

Full wwPDB X-ray Structure Validation Report (i)

Aug 1, 2022 – 06:32 pm BST

:	7Z6N
:	Crystal structure of Zn2+-transporter BbZIP in a metal-stripped state
:	Wiuf, A.; Steffen, J.H.; Becares, E.R.; Groenberg, C.; Mahato, D.R.; Ras-
	mussen, S.G.F.; Andersson, M.; Croll, T.; Gotfryd, K.; Gourdon, P.
:	2022-03-13
:	2.57 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 (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:

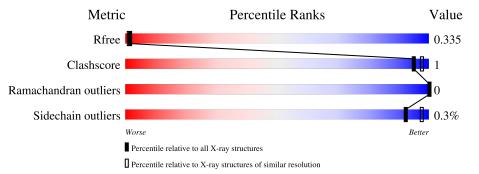
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.57 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)

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%

Mol	Chain	Length	Quality of chain				
1	А	329	82%	•	16%		
1	В	329	75%	•	21%		



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3785 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 Putative membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	275	Total	С	Ν	0	\mathbf{S}	0	0	0
	Л	215	1916	1246	321	337	12	0		
1	В	261	Total	С	Ν	0	S	10	1	0
	D	201	1829	1188	305	324	12	10	1	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	-19	MET	-	initiating methionine	UNP A0A0H3LM39
А	-18	GLY	-	expression tag	UNP A0A0H3LM39
А	-17	SER	-	expression tag	UNP A0A0H3LM39
А	-16	SER	-	expression tag	UNP A0A0H3LM39
A	-15	HIS	-	expression tag	UNP A0A0H3LM39
А	-14	HIS	-	expression tag	UNP A0A0H3LM39
А	-13	HIS	-	expression tag	UNP A0A0H3LM39
А	-12	HIS	-	expression tag	UNP A0A0H3LM39
А	-11	HIS	-	expression tag	UNP A0A0H3LM39
А	-10	HIS	-	expression tag	UNP A0A0H3LM39
А	-9	SER	-	expression tag	UNP A0A0H3LM39
А	-8	SER	-	expression tag	UNP A0A0H3LM39
А	-7	GLY	-	expression tag	UNP A0A0H3LM39
А	-6	LEU	-	expression tag	UNP A0A0H3LM39
А	-5	VAL	-	expression tag	UNP A0A0H3LM39
А	-4	PRO	-	expression tag	UNP A0A0H3LM39
А	-3	ARG	-	expression tag	UNP A0A0H3LM39
А	-2	GLY	-	expression tag	UNP A0A0H3LM39
А	-1	SER	-	expression tag	UNP A0A0H3LM39
А	0	HIS	-	expression tag	UNP A0A0H3LM39
В	-19	MET	-	initiating methionine	UNP A0A0H3LM39
В	-18	GLY	-	expression tag	UNP A0A0H3LM39
В	-17	SER	-	expression tag	UNP A0A0H3LM39
В	-16	SER	-	expression tag	UNP A0A0H3LM39
В	-15	HIS	-	expression tag	UNP A0A0H3LM39

There are 40 discrepancies between the modelled and reference sequences:

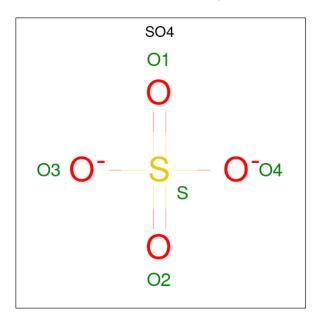
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Chain	Residue	Modelled	Actual	Comment	Reference
В	-14	HIS	-	expression tag	UNP A0A0H3LM39
В	-13	HIS	-	expression tag	UNP A0A0H3LM39
В	-12	HIS	-	expression tag	UNP A0A0H3LM39
В	-11	HIS	-	expression tag	UNP A0A0H3LM39
В	-10	HIS	-	expression tag	UNP A0A0H3LM39
В	-9	SER	-	expression tag	UNP A0A0H3LM39
В	-8	SER	-	expression tag	UNP A0A0H3LM39
В	-7	GLY	-	expression tag	UNP A0A0H3LM39
В	-6	LEU	-	expression tag	UNP A0A0H3LM39
В	-5	VAL	-	expression tag	UNP A0A0H3LM39
В	-4	PRO	-	expression tag	UNP A0A0H3LM39
В	-3	ARG	-	expression tag	UNP A0A0H3LM39
В	-2	GLY	-	expression tag	UNP A0A0H3LM39
В	-1	SER	-	expression tag	UNP A0A0H3LM39
В	0	HIS	-	expression tag	UNP A0A0H3LM39

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• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	4	Total O 4 4	0	0
3	В	6	Total O 6 6	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. 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. 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: Putative membrane protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	111.49Å 122.12Å 101.73Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.17 - 2.57	Depositor
Resolution (A)	43.27 - 2.56	EDS
% Data completeness	63.5(41.17-2.57)	Depositor
(in resolution range)	63.5(43.27-2.56)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.05 (at 2.58 \text{\AA})$	Xtriage
Refinement program	PHENIX dev_4234	Depositor
D D	0.288 , (Not available)	Depositor
R, R_{free}	0.289 , 0.335	DCC
R_{free} test set	745 reflections (5.17%)	wwPDB-VP
Wilson B-factor $(Å^2)$	57.9	Xtriage
Anisotropy	1.093	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$ L > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	3785	wwPDB-VP
Average B, all atoms $(Å^2)$	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 36.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6431e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities 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: SO4

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).

Mal	Mol Chain	Bond	lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.24	0/1948	0.47	0/2658	
1	В	0.25	0/1858	0.49	0/2531	
All	All	0.25	0/3806	0.48	0/5189	

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	А	1916	0	2018	2	0
1	В	1829	0	1913	7	0
2	А	15	0	0	0	0
2	В	15	0	0	1	0
3	А	4	0	0	0	0
3	В	6	0	0	0	0
All	All	3785	0	3931	9	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 1.

All (9) close contacts within the same asymmetric unit are listed below, sorted by their clash



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:VAL:HB	1:B:210:PRO:HD3	1.96	0.47
1:A:209:VAL:HB	1:A:210:PRO:HD3	1.98	0.46
1:B:178:ASN:HB3	1:B:240:GLU:HG3	1.99	0.45
1:B:22:HIS:HB3	1:B:26:THR:HG21	1.98	0.45
1:B:184:ALA:HB1	1:B:200:LEU:HD21	1.98	0.45
1:B:147:THR:HA	1:B:173:THR:HG21	2.01	0.43
1:A:54:VAL:O	1:A:56:VAL:N	2.53	0.42
1:B:286:HIS:ND1	2:B:402:SO4:O2	2.49	0.42
1:B:189:PHE:CE1	1:B:197:GLY:HA3	2.56	0.41

magnitude.

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	\mathbf{ntiles}
1	А	271/329~(82%)	265~(98%)	6(2%)	0	100	100
1	В	254/329~(77%)	246~(97%)	8 (3%)	0	100	100
All	All	525/658~(80%)	511 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	Percentiles		
1	А	187/228~(82%)	186 (100%)	1 (0%)	88 96	
1	В	179/228 (78%)	179 (100%)	0	100 100	
All	All	366/456~(80%)	365 (100%)	1 (0%)	92 97	

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	283	ARG

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Turne	Chain	Res	Link	B	ond leng	gths	В	ond ang	gles
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	SO4	А	403	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0
2	SO4	А	402	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0



Mol	Turne	Chain	Res Link Bond lengths		В	ond ang	gles			
	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	SO4	В	402	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0
2	SO4	В	403	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0
2	SO4	А	401	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0
2	SO4	В	401	-	4,4,4	0.14	0	$6,\!6,\!6$	0.05	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	402	SO4	1	0

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

