

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	2R36
Title	:	Crystal structure of ni human ARG-insulin
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Deposited on	:	2007-08-29
Resolution	:	2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

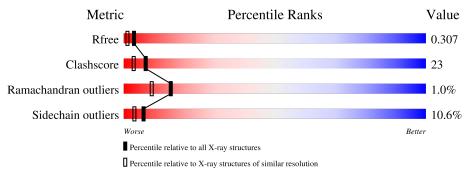
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	8085 (2.00-2.00)
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 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	А	22	68%	27%	5%
1	С	22	77%	18%	5%
2	В	30	63%	27%	10%
2	D	30	83%	139	% •



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 881 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.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	1 A	22	Total	С	Ν	Ο	S	0	0	0
		22	174	105	29	36	4	0		
1	С	22	Total	С	Ν	Ο	S	0	0	0
	U		174	105	29	36	4	0	0	0

• Molecule 1 is a protein called Insulin.

• Molecule 2 is a protein called Insulin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
9	2 B	30	Total	С	Ν	Ο	S	0	1	0
		- 50	243	158	40	43	2	0		
0	Л	30	Total	С	Ν	Ο	\mathbf{S}	0	1	0
	D	- 50	249	165	40	42	2		1	0

• Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	2	Total Ni 2 2	0	0
3	D	2	Total Ni 2 2	0	0

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Na 1 1	0	0

• Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Cl 1 1	0	1



• Molecule 6 is water.

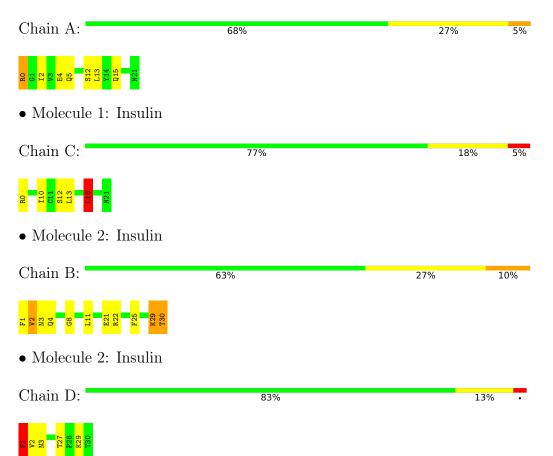
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	6	Total O 6 6	0	0
6	В	16	Total O 16 16	0	0
6	С	2	Total O 2 2	0	0
6	D	11	Total O 11 11	0	1



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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	Н 3	Depositor
Cell constants	83.95Å 83.95Å 40.22Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	$35.20 \ - \ 2.00$	Depositor
Resolution (A)	$35.20 \ - \ 2.00$	EDS
% Data completeness	95.0 (35.20-2.00)	Depositor
(in resolution range)	95.0 (35.20-2.00)	EDS
R _{merge}	0.08	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.27 (at 2.00 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D	0.221 , 0.255	Depositor
R, R_{free}	0.303 , 0.307	DCC
R_{free} test set	680 reflections $(10.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	34.9	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31, 59.0	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	881	wwPDB-VP
Average B, all atoms $(Å^2)$	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.60% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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: NA, NI, CL

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.34	0/175	0.39	0/234	
1	С	0.46	0/175	0.70	1/234~(0.4%)	
2	В	0.35	0/255	0.48	0/343	
2	D	0.42	0/261	0.52	0/351	
All	All	0.39	0/866	0.53	1/1162~(0.1%)	

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
2	D	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	16	LEU	CA-CB-CG	5.16	127.17	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	1[A]	PHE	Peptide
2	D	1[B]	PHE	Peptide



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	А	174	0	162	11	0
1	С	174	0	162	15	0
2	В	243	0	233	12	0
2	D	249	0	235	17	0
3	В	2	0	0	0	0
3	D	2	0	0	0	0
4	D	1	0	0	0	0
5	D	1	0	0	0	0
6	А	6	0	0	1	0
6	В	16	0	0	5	0
6	С	2	0	0	1	0
6	D	11	0	0	0	0
All	All	881	0	792	37	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 23.

The worst 5 of 37 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:13:LEU:HB2	2:D:1[B]:PHE:CE2	1.54	1.40
1:C:13:LEU:HD12	2:D:1[B]:PHE:CZ	1.88	1.08
1:C:13:LEU:CB	2:D:1[B]:PHE:HE2	1.72	1.01
1:C:13:LEU:HB2	2:D:1[B]:PHE:HE2	0.92	0.95
1:C:13:LEU:CB	2:D:1[B]:PHE:CE2	2.47	0.94

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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	20/22~(91%)	18 (90%)	2(10%)	0	100 100
1	С	20/22~(91%)	17 (85%)	3~(15%)	0	100 100
2	В	29/30~(97%)	27~(93%)	1 (3%)	1 (3%)	3 1
2	D	28/30~(93%)	26 (93%)	2(7%)	0	100 100
All	All	97/104 (93%)	88 (91%)	8 (8%)	1 (1%)	15 9

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

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	2	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percent	tiles
1	А	21/21~(100%)	20~(95%)	1 (5%)	25	22
1	С	21/21~(100%)	20~(95%)	1 (5%)	25	22
2	В	27/26 (104%)	22~(82%)	5 (18%)	1 (0
2	D	27/26~(104%)	23~(85%)	4 (15%)	3	1
All	All	96/94 (102%)	85 (88%)	11 (12%)	6	3

 $5~{\rm of}~11$ residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
2	D	1[A]	PHE
2	D	1[B]	PHE
2	D	29	LYS
2	D	27	THR
2	В	29	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such



sidechains are listed below:

Mol	Chain	Res	Type
1	А	15	GLN
2	В	3	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 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 (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.

