

Full wwPDB X-ray Structure Validation Report (i)

Mar 11, 2024 – 08:06 AM EDT

PDB ID	:	3JXJ
Title	:	Crystal structure of the chicken TRPV4 ankyrin repeat domain
Authors	:	Phelps, C.B.; Choo, S.S.; Gaudet, R.
Deposited on		
Resolution	:	2.80 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

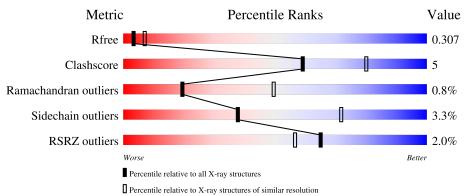
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.80 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569(2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	А	260	83%	15%	
1	В	260	% 	8%	• •



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4027 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.

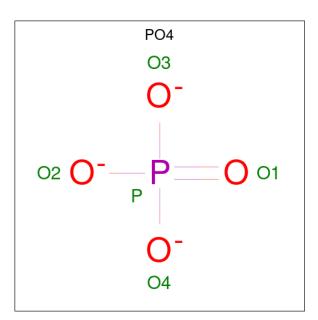
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	257	Total	С	Ν	0	S	0	3	0
		201	2039	1293	367	370	9	0		
1	В	249	Total	С	Ν	0	S	0	3	0
1	В	249	1978	1255	357	357	9	U		0

Chain	Residue	Modelled	Actual	Comment	Reference
А	132	MET	-	expression tag	UNP Q9DFS3
А	383	ALA	-	expression tag	UNP Q9DFS3
A	384	ALA	-	expression tag	UNP Q9DFS3
А	385	ALA	-	expression tag	UNP Q9DFS3
A	386	HIS	-	expression tag	UNP Q9DFS3
А	387	HIS	-	expression tag	UNP Q9DFS3
А	388	HIS	-	expression tag	UNP Q9DFS3
A	389	HIS	-	expression tag	UNP Q9DFS3
А	390	HIS	-	expression tag	UNP Q9DFS3
A	391	HIS	-	expression tag	UNP Q9DFS3
В	132	MET	-	expression tag	UNP Q9DFS3
В	383	ALA	-	expression tag	UNP Q9DFS3
В	384	ALA	-	expression tag	UNP Q9DFS3
В	385	ALA	-	expression tag	UNP Q9DFS3
В	386	HIS	-	expression tag	UNP Q9DFS3
В	387	HIS	-	expression tag	UNP Q9DFS3
В	388	HIS	-	expression tag	UNP Q9DFS3
В	389	HIS	-	expression tag	UNP Q9DFS3
В	390	HIS	-	expression tag	UNP Q9DFS3
В	391	HIS	-	expression tag	UNP Q9DFS3

There are 20 discrepancies between the modelled and reference sequences:

• Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).





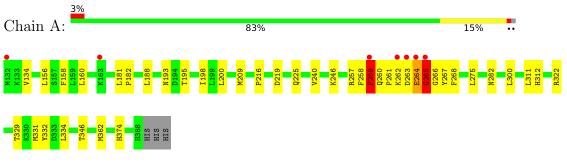
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{P} \\ 5 & 4 & 1 \end{array}$	0	0



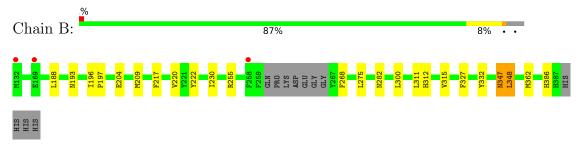
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	47.77Å 77.33Å 186.70Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 - 2.80	Depositor
Resolution (A)	29.78 - 2.80	EDS
% Data completeness	79.7 (29.77-2.80)	Depositor
(in resolution range)	79.7(29.78-2.80)	EDS
R _{merge}	0.14	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$6.47 (at 2.80 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.262 , 0.298	Depositor
It, Itfree	0.266 , 0.307	DCC
R_{free} test set	710 reflections (5.02%)	wwPDB-VP
Wilson B-factor $(Å^2)$	62.9	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.27, 17.0	EDS
L-test for twinning ²	$ L > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4027	wwPDB-VP
Average B, all atoms $(Å^2)$	45.0	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 30.57 % 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 1.2783e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.59	0/2088	0.61	1/2821~(0.0%)	
1	В	0.62	0/2024	0.59	0/2734	
All	All	0.61	0/4112	0.60	1/5555~(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	А	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	265	GLY	N-CA-C	-5.30	99.85	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	259	PHE	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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2039	0	2058	21	0
1	В	1978	0	2004	17	0
2	А	5	0	0	0	0
2	В	5	0	0	0	0
All	All	4027	0	4062	38	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 5.

All (38) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A 4 - 1	A.L. D.	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:275:LEU:HD21	1:B:300:LEU:HD23	1.54	0.87
1:A:219:ASP:O	1:A:257:ARG:NH1	2.11	0.83
1:A:275:LEU:HD21	1:A:300:LEU:HD23	1.76	0.67
1:A:209:MET:HE2	1:A:246:LYS:HD3	1.82	0.60
1:B:220:VAL:HG22	1:B:220:VAL:O	2.05	0.57
1:A:329:THR:HG23	1:A:374:HIS:CD2	2.41	0.56
1:B:347:ASN:HD22	1:B:348:LEU:N	2.06	0.52
1:B:222:TYR:OH	1:B:268:PHE:O	2.25	0.52
1:B:311:LEU:HD11	1:B:348:LEU:HD13	1.92	0.51
1:A:263:ASP:O	1:A:264:GLU:C	2.48	0.51
1:A:265:GLY:C	1:A:267:TYR:H	2.11	0.51
1:A:156:LEU:O	1:A:160:LEU:HD13	2.12	0.50
1:B:311:LEU:HD22	1:B:332:TYR:CD2	2.46	0.50
1:A:265:GLY:O	1:A:267:TYR:N	2.39	0.49
1:B:315:VAL:HB	1:B:362:MET:HE3	1.93	0.49
1:A:181:LEU:HB3	1:A:182:PRO:HD3	1.95	0.48
1:B:311:LEU:HD22	1:B:332:TYR:CE2	2.49	0.48
1:A:259:PHE:CD2	1:A:259:PHE:C	2.88	0.47
1:A:188:LEU:HD23	1:A:193:ASN:HB2	1.96	0.47
1:B:204:GLU:HB2	1:B:209:MET:HE3	1.97	0.47
1:B:312:HIS:O	1:B:362:MET:HE1	2.16	0.46
1:B:188:LEU:HD23	1:B:193:ASN:HB2	1.98	0.46
1:A:311:LEU:HD22	1:A:332:TYR:CD2	2.51	0.46
1:A:312:HIS:O	1:A:362:MET:HE1	2.16	0.46
1:B:196:ILE:N	1:B:197:PRO:CD	2.79	0.46
1:A:134:VAL:HG13	1:A:158:PHE:CE1	2.51	0.46
1:B:347:ASN:HD22	1:B:347:ASN:C	2.20	0.45
1:B:217:PHE:CZ	1:B:230:ILE:HD11	2.53	0.44

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Atom-1	Atom-2	Interatomic	Clash
Atom-1	At0111-2	distance $(Å)$	overlap (Å)
1:B:255:ARG:HH11	1:B:255:ARG:HG2	1.82	0.43
1:A:216:PRO:HA	1:A:225:GLN:O	2.19	0.43
1:B:311:LEU:CD1	1:B:348:LEU:HD13	2.49	0.43
1:A:195:THR:O	1:A:198:ILE:HG22	2.19	0.42
1:A:334:LEU:HD23	1:A:334:LEU:C	2.40	0.42
1:A:329:THR:HG23	1:A:374:HIS:NE2	2.35	0.42
1:A:259:PHE:C	1:A:259:PHE:HD2	2.24	0.41
1:B:311:LEU:HD12	1:B:348:LEU:HD22	2.03	0.41
1:A:200:LEU:O	1:A:209:MET:HE3	2.22	0.40

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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	А	258/260~(99%)	238~(92%)	16~(6%)	4 (2%)	9 31
1	В	248/260~(95%)	240~(97%)	8~(3%)	0	100 100
All	All	506/520~(97%)	478 (94%)	24~(5%)	4 (1%)	19 49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	268	PHE
1	А	266	GLY
1	А	261	PRO
1	А	265	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Analysed Rotameric Outliers		Percentiles		
1	А	218/221~(99%)	209~(96%)	9~(4%)	30 64		
1	В	212/221~(96%)	207~(98%)	5 (2%)	49 81		
All	All	430/442~(97%)	416 (97%)	14 (3%)	38 72		

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	258	PHE
1	А	259	PHE
1	А	260	GLN
1	А	262	LYS
1	А	264	GLU
1	А	282	ASN
1	А	322	ARG
1	А	331	MET
1	А	346	THR
1	В	282	ASN
1	В	327	PHE
1	В	347	ASN
1	В	348	LEU
1	В	386	HIS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such side chains are listed below:

Mol	Chain	Res	Type
1	А	282	ASN
1	А	288	HIS
1	А	297	GLN
1	А	354	ASN
1	А	373	GLN
1	В	225	GLN
1	В	282	ASN
1	В	297	GLN

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Mol	Chain	Res	Type
1	В	347	ASN
1	В	354	ASN
1	В	373	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Dec	Res Link Bond lengths		В	ond ang	gles		
WIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	PO4	А	401	-	4,4,4	0.73	0	$6,\!6,\!6$	0.54	0
2	PO4	В	401	-	4,4,4	0.85	0	$6,\!6,\!6$	0.84	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



No monomer is involved in short contacts.

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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	А	257/260~(98%)	0.09	7 (2%) 54 44	38, 50, 58, 70	0
1	В	249/260~(95%)	-0.19	3 (1%) 79 73	25, 40, 51, 61	0
All	All	506/520~(97%)	-0.05	10 (1%) 65 56	25, 46, 57, 70	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	264	GLU	6.6
1	В	132	MET	5.9
1	А	132	MET	3.3
1	В	258	PHE	3.1
1	А	265	GLY	2.7
1	А	263	ASP	2.6
1	В	169	GLU	2.6
1	А	163	LYS	2.4
1	А	262	LYS	2.2
1	А	259	PHE	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 monosaccharides in this entry.



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	PO4	А	401	5/5	0.94	0.15	77,77,78,80	0
2	PO4	В	401	5/5	0.96	0.17	57,58,59,62	0

6.5 Other polymers (i)

There are no such residues in this entry.

