



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 20, 2018 – 01:37 am GMT

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/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

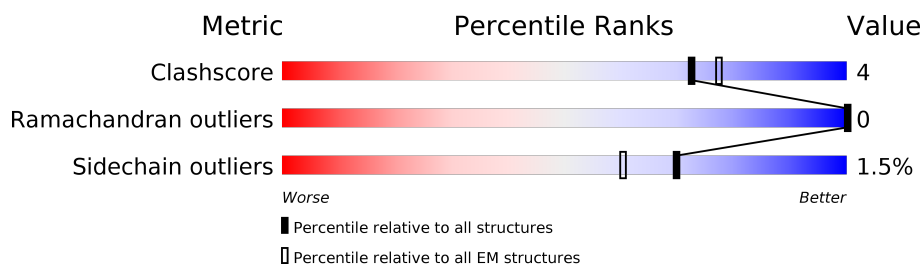
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

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  $\geq 3$ , 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	 68% 8% 24%
1	B	1254	 68% 7% 24%
1	C	1254	 68% 8% 24%
1	D	1254	 68% 7% 24%

## 2 Entry composition

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
1	B	952	Total	C	N	O	S	0	0
			7577	4884	1322	1336	35		
1	A	952	Total	C	N	O	S	0	0
			7577	4884	1322	1336	35		
1	C	952	Total	C	N	O	S	0	0
			7577	4884	1322	1336	35		
1	D	952	Total	C	N	O	S	0	0
			7577	4884	1322	1336	35		

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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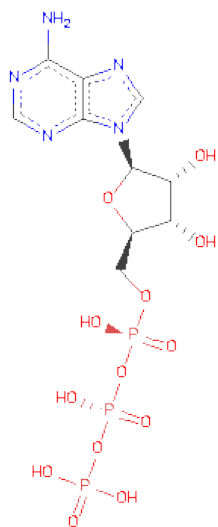
Chain	Residue	Modelled	Actual	Comment	Reference
C	1237	ASP	-	expression tag	UNP Q7TN37
C	1238	TYR	-	expression tag	UNP Q7TN37
C	1239	LYS	-	expression tag	UNP Q7TN37
C	1240	ASP	-	expression tag	UNP Q7TN37
C	1241	ASP	-	expression tag	UNP Q7TN37
C	1242	ASP	-	expression tag	UNP Q7TN37
C	1243	ASP	-	expression 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
2	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
2	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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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	

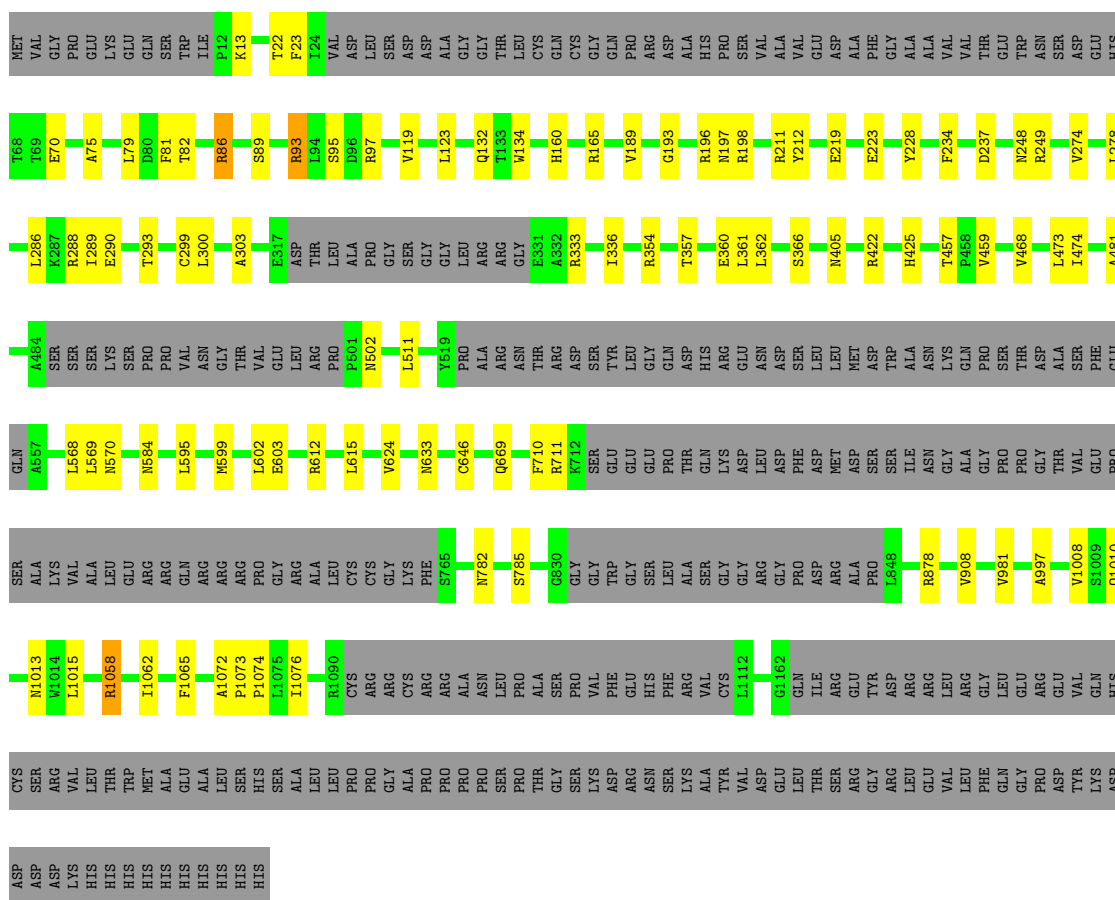


### 3 Residue-property plots

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.

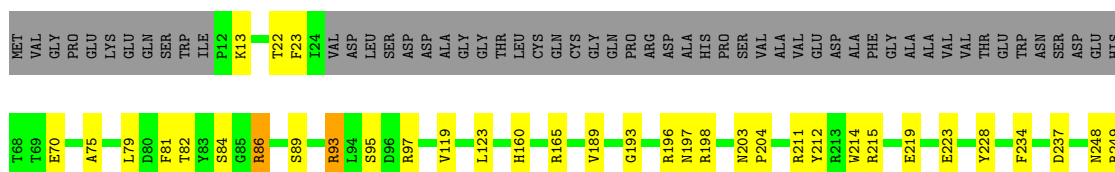
- Molecule 1: Transient receptor potential cation channel subfamily M member 4

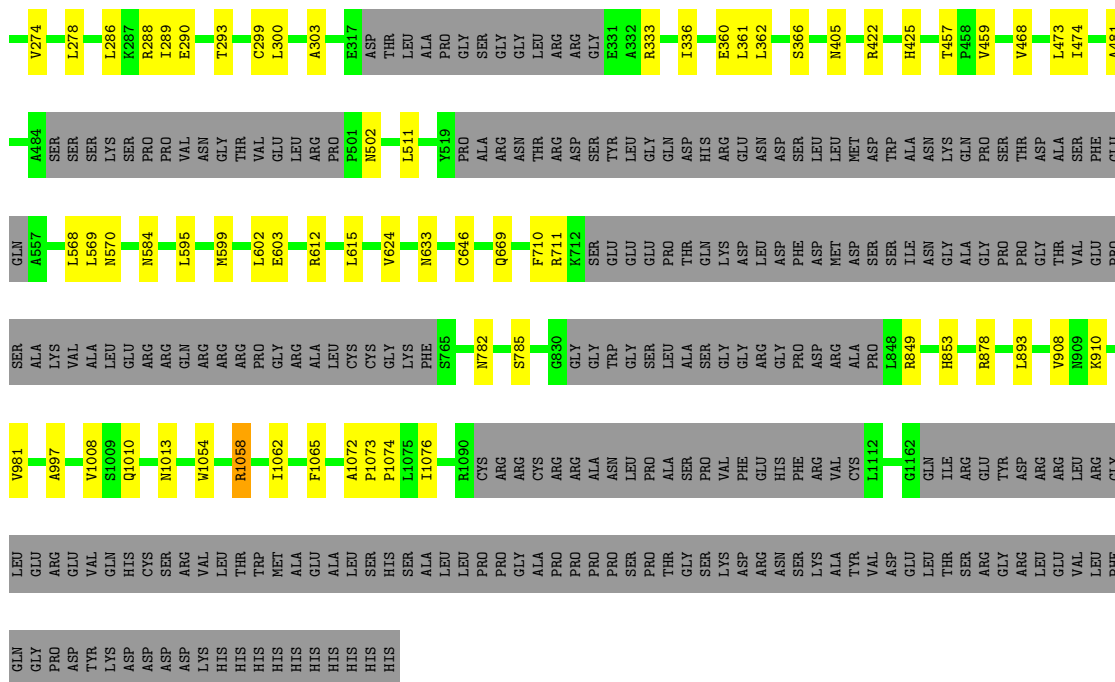
Chain B: 



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

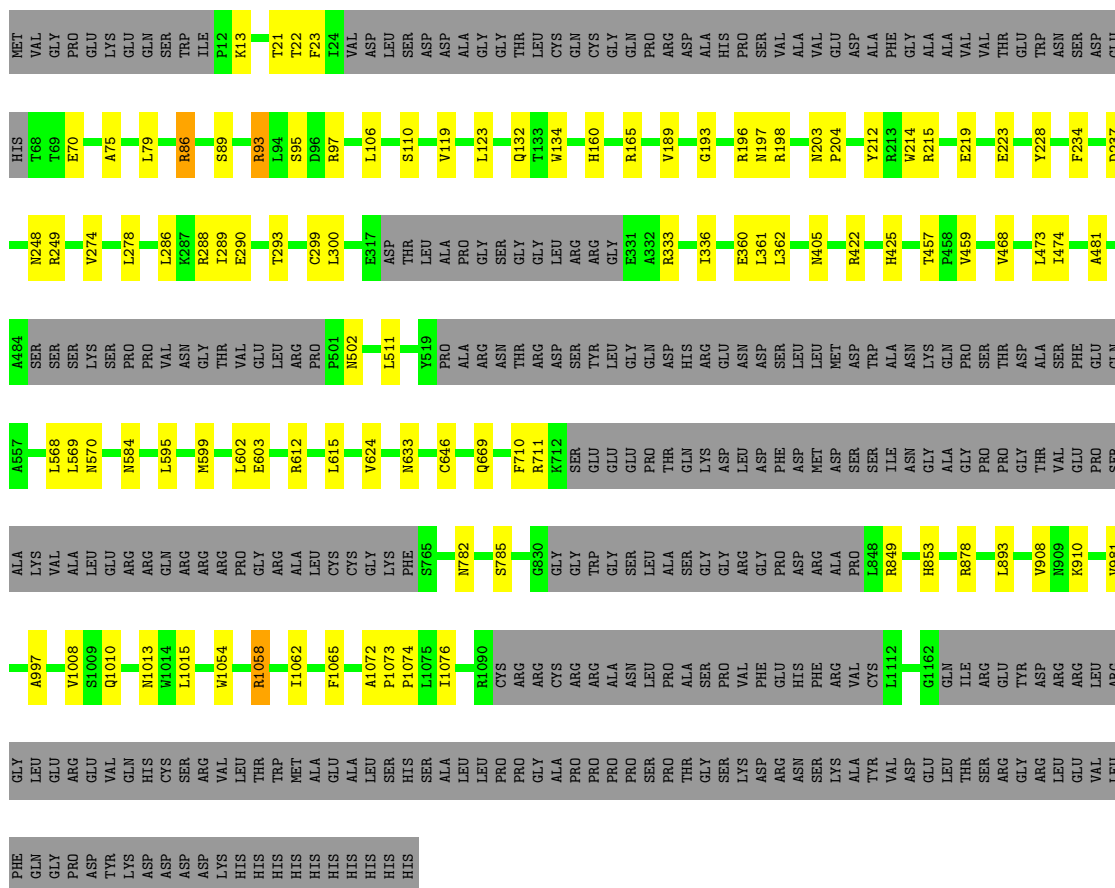
Chain A: 





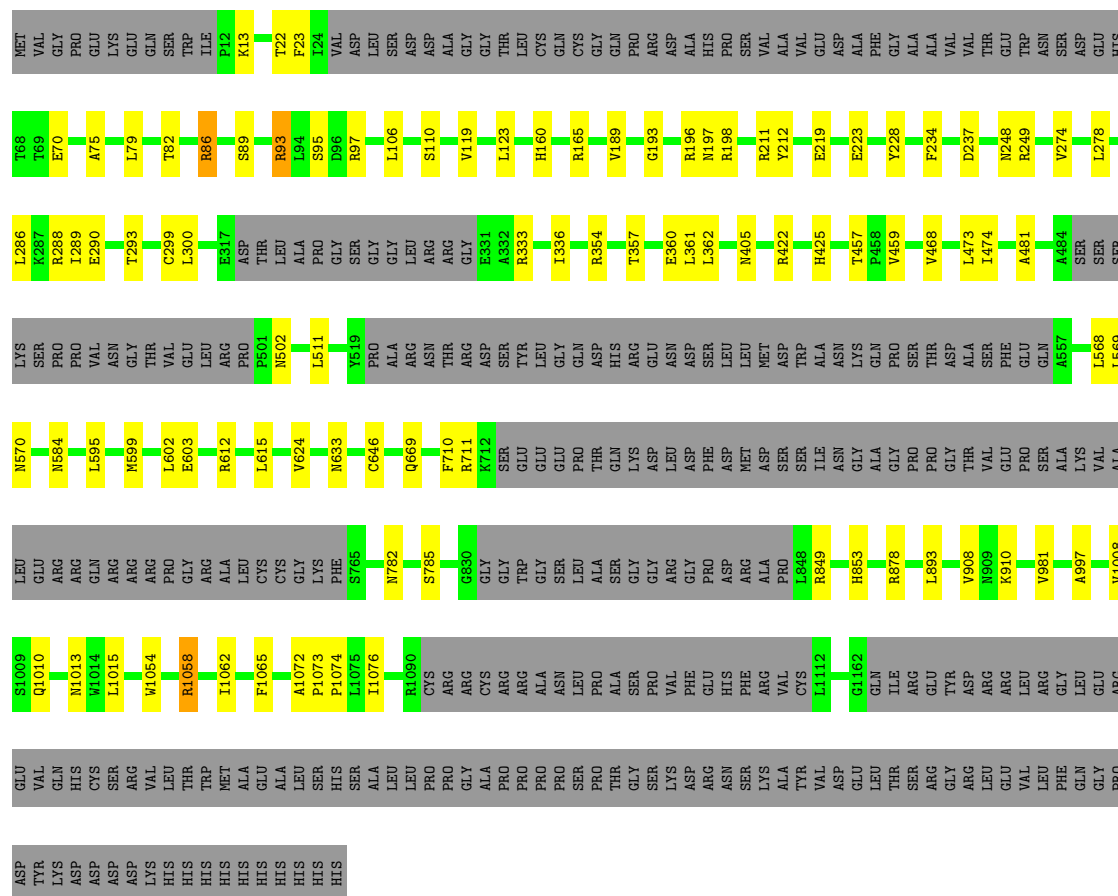
- Molecule 1: Transient receptor potential cation channel subfamily M member 4

Chain C:



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

Chain D:  68% 7% 24%



## 4 Experimental information

Property	Value	Source
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 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: 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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
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:A:422:ARG:HB2	1:A:425:HIS:HD2	1.66	0.60
1:B:473:LEU:HD11	1:B:602:LEU:HD22	1.84	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:N	1:C:86:ARG:HE	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:A:123:LEU:HB2	1:A:278:LEU:HD23	1.91	0.52
1:B:123:LEU:HB2	1:B: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:1073:PRO:N	1:C:1074:PRO:CD	2.73	0.51
1:C:584:ASN:ND2	1:C:646:CYS:SG	2.81	0.51
1:A:299:CYS:SG	1:A:300:LEU:N	2.84	0.51
1:B:360:GLU:HG3	1:B:361:LEU:HD12	1.92	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:A:23:PHE:HA	1:A:70:GLU:HA	1.94	0.50
1:B:584:ASN:ND2	1:B:646:CYS:SG	2.81	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:NE	1:D:86:ARG:N	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:299:CYS:HB3	1:B:362:LEU:HD23	1.97	0.46
1:B:86:ARG:N	1:B:86:ARG:NE	2.62	0.46
1:A:160:HIS:HD2	2:A:2000:ATP:C2	2.32	0.46
1:A:86:ARG:N	1:A:86:ARG:NE	2.62	0.46
1:C:93:ARG:NH1	1:C:237:ASP:OD2	2.44	0.46
1:D:1072:ALA:C	1:D:1074:PRO:HD2	2.36	0.46
1:D:119:VAL:HB	1:D:274:VAL:HG22	1.98	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:119:VAL:HB	1:C:274:VAL:HG22	1.97	0.45
1:C:79:LEU:HD21	1:C:212:TYR:HB2	1.99	0.45
1:A:119:VAL:HB	1:A:274:VAL:HG22	1.98	0.45
1:B:81:PHE:CZ	1:B:228:TYR:HA	2.51	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:160:HIS:HD2	2:B:2000:ATP:C2	2.34	0.44
1:B:79:LEU:HD21	1:B:212:TYR:HB2	1.99	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:A:248:ASN:HB3	1:A:288:ARG:HH21	1.82	0.44
1:B:457:THR:HG22	1:B:459:VAL:H	1.83	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:A:75:ALA:HB3	1:A:93:ARG:HB3	2.00	0.43
1:B:333:ARG:HA	1:B:336:ILE:HD12	2.00	0.43
1:C:160:HIS:CD2	2:C:2000:ATP:C2	3.06	0.43
1:C:457:THR:HG22	1:C:459:VAL:H	1.83	0.43
1:C:97:ARG:HH21	1:C:249:ARG:HH12	1.67	0.43
1:D:457:THR:HG22	1:D:459:VAL:H	1.83	0.43
1:D:97:ARG:HH21	1:D:249:ARG:HH12	1.67	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: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:B:75:ALA:HB3	1:B:93:ARG:HB3	2.00	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:893:LEU:HD11	1:C:1015:LEU:HD21	2.01	0.42
1:A:79:LEU:N	1:A:89:SER:O	2.52	0.42
1:C:1058:ARG:HE	1:C:1062:ILE:HD11	1.84	0.42
1:C:893:LEU:HD11	1:D:1015:LEU:HD21	2.01	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: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:B:86:ARG:HG2	1:B:228:TYR:HD2	1.85	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:A:290:GLU:HA	1:A:293:THR:HG22	2.02	0.42
1:B:286:LEU:HA	1:B:289:ILE:HD12	2.01	0.42
1:D:1058:ARG:HE	1:D:1062:ILE:HD11	1.84	0.42
1:D:79:LEU:N	1:D:89:SER:O	2.52	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:1058:ARG:HE	1:A:1062:ILE:HD11	1.84	0.41
1:A:203:ASN:HA	1:A:204:PRO:HD3	1.81	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:C:290:GLU:HA	1:C:293:THR:HG22	2.02	0.41
1:A:511:LEU:HD11	1:A:595:LEU:HD13	2.02	0.41
1:B:710:PHE:O	1:B:711:ARG:HB2	2.21	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:1015:LEU:HD21	1:D:893:LEU:HD11	2.03	0.40
1:B:132:GLN:HG2	1:B:134:TRP:H	1.86	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:A:214:TRP:CE3	1:A:215:ARG:HB2	2.57	0.40
1:B:82:THR:HG22	1:B:211:ARG:HB3	2.04	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:106:LEU:HD12	1:D:110:SER:HB3	2.03	0.40
1:D:82:THR:HG22	1:D:211:ARG:HB3	2.03	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	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 ⓘ

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%)	67	88
1	B	811/1063 (76%)	799 (98%)	12 (2%)	67	88
1	C	811/1063 (76%)	799 (98%)	12 (2%)	67	88
1	D	811/1063 (76%)	799 (98%)	12 (2%)	67	88
All	All	3244/4252 (76%)	3196 (98%)	48 (2%)	70	88

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

Some 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 ⓘ

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 [i](#)

There are no carbohydrates 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	A	2000	-	27,33,33	0.99	1 (3%)	27,52,52	1.66	3 (11%)
2	ATP	B	2000	-	27,33,33	0.98	1 (3%)	27,52,52	1.66	3 (11%)
2	ATP	C	2000	-	27,33,33	0.99	1 (3%)	27,52,52	1.67	3 (11%)
2	ATP	D	2000	-	27,33,33	0.99	1 (3%)	27,52,52	1.67	3 (11%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	ATP	C5-C4	2.97	1.47	1.40
2	A	2000	ATP	C5-C4	2.99	1.47	1.40
2	C	2000	ATP	C5-C4	3.01	1.47	1.40
2	D	2000	ATP	C5-C4	3.01	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2000	ATP	N3-C2-N1	-5.05	124.54	128.86
2	D	2000	ATP	N3-C2-N1	-5.00	124.58	128.86
2	B	2000	ATP	N3-C2-N1	-4.94	124.64	128.86
2	A	2000	ATP	N3-C2-N1	-4.92	124.65	128.86
2	D	2000	ATP	PB-O3B-PG	-3.67	120.29	132.63
2	B	2000	ATP	PB-O3B-PG	-3.67	120.30	132.63
2	A	2000	ATP	PB-O3B-PG	-3.67	120.31	132.63
2	C	2000	ATP	PB-O3B-PG	-3.65	120.35	132.63
2	B	2000	ATP	C4-C5-N7	-2.96	106.55	109.41
2	D	2000	ATP	C4-C5-N7	-2.95	106.56	109.41
2	C	2000	ATP	C4-C5-N7	-2.91	106.60	109.41
2	A	2000	ATP	C4-C5-N7	-2.87	106.64	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

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

## 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.