Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:54 AM GMT

PDB ID	:	2ETC
Title	:	Crystal structure of the ankyrin repeat domain of TRPV2
Authors	:	Jin, X.; Gaudet, R.
Deposited on	:	2005-10-27
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

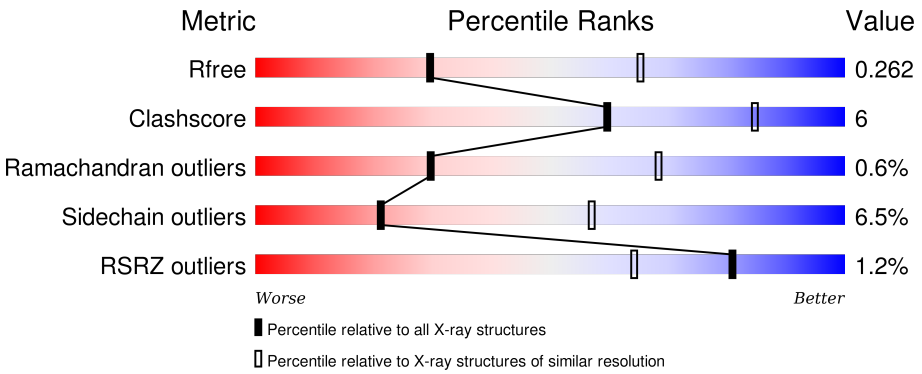
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	274	% 80% 9% • 8%
1	B	274	% 74% 14% • • 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3896 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	252	1975	1246	343	373	13	0	0	0
1	B	248	1921	1210	333	365	13	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

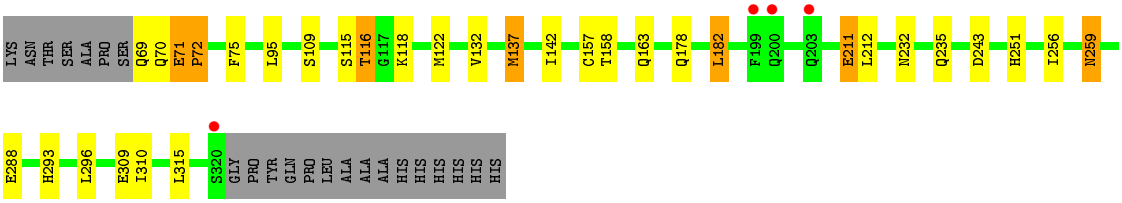
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	PRO	LEU	SEE REMARK 999	UNP Q9WUD2
A	327	ALA	-	CLONING ARTIFACT	UNP Q9WUD2
A	328	ALA	-	CLONING ARTIFACT	UNP Q9WUD2
A	329	ALA	-	CLONING ARTIFACT	UNP Q9WUD2
A	330	HIS	-	CLONING ARTIFACT	UNP Q9WUD2
A	331	HIS	-	CLONING ARTIFACT	UNP Q9WUD2
A	332	HIS	-	CLONING ARTIFACT	UNP Q9WUD2
A	333	HIS	-	CLONING ARTIFACT	UNP Q9WUD2
A	334	HIS	-	CLONING ARTIFACT	UNP Q9WUD2
A	335	HIS	-	CLONING ARTIFACT	UNP Q9WUD2
B	67	PRO	LEU	SEE REMARK 999	UNP Q9WUD2
B	327	ALA	-	CLONING ARTIFACT	UNP Q9WUD2
B	328	ALA	-	CLONING ARTIFACT	UNP Q9WUD2
B	329	ALA	-	CLONING ARTIFACT	UNP Q9WUD2
B	330	HIS	-	CLONING ARTIFACT	UNP Q9WUD2
B	331	HIS	-	CLONING ARTIFACT	UNP Q9WUD2
B	332	HIS	-	CLONING ARTIFACT	UNP Q9WUD2
B	333	HIS	-	CLONING ARTIFACT	UNP Q9WUD2
B	334	HIS	-	CLONING ARTIFACT	UNP Q9WUD2
B	335	HIS	-	CLONING ARTIFACT	UNP Q9WUD2

3 Residue-property plots (i)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

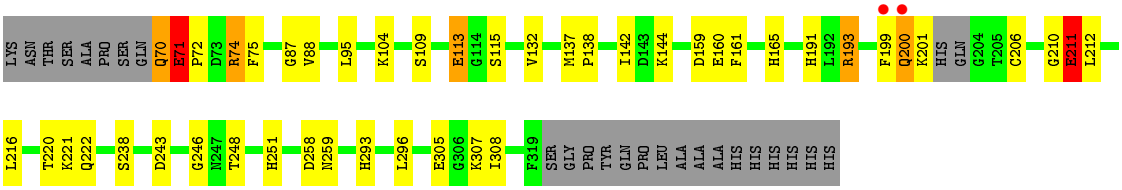
- Molecule 1: Transient receptor potential cation channel subfamily V member 2

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	39.51Å 95.86Å 164.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 47.93 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-3.10) 99.7 (47.93-3.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	5.29 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.210 , 0.262 0.232 , 0.262	Depositor DCC
R_{free} test set	1173 reflections (9.83%)	DCC
Wilson B-factor (Å^2)	50.5	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , -0.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 11944 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	3896	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.40	1/2014 (0.0%)	0.66	4/2729 (0.1%)
1	B	0.34	0/1956	0.61	4/2652 (0.2%)
All	All	0.37	1/3970 (0.0%)	0.64	8/5381 (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	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	PRO	N-CD	10.56	1.62	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	211	GLU	CB-CA-C	-11.90	86.59	110.40
1	B	212	LEU	N-CA-CB	11.04	132.49	110.40
1	A	72	PRO	N-CA-CB	8.18	113.11	103.30
1	A	212	LEU	N-CA-CB	7.90	126.19	110.40
1	A	72	PRO	CA-N-CD	-6.70	102.12	111.50
1	B	201	LYS	N-CA-C	-6.10	94.54	111.00
1	B	159	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	211	GLU	N-CA-C	5.27	125.22	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	200	GLN	Peptide
1	B	211	GLU	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	A	1975	0	1959	17	0
1	B	1921	0	1899	27	0
All	All	3896	0	3858	44	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 6.

All (44) 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:71:GLU:HB2	1:A:72:PRO:HA	1.39	1.00
1:B:193:ARG:HA	1:B:211:GLU:O	1.81	0.79
1:A:116:THR:O	1:A:116:THR:HG23	1.88	0.72
1:A:232:ASN:HD21	1:A:235:GLN:H	1.38	0.71
1:B:74:ARG:HH11	1:B:74:ARG:HG3	1.56	0.70
1:A:116:THR:O	1:A:116:THR:CG2	2.40	0.70
1:B:71:GLU:HB3	1:B:72:PRO:CA	2.25	0.67
1:A:71:GLU:HB2	1:A:72:PRO:CA	2.21	0.64
1:B:258:ASP:O	1:B:259:ASN:HB2	1.98	0.63
1:A:232:ASN:ND2	1:A:235:GLN:H	1.97	0.62
1:B:71:GLU:HB3	1:B:72:PRO:HA	1.82	0.59
1:A:122:MET:SD	1:A:157:CYS:HB2	2.45	0.56
1:B:137:MET:HB3	1:B:138:PRO:HD3	1.88	0.55
1:B:74:ARG:CG	1:B:74:ARG:HH11	2.18	0.55
1:A:71:GLU:CB	1:A:72:PRO:HA	2.27	0.55
1:B:109:SER:HB3	1:B:115:SER:HB3	1.88	0.54
1:B:191:HIS:HE1	1:B:238:SER:H	1.57	0.52
1:B:259:ASN:HD21	1:B:307:LYS:HA	1.75	0.51
1:B:210:GLY:O	1:B:211:GLU:HB2	2.11	0.51
1:A:132:VAL:HG13	1:A:178:GLN:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:PHE:O	1:B:200:GLN:CB	2.60	0.49
1:B:220:THR:CG2	1:B:222:GLN:HE21	2.26	0.49
1:B:248:THR:H	1:B:251:HIS:CD2	2.31	0.49
1:A:259:ASN:HD21	1:A:309:GLU:HB2	1.77	0.49
1:A:115:SER:O	1:A:116:THR:HB	2.12	0.49
1:A:109:SER:OG	1:A:115:SER:HB3	2.14	0.48
1:B:251:HIS:HE1	1:B:296:LEU:O	1.96	0.47
1:B:305:GLU:HB3	1:B:307:LYS:HE2	1.97	0.46
1:B:70:GLN:HA	1:B:71:GLU:HA	1.60	0.44
1:B:71:GLU:HB3	1:B:72:PRO:C	2.37	0.44
1:B:191:HIS:CE1	1:B:238:SER:H	2.35	0.44
1:B:220:THR:HG21	1:B:222:GLN:HE21	1.82	0.44
1:B:216:LEU:O	1:B:220:THR:HG22	2.17	0.43
1:A:211:GLU:CD	1:A:243:ASP:HB2	2.39	0.43
1:B:210:GLY:O	1:B:243:ASP:HB3	2.19	0.42
1:A:251:HIS:HE1	1:A:296:LEU:O	2.01	0.42
1:B:220:THR:HG23	1:B:222:GLN:HG3	2.02	0.42
1:B:246:GLY:HA3	1:B:293:HIS:CD2	2.54	0.42
1:B:165:HIS:HE1	1:B:206:CYS:SG	2.42	0.42
1:B:113:GLU:HG2	1:B:113:GLU:H	1.66	0.41
1:A:158:THR:HG22	1:A:158:THR:O	2.21	0.41
1:B:95:LEU:HD23	1:B:142:ILE:HD13	2.03	0.41
1:A:137:MET:HG2	1:A:182:LEU:HD21	2.02	0.41
1:A:95:LEU:HD23	1:A:142:ILE:HD13	2.03	0.40

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 X-ray entries followed by that with respect to entries of similar resolution.

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	250/274 (91%)	237 (95%)	12 (5%)	1 (0%)	39 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	244/274 (89%)	235 (96%)	7 (3%)	2 (1%)	24	63
All	All	494/548 (90%)	472 (96%)	19 (4%)	3 (1%)	30	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	71	GLU
1	A	71	GLU
1	B	87	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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	218/235 (93%)	204 (94%)	14 (6%)	22	57
1	B	210/235 (89%)	196 (93%)	14 (7%)	20	56
All	All	428/470 (91%)	400 (94%)	28 (6%)	21	57

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	70	GLN
1	A	75	PHE
1	A	116	THR
1	A	118	LYS
1	A	137	MET
1	A	163	GLN
1	A	182	LEU
1	A	256	ILE
1	A	259	ASN
1	A	288	GLU
1	A	293	HIS
1	A	310	ILE

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Mol	Chain	Res	Type
1	A	315	LEU
1	B	70	GLN
1	B	71	GLU
1	B	74	ARG
1	B	75	PHE
1	B	88	VAL
1	B	104	LYS
1	B	113	GLU
1	B	132	VAL
1	B	144	LYS
1	B	160	GLU
1	B	161	PHE
1	B	193	ARG
1	B	221	LYS
1	B	308	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	191	HIS
1	A	232	ASN
1	A	251	HIS
1	B	127	ASN
1	B	129	GLN
1	B	156	GLN
1	B	165	HIS
1	B	191	HIS
1	B	234	HIS
1	B	251	HIS
1	B	259	ASN
1	B	293	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 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.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	252/274 (91%)	-0.07	4 (1%)	74	55	32, 41, 49, 57	0
1	B	248/274 (90%)	-0.12	2 (0%)	87	75	32, 40, 48, 56	0
All	All	500/548 (91%)	-0.09	6 (1%)	81	64	32, 40, 49, 57	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	199	PHE	2.9
1	A	320	SER	2.5
1	A	200	GLN	2.4
1	B	200	GLN	2.4
1	A	199	PHE	2.2
1	A	203	GLN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.