Full wwPDB X-ray Structure Validation Report (i)

May 28, 2020 – 07:42 pm BST

PDB ID	:	1IZB
Title	:	ROLE OF B13 GLU IN INSULIN ASSEMBLY: THE HEXAMER STRUCTURE OF RECOMBINANT MUTANT (B13 GLU-> GLN) INSULIN
Authors	:	Xiao, B.; Dodson, G.G.
Deposited on	:	1992-10-16
Resolution	:	2.00 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 following versions of software and data (see references (i)) were used in the production of this report:

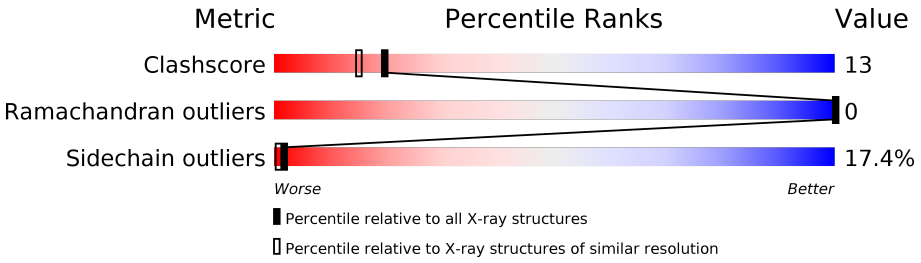
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.00 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 on 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	21	48% 43% 10%
1	C	21	57% 24% 19%
2	B	30	43% 30% 27%
2	D	30	43% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 937 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	C	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			

- Molecule 2 is a protein called INSULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	30	Total	C	N	O	S	0	0	0
			242	158	41	41	2			
2	D	30	Total	C	N	O	S	0	0	0
			242	158	41	41	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	GLN	GLU	ENGINEERED MUTATION	UNP P01315
D	13	GLN	GLU	ENGINEERED MUTATION	UNP P01315

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	38	Total O 38 38	0	0
4	C	42	Total O 42 42	0	0
4	D	28	Total O 28 28	0	0

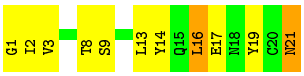
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

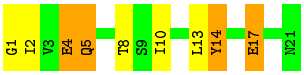
- Molecule 1: INSULIN

Chain A:



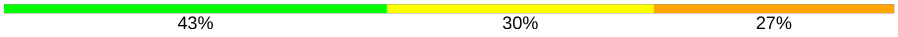
- Molecule 1: INSULIN

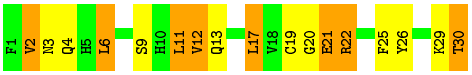
Chain C:



- Molecule 2: INSULIN

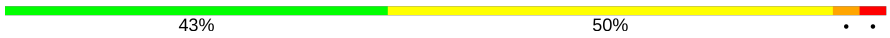
Chain B:

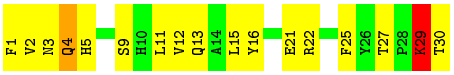




- Molecule 2: INSULIN

Chain D:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	82.85Å 82.85Å 34.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	937	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.34	1/164 (0.6%)	2.31	7/220 (3.2%)
1	C	1.03	0/164	2.22	6/220 (2.7%)
2	B	1.25	0/249	3.92	21/335 (6.3%)
2	D	1.14	0/249	2.75	11/335 (3.3%)
All	All	1.20	1/826 (0.1%)	2.99	45/1110 (4.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	GLU	CD-OE1	-5.71	1.19	1.25

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	22	ARG	NE-CZ-NH2	39.85	140.22	120.30
2	D	22	ARG	NE-CZ-NH1	26.93	133.77	120.30
2	B	22	ARG	NE-CZ-NH1	-25.86	107.37	120.30
2	B	22	ARG	CG-CD-NE	22.38	158.81	111.80
2	D	22	ARG	NE-CZ-NH2	-14.63	112.98	120.30
2	B	29	LYS	C-N-CA	10.94	149.05	121.70
2	B	21	GLU	OE1-CD-OE2	10.43	135.81	123.30
2	B	3	ASN	O-C-N	10.10	138.86	122.70
2	B	22	ARG	CA-CB-CG	9.96	135.32	113.40
1	C	14	TYR	CB-CG-CD2	9.74	126.84	121.00
1	C	14	TYR	CB-CG-CD1	-9.12	115.53	121.00
1	A	17	GLU	CG-CD-OE2	-8.47	101.36	118.30
2	B	6	LEU	CB-CG-CD1	7.56	123.85	111.00
1	A	14	TYR	CB-CG-CD2	6.97	125.18	121.00
2	B	21	GLU	CG-CD-OE2	-6.92	104.45	118.30
2	B	6	LEU	CA-CB-CG	6.77	130.87	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	20	GLY	CA-C-O	6.77	132.78	120.60
2	B	2	VAL	N-CA-CB	-6.68	96.80	111.50
2	B	2	VAL	CB-CA-C	6.54	123.82	111.40
1	A	17	GLU	OE1-CD-OE2	6.52	131.13	123.30
1	C	17	GLU	OE1-CD-OE2	6.41	130.99	123.30
2	B	22	ARG	NH1-CZ-NH2	-6.38	112.38	119.40
2	D	5	HIS	CA-CB-CG	6.25	124.23	113.60
2	B	20	GLY	CA-C-N	-6.20	103.55	117.20
2	B	26	TYR	CZ-CE2-CD2	6.20	125.38	119.80
2	B	12	VAL	CA-C-N	5.86	130.09	117.20
2	B	30	THR	N-CA-C	5.79	126.63	111.00
2	B	3	ASN	OD1-CG-ND2	5.75	135.13	121.90
2	B	3	ASN	CA-C-O	-5.74	108.04	120.10
2	D	22	ARG	NH1-CZ-NH2	-5.60	113.24	119.40
1	C	5	GLN	CA-C-O	-5.56	108.42	120.10
2	D	27	THR	CA-CB-CG2	5.51	120.11	112.40
1	A	3	VAL	CA-CB-CG2	-5.51	102.64	110.90
1	C	4	GLU	CB-CA-C	5.47	121.34	110.40
2	D	4	GLN	CG-CD-OE1	-5.30	111.00	121.60
2	D	25	PHE	N-CA-CB	5.28	120.11	110.60
2	D	29	LYS	CG-CD-CE	5.25	127.64	111.90
2	B	17	LEU	O-C-N	-5.22	114.35	122.70
1	A	1	GLY	CA-C-O	-5.19	111.25	120.60
2	D	25	PHE	CG-CD1-CE1	-5.18	115.10	120.80
2	D	5	HIS	N-CA-CB	5.17	119.91	110.60
2	D	16	TYR	CG-CD2-CE2	-5.14	117.19	121.30
1	A	17	GLU	CB-CA-C	-5.12	100.16	110.40
1	A	8	THR	CA-CB-OG1	-5.11	98.27	109.00
1	C	8	THR	CB-CA-C	5.06	125.26	111.60

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	4	0
1	C	163	0	149	8	0
2	B	242	0	233	7	0
2	D	242	0	234	10	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	17	0	0	0	0
4	B	38	0	0	0	0
4	C	42	0	0	0	0
4	D	28	0	0	1	0
All	All	937	0	765	20	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ILE:HD12	2:D:3:ASN:HB3	1.55	0.86
2:D:29:LYS:HD2	2:D:29:LYS:O	1.88	0.73
1:A:21:ASN:HD21	2:B:25:PHE:HE1	1.46	0.64
2:D:13:GLN:HG3	4:D:103:HOH:O	1.97	0.64
2:B:13:GLN:HG2	2:D:13:GLN:NE2	2.14	0.61
2:B:9:SER:O	2:B:12:VAL:HG22	2.03	0.58
1:A:2:ILE:HB	1:A:19:TYR:CZ	2.39	0.58
1:C:1:GLY:O	1:C:5:GLN:HG3	2.07	0.54
2:B:13:GLN:HE22	2:D:9:SER:HB2	1.73	0.53
1:C:1:GLY:HA3	2:D:30:THR:O	2.08	0.53
1:C:2:ILE:CD1	2:D:15:LEU:HD11	2.39	0.52
1:A:21:ASN:ND2	2:B:25:PHE:CE1	2.80	0.49
2:D:1:PHE:H1	2:D:1:PHE:HD1	1.60	0.49
1:C:2:ILE:HD11	2:D:11:LEU:HD11	1.97	0.47
1:C:14:TYR:O	1:C:17:GLU:HB2	2.16	0.46
1:C:10:ILE:HD13	1:C:10:ILE:HG21	1.82	0.44
2:B:19:CYS:O	2:B:22:ARG:HB2	2.18	0.43
1:C:1:GLY:N	1:C:4:GLU:OE1	2.37	0.43
1:A:16:LEU:HD11	2:B:11:LEU:HD21	2.00	0.43
2:D:9:SER:HA	2:D:12:VAL:HG22	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	Percentiles	
1	A	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
1	C	19/21 (90%)	19 (100%)	0	0	100	100
2	B	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
2	D	28/30 (93%)	28 (100%)	0	0	100	100
All	All	94/102 (92%)	91 (97%)	3 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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%)	16 (80%)	4 (20%)	1	0
1	C	20/20 (100%)	19 (95%)	1 (5%)	24	20
2	B	26/26 (100%)	19 (73%)	7 (27%)	0	0
2	D	26/26 (100%)	22 (85%)	4 (15%)	2	1
All	All	92/92 (100%)	76 (83%)	16 (17%)	2	1

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	13	LEU

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Mol	Chain	Res	Type
1	A	16	LEU
1	A	21	ASN
2	B	2	VAL
2	B	4	GLN
2	B	6	LEU
2	B	11	LEU
2	B	17	LEU
2	B	21	GLU
2	B	30	THR
1	C	13	LEU
2	D	2	VAL
2	D	4	GLN
2	D	21	GLU
2	D	29	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	C	15	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.