

Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 02:34 PM EDT

PDB ID : 6NWV

Title : Insulin Lispro Analog

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2019-02-07 Deposited on

: 1.60 Å(reported) Resolution

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 (i)) were used in the production of this report:

MolProbity **FAILED**

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13

FAILED EDS

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

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: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.60 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 7 unique types of molecules in this entry. The entry contains 2542 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 Insulin A chain.

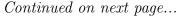
Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	A	21	Total	С	N	О	S	0	0	0
1	Λ	21	161	99	25	33	4	U	U	
1	С	21	Total	С	N	Ο	S	0	2	0
1		21	163	99	25	35	4	0	2	
1	E	21	Total	С	N	Ο	S	0	0	0
1	Ľ	21	160	97	25	34	4			
1	G	21	Total	С	N	Ο	S	0	1	0
1	G	21	171	104	27	36	4	0		
1	Ţ	21	Total	С	N	О	S	0	0	0
1	1	21	163	99	25	35	4	0	U	0
1	K	K 21	Total	С	N	О	S	0	0	0
1	17	21	150	93	23	30	4	U	U	

• Molecule 2 is a protein called Insulin Lispro B chain.

Mol	Chain	Residues		Ato	ms			ZeroOcc	AltConf	Trace
2	В	28	Total	С	N	О	S	0	0	1
	Ъ	20	218	141	37	38	2		0	1
2	D	30	Total	С	N	Ο	S	0	1	1
	D	30	239	155	40	42	2		1	1
2	F	30	Total	С	N	Ο	S	0	1	1
2	I.	30	233	151	40	40	2			
2	Н	30	Total	С	N	Ο	S	0	2	1
2	11	30	244	163	41	38	2		2	1
2	J	26	Total	С	N	Ο	S	0	2	0
	J	20	211	139	35	35	2		2	U
2	T	30	Total	С	N	О	S	0	0	0
	П	30	237	155	40	40	2		U	U

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	28	LYS	PRO	engineered mutation	UNP P01308

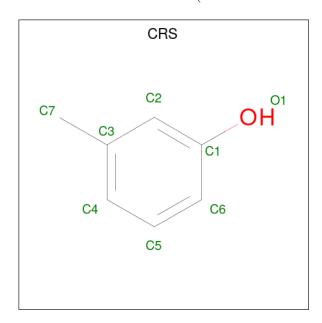




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Chain	Residue	Modelled	Actual	Comment	Reference
В	29	PRO	LYS	engineered mutation	UNP P01308
D	28	LYS	PRO	engineered mutation	UNP P01308
D	29	PRO	LYS	engineered mutation	UNP P01308
F	28	LYS	PRO	engineered mutation	UNP P01308
F	29	PRO	LYS	engineered mutation	UNP P01308
Н	28	LYS	PRO	engineered mutation	UNP P01308
Н	29	PRO	LYS	engineered mutation	UNP P01308
J	28	LYS	PRO	engineered mutation	UNP P01308
J	29	PRO	LYS	engineered mutation	UNP P01308
L	28	LYS	PRO	engineered mutation	UNP P01308
L	29	PRO	LYS	engineered mutation	UNP P01308

 \bullet Molecule 3 is M-CRESOL (three-letter code: CRS) (formula: $\mathrm{C_7H_8O}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 7 1	0	0
3	С	1	Total C O 8 7 1	0	0
3	E	1	Total C O 8 7 1	0	0
3	G	1	Total C O 8 7 1	0	0
3	G	1	Total C O 8 7 1	0	0
3	I	1	Total C O 8 7 1	0	0

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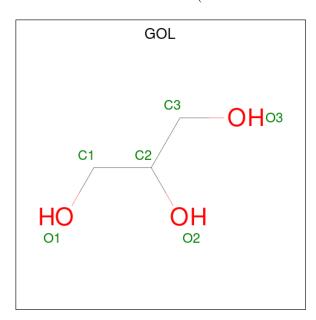
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Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
3	K	1	Total 8	C 7	O 1	0	0

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0

 \bullet Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $\mathrm{C_3H_8O_3}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0

• Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total Cl 1 1	0	0
6	L	1	Total Cl 1 1	0	0



• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	13	Total O 13 13	0	0
7	В	9	Total O 9 9	0	0
7	С	13	Total O 13 13	0	0
7	D	13	Total O 13 13	0	0
7	Е	11	Total O 11 11	0	0
7	F	11	Total O 11 11	0	0
7	G	5	Total O 5 5	0	0
7	Н	15	Total O 15 15	0	0
7	I	7	Total O 7 7	0	0
7	J	8	Total O 8 8	0	0
7	K	3	Total O 3 3	0	0
7	L	12	Total O 12 12	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 1 21 1	Depositor
Cell constants	$46.16\text{\AA} 61.79\text{\AA} 58.62\text{Å}$	Depositor
a, b, c, α , β , γ	90.00° 111.46° 90.00°	Depositor
Resolution (Å)	42.96 - 1.60	Depositor
% Data completeness	99.2 (42.96-1.60)	Depositor
(in resolution range)		-
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.34 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.208 , 0.257	Depositor
Wilson B-factor (A^2)	26.5	Xtriage
Anisotropy	0.222	Xtriage
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
Total number of atoms	2542	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.08% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	ol Type Chain Res Link		Link	В	ond leng	gths	Bond angles			
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	CRS	Е	101	-	8,8,8	0.31	0	10,10,10	0.33	0
3	CRS	I	101	-	8,8,8	0.27	0	10,10,10	0.42	0
3	CRS	G	102	-	8,8,8	0.38	0	10,10,10	0.40	0
3	CRS	С	101	-	8,8,8	0.41	0	10,10,10	0.40	0
3	CRS	A	101	-	8,8,8	0.49	0	10,10,10	0.34	0
3	CRS	G	101	-	8,8,8	0.43	0	10,10,10	0.47	0
3	CRS	K	101	-	8,8,8	0.54	0	10,10,10	0.38	0
5	GOL	D	101	-	5,5,5	0.17	0	5,5,5	0.39	0
5	GOL	F	102	-	5,5,5	0.16	0	5,5,5	0.33	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	CRS	Е	101	-	-	-	0/1/1/1
3	CRS	I	101	-	-	-	0/1/1/1
3	CRS	G	102	-	-	-	0/1/1/1
3	CRS	С	101	-	-	-	0/1/1/1
3	CRS	A	101	-	-	-	0/1/1/1
3	CRS	G	101	-	-	-	0/1/1/1
3	CRS	K	101	-	-	-	0/1/1/1
5	GOL	D	101	-	-	3/4/4/4	-
5	GOL	F	102	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	101	GOL	C1-C2-C3-O3
5	D	101	GOL	O2-C2-C3-O3
5	D	101	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 (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.

