



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 05:02 pm BST

PDB ID : 5UOE
Title : Crystal Structure Analysis of Elbow-Engineered-Fab-Bound Human Insulin
Degrading Enzyme (IDE)
Authors : Liang, W.G.; Bailey, L.; Kossiakoff, T.; Tang, W.J.
Deposited on : 2017-01-31
Resolution : 3.80 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

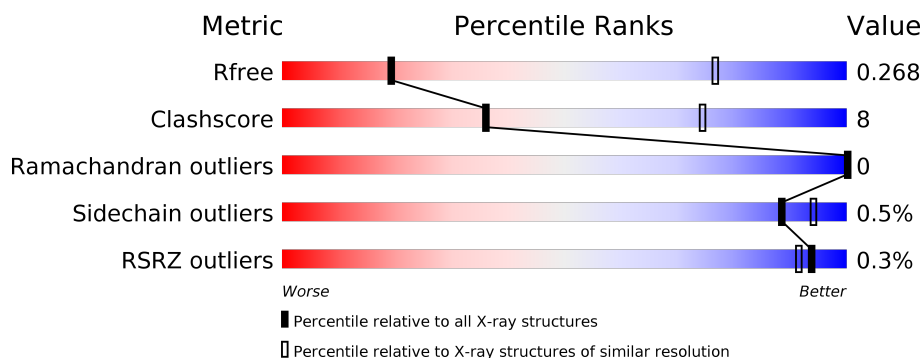
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	990	
1	B	990	
1	C	990	
1	D	990	
1	E	990	
2	H	229	

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Mol	Chain	Length	Quality of chain
2	M	229	 37% 14% 49%
2	P	229	 32% 19% 48%
2	S	229	 43% 8% 49%
2	V	229	 39% 12% 49%
3	L	215	 40% 10% 50%
3	N	215	 41% 9% 49%
3	Q	215	 37% 13% 50%
3	T	215	 34% 14% 50%
3	W	215	 34% 14% 51%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 47331 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.

- Molecule 1 is a protein called Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	953	Total	C	N	O	S	0	0	0
			7762	5003	1302	1435	22			
1	B	952	Total	C	N	O	S	0	0	0
			7752	4997	1303	1430	22			
1	C	953	Total	C	N	O	S	0	0	0
			7770	5009	1308	1431	22			
1	D	953	Total	C	N	O	S	0	0	0
			7764	5006	1307	1429	22			
1	E	953	Total	C	N	O	S	0	0	0
			7764	5006	1307	1429	22			

There are 125 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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	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
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B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735
C	30	MET	-	expression tag	UNP P14735
C	31	HIS	-	expression tag	UNP P14735
C	32	HIS	-	expression tag	UNP P14735
C	33	HIS	-	expression tag	UNP P14735
C	34	HIS	-	expression tag	UNP P14735
C	35	HIS	-	expression tag	UNP P14735
C	36	HIS	-	expression tag	UNP P14735
C	37	ALA	-	expression tag	UNP P14735
C	38	ALA	-	expression tag	UNP P14735
C	39	GLY	-	expression tag	UNP P14735
C	40	ILE	-	expression tag	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
C	41	PRO	-	expression tag	UNP P14735
C	110	LEU	CYS	engineered mutation	UNP P14735
C	171	SER	CYS	engineered mutation	UNP P14735
C	178	ALA	CYS	engineered mutation	UNP P14735
C	257	VAL	CYS	engineered mutation	UNP P14735
C	414	LEU	CYS	engineered mutation	UNP P14735
C	573	ASN	CYS	engineered mutation	UNP P14735
C	590	SER	CYS	engineered mutation	UNP P14735
C	789	SER	CYS	engineered mutation	UNP P14735
C	812	ALA	CYS	engineered mutation	UNP P14735
C	819	ALA	CYS	engineered mutation	UNP P14735
C	904	SER	CYS	engineered mutation	UNP P14735
C	966	ASN	CYS	engineered mutation	UNP P14735
C	974	ALA	CYS	engineered mutation	UNP P14735
D	30	MET	-	expression tag	UNP P14735
D	31	HIS	-	expression tag	UNP P14735
D	32	HIS	-	expression tag	UNP P14735
D	33	HIS	-	expression tag	UNP P14735
D	34	HIS	-	expression tag	UNP P14735
D	35	HIS	-	expression tag	UNP P14735
D	36	HIS	-	expression tag	UNP P14735
D	37	ALA	-	expression tag	UNP P14735
D	38	ALA	-	expression tag	UNP P14735
D	39	GLY	-	expression tag	UNP P14735
D	40	ILE	-	expression tag	UNP P14735
D	41	PRO	-	expression tag	UNP P14735
D	110	LEU	CYS	engineered mutation	UNP P14735
D	171	SER	CYS	engineered mutation	UNP P14735
D	178	ALA	CYS	engineered mutation	UNP P14735
D	257	VAL	CYS	engineered mutation	UNP P14735
D	414	LEU	CYS	engineered mutation	UNP P14735
D	573	ASN	CYS	engineered mutation	UNP P14735
D	590	SER	CYS	engineered mutation	UNP P14735
D	789	SER	CYS	engineered mutation	UNP P14735
D	812	ALA	CYS	engineered mutation	UNP P14735
D	819	ALA	CYS	engineered mutation	UNP P14735
D	904	SER	CYS	engineered mutation	UNP P14735
D	966	ASN	CYS	engineered mutation	UNP P14735
D	974	ALA	CYS	engineered mutation	UNP P14735
E	30	MET	-	expression tag	UNP P14735
E	31	HIS	-	expression tag	UNP P14735
E	32	HIS	-	expression tag	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
E	33	HIS	-	expression tag	UNP P14735
E	34	HIS	-	expression tag	UNP P14735
E	35	HIS	-	expression tag	UNP P14735
E	36	HIS	-	expression tag	UNP P14735
E	37	ALA	-	expression tag	UNP P14735
E	38	ALA	-	expression tag	UNP P14735
E	39	GLY	-	expression tag	UNP P14735
E	40	ILE	-	expression tag	UNP P14735
E	41	PRO	-	expression tag	UNP P14735
E	110	LEU	CYS	engineered mutation	UNP P14735
E	171	SER	CYS	engineered mutation	UNP P14735
E	178	ALA	CYS	engineered mutation	UNP P14735
E	257	VAL	CYS	engineered mutation	UNP P14735
E	414	LEU	CYS	engineered mutation	UNP P14735
E	573	ASN	CYS	engineered mutation	UNP P14735
E	590	SER	CYS	engineered mutation	UNP P14735
E	789	SER	CYS	engineered mutation	UNP P14735
E	812	ALA	CYS	engineered mutation	UNP P14735
E	819	ALA	CYS	engineered mutation	UNP P14735
E	904	SER	CYS	engineered mutation	UNP P14735
E	966	ASN	CYS	engineered mutation	UNP P14735
E	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is a protein called FAB Heavy chain with engineered elbow.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	119	Total	C	N	O	S	0	0	0
			901	568	153	177	3			
2	M	117	Total	C	N	O	S	0	0	0
			882	555	150	174	3			
2	P	118	Total	C	N	O	S	0	0	0
			893	564	151	175	3			
2	S	117	Total	C	N	O	S	0	0	0
			882	555	150	174	3			
2	V	117	Total	C	N	O	S	0	0	0
			881	555	150	173	3			

- Molecule 3 is a protein called FAB light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	108	Total	C	N	O	S	0	0	0
			820	516	136	165	3			

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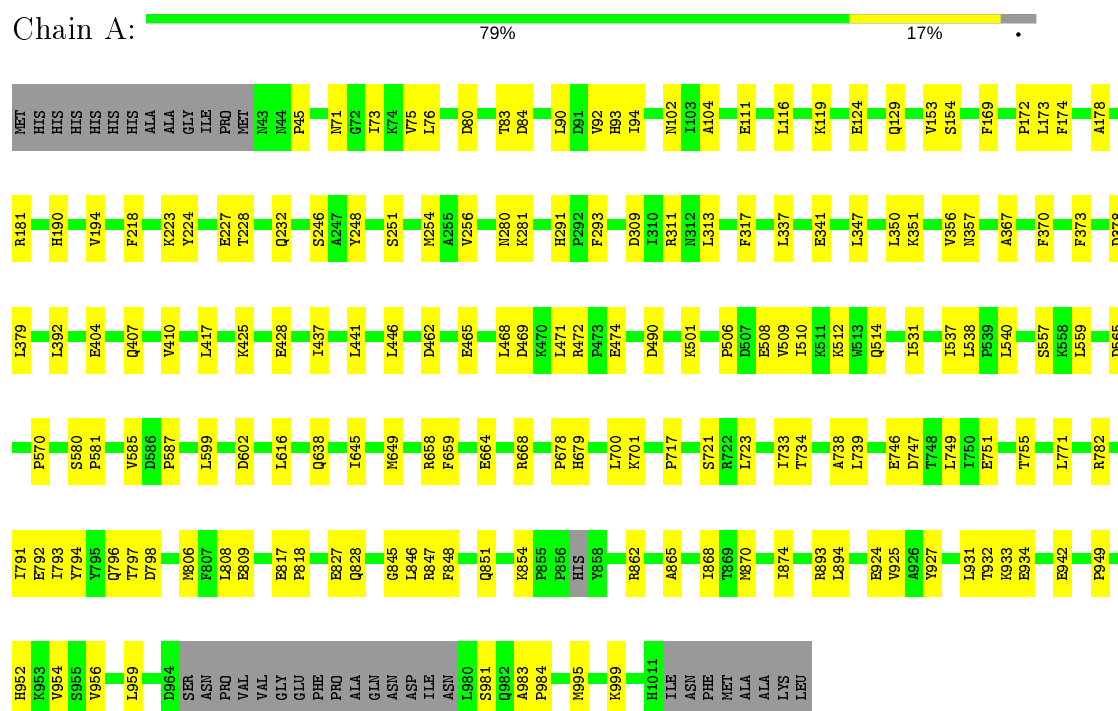
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	109	Total	C	N	O	S	0	0	0
			827	520	137	167	3			
3	Q	108	Total	C	N	O	S	0	0	0
			820	516	136	165	3			
3	T	107	Total	C	N	O	S	0	0	0
			815	513	135	164	3			
3	W	105	Total	C	N	O	S	0	0	0
			798	501	132	162	3			

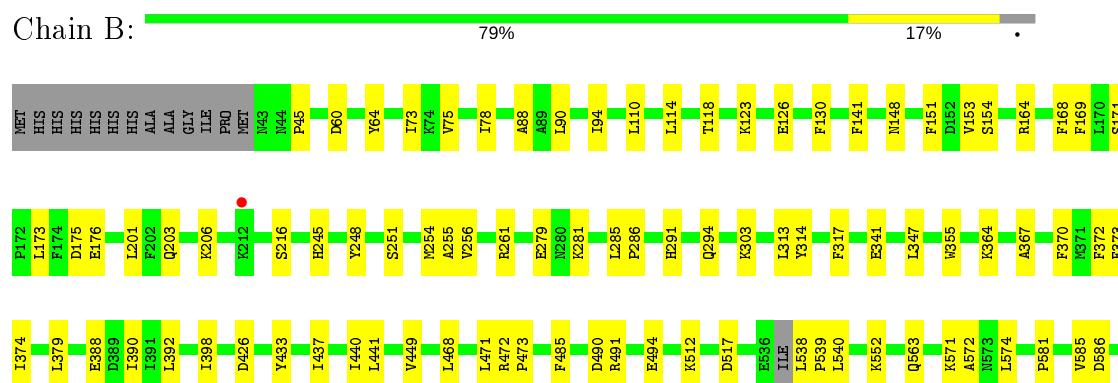
3 Residue-property plots

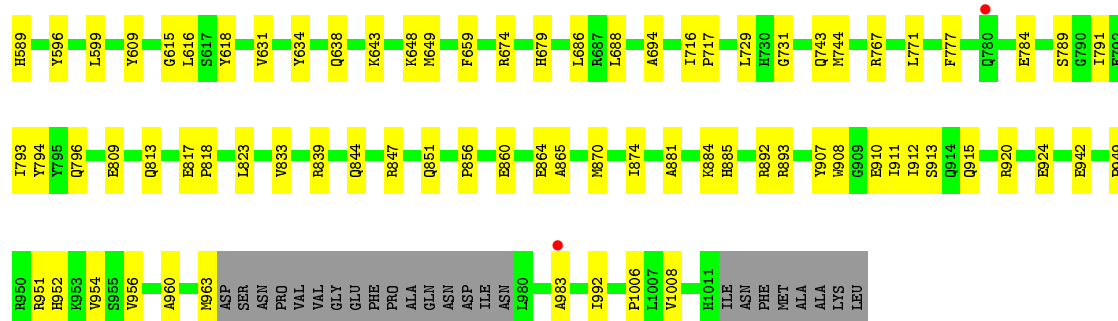
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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



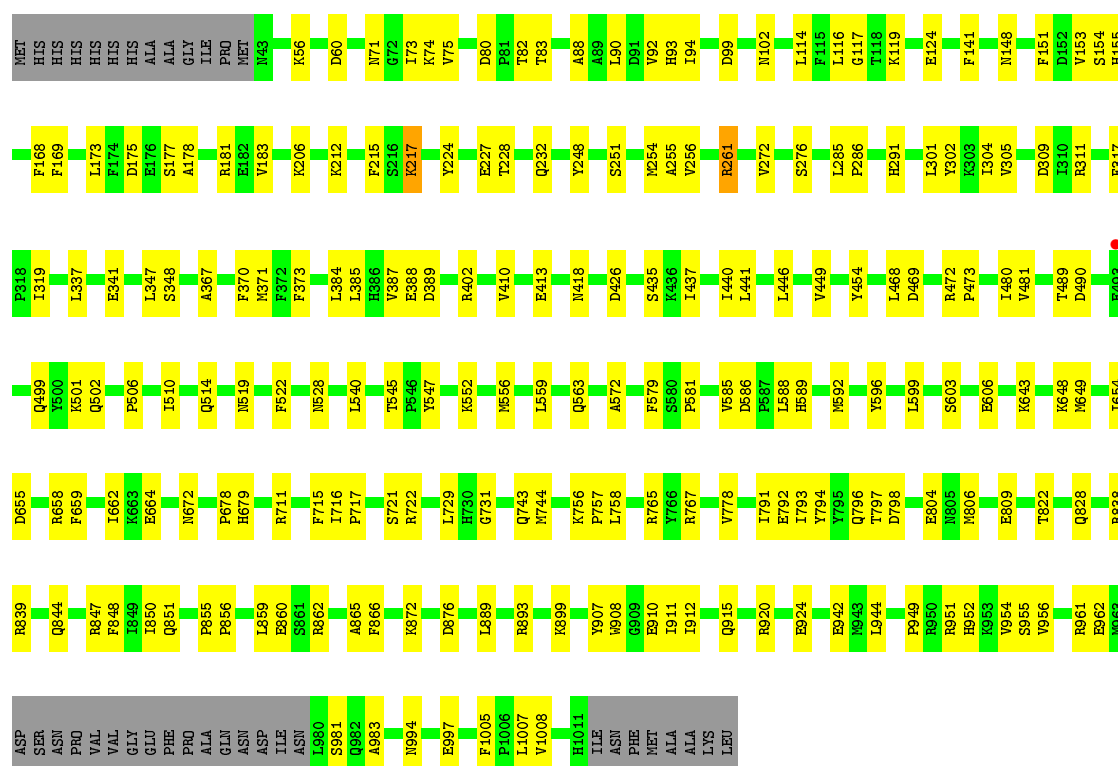
- Molecule 1: Insulin-degrading enzyme





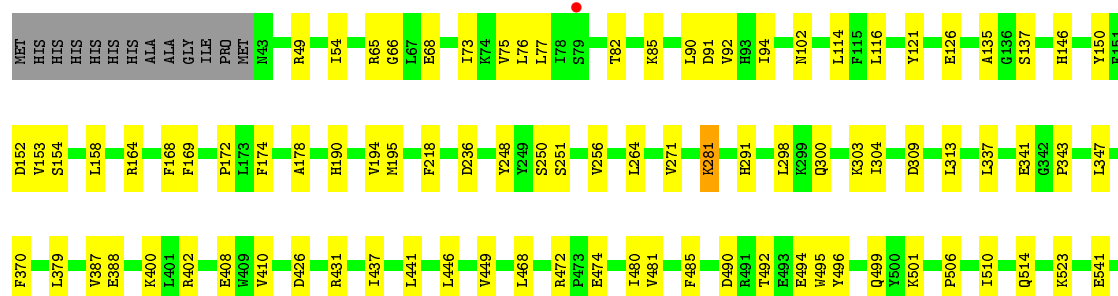
• Molecule 1: Insulin-degrading enzyme

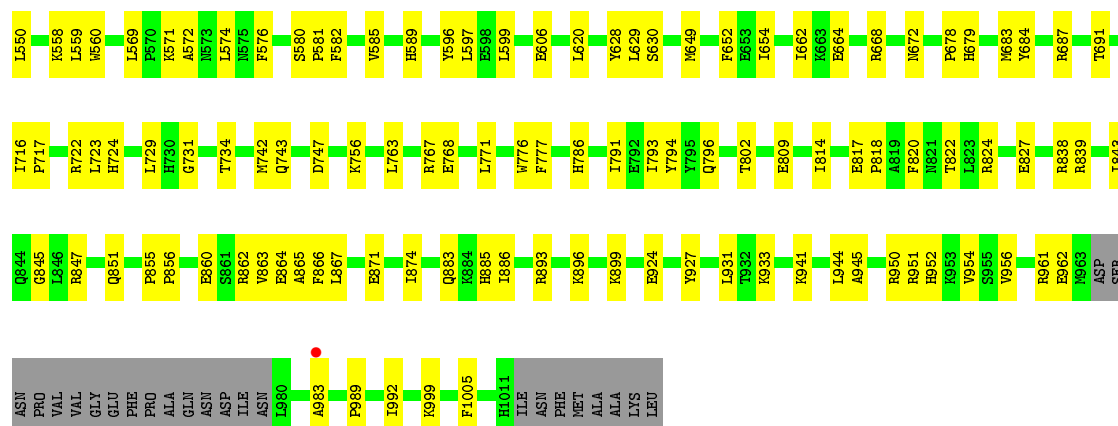
Chain C: 75% 21% .



• Molecule 1: Insulin-degrading enzyme

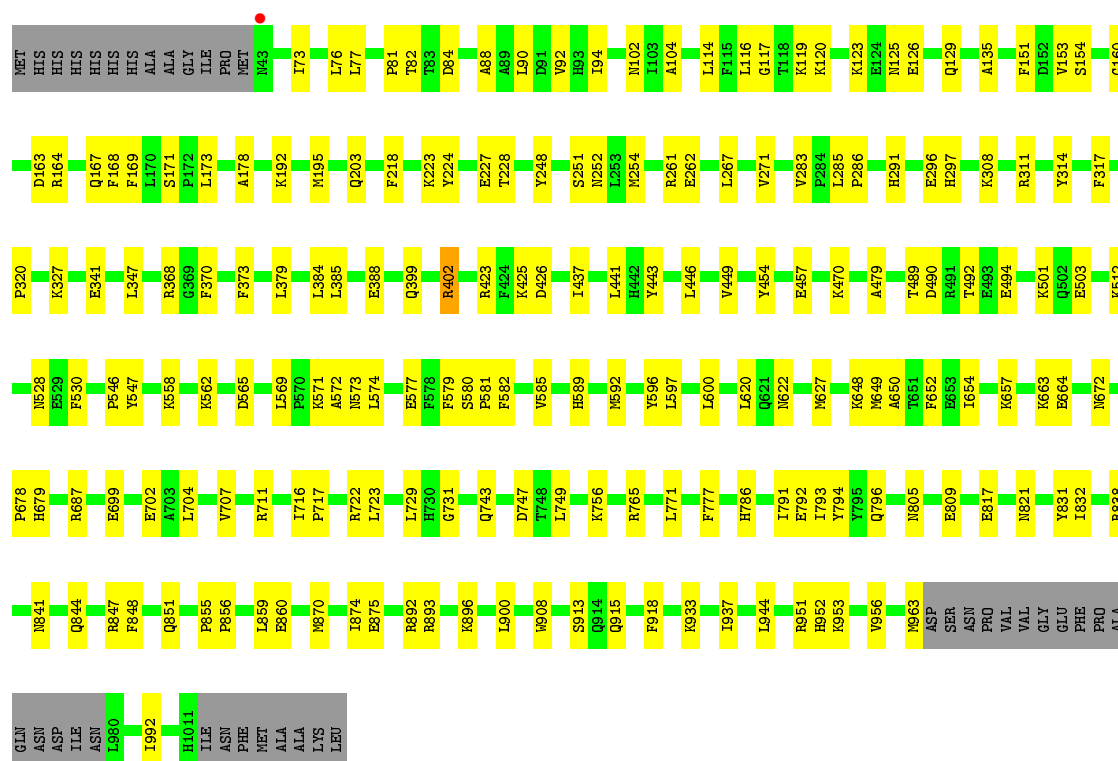
Chain D: 76% 20% .





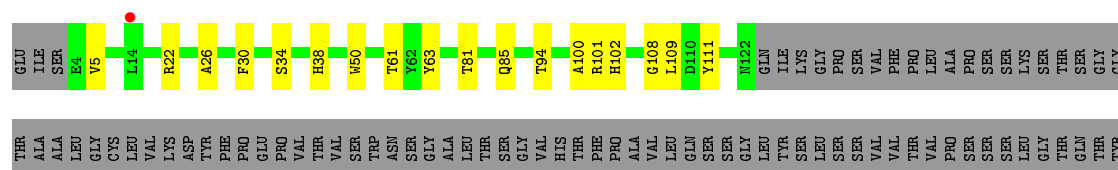
• Molecule 1: Insulin-degrading enzyme

Chain E: 77% 19%



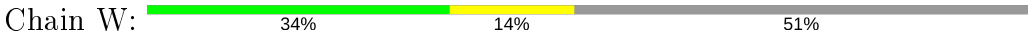
• Molecule 2: FAB Heavy chain with engineered elbow

Chain H: 44% 8% 48%



ALA	ALA	THR	PRO	SER	SER	VAL	PHE	PHE	PRO	PRO	SER	SER	ASP	SER	SER	GLN	LEU	LYS	SER	GLY	THR	ALA	ALA	SER	VAL	VAL	VAL	CYS	LEU	LEU	ASN	ASN	PHE	PRO	TYR	PRO	ARG	GLU	ALA	LYS	VAL	GLN	LYS	TRP	SER	LYS	VAL	ASP	ASN	ALA	LEU	GLN	SER	GLY	ASN	SER	GLN	GLU	THR	THR	GLN	GLU	ASP	SER	LYS	ASP
SER	THR	TYR	SER	SER	SER	LEU	SER	THR	LEU	THR	LEU	SER	LYS	ASP	LYS	ALA	ASP	TYR	GLY	LYS	HIS	LYS	VAL	VAL	THR	HIS	GLN	CYS	GLU	VAL	THR	HIS	GLN	GLY	LEU	SER	SER	SER	PRO	VAL	VAL	THR	THR	LYS	SER	PHE	ASN	ARG	GLY	GLU	CYS															

● Molecule 3: FAB light chain



THR	TYR	SER	LEU	SER	SER	THR	LEU	LEU	THR	LEU	SER	LYS	ALA	ASP	THR	GLY	HIS	LYS	VAL	TYR	CYS	GLU	VAL	THR	HIS	GLN	GLY	LEU	SER	SER	PRO	SER	VAL	THR	LYS	TRP	LYS	VAL	ASN	ARG	GLY	GLU	CYS																			
ALA	PRO	SER	VAL	PHE	ILE	PHE	PRO	PRO	SER	ASP	SER	GLN	LEU	LYS	SER	GLY	THR	ALA	SER	VAL	VAL	CYS	LEU	LEU	ASN	ASN	PHE	TYR	PRO	ARG	GLU	ALA	LYS	VAL	THR	GLN	TRP	LYS	VAL	ASP	ASN	ALA	LEU	GLN	SER	GLY	ASN	SER	GLN	GLU	SER	VAL	THR	GLU	GLN	ASP	SER	LYS	ARG	THR	VAL	ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	131.32Å 242.05Å 310.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 3.80 49.24 – 3.79	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.24-3.80) 91.4 (49.24-3.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 3.77Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.220 , 0.270 0.220 , 0.268	Depositor DCC
R_{free} test set	2000 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	69.1	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	47331	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.68% 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](#)

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	0.26	0/7955	0.42	0/10764
1	B	0.26	0/7946	0.42	0/10752
1	C	0.27	0/7965	0.43	0/10777
1	D	0.26	0/7959	0.42	0/10771
1	E	0.26	0/7959	0.42	0/10771
2	H	0.28	0/922	0.50	0/1253
2	M	0.26	0/902	0.50	0/1226
2	P	0.26	0/914	0.48	0/1242
2	S	0.26	0/902	0.47	0/1226
2	V	0.29	0/901	0.51	0/1224
3	L	0.35	0/838	0.55	1/1137 (0.1%)
3	N	0.28	0/845	0.50	0/1147
3	Q	0.35	0/838	0.53	0/1137
3	T	0.27	0/833	0.49	0/1130
3	W	0.29	0/816	0.54	0/1108
All	All	0.27	0/48495	0.44	1/65665 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	93	TYR	C-N-CA	-5.01	109.18	121.70

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	7762	0	7681	98	0
1	B	7752	0	7669	100	0
1	C	7770	0	7703	132	0
1	D	7764	0	7695	120	0
1	E	7764	0	7695	114	0
2	H	901	0	856	16	0
2	M	882	0	841	28	0
2	P	893	0	850	38	0
2	S	882	0	841	14	0
2	V	881	0	840	21	0
3	L	820	0	797	19	0
3	N	827	0	804	16	0
3	Q	820	0	797	26	0
3	T	815	0	795	29	0
3	W	798	0	771	23	0
All	All	47331	0	46635	755	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 8.

The worst 5 of 755 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:402:ARG:HG3	1:C:468:LEU:HD21	1.46	0.97
1:E:716:ILE:HB	1:E:717:PRO:HD3	1.58	0.86
3:W:3:ILE:HG13	3:W:27:SER:HB3	1.60	0.84
1:C:599:LEU:HD23	1:C:662:ILE:HD12	1.61	0.83
1:C:893:ARG:HH11	1:C:893:ARG:HG3	1.42	0.82

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.

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	947/990 (96%)	924 (98%)	23 (2%)	0	100	100
1	B	946/990 (96%)	922 (98%)	24 (2%)	0	100	100
1	C	949/990 (96%)	923 (97%)	26 (3%)	0	100	100
1	D	949/990 (96%)	926 (98%)	23 (2%)	0	100	100
1	E	949/990 (96%)	919 (97%)	30 (3%)	0	100	100
2	H	117/229 (51%)	110 (94%)	7 (6%)	0	100	100
2	M	115/229 (50%)	109 (95%)	6 (5%)	0	100	100
2	P	116/229 (51%)	110 (95%)	6 (5%)	0	100	100
2	S	115/229 (50%)	109 (95%)	6 (5%)	0	100	100
2	V	115/229 (50%)	108 (94%)	7 (6%)	0	100	100
3	L	106/215 (49%)	97 (92%)	9 (8%)	0	100	100
3	N	107/215 (50%)	103 (96%)	4 (4%)	0	100	100
3	Q	106/215 (49%)	99 (93%)	7 (7%)	0	100	100
3	T	105/215 (49%)	99 (94%)	6 (6%)	0	100	100
3	W	103/215 (48%)	96 (93%)	7 (7%)	0	100	100
All	All	5845/7170 (82%)	5654 (97%)	191 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	837 (100%)	3 (0%)	91	95
1	B	838/879 (95%)	837 (100%)	1 (0%)	93	97
1	C	841/879 (96%)	837 (100%)	4 (0%)	88	94
1	D	840/879 (96%)	838 (100%)	2 (0%)	93	97
1	E	840/879 (96%)	835 (99%)	5 (1%)	86	92
2	H	94/191 (49%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	92/191 (48%)	91 (99%)	1 (1%)	73	85
2	P	93/191 (49%)	92 (99%)	1 (1%)	73	85
2	S	92/191 (48%)	92 (100%)	0	100	100
2	V	92/191 (48%)	92 (100%)	0	100	100
3	L	93/190 (49%)	90 (97%)	3 (3%)	39	65
3	N	94/190 (50%)	92 (98%)	2 (2%)	53	74
3	Q	93/190 (49%)	92 (99%)	1 (1%)	73	85
3	T	93/190 (49%)	90 (97%)	3 (3%)	39	65
3	W	91/190 (48%)	90 (99%)	1 (1%)	73	85
All	All	5126/6300 (81%)	5099 (100%)	27 (0%)	88	94

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	648	LYS
3	L	5	MET
3	T	93	TYR
1	E	687	ARG
1	C	217	LYS

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

Mol	Chain	Res	Type
1	B	519	ASN
1	D	190	HIS
2	H	42	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 [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.

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	953/990 (96%)	-0.28	0 100 100	55, 72, 89, 121	0
1	B	952/990 (96%)	-0.18	3 (0%) 94 91	56, 76, 92, 128	0
1	C	953/990 (96%)	-0.28	1 (0%) 95 95	55, 72, 90, 117	0
1	D	953/990 (96%)	-0.20	2 (0%) 95 94	54, 77, 93, 121	0
1	E	953/990 (96%)	-0.25	1 (0%) 95 95	51, 73, 90, 120	0
2	H	119/229 (51%)	0.02	1 (0%) 86 81	64, 78, 98, 106	0
2	M	117/229 (51%)	0.24	2 (1%) 70 62	73, 92, 106, 125	0
2	P	118/229 (51%)	0.14	1 (0%) 86 81	71, 88, 105, 112	0
2	S	117/229 (51%)	0.17	1 (0%) 84 79	71, 89, 105, 116	0
2	V	117/229 (51%)	0.03	1 (0%) 84 79	70, 89, 110, 119	0
3	L	108/215 (50%)	0.08	1 (0%) 84 79	64, 77, 96, 113	0
3	N	109/215 (50%)	0.28	1 (0%) 84 79	71, 89, 103, 109	0
3	Q	108/215 (50%)	0.15	0 100 100	63, 81, 96, 100	0
3	T	107/215 (49%)	0.25	1 (0%) 84 79	64, 82, 95, 104	0
3	W	105/215 (48%)	0.20	1 (0%) 82 76	70, 85, 99, 108	0
All	All	5889/7170 (82%)	-0.16	17 (0%) 94 91	51, 76, 96, 128	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	14	LEU	3.5
2	M	20	SER	2.8
1	C	493	GLU	2.8
1	E	43	ASN	2.6
2	S	14	LEU	2.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.