



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jan 10, 2018 – 03:43 PM EST

PDB ID : 6BFC
EMDB ID: : EMD-7041
Title : Cryo-EM structure of human insulin degrading enzyme in complex with insulin
Authors : Liang, W.G.; Zhang, Z.; Bailey, L.J.; Kossiakoff, A.A.; Tan, Y.Z.; Wei, H.;
Carragher, B.; Potter, S.C.; Tang, W.J.
Deposited on : 2017-10-26
Resolution : 3.70 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

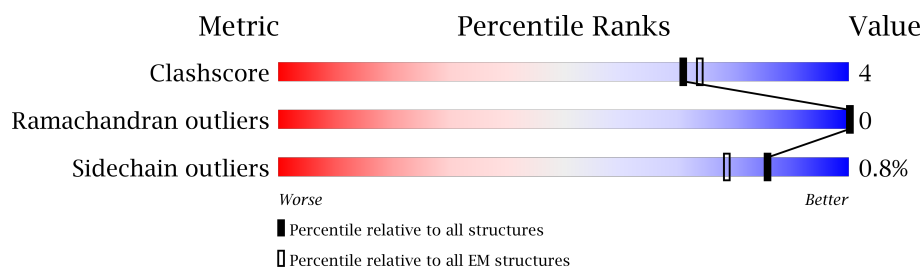
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	966	
1	B	966	
2	a	110	
2	b	110	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15762 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-degrading enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	948	Total	C	N	O	S	0	0
			7737	4986	1301	1428	22		
1	B	938	Total	C	N	O	S	0	0
			7662	4940	1286	1415	21		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	LEU	CYS	conflict	UNP P14735
A	171	SER	CYS	conflict	UNP P14735
A	178	ALA	CYS	conflict	UNP P14735
A	257	VAL	CYS	conflict	UNP P14735
A	414	LEU	CYS	conflict	UNP P14735
A	573	ASN	CYS	conflict	UNP P14735
A	590	SER	CYS	conflict	UNP P14735
A	789	SER	CYS	conflict	UNP P14735
A	812	ALA	CYS	conflict	UNP P14735
A	819	ALA	CYS	conflict	UNP P14735
A	904	SER	CYS	conflict	UNP P14735
B	110	LEU	CYS	conflict	UNP P14735
B	171	SER	CYS	conflict	UNP P14735
B	178	ALA	CYS	conflict	UNP P14735
B	257	VAL	CYS	conflict	UNP P14735
B	414	LEU	CYS	conflict	UNP P14735
B	573	ASN	CYS	conflict	UNP P14735
B	590	SER	CYS	conflict	UNP P14735
B	789	SER	CYS	conflict	UNP P14735
B	812	ALA	CYS	conflict	UNP P14735
B	819	ALA	CYS	conflict	UNP P14735
B	904	SER	CYS	conflict	UNP P14735

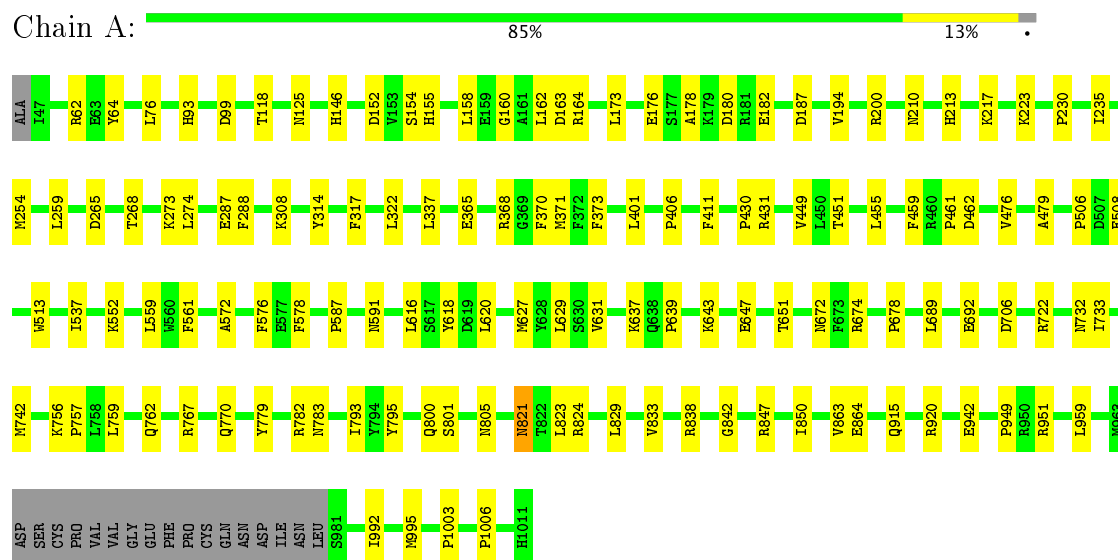
- Molecule 2 is a protein called Insulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	27	Total	C	N	O	S	0	0
			200	124	32	40	4		
2	b	22	Total	C	N	O	S	0	0
			163	104	26	30	3		

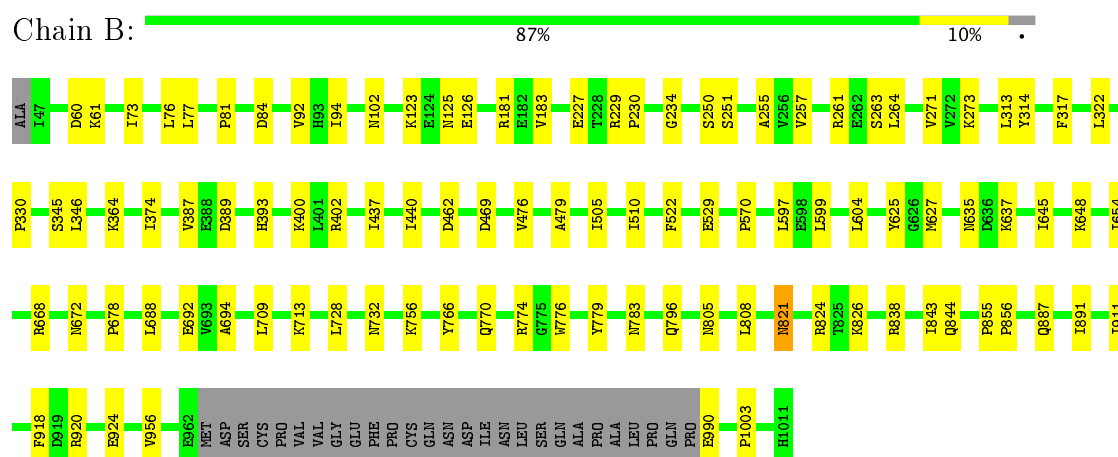
3 Residue-property plots

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.

- Molecule 1: Insulin-degrading enzyme



- Molecule 1: Insulin-degrading enzyme



- Molecule 2: Insulin



MET ALA LEU TRP MET ARG LEU LEU LEU LEU LEU ALA LEU LEU ALA TRP GLY PRO GLY ASP ASP ALA ALA F1 F1 E21 ARG GLY PHE PHE TYR THR PRO LYS THR ARG ARG GLU ALA ALA ASP LEU GLN VAL GLY GLN VAL GLU LEU GLY GLY PRO GLY ALA GLY SER LEU GLN

PRO LEU ALA LEU TRP MET GLY SER LEU PRO GLN LYS ARG GLY ILE VAL E44 E49 ILE CYS SER LEU TYR ALA GLN LEU GLU ASN CYS TYR ASN

● Molecule 2: Insulin



MET ALA LEU TRP MET ARG LEU LEU LEU LEU LEU ALA LEU LEU ALA TRP GLY PRO GLY ASP ASP ALA ALA F1 F1 C19 GLY GLU ARG GLY PHE PHE TYR THR PRO LYS THR ARG ARG GLU ALA ALA ASP LEU GLN VAL GLY GLN VAL GLU LEU GLY GLY PRO GLY ALA GLY SER LEU GLN

LEU GLN PRO LEU ALA LEU GLY SER LEU LEU GLN LYS ARG GLY ILE VAL GLU GLN CYS C47 T48 S49 ILE CYS SER LEU TYR GLN LEU GLU ASN TYR CYS ASN

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	148392	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	71.4	Depositor
Minimum defocus (nm)	940	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	46598	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 >2	RMSZ	# Z >2
1	A	0.34	0/7931	0.60	0/10729
1	B	0.32	0/7853	0.59	0/10621
2	a	0.36	0/201	0.91	0/270
2	b	0.32	0/164	0.73	0/221
All	All	0.33	0/16149	0.60	0/21841

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	7737	0	7663	67	0
1	B	7662	0	7584	56	0
2	a	200	0	185	0	0
2	b	163	0	157	0	0
All	All	15762	0	15589	121	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 4.

The worst 5 of 121 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:B:668:ARG:O	1:B:672:ASN:HB2	1.92	0.69
1:A:770:GLN:HB3	1:A:1003:PRO:HG2	1.77	0.66
1:B:920:ARG:O	1:B:924:GLU:HB3	1.98	0.63
1:A:620:LEU:HD12	1:A:629:LEU:HD13	1.80	0.62
1:B:776:TRP:O	1:B:990:GLU:N	2.33	0.61

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	944/966 (98%)	918 (97%)	26 (3%)	0	100	100
1	B	934/966 (97%)	910 (97%)	24 (3%)	0	100	100
2	a	23/110 (21%)	20 (87%)	3 (13%)	0	100	100
2	b	18/110 (16%)	16 (89%)	2 (11%)	0	100	100
All	All	1919/2152 (89%)	1864 (97%)	55 (3%)	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 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	838/861 (97%)	831 (99%)	7 (1%)	85	93
1	B	829/861 (96%)	823 (99%)	6 (1%)	87	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	a	23/88 (26%)	23 (100%)	0	100	100
2	b	19/88 (22%)	19 (100%)	0	100	100
All	All	1709/1898 (90%)	1696 (99%)	13 (1%)	86	93

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	920	ARG
1	A	951	ARG
1	B	821	ASN
1	A	821	ASN
1	B	774	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	762	GLN
1	A	915	GLN
1	B	475	ASN
1	B	844	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.