



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:51 PM BST

PDB ID : 3J9P
EMDB ID: : EMD-6267
Title : Structure of the TRPA1 ion channel determined by electron cryo-microscopy
Authors : Paulsen, C.E.; Armache, J.-P.; Gao, Y.; Cheng, Y.; Julius, D.
Deposited on : 2015-02-14
Resolution : 4.24 Å(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

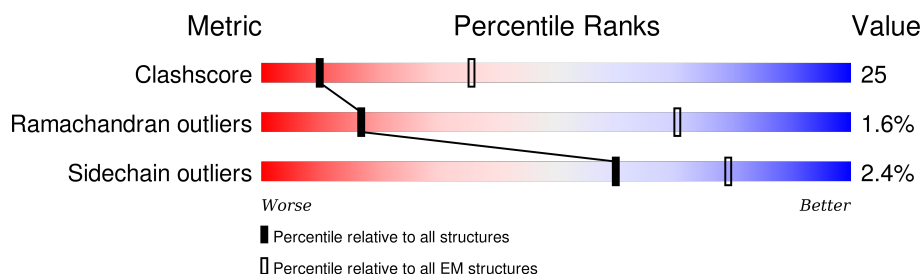
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.24 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	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	1528	 20% 15% • 63%
1	B	1528	 20% 15% • 63%
1	C	1528	 20% 15% • 63%
1	D	1528	 19% 16% • 63%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16952 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 Maltose-binding periplasmic protein, Transient receptor potential cation channel subfamily A member 1 chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	560	Total	C	N	O	S	0	0
			4238	2775	711	722	30		
1	A	560	Total	C	N	O	S	0	0
			4238	2775	711	722	30		
1	B	560	Total	C	N	O	S	0	0
			4238	2775	711	722	30		
1	C	560	Total	C	N	O	S	0	0
			4238	2775	711	722	30		

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-408	MET	-	EXPRESSION TAG	UNP P0AEX9
D	-407	GLY	-	EXPRESSION TAG	UNP P0AEX9
D	-406	SER	-	EXPRESSION TAG	UNP P0AEX9
D	-405	SER	-	EXPRESSION TAG	UNP P0AEX9
D	-404	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-403	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-402	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-401	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-400	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-399	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-398	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-397	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-396	GLY	-	EXPRESSION TAG	UNP P0AEX9
D	-395	SER	-	EXPRESSION TAG	UNP P0AEX9
D	-394	SER	-	EXPRESSION TAG	UNP P0AEX9
D	-393	MET	-	EXPRESSION TAG	UNP P0AEX9
D	-26	ASN	-	LINKER	UNP O75762
D	-25	SER	-	LINKER	UNP O75762
D	-24	SER	-	LINKER	UNP O75762
D	-23	SER	-	LINKER	UNP O75762
D	-22	ASN	-	LINKER	UNP O75762

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-21	ASN	-	LINKER	UNP O75762
D	-20	ASN	-	LINKER	UNP O75762
D	-19	ASN	-	LINKER	UNP O75762
D	-18	ASN	-	LINKER	UNP O75762
D	-17	ASN	-	LINKER	UNP O75762
D	-16	ASN	-	LINKER	UNP O75762
D	-15	ASN	-	LINKER	UNP O75762
D	-14	ASN	-	LINKER	UNP O75762
D	-13	ASN	-	LINKER	UNP O75762
D	-12	LEU	-	LINKER	UNP O75762
D	-11	GLY	-	LINKER	UNP O75762
D	-10	ILE	-	LINKER	UNP O75762
D	-9	GLU	-	LINKER	UNP O75762
D	-8	GLU	-	LINKER	UNP O75762
D	-7	ASN	-	LINKER	UNP O75762
D	-6	LEU	-	LINKER	UNP O75762
D	-5	TYR	-	LINKER	UNP O75762
D	-4	PHE	-	LINKER	UNP O75762
D	-3	GLN	-	LINKER	UNP O75762
D	-2	GLY	-	LINKER	UNP O75762
D	-1	ALA	-	LINKER	UNP O75762
D	0	GLY	-	LINKER	UNP O75762
D	1	SER	-	LINKER	UNP O75762
D	966	ASP	GLU	CONFLICT	UNP O75762
A	-408	MET	-	EXPRESSION TAG	UNP P0AEX9
A	-407	GLY	-	EXPRESSION TAG	UNP P0AEX9
A	-406	SER	-	EXPRESSION TAG	UNP P0AEX9
A	-405	SER	-	EXPRESSION TAG	UNP P0AEX9
A	-404	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-403	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-402	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-401	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-400	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-399	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-398	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-397	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-396	GLY	-	EXPRESSION TAG	UNP P0AEX9
A	-395	SER	-	EXPRESSION TAG	UNP P0AEX9
A	-394	SER	-	EXPRESSION TAG	UNP P0AEX9
A	-393	MET	-	EXPRESSION TAG	UNP P0AEX9
A	-26	ASN	-	LINKER	UNP O75762
A	-25	SER	-	LINKER	UNP O75762

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	SER	-	LINKER	UNP O75762
A	-23	SER	-	LINKER	UNP O75762
A	-22	ASN	-	LINKER	UNP O75762
A	-21	ASN	-	LINKER	UNP O75762
A	-20	ASN	-	LINKER	UNP O75762
A	-19	ASN	-	LINKER	UNP O75762
A	-18	ASN	-	LINKER	UNP O75762
A	-17	ASN	-	LINKER	UNP O75762
A	-16	ASN	-	LINKER	UNP O75762
A	-15	ASN	-	LINKER	UNP O75762
A	-14	ASN	-	LINKER	UNP O75762
A	-13	ASN	-	LINKER	UNP O75762
A	-12	LEU	-	LINKER	UNP O75762
A	-11	GLY	-	LINKER	UNP O75762
A	-10	ILE	-	LINKER	UNP O75762
A	-9	GLU	-	LINKER	UNP O75762
A	-8	GLU	-	LINKER	UNP O75762
A	-7	ASN	-	LINKER	UNP O75762
A	-6	LEU	-	LINKER	UNP O75762
A	-5	TYR	-	LINKER	UNP O75762
A	-4	PHE	-	LINKER	UNP O75762
A	-3	GLN	-	LINKER	UNP O75762
A	-2	GLY	-	LINKER	UNP O75762
A	-1	ALA	-	LINKER	UNP O75762
A	0	GLY	-	LINKER	UNP O75762
A	1	SER	-	LINKER	UNP O75762
A	966	ASP	GLU	CONFLICT	UNP O75762
B	-408	MET	-	EXPRESSION TAG	UNP P0AEX9
B	-407	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	-406	SER	-	EXPRESSION TAG	UNP P0AEX9
B	-405	SER	-	EXPRESSION TAG	UNP P0AEX9
B	-404	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-403	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-402	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-401	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-400	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-399	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-398	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-397	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-396	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	-395	SER	-	EXPRESSION TAG	UNP P0AEX9
B	-394	SER	-	EXPRESSION TAG	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-393	MET	-	EXPRESSION TAG	UNP P0AEX9
B	-26	ASN	-	LINKER	UNP O75762
B	-25	SER	-	LINKER	UNP O75762
B	-24	SER	-	LINKER	UNP O75762
B	-23	SER	-	LINKER	UNP O75762
B	-22	ASN	-	LINKER	UNP O75762
B	-21	ASN	-	LINKER	UNP O75762
B	-20	ASN	-	LINKER	UNP O75762
B	-19	ASN	-	LINKER	UNP O75762
B	-18	ASN	-	LINKER	UNP O75762
B	-17	ASN	-	LINKER	UNP O75762
B	-16	ASN	-	LINKER	UNP O75762
B	-15	ASN	-	LINKER	UNP O75762
B	-14	ASN	-	LINKER	UNP O75762
B	-13	ASN	-	LINKER	UNP O75762
B	-12	LEU	-	LINKER	UNP O75762
B	-11	GLY	-	LINKER	UNP O75762
B	-10	ILE	-	LINKER	UNP O75762
B	-9	GLU	-	LINKER	UNP O75762
B	-8	GLU	-	LINKER	UNP O75762
B	-7	ASN	-	LINKER	UNP O75762
B	-6	LEU	-	LINKER	UNP O75762
B	-5	TYR	-	LINKER	UNP O75762
B	-4	PHE	-	LINKER	UNP O75762
B	-3	GLN	-	LINKER	UNP O75762
B	-2	GLY	-	LINKER	UNP O75762
B	-1	ALA	-	LINKER	UNP O75762
B	0	GLY	-	LINKER	UNP O75762
B	1	SER	-	LINKER	UNP O75762
B	966	ASP	GLU	CONFLICT	UNP O75762
C	-408	MET	-	EXPRESSION TAG	UNP P0AEX9
C	-407	GLY	-	EXPRESSION TAG	UNP P0AEX9
C	-406	SER	-	EXPRESSION TAG	UNP P0AEX9
C	-405	SER	-	EXPRESSION TAG	UNP P0AEX9
C	-404	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-403	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-402	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-401	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-400	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-399	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-398	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-397	HIS	-	EXPRESSION TAG	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-396	GLY	-	EXPRESSION TAG	UNP P0AEX9
C	-395	SER	-	EXPRESSION TAG	UNP P0AEX9
C	-394	SER	-	EXPRESSION TAG	UNP P0AEX9
C	-393	MET	-	EXPRESSION TAG	UNP P0AEX9
C	-26	ASN	-	LINKER	UNP O75762
C	-25	SER	-	LINKER	UNP O75762
C	-24	SER	-	LINKER	UNP O75762
C	-23	SER	-	LINKER	UNP O75762
C	-22	ASN	-	LINKER	UNP O75762
C	-21	ASN	-	LINKER	UNP O75762
C	-20	ASN	-	LINKER	UNP O75762
C	-19	ASN	-	LINKER	UNP O75762
C	-18	ASN	-	LINKER	UNP O75762
C	-17	ASN	-	LINKER	UNP O75762
C	-16	ASN	-	LINKER	UNP O75762
C	-15	ASN	-	LINKER	UNP O75762
C	-14	ASN	-	LINKER	UNP O75762
C	-13	ASN	-	LINKER	UNP O75762
C	-12	LEU	-	LINKER	UNP O75762
C	-11	GLY	-	LINKER	UNP O75762
C	-10	ILE	-	LINKER	UNP O75762
C	-9	GLU	-	LINKER	UNP O75762
C	-8	GLU	-	LINKER	UNP O75762
C	-7	ASN	-	LINKER	UNP O75762
C	-6	LEU	-	LINKER	UNP O75762
C	-5	TYR	-	LINKER	UNP O75762
C	-4	PHE	-	LINKER	UNP O75762
C	-3	GLN	-	LINKER	UNP O75762
C	-2	GLY	-	LINKER	UNP O75762
C	-1	ALA	-	LINKER	UNP O75762
C	0	GLY	-	LINKER	UNP O75762
C	1	SER	-	LINKER	UNP O75762
C	966	ASP	GLU	CONFLICT	UNP O75762



- Molecule 1: Maltose-binding periplasmic protein, Transient receptor potential cation channel subfamily A member 1 chimera

Response	Percentage
Yes	20%
No	15%
Don't know	63%

[illegible]




4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	43585	Depositor
Resolution determination method	FSC 0.143	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)	2800	Depositor
Magnification	31000	Depositor
Image detector	Gatan K2 (4k x 4k)	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	0.41	0/4326	0.82	1/5872 (0.0%)
1	B	0.41	0/4326	0.82	1/5872 (0.0%)
1	C	0.42	0/4326	0.82	1/5872 (0.0%)
1	D	0.41	0/4326	0.82	1/5872 (0.0%)
All	All	0.41	0/17304	0.82	4/23488 (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	A	0	23
1	B	0	23
1	C	0	23
1	D	0	24
All	All	0	93

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	766	ASN	N-CA-CB	9.05	126.89	110.60
1	D	766	ASN	N-CA-CB	9.02	126.84	110.60
1	C	766	ASN	N-CA-CB	9.02	126.84	110.60
1	B	766	ASN	N-CA-CB	9.00	126.80	110.60

There are no chirality outliers.

5 of 93 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	547	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	D	593	LYS	Peptide
1	D	604	ARG	Peptide
1	D	609	LEU	Peptide
1	D	610	LYS	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	4238	0	4110	232	0
1	B	4238	0	4110	230	0
1	C	4238	0	4110	233	0
1	D	4238	0	4110	239	0
All	All	16952	0	16440	851	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 25.

The worst 5 of 851 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:D:1051:LEU:HD13	1:A:1047:GLN:NE2	1.39	1.37
1:A:1051:LEU:HD13	1:B:1047:GLN:NE2	1.40	1.32
1:B:1051:LEU:HD13	1:C:1047:GLN:NE2	1.41	1.32
1:D:1047:GLN:NE2	1:C:1051:LEU:HD13	1.40	1.30
1:D:1051:LEU:CD1	1:A:1047:GLN:NE2	2.26	0.97

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	550/1528 (36%)	485 (88%)	56 (10%)	9 (2%)	12	57
1	B	550/1528 (36%)	485 (88%)	56 (10%)	9 (2%)	12	57
1	C	550/1528 (36%)	485 (88%)	56 (10%)	9 (2%)	12	57
1	D	550/1528 (36%)	485 (88%)	56 (10%)	9 (2%)	12	57
All	All	2200/6112 (36%)	1940 (88%)	224 (10%)	36 (2%)	17	57

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	580	GLN
1	D	639	ASP
1	A	580	GLN
1	A	639	ASP
1	B	580	GLN

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	415/1325 (31%)	405 (98%)	10 (2%)	57	83
1	B	415/1325 (31%)	405 (98%)	10 (2%)	57	83
1	C	415/1325 (31%)	405 (98%)	10 (2%)	57	83
1	D	415/1325 (31%)	405 (98%)	10 (2%)	57	83
All	All	1660/5300 (31%)	1620 (98%)	40 (2%)	60	83

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	832	TRP
1	B	620	LYS
1	C	785	TYR

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Mol	Chain	Res	Type
1	B	480	LEU
1	B	690	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1047	GLN
1	C	1047	GLN
1	B	1047	GLN
1	D	1047	GLN
1	B	1061	GLN

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.