

# Full wwPDB X-ray Structure Validation Report (i)

#### Oct 4, 2023 – 10:56 PM EDT

PDB ID	:	6VET
Title	:	Human insulin analog: [GluB10,HisA8,ArgA9,TyrB20]-DOI
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Deposited on		
Resolution	:	1.46  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 (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 1.46 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 2072 atoms, of which 903 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	А	20		С		Ν	Ο	$\mathbf{S}$	0	0	0
		20	309	100	147	28	30	4	0	0	
1	C	20	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0	0
		20	310	100	148	28	30	4	0	0	
1	Е	20	Total	С	Н	Ν	Ο	S	0	0	0
		20	311	100	149	28	30	4	0	U	

• Molecule 1 is a protein called Insulin A chain.

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	8	HIS	THR	engineered mutation	UNP P01308
А	9	ARG	SER	engineered mutation	UNP P01308
С	8	HIS	THR	engineered mutation	UNP P01308
С	9	ARG	SER	engineered mutation	UNP P01308
Е	8	HIS	THR	engineered mutation	UNP P01308
Е	9	ARG	SER	engineered mutation	UNP P01308

• Molecule 2 is a protein called Insulin B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
9	В	22	Total	С	Η	Ν	Ο	S	0	1	0
	D		359	121	171	30	35	2	0	1	
0	П	22	Total	С	Η	Ν	Ο	S	0	0	0
			334	116	153	29	34	2	0		
9	F	22	Total	С	Η	Ν	Ο	S	0	ე	0
	Ľ		330	123	135	32	38	2	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	10	GLU	HIS	engineered mutation	UNP P01308
В	20	TYR	GLY	engineered mutation	UNP P01308

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Chain	Residue	Modelled	Actual	Comment	Reference
D	10	GLU	HIS	engineered mutation	UNP P01308
D	20	TYR	GLY	engineered mutation	UNP P01308
F	10	GLU	HIS	engineered mutation	UNP P01308
F	20	TYR	GLY	engineered mutation	UNP P01308

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• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	20	TotalO2020	0	0
3	В	21	Total O 21 21	0	0
3	С	15	Total O   15 15	0	0
3	D	31	$\begin{array}{cc} \text{Total} & \text{O} \\ 31 & 31 \end{array}$	0	0
3	Е	14	Total O   14 14	0	0
3	F	18	Total O   18 18	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 21 21 21	Depositor	
Cell constants	28.37Å $52.12$ Å $80.50$ Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	43.75 - 1.46	Depositor	
% Data completeness	99.1 (43.75-1.46)	Depositor	
(in resolution range)		Depositor	
R <sub>merge</sub>	0.14	Depositor	
R <sub>sym</sub>	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$1.10 (at 1.46 \text{\AA})$	Xtriage	
Refinement program	PHENIX (1.13-2998_1692)	Depositor	
$R, R_{free}$	0.201 , $0.238$	Depositor	
Wilson B-factor $(Å^2)$	20.2	Xtriage	
Anisotropy	0.418	Xtriage	
L-test for twinning <sup>2</sup>	$ < L >=0.49, < L^2>=0.32$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	2072	wwPDB-VP	
Average B, all atoms $(Å^2)$	32.0	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 11.32% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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.

