



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 17, 2017 – 06:08 PM 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 : unknown
Resolution : 3.54 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

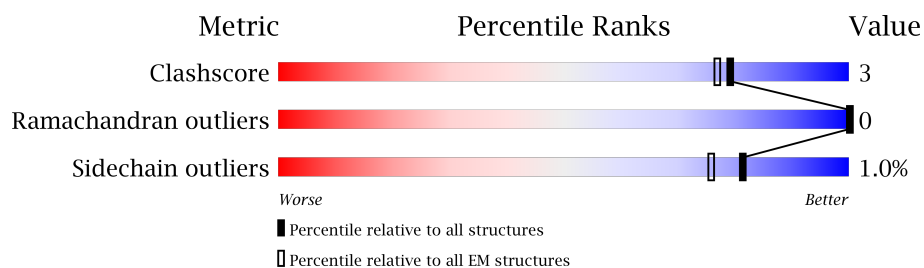
1 Overall quality at a glance

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1254	70% 7% 23%
1	B	1254	70% 7% 23%
1	C	1254	70% 7% 23%
1	D	1254	70% 7% 23%

2 Entry composition

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

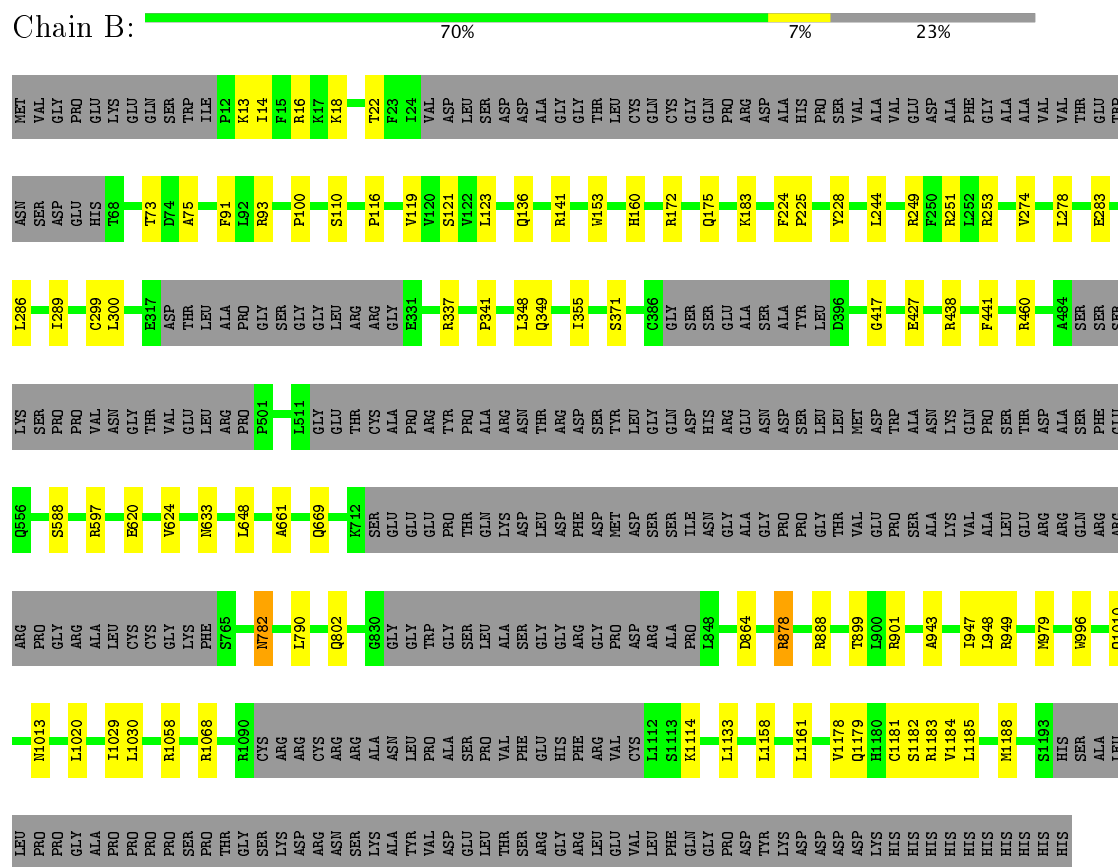
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

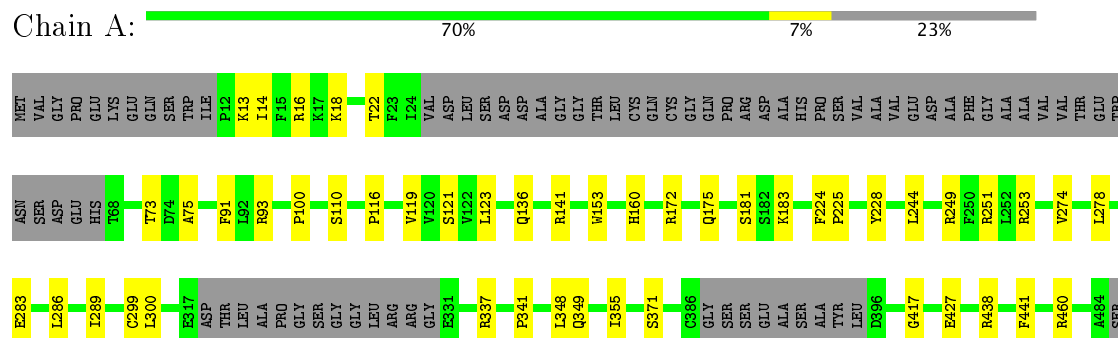
3 Residue-property plots

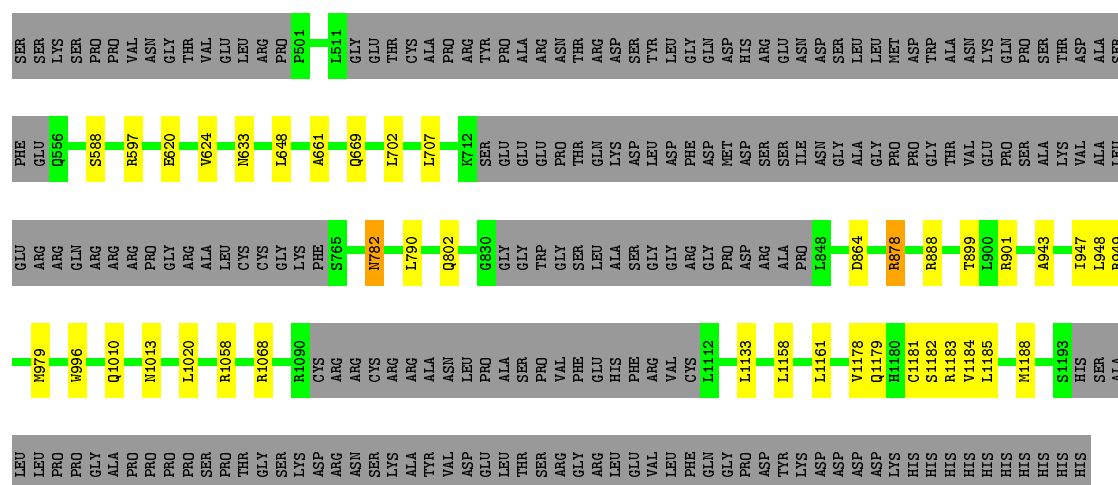
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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



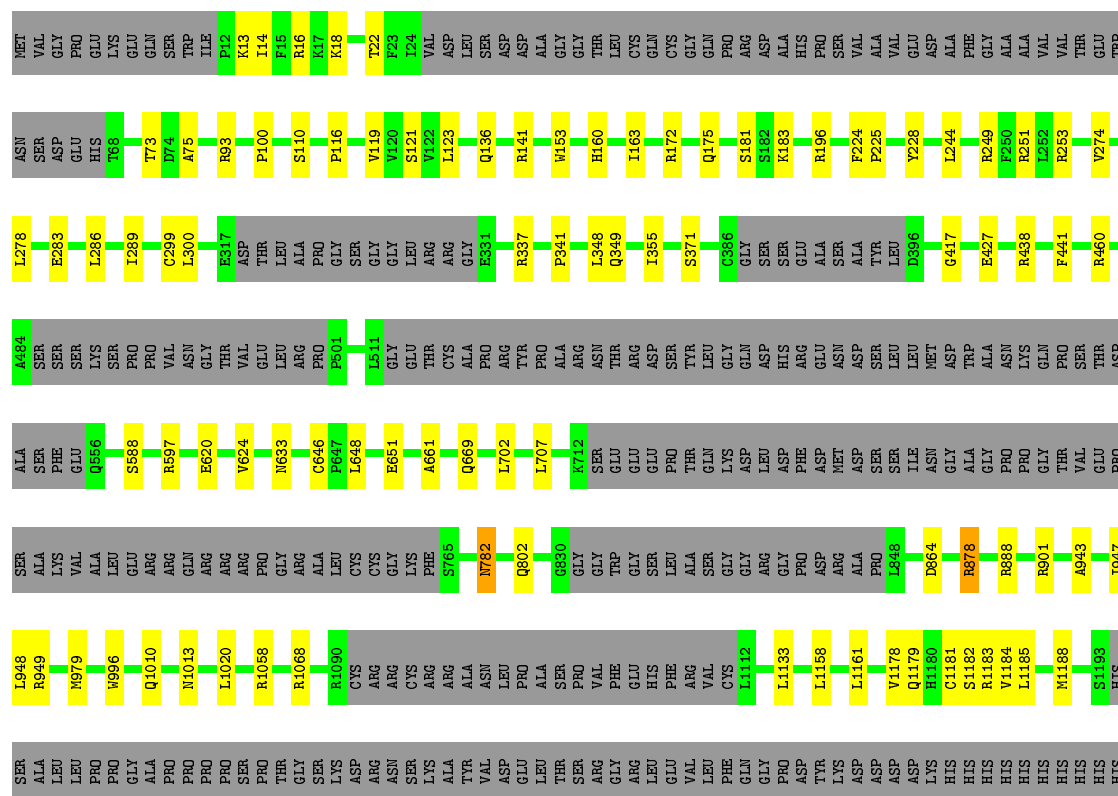
- Molecule 1: Transient receptor potential cation channel subfamily M member 4





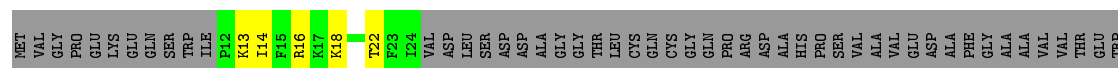
- Molecule 1: Transient receptor potential cation channel subfamily M member 4

Chain C: 70% 7% 23%



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

Chain D: 70% 7% 23%



[illegible]

4 Experimental information

Property	Value	Source
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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	46730	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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: 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	$\# Z > 2$	RMSZ	$\# Z > 2$
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 [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	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:HD12	1:D:948:LEU:O	1.84	0.78
1:B:948:LEU:O	1:B:948:LEU:HD12	1.84	0.77
1:C:948:LEU:HD12	1:C:948:LEU:O	1.85	0.76
1:A:948:LEU:O	1:A:948:LEU:HD12	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:A:14:ILE:HG22	1:A: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: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:996:TRP:O	1:D:1010:GLN:NE2	2.41	0.54
1:D:75:ALA:HB3	1:D:93:ARG:HB2	1.89	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:A:175:GLN:HG3	1:A:183:LYS:HE2	1.94	0.50
1:A:141:ARG:HB2	1:A:371:SER:HB2	1.94	0.50
1:B:175:GLN:HG3	1:B: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:1179:GLN:O	1:B:1183:ARG:N	2.42	0.49
1:B:299:CYS:SG	1:B:300:LEU:N	2.85	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:A:597:ARG:NH2	1:A:620:GLU:OE1	2.49	0.46
1:B:597:ARG:NH2	1:B: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:C:100:PRO:HG3	1:C:253:ARG:HG2	1.98	0.45
1:A:1133:LEU:HD13	1:C:181:SER:HB2	1.99	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:A:1184:VAL:O	1:A:1188:MET:N	2.44	0.44
1:A:224:PHE:HE2	1:A:244:LEU:HD11	1.83	0.44
1:B:100:PRO:HG3	1:B:253:ARG:HG2	1.98	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: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: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: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:A:1158:LEU:HD23	1:A:1161:LEU:HD12	2.02	0.42
1:B:116:PRO:HG3	1:B:153:TRP:CE2	2.55	0.42
1:D:121:SER:HB2	1:D:251:ARG:HH21	1.85	0.42
1:D:948:LEU:C	1:D:948:LEU:HD12	2.39	0.42
1:C:163:ILE:HG13	1:C:163:ILE:H	1.59	0.41
1:C:948:LEU:C	1:C:948:LEU:HD12	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:160:HIS:HD2	1:C:225:PRO:HG2	1.85	0.41
1:C:121:SER:HB2	1:C:251:ARG:HH21	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:A:121:SER:HB2	1:A:251:ARG:HH21	1.85	0.41
1:A:948:LEU:C	1:A:948:LEU:HD12	2.39	0.41
1:B:1181:CYS:O	1:B:1185:LEU:N	2.44	0.41
1:A:979:MET:HE1	1:A:1020:LEU:HD13	2.03	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:C:438:ARG:HB3	1:C:441:PHE:HD2	1.86	0.41
1:D:1180:HIS:O	1:D:1184:VAL:N	2.49	0.41
1:D:979:MET:HE1	1:D:1020:LEU:HD13	2.03	0.41
1:C:702:LEU:HD21	1:C:707:LEU:HD12	2.03	0.41
1:A:75:ALA:HB1	1:A:91:PHE:HE2	1.85	0.40
1:B:979:MET:HE1	1:B:1020:LEU:HD13	2.03	0.40
1:C:979:MET:HE1	1:C:1020:LEU:HD13	2.03	0.40
1:A:702:LEU:HD21	1:A:707:LEU:HD12	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: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:HD2	1:B:1114:LYS:HA	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 ⓘ

5.3.1 Protein backbone ⓘ

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 ⓘ

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%)	80	91
1	B	800/1063 (75%)	792 (99%)	8 (1%)	80	91
1	C	800/1063 (75%)	792 (99%)	8 (1%)	80	91
1	D	800/1063 (75%)	792 (99%)	8 (1%)	80	91
All	All	3200/4252 (75%)	3168 (99%)	32 (1%)	81	91

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

Some 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 carbohydrates 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.