
1:A:1073:PRO:N	1:A:1074:PRO:HD2	2.08	0.67
1:D:22:THR:HA	1:D:95:SER:HB3	1.78	0.66
1:C:22:THR:HA	1:C:95:SER:HB3	1.78	0.66
1:A:997:ALA:HB2	1:A:1010:GLN:HE21	1.62	0.65
1:C:997:ALA:HB2	1:C:1010:GLN:HE21	1.62	0.65
1:D:997:ALA:HB2	1:D:1010:GLN:HE21	1.62	0.65
1:B:22:THR:HA	1:B:95:SER:HB3	1.78	0.64
1:A:22:THR:HA	1:A:95:SER:HB3	1.78	0.64
1:B:997:ALA:HB2	1:B:1010:GLN:HE21	1.62	0.63
1:A:785:SER:OG	1:A:1073:PRO:HD2	2.00	0.62
1:D:785:SER:OG	1:D:1073:PRO:HD2	2.00	0.62
1:B:785:SER:OG	1:B:1073:PRO:HD2	2.00	0.61
1:C:785:SER:OG	1:C:1073:PRO:HD2	2.00	0.61
1:B:422:ARG:HB2	1:B:425:HIS:HD2	1.66	0.61
1:D:624:VAL:HG13	1:D:669:GLN:HE21	1.65	0.61
1:A:624:VAL:HG13	1:A:669:GLN:HE21	1.65	0.61
1:C:624:VAL:HG13	1:C:669:GLN:HE21	1.65	0.61
1:D:86:ARG:N	1:D:86:ARG:HE	1.98	0.60
1:D:422:ARG:HB2	1:D:425:HIS:HD2	1.66	0.60
1:B:624:VAL:HG13	1:B:669:GLN:HE21	1.66	0.60
1:B:473:LEU:HD11	1:B:602:LEU:HD22	1.84	0.60
1:A:422:ARG:HB2	1:A:425:HIS:HD2	1.66	0.60
1:B:86:ARG:N	1:B:86:ARG:HE	1.99	0.60
1:C:422:ARG:HB2	1:C:425:HIS:HD2	1.66	0.60
1:D:473:LEU:HD11	1:D:602:LEU:HD22	1.84	0.60
1:A:86:ARG:HE	1:A:86:ARG:N	1.99	0.59
1:A:81:PHE:CE2	1:A:228:TYR:HA	2.37	0.59
1:D:189:VAL:HG12	1:D:234:PHE:HB2	1.85	0.58
1:C:189:VAL:HG12	1:C:234:PHE:HB2	1.85	0.58
1:C:473:LEU:HD11	1:C:602:LEU:HD22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ARG:HE	1:C:86:ARG:N	2.01	0.58
1:A:189:VAL:HG12	1:A:234:PHE:HB2	1.85	0.57
1:A:473:LEU:HD11	1:A:602:LEU:HD22	1.84	0.57
1:B:189:VAL:HG12	1:B:234:PHE:HB2	1.85	0.57
1:B:474:ILE:HD12	1:B:568:LEU:HB3	1.88	0.56
1:A:474:ILE:HD12	1:A:568:LEU:HB3	1.88	0.55
1:A:81:PHE:CZ	1:A:228:TYR:HA	2.42	0.55
1:D:474:ILE:HD12	1:D:568:LEU:HB3	1.88	0.55
1:A:481:ALA:O	1:A:502:ASN:ND2	2.41	0.54
1:C:474:ILE:HD12	1:C:568:LEU:HB3	1.88	0.54
1:B:481:ALA:O	1:B:502:ASN:ND2	2.41	0.54
1:B:599:MET:SD	1:B:612:ARG:NH1	2.81	0.54
1:A:599:MET:SD	1:A:612:ARG:NH1	2.81	0.53
1:D:599:MET:SD	1:D:612:ARG:NH1	2.81	0.53
1:C:123:LEU:HB2	1:C:278:LEU:HD23	1.91	0.53
1:A:981:VAL:H	1:A:1013:ASN:HD21	1.57	0.53
1:C:599:MET:SD	1:C:612:ARG:NH1	2.81	0.53
1:D:123:LEU:HB2	1:D:278:LEU:HD23	1.91	0.53
1:C:481:ALA:O	1:C:502:ASN:ND2	2.41	0.53
1:D:481:ALA:O	1:D:502:ASN:ND2	2.41	0.52
1:B:123:LEU:HB2	1:B:278:LEU:HD23	1.91	0.52
1:A:123:LEU:HB2	1:A:278:LEU:HD23	1.91	0.52
1:D:196:ARG:NH2	1:D:219:GLU:O	2.43	0.52
1:B:193:GLY:O	1:B:198:ARG:NH2	2.43	0.52
1:B:981:VAL:H	1:B:1013:ASN:HD21	1.56	0.52
1:D:193:GLY:O	1:D:198:ARG:NH2	2.43	0.52
1:A:584:ASN:ND2	1:A:646:CYS:SG	2.81	0.52
1:A:193:GLY:O	1:A:198:ARG:NH2	2.43	0.52
1:C:193:GLY:O	1:C:198:ARG:NH2	2.43	0.52
1:A:196:ARG:NH2	1:A:219:GLU:O	2.43	0.52
1:A:360:GLU:HG3	1:A:361:LEU:HD12	1.92	0.52
1:C:981:VAL:H	1:C:1013:ASN:HD21	1.57	0.52
1:C:584:ASN:ND2	1:C:646:CYS:SG	2.81	0.51
1:C:1073:PRO:N	1:C:1074:PRO:CD	2.73	0.51
1:B:360:GLU:HG3	1:B:361:LEU:HD12	1.92	0.51
1:A:299:CYS:SG	1:A:300:LEU:N	2.84	0.51
1:C:196:ARG:NH2	1:C:219:GLU:O	2.43	0.51
1:C:299:CYS:SG	1:C:300:LEU:N	2.84	0.51
1:D:981:VAL:H	1:D:1013:ASN:HD21	1.57	0.51
1:B:81:PHE:CE2	1:B:228:TYR:HA	2.46	0.51
1:D:299:CYS:SG	1:D:300:LEU:N	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ARG:NH2	1:B:219:GLU:O	2.43	0.51
1:A:473:LEU:HD22	1:A:603:GLU:OE1	2.11	0.51
1:B:299:CYS:SG	1:B:300:LEU:N	2.84	0.51
1:D:360:GLU:HG3	1:D:361:LEU:HD12	1.92	0.51
1:B:1073:PRO:N	1:B:1074:PRO:CD	2.73	0.50
1:C:23:PHE:HA	1:C:70:GLU:HA	1.94	0.50
1:B:584:ASN:ND2	1:B:646:CYS:SG	2.81	0.50
1:A:23:PHE:HA	1:A:70:GLU:HA	1.94	0.50
1:D:1073:PRO:N	1:D:1074:PRO:CD	2.73	0.50
1:C:473:LEU:HD22	1:C:603:GLU:OE1	2.11	0.50
1:B:93:ARG:NH1	1:B:237:ASP:OD2	2.44	0.50
1:C:360:GLU:HG3	1:C:361:LEU:HD12	1.92	0.50
1:B:23:PHE:HA	1:B:70:GLU:HA	1.94	0.49
1:D:584:ASN:ND2	1:D:646:CYS:SG	2.81	0.49
1:A:1073:PRO:N	1:A:1074:PRO:CD	2.73	0.49
1:D:23:PHE:HA	1:D:70:GLU:HA	1.94	0.49
1:D:473:LEU:HD22	1:D:603:GLU:OE1	2.12	0.49
1:A:93:ARG:NH1	1:A:237:ASP:OD2	2.44	0.49
1:B:473:LEU:HD22	1:B:603:GLU:OE1	2.12	0.48
1:C:981:VAL:H	1:C:1013:ASN:ND2	2.12	0.48
1:D:981:VAL:H	1:D:1013:ASN:ND2	2.12	0.48
1:B:981:VAL:H	1:B:1013:ASN:ND2	2.12	0.48
1:A:981:VAL:H	1:A:1013:ASN:ND2	2.12	0.47
1:D:86:ARG:N	1:D:86:ARG:NE	2.61	0.47
1:C:299:CYS:HB3	1:C:362:LEU:HD23	1.97	0.47
1:A:1072:ALA:C	1:A:1074:PRO:HD2	2.35	0.47
1:C:849:ARG:O	1:C:853:HIS:ND1	2.37	0.47
1:B:86:ARG:N	1:B:86:ARG:NE	2.62	0.46
1:B:299:CYS:HB3	1:B:362:LEU:HD23	1.97	0.46
1:A:86:ARG:N	1:A:86:ARG:NE	2.62	0.46
1:A:160:HIS:HD2	2:A:2000:ATP:C2	2.32	0.46
1:C:93:ARG:NH1	1:C:237:ASP:OD2	2.44	0.46
1:D:119:VAL:HB	1:D:274:VAL:HG22	1.98	0.46
1:D:1072:ALA:C	1:D:1074:PRO:HD2	2.36	0.46
1:B:119:VAL:HB	1:B:274:VAL:HG22	1.98	0.46
1:C:1072:ALA:C	1:C:1074:PRO:HD2	2.35	0.46
1:D:93:ARG:NH1	1:D:237:ASP:OD2	2.44	0.46
1:B:1072:ALA:C	1:B:1074:PRO:HD2	2.36	0.46
1:C:86:ARG:N	1:C:86:ARG:NE	2.64	0.46
1:D:160:HIS:HD2	2:D:2000:ATP:C2	2.34	0.46
1:D:299:CYS:HB3	1:D:362:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:HIS:HD2	2:C:2000:ATP:C2	2.35	0.45
1:A:82:THR:HG22	1:A:211:ARG:HB3	1.98	0.45
1:A:79:LEU:HD21	1:A:212:TYR:HB2	1.99	0.45
1:C:79:LEU:HD21	1:C:212:TYR:HB2	1.99	0.45
1:C:119:VAL:HB	1:C:274:VAL:HG22	1.97	0.45
1:B:81:PHE:CZ	1:B:228:TYR:HA	2.51	0.45
1:A:119:VAL:HB	1:A:274:VAL:HG22	1.98	0.45
1:D:248:ASN:HB3	1:D:288:ARG:HH21	1.82	0.45
1:A:160:HIS:O	1:A:165:ARG:HB2	2.17	0.45
1:A:299:CYS:HB3	1:A:362:LEU:HD23	1.97	0.45
1:B:160:HIS:O	1:B:165:ARG:HB2	2.17	0.45
1:D:160:HIS:CD2	2:D:2000:ATP:C2	3.05	0.45
1:A:333:ARG:HA	1:A:336:ILE:HD12	2.00	0.44
1:C:248:ASN:HB3	1:C:288:ARG:HH21	1.82	0.44
1:B:79:LEU:HD21	1:B:212:TYR:HB2	1.99	0.44
1:B:160:HIS:HD2	2:B:2000:ATP:C2	2.34	0.44
1:B:248:ASN:HB3	1:B:288:ARG:HH21	1.82	0.44
1:B:160:HIS:CD2	2:B:2000:ATP:C2	3.05	0.44
1:B:908:VAL:HG21	1:B:1065:PHE:HE2	1.83	0.44
1:D:333:ARG:HA	1:D:336:ILE:HD12	2.00	0.44
1:D:354:ARG:O	1:D:357:THR:OG1	2.29	0.44
1:D:908:VAL:HG21	1:D:1065:PHE:HE2	1.83	0.44
1:A:908:VAL:HG21	1:A:1065:PHE:HE2	1.83	0.44
1:A:457:THR:HG22	1:A:459:VAL:H	1.83	0.44
1:C:333:ARG:HA	1:C:336:ILE:HD12	2.00	0.44
1:D:79:LEU:HD21	1:D:212:TYR:HB2	1.99	0.44
1:B:457:THR:HG22	1:B:459:VAL:H	1.83	0.44
1:A:248:ASN:HB3	1:A:288:ARG:HH21	1.82	0.44
1:C:908:VAL:HG21	1:C:1065:PHE:HE2	1.83	0.44
1:A:160:HIS:CD2	2:A:2000:ATP:C2	3.05	0.44
1:C:160:HIS:O	1:C:165:ARG:HB2	2.17	0.44
1:C:203:ASN:HA	1:C:204:PRO:HD3	1.81	0.43
1:B:333:ARG:HA	1:B:336:ILE:HD12	2.00	0.43
1:A:75:ALA:HB3	1:A:93:ARG:HB3	2.00	0.43
1:C:160:HIS:CD2	2:C:2000:ATP:C2	3.06	0.43
1:C:97:ARG:HH21	1:C:249:ARG:HH12	1.67	0.43
1:C:457:THR:HG22	1:C:459:VAL:H	1.83	0.43
1:D:97:ARG:HH21	1:D:249:ARG:HH12	1.67	0.43
1:D:457:THR:HG22	1:D:459:VAL:H	1.83	0.43
1:C:286:LEU:HA	1:C:289:ILE:HD12	2.01	0.43
1:A:97:ARG:HH21	1:A:249:ARG:HH12	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ARG:HG2	1:C:228:TYR:HD2	1.83	0.43
1:C:286:LEU:HG	1:C:289:ILE:HD12	2.01	0.43
1:B:75:ALA:HB3	1:B:93:ARG:HB3	2.00	0.43
1:B:97:ARG:HH21	1:B:249:ARG:HH12	1.67	0.43
1:B:286:LEU:HG	1:B:289:ILE:HD12	2.01	0.43
1:C:79:LEU:N	1:C:89:SER:O	2.52	0.43
1:A:196:ARG:HA	1:A:223:GLU:HB3	2.01	0.43
1:D:286:LEU:HA	1:D:289:ILE:HD12	2.01	0.43
1:A:79:LEU:N	1:A:89:SER:O	2.52	0.42
1:A:893:LEU:HD11	1:C:1015:LEU:HD21	2.01	0.42
1:C:893:LEU:HD11	1:D:1015:LEU:HD21	2.01	0.42
1:C:1058:ARG:HE	1:C:1062:ILE:HD11	1.84	0.42
1:D:286:LEU:HG	1:D:289:ILE:HD12	2.01	0.42
1:C:75:ALA:HB3	1:C:93:ARG:HB3	2.00	0.42
1:D:75:ALA:HB3	1:D:93:ARG:HB3	2.00	0.42
1:B:86:ARG:HG2	1:B:228:TYR:HD2	1.85	0.42
1:A:286:LEU:HG	1:A:289:ILE:HD12	2.01	0.42
1:A:468:VAL:HG22	1:A:569:LEU:HD21	2.02	0.42
1:D:160:HIS:O	1:D:165:ARG:HB2	2.17	0.42
1:B:79:LEU:N	1:B:89:SER:O	2.52	0.42
1:D:196:ARG:HA	1:D:223:GLU:HB3	2.01	0.42
1:B:286:LEU:HA	1:B:289:ILE:HD12	2.01	0.42
1:A:290:GLU:HA	1:A:293:THR:HG22	2.02	0.42
1:D:79:LEU:N	1:D:89:SER:O	2.52	0.42
1:D:1058:ARG:HE	1:D:1062:ILE:HD11	1.84	0.42
1:B:468:VAL:HG22	1:B:569:LEU:HD21	2.02	0.42
1:D:468:VAL:HG22	1:D:569:LEU:HD21	2.02	0.42
1:C:196:ARG:HA	1:C:223:GLU:HB3	2.01	0.42
1:C:468:VAL:HG22	1:C:569:LEU:HD21	2.02	0.42
1:D:710:PHE:O	1:D:711:ARG:HB2	2.20	0.42
1:B:290:GLU:HA	1:B:293:THR:HG22	2.02	0.42
1:B:1058:ARG:HE	1:B:1062:ILE:HD11	1.84	0.41
1:C:511:LEU:HD11	1:C:595:LEU:HD13	2.02	0.41
1:A:286:LEU:HA	1:A:289:ILE:HD12	2.01	0.41
1:B:196:ARG:HA	1:B:223:GLU:HB3	2.01	0.41
1:B:354:ARG:O	1:B:357:THR:OG1	2.29	0.41
1:C:21:THR:OG1	1:C:70:GLU:OE2	2.29	0.41
1:A:203:ASN:HA	1:A:204:PRO:HD3	1.81	0.41
1:A:1058:ARG:HE	1:A:1062:ILE:HD11	1.84	0.41
1:B:511:LEU:HD11	1:B:595:LEU:HD13	2.02	0.41
1:C:910:LYS:HD2	1:C:1054:TRP:HH2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:ARG:HG2	1:D:228:TYR:HD2	1.85	0.41
1:A:710:PHE:O	1:A:711:ARG:HB2	2.20	0.41
1:B:710:PHE:O	1:B:711:ARG:HB2	2.21	0.41
1:A:511:LEU:HD11	1:A:595:LEU:HD13	2.02	0.41
1:C:290:GLU:HA	1:C:293:THR:HG22	2.02	0.41
1:D:849:ARG:O	1:D:853:HIS:ND1	2.37	0.41
1:A:303:ALA:HB2	1:A:366:SER:HB2	2.03	0.41
1:B:132:GLN:HG2	1:B:134:TRP:H	1.86	0.40
1:B:1015:LEU:HD21	1:D:893:LEU:HD11	2.03	0.40
1:D:290:GLU:HA	1:D:293:THR:HG22	2.02	0.40
1:D:910:LYS:HD2	1:D:1054:TRP:HH2	1.86	0.40
1:A:81:PHE:HB2	1:A:84:SER:OG	2.21	0.40
1:C:106:LEU:HD12	1:C:110:SER:HB3	2.03	0.40
1:C:710:PHE:O	1:C:711:ARG:HB2	2.20	0.40
1:A:86:ARG:HG2	1:A:228:TYR:HD2	1.86	0.40
1:A:849:ARG:O	1:A:853:HIS:ND1	2.37	0.40
1:A:910:LYS:HD2	1:A:1054:TRP:HH2	1.86	0.40
1:D:511:LEU:HD11	1:D:595:LEU:HD13	2.02	0.40
1:B:303:ALA:HB2	1:B:366:SER:HB2	2.04	0.40
1:C:1073:PRO:CD	1:C:1074:PRO:HD2	2.51	0.40
1:B:82:THR:HG22	1:B:211:ARG:HB3	2.04	0.40
1:A:214:TRP:CE3	1:A:215:ARG:HB2	2.57	0.40
1:C:132:GLN:HG2	1:C:134:TRP:H	1.87	0.40
1:C:214:TRP:CE3	1:C:215:ARG:HB2	2.57	0.40
1:D:82:THR:HG22	1:D:211:ARG:HB3	2.03	0.40
1:D:106:LEU:HD12	1:D:110:SER:HB3	2.03	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	936/1254 (75%)	881 (94%)	55 (6%)	0	100	100
1	B	936/1254 (75%)	881 (94%)	55 (6%)	0	100	100
1	C	936/1254 (75%)	881 (94%)	55 (6%)	0	100	100
1	D	936/1254 (75%)	882 (94%)	54 (6%)	0	100	100
All	All	3744/5016 (75%)	3525 (94%)	219 (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	811/1063 (76%)	799 (98%)	12 (2%)	65	86
1	B	811/1063 (76%)	799 (98%)	12 (2%)	65	86
1	C	811/1063 (76%)	799 (98%)	12 (2%)	65	86
1	D	811/1063 (76%)	799 (98%)	12 (2%)	65	86
All	All	3244/4252 (76%)	3196 (98%)	48 (2%)	66	86

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	13	LYS
1	B	86	ARG
1	B	93	ARG
1	B	197	ASN
1	B	405	ASN
1	B	570	ASN
1	B	615	LEU
1	B	633	ASN
1	B	782	ASN
1	B	878	ARG
1	B	1008	VAL
1	B	1058	ARG
1	A	13	LYS

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Mol	Chain	Res	Type
1	A	86	ARG
1	A	93	ARG
1	A	197	ASN
1	A	405	ASN
1	A	570	ASN
1	A	615	LEU
1	A	633	ASN
1	A	782	ASN
1	A	878	ARG
1	A	1008	VAL
1	A	1058	ARG
1	C	13	LYS
1	C	86	ARG
1	C	93	ARG
1	C	197	ASN
1	C	405	ASN
1	C	570	ASN
1	C	615	LEU
1	C	633	ASN
1	C	782	ASN
1	C	878	ARG
1	C	1008	VAL
1	C	1058	ARG
1	D	13	LYS
1	D	86	ARG
1	D	93	ARG
1	D	197	ASN
1	D	405	ASN
1	D	570	ASN
1	D	615	LEU
1	D	633	ASN
1	D	782	ASN
1	D	878	ARG
1	D	1008	VAL
1	D	1058	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	197	ASN
1	B	405	ASN
1	B	425	HIS

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Mol	Chain	Res	Type
1	B	633	ASN
1	B	782	ASN
1	B	1010	GLN
1	B	1013	ASN
1	B	1047	HIS
1	A	197	ASN
1	A	405	ASN
1	A	425	HIS
1	A	633	ASN
1	A	782	ASN
1	A	1010	GLN
1	A	1013	ASN
1	A	1047	HIS
1	C	197	ASN
1	C	405	ASN
1	C	425	HIS
1	C	633	ASN
1	C	669	GLN
1	C	782	ASN
1	C	1010	GLN
1	C	1013	ASN
1	C	1047	HIS
1	D	197	ASN
1	D	405	ASN
1	D	425	HIS
1	D	633	ASN
1	D	782	ASN
1	D	1010	GLN
1	D	1013	ASN
1	D	1047	HIS

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)

4 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	ATP	C	2000	-	26,33,33	0.90	1 (3%)	31,52,52	1.47	4 (12%)
2	ATP	D	2000	-	26,33,33	0.90	1 (3%)	31,52,52	1.47	4 (12%)
2	ATP	B	2000	-	26,33,33	0.89	1 (3%)	31,52,52	1.47	4 (12%)
2	ATP	A	2000	-	26,33,33	0.90	1 (3%)	31,52,52	1.46	4 (12%)

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	ATP	C	2000	-	-	3/18/38/38	0/3/3/3
2	ATP	D	2000	-	-	3/18/38/38	0/3/3/3
2	ATP	B	2000	-	-	3/18/38/38	0/3/3/3
2	ATP	A	2000	-	-	3/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2000	ATP	C5-C4	2.40	1.47	1.40
2	D	2000	ATP	C5-C4	2.40	1.47	1.40
2	A	2000	ATP	C5-C4	2.38	1.47	1.40
2	B	2000	ATP	C5-C4	2.37	1.47	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2000	ATP	PB-O3B-PG	-3.65	120.29	132.83
2	B	2000	ATP	PB-O3B-PG	-3.65	120.30	132.83
2	A	2000	ATP	PB-O3B-PG	-3.65	120.31	132.83
2	C	2000	ATP	PB-O3B-PG	-3.64	120.35	132.83
2	C	2000	ATP	C3'-C2'-C1'	3.36	106.03	100.98
2	D	2000	ATP	C3'-C2'-C1'	3.34	106.01	100.98
2	A	2000	ATP	C3'-C2'-C1'	3.30	105.94	100.98
2	B	2000	ATP	C3'-C2'-C1'	3.30	105.94	100.98
2	B	2000	ATP	C4-C5-N7	-2.73	106.55	109.40
2	D	2000	ATP	C4-C5-N7	-2.73	106.56	109.40
2	C	2000	ATP	C4-C5-N7	-2.68	106.60	109.40
2	A	2000	ATP	C4-C5-N7	-2.65	106.64	109.40
2	C	2000	ATP	N3-C2-N1	-2.65	124.54	128.68
2	D	2000	ATP	N3-C2-N1	-2.62	124.58	128.68
2	B	2000	ATP	N3-C2-N1	-2.59	124.64	128.68
2	A	2000	ATP	N3-C2-N1	-2.58	124.65	128.68

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2000	ATP	C3'-C4'-C5'-O5'
2	A	2000	ATP	C3'-C4'-C5'-O5'
2	C	2000	ATP	C3'-C4'-C5'-O5'
2	D	2000	ATP	C3'-C4'-C5'-O5'
2	B	2000	ATP	O4'-C4'-C5'-O5'
2	A	2000	ATP	O4'-C4'-C5'-O5'
2	C	2000	ATP	O4'-C4'-C5'-O5'
2	D	2000	ATP	O4'-C4'-C5'-O5'
2	B	2000	ATP	C5'-O5'-PA-O1A
2	A	2000	ATP	C5'-O5'-PA-O1A
2	C	2000	ATP	C5'-O5'-PA-O1A
2	D	2000	ATP	C5'-O5'-PA-O1A

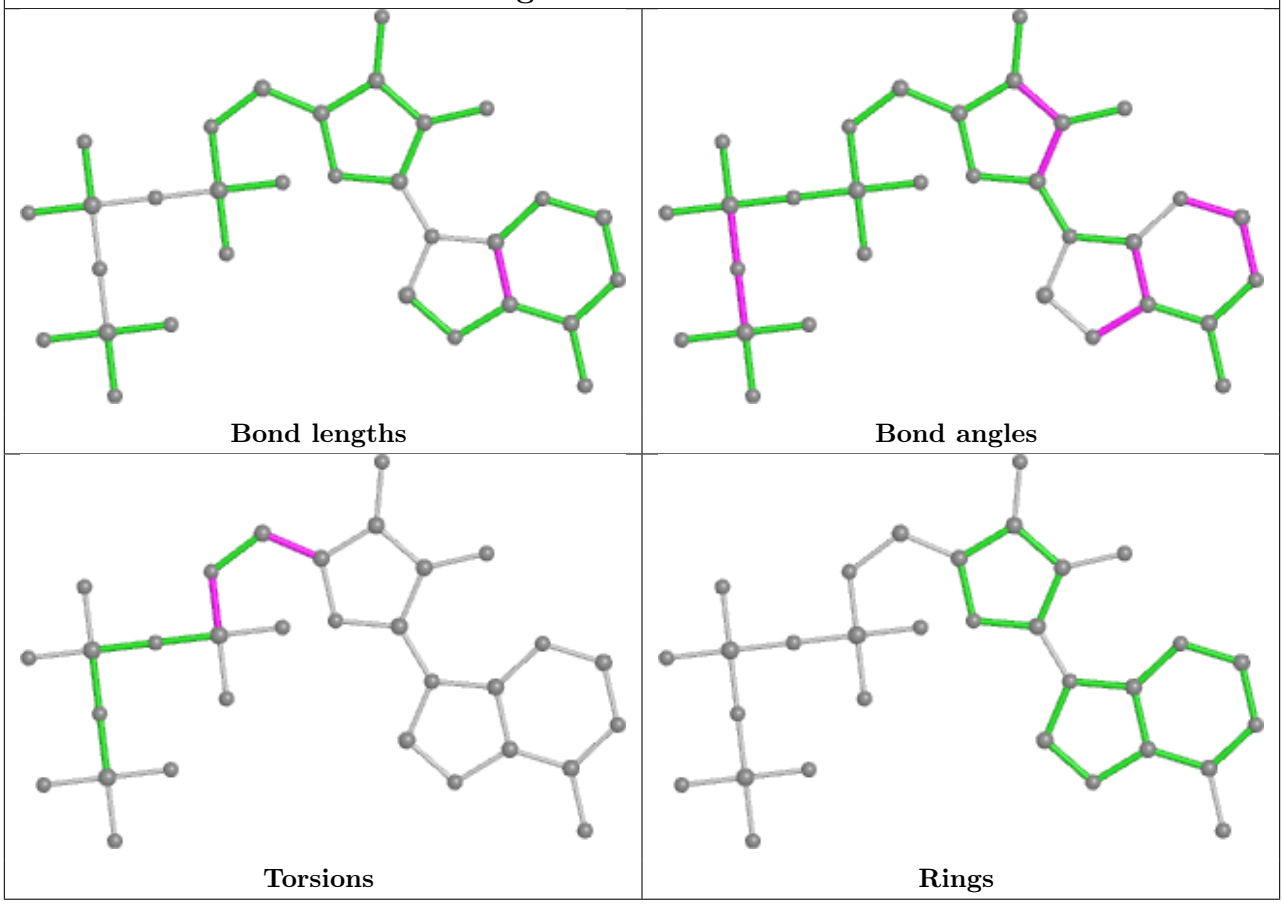
There are no ring outliers.

4 monomers are involved in 8 short contacts:

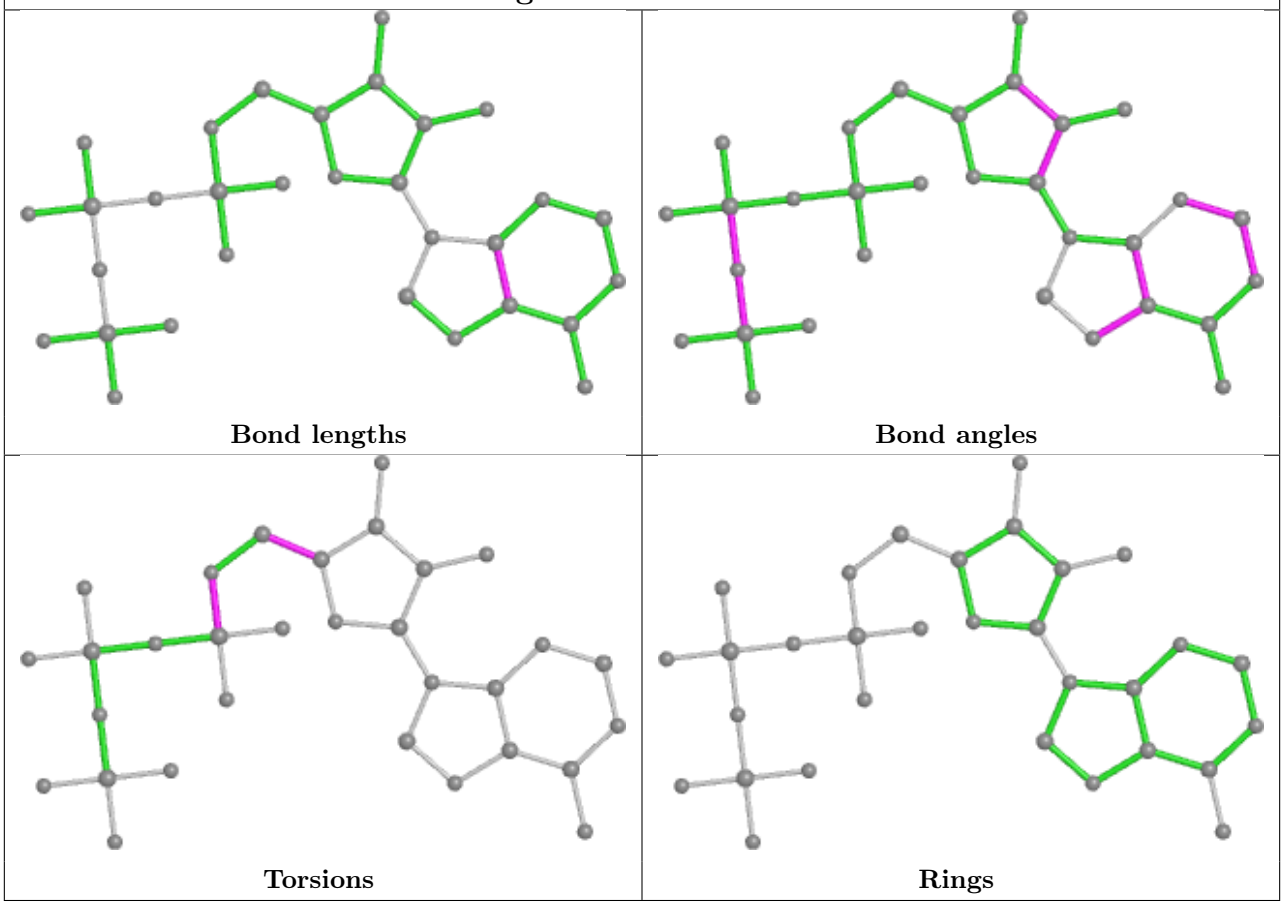
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2000	ATP	2	0
2	D	2000	ATP	2	0
2	B	2000	ATP	2	0
2	A	2000	ATP	2	0

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.

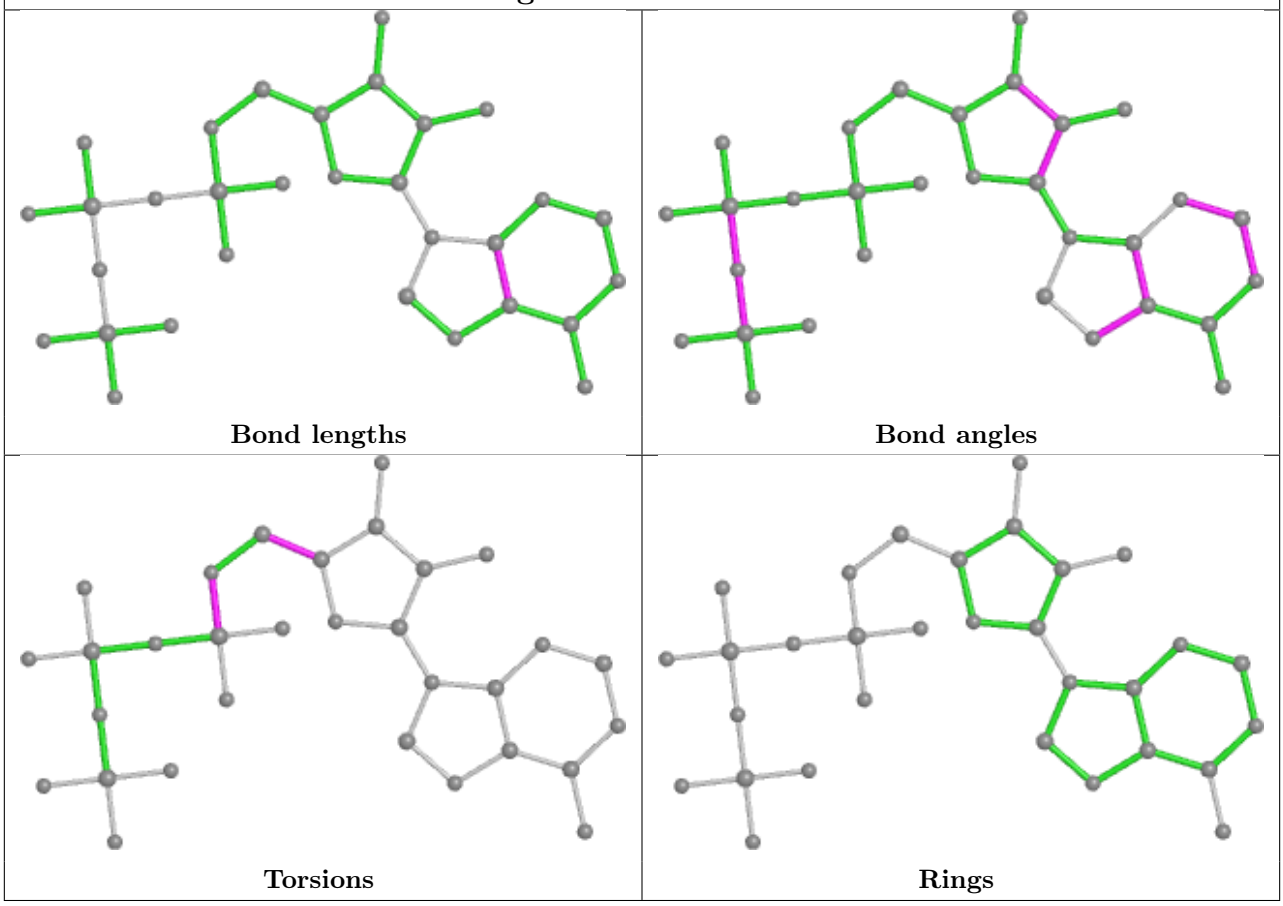
Ligand ATP C 2000

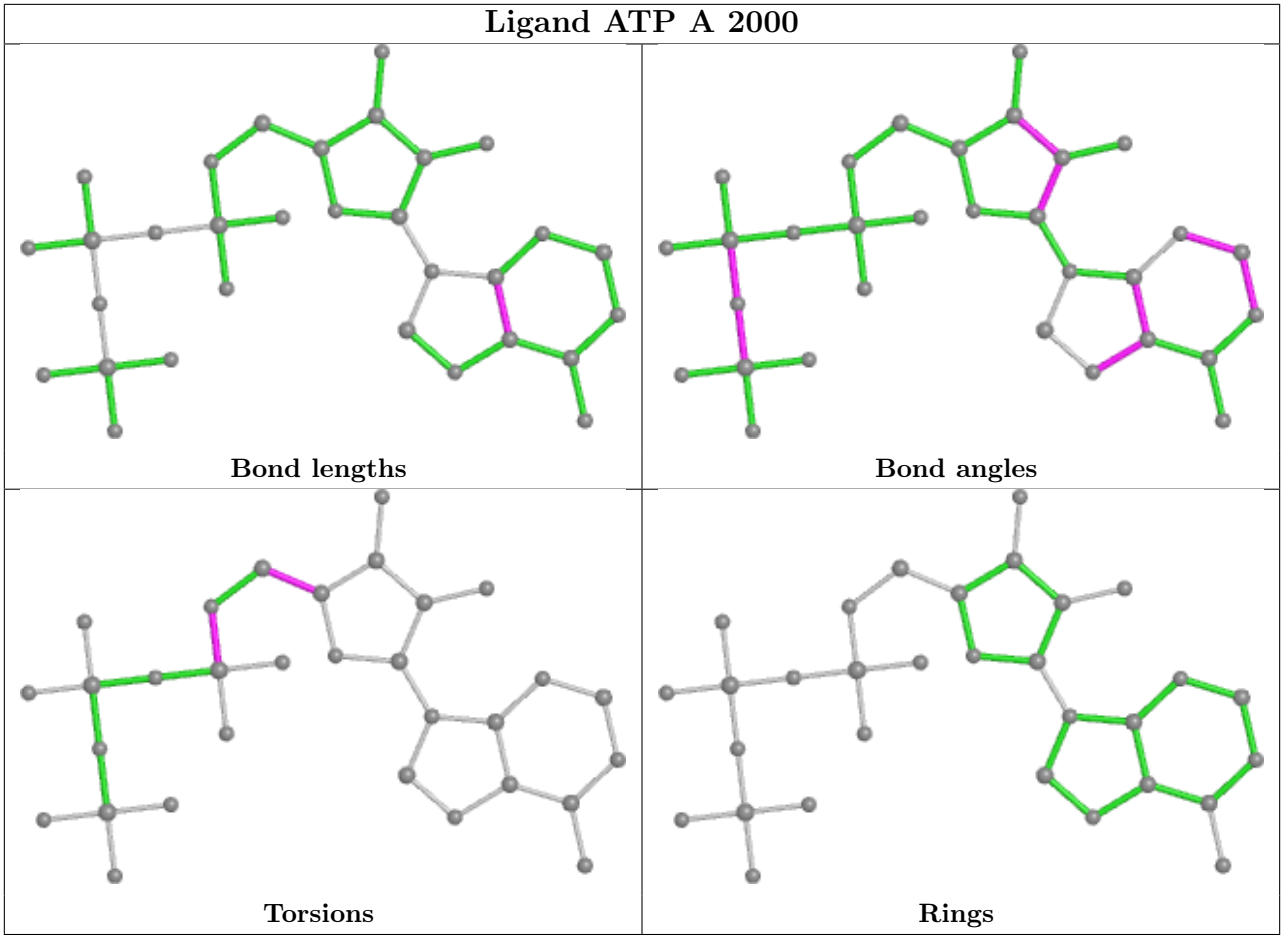


Ligand ATP D 2000



Ligand ATP B 2000





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.

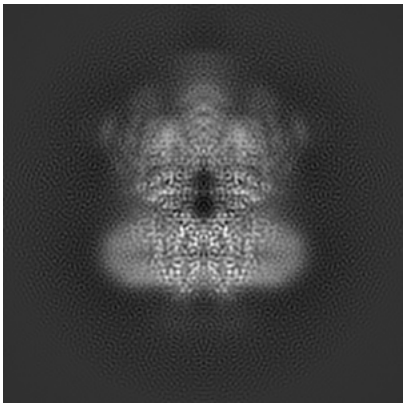
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7083. These allow visual inspection of the internal detail of the map and identification of artifacts.

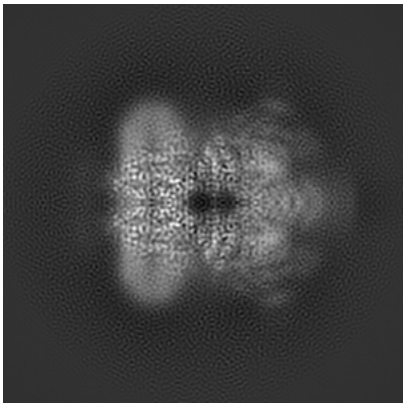
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

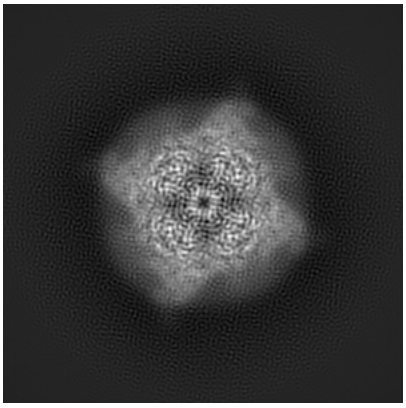
6.1.1 Primary map



X



Y

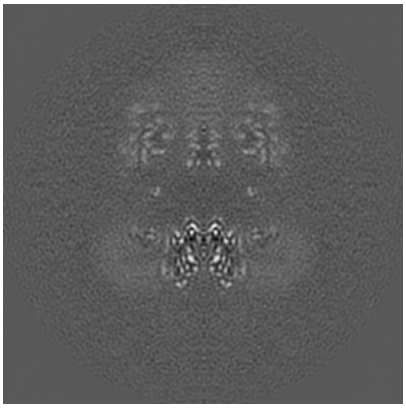


Z

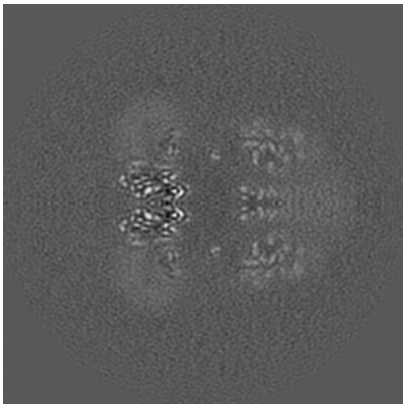
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

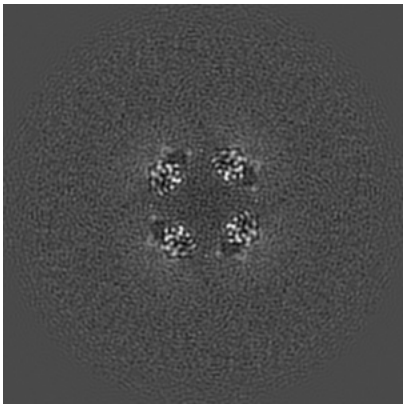
6.2.1 Primary map



X Index: 129



Y Index: 129

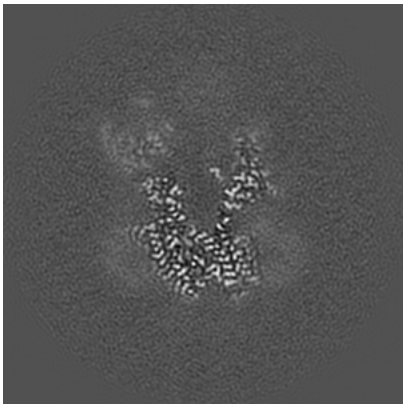


Z Index: 129

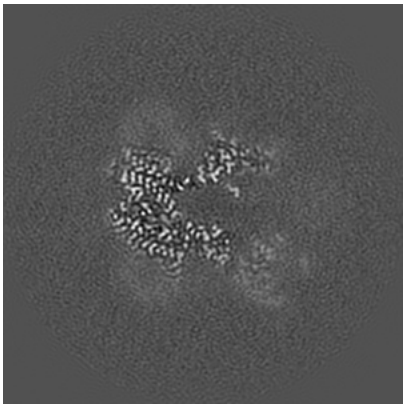
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

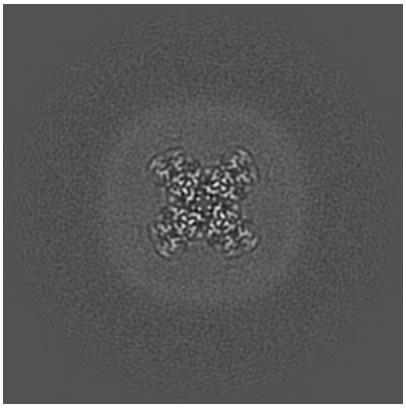
6.3.1 Primary map



X Index: 113



Y Index: 145

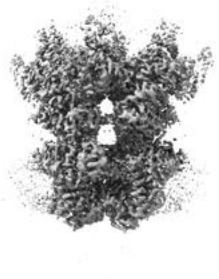


Z Index: 89

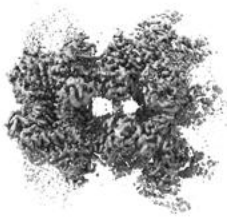
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

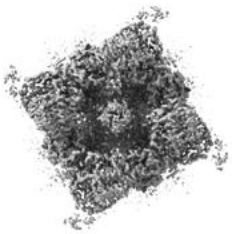
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0313. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

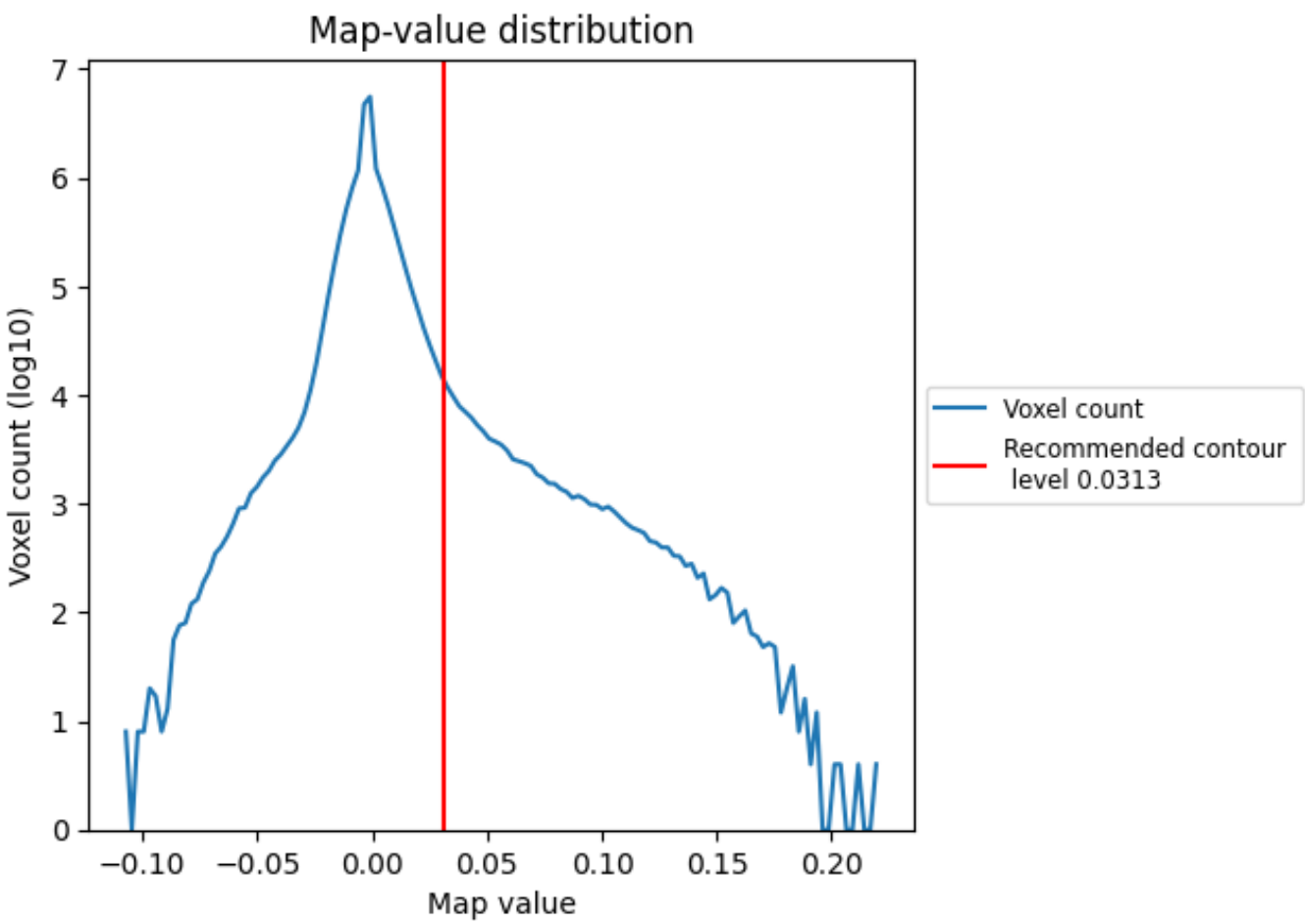
6.5 Mask visualisation (i)

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

7 Map analysis (i)

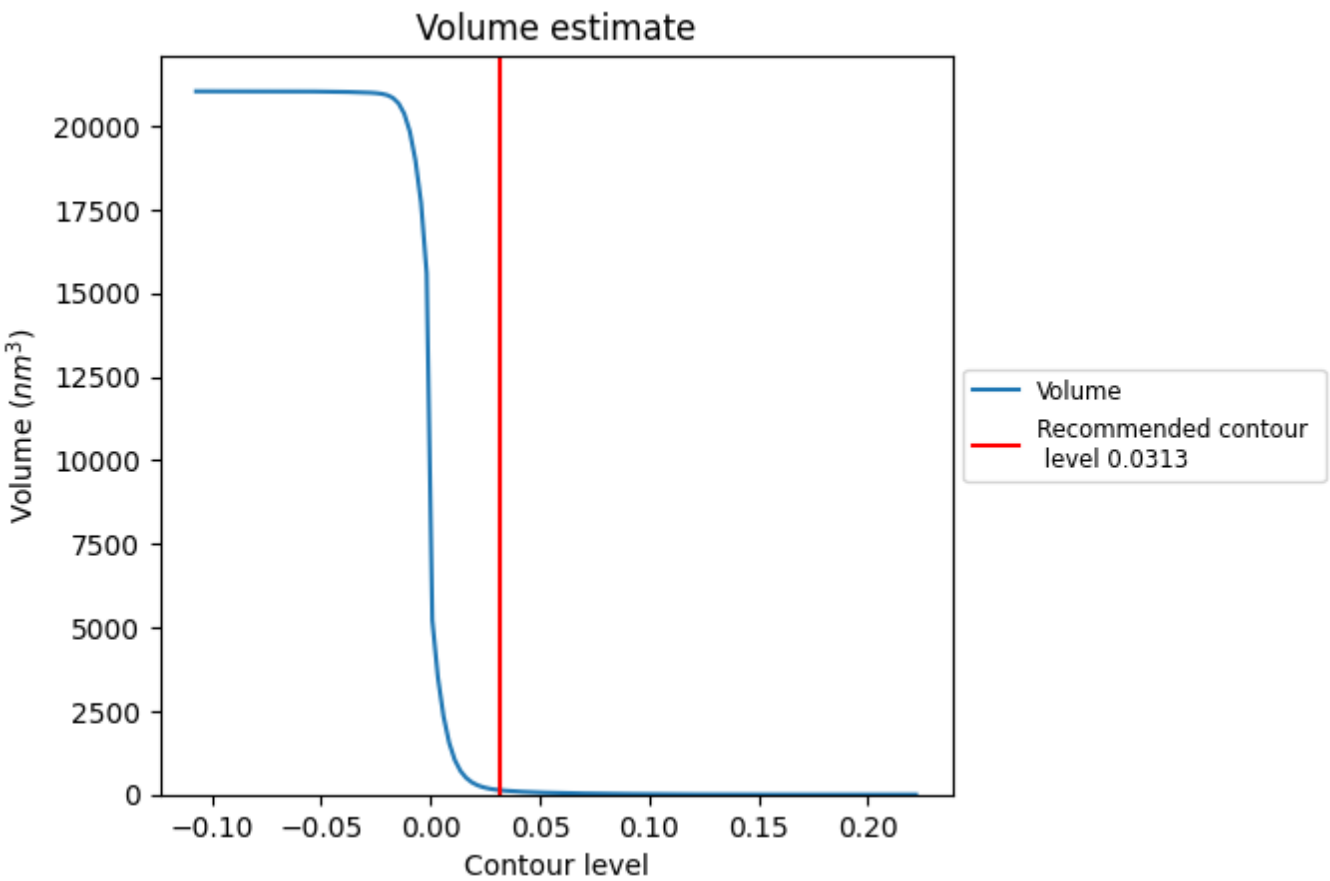
This section contains the results of statistical analysis of the map.

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.

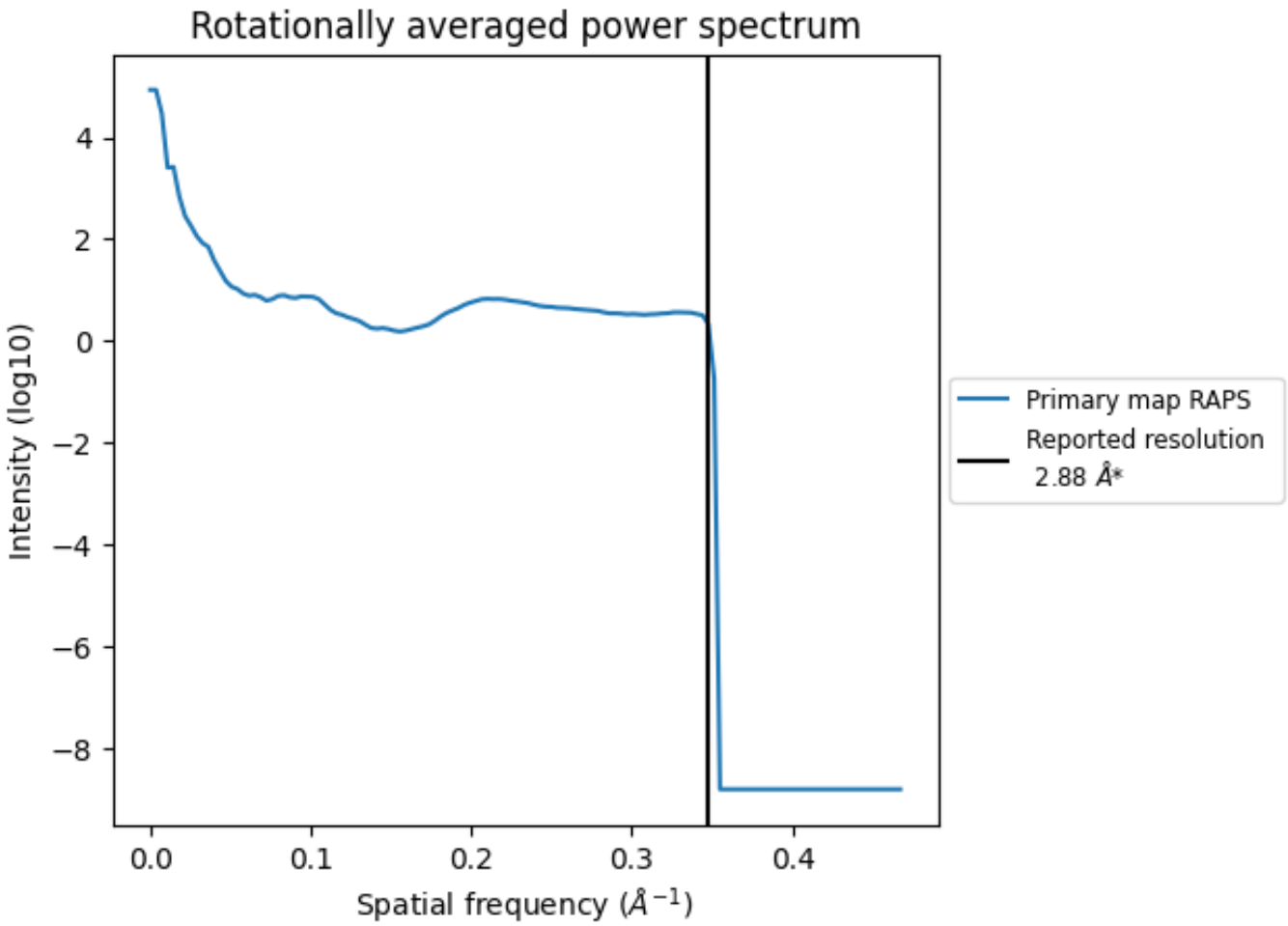
7.2 Volume estimate (i)



The volume at the recommended contour level is 135 nm^3; this corresponds to an approximate mass of 122 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 0.347 Å^{-1}

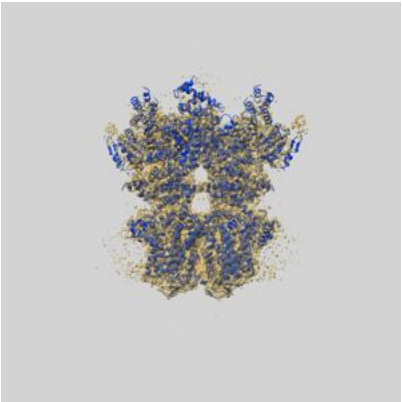
8 Fourier-Shell correlation (i)

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

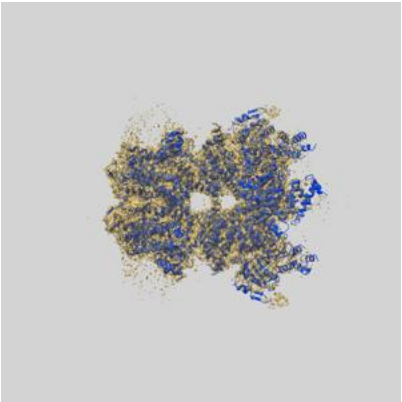
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7083 and PDB model 6BCO. Per-residue inclusion information can be found in section 3 on page 9.

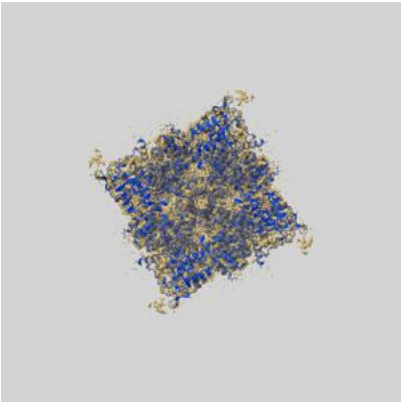
9.1 Map-model overlay (i)



X



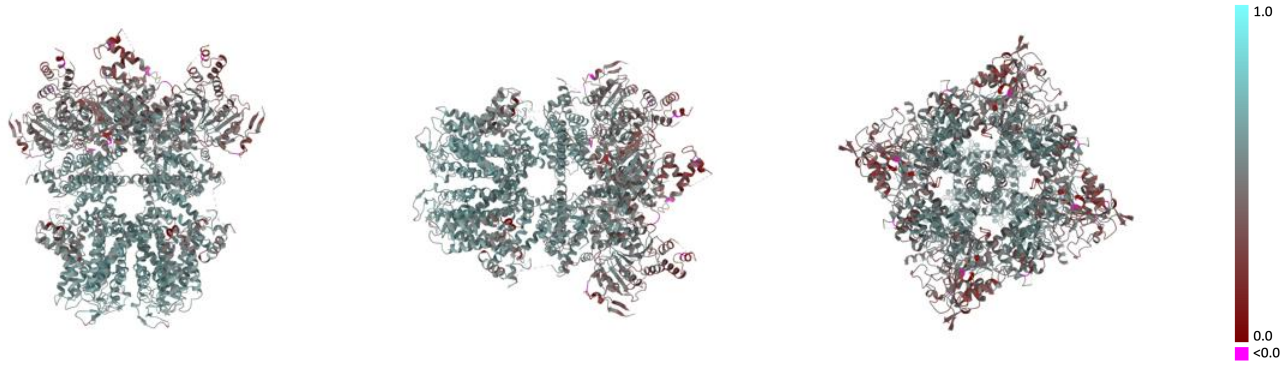
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0313 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.

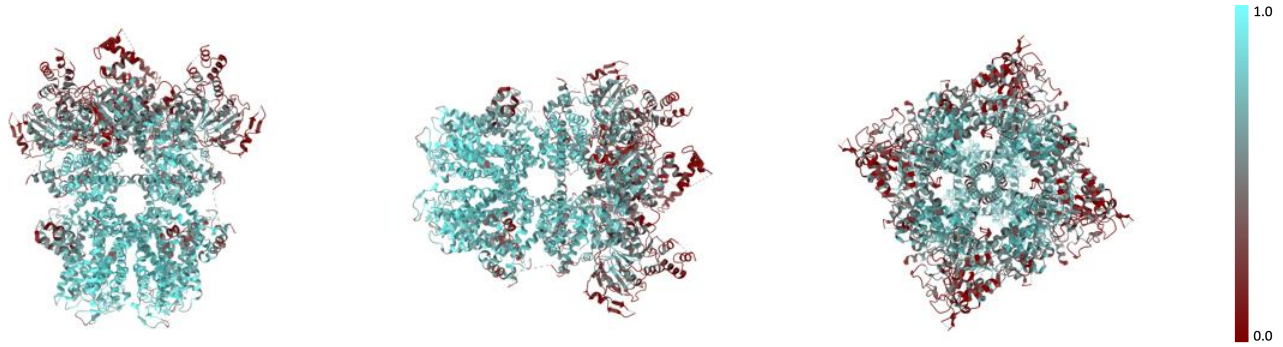
9.2 Q-score mapped to coordinate model (i)



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.

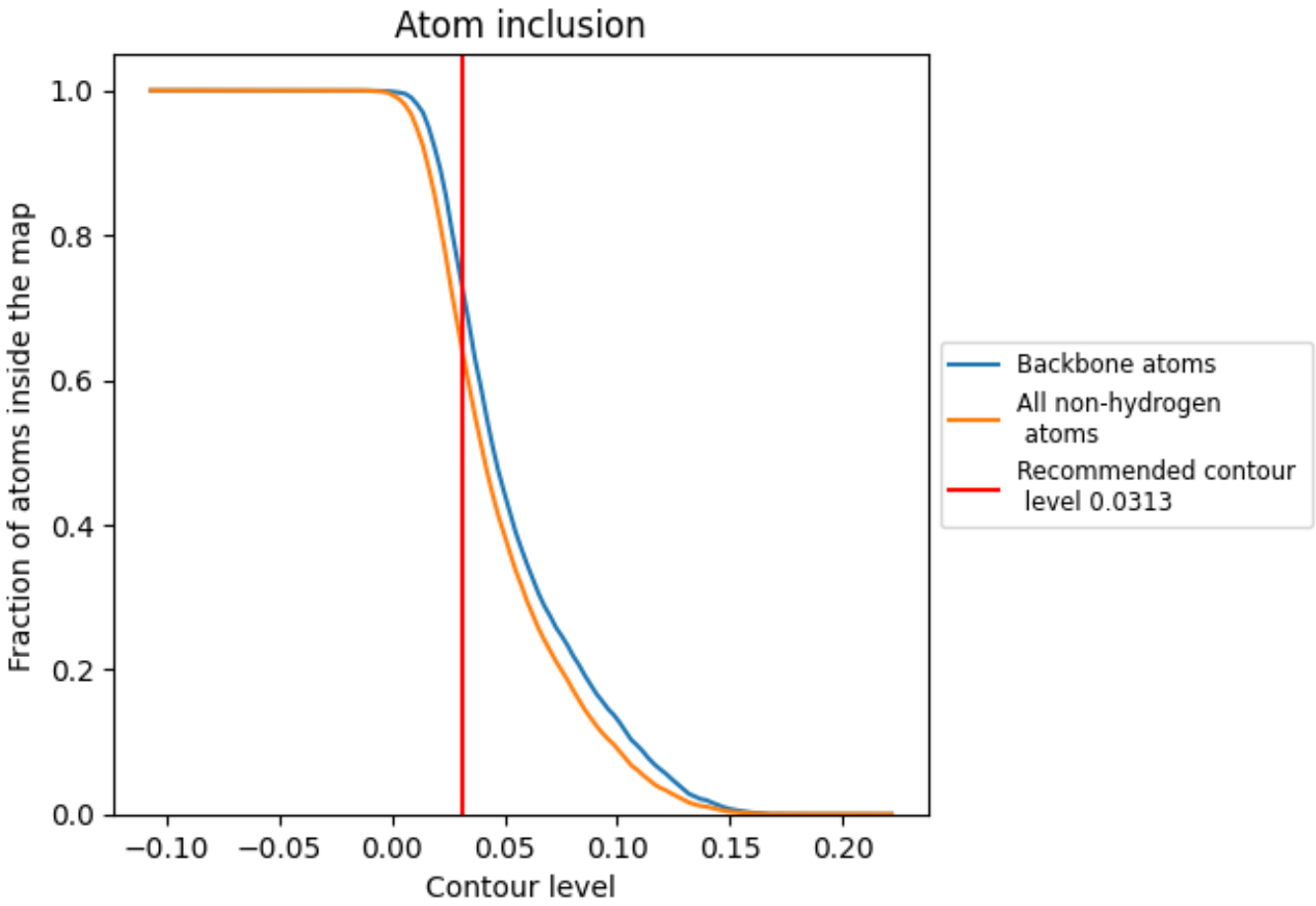
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0313).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 64% 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 (0.0313) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6396	0.5090
A	0.6398	0.5090
B	0.6398	0.5100
C	0.6394	0.5090
D	0.6395	0.5090