



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:31 am GMT

PDB ID : 3J5Q
EMDB ID: : EMD-5776
Title : Structure of TRPV1 ion channel in complex with DkTx and RTX determined
by single particle electron cryo-microscopy
Authors : Liao, M.; Cao, E.; Julius, D.; Cheng, Y.
Deposited on : 2013-10-28
Resolution : 3.80 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary 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) : recalc29047

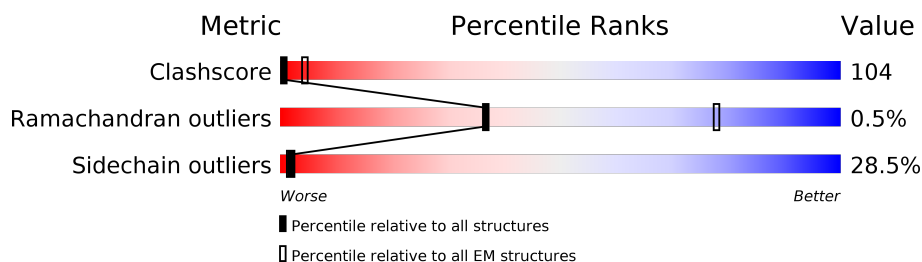
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	B	598	39% 42% 18% .
1	D	598	39% 42% 18% .
1	E	598	39% 42% 18% .
1	G	598	39% 42% 18% .
2	A	31	32% 68%
2	C	31	32% 68%
2	F	31	32% 68%
2	H	31	32% 68%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18556 atoms, of which 292 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	D	592	Total	C	N	O	S	0	0
			4409	2860	730	796	23		
1	B	592	Total	C	N	O	S	0	0
			4409	2860	730	796	23		
1	E	592	Total	C	N	O	S	0	0
			4409	2860	730	796	23		
1	G	592	Total	C	N	O	S	0	0
			4409	2860	730	796	23		

- Molecule 2 is a protein called Double-knot toxin.

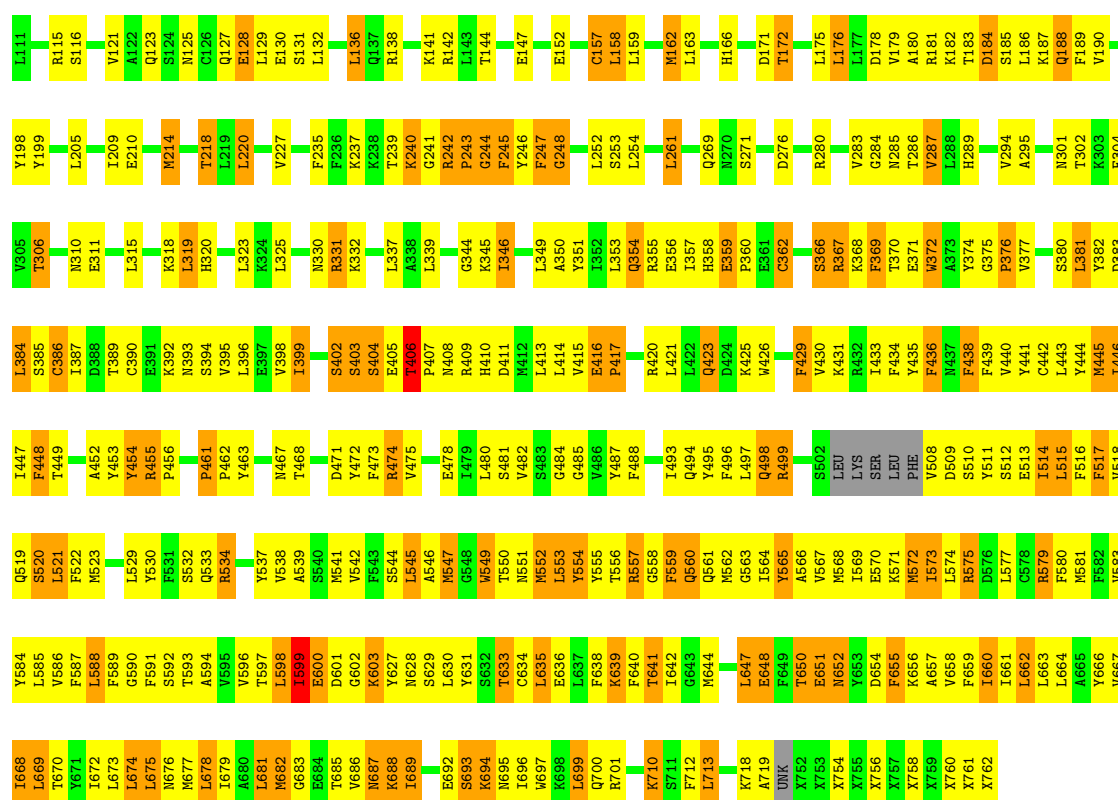
Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	31	Total 230	C 89	H 73	N 31	O 31	S 6	0	0
2	C	31	Total 230	C 89	H 73	N 31	O 31	S 6	0	0
2	F	31	Total 230	C 89	H 73	N 31	O 31	S 6	0	0
2	H	31	Total 230	C 89	H 73	N 31	O 31	S 6	0	0

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.

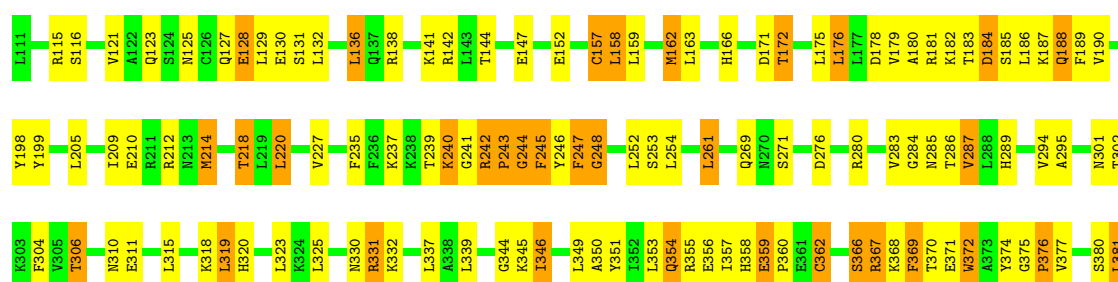
- Molecule 1: Transient receptor potential cation channel subfamily V member 1

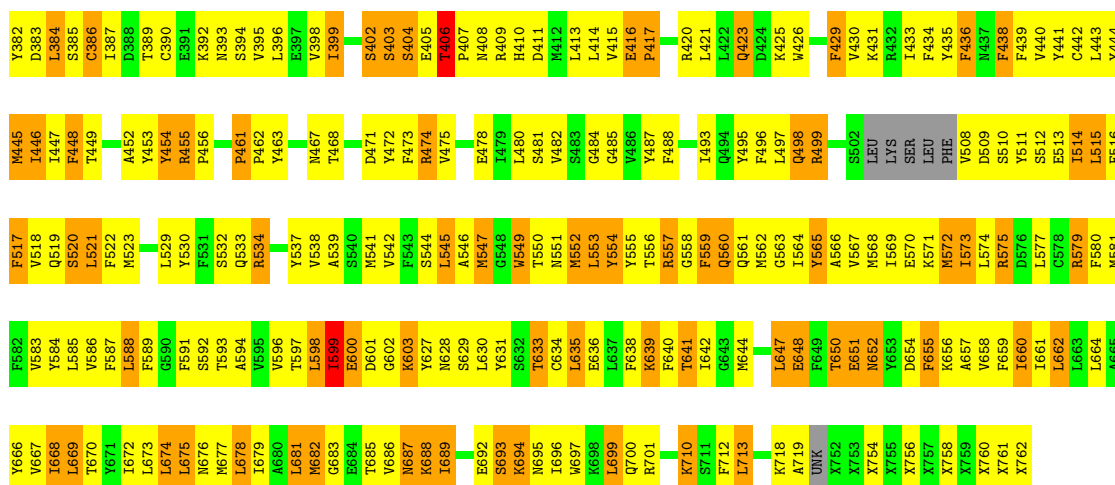
Chain D: 



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

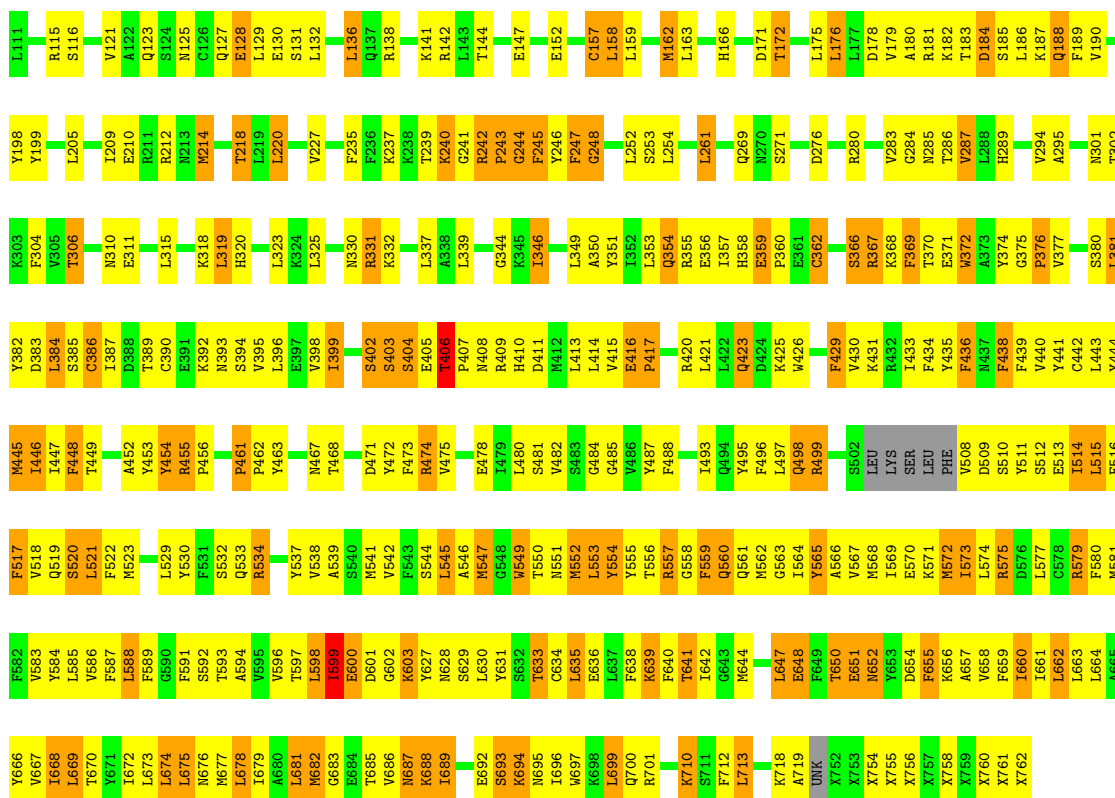
Chain B: 





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

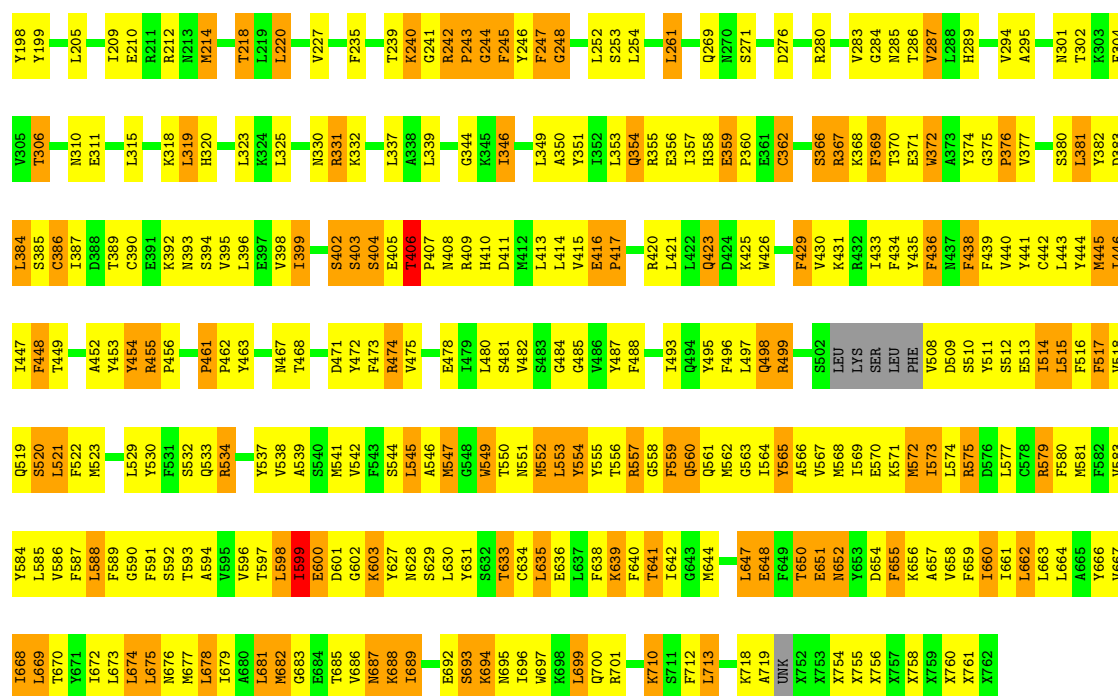
Chain E: 39% 42% 18%



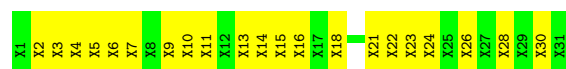
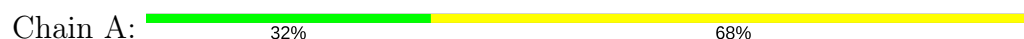
• Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain G: 39% 42% 18%





- Molecule 2: Double-knot toxin



- Molecule 2: Double-knot toxin



- Molecule 2: Double-knot toxin



- Molecule 2: Double-knot toxin



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	36158	Depositor
Resolution determination method	Gold standard FSC at 0.143 cut-off	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	21	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	31000	Depositor
Image detector	K2 Summit	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	B	0.47	3/4448 (0.1%)	0.64	3/6041 (0.0%)
1	D	0.47	3/4448 (0.1%)	0.64	3/6041 (0.0%)
1	E	0.47	3/4448 (0.1%)	0.64	3/6041 (0.0%)
1	G	0.47	3/4448 (0.1%)	0.64	3/6041 (0.0%)
All	All	0.47	12/17792 (0.1%)	0.64	12/24164 (0.0%)

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	B	0	7
1	D	0	7
1	E	0	7
1	G	0	7
All	All	0	28

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	162	MET	CG-SD	7.66	2.01	1.81
1	E	162	MET	CG-SD	7.66	2.01	1.81
1	G	162	MET	CG-SD	7.66	2.01	1.81
1	B	162	MET	CG-SD	7.64	2.01	1.81
1	E	214	MET	CG-SD	6.37	1.97	1.81

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	406	THR	C-N-CD	6.28	141.60	128.40
1	B	406	THR	C-N-CD	6.27	141.57	128.40
1	G	406	THR	C-N-CD	6.27	141.56	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	406	THR	C-N-CD	6.26	141.54	128.40
1	D	416	GLU	C-N-CD	5.90	140.80	128.40

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	243	PRO	Peptide
1	D	244	GLY	Peptide
1	D	247	PHE	Peptide
1	D	248	GLY	Peptide
1	D	376	PRO	Peptide

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	B	4409	0	4101	960	0
1	D	4409	0	4101	971	0
1	E	4409	0	4101	976	0
1	G	4409	0	4101	985	0
2	A	157	73	28	40	0
2	C	157	73	28	40	0
2	F	157	73	28	41	0
2	H	157	73	28	43	0
All	All	18264	292	16516	3602	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 104.

The worst 5 of 3602 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:E:426:TRP:HD1	1:E:430:VAL:CB	1.07	1.66
1:B:443:LEU:HA	1:B:446:ILE:CD1	1.18	1.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:TYR:CD2	1:G:372:TRP:CZ3	1.76	1.64
1:G:426:TRP:HD1	1:G:430:VAL:CB	1.07	1.63
1:G:426:TRP:CD1	1:G:430:VAL:HB	1.11	1.62

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	B	577/598 (96%)	537 (93%)	37 (6%)	3 (0%)	32	73
1	D	577/598 (96%)	537 (93%)	37 (6%)	3 (0%)	32	73
1	E	577/598 (96%)	537 (93%)	37 (6%)	3 (0%)	32	73
1	G	577/598 (96%)	537 (93%)	37 (6%)	3 (0%)	32	73
All	All	2308/2392 (96%)	2148 (93%)	148 (6%)	12 (0%)	37	73

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	406	THR
1	D	461	PRO
1	B	406	THR
1	B	461	PRO
1	E	406	THR

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	B	418/519 (80%)	299 (72%)	119 (28%)	0	3
1	D	418/519 (80%)	299 (72%)	119 (28%)	0	3
1	E	418/519 (80%)	299 (72%)	119 (28%)	0	3
1	G	418/519 (80%)	299 (72%)	119 (28%)	0	3
All	All	1672/2076 (80%)	1196 (72%)	476 (28%)	2	3

5 of 476 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	641	THR
1	E	304	PHE
1	G	565	TYR
1	B	655	PHE
1	E	131	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	676	ASN
1	E	269	GLN
1	G	498	GLN
1	B	687	ASN
1	E	125	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 [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.