



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:30 AM UTC

PDB ID : 5UOE / pdb_00005uoe
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 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

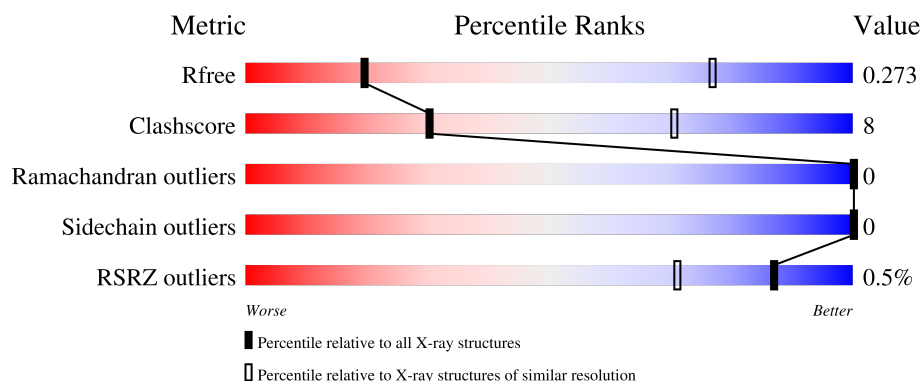
1 Overall quality at a glance

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.



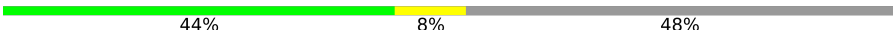
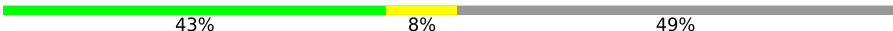
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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 of 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	 78% 18% .
1	B	990	 79% 17% .
1	C	990	 75% 21% .
1	D	990	 % 76% 20% .
1	E	990	 77% 20% .

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Mol	Chain	Length	Quality of chain
2	H	229	
2	M	229	
2	P	229	
2	S	229	
2	V	229	
3	L	215	
3	N	215	
3	Q	215	
3	T	215	
3	W	215	

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
B	819	ALA	CYS	engineered mutation	UNP P14735
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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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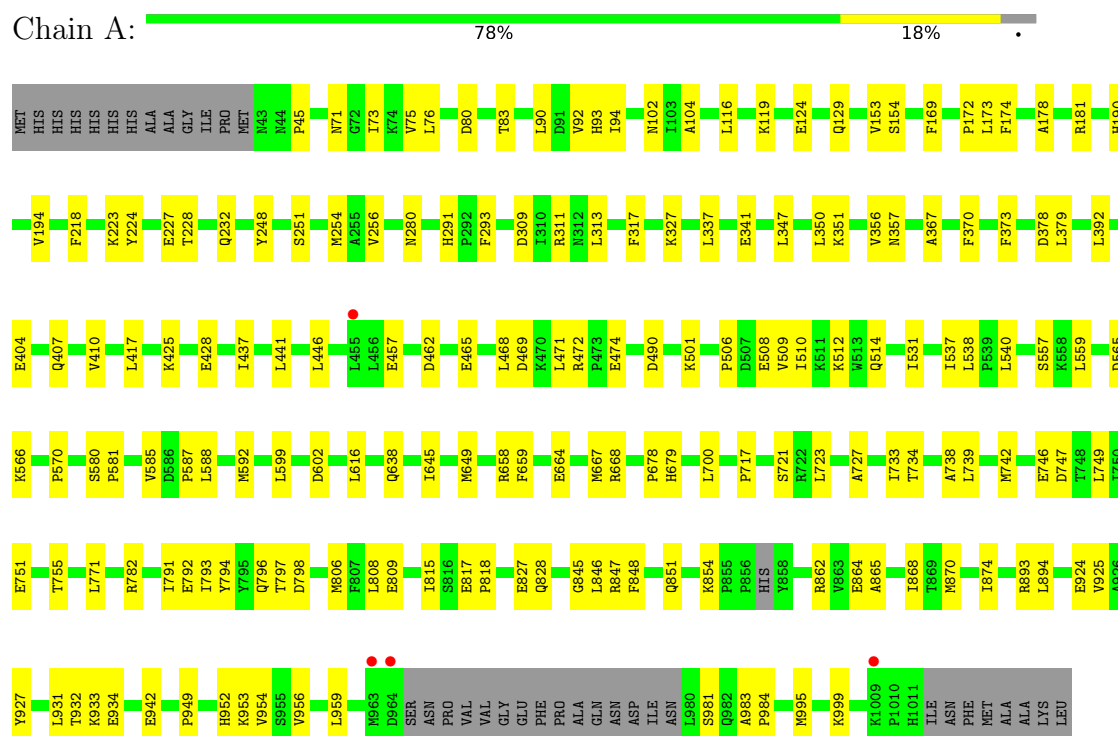
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	109	Total	C	N	O	S	0	0	0
			827	520	137	167	3			
3	Q	108	Total	C	N	O	S	0	0	0
			820	516	136	165	3			
3	T	107	Total	C	N	O	S	0	0	0
			815	513	135	164	3			
3	W	105	Total	C	N	O	S	0	0	0
			798	501	132	162	3			

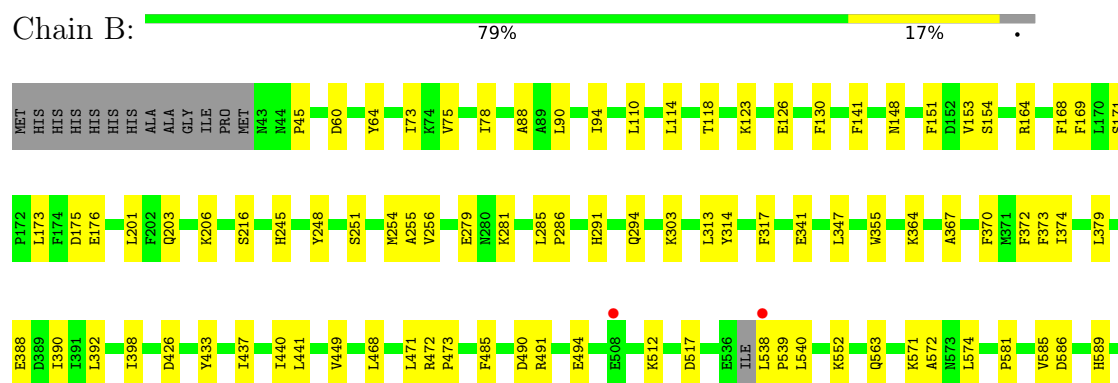
3 Residue-property plots

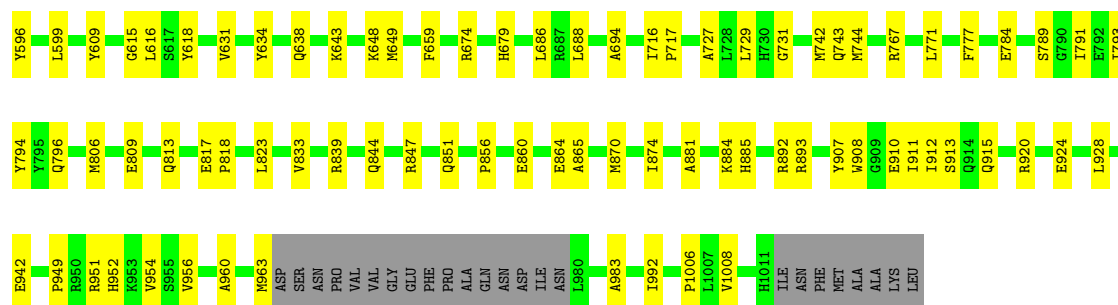
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



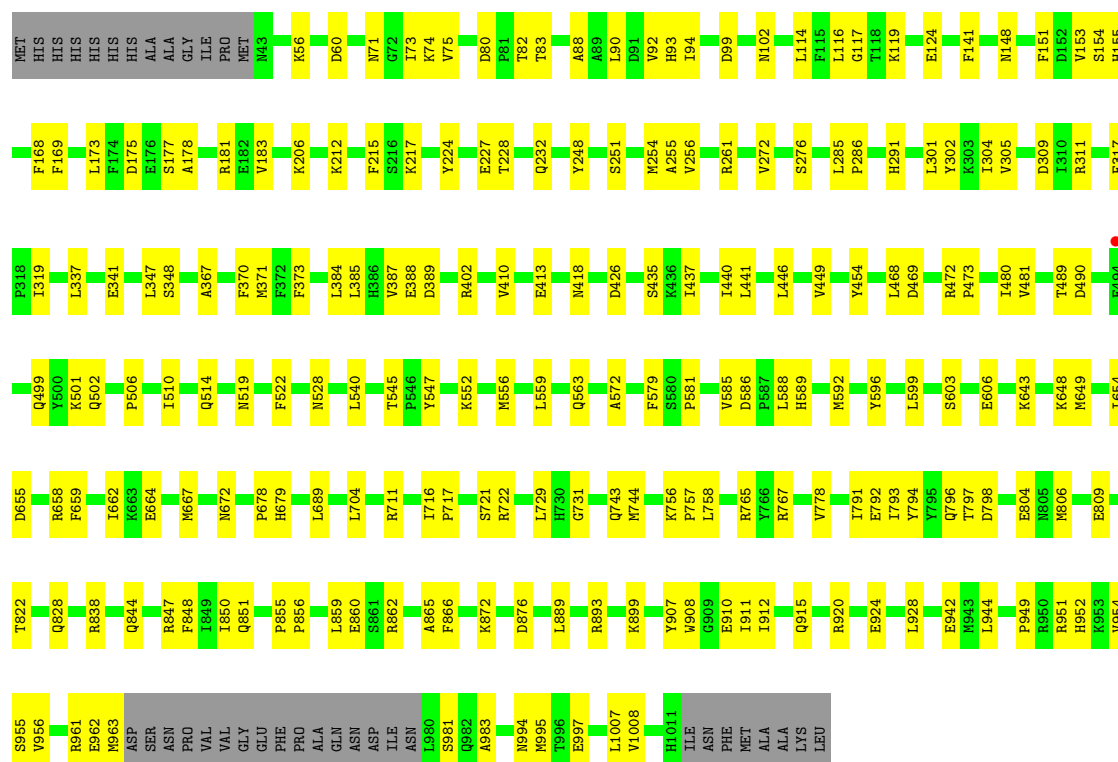
• Molecule 1: Insulin-degrading enzyme





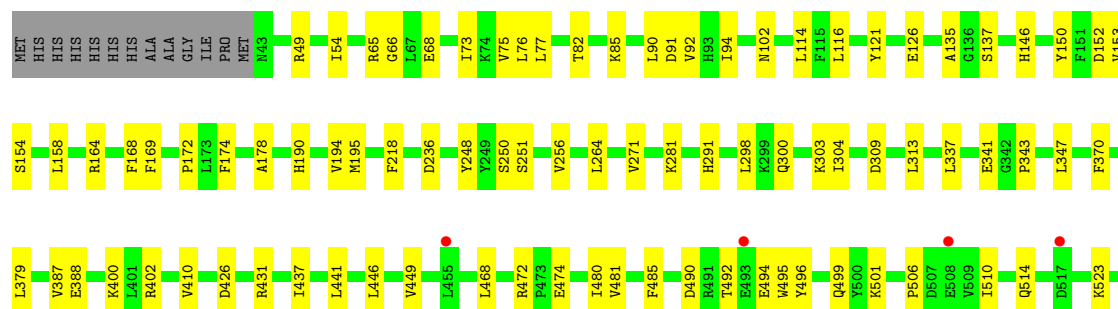
• Molecule 1: Insulin-degrading enzyme

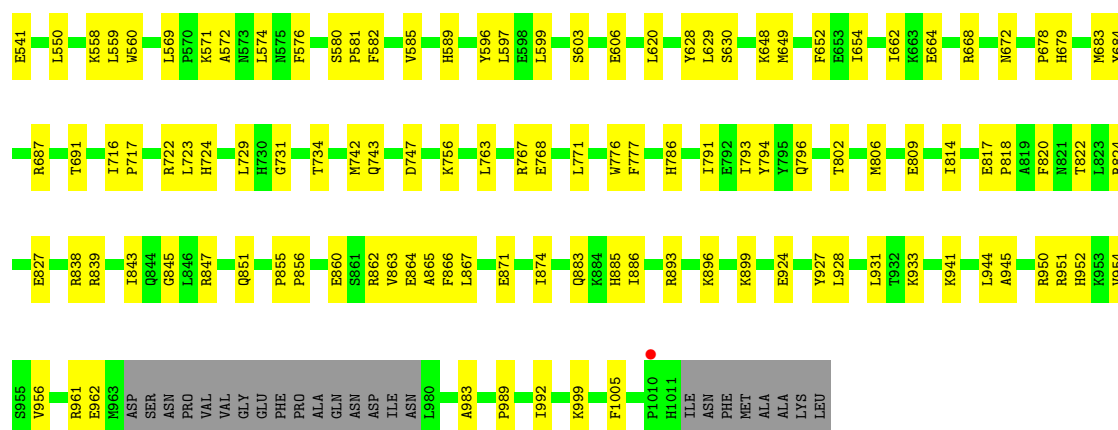
Chain C: 75% 21% .



• Molecule 1: Insulin-degrading enzyme

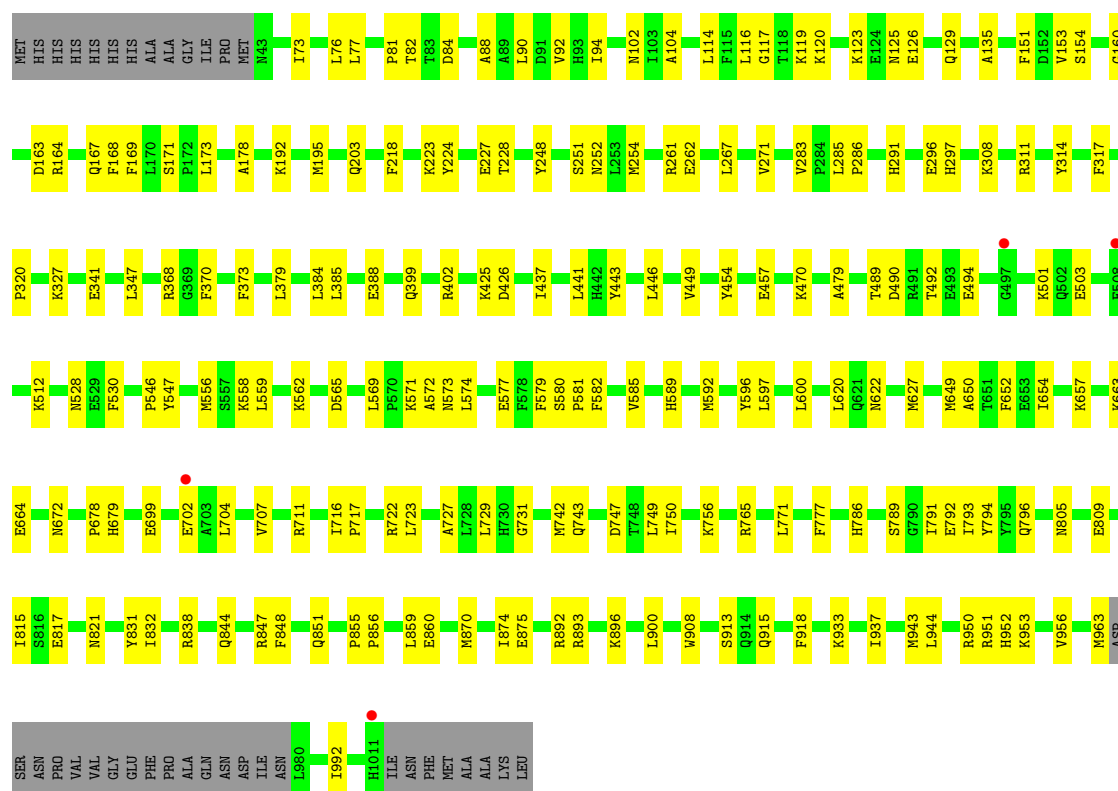
Chain D: 76% 20% .





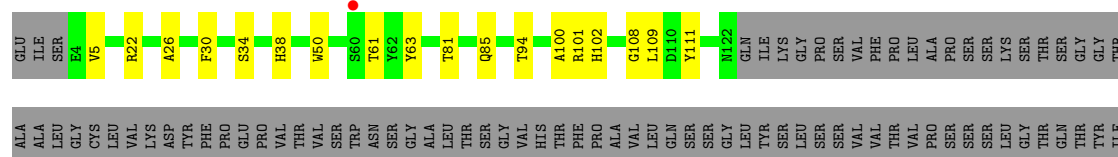
• Molecule 1: Insulin-degrading enzyme

Chain E: 77% 20% .



• Molecule 2: FAB Heavy chain with engineered elbow

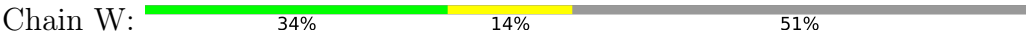
Chain H: 44% 8% 48%



GLU	ILE	SER	E4	E9	Q16	P17	I32	S35	S36	I37	P44	W50	V51	A52	S53	I54	S60	T61	Y62	Y63	V67	R70	K79	Y83	M86	L89	R90	A91	T94	A95	V96	Y97	Y98	C99	A100	R101	A107	G108	L109	T116	V120	RFE
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SER	THR	TYR	SER	LEU	SER	SER	SER	THR	THR	LEU	LEU	LEU	SER	LYS	ALA	ASP	TYR	GLU	LYS	HIS	LYS	VAL	TYR	ALA	ALA	CYS	GLU	VAL	THR	HIS	GLN	GLY	LEU	SER	SER	PRO	VAL	THR	LYS	SER	PHE	ASN	ARG	GLY	GLU	CYS
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● Molecule 3: FAB light chain



SER	D2	I3	S8	P9	L12	S15	D18	R19	I22	R25	A26	S27	Q28	A33	Y37	Q38	Q39	K40	P45	K46	S51	A52	D71	T75	L79	Q90	Q91	S92	Y93	F94	I97	T98	T103	K104	V105	E106	I107	LYS	ARG	THR	VAL	ALA	ALA
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PRO	SER	VAL	PHE	ILE	PHE	PRO	PRO	SER	ASP	SER	GLN	LEU	LYS	SER	THR	ALA	SER	VAL	VAL	CYS	LEU	LEU	ASN	ASN	PHE	TYR	PRO	ARG	GLU	ALA	S51	A52	LYS	VAL	GLN	TRP	LYS	VAL	ASP	ASN	ALA	LEU	GLN	SER	GLY	ASN	GLN	GLU	SER	VAL	THR	GLU	GLN	ASP	SER	LYS	ASP	SER	THR	ALA	ALA
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TYR	SER	LEU	SER	SER	THR	LEU	THR	LEU	SER	SER	LYS	ALA	ASP	TYR	GLU	LYS	HIS	LYS	VAL	TYR	ALA	CYS	GLU	VAL	THR	HIS	GLN	GLY	LEU	SER	SER	PRO	VAL	THR	LYS	SER	PHE	ASN	ARG	GLY	GLU	CYS
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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 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.24-3.80) 91.6 (49.24-3.80)	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 0.225 , 0.273	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)	0.31 , 36.3	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	0.13	0/7955	0.32	0/10764
1	B	0.12	0/7946	0.32	0/10752
1	C	0.15	0/7965	0.34	0/10777
1	D	0.13	0/7959	0.33	0/10771
1	E	0.13	0/7959	0.33	0/10771
2	H	0.14	0/922	0.39	0/1253
2	M	0.13	0/902	0.38	0/1226
2	P	0.13	0/914	0.39	0/1242
2	S	0.12	0/902	0.34	0/1226
2	V	0.16	0/901	0.42	0/1224
3	L	0.23	0/838	0.50	0/1137
3	N	0.16	0/845	0.43	0/1147
3	Q	0.26	0/838	0.47	0/1137
3	T	0.15	0/833	0.42	0/1130
3	W	0.21	0/816	0.44	0/1108
All	All	0.14	0/48495	0.35	0/65665

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	7762	0	7681	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7752	0	7669	104	0
1	C	7770	0	7703	138	0
1	D	7764	0	7695	122	0
1	E	7764	0	7695	121	0
2	H	901	0	856	16	0
2	M	882	0	841	28	0
2	P	893	0	850	40	0
2	S	882	0	841	14	0
2	V	881	0	840	23	0
3	L	820	0	797	19	0
3	N	827	0	804	18	0
3	Q	820	0	797	27	0
3	T	815	0	795	30	0
3	W	798	0	771	24	0
All	All	47331	0	46635	790	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 790 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:HG3	1:C:893:ARG:HH11	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%)	840 (100%)	0	100	100
1	B	838/879 (95%)	838 (100%)	0	100	100
1	C	841/879 (96%)	841 (100%)	0	100	100
1	D	840/879 (96%)	840 (100%)	0	100	100
1	E	840/879 (96%)	840 (100%)	0	100	100
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%)	92 (100%)	0	100	100
2	P	93/191 (49%)	93 (100%)	0	100	100
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%)	93 (100%)	0	100	100
3	N	94/190 (50%)	94 (100%)	0	100	100
3	Q	93/190 (49%)	93 (100%)	0	100	100
3	T	93/190 (49%)	93 (100%)	0	100	100
3	W	91/190 (48%)	91 (100%)	0	100	100
All	All	5126/6300 (81%)	5126 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	851	GLN
3	L	80	GLN
1	E	184	ASN
2	H	42	GLN
2	S	87	ASN

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 oligosaccharides 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%)	-0.04	4 (0%) 88 74	55, 72, 89, 121	0
1	B	952/990 (96%)	0.01	2 (0%) 91 81	56, 76, 92, 128	0
1	C	953/990 (96%)	-0.05	1 (0%) 92 87	55, 72, 90, 117	0
1	D	953/990 (96%)	-0.00	5 (0%) 87 71	54, 77, 93, 121	0
1	E	953/990 (96%)	-0.05	4 (0%) 88 74	51, 73, 90, 120	0
2	H	119/229 (51%)	0.16	1 (0%) 82 62	64, 78, 98, 106	0
2	M	117/229 (51%)	0.36	4 (3%) 48 33	73, 92, 106, 125	0
2	P	118/229 (51%)	0.27	1 (0%) 82 62	71, 88, 105, 112	0
2	S	117/229 (51%)	0.11	1 (0%) 81 60	71, 89, 105, 116	0
2	V	117/229 (51%)	0.27	2 (1%) 69 47	70, 89, 110, 119	0
3	L	108/215 (50%)	0.21	1 (0%) 81 60	64, 77, 96, 113	0
3	N	109/215 (50%)	0.22	2 (1%) 67 46	71, 89, 103, 109	0
3	Q	108/215 (50%)	0.07	0 100 100	63, 81, 96, 100	0
3	T	107/215 (49%)	0.11	0 100 100	64, 82, 95, 104	0
3	W	105/215 (48%)	0.28	0 100 100	70, 85, 99, 108	0
All	All	5889/7170 (82%)	0.02	28 (0%) 87 71	51, 76, 96, 128	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	93	TYR	3.5
1	C	494	GLU	3.3
1	D	1010	PRO	2.8
1	A	963	MET	2.8
2	P	36	SER	2.7

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 oligosaccharides 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.