WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Sep 18, 2023 – 05:24 PM EDT

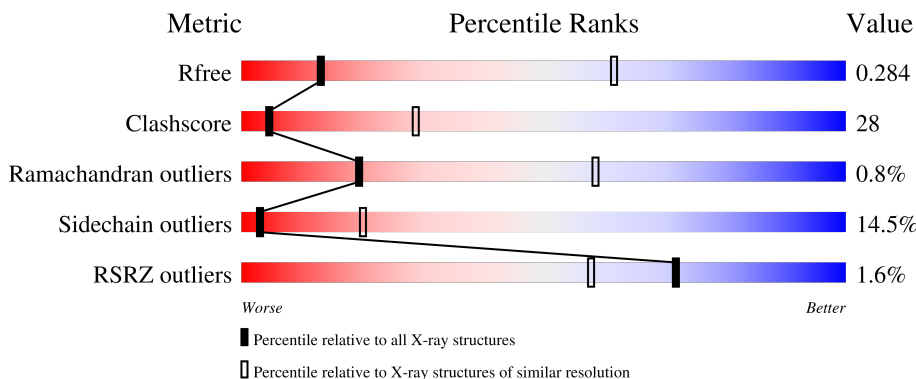|		
PDB ID	:	5CBF
Title	:	Structural and Functional Characterization of a Calcium-activated Cation channel from Tsukamurella Paurometabola
Authors	:	Dhakshnamoorthy, B.; Rohaim, A.; Rui, H.; Blachowicz, L.; Roux, B.
Deposited on	:	2015-06-30
Resolution	:	3.61 Å(reported)

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 3.61 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.
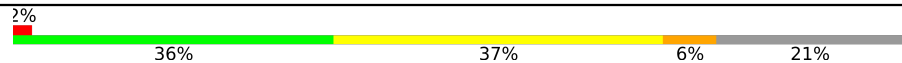
Metric	Percentile Ranks	Value
Rfree		0.284
Clashscore		28
Ramachandran outliers		0.8%
Sidechain outliers		14.5%
RSRZ outliers		1.6%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)

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 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	A	129	40% 30% 9% • 21%
1	B	129	2% 40% 32% 7% 21%
1	C	129	4% 43% 27% 8% • 21%
1	D	129	39% 33% 6% • 21%
1	E	129	43% 29% 7% 21%

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Mol	Chain	Length	Quality of chain
1	F	129	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 4623 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 2 domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	S	0	0	0
			770	510	123	135	2			
1	B	102	Total	C	N	O	S	0	0	0
			770	510	123	135	2			
1	C	102	Total	C	N	O	S	0	0	0
			770	510	123	135	2			
1	D	102	Total	C	N	O	S	0	0	0
			770	510	123	135	2			
1	E	102	Total	C	N	O	S	0	0	0
			770	510	123	135	2			
1	F	102	Total	C	N	O	S	0	0	0
			770	510	123	135	2			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	HIS	-	expression tag	UNP D5UM26
A	125	HIS	-	expression tag	UNP D5UM26
A	126	HIS	-	expression tag	UNP D5UM26
A	127	HIS	-	expression tag	UNP D5UM26
A	128	HIS	-	expression tag	UNP D5UM26
A	129	HIS	-	expression tag	UNP D5UM26
B	124	HIS	-	expression tag	UNP D5UM26
B	125	HIS	-	expression tag	UNP D5UM26
B	126	HIS	-	expression tag	UNP D5UM26
B	127	HIS	-	expression tag	UNP D5UM26
B	128	HIS	-	expression tag	UNP D5UM26
B	129	HIS	-	expression tag	UNP D5UM26
C	124	HIS	-	expression tag	UNP D5UM26
C	125	HIS	-	expression tag	UNP D5UM26
C	126	HIS	-	expression tag	UNP D5UM26
C	127	HIS	-	expression tag	UNP D5UM26
C	128	HIS	-	expression tag	UNP D5UM26

W O R L D W I D E
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Chain	Residue	Modelled	Actual	Comment	Reference
C	129	HIS	-	expression tag	UNP D5UM26
D	124	HIS	-	expression tag	UNP D5UM26
D	125	HIS	-	expression tag	UNP D5UM26
D	126	HIS	-	expression tag	UNP D5UM26
D	127	HIS	-	expression tag	UNP D5UM26
D	128	HIS	-	expression tag	UNP D5UM26
D	129	HIS	-	expression tag	UNP D5UM26
E	124	HIS	-	expression tag	UNP D5UM26
E	125	HIS	-	expression tag	UNP D5UM26
E	126	HIS	-	expression tag	UNP D5UM26
E	127	HIS	-	expression tag	UNP D5UM26
E	128	HIS	-	expression tag	UNP D5UM26
E	129	HIS	-	expression tag	UNP D5UM26
F	124	HIS	-	expression tag	UNP D5UM26
F	125	HIS	-	expression tag	UNP D5UM26
F	126	HIS	-	expression tag	UNP D5UM26
F	127	HIS	-	expression tag	UNP D5UM26
F	128	HIS	-	expression tag	UNP D5UM26
F	129	HIS	-	expression tag	UNP D5UM26

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

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

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.
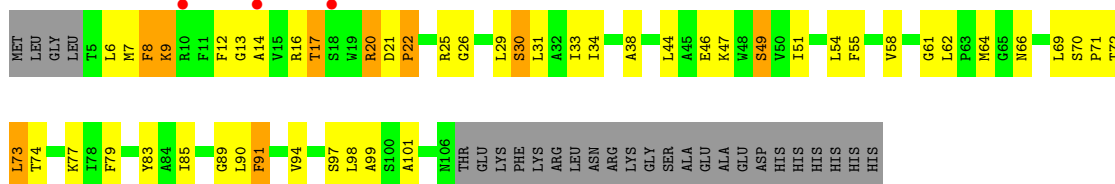
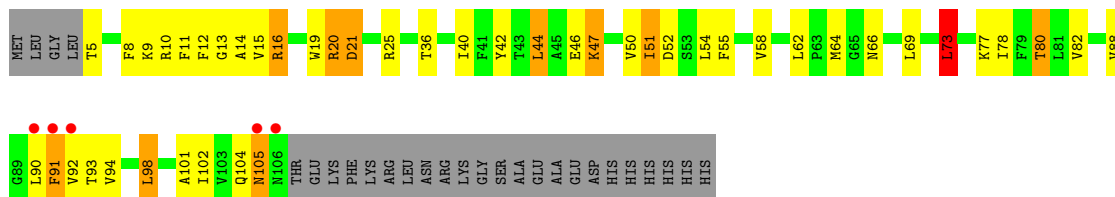• Molecule 1: Ion transport 2 domain protein

Chain A:
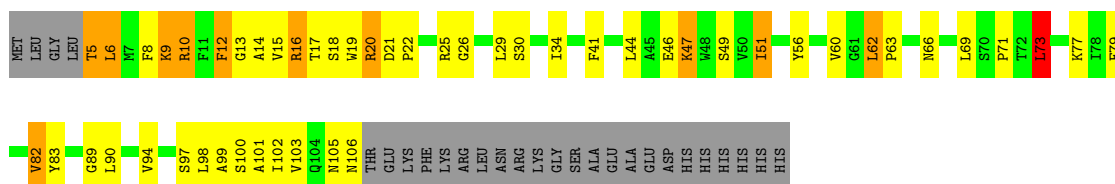
• Molecule 1: Ion transport 2 domain protein

Chain B:

• Molecule 1: Ion transport 2 domain protein

Chain C:

• Molecule 1: Ion transport 2 domain protein

Chain D:

I78 L81 V82 Y83 L86 V87 V88 G89 V92 L98 A99 S100 A101 I102 V103 Q104 N105 N106 THR GLU LYS PHE LYS ARG LEU ASN ARG LYS GLY SER ALA GLU ALA GLU ASP HIS HIS HIS HIS HIS HIS

• Molecule 1: Ion transport 2 domain protein

Chain E:

43%   29%   7%   21%

MET LEU GLY LEU T5 L6 K9 R10 G13 A14 V15 R16 R20 R25 G26 A27 V28 L29 I33 I34 V35 F41 S49 V50 I51 Y56 V60 M64 G65 N66 L69 S70 P71 T72 L73 T74 L75 S76 K77 I78 F79 T80 L81 V82 Y83 A84 I85 L86 V87

V88 G89 L90 V94 S97 L98 A99 I102 N105 N106 THR GLU LYS PHE LYS ARG LEU ASN ARG LYS GLY SER ALA GLU ALA GLU ASP HIS HIS HIS HIS HIS HIS

• Molecule 1: Ion transport 2 domain protein

Chain F:

2%
36%   37%   6%   21%

MET LEU GLY LEU T5 L6 K9 R10 F11 F12 G13 A14 V15 R16 T17 S18 W19 R20 D21 P22 R25 V28 L29 S30 L31 A32 I33 I34 V35 T36 I40 L44 A45 E46 K47 W48 S49 V50 I51 D52 S53 L54 F55 Y56 A57 V58 S59 V60 G61 L62 N66 L69 S70

P71 T72 L73 T74 L75 I78 F79 V82 Y83 L86 V87 L90 F91 V92 T93 V94 G95 L98 A101 I102 N105 N106 THR GLU LYS PHE LYS ARG LEU ASN ARG LYS GLY SER ALA GLU ALA GLU ASP HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	116.05Å 116.05Å 132.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.61 48.33 – 3.61	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-3.61) 99.1 (48.33-3.61)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.239 , 0.279 0.241 , 0.284	Depositor DCC
R_{free} test set	489 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	122.1	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 40.2	EDS
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.206 for -h,k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4623	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.76	0/787	1.11	2/1075 (0.2%)
1	B	0.78	0/787	1.09	1/1075 (0.1%)
1	C	0.77	0/787	1.12	2/1075 (0.2%)
1	D	0.77	0/787	1.08	2/1075 (0.2%)
1	E	0.77	0/787	1.11	1/1075 (0.1%)
1	F	0.79	0/787	1.11	2/1075 (0.2%)
All	All	0.77	0/4722	1.10	10/6450 (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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	73	LEU	CA-CB-CG	7.34	132.18	115.30
1	C	20	ARG	N-CA-C	-6.54	93.34	111.00
1	D	13	GLY	N-CA-C	6.48	129.30	113.10
1	A	73	LEU	CA-CB-CG	5.96	129.01	115.30
1	C	73	LEU	CA-CB-CG	5.56	128.09	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ALA	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	770	0	808	52	0
1	B	770	0	808	49	0
1	C	770	0	808	44	0
1	D	770	0	808	62	0
1	E	770	0	808	48	0
1	F	770	0	808	52	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	E	1	0	0	0	0
All	All	4623	0	4848	268	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 268 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:10:ARG:NH2	1:A:15:VAL:HG21	1.25	1.45
1:C:40:ILE:O	1:C:44:LEU:HD12	1.40	1.19
1:A:10:ARG:NH2	1:A:15:VAL:CG2	2.07	1.18
1:F:90:LEU:O	1:F:94:VAL:HG23	1.44	1.15
1:A:20:ARG:HB3	1:A:25:ARG:NH2	1.63	1.10

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	100/129 (78%)	89 (89%)	11 (11%)	0	100	100
1	B	100/129 (78%)	89 (89%)	9 (9%)	2 (2%)	7	41
1	C	100/129 (78%)	92 (92%)	8 (8%)	0	100	100
1	D	100/129 (78%)	88 (88%)	10 (10%)	2 (2%)	7	41
1	E	100/129 (78%)	90 (90%)	10 (10%)	0	100	100
1	F	100/129 (78%)	90 (90%)	9 (9%)	1 (1%)	15	54
All	All	600/774 (78%)	538 (90%)	57 (10%)	5 (1%)	19	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	MET
1	B	22	PRO
1	D	22	PRO
1	D	13	GLY
1	F	22	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	84/107 (78%)	66 (79%)	18 (21%)	1	7
1	B	84/107 (78%)	73 (87%)	11 (13%)	4	23
1	C	84/107 (78%)	72 (86%)	12 (14%)	3	21
1	D	84/107 (78%)	74 (88%)	10 (12%)	5	27
1	E	84/107 (78%)	73 (87%)	11 (13%)	4	23
1	F	84/107 (78%)	73 (87%)	11 (13%)	4	23
All	All	504/642 (78%)	431 (86%)	73 (14%)	3	20

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	69	LEU
1	F	75	LEU
1	E	85	ILE
1	F	16	ARG
1	B	30	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	104	GLN
1	F	105	ASN
1	D	106	ASN
1	E	104	GLN
1	E	105	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 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 ⓘ

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 ⓘ

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(Å²)	Q<0.9
1	A	102/129 (79%)	-0.57	0	100	100	66, 99, 136, 163	0
1	B	102/129 (79%)	-0.31	3 (2%)	51	35	70, 104, 157, 201	0
1	C	102/129 (79%)	-0.29	5 (4%)	29	19	91, 126, 178, 208	0
1	D	102/129 (79%)	-0.46	0	100	100	66, 102, 145, 178	0
1	E	102/129 (79%)	-0.44	0	100	100	74, 102, 157, 170	0
1	F	102/129 (79%)	-0.30	2 (1%)	65	50	63, 119, 166, 197	0
All	All	612/774 (79%)	-0.39	10 (1%)	72	58	63, 109, 164, 208	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	90	LEU	4.5
1	C	92	VAL	4.1
1	C	105	ASN	3.5
1	C	106	ASN	3.5
1	B	10	ARG	2.6

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
2	CA	E	201	1/1	0.88	0.25	76,76,76,76	0
2	CA	B	201	1/1	0.92	0.23	148,148,148,148	0
2	CA	A	201	1/1	0.94	0.13	97,97,97,97	0

6.5 Other polymers ⓘ

There are no such residues in this entry.