

Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 06:24 AM EDT

PDB ID : 3JSD

Title: Insulin's biosynthesis and activity have opposing structural requirements: a

new factor in neonatal diabetes mellitus

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Deposited on : 2009-09-10

Resolution : 2.50 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:

MolProbity: 4.02b-467

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

Parkinson et al. (1996)

Xtriage (Phenix) : 1.13

Ideal geometry (DNA, RNA)

EDS : 2.35

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

Refmac : 5.8.0158

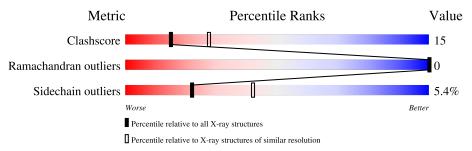
 $\begin{array}{cccc} & CCP4 & : & 7.0.044 \; (Gargrove) \\ Ideal \; geometry \; (proteins) & : & Engh \; \& \; Huber \; (2001) \end{array}$

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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain		
1	A	21	67%	29%	5%
1	С	21	71%	24%	5%
2	В	30	87%		13%
2	D	30	83%	1	.3% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DAL	D	8	_	-	X	-



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 841 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		
Ī	1	Λ	21	Total	С	N	О	S	0	0	0
	1	А	21	163	99	25	35	4	U		
Ī	1	C	21	Total	С	N	О	S	0	0	0
	1	C	21	163	99	25	35	4	U		

• Molecule 2 is a protein called Insulin B chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	B	30	Total	С	N	О	S	0	0	0
2	Б	30	243	159	40	42	2			
2	D	30	Total	С	N	О	S	0	0	0
	D	30	243	159	40	42	2	0	U	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	8	DAL	GLY	engineered mutation	UNP P01308
D	8	DAL	GLY	engineered mutation	UNP P01308

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total Cl 1 1	0	0

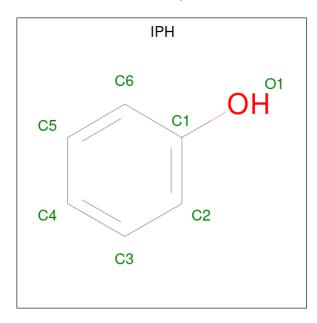
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\mathbf{Mol}	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0

• Molecule 5 is PHENOL (three-letter code: IPH) (formula: C₆H₆O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	1	Total C O 7 6 1	0	0

• Molecule 6 is water.

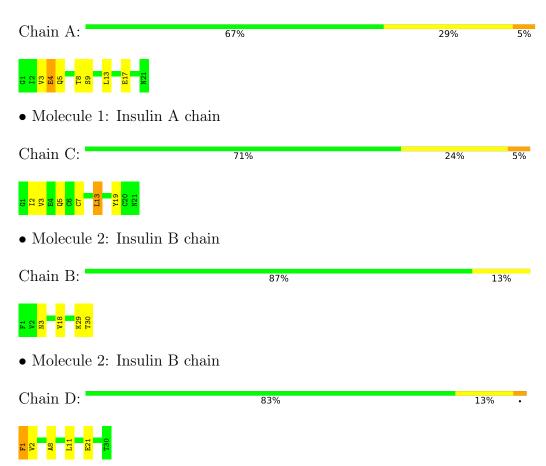
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total O 4 4	0	0
6	В	9	Total O 9 9	0	0
6	D	5	Total O 5 5	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Insulin A chain





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants	80.84Å 80.84Å 38.84Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	17.37 - 2.50	Depositor
Resolution (A)	21.87 - 2.00	EDS
% Data completeness	97.6 (17.37-2.50)	Depositor
(in resolution range)	92.1 (21.87-2.00)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.30 \; (at \; 2.01\text{Å})$	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.274	Depositor
it, it free	0.235 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 54.0	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	841	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.66% 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.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CL, DAL, IPH

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| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond	lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.51	0/164	0.60	0/220	
1	С	0.39	0/164	0.61	0/220	
2	В	0.51	0/244	0.75	0/327	
2	D	0.51	0/244	0.63	0/327	
All	All	0.49	0/816	0.66	0/1094	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	163	0	149	9	0
1	С	163	0	149	6	0
2	В	243	0	233	5	0
2	D	243	0	233	8	0
3	В	1	0	0	0	0
3	D	1	0	0	0	0
4	В	1	0	0	0	0
4	D	1	0	0	0	0
5	С	7	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	4	0	0	0	0
6	В	9	0	0	0	0
6	D	5	0	0	1	0
All	All	841	0	770	24	0

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 15.

All (24) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A	A	Interatomic	Clash	
Atom-1	Atom-2	${\rm distance}(\mathring{\rm A})$	overlap (Å)	
1:C:13:LEU:HD22	1:C:13:LEU:H	1.41	0.83	
2:D:8:DAL:HB3	2:D:11:LEU:HB2	1.67	0.75	
2:D:2:VAL:HG23	2:D:2:VAL:O	1.88	0.71	
1:C:13:LEU:HD22	1:C:13:LEU:N	2.10	0.66	
1:C:13:LEU:H	1:C:13:LEU:CD2	2.10	0.64	
2:D:8:DAL:CB	2:D:11:LEU:HB2	2.27	0.63	
2:D:8:DAL:CB	2:D:11:LEU:HD12	2.31	0.61	
2:D:1:PHE:HB2	6:D:38:HOH:O	2.01	0.60	
2:D:21:GLU:H	2:D:21:GLU:CD	2.06	0.59	
1:A:17:GLU:HG2	2:B:18:VAL:HG11	1.85	0.57	
1:A:13:LEU:O	1:A:17:GLU:HG3	2.07	0.55	
1:A:4:GLU:HB2	2:B:30:THR:OXT	2.09	0.53	
2:D:21:GLU:CD	2:D:21:GLU:N	2.65	0.50	
2:D:8:DAL:HB2	2:D:11:LEU:HD12	1.94	0.49	
2:B:29:LYS:O	2:B:30:THR:HB	2.12	0.49	
1:A:3:VAL:HB	2:B:30:THR:HA	1.96	0.47	
1:A:4:GLU:O	1:A:8:THR:HB	2.15	0.46	
1:A:8:THR:O	1:A:8:THR:HG22	2.16	0.46	
1:A:4:GLU:HA	1:A:8:THR:HB	1.98	0.44	
1:C:2:ILE:HD12	1:C:19:TYR:CD2	2.53	0.44	
1:A:17:GLU:HG2	2:B:18:VAL:CG1	2.47	0.44	
1:C:3:VAL:O	1:C:7:CYS:HB2	2.19	0.43	
1:A:5:GLN:O	1:A:9:SER:HB2	2.19	0.41	
1:C:2:ILE:HD12	1:C:19:TYR:CG	2.57	0.41	

There are no symmetry-related clashes.



5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	A	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
1	C	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
2	В	27/30 (90%)	24 (89%)	3 (11%)	0	100	100
2	D	27/30 (90%)	24 (89%)	3 (11%)	0	100	100
All	All	92/102~(90%)	84 (91%)	8 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	20/20 (100%)	19 (95%)	1 (5%)	24 46
1	С	20/20 (100%)	18 (90%)	2 (10%)	7 15
2	В	26/26 (100%)	25 (96%)	1 (4%)	33 58
2	D	26/26 (100%)	25 (96%)	1 (4%)	33 58
All	All	92/92 (100%)	87 (95%)	5 (5%)	22 42

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
2	В	3	ASN

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Mol	Chain	Res	Type
1	С	5	GLN
1	С	13	LEU
2	D	1	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
2	В	3	ASN
1	С	21	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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2 non-standard protein/DNA/RNA residues are modelled in this entry.

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.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	Type Chain	Chain Res	Link	Bond lengths			Bond angles		
	WIOI	туре				Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
Ī	5	IPH	С	200	-	7,7,7	2.06	3 (42%)	8,8,8	1.75	2 (25%)

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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IPH	С	200	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
5	С	200	IPH	C5-C6	2.88	1.45	1.38
5	С	200	IPH	C2-C1	2.71	1.44	1.38
5	С	200	IPH	C3-C2	2.64	1.44	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
5	С	200	IPH	C6-C1-C2	3.43	125.54	119.77
5	С	200	IPH	C3-C2-C1	-2.43	115.88	119.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

