wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 01:54 PM EDT

PDB ID	:	6NPS
Title	:	Crystal structure of GH115 enzyme AxyAgu115A from Amphibacillus xylanus
Authors	:	Stogios, P.J.; Skarina, T.; Di Leo, R.; Yan, R.; Master, E.; Savchenko, A.
Deposited on	:	2019-01-18
Resolution	:	1.99 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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 1.99 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 4 unique types of molecules in this entry. The entry contains 17523 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 AxyAgu115A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	968	Total	C	N	O	S	0	4	0
			7797	4987	1295	1489	26			
1	B	958	Total	C	N	O	S	0	5	0
			7725	4945	1279	1475	26			

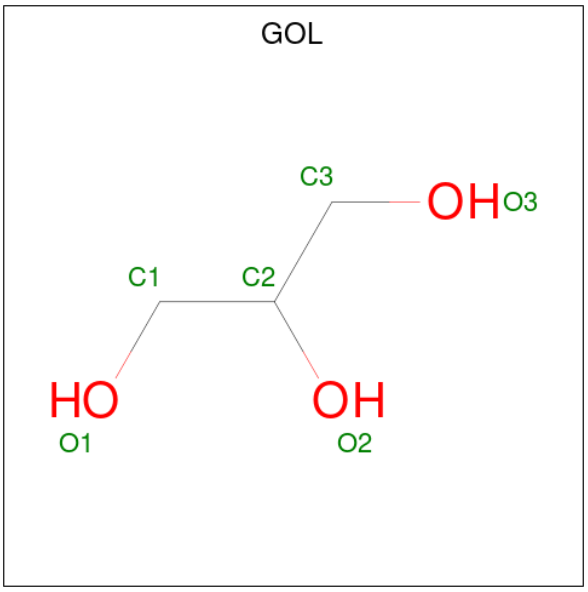
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP K0J4X5
A	0	GLY	-	expression tag	UNP K0J4X5
A	79	ALA	LYS	engineered mutation	UNP K0J4X5
A	80	ALA	LYS	engineered mutation	UNP K0J4X5
A	81	ALA	GLU	engineered mutation	UNP K0J4X5
B	-1	GLN	-	expression tag	UNP K0J4X5
B	0	GLY	-	expression tag	UNP K0J4X5
B	79	ALA	LYS	engineered mutation	UNP K0J4X5
B	80	ALA	LYS	engineered mutation	UNP K0J4X5
B	81	ALA	GLU	engineered mutation	UNP K0J4X5

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	2	Total	Cl	0	0
			2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	861	Total O 876 876	0	15
4	B	976	Total O 1002 1002	0	26

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 1	Depositor
Cell constants a, b, c, α, β, γ	63.08Å 96.21Å 111.75Å 84.37° 78.37° 83.32°	Depositor
Resolution (Å)	47.64 – 1.99	Depositor
% Data completeness (in resolution range)	94.6 (47.64-1.99)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.147 , 0.190	Depositor
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.494	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17523	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 for Mogul analysis.

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	1007	-	5,5,5	1.11	0	5,5,5	0.82	0
3	GOL	A	1008[B]	-	5,5,5	1.24	0	5,5,5	1.04	0
3	GOL	A	1006	-	5,5,5	0.96	0	5,5,5	1.01	0
3	GOL	A	1002	-	5,5,5	1.01	0	5,5,5	0.90	0
3	GOL	A	1009	-	5,5,5	0.99	0	5,5,5	0.91	0
3	GOL	A	1011	-	5,5,5	1.05	0	5,5,5	0.77	0
3	GOL	B	1009	-	5,5,5	1.48	1 (20%)	5,5,5	0.83	0
3	GOL	B	1005	-	5,5,5	0.94	0	5,5,5	0.91	0
3	GOL	B	1003	-	5,5,5	1.18	0	5,5,5	0.90	0
3	GOL	A	1003	-	5,5,5	0.90	0	5,5,5	1.21	1 (20%)
3	GOL	B	1004	-	5,5,5	1.35	1 (20%)	5,5,5	0.71	0
3	GOL	B	1010	-	5,5,5	1.30	1 (20%)	5,5,5	0.88	0
3	GOL	A	1004	-	5,5,5	1.10	0	5,5,5	0.81	0
3	GOL	A	1005	-	5,5,5	1.01	0	5,5,5	1.01	0
3	GOL	B	1008	-	5,5,5	1.06	0	5,5,5	0.89	0
3	GOL	B	1011	-	5,5,5	1.07	0	5,5,5	0.91	0
3	GOL	A	1010	-	5,5,5	1.12	0	5,5,5	0.91	0
3	GOL	B	1007	-	5,5,5	0.97	0	5,5,5	0.97	0
3	GOL	B	1006	-	5,5,5	0.92	0	5,5,5	0.93	0
3	GOL	A	1008[A]	-	5,5,5	1.18	0	5,5,5	1.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1007	-	-	2/4/4/4	-
3	GOL	A	1008[B]	-	-	2/4/4/4	-
3	GOL	A	1006	-	-	2/4/4/4	-
3	GOL	A	1002	-	-	2/4/4/4	-
3	GOL	A	1009	-	-	4/4/4/4	-
3	GOL	A	1011	-	-	0/4/4/4	-
3	GOL	B	1009	-	-	2/4/4/4	-
3	GOL	B	1005	-	-	1/4/4/4	-
3	GOL	B	1003	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1003	-	-	2/4/4/4	-
3	GOL	B	1004	-	-	0/4/4/4	-
3	GOL	B	1010	-	-	4/4/4/4	-
3	GOL	A	1004	-	-	0/4/4/4	-
3	GOL	A	1005	-	-	0/4/4/4	-
3	GOL	B	1008	-	-	4/4/4/4	-
3	GOL	B	1011	-	-	2/4/4/4	-
3	GOL	A	1010	-	-	4/4/4/4	-
3	GOL	B	1007	-	-	0/4/4/4	-
3	GOL	B	1006	-	-	2/4/4/4	-
3	GOL	A	1008[A]	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1009	GOL	C1-C2	2.79	1.63	1.51
3	B	1010	GOL	C1-C2	2.32	1.61	1.51
3	B	1004	GOL	O2-C2	-2.32	1.36	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1003	GOL	C3-C2-C1	-2.03	103.79	111.70

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	GOL	O1-C1-C2-C3
3	A	1006	GOL	O1-C1-C2-C3
3	A	1008[A]	GOL	O1-C1-C2-C3
3	A	1008[B]	GOL	O1-C1-C2-C3
3	A	1009	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

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.