



Full wwPDB X-ray Structure Validation Report ⓘ

May 30, 2020 – 01:49 am BST

PDB ID : 6IZ6
Title : Crystal Structure Analysis of TRIC counter-ion channels in calcium release
Authors : Liu, X.L.; Wang, X.H.; Su, M.; Hendrickson, W.A.; Chen, Y.H.
Deposited on : 2018-12-18
Resolution : 3.29 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

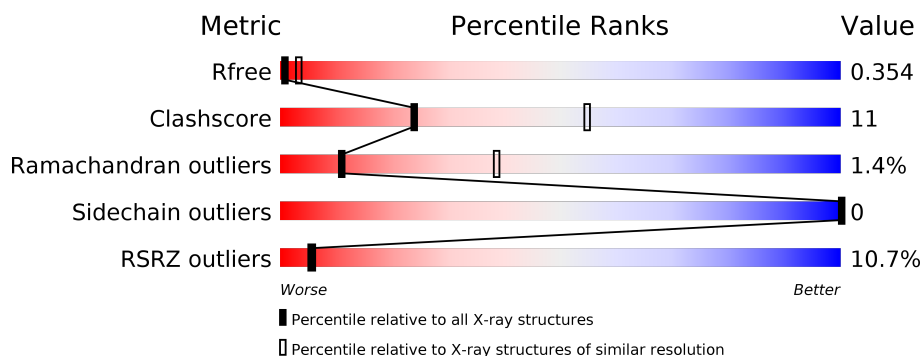
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 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	314	<div> <div>8%</div> <div>51%</div> <div>21%</div> <div>29%</div> </div>

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	CA	A	401	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1769 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 Trimeric intracellular cation channel type B-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1766	1166	285	299	16			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	285	ALA	-	expression tag	UNP Q6GN30
A	286	ALA	-	expression tag	UNP Q6GN30
A	287	ALA	-	expression tag	UNP Q6GN30
A	288	GLU	-	expression tag	UNP Q6GN30
A	289	ASN	-	expression tag	UNP Q6GN30
A	290	LEU	-	expression tag	UNP Q6GN30
A	291	TYR	-	expression tag	UNP Q6GN30
A	292	PHE	-	expression tag	UNP Q6GN30
A	293	GLN	-	expression tag	UNP Q6GN30
A	294	GLY	-	expression tag	UNP Q6GN30
A	295	LEU	-	expression tag	UNP Q6GN30
A	296	GLU	-	expression tag	UNP Q6GN30
A	297	ASP	-	expression tag	UNP Q6GN30
A	298	TYR	-	expression tag	UNP Q6GN30
A	299	LYS	-	expression tag	UNP Q6GN30
A	300	ASP	-	expression tag	UNP Q6GN30
A	301	ASP	-	expression tag	UNP Q6GN30
A	302	ASP	-	expression tag	UNP Q6GN30
A	303	ASP	-	expression tag	UNP Q6GN30
A	304	LYS	-	expression tag	UNP Q6GN30
A	305	HIS	-	expression tag	UNP Q6GN30
A	306	HIS	-	expression tag	UNP Q6GN30
A	307	HIS	-	expression tag	UNP Q6GN30
A	308	HIS	-	expression tag	UNP Q6GN30
A	309	HIS	-	expression tag	UNP Q6GN30
A	310	HIS	-	expression tag	UNP Q6GN30
A	311	HIS	-	expression tag	UNP Q6GN30

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	HIS	-	expression tag	UNP Q6GN30
A	313	HIS	-	expression tag	UNP Q6GN30
A	314	HIS	-	expression tag	UNP Q6GN30

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

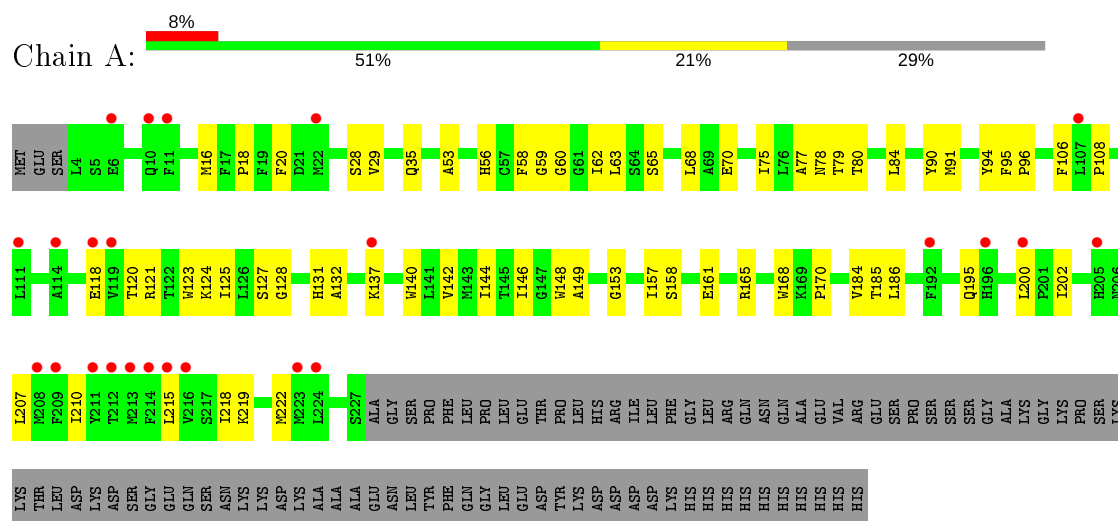
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 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 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: Trimeric intracellular cation channel type B-B



4 Data and refinement statistics

Property	Value	Source
Space group	F 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	250.11Å 250.11Å 250.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.13 – 3.29 48.13 – 3.29	Depositor EDS
% Data completeness (in resolution range)	91.8 (48.13-3.29) 91.8 (48.13-3.29)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.14rc2_3191	Depositor
R, R_{free}	0.326 , 0.354 0.326 , 0.354	Depositor DCC
R_{free} test set	456 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	154.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 109.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	1769	wwPDB-VP
Average B, all atoms (Å ²)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: CA

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	0.26	0/1820	0.39	0/2470

There are no bond length outliers.

There are no bond angle outliers.

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	1766	0	1763	39	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
All	All	1769	0	1763	39	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.

All (39) 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:184:VAL:HG11	1:A:215:LEU:HD13	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:SER:HB3	1:A:56:HIS:HB3	1.82	0.60
1:A:118:GLU:HB3	1:A:215:LEU:HG	1.84	0.59
1:A:70:GLU:OE2	1:A:131:HIS:NE2	2.36	0.59
1:A:16:MET:HA	1:A:20:PHE:HB2	1.85	0.59
1:A:168:TRP:NE1	1:A:170:PRO:HG3	2.19	0.57
1:A:157:ILE:O	1:A:161:GLU:N	2.37	0.56
1:A:207:LEU:HA	1:A:210:ILE:HG22	1.88	0.55
1:A:148:TRP:CZ2	1:A:186:LEU:HB2	2.42	0.55
1:A:35:GLN:OE1	1:A:165:ARG:NH1	2.39	0.55
1:A:29:VAL:HG22	1:A:53:ALA:HB1	1.90	0.54
1:A:123:TRP:O	1:A:127:SER:N	2.43	0.51
1:A:106:PHE:CD2	1:A:108:PRO:HD2	2.45	0.51
1:A:58:PHE:HB3	1:A:75:ILE:HG21	1.92	0.50
1:A:195:GLN:NE2	1:A:202:ILE:O	2.35	0.48
1:A:120:THR:HG22	1:A:124:LYS:HE3	1.96	0.47
1:A:121:ARG:HD2	1:A:215:LEU:HD21	1.96	0.47
1:A:90:TYR:O	1:A:94:TYR:N	2.47	0.47
1:A:60:GLY:HA2	1:A:153:GLY:HA3	1.97	0.47
1:A:91:MET:O	1:A:95:PHE:HB2	2.15	0.46
1:A:121:ARG:O	1:A:125:ILE:HG13	2.15	0.46
1:A:80:THR:O	1:A:84:LEU:HB2	2.15	0.46
1:A:68:LEU:HD11	1:A:146:ILE:HG21	1.98	0.45
1:A:148:TRP:CZ3	1:A:186:LEU:HD13	2.51	0.45
1:A:158:SER:HA	1:A:161:GLU:HB3	1.98	0.45
1:A:132:ALA:HB1	1:A:142:VAL:HG12	1.98	0.45
1:A:59:GLY:HA2	1:A:62:ILE:HB	1.99	0.45
1:A:63:LEU:HB2	1:A:157:ILE:HD11	2.00	0.44
1:A:77:ALA:O	1:A:79:THR:N	2.50	0.44
1:A:148:TRP:HE1	1:A:185:THR:HG1	1.65	0.44
1:A:95:PHE:CG	1:A:96:PRO:HD2	2.53	0.44
1:A:140:TRP:O	1:A:144:ILE:HG13	2.19	0.43
1:A:219:LYS:HA	1:A:222:MET:HB2	2.01	0.43
1:A:128:GLY:HA2	1:A:131:HIS:HB3	2.00	0.42
1:A:60:GLY:HA2	1:A:149:ALA:O	2.20	0.42
1:A:218:ILE:O	1:A:222:MET:N	2.46	0.41
1:A:200:LEU:HD23	1:A:207:LEU:HD22	2.02	0.41
1:A:65:SER:OG	1:A:75:ILE:HD11	2.20	0.40
1:A:153:GLY:O	1:A:157:ILE:HG13	2.21	0.40

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	222/314 (71%)	209 (94%)	10 (4%)	3 (1%)	11	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	PRO
1	A	137	LYS
1	A	78	ASN

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	189/268 (70%)	189 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	224/314 (71%)	0.66	24 (10%) 6 5	95, 145, 187, 206	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	TYR	5.9
1	A	114	ALA	4.7
1	A	214	PHE	4.4
1	A	212	THR	4.0
1	A	192	PHE	4.0
1	A	209	PHE	4.0
1	A	200	LEU	3.8
1	A	118	GLU	3.4
1	A	196	HIS	3.4
1	A	208	MET	3.4
1	A	6	GLU	3.3
1	A	11	PHE	3.3
1	A	137	LYS	3.1
1	A	224	LEU	3.0
1	A	119	VAL	3.0
1	A	10	GLN	2.9
1	A	215	LEU	2.8
1	A	205	HIS	2.6
1	A	111	LEU	2.4
1	A	107	LEU	2.4
1	A	223	MET	2.4
1	A	213	MET	2.4
1	A	216	VAL	2.2
1	A	22	MET	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 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. 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(\AA^2)	Q<0.9
2	CA	A	401	1/1	0.52	0.71	182,182,182,182	1

6.5 Other polymers [i](#)

There are no such residues in this entry.