



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2023 – 05:24 pm GMT

PDB ID : 3ZCN
Title : Fic protein from SHEWANELLA ONEIDENSIS in complex with ATP
Authors : Goepfert, A.; Schirmer, T.
Deposited on : 2012-11-21
Resolution : 1.70 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 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 : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

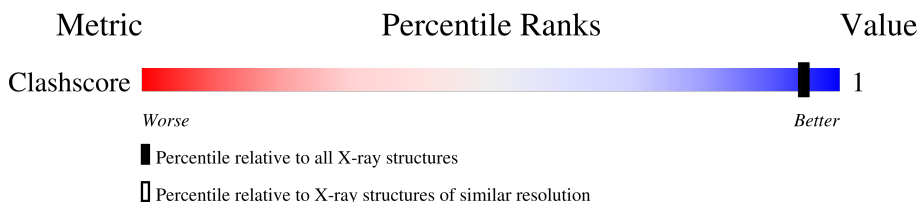
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

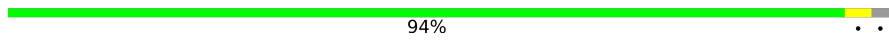
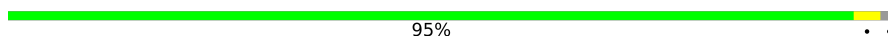
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4695 (1.70-1.70)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	378	 94% . .
1	B	378	 95% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7004 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 ADENOSINE MONOPHOSPHATE-PROTEIN TRANSFERASE SOFIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	369	2982	1911	502	558	11	63	5	0
1	B	369	2979	1910	501	557	11	57	5	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP Q8E9K5
A	-4	HIS	-	expression tag	UNP Q8E9K5
A	-3	HIS	-	expression tag	UNP Q8E9K5
A	-2	HIS	-	expression tag	UNP Q8E9K5
A	-1	HIS	-	expression tag	UNP Q8E9K5
A	0	HIS	-	expression tag	UNP Q8E9K5
A	1	HIS	-	expression tag	UNP Q8E9K5
A	109	CYS	GLY	engineered mutation	UNP Q8E9K5
B	-5	MET	-	expression tag	UNP Q8E9K5
B	-4	HIS	-	expression tag	UNP Q8E9K5
B	-3	HIS	-	expression tag	UNP Q8E9K5
B	-2	HIS	-	expression tag	UNP Q8E9K5
B	-1	HIS	-	expression tag	UNP Q8E9K5
B	0	HIS	-	expression tag	UNP Q8E9K5
B	1	HIS	-	expression tag	UNP Q8E9K5
B	109	CYS	GLY	engineered mutation	UNP Q8E9K5

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	5	13	3	0	0
2	B	1	31	10	5	13	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	485	485	485	0	0
3	B	496	496	496	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.

Note EDS failed to run properly.

- Molecule 1: ADENOSINE MONOPHOSPHATE-PROTEIN TRANSFERASE SOFIC

Chain A:  94%



- Molecule 1: ADENOSINE MONOPHOSPHATE-PROTEIN TRANSFERASE SOFIC

Chain B:  95%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	37.79Å 164.91Å 70.23Å 90.00° 94.43° 90.00°	Depositor
Resolution (Å)	14.99 – 1.70	Depositor
% Data completeness (in resolution range)	99.5 (14.99-1.70)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 1.70Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.166 , 0.202	Depositor
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.651	Xtriage
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
Total number of atoms	7004	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% 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: ATP

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	0.35	0/3057	0.51	0/4161
1	B	0.36	0/3054	0.54	0/4158
All	All	0.36	0/6111	0.53	0/8319

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	2982	0	3017	7	0
1	B	2979	0	3019	7	0
2	A	31	0	10	0	0
2	B	31	0	10	0	0
3	A	485	0	0	2	0
3	B	496	0	0	1	0
All	All	7004	0	6056	14	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 (14) 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:B:301:LEU:HA	1:B:321:LEU:HD21	1.84	0.58
1:B:312:ARG:NH2	3:B:2170:HOH:O	2.39	0.56
1:A:116:ARG:NH2	1:A:125:GLU:OE1	2.46	0.48
1:A:293:LEU:HD13	1:A:296:ILE:HD11	1.96	0.48
1:A:251:GLN:NE2	3:A:2374:HOH:O	2.44	0.48
1:A:312:ARG:NH2	3:A:2176:HOH:O	2.30	0.45
1:B:25:ALA:HB1	1:B:185:ILE:HG21	1.99	0.44
1:A:244:LEU:HG	1:A:256:TRP:CZ3	2.54	0.42
1:B:21:LEU:HG	1:B:181:VAL:HG21	2.03	0.41
1:B:358:THR:HG23	1:B:362:LYS:HD3	2.03	0.41
1:A:25:ALA:HB1	1:A:185:ILE:HG21	2.02	0.41
1:A:107:TYR:O	1:A:111:THR:HG23	2.22	0.40
1:B:355:LYS:HE2	1:B:355:LYS:HB2	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

2 ligands are modelled in this entry.

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.