

wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 11:42 PM EDT

PDB ID	:	6VSS
Title	:	Arginase from Medicago truncatula
Authors	:	Sekula, B.
Deposited on	:	2020-02-11
Resolution	:	1.93 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 (1)) 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: $X\hbox{-}RAY\,DIFFRACTION$

The reported resolution of this entry is 1.93 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 3 unique types of molecules in this entry. The entry contains 15295 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.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace											
1	А	316	Total	С	Ν	Ο	S	0	0	0											
	A	510	2441	1531	439	464	7	0	0	0											
1	В	319	Total	С	Ν	0	S	0	1	0											
1	D	519	2470	1547	445	471	7	0	L												
1	С	318	Total	С	Ν	0	S	0	0	0											
1	U	510	2455	1537	441	470	7														
1	D	318	Total	С	Ν	0	S	0	1	0											
1	D	510	2463	1542	444	470	7	0	T	0											
1	Е	316	Total	С	Ν	0	S	$\frac{S}{0}$	1	0											
1			2449	1535	442	465	7	0	T	0											
1	1 F	F 318	Total	С	Ν	Ο	S	0	0	0											
		Г	Г	Г	Г	Г	Г	Г	Г	Г	Ľ	Ľ	F	510	2455	1537	441	470	$\overline{7}$		0

• Molecule 1 is a protein called Arginase.

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference	
А	-2	SER	-	expression tag	UNP G7JFU5	
А	-1	ASN	-	expression tag	UNP G7JFU5	
А	0	ALA	-	expression tag	UNP G7JFU5	
В	-2	SER	-	expression tag	UNP G7JFU5	
В	-1	ASN	-	expression tag	UNP G7JFU5	
В	0	ALA	-	expression tag	UNP G7JFU5	
С	-2	SER	-	expression tag	UNP G7JFU5	
С	-1	ASN	-	expression tag	UNP G7JFU5	
С	0	ALA	-	expression tag	UNP G7JFU5	
D	-2	SER	-	expression tag	UNP G7JFU5	
D	-1	ASN	-	expression tag	UNP G7JFU5	
D	0	ALA	-	expression tag	UNP G7JFU5	
Е	-2	SER	-	expression tag	UNP G7JFU5	
Е	-1	ASN	-	expression tag	UNP G7JFU5	
Е	0	ALA	-	expression tag	UNP G7JFU5	
F	-2	SER	-	expression tag	UNP G7JFU5	
F	-1	ASN	-	expression tag	UNP G7JFU5	
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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP G7JFU5

• Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Mn 2 2	0	0
2	В	2	Total Mn 2 2	0	0
2	С	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0
2	Е	2	Total Mn 2 2	0	0
2	F	2	Total Mn 2 2	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	104	Total O 105 105	0	1
3	В	91	Total O 92 92	0	1
3	С	78	Total O 78 78	0	0
3	D	78	Total O 78 78	0	0
3	Е	95	Total O 96 96	0	1
3	F	101	Total O 101 101	0	0

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



3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	79.33Å 142.91Å 90.05Å	Depositor
a, b, c, α , β , γ	90.00° 115.90° 90.00°	Depositor
Resolution (Å)	44.55 - 1.93	Depositor
% Data completeness	95.9 (44.55-1.93)	Depositor
(in resolution range)		-
R _{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.75 (at 1.92 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.182 , 0.218	Depositor
Wilson B-factor ($Å^2$)	28.2	Xtriage
Anisotropy	0.207	Xtriage
L-test for twinning ²	$< L > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.240 for h,-k,-h-l	Xtriage
Total number of atoms	15295	wwPDB-VP
Average B, all atoms $(Å^2)$	36.0	wwPDB-VP

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

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.

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.

4 Model quality (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains (i)

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

4.3.3 RNA (i)

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

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 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.

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 (i)

5.1 Protein, DNA and RNA chains (i)

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

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

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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

