



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2016 – 06:23 PM EDT

PDB ID : 5IWN  
Title : Bacterial sodium channel pore domain, high bromide  
Authors : Shaya, D.; Findeisen, F.; Rohaim, A.; Minor, D.L.  
Deposited on : 2016-03-22  
Resolution : 3.75 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

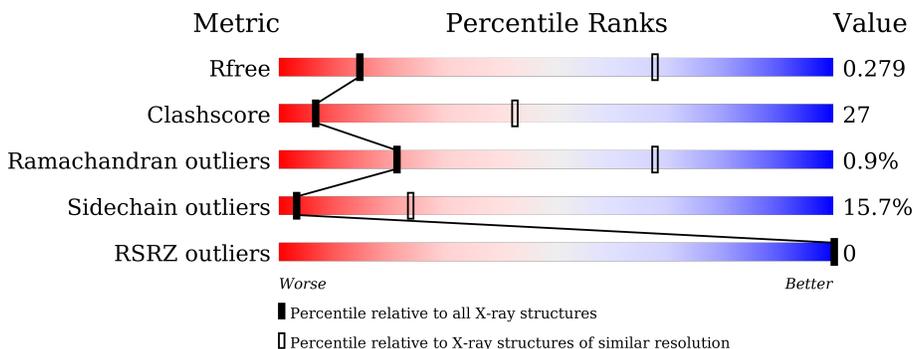
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.75 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	1268 (4.02-3.50)
Clashscore	102246	1407 (4.02-3.50)
Ramachandran outliers	100387	1346 (4.02-3.50)
Sidechain outliers	100360	1342 (4.02-3.50)
RSRZ outliers	91569	1276 (4.02-3.50)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	152	
1	B	152	
1	C	152	
1	D	152	

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 crite-

ria:

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 4502 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
			Total	C	N	O	S			
1	A	139	1124	742	181	195	6	0	0	0
1	B	138	1126	745	180	195	6	0	1	0
1	C	138	1122	742	178	196	6	0	0	0
1	D	138	1128	745	181	196	6	0	0	0

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
B	137	GLY	-	expression tag	UNP Q0ABW0
B	138	PRO	-	expression tag	UNP Q0ABW0
B	139	SER	-	expression tag	UNP Q0ABW0
B	140	SER	-	expression tag	UNP Q0ABW0
B	141	PRO	-	expression tag	UNP Q0ABW0
B	142	SER	-	expression tag	UNP Q0ABW0
C	137	GLY	-	expression tag	UNP Q0ABW0
C	138	PRO	-	expression tag	UNP Q0ABW0
C	139	SER	-	expression tag	UNP Q0ABW0
C	140	SER	-	expression tag	UNP Q0ABW0
C	141	PRO	-	expression tag	UNP Q0ABW0
C	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

*Continued on next page...*

*Continued from previous page...*

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

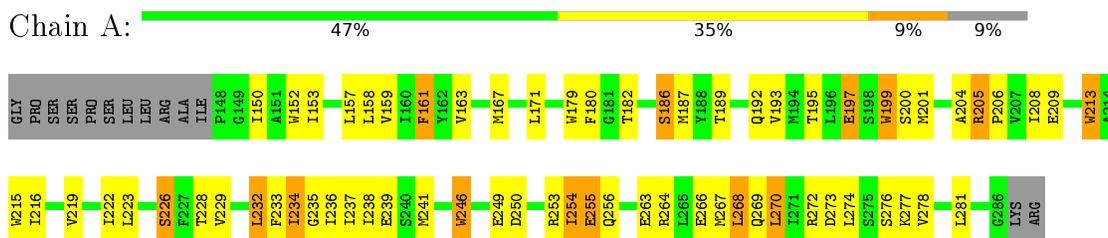
- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

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

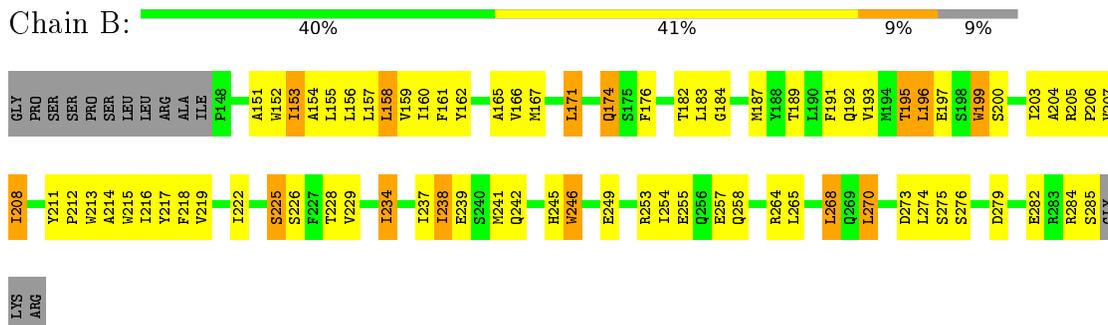
### 3 Residue-property plots [i](#)

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.

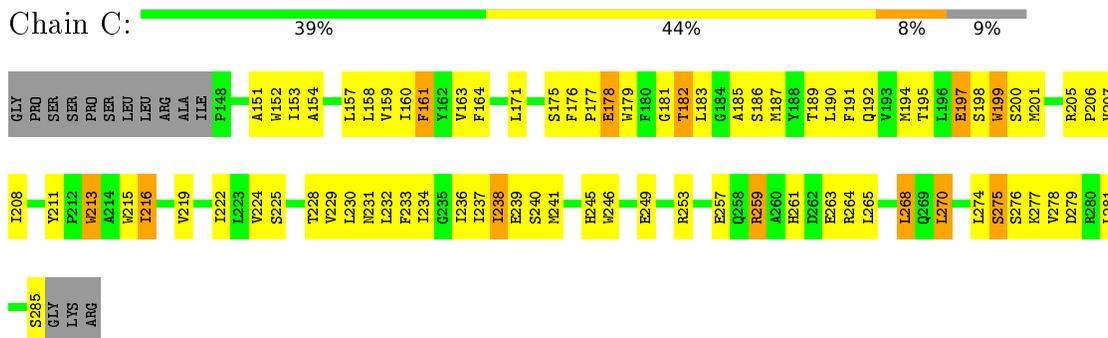
- Molecule 1: Ion transport protein



- Molecule 1: Ion transport protein



- Molecule 1: Ion transport protein



- Molecule 1: Ion transport protein



GLY	V207	S275
PRO	I208	V278
SER	E209	D279
SER	A210	R280
PRO	Y211	L281
SER	P212	E282
LEU	W213	R283
LEU	A214	R284
ARG	W215	S285
ALA	I216	GLY
ILE	Y217	LYS
P148	F218	ARG
G149	V219	
I150	S220	
A151	F221	
W152	I222	
I153	L223	
A154	V224	
L155	S225	
L156		
L157	V229	
L158	L230	
V159	N231	
I160	L232	
F161	F233	
Y162	L234	
	G235	
L171	I236	
F172	I237	
A173	I238	
Q174	E239	
S175	S240	
F176	M241	
	Q242	
W179	S243	
F180	A244	
G181	H245	
T182	W246	
L183	E247	
G184	A248	
	E249	
M187	D250	
Y188	A251	
T189	K252	
L190	R253	
F191	I254	
Q192	E255	
V193	Q256	
M194		
T195	R259	
L196	A260	
E197	H261	
S198	D262	
W199	E263	
R264	R264	
S200	L265	
I203	L270	
A204		
R205		
P206	L274	

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.40Å 160.87Å 167.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.75 14.98 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (15.00-3.75) 99.5 (14.98-3.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.26	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 3.77Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.228 , 0.280 0.222 , 0.279	Depositor DCC
$R_{free}$ test set	1126 reflections (5.49%)	DCC
Wilson B-factor (Å <sup>2</sup> )	144.1	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 101.9	EDS
Estimated twinning fraction	0.129 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	0 of 21634 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4502	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	169.0	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>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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](#)

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	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.70	3/1155 (0.3%)	0.78	1/1569 (0.1%)
1	B	0.70	3/1160 (0.3%)	0.77	1/1575 (0.1%)
1	C	0.76	4/1153 (0.3%)	0.81	0/1566
1	D	0.72	5/1159 (0.4%)	0.80	3/1573 (0.2%)
All	All	0.72	15/4627 (0.3%)	0.79	5/6283 (0.1%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	199	TRP	CD2-CE2	6.69	1.49	1.41
1	C	152	TRP	CD2-CE2	5.74	1.48	1.41
1	D	179	TRP	CD2-CE2	5.50	1.48	1.41
1	A	152	TRP	CD2-CE2	5.50	1.48	1.41
1	C	213	TRP	CD2-CE2	5.43	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	D	196	LEU	CB-CG-CD1	-5.73	101.26	111.00
1	D	223	LEU	CA-CB-CG	-5.49	102.67	115.30
1	D	151	ALA	CB-CA-C	5.29	118.04	110.10
1	A	270	LEU	CB-CG-CD1	-5.02	102.47	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	71	0
1	B	1126	0	1119	61	0
1	C	1122	0	1112	85	0
1	D	1128	0	1123	78	0
2	A	2	0	0	6	0
All	All	4502	0	4465	244	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 27.

The worst 5 of 244 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)
2:A:301:BR:BR	1:C:264:ARG:HD3	1.81	1.33
1:A:264:ARG:HD3	2:A:301:BR:BR	1.87	1.28
1:A:264:ARG:NE	2:A:301:BR:BR	2.25	1.23
1:A:264:ARG:CD	2:A:301:BR:BR	2.44	1.21
1:B:208:ILE:HD11	1:B:215:TRP:HB3	1.25	1.17

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	137/152 (90%)	117 (85%)	19 (14%)	1 (1%)	26 72

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	137/152 (90%)	119 (87%)	16 (12%)	2 (2%)	13	59
1	C	136/152 (90%)	114 (84%)	21 (15%)	1 (1%)	26	72
1	D	136/152 (90%)	115 (85%)	20 (15%)	1 (1%)	26	72
All	All	546/608 (90%)	465 (85%)	76 (14%)	5 (1%)	21	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	151	ALA
1	A	199	TRP
1	B	151	ALA
1	B	212	PRO
1	C	216	ILE

### 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%)	101 (86%)	16 (14%)	4	30
1	B	118/131 (90%)	98 (83%)	20 (17%)	2	19
1	C	118/131 (90%)	100 (85%)	18 (15%)	3	25
1	D	119/131 (91%)	99 (83%)	20 (17%)	2	19
All	All	472/524 (90%)	398 (84%)	74 (16%)	3	24

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	273	ASP
1	C	197	GLU
1	D	256	GLN
1	B	276	SER
1	C	159	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	B	242	GLN
1	D	245	HIS
1	C	242	GLN
1	B	174	GLN
1	C	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are 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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	139/152 (91%)	-0.81	0 100 100	125, 169, 207, 233	0
1	B	138/152 (90%)	-0.79	0 100 100	130, 171, 213, 242	0
1	C	138/152 (90%)	-0.76	0 100 100	117, 165, 214, 258	0
1	D	138/152 (90%)	-0.78	0 100 100	115, 160, 203, 246	0
All	All	553/608 (90%)	-0.78	0 100 100	115, 166, 211, 258	0

There are no RSRZ outliers to report.

### 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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	BR	A	301	1/1	0.92	0.50	-	178,178,178,178	0
2	BR	A	302	1/1	0.92	0.31	-	195,195,195,195	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.