



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:57 PM GMT

PDB ID : 4Q5Z
Title : Crystal Structure Analysis of Fab-Bound Human Insulin Degrading Enzyme (IDE) in Complex with Insulin
Authors : McCord, L.A.; Liang, W.G.; Farcasanu, M.; Wang, A.G.; Koide, S.; Tang, W.J.
Deposited on : 2014-04-18
Resolution : 3.93 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

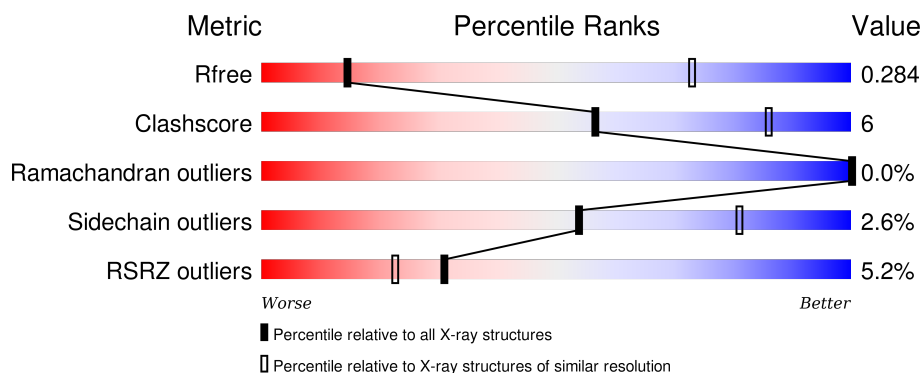
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.93 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}	91344	1007 (4.34-3.54)
Clashscore	102246	1042 (4.30-3.58)
Ramachandran outliers	100387	1000 (4.30-3.58)
Sidechain outliers	100360	1021 (4.32-3.56)
RSRZ outliers	91569	1011 (4.34-3.54)

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. 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	 2% 82% 13% • 5%
1	B	990	 % 81% 13% • •
1	C	990	 5% 79% 16% • •
1	D	990	 8% 79% 16% • •
1	E	990	 5% 80% 15% • 5%

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Mol	Chain	Length	Quality of chain
1	F	990	
1	G	990	
1	H	990	
2	I	263	
2	K	263	
2	M	263	
2	O	263	
2	Q	263	
2	S	263	
2	U	263	
2	W	263	
3	J	239	
3	L	239	
3	N	239	
3	P	239	
3	R	239	
3	T	239	
3	V	239	
3	X	239	
4	a	20	
4	b	20	
4	c	20	
4	d	20	
4	e	20	
4	f	20	

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Mol	Chain	Length	Quality of chain
4	g	20	<div><div><div>5%</div><div>35%</div><div>5%</div><div>60%</div></div></div>
4	h	20	<div><div><div>30%</div><div>5%</div><div>65%</div></div></div>
5	x	19	<div><div><div>16%</div><div>84%</div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 86673 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	941	Total	C	N	O	S	0	0	0
			7708	4971	1294	1422	21			
1	B	946	Total	C	N	O	S	0	0	0
			7754	4995	1301	1436	22			
1	C	950	Total	C	N	O	S	0	0	0
			7772	5009	1304	1437	22			
1	D	952	Total	C	N	O	S	0	0	0
			7790	5018	1307	1443	22			
1	E	942	Total	C	N	O	S	0	0	0
			7709	4967	1293	1427	22			
1	F	944	Total	C	N	O	S	0	0	0
			7735	4988	1301	1425	21			
1	G	943	Total	C	N	O	S	0	0	0
			7722	4975	1298	1427	22			
1	H	936	Total	C	N	O	S	0	0	0
			7663	4945	1288	1410	20			

There are 208 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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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
C	30	MET	-	EXPRESSION TAG	UNP P14735
C	31	HIS	-	EXPRESSION TAG	UNP P14735
C	32	HIS	-	EXPRESSION TAG	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
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
C	41	PRO	-	EXPRESSION TAG	UNP P14735
C	110	LEU	CYS	Engineered Mutation	UNP P14735
C	111	GLN	GLU	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	111	GLN	GLU	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	111	GLN	GLU	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
F	30	MET	-	EXPRESSION TAG	UNP P14735
F	31	HIS	-	EXPRESSION TAG	UNP P14735
F	32	HIS	-	EXPRESSION TAG	UNP P14735
F	33	HIS	-	EXPRESSION TAG	UNP P14735
F	34	HIS	-	EXPRESSION TAG	UNP P14735
F	35	HIS	-	EXPRESSION TAG	UNP P14735
F	36	HIS	-	EXPRESSION TAG	UNP P14735
F	37	ALA	-	EXPRESSION TAG	UNP P14735
F	38	ALA	-	EXPRESSION TAG	UNP P14735

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	215	Total	C	N	O	S	0	0	0
			1632	1041	267	317	7			
2	K	207	Total	C	N	O	S	0	0	0
			1582	1009	259	307	7			
2	M	214	Total	C	N	O	S	0	0	0
			1623	1035	265	316	7			
2	O	209	Total	C	N	O	S	0	0	0
			1587	1011	261	309	6			
2	Q	201	Total	C	N	O	S	0	0	0
			1539	984	252	297	6			
2	S	215	Total	C	N	O	S	0	0	0
			1632	1041	267	317	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	199	Total	C	N	O	S	0	0	0
			1514	968	248	291	7			
2	W	204	Total	C	N	O	S	0	0	0
			1544	985	252	301	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	198	Total	C	N	O	S	0	0	0
			1523	959	254	305	5			
3	L	176	Total	C	N	O	S	0	0	0
			1356	854	226	272	4			
3	N	200	Total	C	N	O	S	0	0	0
			1532	964	256	307	5			
3	P	184	Total	C	N	O	S	0	0	0
			1416	891	239	281	5			
3	R	177	Total	C	N	O	S	0	0	0
			1350	846	224	276	4			
3	T	198	Total	C	N	O	S	0	0	0
			1518	952	255	306	5			
3	V	186	Total	C	N	O	S	0	0	0
			1432	900	239	289	4			
3	X	198	Total	C	N	O	S	0	0	0
			1515	949	255	307	4			

- Molecule 4 is a protein called Insulin A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	a	17	Total	C	N	O	S	0	0	0
			128	79	19	27	3			
4	b	3	Total	C	N	O		0	0	0
			19	13	3	3				
4	c	11	Total	C	N	O	S	0	0	0
			83	50	13	18	2			
4	d	5	Total	C	N	O		0	0	0
			37	23	6	8				
4	e	9	Total	C	N	O		0	0	0
			74	49	11	14				
4	f	7	Total	C	N	O	S	0	0	0
			49	29	8	10	2			
4	g	8	Total	C	N	O	S	0	0	0
			60	39	8	12	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	h	7	Total	C	N	O	S	0	0	0
			49	29	8	10	2			

- Molecule 5 is a protein called Insulin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	x	3	Total	C	N	O	S	0	0	0
			18	11	3	3	1			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Zn	0	0
			1	1		
6	D	1	Total	Zn	0	0
			1	1		
6	E	1	Total	Zn	0	0
			1	1		
6	H	1	Total	Zn	0	0
			1	1		
6	B	1	Total	Zn	0	0
			1	1		
6	C	1	Total	Zn	0	0
			1	1		
6	A	1	Total	Zn	0	0
			1	1		
6	F	1	Total	Zn	0	0
			1	1		

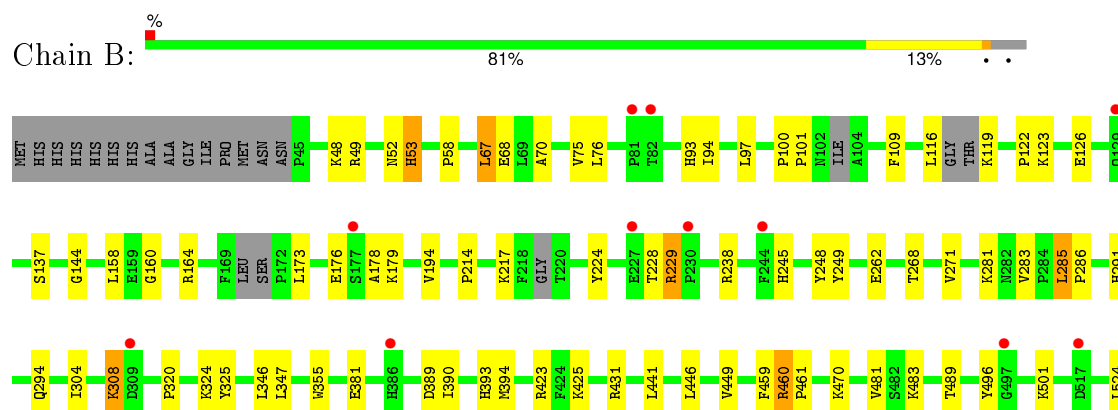
3 Residue-property plots [i](#)

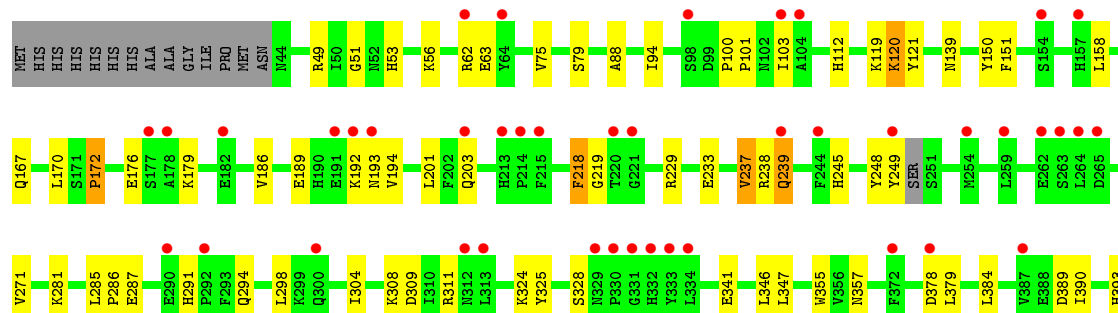
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

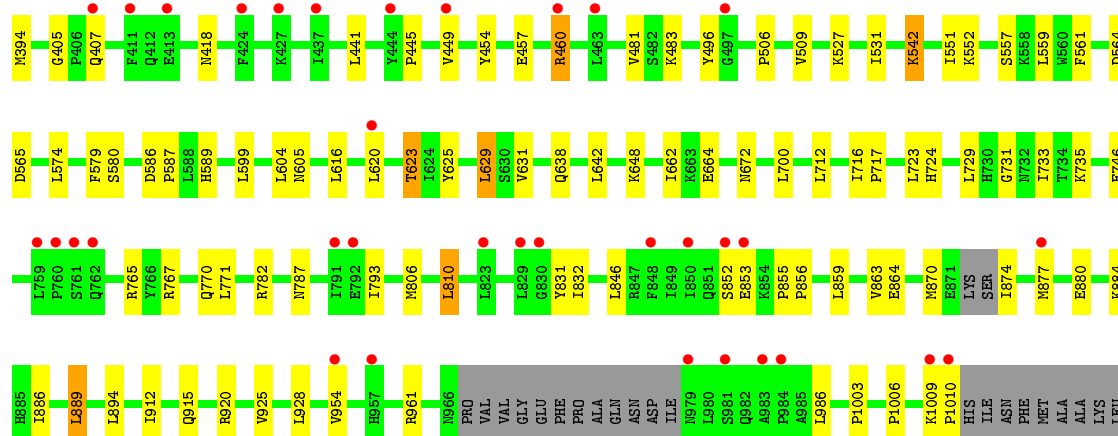
- Molecule 1: Insulin-degrading enzyme



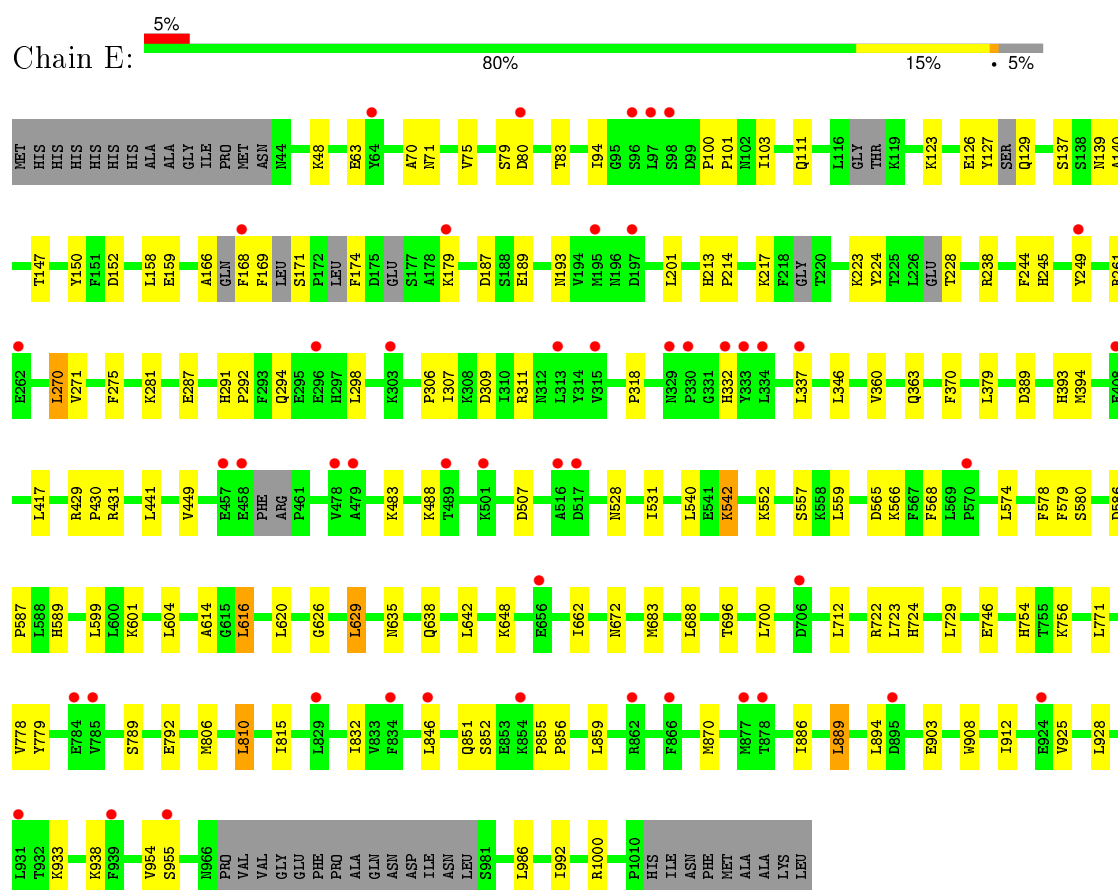
- Molecule 1: Insulin-degrading enzyme



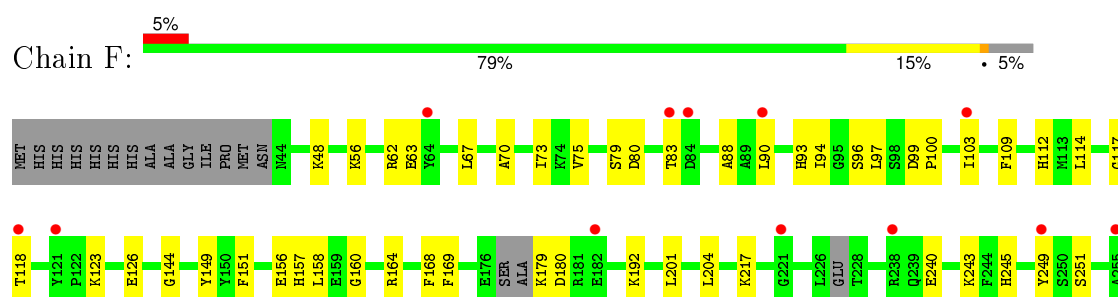


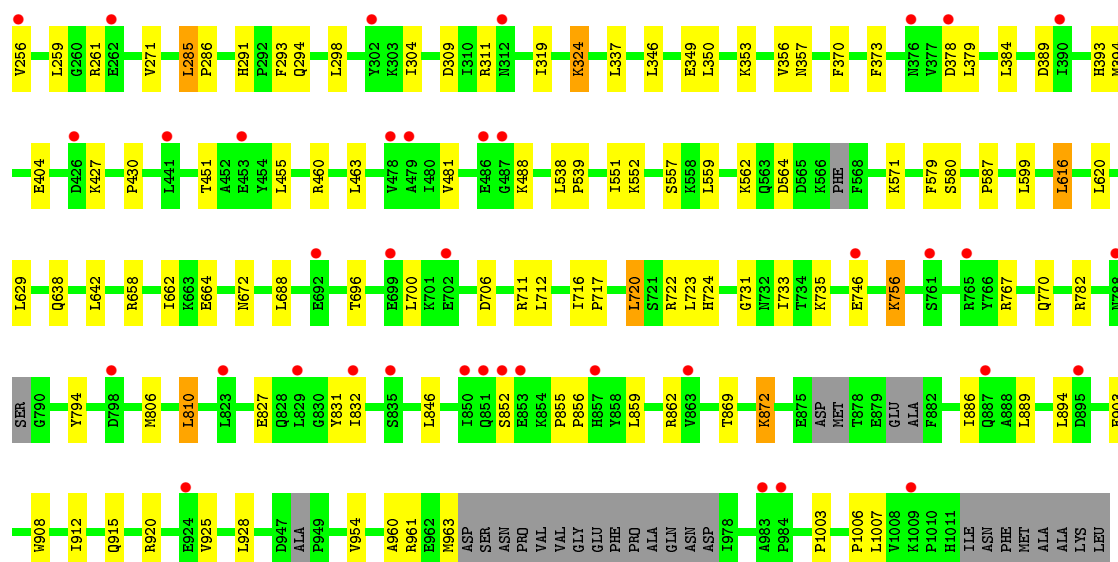


• Molecule 1: Insulin-degrading enzyme

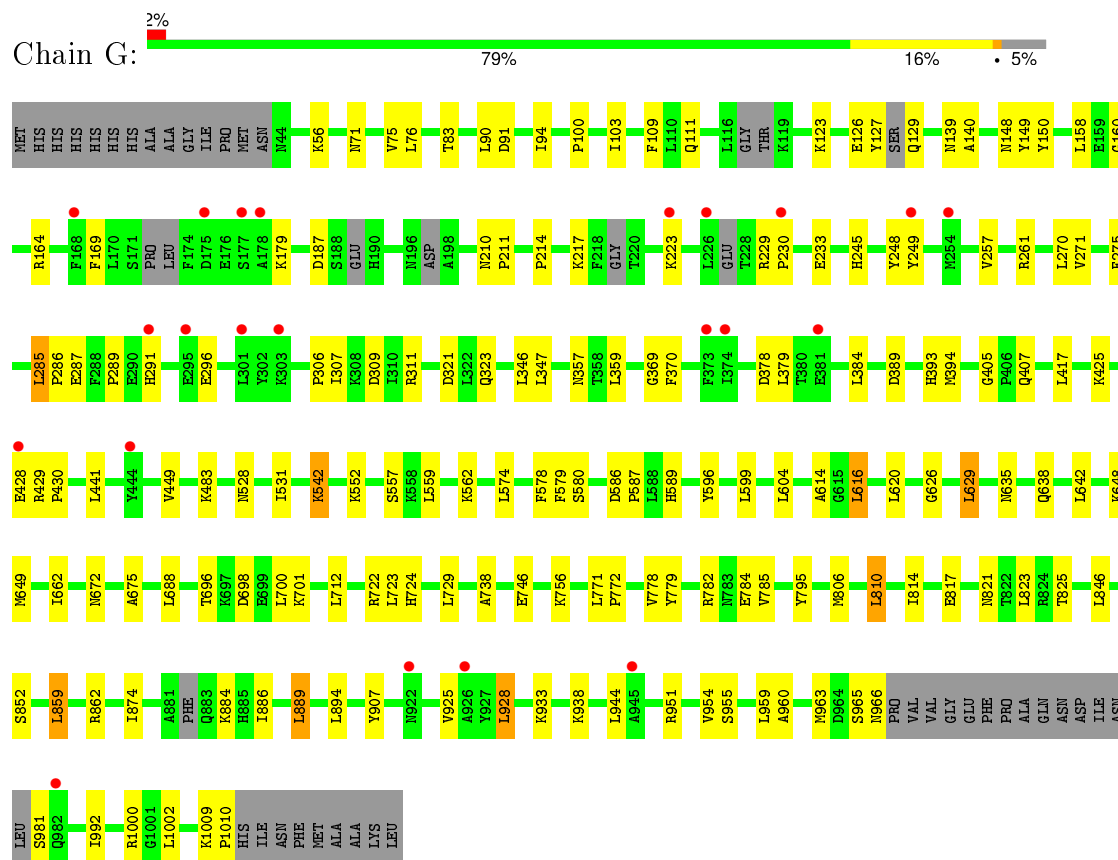


• Molecule 1: Insulin-degrading enzyme

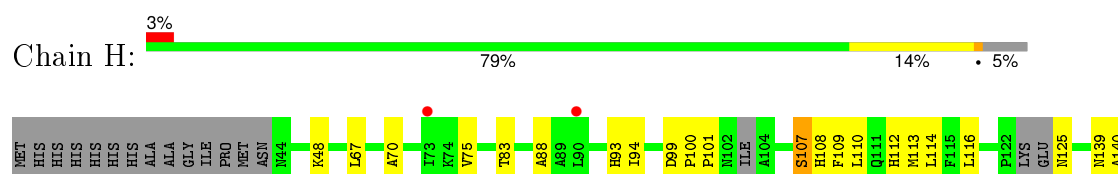




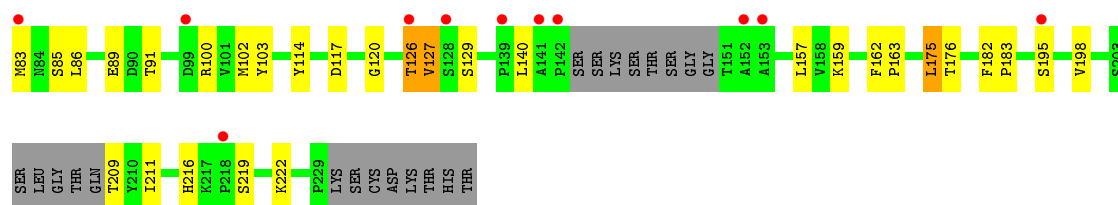
• Molecule 1: Insulin-degrading enzyme



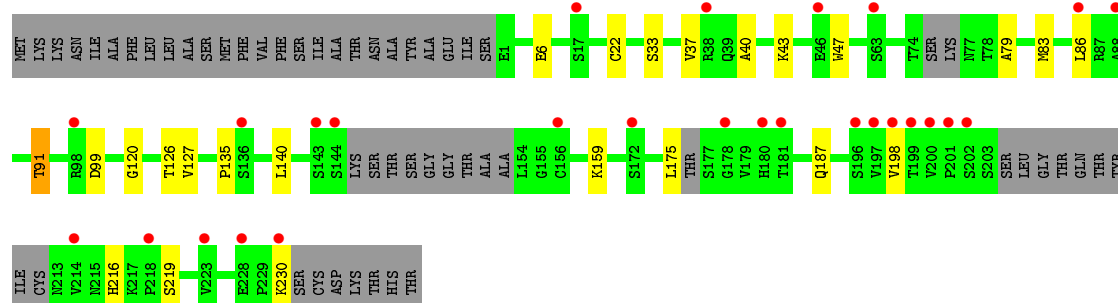
• Molecule 1: Insulin-degrading enzyme



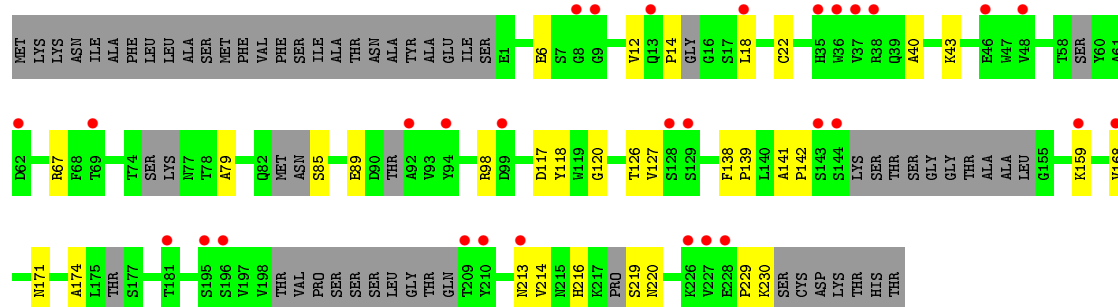




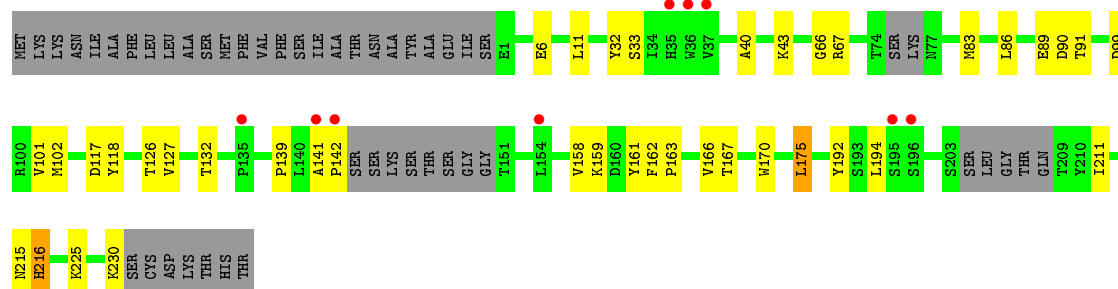
- Molecule 2: IDE-bound Fab, heavy chain



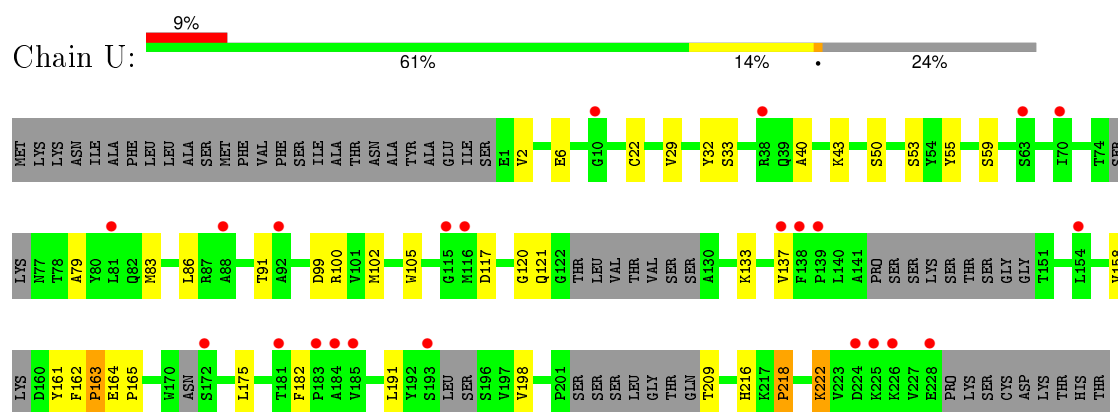
- Molecule 2: IDE-bound Fab, heavy chain



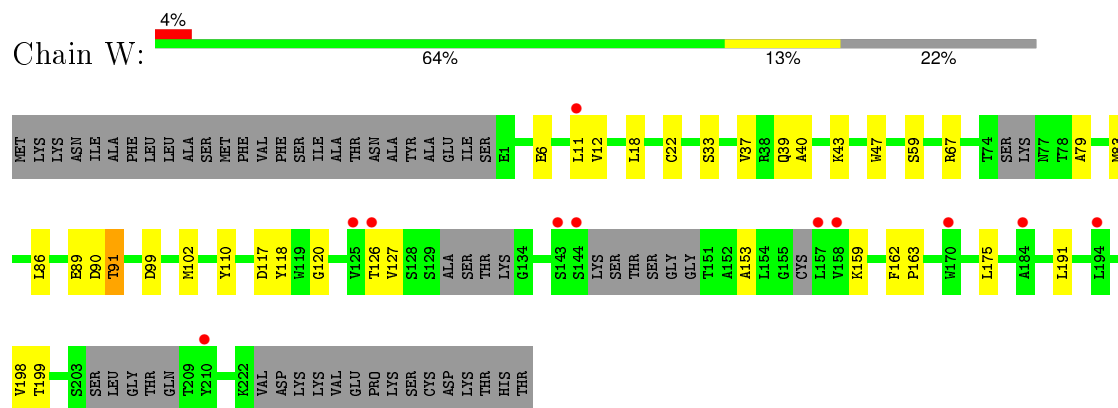
- Molecule 2: IDE-bound Fab, heavy chain



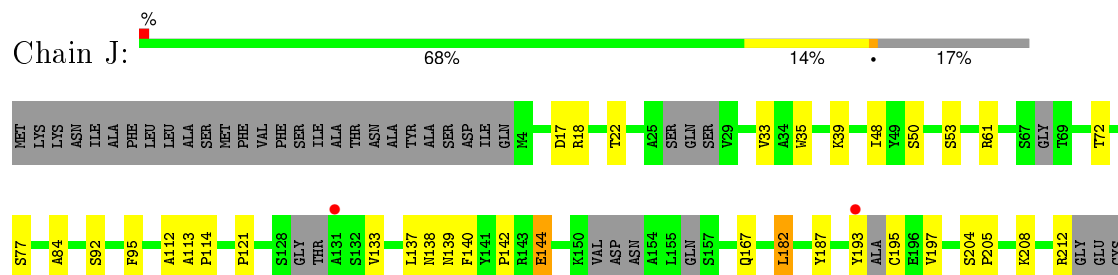
- Molecule 2: IDE-bound Fab, heavy chain



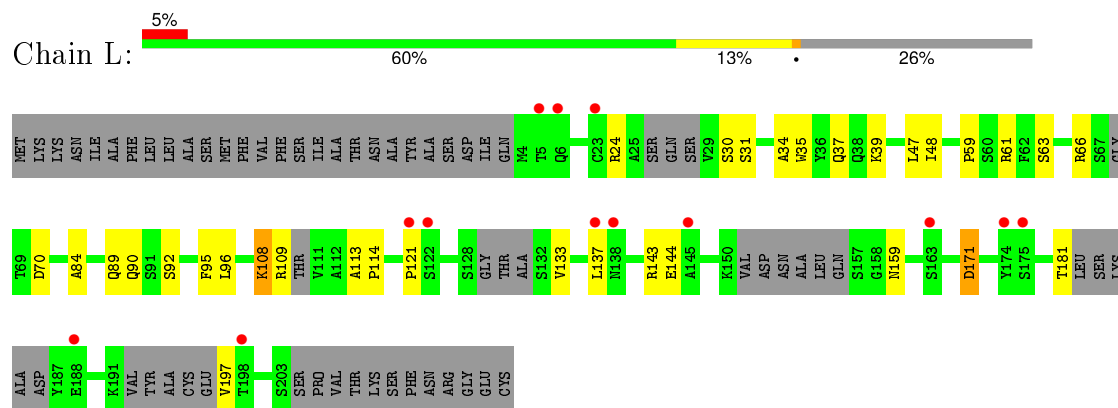
• Molecule 2: IDE-bound Fab, heavy chain



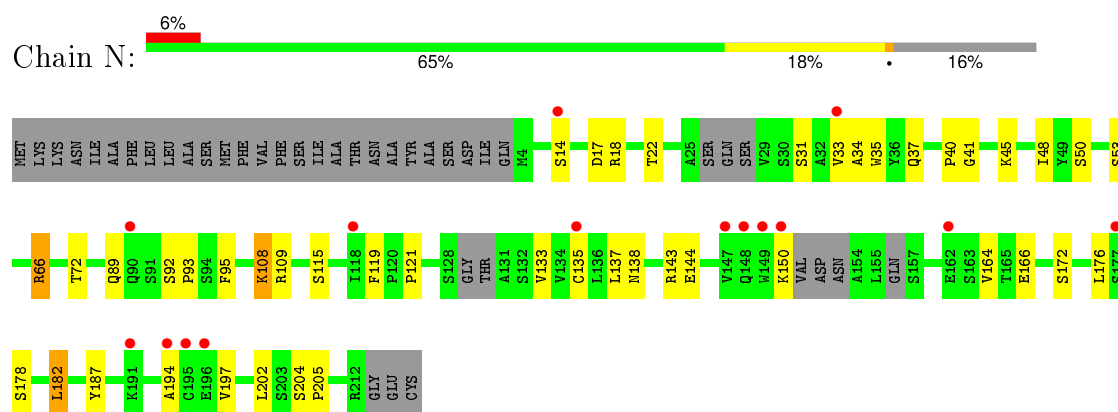
• Molecule 3: IDE-bound Fab, light chain



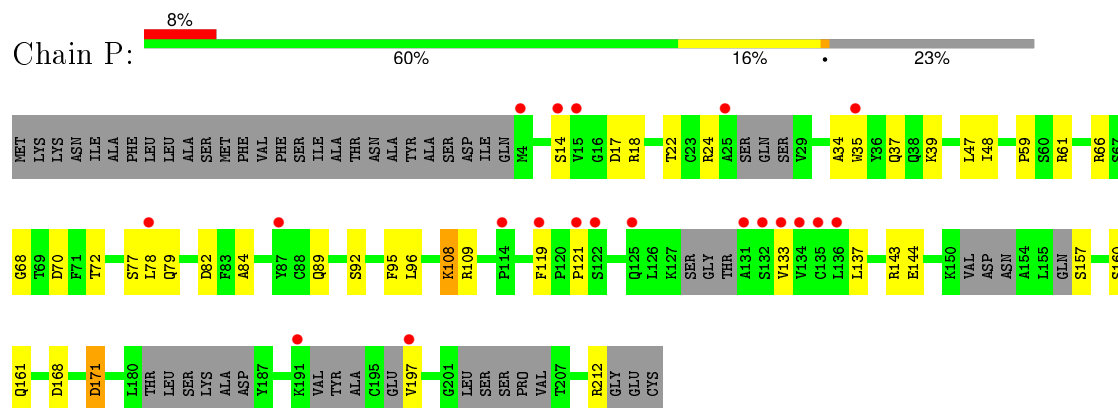
• Molecule 3: IDE-bound Fab, light chain



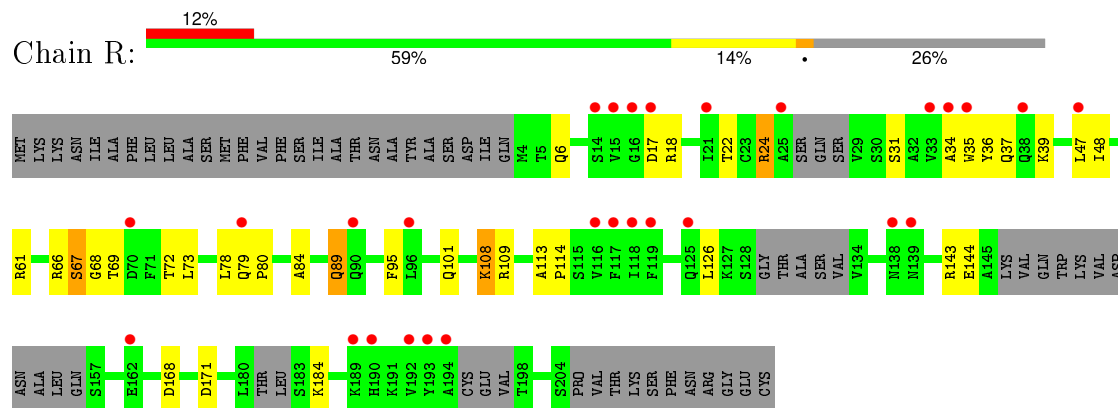
• Molecule 3: IDE-bound Fab, light chain



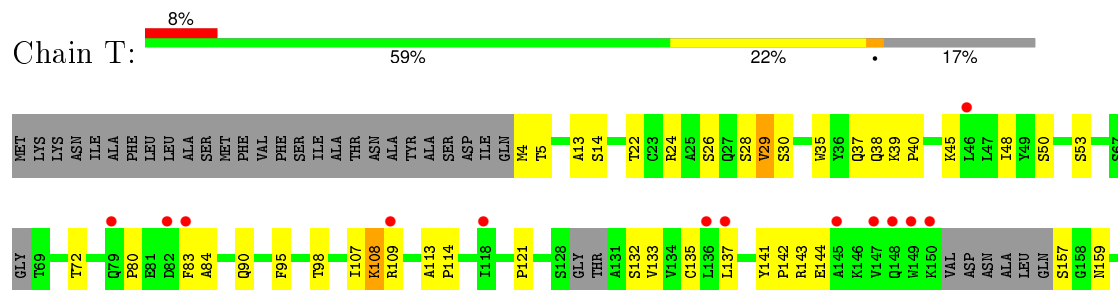
• Molecule 3: IDE-bound Fab, light chain

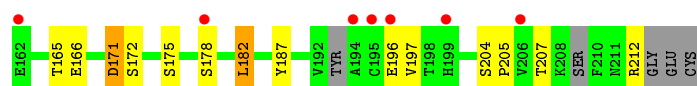


• Molecule 3: IDE-bound Fab, light chain

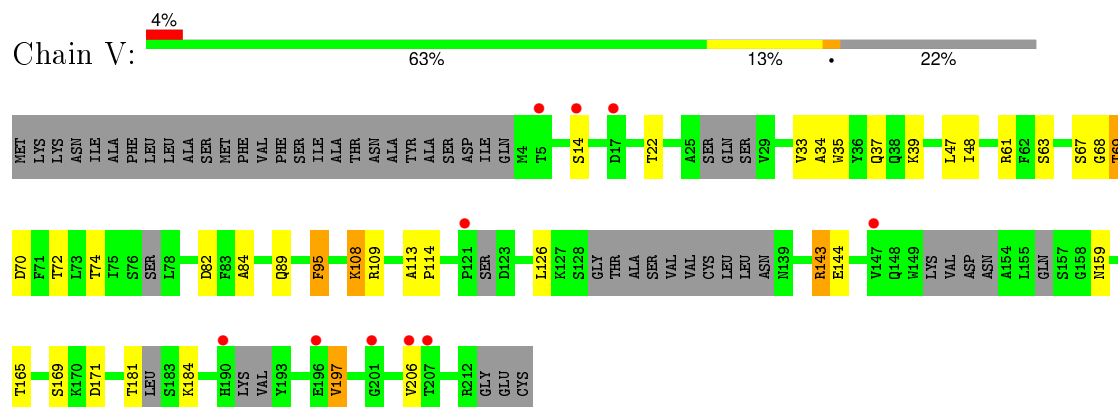


• Molecule 3: IDE-bound Fab, light chain

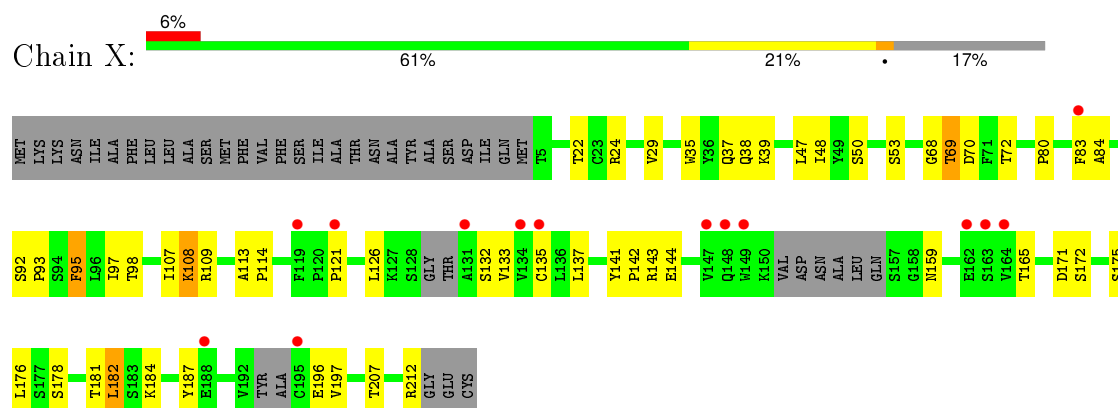




- Molecule 3: IDE-bound Fab, light chain



- Molecule 3: IDE-bound Fab, light chain



- Molecule 4: Insulin A chain



- Molecule 4: Insulin A chain

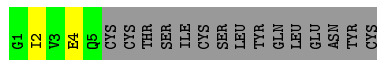


- Molecule 4: Insulin A chain




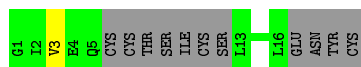
- Molecule 4: Insulin A chain

Chain d:  15% 10% 75%



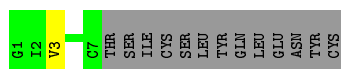
- Molecule 4: Insulin A chain

Chain e:  40% 5% 55%




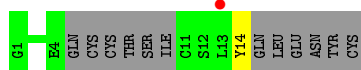
- Molecule 4: Insulin A chain

Chain f:  30% 5% 65%



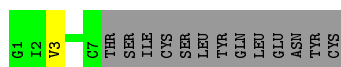
- Molecule 4: Insulin A chain

Chain g:  5% 35% 5% 60%



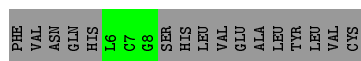
- Molecule 4: Insulin A chain

Chain h:  30% 5% 65%



- Molecule 5: Insulin B chain

Chain x:  16% 84%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.59Å 138.19Å 376.51Å 90.00° 99.36° 90.00°	Depositor
Resolution (Å)	49.54 – 3.93 49.54 – 3.93	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.54-3.93) 93.6 (49.54-3.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.246 , 0.288 0.243 , 0.284	Depositor DCC
R_{free} test set	1892 reflections (1.84%)	DCC
Wilson B-factor (Å ²)	81.6	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.5	EDS
Estimated twinning fraction	0.377 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	3 of 108371 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	86673	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.89 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.4254e-03.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0/7898	0.37	0/10677
1	B	0.21	0/7942	0.39	1/10731 (0.0%)
1	C	0.21	0/7965	0.37	0/10772
1	D	0.22	0/7982	0.40	3/10795 (0.0%)
1	E	0.21	0/7893	0.37	0/10662
1	F	0.21	0/7922	0.37	0/10704
1	G	0.22	0/7906	0.37	0/10680
1	H	0.22	0/7853	0.37	0/10618
2	I	0.22	0/1675	0.41	0/2282
2	K	0.22	0/1623	0.37	0/2206
2	M	0.21	0/1666	0.38	0/2271
2	O	0.21	0/1628	0.37	0/2214
2	Q	0.21	0/1574	0.35	0/2131
2	S	0.24	0/1675	0.40	0/2282
2	U	0.26	1/1551 (0.1%)	0.41	0/2106
2	W	0.21	0/1584	0.37	0/2157
3	J	0.21	0/1551	0.38	0/2096
3	L	0.21	0/1380	0.38	0/1862
3	N	0.22	0/1562	0.40	0/2114
3	P	0.21	0/1440	0.37	0/1940
3	R	0.22	0/1375	0.39	0/1858
3	T	0.21	0/1546	0.38	0/2090
3	V	0.21	0/1458	0.37	0/1967
3	X	0.22	0/1545	0.37	0/2092
4	a	0.26	0/128	0.50	0/172
4	b	0.17	0/18	0.44	0/23
4	c	0.22	0/82	0.37	0/108
4	d	0.20	0/36	0.54	0/47
4	e	0.24	0/73	0.96	0/96
4	f	0.18	0/48	0.40	0/63
4	g	0.20	0/59	0.44	0/77
4	h	0.18	0/48	0.37	0/63

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	x	0.23	0/17	0.33	0/21
All	All	0.22	1/88703 (0.0%)	0.38	4/119977 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	163	PRO	N-CD	5.91	1.56	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	732	ASN	N-CA-C	-5.99	94.83	111.00
1	D	457	GLU	N-CA-CB	-5.90	99.98	110.60
1	D	457	GLU	N-CA-C	5.77	126.57	111.00
1	D	120	LYS	CB-CA-C	-5.61	99.18	110.40

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	7708	0	7652	66	0
1	B	7754	0	7692	81	0
1	C	7772	0	7714	95	0
1	D	7790	0	7728	91	0
1	E	7709	0	7646	82	0
1	F	7735	0	7691	91	0
1	G	7722	0	7667	91	0
1	H	7663	0	7617	84	0
2	I	1632	0	1575	17	0
2	K	1582	0	1517	25	0
2	M	1623	0	1562	26	0
2	O	1587	0	1530	14	0
2	Q	1539	0	1474	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	1632	0	1575	34	0
2	U	1514	0	1442	21	0
2	W	1544	0	1471	22	0
3	J	1523	0	1495	18	0
3	L	1356	0	1327	19	0
3	N	1532	0	1505	24	0
3	P	1416	0	1385	24	0
3	R	1350	0	1311	24	0
3	T	1518	0	1489	31	0
3	V	1432	0	1386	21	0
3	X	1515	0	1485	29	0
4	a	128	0	124	0	0
4	b	19	0	25	0	0
4	c	83	0	77	0	0
4	d	37	0	39	0	0
4	e	74	0	77	0	0
4	f	49	0	49	0	0
4	g	60	0	60	0	0
4	h	49	0	49	0	0
5	x	18	0	17	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
All	All	86673	0	85453	1021	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 6.

The worst 5 of 1021 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)
2:S:162:PHE:CE2	2:S:163:PRO:HB3	1.81	1.15
2:S:162:PHE:CZ	2:S:163:PRO:HB3	2.09	0.87
1:E:565:ASP:OD1	1:E:566:LYS:NZ	2.14	0.80
1:B:731:GLY:O	1:B:733:ILE:HG22	1.83	0.79
2:S:162:PHE:CG	2:S:163:PRO:HA	2.19	0.78

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	929/990 (94%)	919 (99%)	10 (1%)	0	100	100
1	B	932/990 (94%)	919 (99%)	13 (1%)	0	100	100
1	C	942/990 (95%)	929 (99%)	13 (1%)	0	100	100
1	D	944/990 (95%)	926 (98%)	16 (2%)	2 (0%)	52	86
1	E	920/990 (93%)	910 (99%)	10 (1%)	0	100	100
1	F	926/990 (94%)	912 (98%)	14 (2%)	0	100	100
1	G	923/990 (93%)	903 (98%)	20 (2%)	0	100	100
1	H	924/990 (93%)	907 (98%)	17 (2%)	0	100	100
2	I	207/263 (79%)	201 (97%)	6 (3%)	0	100	100
2	K	195/263 (74%)	189 (97%)	6 (3%)	0	100	100
2	M	206/263 (78%)	196 (95%)	10 (5%)	0	100	100
2	O	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
2	Q	181/263 (69%)	176 (97%)	5 (3%)	0	100	100
2	S	207/263 (79%)	202 (98%)	5 (2%)	0	100	100
2	U	183/263 (70%)	176 (96%)	6 (3%)	1 (0%)	34	76
2	W	192/263 (73%)	187 (97%)	5 (3%)	0	100	100
3	J	184/239 (77%)	178 (97%)	6 (3%)	0	100	100
3	L	160/239 (67%)	152 (95%)	8 (5%)	0	100	100
3	N	190/239 (80%)	184 (97%)	6 (3%)	0	100	100
3	P	167/239 (70%)	158 (95%)	9 (5%)	0	100	100
3	R	165/239 (69%)	156 (94%)	9 (6%)	0	100	100
3	T	186/239 (78%)	182 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	V	168/239 (70%)	162 (96%)	6 (4%)	0	100	100
3	X	190/239 (80%)	183 (96%)	7 (4%)	0	100	100
4	a	15/20 (75%)	14 (93%)	1 (7%)	0	100	100
4	b	1/20 (5%)	1 (100%)	0	0	100	100
4	c	7/20 (35%)	7 (100%)	0	0	100	100
4	d	3/20 (15%)	3 (100%)	0	0	100	100
4	e	5/20 (25%)	5 (100%)	0	0	100	100
4	f	5/20 (25%)	4 (80%)	1 (20%)	0	100	100
4	g	4/20 (20%)	3 (75%)	1 (25%)	0	100	100
4	h	5/20 (25%)	4 (80%)	1 (20%)	0	100	100
5	x	1/19 (5%)	1 (100%)	0	0	100	100
All	All	10466/12115 (86%)	10242 (98%)	221 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	U	218	PRO
1	D	172	PRO
1	D	237	VAL

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	838/879 (95%)	821 (98%)	17 (2%)	63	86
1	B	845/879 (96%)	825 (98%)	20 (2%)	57	83
1	C	846/879 (96%)	828 (98%)	18 (2%)	61	85
1	D	848/879 (96%)	830 (98%)	18 (2%)	61	85
1	E	840/879 (96%)	820 (98%)	20 (2%)	57	83
1	F	843/879 (96%)	821 (97%)	22 (3%)	54	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	841/879 (96%)	824 (98%)	17 (2%)	63	86
1	H	833/879 (95%)	815 (98%)	18 (2%)	60	84
2	I	180/220 (82%)	177 (98%)	3 (2%)	68	88
2	K	176/220 (80%)	173 (98%)	3 (2%)	68	88
2	M	179/220 (81%)	171 (96%)	8 (4%)	34	71
2	O	176/220 (80%)	174 (99%)	2 (1%)	80	91
2	Q	169/220 (77%)	167 (99%)	2 (1%)	78	90
2	S	180/220 (82%)	174 (97%)	6 (3%)	45	78
2	U	163/220 (74%)	157 (96%)	6 (4%)	41	75
2	W	169/220 (77%)	167 (99%)	2 (1%)	78	90
3	J	178/210 (85%)	173 (97%)	5 (3%)	51	79
3	L	159/210 (76%)	153 (96%)	6 (4%)	40	75
3	N	178/210 (85%)	172 (97%)	6 (3%)	44	77
3	P	164/210 (78%)	159 (97%)	5 (3%)	48	79
3	R	157/210 (75%)	148 (94%)	9 (6%)	25	65
3	T	178/210 (85%)	170 (96%)	8 (4%)	34	71
3	V	165/210 (79%)	157 (95%)	8 (5%)	31	69
3	X	178/210 (85%)	168 (94%)	10 (6%)	26	65
4	a	16/19 (84%)	13 (81%)	3 (19%)	2	15
4	b	2/19 (10%)	1 (50%)	1 (50%)	0	0
4	c	10/19 (53%)	9 (90%)	1 (10%)	9	42
4	d	4/19 (21%)	2 (50%)	2 (50%)	0	0
4	e	8/19 (42%)	7 (88%)	1 (12%)	6	32
4	f	6/19 (32%)	5 (83%)	1 (17%)	3	20
4	g	7/19 (37%)	6 (86%)	1 (14%)	4	27
4	h	6/19 (32%)	5 (83%)	1 (17%)	3	20
5	x	2/17 (12%)	2 (100%)	0	100	100
All	All	9544/10641 (90%)	9294 (97%)	250 (3%)	54	81

5 of 250 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	862	ARG

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Mol	Chain	Res	Type
1	H	226	LEU
3	X	69	THR
1	G	158	LEU
1	G	846	LEU

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	H	190	HIS
1	H	329	ASN
3	P	139	ASN
1	E	442	HIS
3	J	139	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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.

No monomer is involved in short contacts.

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	941/990 (95%)	-0.05	16 (1%) 73 62	61, 82, 101, 122	0
1	B	946/990 (95%)	-0.03	13 (1%) 78 68	57, 78, 99, 121	0
1	C	950/990 (95%)	0.23	48 (5%) 32 23	95, 122, 138, 149	0
1	D	952/990 (96%)	0.42	76 (7%) 15 10	125, 142, 153, 166	0
1	E	942/990 (95%)	0.38	48 (5%) 32 23	121, 136, 149, 161	0
1	F	944/990 (95%)	0.28	50 (5%) 30 22	110, 127, 139, 150	0
1	G	943/990 (95%)	0.16	22 (2%) 64 52	69, 96, 111, 129	0
1	H	936/990 (94%)	0.12	31 (3%) 50 38	68, 94, 111, 124	0
2	I	215/263 (81%)	0.21	4 (1%) 70 59	81, 98, 115, 123	0
2	K	207/263 (78%)	0.28	14 (6%) 20 13	69, 98, 116, 123	0
2	M	214/263 (81%)	0.36	15 (7%) 19 13	104, 120, 133, 141	0
2	O	209/263 (79%)	0.68	27 (12%) 5 5	141, 156, 170, 183	0
2	Q	201/263 (76%)	0.82	30 (14%) 3 3	137, 160, 172, 180	0
2	S	215/263 (81%)	0.27	9 (4%) 40 29	105, 123, 146, 160	0
2	U	199/263 (75%)	0.51	23 (11%) 6 6	83, 113, 134, 140	0
2	W	204/263 (77%)	0.29	11 (5%) 29 21	89, 110, 128, 142	0
3	J	198/239 (82%)	0.03	2 (1%) 84 77	83, 98, 113, 127	0
3	L	176/239 (73%)	0.30	13 (7%) 17 12	67, 95, 115, 122	0
3	N	200/239 (83%)	0.46	15 (7%) 17 12	109, 124, 136, 141	0
3	P	184/239 (76%)	0.71	20 (10%) 7 6	137, 153, 169, 182	0
3	R	177/239 (74%)	0.82	28 (15%) 3 3	147, 159, 174, 184	0
3	T	198/239 (82%)	0.48	20 (10%) 9 7	109, 134, 156, 170	0
3	V	186/239 (77%)	0.42	10 (5%) 29 21	87, 112, 128, 136	0
3	X	198/239 (82%)	0.31	14 (7%) 19 13	83, 106, 131, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
4	a	17/20 (85%)	-0.25	0 100 100	75, 102, 113, 117	0
4	b	3/20 (15%)	-0.59	0 100 100	64, 64, 67, 67	0
4	c	11/20 (55%)	-0.19	0 100 100	105, 121, 129, 133	0
4	d	5/20 (25%)	-0.24	0 100 100	135, 139, 143, 151	0
4	e	9/20 (45%)	-0.03	0 100 100	127, 132, 137, 141	0
4	f	7/20 (35%)	-0.18	0 100 100	119, 126, 134, 136	0
4	g	8/20 (40%)	0.60	1 (12%) 5 5	90, 97, 116, 117	0
4	h	7/20 (35%)	-0.25	0 100 100	89, 102, 110, 115	0
5	x	3/19 (15%)	0.26	0 100 100	94, 94, 103, 110	0
All	All	10805/12115 (89%)	0.26	560 (5%) 31 23	57, 115, 154, 184	0

The worst 5 of 560 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	852	SER	8.2
3	X	148	GLN	7.6
2	O	199	THR	5.8
3	R	79	GLN	5.8
1	D	262	GLU	5.7

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	ZN	A	1101	1/1	0.96	0.17	-0.62	87,87,87,87	0
6	ZN	C	1101	1/1	0.86	0.15	-0.78	125,125,125,125	0
6	ZN	E	2001	1/1	0.89	0.14	-1.81	162,162,162,162	0
6	ZN	F	1101	1/1	0.87	0.17	-	116,116,116,116	0
6	ZN	B	2001	1/1	0.97	0.17	-	89,89,89,89	0
6	ZN	G	2001	1/1	0.98	0.21	-	86,86,86,86	0
6	ZN	D	2001	1/1	0.91	0.11	-	137,137,137,137	0
6	ZN	H	1101	1/1	0.98	0.17	-	93,93,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.