

Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 12:32 AM EDT

Acine-

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:

:	FAILED
:	1.13
:	FAILED
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	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 1.90 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.



6 UDS

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7362 atoms, of which 3493 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	Atoms					ZeroOcc	AltConf	Trace		
1	Δ	244	Total	С	Η	Ν	0	S	0	1	0 1	0
	A	244	3633	1136	1815	318	358	6	0		U	
1	D	240	Total	С	Н	Ν	0	S	0	0	0	
	D	240	3403	1083	1678	300	337	5		U	U	

• Molecule 1 is a protein called 3-oxoacyl-(Acyl-carrier-protein) reductase.

Chain	Residue	Modelled	Actual	Comment	Reference
А	-23	MET	-	expression tag	UNP V5VHN7
А	-22	HIS	-	expression tag	UNP V5VHN7
А	-21	HIS	-	expression tag	UNP V5VHN7
А	-20	HIS	-	expression tag	UNP V5VHN7
А	-19	HIS	-	expression tag	UNP V5VHN7
А	-18	HIS	-	expression tag	UNP V5VHN7
А	-17	HIS	-	expression tag	UNP V5VHN7
А	-16	SER	-	expression tag	UNP V5VHN7
А	-15	SER	-	expression tag	UNP V5VHN7
А	-14	GLY	-	expression tag	UNP V5VHN7
А	-13	VAL	-	expression tag	UNP V5VHN7
А	-12	ASP	-	expression tag	UNP V5VHN7
А	-11	LEU	-	expression tag	UNP V5VHN7
А	-10	GLY	-	expression tag	UNP V5VHN7
А	-9	THR	-	expression tag	UNP V5VHN7
А	-8	GLU	-	expression tag	UNP V5VHN7
А	-7	ASN	-	expression tag	UNP V5VHN7
А	-6	LEU	-	expression tag	UNP V5VHN7
А	-5	TYR	-	expression tag	UNP V5VHN7
А	-4	PHE	-	expression tag	UNP V5VHN7
А	-3	GLN	-	expression tag	UNP V5VHN7
A	-2	SER	-	expression tag	UNP V5VHN7
А	-1	ASN	-	expression tag	UNP V5VHN7
A	0	ALA	-	expression tag	UNP V5VHN7
В	-23	MET	_	expression tag	UNP V5VHN7

There are 48 discrepancies between the modelled and reference sequences:

Continued on next page...



Chain	Residue	Modelled	Actual	Comment	Reference
В	-22	HIS	-	expression tag	UNP V5VHN7
В	-21	HIS	-	expression tag	UNP V5VHN7
В	-20	HIS	-	expression tag	UNP V5VHN7
В	-19	HIS	-	expression tag	UNP V5VHN7
В	-18	HIS	-	expression tag	UNP V5VHN7
В	-17	HIS	-	expression tag	UNP V5VHN7
В	-16	SER	-	expression tag	UNP V5VHN7
В	-15	SER	-	expression tag	UNP V5VHN7
В	-14	GLY	-	expression tag	UNP V5VHN7
В	-13	VAL	-	expression tag	UNP V5VHN7
В	-12	ASP	-	expression tag	UNP V5VHN7
В	-11	LEU	-	expression tag	UNP V5VHN7
В	-10	GLY	-	expression tag	UNP V5VHN7
В	-9	THR	-	expression tag	UNP V5VHN7
В	-8	GLU	-	expression tag	UNP V5VHN7
В	-7	ASN	-	expression tag	UNP V5VHN7
В	-6	LEU	-	expression tag	UNP V5VHN7
В	-5	TYR	-	expression tag	UNP V5VHN7
В	-4	PHE	-	expression tag	UNP V5VHN7
В	-3	GLN	-	expression tag	UNP V5VHN7
В	-2	SER	-	expression tag	UNP V5VHN7
В	-1	ASN	-	expression tag	UNP V5VHN7
В	0	ALA	-	expression tag	UNP V5VHN7

Continued from previous page...

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	204	Total O 204 204	0	0
2	В	122	Total O 122 122	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 43 21 2	Depositor	
Cell constants	87.39Å 87.39Å 151.29Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°		
Resolution (Å)	29.13 - 1.90	Depositor	
% Data completeness	99.7 (29.13-1.90)	Depositor	
(in resolution range)		Depositor	
R _{merge}	0.16	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$2.26 (at 1.91 \text{\AA})$	Xtriage	
Refinement program	PHENIX 1.14_3260	Depositor	
R, R_{free}	0.188 , 0.206	Depositor	
Wilson B-factor $(Å^2)$	31.1	Xtriage	
Anisotropy	0.465	Xtriage	
L-test for twinning ²	$ < L >=0.47, < L^2>=0.30$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	7362	wwPDB-VP	
Average B, all atoms $(Å^2)$	42.0	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 7.17% 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)

There are no ligands in this entry.

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.

