



## wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 09:39 AM EDT

PDB ID : 6MJ2  
EMDB ID : EMD-9134  
Title : Human TRPM2 ion channel in a calcium- and ADPR-bound state  
Authors : Wang, L.; Fu, T.M.; Xia, S.; Wu, H.  
Deposited on : 2018-09-20  
Resolution : 6.36 Å(reported)

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

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

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

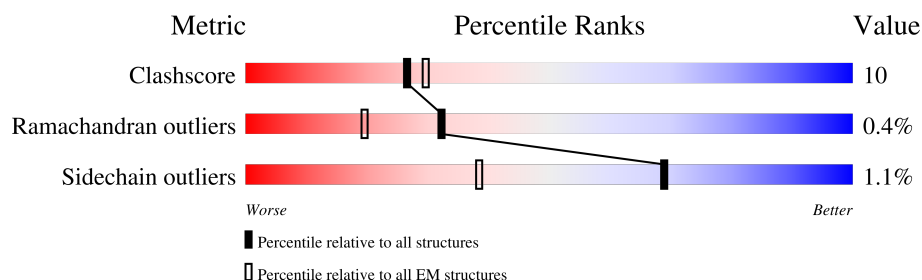
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.36 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1503	
1	B	1503	
1	C	1503	
1	D	1503	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 43124 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1337	Total	C	N	O	S	0	0
			10780	6942	1865	1919	54		
1	B	1337	Total	C	N	O	S	0	0
			10780	6942	1865	1919	54		
1	C	1337	Total	C	N	O	S	0	0
			10780	6942	1865	1919	54		
1	D	1337	Total	C	N	O	S	0	0
			10780	6942	1865	1919	54		

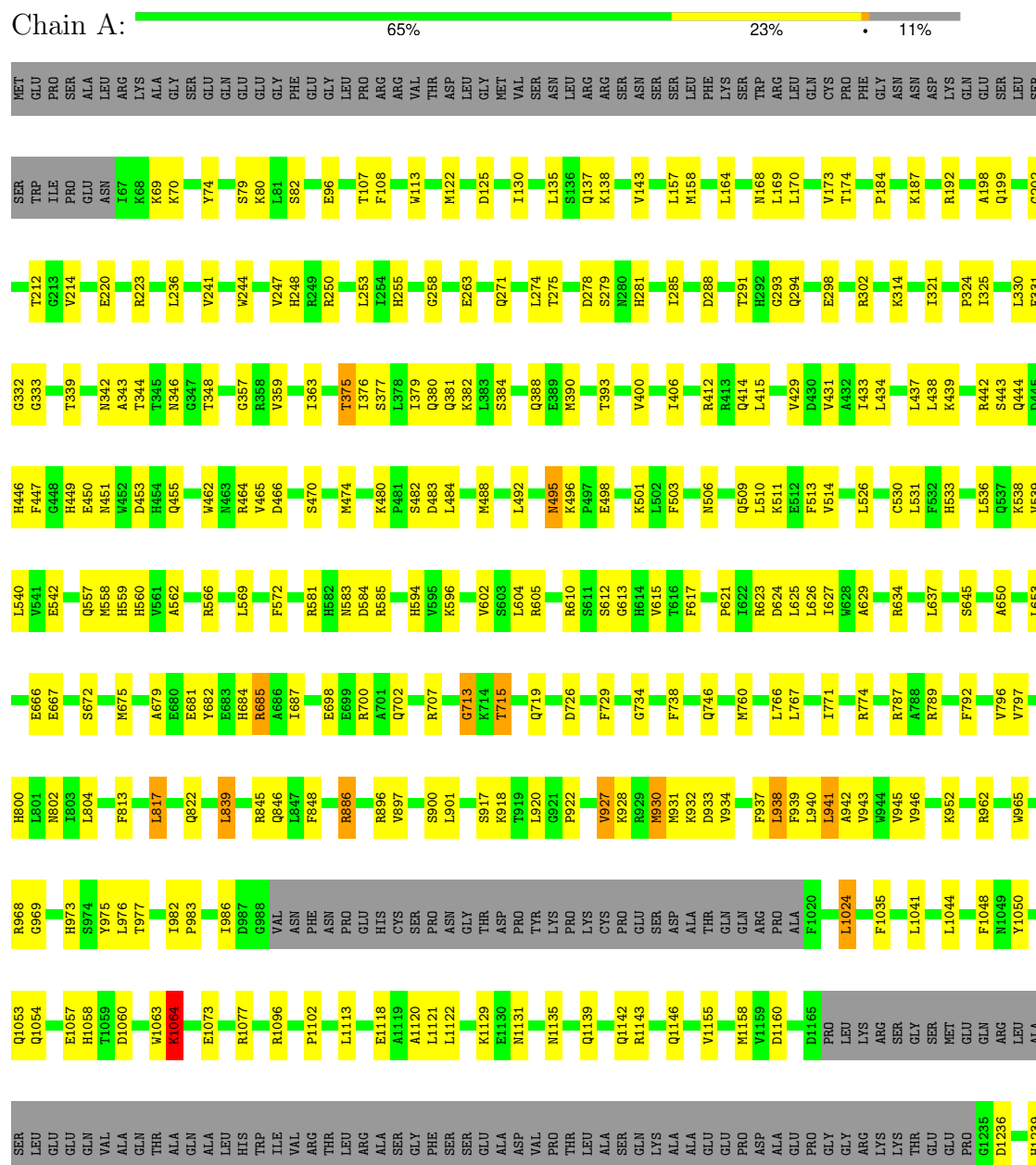
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

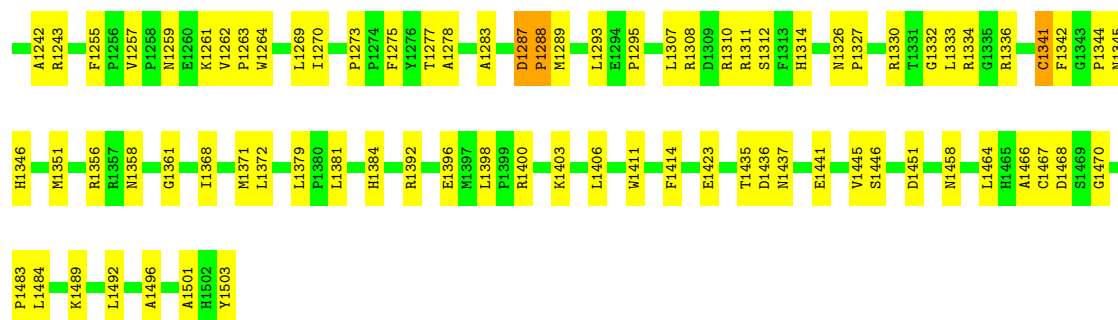
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Ca	0
			1	1	
2	B	1	Total	Ca	0
			1	1	
2	C	1	Total	Ca	0
			1	1	
2	D	1	Total	Ca	0
			1	1	

### 3 Residue-property plots

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. 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.

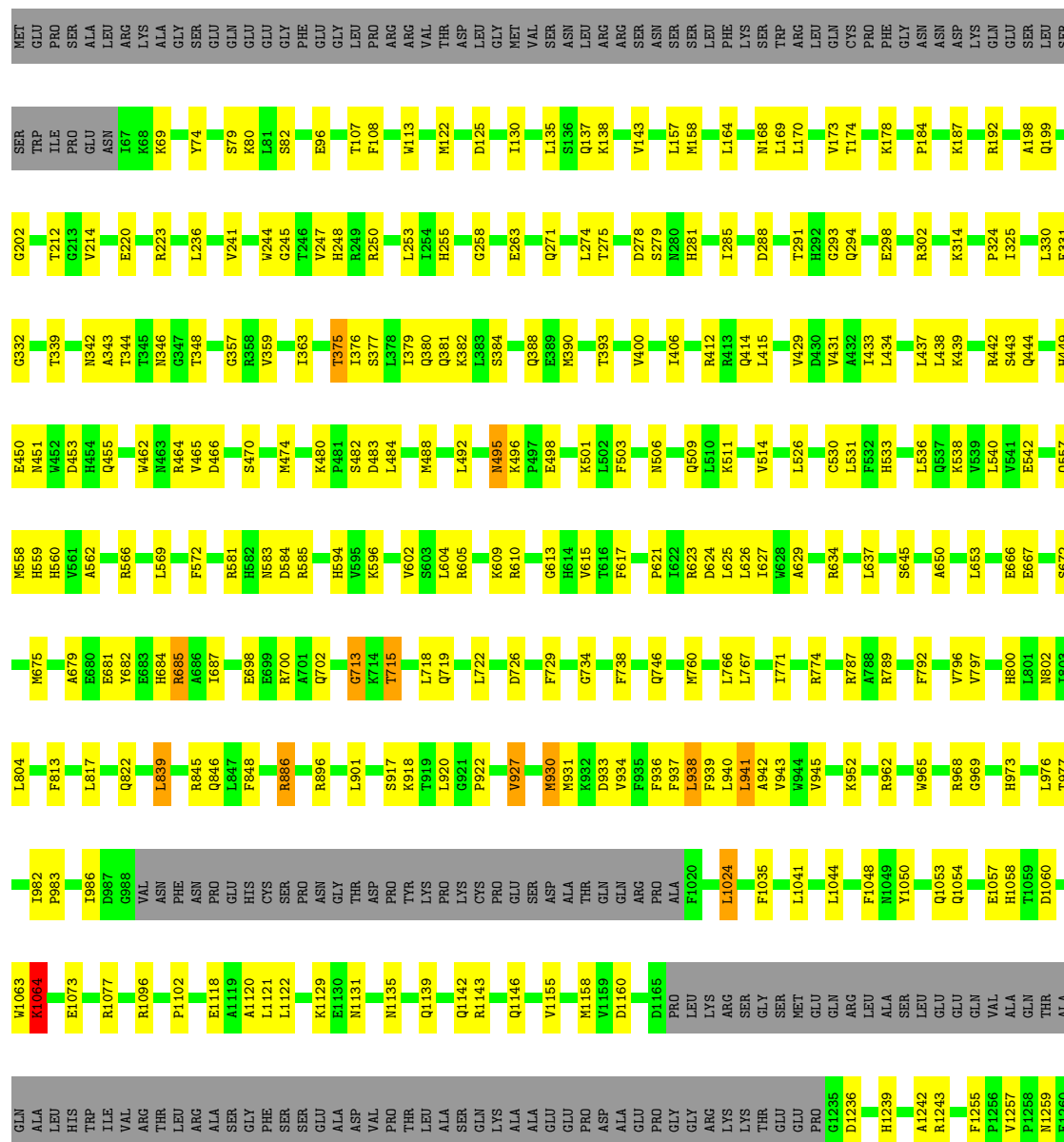
- Molecule 1: Transient receptor potential cation channel subfamily M member 2

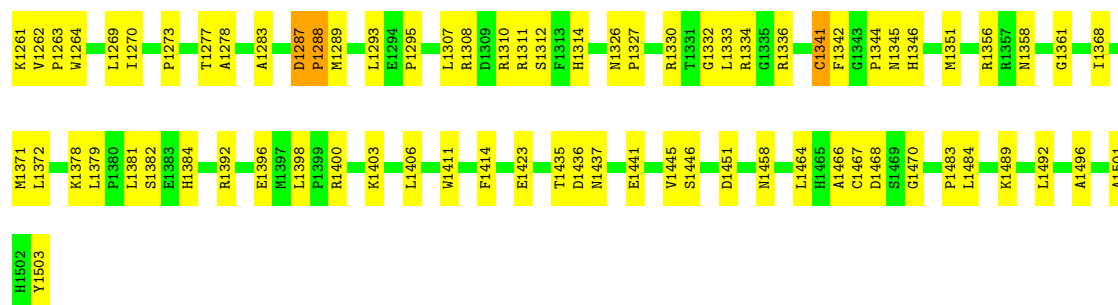




● Molecule 1: Transient receptor potential cation channel subfamily M member 2

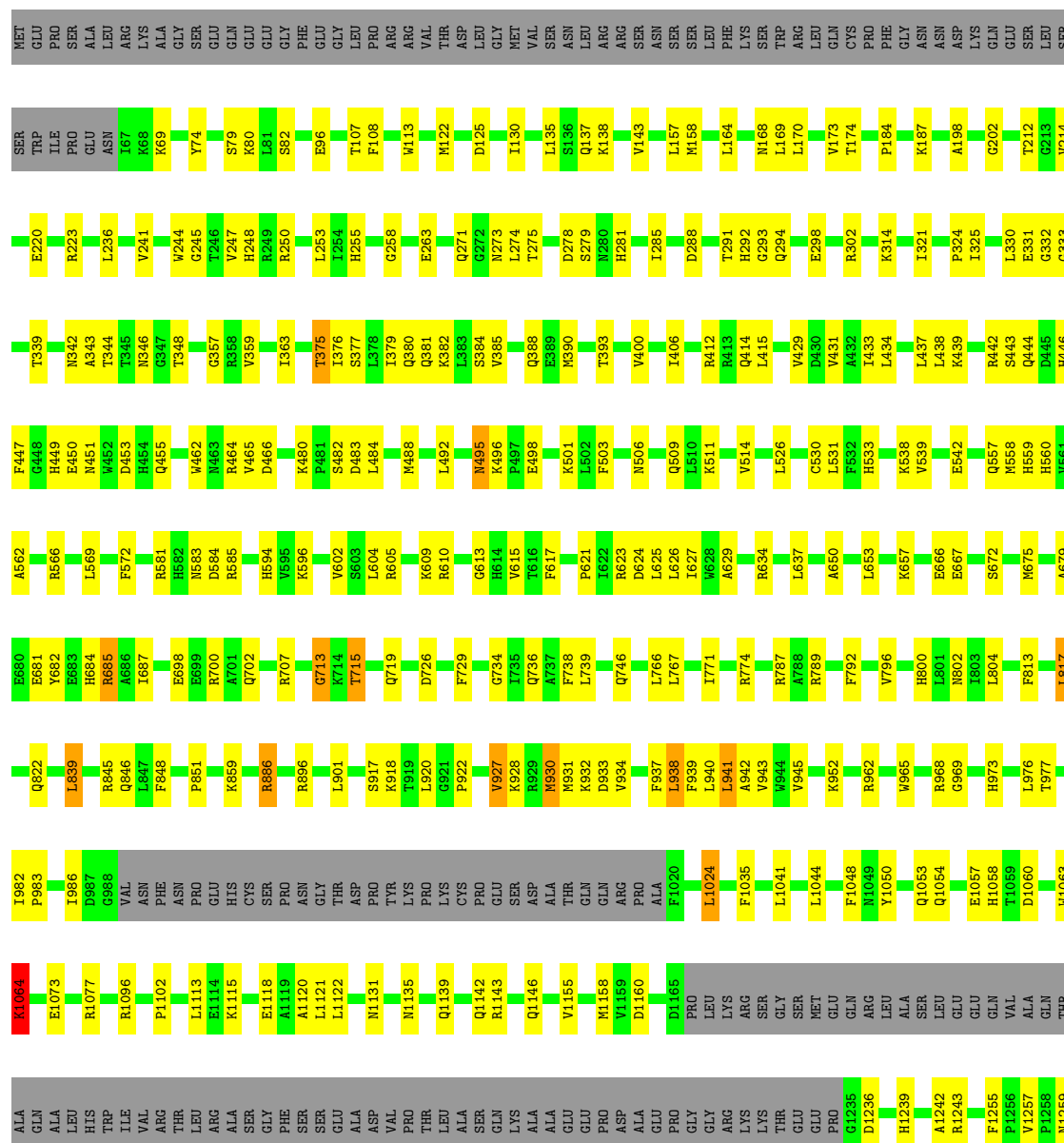
Chain B: 65% 23% 11%





- Molecule 1: Transient receptor potential cation channel subfamily M member 2

Chain C: 65% 23% 11%









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14199	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	70.072	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
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: CA

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	0.30	0/11050	0.67	19/14990 (0.1%)
1	B	0.30	0/11050	0.67	19/14990 (0.1%)
1	C	0.30	0/11050	0.67	19/14990 (0.1%)
1	D	0.30	0/11050	0.67	19/14990 (0.1%)
All	All	0.30	0/44200	0.67	76/59960 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	13
1	B	0	13
1	C	0	13
1	D	0	13
All	All	0	52

There are no bond length outliers.

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	933	ASP	CB-CG-OD2	-8.80	110.38	118.30
1	D	933	ASP	CB-CG-OD2	-8.77	110.41	118.30
1	C	933	ASP	CB-CG-OD2	-8.77	110.41	118.30
1	A	933	ASP	CB-CG-OD2	-8.74	110.44	118.30
1	C	933	ASP	CB-CG-OD1	8.54	125.99	118.30

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	375	THR	Peptide
1	A	388	GLN	Peptide
1	A	495	ASN	Peptide
1	A	615	VAL	Peptide
1	A	82	SER	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10780	0	10822	212	0
1	B	10780	0	10822	209	0
1	C	10780	0	10822	215	0
1	D	10780	0	10822	215	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	43124	0	43288	843	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 10.

The worst 5 of 843 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:569:LEU:HD13	1:A:572:PHE:HB2	1.76	0.68
1:D:569:LEU:HD13	1:D:572:PHE:HB2	1.77	0.67
1:B:569:LEU:HD13	1:B:572:PHE:HB2	1.76	0.67
1:C:569:LEU:HD13	1:C:572:PHE:HB2	1.76	0.66
1:B:962:ARG:H	1:B:965:TRP:HB2	1.60	0.66

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	1331/1503 (89%)	1131 (85%)	195 (15%)	5 (0%)	30	68
1	B	1331/1503 (89%)	1133 (85%)	193 (14%)	5 (0%)	30	68
1	C	1331/1503 (89%)	1131 (85%)	195 (15%)	5 (0%)	30	68
1	D	1331/1503 (89%)	1131 (85%)	195 (15%)	5 (0%)	30	68
All	All	5324/6012 (89%)	4526 (85%)	778 (15%)	20 (0%)	32	68

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ILE
1	B	376	ILE
1	C	376	ILE
1	D	376	ILE
1	A	384	SER

### 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	1176/1318 (89%)	1163 (99%)	13 (1%)	70	80
1	B	1176/1318 (89%)	1163 (99%)	13 (1%)	70	80
1	C	1176/1318 (89%)	1163 (99%)	13 (1%)	70	80
1	D	1176/1318 (89%)	1163 (99%)	13 (1%)	70	80
All	All	4704/5272 (89%)	4652 (99%)	52 (1%)	69	80

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	566	ARG
1	C	930	MET
1	D	941	LEU
1	C	610	ARG
1	C	839	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	446	HIS
1	D	506	ASN
1	D	684	HIS
1	B	506	ASN
1	B	454	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9134. 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

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

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

## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



## 8 Fourier-Shell correlation

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

## 9 Map-model fit

This section was not generated.