Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 11:48 PM EDT

PDB ID	:	2INS
Title	:	THE STRUCTURE OF DES-PHE B1 BOVINE INSULIN
Authors	:	Smith, G.D.; Duax, W.L.; Dodson, E.J.; Dodson, G.G.; Degraaf, R.A.G.; Reynolds, C.D.
Deposited on	:	1982-05-10
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:

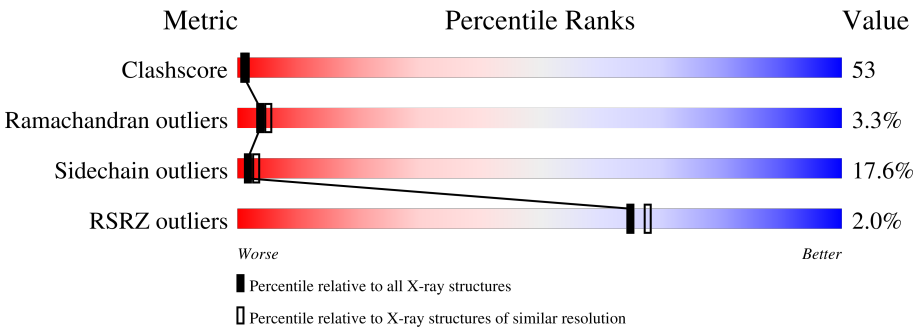
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	21	5%, 43%, 33%, 14%, 10%
1	C	21	33%, 48%, 10%, 10%
2	B	29	24%, 59%, 14%, •
2	D	29	3%, 45%, 38%, 7%, 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 964 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 DES-PHE B1 INSULIN (CHAIN A).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	21	160	97	25	34	4	0	0	0
1	C	21	152	90	25	33	4	0	0	0

- Molecule 2 is a protein called DES-PHE B1 INSULIN (CHAIN B).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	29	233	149	42	40	2	0	1	0
2	D	29	233	151	40	40	2	0	1	0

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	19	19	19	0	0
4	B	58	58	58	0	0
4	D	107	107	107	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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: DES-PHE B1 INSULIN (CHAIN A)

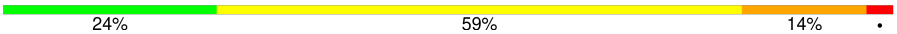
Chain A:

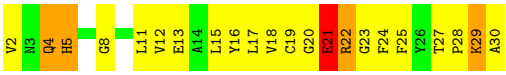
• Molecule 1: DES-PHE B1 INSULIN (CHAIN A)

Chain C:

• Molecule 2: DES-PHE B1 INSULIN (CHAIN B)

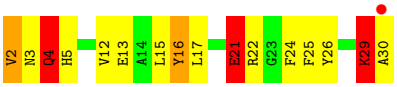
Chain B:





• Molecule 2: DES-PHE B1 INSULIN (CHAIN B)

Chain D:



4 Data and refinement statistics (i)

Property	Value
Space group	H 3
Cell constants a, b, c, α, β, γ	81.60Å 81.60Å 34.00Å 90.00° 90.00° 120.00°
Resolution (Å)	(Not available) – 2.50 5.95 – 2.56
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50 85.0 (5.95-2.56)
R_{merge}	(Not available)
R_{sym}	(Not available)
$< I/\sigma(I) >$ [1]	1.83 (at 2.55Å)
Refinement program	FAST FOURIER LEAST-SQUARES REFINEMENT, FAST-FOURIER
R, R_{free}	0.180 , (Not available) 0.174 , (Not available)
R_{free} test set	No test flags present.
Wilson B-factor (Å^2)	24.3
Anisotropy	0.062
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 118.0
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.31$
Estimated twinning fraction	0.053 for h,-h-k,-l
F_o,F_c correlation	0.94
Total number of atoms	964
Average B, all atoms (Å^2)	26.0

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical 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.

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

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	0.74	0/161	2.45	11/216 (5.1%)
1	C	0.68	0/152	2.67	9/203 (4.4%)
2	B	1.18	2/246 (0.8%)	2.10	9/330 (2.7%)
2	D	0.76	0/244	2.37	9/327 (2.8%)
All	All	0.90	2/803 (0.2%)	2.36	38/1076 (3.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	22[A]	ARG	CD-NE	-9.71	1.29	1.46
2	B	22[B]	ARG	CD-NE	-9.71	1.29	1.46

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	5	GLN	CA-CB-CG	21.66	161.05	113.40
2	D	29[A]	LYS	CB-CG-CD	15.16	151.01	111.60
2	D	29[B]	LYS	CB-CG-CD	15.16	151.01	111.60
1	A	2	ILE	CA-CB-CG2	9.84	130.58	110.90
2	B	21	GLU	CB-CG-CD	-9.54	88.45	114.20
1	A	21	ASN	N-CA-CB	-9.53	93.45	110.60
2	B	21	GLU	N-CA-CB	-9.19	94.05	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	22[A]	ARG	CG-CD-NE	9.17	131.06	111.80
2	B	22[B]	ARG	CG-CD-NE	9.17	131.06	111.80
1	C	5	GLN	CB-CA-C	9.06	128.51	110.40
2	B	22[A]	ARG	NE-CZ-NH2	-7.86	116.37	120.30
2	B	22[B]	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	C	9	SER	N-CA-CB	7.81	122.21	110.50
1	C	9	SER	CB-CA-C	7.66	124.65	110.10
2	B	21	GLU	OE1-CD-OE2	7.48	132.28	123.30
1	C	5	GLN	CB-CG-CD	-7.42	92.31	111.60
1	A	19	TYR	CB-CG-CD2	-7.24	116.66	121.00
1	A	19	TYR	CA-CB-CG	-7.02	100.07	113.40
1	A	14	TYR	CA-CB-CG	-6.84	100.41	113.40
2	D	30	ALA	N-CA-C	6.79	129.34	111.00
1	A	21	ASN	CB-CA-C	-6.74	96.92	110.40
1	A	21	ASN	CA-CB-CG	6.40	127.47	113.40
1	A	19	TYR	C-N-CA	-6.08	106.50	121.70
1	C	6	CYS	N-CA-C	6.08	127.41	111.00
2	B	5	HIS	CA-CB-CG	-6.03	103.35	113.60
1	C	16	LEU	N-CA-CB	5.97	122.33	110.40
2	D	16	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	C	20	CYS	N-CA-CB	5.88	121.18	110.60
2	D	29[A]	LYS	CG-CD-CE	5.67	128.91	111.90
2	D	29[B]	LYS	CG-CD-CE	5.67	128.91	111.90
2	B	21	GLU	CA-CB-CG	-5.65	100.98	113.40
2	D	21	GLU	OE1-CD-OE2	5.38	129.76	123.30
1	A	21	ASN	N-CA-C	-5.36	96.52	111.00
1	C	17	GLU	CA-CB-CG	-5.26	101.83	113.40
2	D	16	TYR	CB-CA-C	-5.25	99.91	110.40
1	A	4	GLU	OE1-CD-OE2	5.23	129.58	123.30
2	D	4	GLN	CB-CA-C	-5.02	100.35	110.40
1	A	4	GLU	CB-CA-C	5.00	120.41	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	9	SER	CA

There are no planarity outliers.

CLOSE-CONTACTS INFOmissingINFO

5.2 Torsion angles (i)

5.2.1 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	Percentiles
1	A	19/21 (90%)	14 (74%)	4 (21%)	1 (5%)	2 2
1	C	19/21 (90%)	18 (95%)	0	1 (5%)	2 2
2	B	28/29 (97%)	26 (93%)	1 (4%)	1 (4%)	3 4
2	D	28/29 (97%)	27 (96%)	1 (4%)	0	100 100
All	All	94/100 (94%)	85 (90%)	6 (6%)	3 (3%)	4 5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	9	SER
1	A	2	ILE
2	B	21	GLU

5.2.2 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	19/19 (100%)	15 (79%)	4 (21%)	1 2
1	C	18/19 (95%)	16 (89%)	2 (11%)	6 11
2	B	25/24 (104%)	21 (84%)	4 (16%)	2 4
2	D	25/24 (104%)	19 (76%)	6 (24%)	0 1
All	All	87/86 (101%)	71 (82%)	16 (18%)	2 2

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

Mol	Chain	Res	Type
1	A	2	ILE
1	A	4	GLU
1	A	5	GLN
1	A	18	ASN
2	B	2	VAL
2	B	4	GLN
2	B	17	LEU
2	B	29	LYS
1	C	13	LEU
1	C	16	LEU
2	D	2	VAL
2	D	4	GLN
2	D	17	LEU
2	D	21	GLU
2	D	29[A]	LYS
2	D	29[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	18	ASN
1	A	21	ASN
2	B	4	GLN
1	C	15	GLN
1	C	18	ASN
1	C	21	ASN
2	D	5	HIS

5.2.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.4 Carbohydrates (i)

There are no monosaccharides in this entry.

5.5 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.

5.6 Other polymers (i)

There are no such residues in this entry.

5.7 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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	21/21 (100%)	0.08	1 (4%) 30 32	10, 19, 30, 33	0
1	C	21/21 (100%)	-0.00	0 100 100	16, 20, 31, 35	0
2	B	29/29 (100%)	-0.13	0 100 100	7, 14, 32, 41	0
2	D	29/29 (100%)	-0.30	1 (3%) 45 48	9, 16, 34, 38	0
All	All	100/100 (100%)	-0.11	2 (2%) 65 68	7, 19, 34, 41	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	GLY	2.1
2	D	30	ALA	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	D	31	1/1	0.96	0.04	13,13,13,13	1
3	ZN	B	1	1/1	1.00	0.05	10,10,10,10	1

6.5 Other polymers (i)

There are no such residues in this entry.