

# wwPDB X-ray Structure Validation Summary Report (i)

#### Sep 20, 2023 – 01:44 PM EDT

PDB ID : 5IWO

Title : Bacterial sodium channel pore domain, low bromide Authors : Shaya, D.; Findeisen, F.; Rohaim, A.; Minor, D.L.

Deposited on : 2016-03-22

Resolution : 3.33 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 Xtriage (Phenix): 1.13

EDS : 2.35.1

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)

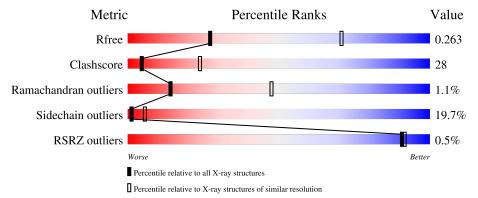
Validation Pipeline (wwPDB-VP) : 2.35.1

## 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 3.33 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

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 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	C	Quality of chain	
1	A	152	38%	43%	11% • 9%
1	В	152	37%	41%	12% • 9%
1	С	152	46%	32%	13% 9%
1	D	152	40%	43%	7% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	A	301	-	-	X	-



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4501 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 Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	139	Total	С	N	О	S	0	0	0
1	A	139	1124	742	181	195	6	0	0	
1	D	138	Total	С	N	О	S	0	1	0
1	Ъ	130	1126	745	180	195	6	0	1	
1	С	138	Total	С	N	О	S	0	0	0
1		130	1122	742	178	196	6	0		
1	1 D	128	Total	С	N	О	S	0	0	0
	ש	138	1128	745	181	196	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	GLY	-	expression tag	UNP Q0ABW0
A	138	PRO	-	expression tag	UNP Q0ABW0
A	139	SER	-	expression tag	UNP Q0ABW0
A	140	SER	-	expression tag	UNP Q0ABW0
A	141	PRO	-	expression tag	UNP Q0ABW0
A	142	SER	-	expression tag	UNP Q0ABW0
В	137	GLY	-	expression tag	UNP Q0ABW0
В	138	PRO	-	expression tag	UNP Q0ABW0
В	139	SER	-	expression tag	UNP Q0ABW0
В	140	SER	-	expression tag	UNP Q0ABW0
В	141	PRO	-	expression tag	UNP Q0ABW0
В	142	SER	-	expression tag	UNP Q0ABW0
С	137	GLY	-	expression tag	UNP Q0ABW0
С	138	PRO	-	expression tag	UNP Q0ABW0
С	139	SER	-	expression tag	UNP Q0ABW0
С	140	SER	-	expression tag	UNP Q0ABW0
С	141	PRO	-	expression tag	UNP Q0ABW0
С	142	SER	-	expression tag	UNP Q0ABW0
D	137	GLY	-	expression tag	UNP Q0ABW0
D	138	PRO	-	expression tag	UNP Q0ABW0
D	139	SER	-	expression tag	UNP Q0ABW0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	140	SER	-	expression tag	UNP Q0ABW0
D	141	PRO	-	expression tag	UNP Q0ABW0
D	142	SER	-	expression tag	UNP Q0ABW0

• Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

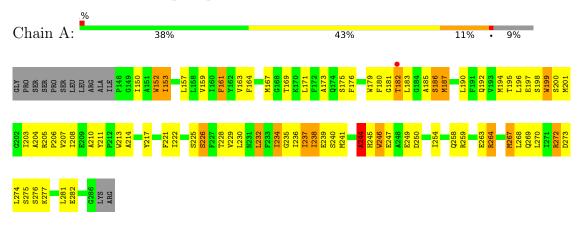
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Br 1 1	0	0



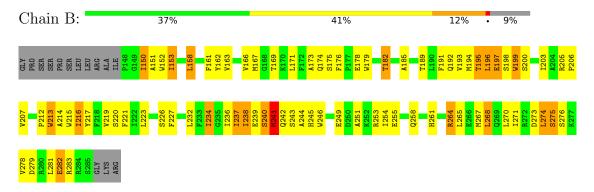
## 3 Residue-property plots (i)

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.

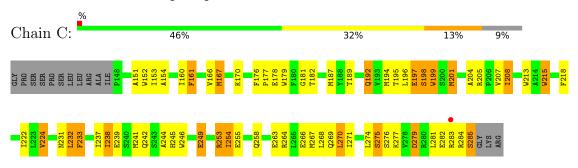
• Molecule 1: Ion transport protein



• Molecule 1: Ion transport protein

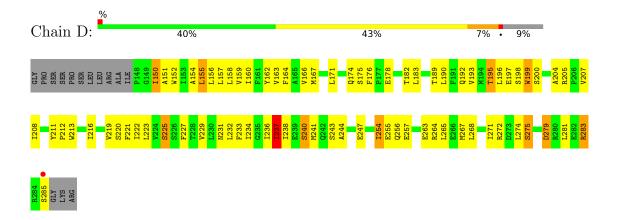


• Molecule 1: Ion transport protein



• Molecule 1: Ion transport protein







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	151.72Å 159.95Å 168.57Å	Donogitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 - 3.33	Depositor
Resolution (A)	14.98 - 3.33	EDS
% Data completeness	98.2 (15.00-3.33)	Depositor
(in resolution range)	98.4 (14.98-3.33)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.23	Depositor
$< I/\sigma(I) > 1$	1.55 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
D D.	0.209 , 0.262	Depositor
$R, R_{free}$	0.209 , $0.263$	DCC
$R_{free}$ test set	1520 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	103.9	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.31, 87.9	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.41, < L^2>=0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4501	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: BR

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	Bo	nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.84	3/1155 (0.3%)	0.96	4/1569 (0.3%)	
1	В	0.75	4/1160 (0.3%)	0.94	4/1575 (0.3%)	
1	С	0.81	4/1153 (0.3%)	0.93	2/1566 (0.1%)	
1	D	0.81	3/1159 (0.3%)	0.89	1/1573 (0.1%)	
All	All	0.80	$14/4627 \ (0.3\%)$	0.93	11/6283 (0.2%)	

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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	В	0	1
All	All	0	2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$Ideal(\AA)$
1	С	199	TRP	CD2-CE2	6.94	1.49	1.41
1	A	199	TRP	CD2-CE2	6.86	1.49	1.41
1	С	152	TRP	CD2-CE2	6.06	1.48	1.41
1	A	152	TRP	CD2-CE2	5.94	1.48	1.41
1	D	213	TRP	CD2-CE2	5.83	1.48	1.41

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
1	A	244	ALA	CB-CA-C	11.00	126.60	110.10
1	В	244	ALA	CB-CA-C	7.52	121.38	110.10

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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
1	D	196	LEU	CB-CG-CD1	-6.48	99.98	111.00
1	В	158	LEU	CB-CG-CD2	-6.22	100.42	111.00
1	В	196	LEU	CB-CG-CD1	-6.15	100.55	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	ALA	Peptide
1	В	241	MET	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	1124	0	1111	91	0
1	В	1126	0	1119	71	0
1	С	1122	0	1112	72	0
1	D	1128	0	1123	76	0
2	A	1	0	0	7	0
All	All	4501	0	4465	253	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 28.

The worst 5 of 253 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:264:ARG:HD3	2:A:301:BR:BR	1.67	1.48
2:A:301:BR:BR	1:C:264:ARG:HD3	1.88	1.27
1:A:204:ALA:O	1:A:208:ILE:HG13	1.49	1.11
1:A:264:ARG:CD	2:A:301:BR:BR	2.56	1.08
1:C:270:LEU:HD23	1:C:270:LEU:H	1.11	1.06

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	Perce	entiles
1	A	$137/152 \ (90\%)$	113 (82%)	24 (18%)	0	100	100
1	В	137/152~(90%)	116 (85%)	19 (14%)	2 (2%)	10	40
1	C	$136/152 \ (90\%)$	110 (81%)	24 (18%)	2 (2%)	10	40
1	D	$136/152 \ (90\%)$	110 (81%)	24 (18%)	2 (2%)	10	40
All	All	546/608 (90%)	449 (82%)	91 (17%)	6 (1%)	14	47

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	151	ALA
1	С	284	ARG
1	С	224	VAL
1	D	237	ILE
1	D	212	PRO

#### 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	117/131 (89%)	96 (82%)	21 (18%)	2 8
1	В	118/131 (90%)	92 (78%)	26 (22%)	1 4
1	С	118/131 (90%)	96 (81%)	22 (19%)	1 7
1	D	119/131 (91%)	95 (80%)	24 (20%)	1 5
All	All	472/524 (90%)	379 (80%)	93 (20%)	1 6



5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	233	PHE
1	D	167	MET
1	С	242	GLN
1	С	275	SER
1	D	178	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	245	HIS
1	С	242	GLN
1	В	242	GLN
1	В	231	ASN
1	В	245	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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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	<rsrz></rsrz>	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	139/152 (91%)	-0.57	1 (0%) 87 90	58, 111, 150, 178	0
1	В	138/152 (90%)	-0.55	0 100 100	59, 115, 152, 178	0
1	С	138/152 (90%)	-0.54	1 (0%) 87 90	70, 108, 158, 186	0
1	D	138/152 (90%)	-0.61	1 (0%) 87 90	68, 104, 152, 167	0
All	All	553/608 (90%)	-0.57	3 (0%) 91 91	58, 110, 154, 186	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	THR	2.8
1	D	285	SER	2.6
1	С	283	ARG	2.0

#### 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
2	BR	A	301	1/1	0.94	0.18	170,170,170,170	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

