



Full wwPDB EM Validation Report ⓘ

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PDB ID : 6ZHB
Title : 3D electron diffraction structure of bovine insulin
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Deposited on : 2020-06-22
Resolution : 3.25 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
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) : 2.35

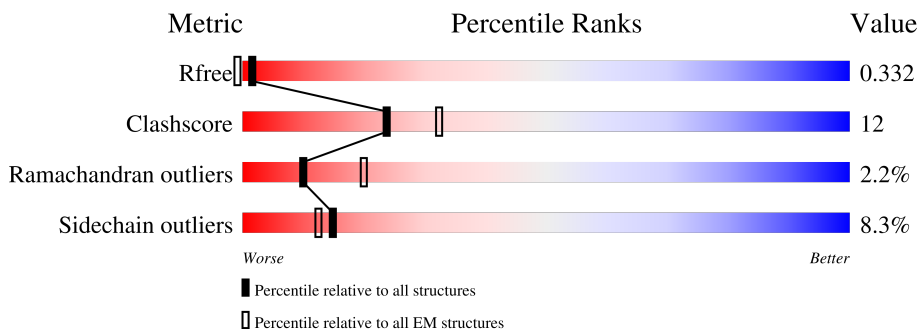
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.25 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)	EM structures (#Entries)
R_{free}	130704	0
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	21	86% (green), 14% (yellow)
1	C	21	67% (green), 29% (yellow), 5% (orange)
2	B	30	50% (green), 40% (yellow), 7% (orange), 3% (grey)
2	D	30	70% (green), 20% (yellow), 7% (orange), 3% (grey)

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 775 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
			Total	C	N	O	S		
1	A	21	160	97	25	34	4	0	0
1	C	21	160	97	25	34	4	0	0

- Molecule 2 is a protein called Insulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	28	221	146	37	36	2	0	0
2	D	29	233	150	39	42	2	1	0


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

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

Chain A:  86% 14%



- Molecule 1: Insulin

Chain C:  67% 29% 5%



- Molecule 2: Insulin

Chain B:  50% 40% 7%



- Molecule 2: Insulin

Chain D:  70% 20% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	82.40Å 82.40Å 33.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.30 – 3.25 30.30 – 3.25	Depositor EDS
% Data completeness (in resolution range)	84.4 (30.30-3.25) 84.4 (30.30-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.24Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.181 , 0.319 0.204 , 0.332	Depositor DCC
R_{free} test set	114 reflections (9.49%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtrriage
Anisotropy	0.195	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 0.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.069 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	775	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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	0.39	0/161	0.59	0/216
1	C	0.47	0/161	0.58	0/216
2	B	0.39	0/228	0.55	0/309
2	D	0.41	0/242	0.62	0/325
All	All	0.41	0/792	0.59	0/1066

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	160	0	145	2	0
1	C	160	0	145	4	0
2	B	221	0	208	12	0
2	D	233	0	217	6	0
3	D	1	0	0	0	0
All	All	775	0	715	18	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 12.

All (18) 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)
2:B:13:GLU:OE2	2:D:13[B]:GLU:OE2	1.62	1.17
2:B:2:VAL:CG2	2:B:4:GLN:HE21	2.02	0.73
2:B:2:VAL:HG23	2:B:4:GLN:HE21	1.64	0.64
2:B:2:VAL:HG21	2:B:4:GLN:HE21	1.70	0.57
1:C:5:GLN:NE2	1:C:19:TYR:OH	2.38	0.56
1:C:6:CYS:O	1:C:7:CYS:HB2	2.11	0.49
1:C:5:GLN:O	1:C:9:SER:HB3	2.13	0.47
2:B:9:SER:HB2	2:D:13[A]:GLU:HG2	1.95	0.47
2:B:15:LEU:HD13	2:B:24:PHE:CD1	2.49	0.47
1:A:14:TYR:CZ	2:B:1:PHE:CE2	3.06	0.44
1:A:14:TYR:CE2	2:B:1:PHE:CD2	3.06	0.44
2:B:9:SER:O	2:B:12:VAL:HG22	2.18	0.44
1:C:20:CYS:HB3	2:D:19:CYS:HB3	1.76	0.43
2:B:23:GLY:O	2:B:24:PHE:HB3	2.18	0.42
2:D:2:VAL:O	2:D:3:ASN:ND2	2.53	0.41
2:B:16:TYR:OH	2:D:8:GLY:HA2	2.21	0.41
2:D:11:LEU:O	2:D:14:ALA:N	2.54	0.41
2:B:8:GLY:O	2:B:10:HIS:N	2.54	0.40

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 PDB entries followed by that with respect to all EM entries.

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%)	17 (90%)	2 (10%)	0	100	100
1	C	19/21 (90%)	14 (74%)	4 (21%)	1 (5%)	2	12
2	B	26/30 (87%)	22 (85%)	3 (12%)	1 (4%)	3	19
2	D	28/30 (93%)	23 (82%)	5 (18%)	0	100	100
All	All	92/102 (90%)	76 (83%)	14 (15%)	2 (2%)	10	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	7	CYS
2	B	9	SER

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 PDB entries followed by that with respect to all EM entries.

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%)	17 (90%)	2 (10%)	7 25
1	C	19/19 (100%)	18 (95%)	1 (5%)	22 53
2	B	23/25 (92%)	22 (96%)	1 (4%)	29 59
2	D	24/25 (96%)	21 (88%)	3 (12%)	4 19
All	All	85/88 (97%)	78 (92%)	7 (8%)	15 36

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	13	LEU
2	B	27	THR
1	C	4	GLU
2	D	11	LEU
2	D	19	CYS
2	D	27	THR

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

Mol	Chain	Res	Type
2	B	4	GLN
1	C	5	GLN
2	D	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 1 ligands modelled in this entry, 1 is 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.