



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 29, 2017 – 08:22 PM EST

PDB ID : 6B7Y
EMDB ID: : EMD-7065
Title : Cryo-EM structure of human insulin degrading enzyme
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 : unknown
Resolution : 6.50 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-20030345

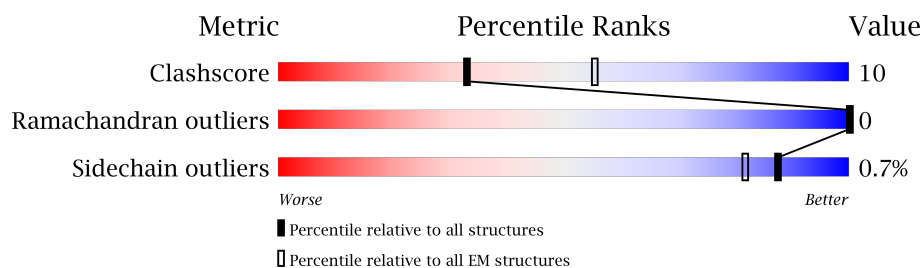
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.50 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)	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 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15410 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	949	Total	C	N	O	S	0	0
			7748	4995	1302	1429	22		
1	B	939	Total	C	N	O	S	0	0
			7662	4942	1284	1415	21		

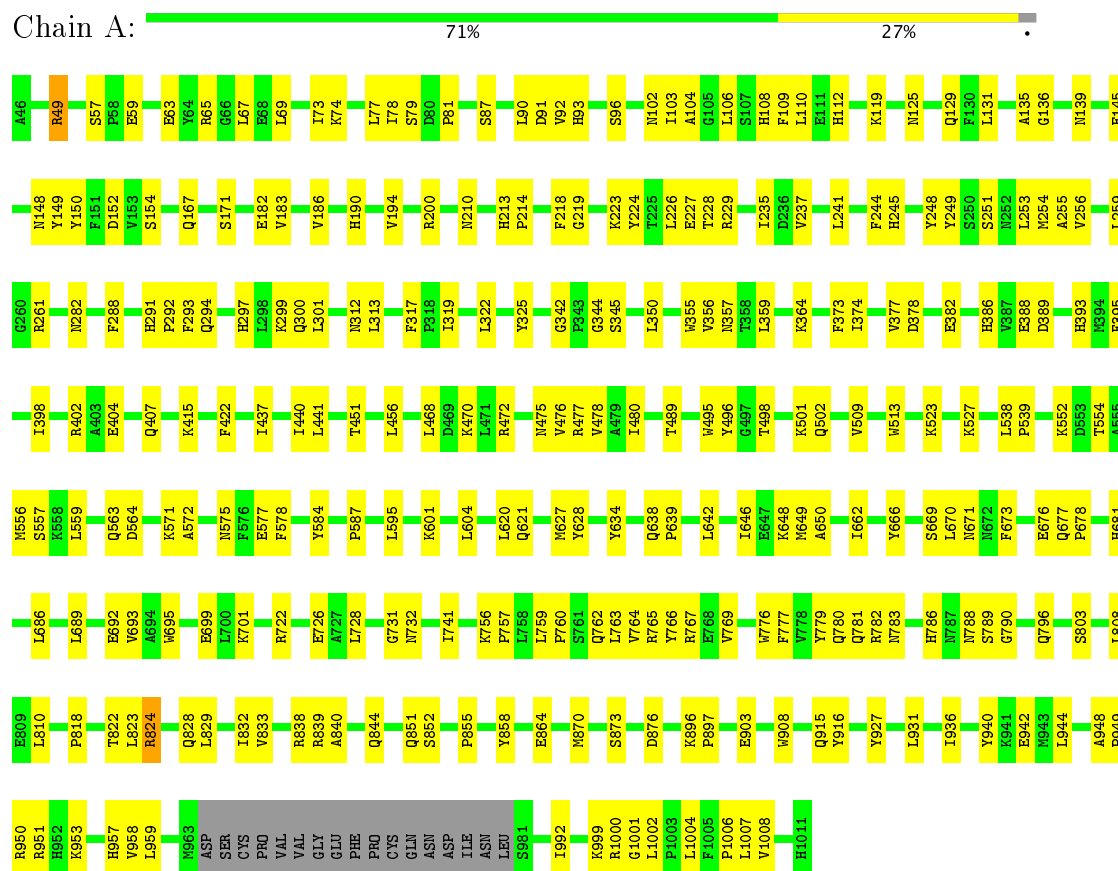
There are 22 discrepancies between the modelled and reference sequences:

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

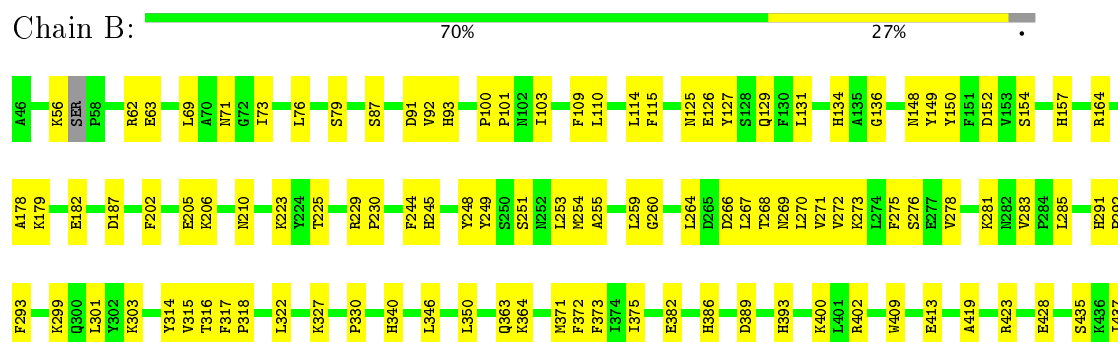
3 Residue-property plots

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



V958	F834	V707	F568	V449
L959	L346	R711	K571	L450
E962	I349	L712	A572	E457
MET	I850	H724	N573	E458
ASP	Q851	L725	L574	
SER		E726	N575	P461
CYS	P855	A727	F576	
PRO	P856	L728	E577	I464
VAL	H857		F578	
VAL	Y858	G731	F579	L468
GLY		N732		D469
GLU	F866		D586	
GLU		Q743	P587	R472
PHE	M870		L588	P473
PRO		E746	H589	E474
CYS	S873	D747	N475	N475
GLN		T748	V476	V476
ASN	Q883	L749	M592	R477
ASP			Y596	V478
ILE	I886	L758	L600	A479
ASN	Q887	L759	K601	I480
LEU	A888			
GLN		V764	L604	T489
ALA	R892	R765	M605	
PRO	R893	Y766	A608	I505
ALA	L894			
LEU	D895	W776	A611	E508
PRO	K896			V509
GLN		Q780	L616	I510
P989	L900	Q781	D619	Q514
		R782	L620	F522
K999	E903	N783	T623	
R1000	S904	E784	I624	P530
G1001	A905		Y625	
L1002	K906	N788	G626	I537
P1003		S789	M627	L538
L1004	F918	G790	Y628	
	V925	Y795	L629	Y547
L1007	A926		S630	P546
	Y927	D798	G633	A549
			Y634	L550
	L931	S803	I551	K552
	E934	E804	D553	T554
	I937	L810	Q638	
		I815	L642	S557
	Y940		M649	K558
	M943	T822	P678	L559
	L944	L823		I560
		R824	E592	F561
		T825	D706	K562
	R950	K826		Q563
		E827		D564
	K953	I832		
	H957	W833		

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24425	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 ($e^-/\text{\AA}^2$)	7.9, 6.8	Depositor
Minimum defocus (nm)	940	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	46598	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	0.39	0/7942	0.65	0/10744
1	B	0.39	0/7853	0.64	0/10620
All	All	0.39	0/15795	0.65	0/21364

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

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	7748	0	7686	165	0
1	B	7662	0	7581	163	0
All	All	15410	0	15267	321	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 10.

The worst 5 of 321 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:244:PHE:O	1:B:248:TYR:HB2	1.84	0.78
1:B:419:ALA:O	1:B:423:ARG:HB2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:ARG:HG2	1:A:844:GLN:HA	1.71	0.71
1:B:245:HIS:HA	1:B:249:TYR:HB2	1.72	0.70
1:A:317:PHE:HB2	1:A:373:PHE:HB3	1.73	0.69

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	945/966 (98%)	906 (96%)	39 (4%)	0	100	100
1	B	933/966 (97%)	902 (97%)	31 (3%)	0	100	100
All	All	1878/1932 (97%)	1808 (96%)	70 (4%)	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	840/861 (98%)	833 (99%)	7 (1%)	85	92
1	B	828/861 (96%)	824 (100%)	4 (0%)	91	95
All	All	1668/1722 (97%)	1657 (99%)	11 (1%)	87	93

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	732	ASN
1	A	824	ARG
1	B	649	MET
1	A	649	MET
1	B	56	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	502	GLN
1	A	575	ASN
1	A	844	GLN
1	A	300	GLN
1	A	762	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](#)

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.