wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 08:33 PM EDT

PDB ID	:	8G83
Title	:	Structure of NAD+ consuming protein Acinetobacter baumannii TIR domain
Authors	:	Klontz, E.H.; Wang, Y.; Glendening, G.; Carr, J.; Tsibouris, T.; Buddula, S.; Nallar, S.; Soares, A.; Snyder, G.A.
Deposited on	:	2023-02-17
Resolution	:	3.03 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 (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 (i)) were used in the production of this report:

MolProbity	:	FAILED
Xtriage (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)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4154 atoms, of which 2025 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 NAD(+) hydrolase AbTIR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	138	Total	C	H	N	O	S	0	0	0
			2055	669	1006	174	204	2			
1	B	139	Total	C	H	N	O	S	0	0	0
			2092	684	1019	182	205	2			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	HIS	-	expression tag	UNP A0A009IHW8
A	93	MET	-	expression tag	UNP A0A009IHW8
A	94	SER	-	expression tag	UNP A0A009IHW8
A	95	ALA	-	expression tag	UNP A0A009IHW8
A	96	TRP	-	expression tag	UNP A0A009IHW8
A	97	SER	-	expression tag	UNP A0A009IHW8
A	98	HIS	-	expression tag	UNP A0A009IHW8
A	99	PRO	-	expression tag	UNP A0A009IHW8
A	100	GLN	-	expression tag	UNP A0A009IHW8
A	101	PHE	-	expression tag	UNP A0A009IHW8
A	102	GLU	-	expression tag	UNP A0A009IHW8
A	103	LYS	-	expression tag	UNP A0A009IHW8
A	104	GLY	-	expression tag	UNP A0A009IHW8
A	105	GLY	-	expression tag	UNP A0A009IHW8
A	106	GLY	-	expression tag	UNP A0A009IHW8
A	107	SER	-	expression tag	UNP A0A009IHW8
A	108	GLY	-	expression tag	UNP A0A009IHW8
A	109	GLY	-	expression tag	UNP A0A009IHW8
A	110	GLY	-	expression tag	UNP A0A009IHW8
A	111	SER	-	expression tag	UNP A0A009IHW8
A	112	GLY	-	expression tag	UNP A0A009IHW8
A	113	GLY	-	expression tag	UNP A0A009IHW8
A	114	SER	-	expression tag	UNP A0A009IHW8
A	115	ALA	-	expression tag	UNP A0A009IHW8
A	116	TRP	-	expression tag	UNP A0A009IHW8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	117	SER	-	expression tag	UNP A0A009IHW8
A	118	HIS	-	expression tag	UNP A0A009IHW8
A	119	PRO	-	expression tag	UNP A0A009IHW8
A	120	GLN	-	expression tag	UNP A0A009IHW8
A	121	PHE	-	expression tag	UNP A0A009IHW8
A	122	GLU	-	expression tag	UNP A0A009IHW8
A	123	LYS	-	expression tag	UNP A0A009IHW8
A	124	GLY	-	expression tag	UNP A0A009IHW8
A	125	GLY	-	expression tag	UNP A0A009IHW8
A	126	GLY	-	expression tag	UNP A0A009IHW8
A	127	SER	-	expression tag	UNP A0A009IHW8
A	128	SER	-	expression tag	UNP A0A009IHW8
A	129	GLY	-	expression tag	UNP A0A009IHW8
A	130	GLY	-	expression tag	UNP A0A009IHW8
A	131	GLY	-	expression tag	UNP A0A009IHW8
A	132	ALA	-	expression tag	UNP A0A009IHW8
A	133	SER	-	expression tag	UNP A0A009IHW8
A	270	HIS	-	expression tag	UNP A0A009IHW8
A	271	HIS	-	expression tag	UNP A0A009IHW8
A	272	HIS	-	expression tag	UNP A0A009IHW8
A	273	HIS	-	expression tag	UNP A0A009IHW8
A	274	HIS	-	expression tag	UNP A0A009IHW8
A	275	HIS	-	expression tag	UNP A0A009IHW8
B	92	HIS	-	expression tag	UNP A0A009IHW8
B	93	MET	-	expression tag	UNP A0A009IHW8
B	94	SER	-	expression tag	UNP A0A009IHW8
B	95	ALA	-	expression tag	UNP A0A009IHW8
B	96	TRP	-	expression tag	UNP A0A009IHW8
B	97	SER	-	expression tag	UNP A0A009IHW8
B	98	HIS	-	expression tag	UNP A0A009IHW8
B	99	PRO	-	expression tag	UNP A0A009IHW8
B	100	GLN	-	expression tag	UNP A0A009IHW8
B	101	PHE	-	expression tag	UNP A0A009IHW8
B	102	GLU	-	expression tag	UNP A0A009IHW8
B	103	LYS	-	expression tag	UNP A0A009IHW8
B	104	GLY	-	expression tag	UNP A0A009IHW8
B	105	GLY	-	expression tag	UNP A0A009IHW8
B	106	GLY	-	expression tag	UNP A0A009IHW8
B	107	SER	-	expression tag	UNP A0A009IHW8
B	108	GLY	-	expression tag	UNP A0A009IHW8
B	109	GLY	-	expression tag	UNP A0A009IHW8
B	110	GLY	-	expression tag	UNP A0A009IHW8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	111	SER	-	expression tag	UNP A0A009IHW8
B	112	GLY	-	expression tag	UNP A0A009IHW8
B	113	GLY	-	expression tag	UNP A0A009IHW8
B	114	SER	-	expression tag	UNP A0A009IHW8
B	115	ALA	-	expression tag	UNP A0A009IHW8
B	116	TRP	-	expression tag	UNP A0A009IHW8
B	117	SER	-	expression tag	UNP A0A009IHW8
B	118	HIS	-	expression tag	UNP A0A009IHW8
B	119	PRO	-	expression tag	UNP A0A009IHW8
B	120	GLN	-	expression tag	UNP A0A009IHW8
B	121	PHE	-	expression tag	UNP A0A009IHW8
B	122	GLU	-	expression tag	UNP A0A009IHW8
B	123	LYS	-	expression tag	UNP A0A009IHW8
B	124	GLY	-	expression tag	UNP A0A009IHW8
B	125	GLY	-	expression tag	UNP A0A009IHW8
B	126	GLY	-	expression tag	UNP A0A009IHW8
B	127	SER	-	expression tag	UNP A0A009IHW8
B	128	SER	-	expression tag	UNP A0A009IHW8
B	129	GLY	-	expression tag	UNP A0A009IHW8
B	130	GLY	-	expression tag	UNP A0A009IHW8
B	131	GLY	-	expression tag	UNP A0A009IHW8
B	132	ALA	-	expression tag	UNP A0A009IHW8
B	133	SER	-	expression tag	UNP A0A009IHW8
B	270	HIS	-	expression tag	UNP A0A009IHW8
B	271	HIS	-	expression tag	UNP A0A009IHW8
B	272	HIS	-	expression tag	UNP A0A009IHW8
B	273	HIS	-	expression tag	UNP A0A009IHW8
B	274	HIS	-	expression tag	UNP A0A009IHW8
B	275	HIS	-	expression tag	UNP A0A009IHW8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total O 2 2	0	0
2	B	5	Total O 5 5	0	0

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

3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	44.20Å 76.19Å 97.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.86 – 3.03	Depositor
% Data completeness (in resolution range)	98.2 (28.86-3.03)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 3.05Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.228 , 0.274	Depositor
Wilson B-factor (Å^2)	63.3	Xtriage
Anisotropy	0.532	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4154	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[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.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

There are no ligands in this entry.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

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

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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