W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 27, 2017 – 11:02 PM EDT

PDB ID	:	3JXI
Title	:	Crystal structure of the chicken TRPV4 ankyrin repeat domain
Authors	:	Phelps, C.B.; Wang, R.R.; Gaudet, R.
Deposited on	:	unknown
Resolution	:	2.30 Å(reported)

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

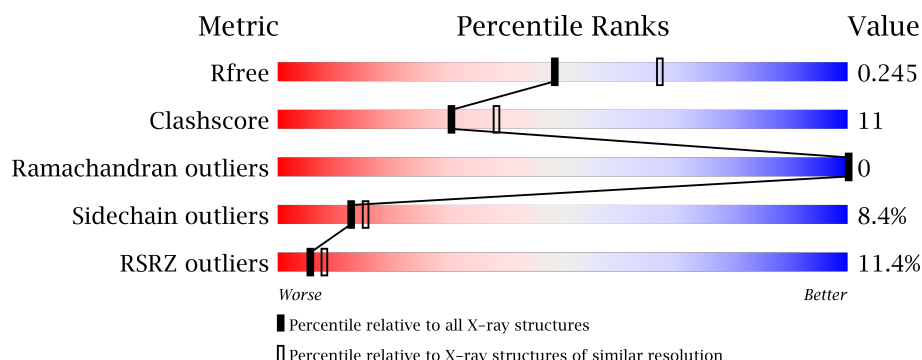|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

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 2.30 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 | Percentile Ranks | Value

Rfree 0.245
Clashscore 11
Ramachandran outliers 0
Sidechain outliers 8.4%
RSRZ outliers 11.4%

Worse .... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	260	5% / 77% / 17% · ·
1	B	260	7% / 75% / 19% / 5% ·
1	C	260	4% / 72% / 20% · ·
1	D	260	29% / 72% / 21% · ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8556 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 Vanilloid receptor-related osmotically activated channel protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total 2017	C 1280	N 361	O 366	S 10	0	3	0
1	B	256	Total 2033	C 1289	N 368	O 367	S 9	0	0	0
1	C	249	Total 1990	C 1262	N 364	O 355	S 9	0	1	0
1	D	249	Total 1982	C 1257	N 361	O 355	S 9	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	MET	-	EXPRESSION TAG	UNP Q9DFS3
A	383	ALA	-	EXPRESSION TAG	UNP Q9DFS3
A	384	ALA	-	EXPRESSION TAG	UNP Q9DFS3
A	385	ALA	-	EXPRESSION TAG	UNP Q9DFS3
A	386	HIS	-	EXPRESSION TAG	UNP Q9DFS3
A	387	HIS	-	EXPRESSION TAG	UNP Q9DFS3
A	388	HIS	-	EXPRESSION TAG	UNP Q9DFS3
A	389	HIS	-	EXPRESSION TAG	UNP Q9DFS3
A	390	HIS	-	EXPRESSION TAG	UNP Q9DFS3
A	391	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	132	MET	-	EXPRESSION TAG	UNP Q9DFS3
B	383	ALA	-	EXPRESSION TAG	UNP Q9DFS3
B	384	ALA	-	EXPRESSION TAG	UNP Q9DFS3
B	385	ALA	-	EXPRESSION TAG	UNP Q9DFS3
B	386	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	387	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	388	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	389	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	390	HIS	-	EXPRESSION TAG	UNP Q9DFS3
B	391	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	132	MET	-	EXPRESSION TAG	UNP Q9DFS3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	383	ALA	-	EXPRESSION TAG	UNP Q9DFS3
C	384	ALA	-	EXPRESSION TAG	UNP Q9DFS3
C	385	ALA	-	EXPRESSION TAG	UNP Q9DFS3
C	386	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	387	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	388	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	389	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	390	HIS	-	EXPRESSION TAG	UNP Q9DFS3
C	391	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	132	MET	-	EXPRESSION TAG	UNP Q9DFS3
D	383	ALA	-	EXPRESSION TAG	UNP Q9DFS3
D	384	ALA	-	EXPRESSION TAG	UNP Q9DFS3
D	385	ALA	-	EXPRESSION TAG	UNP Q9DFS3
D	386	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	387	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	388	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	389	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	390	HIS	-	EXPRESSION TAG	UNP Q9DFS3
D	391	HIS	-	EXPRESSION TAG	UNP Q9DFS3

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	171	Total O 171 171	0	0
2	B	178	Total O 178 178	0	0
2	C	124	Total O 124 124	0	0
2	D	61	Total O 61 61	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 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: Vanilloid receptor-related osmotically activated channel protein
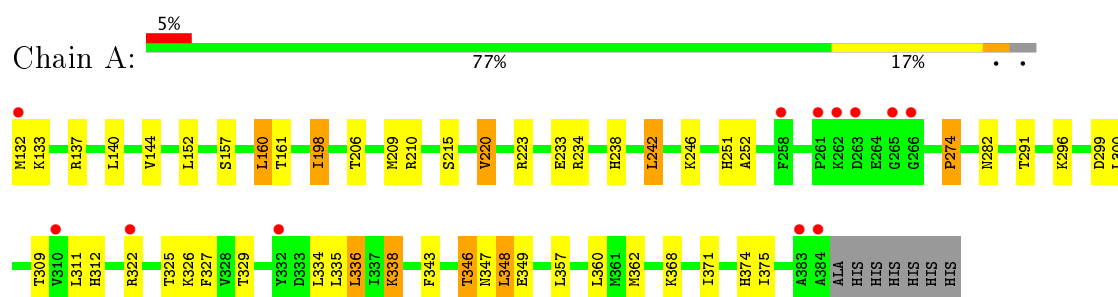
- Molecule 1: Vanilloid receptor-related osmotically activated channel protein
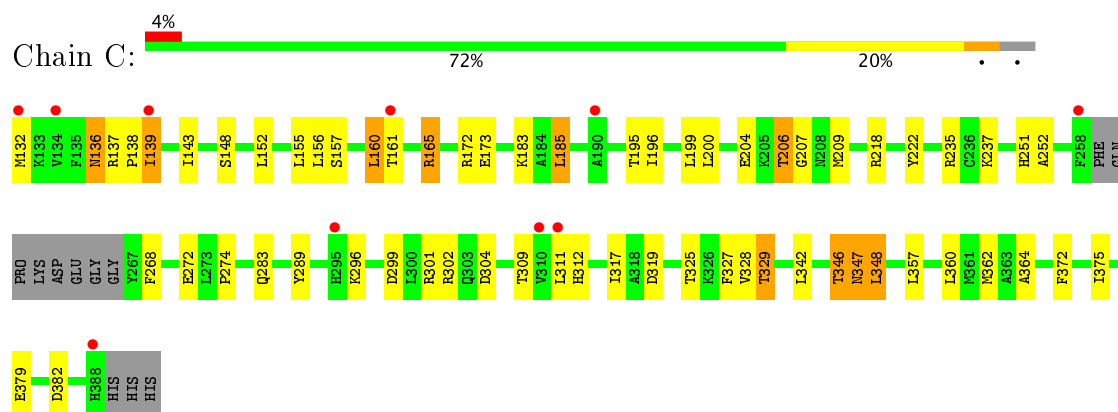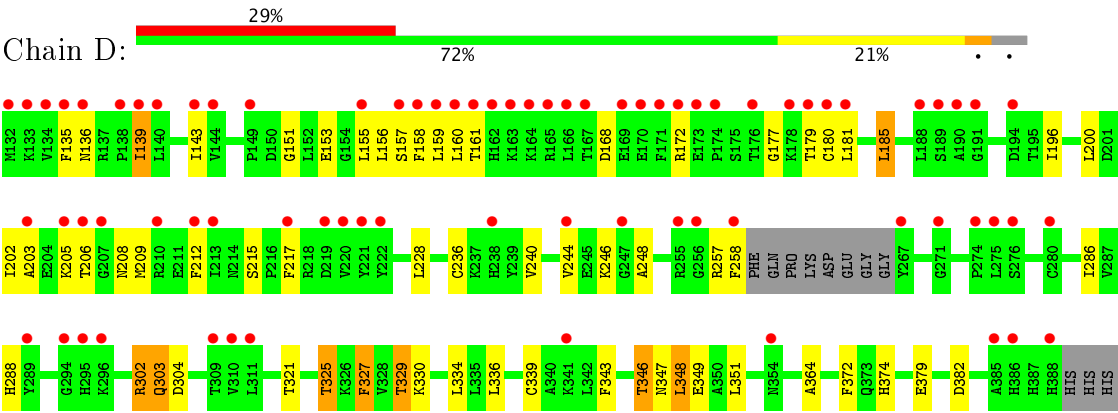

- Molecule 1: Vanilloid receptor-related osmotically activated channel protein

- Molecule 1: Vanilloid receptor-related osmotically activated channel protein

Chain D:

29%

72%   21%
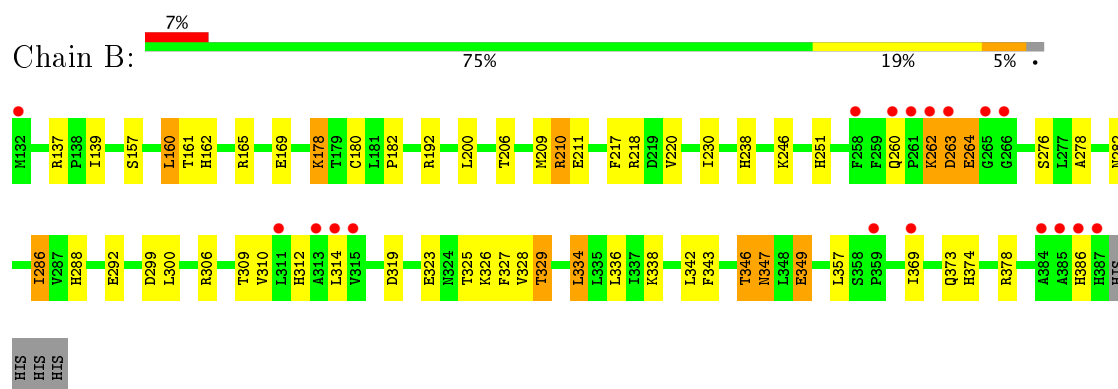
4　Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.26Å　　48.12Å　　133.89Å 90.00°　　101.89°　　90.00°	Depositor
Resolution (Å)	29.51　–　2.30 29.51　–　2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.51-2.30) 97.6 (29.51-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.203　,　0.243 0.206　,　0.245	Depositor DCC
R_{free} test set	1178 reflections (2.08%)	DCC
Wilson B-factor (Å²)	37.4	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.32 , 50.1	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8556	wwPDB-VP
Average B, all atoms (Å²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.08 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3910e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.77	0/2065	0.83	3/2788 (0.1%)
1	B	0.79	2/2074 (0.1%)	0.87	3/2799 (0.1%)
1	C	0.56	0/2032	0.70	1/2741 (0.0%)
1	D	0.46	0/2021	0.61	0/2727
All	All	0.66	2/8192 (0.0%)	0.76	7/11055 (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
1	C	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	180	CYS	CB-SG	-5.83	1.72	1.81
1	B	349	GLU	CB-CG	-5.29	1.42	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	B	378	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	137	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	A	137	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	137	ARG	NE-CZ-NH1	5.66	123.13	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	262	LYS	Peptide
1	B	263	ASP	Peptide
1	C	207	GLY	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	2017	0	2049	39	0
1	B	2033	0	2053	41	0
1	C	1990	0	2019	44	0
1	D	1982	0	2006	48	0
2	A	171	0	0	6	0
2	B	178	0	0	7	0
2	C	124	0	0	6	0
2	D	61	0	0	5	0
All	All	8556	0	8127	170	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 11.

The worst 5 of 170 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:257:ARG:O	1:D:258:PHE:CG	2.11	1.04
1:C:218[B]:ARG:CG	1:C:218[B]:ARG:HH11	1.71	1.03
1:D:158:PHE:HA	1:D:161:THR:HG22	1.44	0.97
1:C:218[B]:ARG:HH11	1:C:218[B]:ARG:HG2	1.24	0.97
1:D:257:ARG:O	1:D:258:PHE:CD2	2.24	0.90

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	254/260 (98%)	246 (97%)	8 (3%)	0	100	100
1	B	254/260 (98%)	242 (95%)	12 (5%)	0	100	100
1	C	246/260 (95%)	235 (96%)	11 (4%)	0	100	100
1	D	245/260 (94%)	228 (93%)	17 (7%)	0	100	100
All	All	999/1040 (96%)	951 (95%)	48 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	218/221 (99%)	197 (90%)	21 (10%)	10	11
1	B	217/221 (98%)	197 (91%)	20 (9%)	11	12
1	C	213/221 (96%)	198 (93%)	15 (7%)	18	22
1	D	212/221 (96%)	195 (92%)	17 (8%)	14	17
All	All	860/884 (97%)	787 (92%)	73 (8%)	13	15

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	327	PHE
1	B	386	HIS
1	D	339	CYS

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Mol	Chain	Res	Type
1	B	342	LEU
1	C	139	ILE

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	C	136	ASN
1	C	282	ASN
1	D	354	ASN
1	C	208	ASN
1	C	251	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(Å²)	Q<0.9
1	A	253/260 (97%)	0.16	12 (4%)	32	39	9, 17, 28, 35	0
1	B	256/260 (98%)	0.19	18 (7%)	17	23	9, 18, 35, 64	0
1	C	249/260 (95%)	0.22	10 (4%)	39	46	16, 25, 32, 44	0
1	D	249/260 (95%)	1.63	75 (30%)	1	0	23, 39, 62, 70	0
All	All	1007/1040 (96%)	0.55	115 (11%)	6	8	9, 24, 51, 70	0

The worst 5 of 115 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	134	VAL	15.1
1	D	135	PHE	15.1
1	D	132	MET	10.8
1	D	258	PHE	10.7
1	D	139	ILE	10.5

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.