



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:50 PM BST

PDB ID : 3J9J
EMDB ID: : EMD-5778
Title : Structure of the capsaicin receptor, TRPV1, determined by single particle electron cryo-microscopy
Authors : Wang, R.Y.-R.; Barad, B.A.; Fraser, J.S.; DiMaio, F.
Deposited on : 2015-02-02
Resolution : unknown (reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

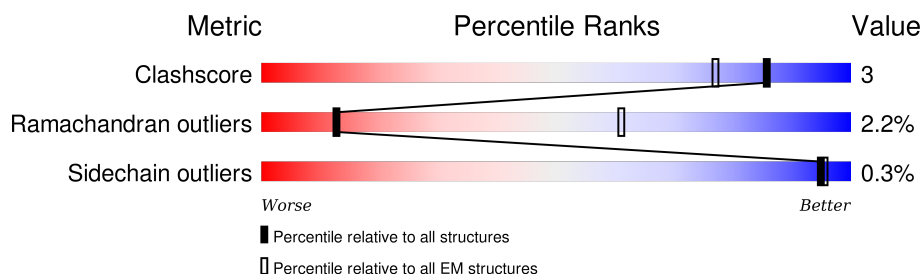
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	586	<div> <div>50%</div> <div>•</div> <div>46%</div> </div>
1	B	586	<div> <div>50%</div> <div>•</div> <div>46%</div> </div>
1	C	586	<div> <div>50%</div> <div>•</div> <div>46%</div> </div>
1	D	586	<div> <div>50%</div> <div>•</div> <div>46%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21068 atoms, of which 10624 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 V member 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	315	Total	C	H	N	O	S	0	0
			5267	1738	2656	402	451	20		
1	B	315	Total	C	H	N	O	S	0	0
			5267	1738	2656	402	451	20		
1	C	315	Total	C	H	N	O	S	0	0
			5267	1738	2656	402	451	20		
1	D	315	Total	C	H	N	O	S	0	0
			5267	1738	2656	402	451	20		

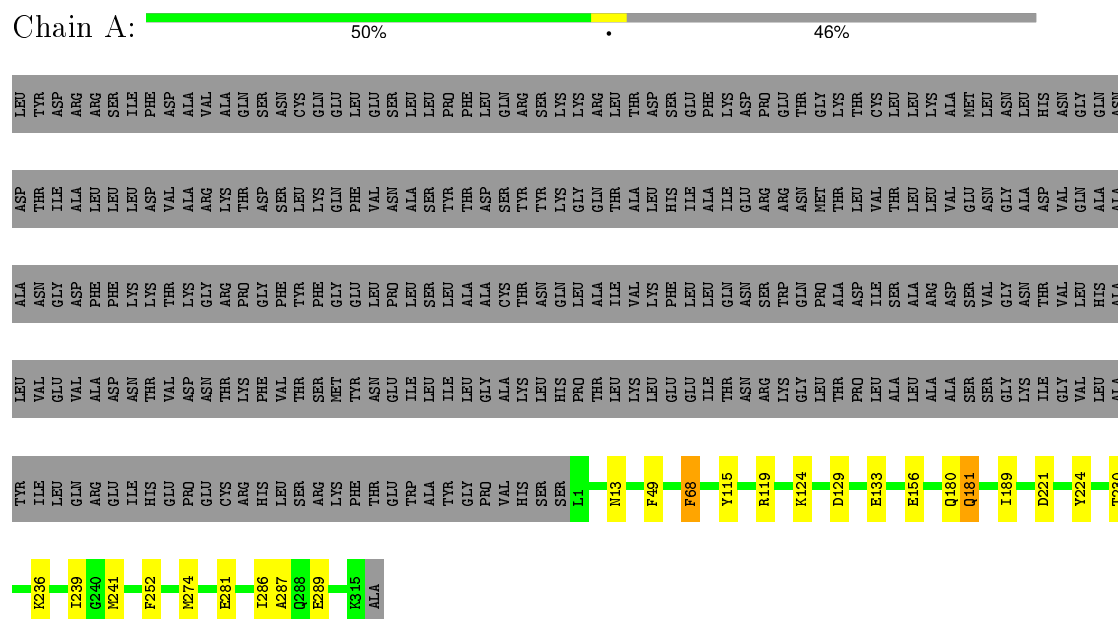
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	273	GLN	ASN	CONFLICT	UNP O35433
B	273	GLN	ASN	CONFLICT	UNP O35433
C	273	GLN	ASN	CONFLICT	UNP O35433
D	273	GLN	ASN	CONFLICT	UNP O35433

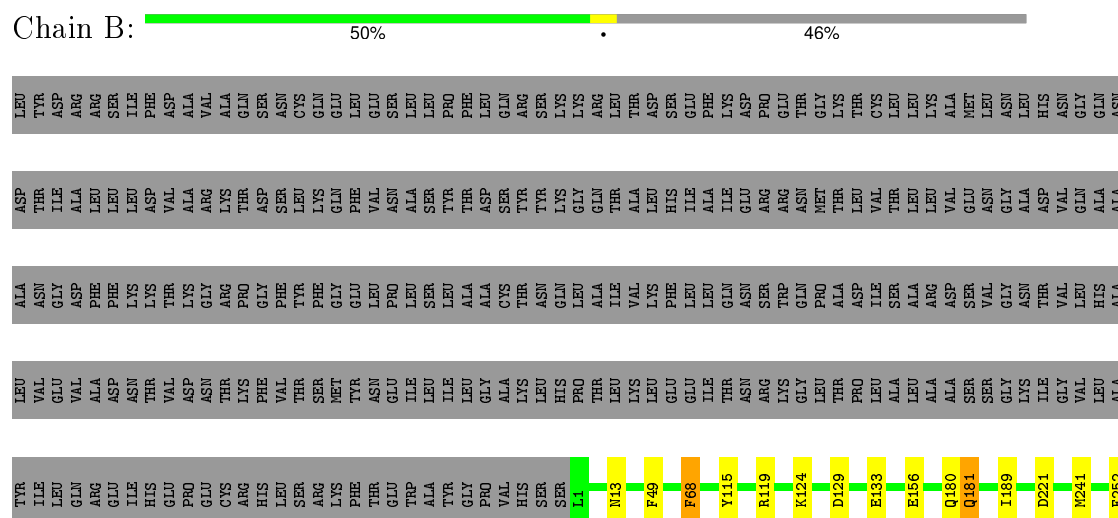
3 Residue-property plots

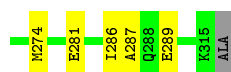
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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 V member 1



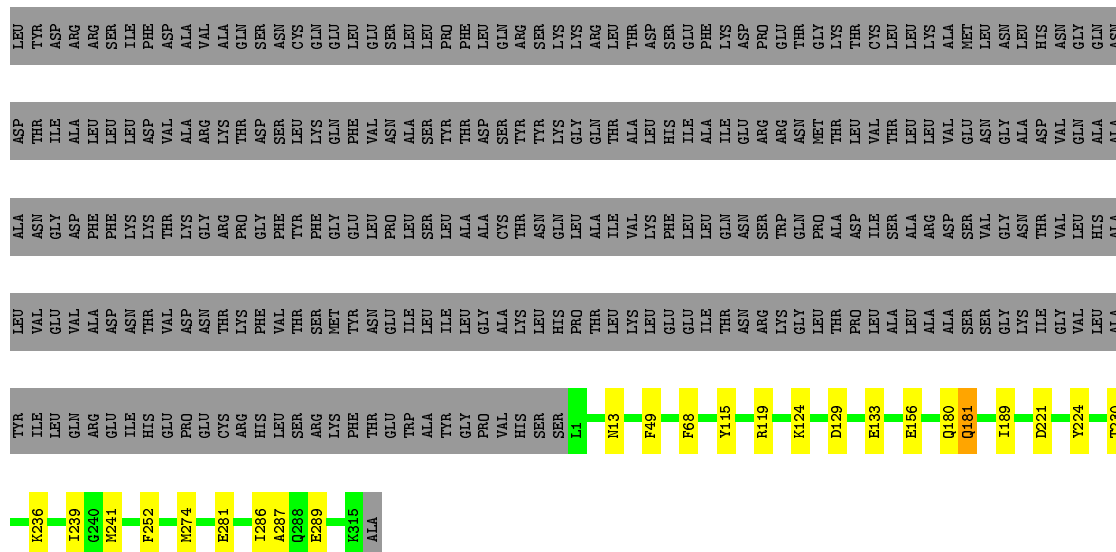
- Molecule 1: Transient receptor potential cation channel subfamily V member 1





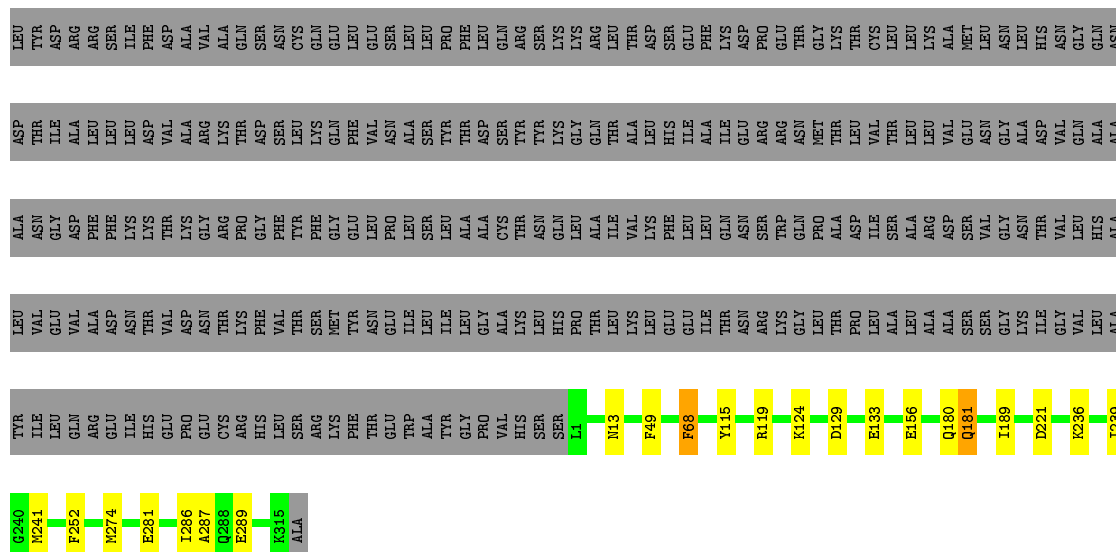
- Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain C: 50% 46%



- Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain D: 50% 46%



4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.83	0/2675	0.57	0/3613
1	B	0.83	0/2675	0.57	0/3613
1	C	0.83	0/2675	0.57	0/3613
1	D	0.83	0/2675	0.57	0/3613
All	All	0.83	0/10700	0.57	0/14452

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2611	2656	2658	19	0
1	B	2611	2656	2658	17	0
1	C	2611	2656	2658	19	0
1	D	2611	2656	2658	18	0
All	All	10444	10624	10632	57	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 (57) 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:C:156:GLU:OE1	1:C:156:GLU:N	2.27	0.65
1:D:156:GLU:N	1:D:156:GLU:OE1	2.27	0.61
1:B:156:GLU:N	1:B:156:GLU:OE1	2.27	0.59
1:A:156:GLU:OE1	1:A:156:GLU:N	2.27	0.58
1:B:281:GLU:HA	1:B:281:GLU:OE1	2.10	0.52
1:A:281:GLU:OE1	1:A:281:GLU:HA	2.10	0.52
1:C:281:GLU:HA	1:C:281:GLU:OE1	2.10	0.52
1:D:281:GLU:OE1	1:D:281:GLU:HA	2.10	0.51
1:C:189:ILE:HA	1:D:274:MET:HE1	1.94	0.50
1:A:274:MET:HE1	1:B:189:ILE:HA	1.94	0.49
1:B:274:MET:HE1	1:D:189:ILE:HA	1.94	0.49
1:A:189:ILE:HA	1:C:274:MET:HE1	1.95	0.48
1:D:289:GLU:HA	1:D:289:GLU:OE1	2.15	0.47
1:B:289:GLU:HA	1:B:289:GLU:OE1	2.15	0.46
1:B:68:PHE:C	1:B:68:PHE:CD1	2.89	0.46
1:B:68:PHE:CD1	1:B:68:PHE:O	2.69	0.46
1:D:68:PHE:O	1:D:68:PHE:CD1	2.69	0.46
1:C:189:ILE:HG12	1:D:274:MET:SD	2.56	0.46
1:A:68:PHE:O	1:A:68:PHE:CD1	2.69	0.45
1:D:68:PHE:C	1:D:68:PHE:CD1	2.89	0.45
1:A:68:PHE:C	1:A:68:PHE:CD1	2.89	0.45
1:C:289:GLU:HA	1:C:289:GLU:OE1	2.15	0.45
1:A:289:GLU:OE1	1:A:289:GLU:HA	2.15	0.45
1:A:241:MET:HA	1:B:241:MET:SD	2.57	0.45
1:C:241:MET:SD	1:D:241:MET:HA	2.57	0.45
1:C:68:PHE:CD1	1:C:68:PHE:O	2.69	0.44
1:B:241:MET:HA	1:D:241:MET:SD	2.58	0.44
1:A:189:ILE:HG12	1:C:274:MET:SD	2.57	0.44
1:B:274:MET:SD	1:D:189:ILE:HG12	2.57	0.44
1:C:68:PHE:CD1	1:C:68:PHE:C	2.89	0.43
1:D:115:TYR:O	1:D:119:ARG:N	2.52	0.43
1:A:124:LYS:NZ	1:A:133:GLU:OE1	2.52	0.43
1:D:124:LYS:NZ	1:D:133:GLU:OE1	2.52	0.43
1:B:115:TYR:O	1:B:119:ARG:N	2.52	0.43
1:C:115:TYR:O	1:C:119:ARG:N	2.52	0.43
1:A:274:MET:SD	1:B:189:ILE:HG12	2.58	0.43
1:A:241:MET:SD	1:C:241:MET:HA	2.59	0.42
1:C:124:LYS:NZ	1:C:133:GLU:OE1	2.52	0.42
1:A:115:TYR:O	1:A:119:ARG:N	2.52	0.42
1:B:124:LYS:NZ	1:B:133:GLU:OE1	2.52	0.42
1:A:68:PHE:HD1	1:A:68:PHE:O	2.03	0.42
1:B:252:PHE:CZ	1:D:156:GLU:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:PHE:HD1	1:B:68:PHE:O	2.03	0.41
1:D:68:PHE:O	1:D:68:PHE:HD1	2.03	0.41
1:A:252:PHE:CZ	1:B:156:GLU:HA	2.56	0.41
1:C:68:PHE:HD1	1:C:68:PHE:O	2.03	0.41
1:C:224:TYR:O	1:C:230:THR:OG1	2.36	0.41
1:C:236:LYS:HA	1:C:239:ILE:HG12	2.03	0.41
1:D:236:LYS:HA	1:D:239:ILE:HG12	2.03	0.41
1:A:156:GLU:HA	1:C:252:PHE:CZ	2.56	0.40
1:B:180:GLN:O	1:B:181:GLN:HB3	2.21	0.40
1:A:180:GLN:O	1:A:181:GLN:HB3	2.21	0.40
1:A:236:LYS:HA	1:A:239:ILE:HG12	2.03	0.40
1:C:156:GLU:HA	1:D:252:PHE:CZ	2.56	0.40
1:C:180:GLN:O	1:C:181:GLN:HB3	2.21	0.40
1:D:180:GLN:O	1:D:181:GLN:HB3	2.21	0.40
1:A:224:TYR:O	1:A:230:THR:OG1	2.36	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	313/586 (53%)	295 (94%)	11 (4%)	7 (2%)	8	8
1	B	313/586 (53%)	296 (95%)	10 (3%)	7 (2%)	8	8
1	C	313/586 (53%)	296 (95%)	10 (3%)	7 (2%)	8	8
1	D	313/586 (53%)	296 (95%)	10 (3%)	7 (2%)	8	8
All	All	1252/2344 (53%)	1183 (94%)	41 (3%)	28 (2%)	13	8

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	B	181	GLN
1	C	181	GLN
1	D	181	GLN
1	A	129	ASP
1	A	221	ASP
1	B	129	ASP
1	B	221	ASP
1	C	129	ASP
1	C	221	ASP
1	D	129	ASP
1	D	221	ASP
1	A	13	ASN
1	A	287	ALA
1	B	13	ASN
1	B	287	ALA
1	C	13	ASN
1	C	287	ALA
1	D	13	ASN
1	D	287	ALA
1	A	49	PHE
1	B	49	PHE
1	C	49	PHE
1	D	49	PHE
1	A	286	ILE
1	B	286	ILE
1	C	286	ILE
1	D	286	ILE

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	288/519 (56%)	287 (100%)	1 (0%)	94	94
1	B	288/519 (56%)	287 (100%)	1 (0%)	94	94
1	C	288/519 (56%)	288 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	288/519 (56%)	287 (100%)	1 (0%)	94	94
All	All	1152/2076 (56%)	1149 (100%)	3 (0%)	95	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	PHE
1	B	68	PHE
1	D	68	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.