



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 08:24 PM UTC

PDB ID : 1P7B / pdb_00001p7b
Title : Crystal structure of an inward rectifier potassium channel
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Deposited on : 2003-05-01
Resolution : 3.65 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

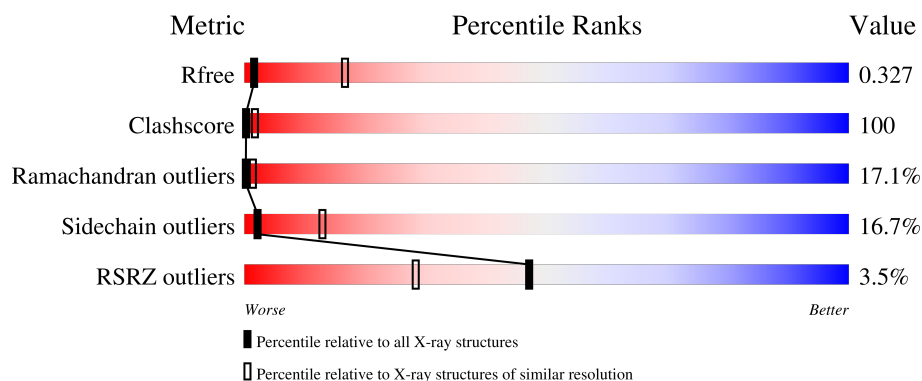
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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}	180053	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

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 $\leq 5\%$. 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	333	
1	B	333	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4059 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 integral membrane channel and cytosolic domains.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2024	1313	349	348	14			
1	B	258	Total	C	N	O	S	0	0	0
			2024	1313	349	348	14			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	K	0	0
			3	3		
2	B	1	Total	K	0	0
			1	1		

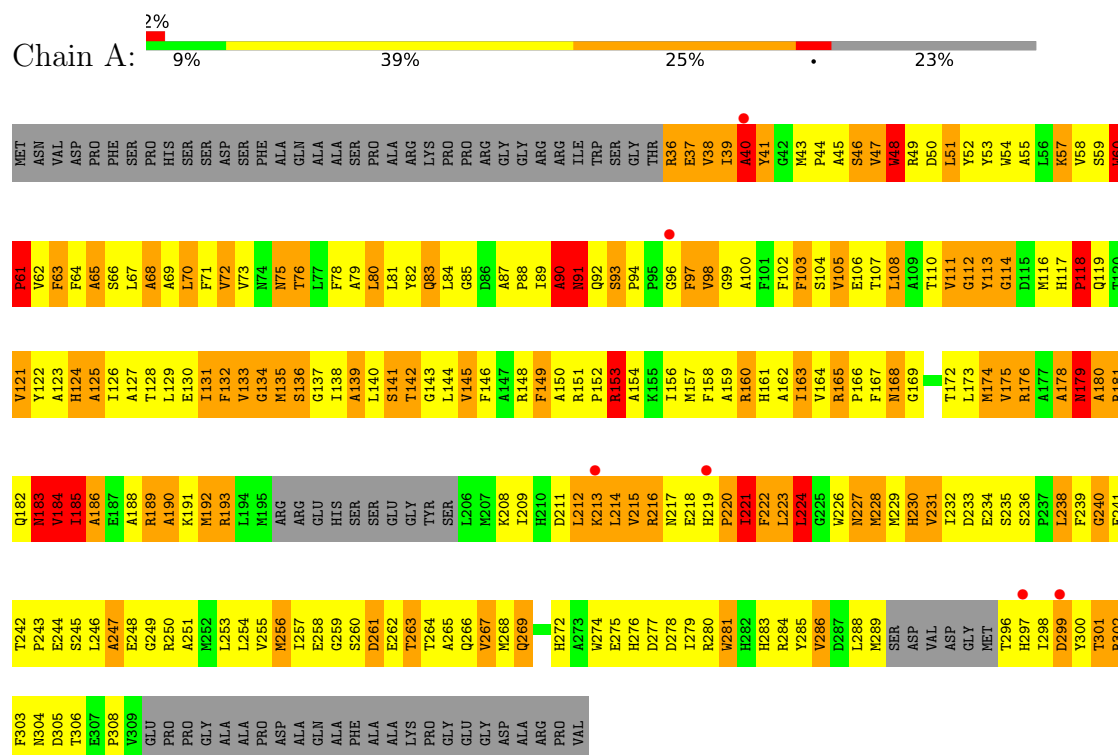
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	3	Total	O	0	0
			3	3		

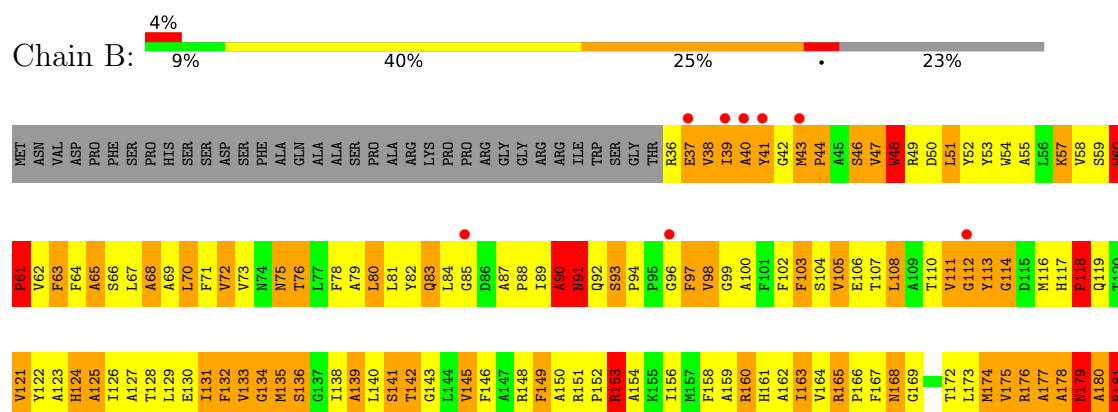
3 Residue-property plots

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: integral membrane channel and cytosolic domains



- Molecule 1: integral membrane channel and cytosolic domains



R302	F303	N304	D305	T306	E307	P308	V309	GLU	PRO	PRO	GLY	ALA	ALA	ALA	ALA	ALA	LYS	PRO	GLY	GLU	GLY	ASP	ALA	GLN	ALA	PHE	ALA	ALA	ALA	ALA	LYS	PRO	VAL																											
T242	E243	E244	S245	L246	A247	E248	G249	R250	A251	M252	L253	L254	V255	M256	I257	E258	G259	A260	D261	E262	T263	T264	A265	A266	T267	M268	Q269	A270	R271	A272	T273	T274	E275	H276	D277	D278	I279	R280	Z281	H282	H283	R284	T285	V286	D287	L288	M289	SER	ASP	VAL	ASP	GLY	GLY	MET	T296	H297	L298	D299	T300	T301
Q182	M183	V184	L185	A186	E187	A188	R189	A190	K191	M192	R193	L194	M195	ARG	ARG	GLU	HIS	SER	SER	GLU	GLY	TVR	SER	L206	M207	T208	L209	H210	D211	L212	L213	L214	V215	R216	K217	E218	H219	P220	L221	F222	L223	L224	G225	V226	N227	N228	N229	H230	V231	L232	D233	E234	S235	S236	P237	L238	F239	G240	E241	

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	92.84Å 105.62Å 258.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.50 – 3.65 7.50 – 3.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (7.50-3.65) 87.6 (7.50-3.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 3.62Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.295 , 0.329 0.295 , 0.327	Depositor DCC
R_{free} test set	725 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	127.3	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 137.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4059	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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:
K

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	1.30	18/2079 (0.9%)	1.65	48/2827 (1.7%)
1	B	1.35	20/2079 (1.0%)	1.63	45/2827 (1.6%)
All	All	1.33	38/4158 (0.9%)	1.64	93/5654 (1.6%)

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	A	0	1
1	B	0	1
All	All	0	2

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	VAL	C-N	-15.90	1.12	1.33
1	A	38	VAL	C-N	-15.85	1.12	1.33
1	B	41	TYR	C-N	-13.15	1.14	1.33
1	B	42	GLY	C-N	12.93	1.60	1.33
1	A	184	VAL	CA-C	7.87	1.62	1.52

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	VAL	CA-C-O	-21.67	98.07	122.13
1	A	38	VAL	CA-C-O	-21.66	98.09	122.13
1	B	38	VAL	CA-C-N	18.32	154.95	121.97
1	B	38	VAL	C-N-CA	18.32	154.95	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	38	VAL	CA-C-N	18.31	154.93	121.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	38	VAL	Mainchain
1	B	38	VAL	Mainchain

5.2 Too-close contacts ⓘ

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	2024	0	1974	428	2
1	B	2024	0	1974	425	2
2	A	3	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	0	0	0
3	B	3	0	0	2	0
All	All	4059	0	3948	804	2

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 100.

The worst 5 of 804 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:190:ALA:CB	1:A:214:LEU:H	1.60	1.15
1:A:190:ALA:HB3	1:A:214:LEU:H	1.00	1.13
1:A:213:LYS:HB3	1:A:215:VAL:HG22	1.30	1.12
1:B:190:ALA:HB3	1:B:214:LEU:H	0.98	1.11
1:B:213:LYS:HB3	1:B:215:VAL:HG22	1.31	1.10

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:CD2	1:B:37:GLU:OE2[2_665]	1.99	0.21
1:A:262:GLU:OE2	1:B:271:ARG:NE[2_665]	2.10	0.10

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	252/333 (76%)	154 (61%)	55 (22%)	43 (17%)	0	1
1	B	252/333 (76%)	153 (61%)	56 (22%)	43 (17%)	0	1
All	All	504/666 (76%)	307 (61%)	111 (22%)	86 (17%)	0	1

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ALA
1	A	47	VAL
1	A	90	ALA
1	A	97	PHE
1	A	105	VAL

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	204/269 (76%)	170 (83%)	34 (17%)	2	13
1	B	204/269 (76%)	170 (83%)	34 (17%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	408/538 (76%)	340 (83%)	68 (17%)	2 13

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	227	ASN
1	B	255	VAL
1	B	269	GLN
1	A	230	HIS
1	A	227	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	168	ASN
1	B	272	HIS
1	B	283	HIS
1	A	269	GLN
1	A	168	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	41:TYR	C	42:GLY	N	1.14
1	A	38:VAL	C	39:ILE	N	1.12
1	B	38:VAL	C	39:ILE	N	1.12

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	258/333 (77%)	0.06	6 (2%) 61 36	45, 89, 138, 159	0
1	B	258/333 (77%)	0.06	12 (4%) 36 22	43, 89, 137, 157	0
All	All	516/666 (77%)	0.06	18 (3%) 47 28	43, 89, 138, 159	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	HIS	7.2
1	A	299	ASP	3.9
1	B	43	MET	3.1
1	B	40	ALA	2.9
1	B	39	ILE	2.7

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 oligosaccharides 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, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	K	B	401	1/1	0.47	0.25	22,22,22,22	1
2	K	A	403	1/1	0.83	0.19	5,5,5,5	1
2	K	A	404	1/1	0.84	0.29	56,56,56,56	1
2	K	A	402	1/1	0.90	0.36	57,57,57,57	1

6.5 Other polymers [i](#)

There are no such residues in this entry.