



wwPDB X-ray Structure Validation Summary Report i

Sep 30, 2014 – 04:56 PM EDT

PDB ID : 4M1C
Title : Crystal Structure Analysis of Fab-Bound Human Insulin Degrading Enzyme (IDE) in Complex with Amyloid-Beta (1-40)
Authors : McCord, L.M.; Liang, W.; Farcasanu, M.; Scherpelz, K.; Meredith, S.C.; Koide, S.; Tang, W.J.
Deposited on : 2013-08-02
Resolution : 3.50 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

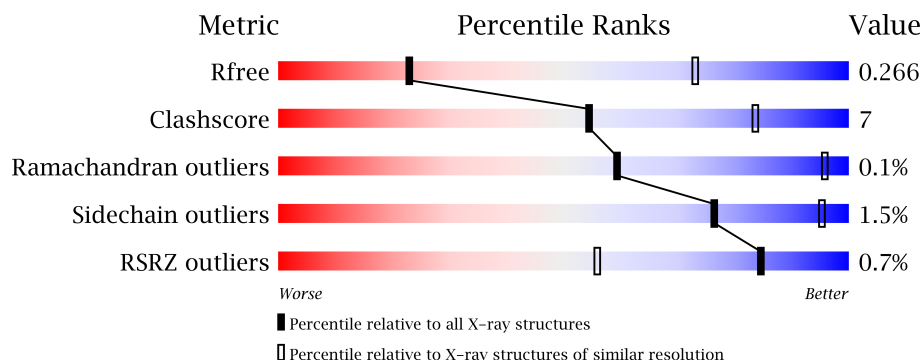
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable23828
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23828

1 Overall quality at a glance

The reported resolution of this entry is 3.50 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))
R_{free}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	990	
1	B	990	
2	C	263	
2	E	263	
3	D	239	
3	F	239	
4	G	40	
4	H	40	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21509 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	957	Total	C	N	O	S	0	0	0
			7779	5014	1309	1434	22			
1	B	952	Total	C	N	O	S	0	0	0
			7745	4992	1301	1430	22			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	EXPRESSION TAG	UNP P14735
A	31	HIS	-	EXPRESSION TAG	UNP P14735
A	32	HIS	-	EXPRESSION TAG	UNP P14735
A	33	HIS	-	EXPRESSION TAG	UNP P14735
A	34	HIS	-	EXPRESSION TAG	UNP P14735
A	35	HIS	-	EXPRESSION TAG	UNP P14735
A	36	HIS	-	EXPRESSION TAG	UNP P14735
A	37	ALA	-	EXPRESSION TAG	UNP P14735
A	38	ALA	-	EXPRESSION TAG	UNP P14735
A	39	GLY	-	EXPRESSION TAG	UNP P14735
A	40	ILE	-	EXPRESSION TAG	UNP P14735
A	41	PRO	-	EXPRESSION TAG	UNP P14735
A	110	LEU	CYS	ENGINEERED MUTATION	UNP P14735
A	111	GLN	GLU	ENGINEERED MUTATION	UNP P14735
A	171	SER	CYS	ENGINEERED MUTATION	UNP P14735
A	178	ALA	CYS	ENGINEERED MUTATION	UNP P14735
A	257	VAL	CYS	ENGINEERED MUTATION	UNP P14735
A	414	LEU	CYS	ENGINEERED MUTATION	UNP P14735
A	573	ASN	CYS	ENGINEERED MUTATION	UNP P14735
A	590	SER	CYS	ENGINEERED MUTATION	UNP P14735
A	789	SER	CYS	ENGINEERED MUTATION	UNP P14735
A	812	ALA	CYS	ENGINEERED MUTATION	UNP P14735
A	819	ALA	CYS	ENGINEERED MUTATION	UNP P14735
A	904	SER	CYS	ENGINEERED MUTATION	UNP P14735
A	966	ASN	CYS	ENGINEERED MUTATION	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
A	974	ALA	CYS	ENGINEERED MUTATION	UNP P14735
B	30	MET	-	EXPRESSION TAG	UNP P14735
B	31	HIS	-	EXPRESSION TAG	UNP P14735
B	32	HIS	-	EXPRESSION TAG	UNP P14735
B	33	HIS	-	EXPRESSION TAG	UNP P14735
B	34	HIS	-	EXPRESSION TAG	UNP P14735
B	35	HIS	-	EXPRESSION TAG	UNP P14735
B	36	HIS	-	EXPRESSION TAG	UNP P14735
B	37	ALA	-	EXPRESSION TAG	UNP P14735
B	38	ALA	-	EXPRESSION TAG	UNP P14735
B	39	GLY	-	EXPRESSION TAG	UNP P14735
B	40	ILE	-	EXPRESSION TAG	UNP P14735
B	41	PRO	-	EXPRESSION TAG	UNP P14735
B	110	LEU	CYS	ENGINEERED MUTATION	UNP P14735
B	111	GLN	GLU	ENGINEERED MUTATION	UNP P14735
B	171	SER	CYS	ENGINEERED MUTATION	UNP P14735
B	178	ALA	CYS	ENGINEERED MUTATION	UNP P14735
B	257	VAL	CYS	ENGINEERED MUTATION	UNP P14735
B	414	LEU	CYS	ENGINEERED MUTATION	UNP P14735
B	573	ASN	CYS	ENGINEERED MUTATION	UNP P14735
B	590	SER	CYS	ENGINEERED MUTATION	UNP P14735
B	789	SER	CYS	ENGINEERED MUTATION	UNP P14735
B	812	ALA	CYS	ENGINEERED MUTATION	UNP P14735
B	819	ALA	CYS	ENGINEERED MUTATION	UNP P14735
B	904	SER	CYS	ENGINEERED MUTATION	UNP P14735
B	966	ASN	CYS	ENGINEERED MUTATION	UNP P14735
B	974	ALA	CYS	ENGINEERED MUTATION	UNP P14735

- Molecule 2 is a protein called Fab-bound IDE, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	205	Total	C	N	O	S	0	0	0
			1562	999	256	300	7			
2	E	206	Total	C	N	O	S	0	0	0
			1567	999	258	303	7			

- Molecule 3 is a protein called Fab-bound IDE, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	175	Total	C	N	O	S	0	0	0
			1339	846	220	269	4			

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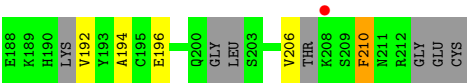
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	184	Total	C	N	O	S	0	0	0
			1409	883	237	284	5			

- Molecule 4 is a protein called Amyloid beta A4 protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	10	Total	C	N	O	0	0	0
			84	59	11	14			
4	H	3	Total	C	N	O	0	0	0
			22	12	3	7			

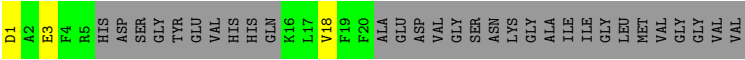
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	A	1	Total	Zn	0	0
			1	1		



- Molecule 4: Amyloid beta A4 protein

Chain G:



- Molecule 4: Amyloid beta A4 protein

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.58Å 135.32Å 368.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.06 – 3.50 49.84 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.2 (49.06-3.50) 92.7 (49.84-3.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.42 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.228 , 0.270 0.225 , 0.266	Depositor DCC
R_{free} test set	1909 reflections (5.59%)	DCC
Wilson B-factor (Å ²)	77.8	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 0.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 35539 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	21509	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.22	0/7974	0.37	1/10793 (0.0%)
1	B	0.23	0/7938	0.38	1/10743 (0.0%)
2	C	0.20	0/1602	0.40	1/2179 (0.0%)
2	E	0.21	0/1605	0.39	0/2180
3	D	0.22	0/1362	0.44	0/1839
3	F	0.23	0/1433	0.41	0/1931
4	G	0.26	0/85	0.34	0/111
4	H	0.18	0/21	0.32	0/27
All	All	0.22	0/22020	0.39	3/29803 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457	GLU	N-CA-C	5.98	127.16	111.00
2	C	43	LYS	N-CA-CB	5.80	121.04	110.60
1	B	564	ASP	CB-CA-C	-5.01	100.37	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7779	0	7689	92	0
1	B	7745	0	7654	99	0
2	C	1562	0	1501	34	0
2	E	1567	0	1503	38	0
3	D	1339	0	1306	11	0
3	F	1409	0	1351	21	0
4	G	84	0	78	2	0
4	H	22	0	17	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	21509	0	21099	289	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 289 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:510:ILE:O	1:B:514:GLN:HG3	1.65	0.97
1:B:862:ARG:HH12	1:B:981:SER:HB2	1.38	0.87
1:B:510:ILE:HG22	1:B:514:GLN:HE21	1.47	0.79
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.71	0.73
1:A:429:ARG:HD3	1:A:898:LYS:HE2	1.71	0.73

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	951/990 (96%)	926 (97%)	23 (2%)	2 (0%)	56	94
1	B	946/990 (96%)	917 (97%)	29 (3%)	0	100	100
2	C	191/263 (73%)	183 (96%)	8 (4%)	0	100	100
2	E	192/263 (73%)	182 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	156/239 (65%)	147 (94%)	9 (6%)	0	100	100
3	F	164/239 (69%)	156 (95%)	8 (5%)	0	100	100
4	G	6/40 (15%)	5 (83%)	1 (17%)	0	100	100
4	H	1/40 (2%)	1 (100%)	0	0	100	100
All	All	2607/3064 (85%)	2517 (96%)	88 (3%)	2 (0%)	59	96

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	570	PRO
1	A	172	PRO

5.3.2 Protein sidechains ⓘ

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	840/879 (96%)	835 (99%)	5 (1%)	92	98
1	B	837/879 (95%)	826 (99%)	11 (1%)	80	96
2	C	172/220 (78%)	165 (96%)	7 (4%)	41	84
2	E	173/220 (79%)	170 (98%)	3 (2%)	73	94
3	D	157/210 (75%)	154 (98%)	3 (2%)	69	93
3	F	162/210 (77%)	157 (97%)	5 (3%)	52	90
4	G	8/31 (26%)	7 (88%)	1 (12%)	7	35
4	H	2/31 (6%)	2 (100%)	0	100	100
All	All	2351/2680 (88%)	2316 (98%)	35 (2%)	76	95

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	959	LEU
2	C	48	VAL
3	F	192	VAL
2	C	11	LEU

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Mol	Chain	Res	Type
2	C	12	VAL

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

Mol	Chain	Res	Type
1	B	514	GLN
1	B	515	ASN
1	B	677	GLN
2	C	77	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	957/990 (96%)	-0.05	1 (0%) 93 84	50, 73, 96, 117	0
1	B	952/990 (96%)	-0.04	0 100 100	48, 68, 88, 107	0
2	C	205/263 (77%)	0.33	2 (0%) 79 47	74, 104, 124, 136	0
2	E	206/263 (78%)	0.33	6 (2%) 49 23	69, 92, 114, 126	0
3	D	175/239 (73%)	0.44	9 (5%) 27 11	77, 102, 132, 143	0
3	F	184/239 (76%)	0.25	1 (0%) 88 64	71, 94, 117, 128	0
4	G	10/40 (25%)	0.23	0 100 100	81, 97, 109, 110	0
4	H	3/40 (7%)	0.10	0 100 100	74, 74, 96, 98	0
All	All	2692/3064 (87%)	0.07	19 (0%) 84 56	48, 76, 113, 143	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	153	ALA	3.0
2	E	130	ALA	2.9
3	D	109	ARG	2.8
2	E	131	SER	2.6
3	D	181	THR	2.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	ZN	A	1101	1/1	0.12	-1.87	68,68,68,68	0
5	ZN	B	2001	1/1	0.08	-2.62	59,59,59,59	0

6.5 Other polymers

There are no such residues in this entry.