



Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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

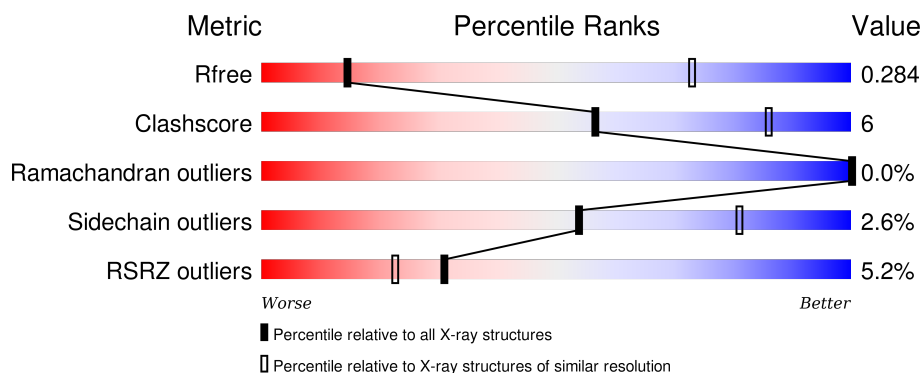
1 Overall quality at a glance

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	<div> <div>2%</div> <div>82% 13% • 5%</div> </div>
1	B	990	<div> <div>%</div> <div>81% 13% • •</div> </div>
1	C	990	<div> <div>5%</div> <div>79% 16% • •</div> </div>
1	D	990	<div> <div>8%</div> <div>79% 16% • •</div> </div>
1	E	990	<div> <div>5%</div> <div>80% 15% • 5%</div> </div>

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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
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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
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		

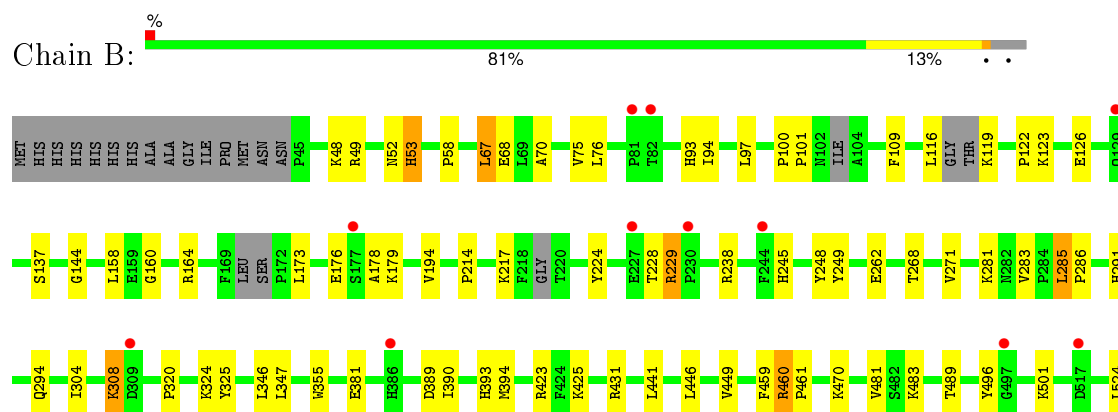
3 Residue-property plots

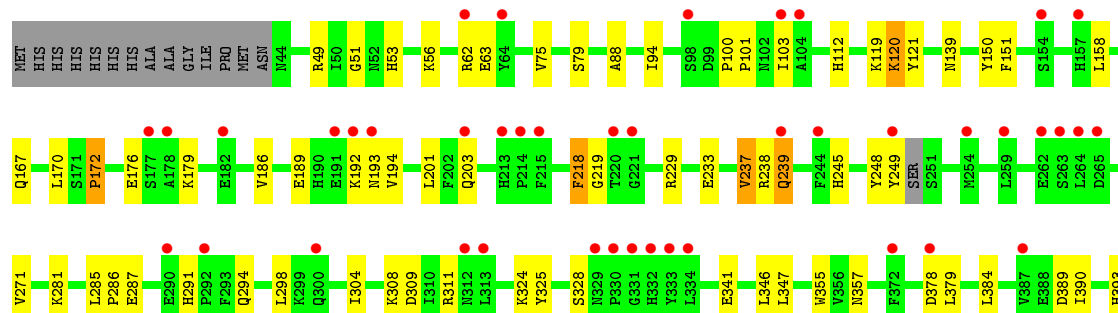
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

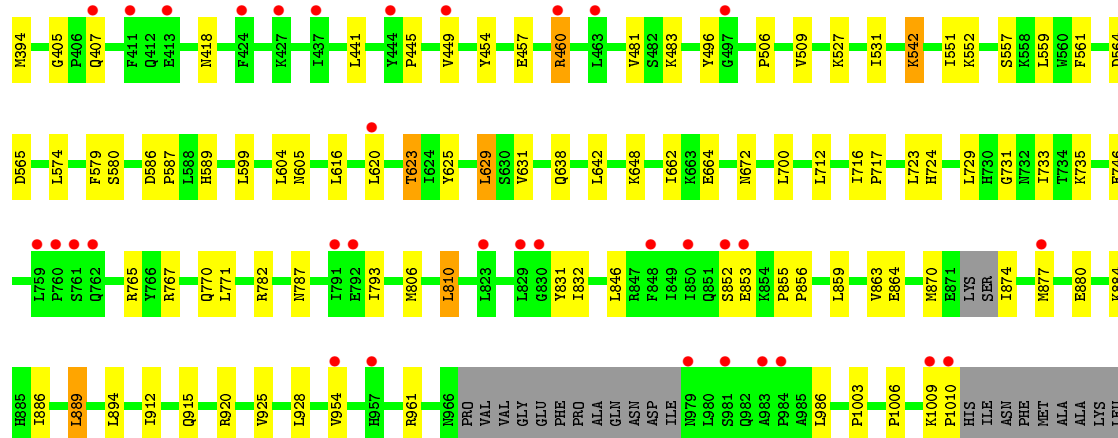
- Molecule 1: Insulin-degrading enzyme



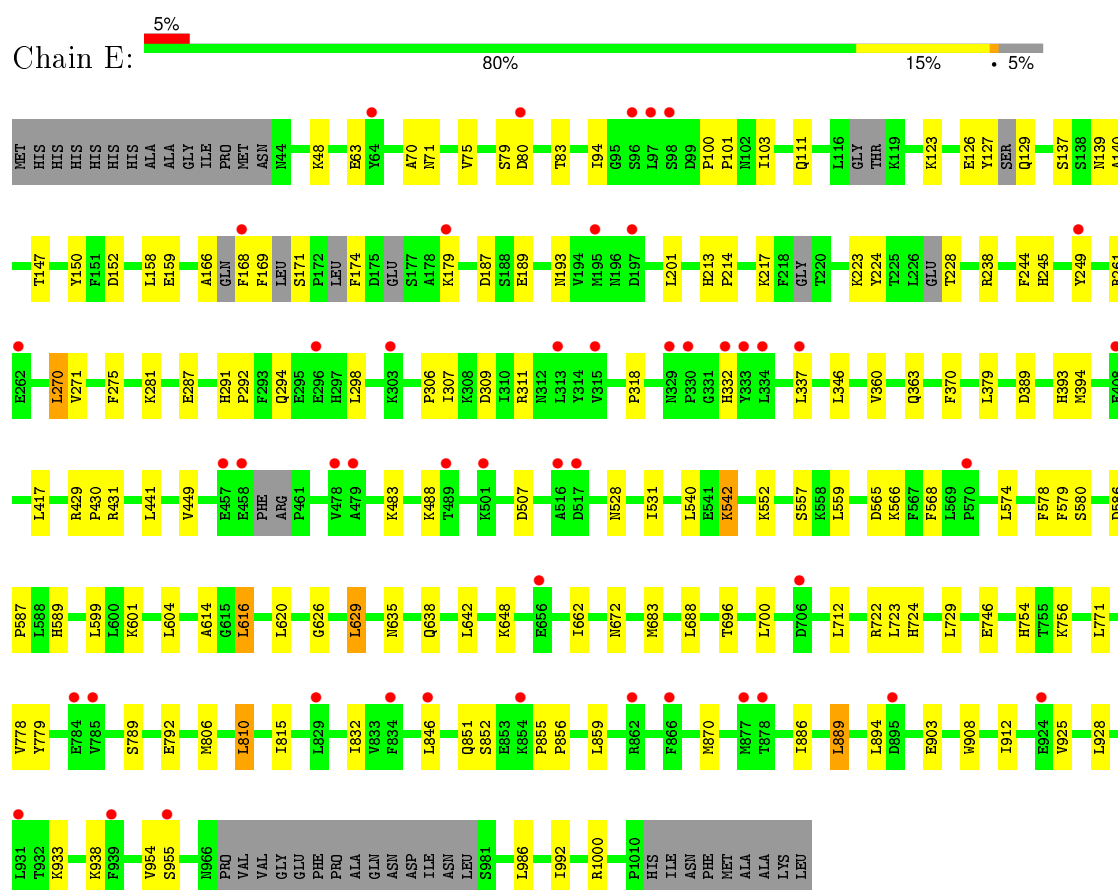
- Molecule 1: Insulin-degrading enzyme



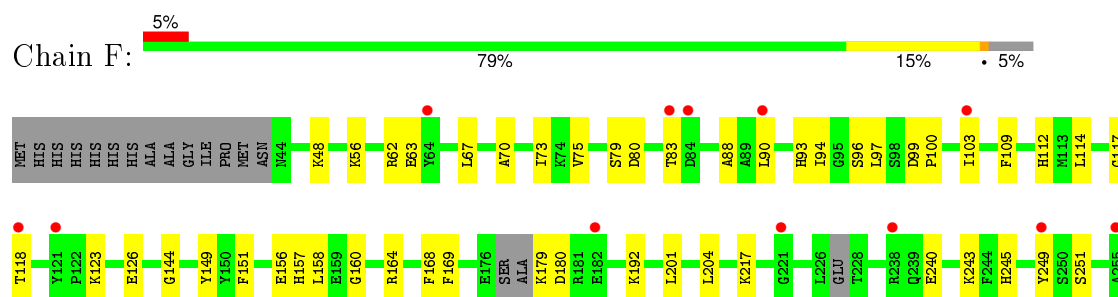


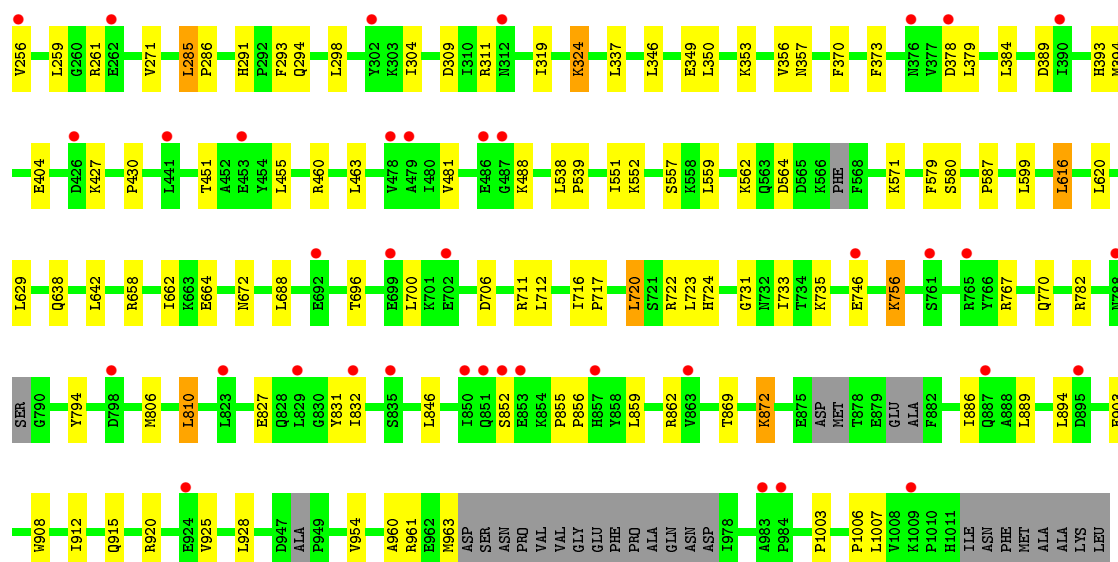


- Molecule 1: Insulin-degrading enzyme

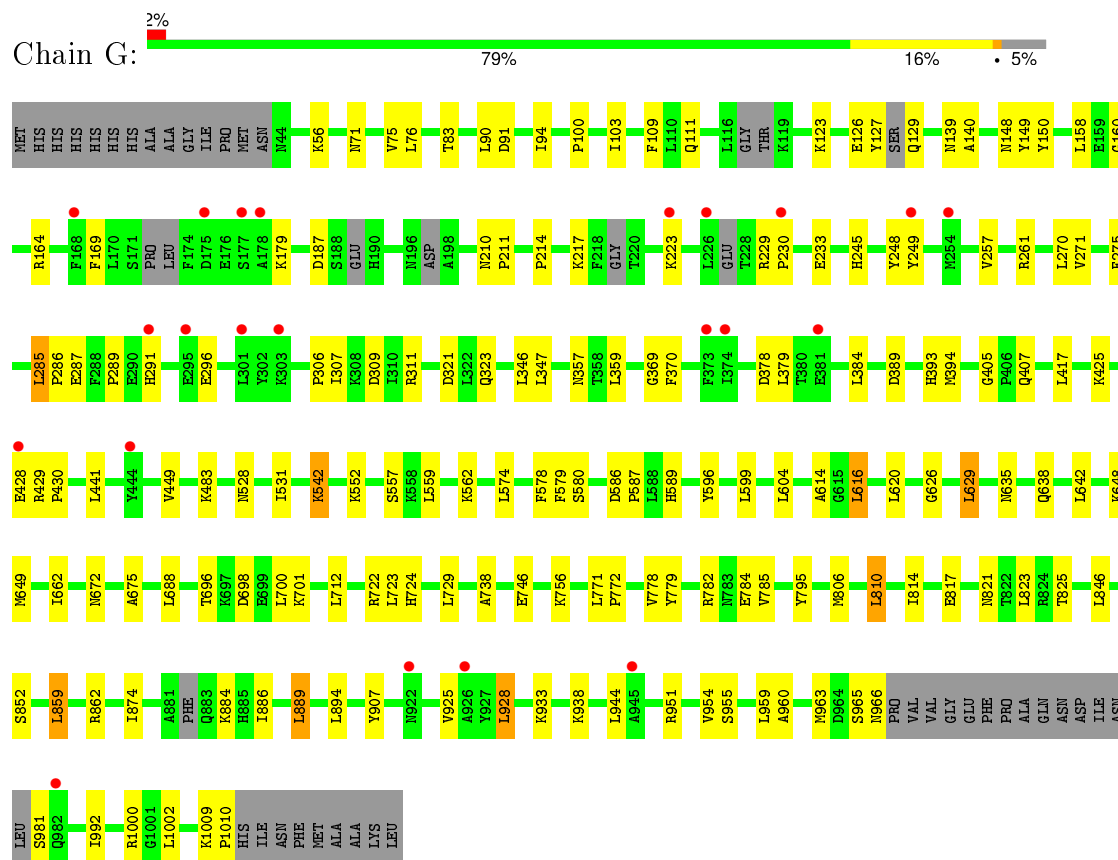


- Molecule 1: Insulin-degrading enzyme

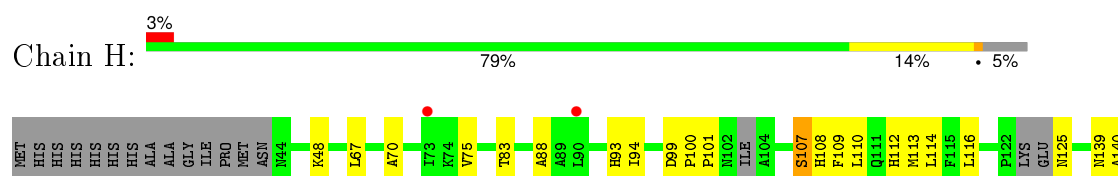




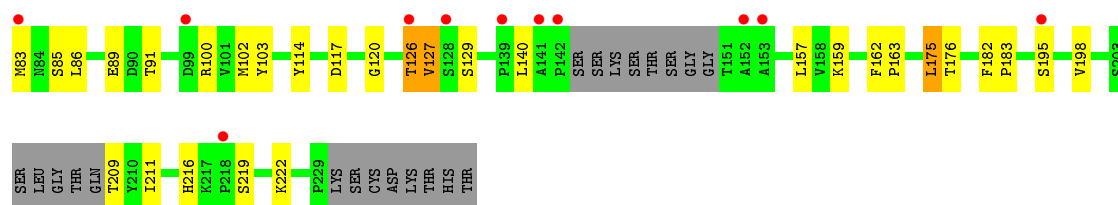
• Molecule 1: Insulin-degrading enzyme



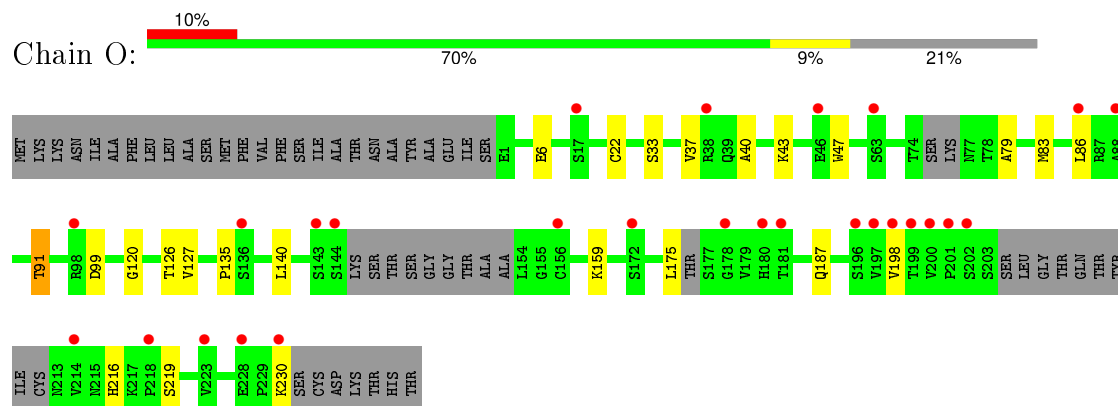
• Molecule 1: Insulin-degrading enzyme



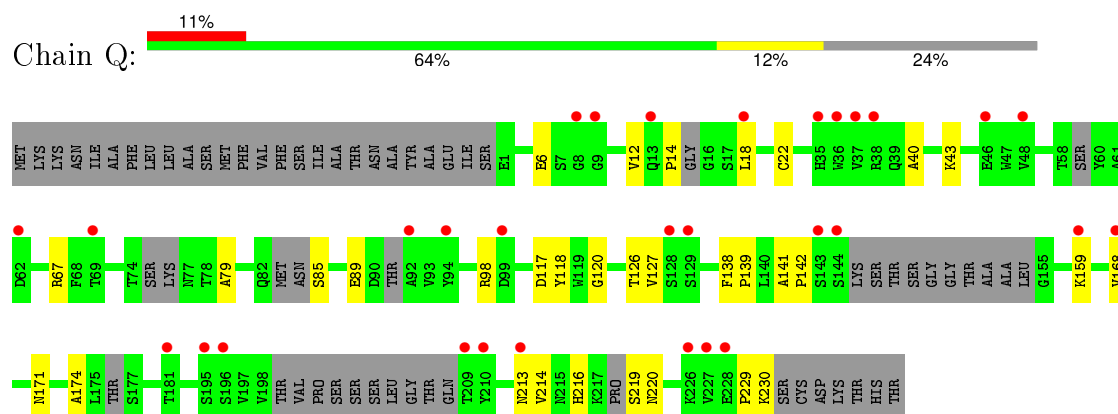




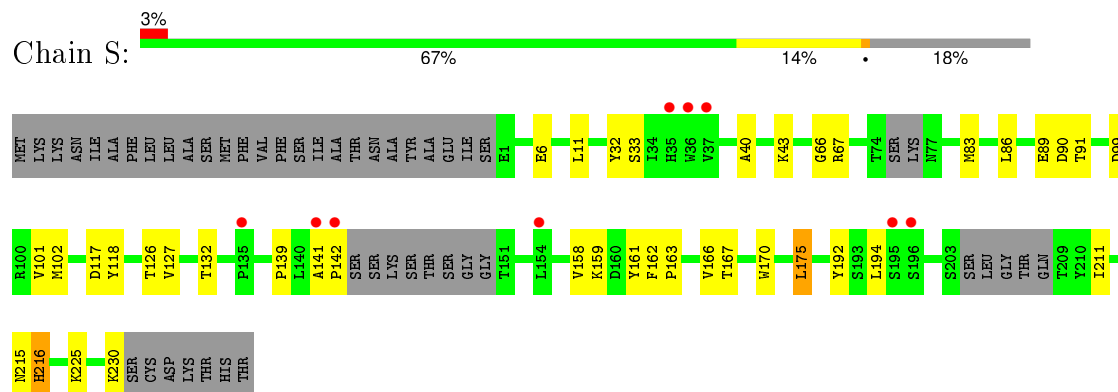
• Molecule 2: IDE-bound Fab, heavy chain



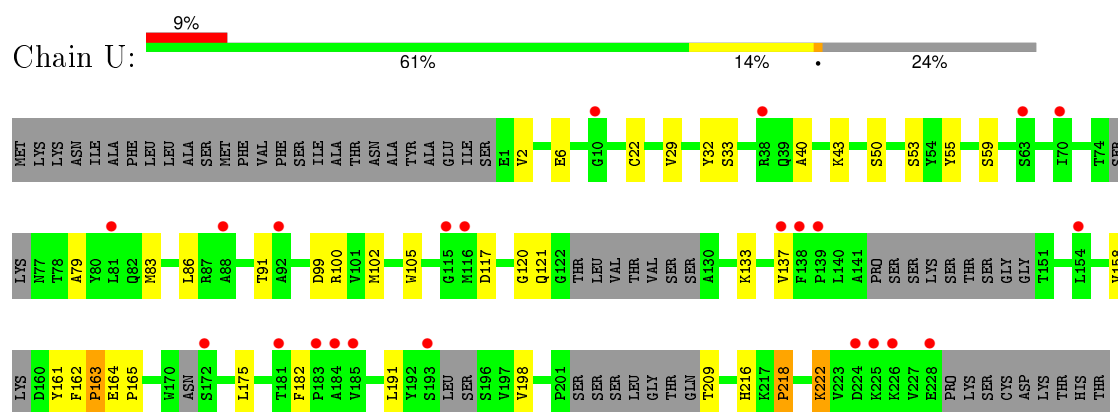
• Molecule 2: IDE-bound Fab, heavy chain



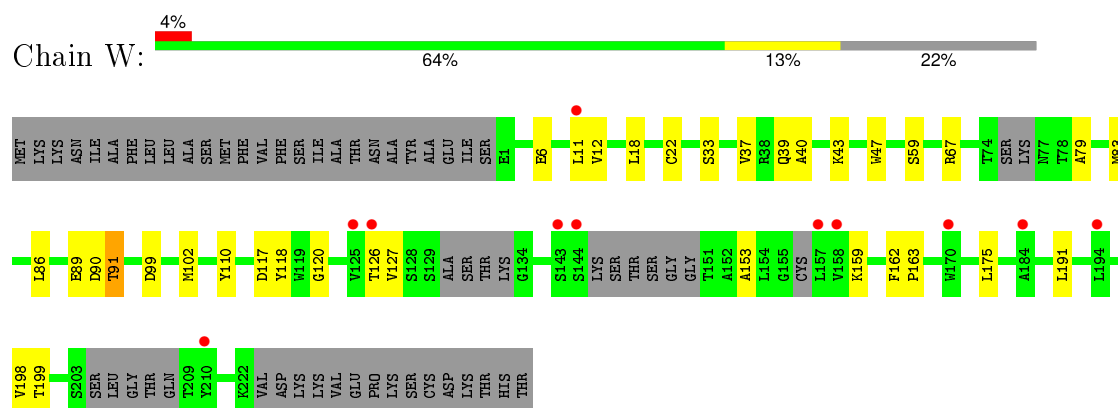
• Molecule 2: IDE-bound Fab, heavy chain



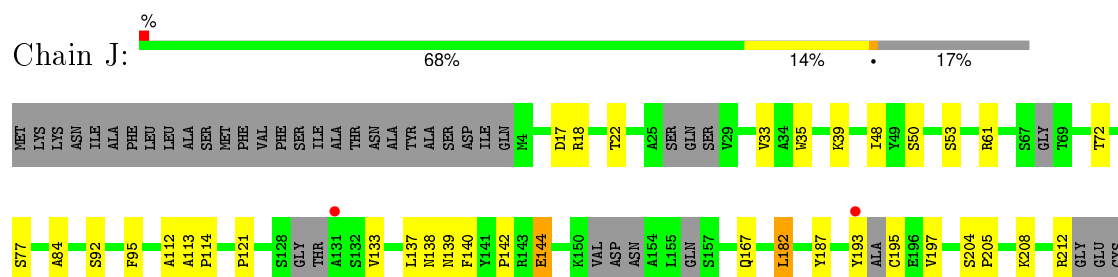
• Molecule 2: IDE-bound Fab, heavy chain



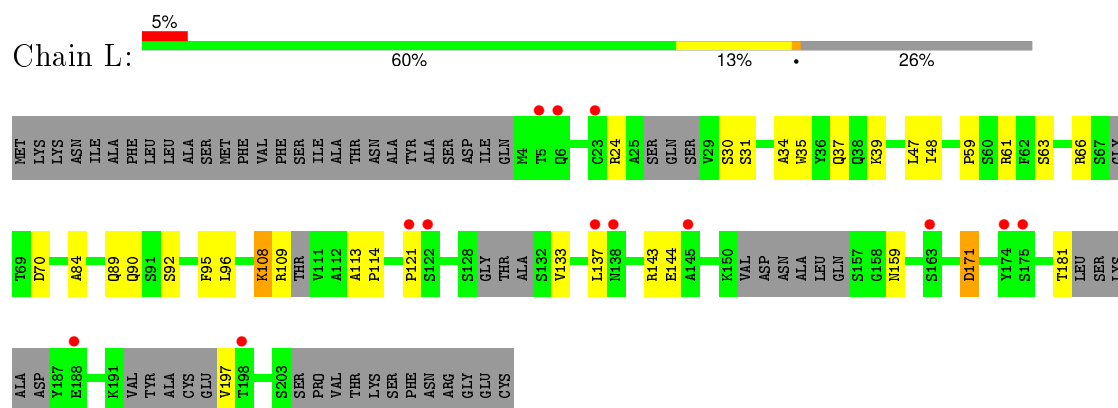
• Molecule 2: IDE-bound Fab, heavy chain



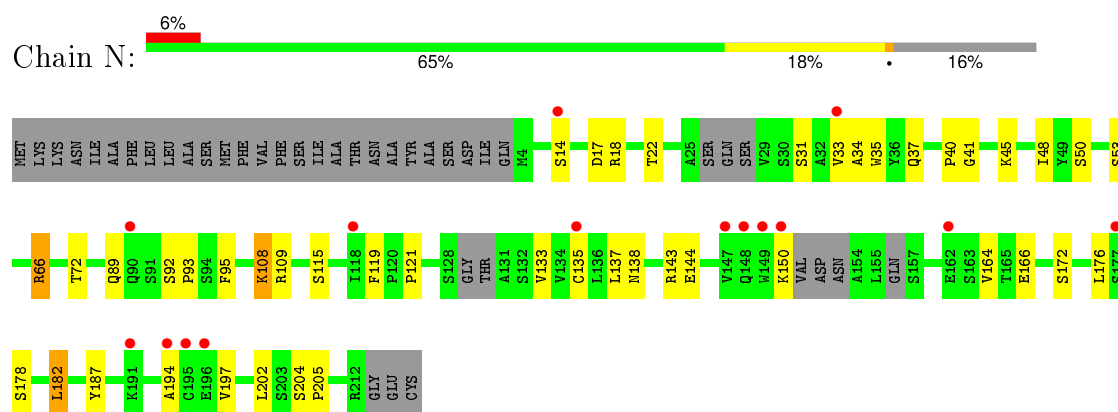
• Molecule 3: IDE-bound Fab, light chain



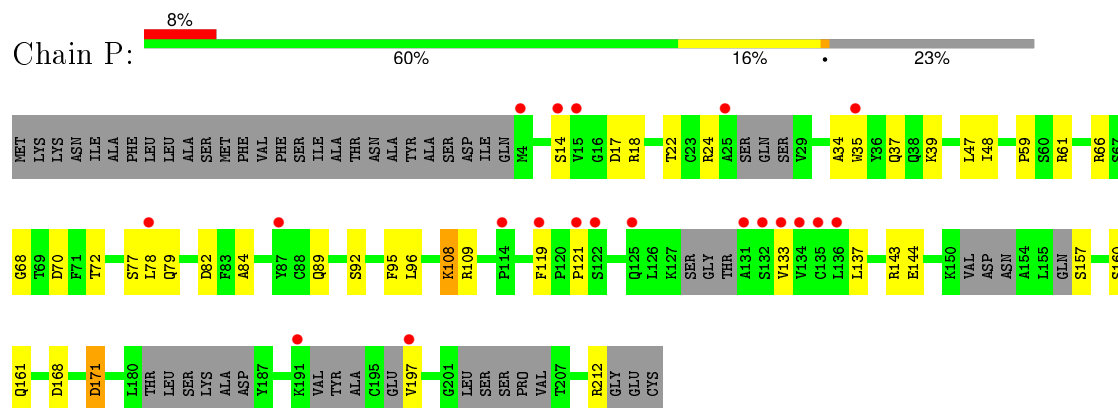
• Molecule 3: IDE-bound Fab, light chain



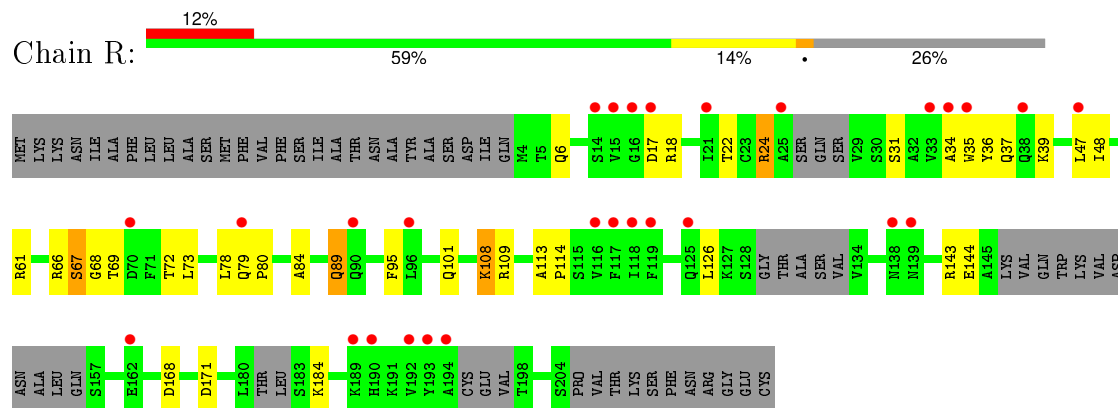
• Molecule 3: IDE-bound Fab, light chain



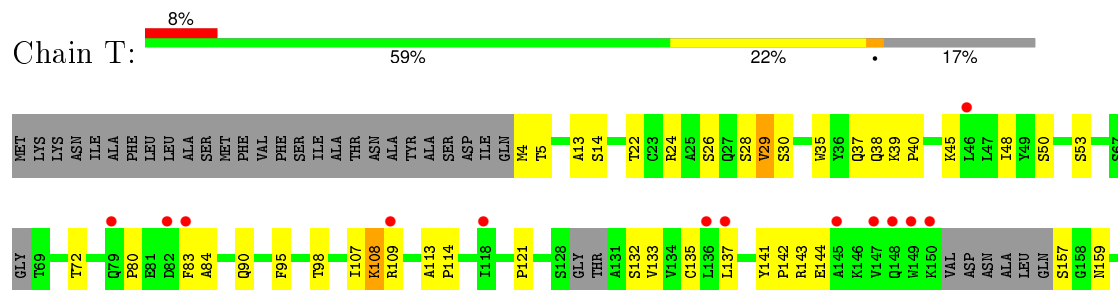
• Molecule 3: IDE-bound Fab, light chain

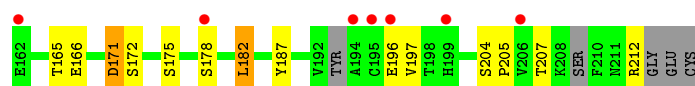


• Molecule 3: IDE-bound Fab, light chain

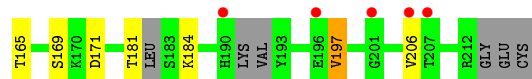
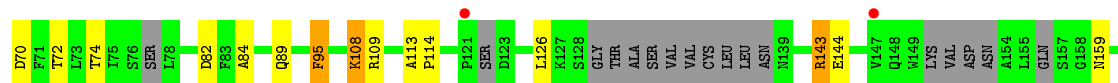
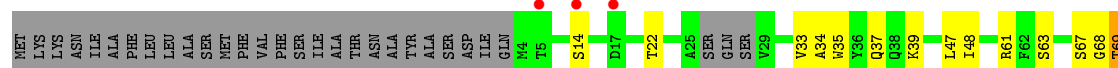


• Molecule 3: IDE-bound Fab, light chain

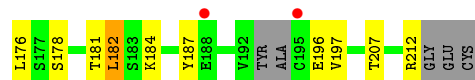
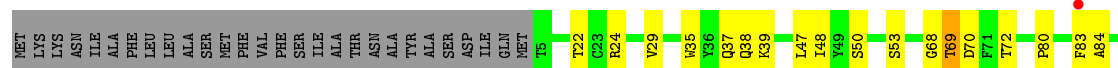




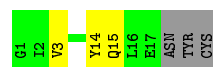
- Molecule 3: IDE-bound Fab, light chain



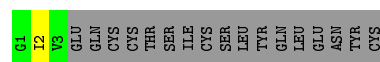
- Molecule 3: IDE-bound Fab, light chain



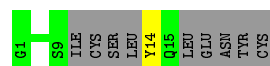
- Molecule 4: Insulin A chain



- Molecule 4: Insulin A chain

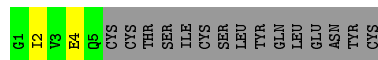


- Molecule 4: Insulin A chain




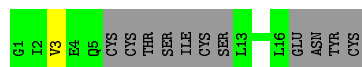
- Molecule 4: Insulin A chain

Chain d: 



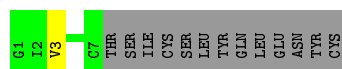
- Molecule 4: Insulin A chain

Chain e: 




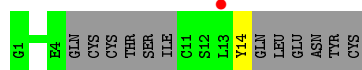
- Molecule 4: Insulin A chain

Chain f: 



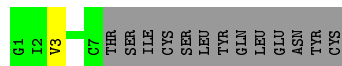
- Molecule 4: Insulin A chain

Chain g: 



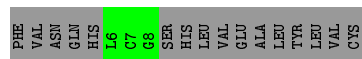
- Molecule 4: Insulin A chain

Chain h: 



- Molecule 5: Insulin B chain

Chain x: 



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.

All (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:162:PHE:CD2	2:S:163:PRO:HB3	2.21	0.75
1:B:308:LYS:O	1:B:483:LYS:NZ	2.23	0.70
3:V:14:SER:OG	3:V:108:LYS:NZ	2.24	0.70
2:S:162:PHE:CD1	2:S:163:PRO:HA	2.26	0.70
1:G:429:ARG:NH1	1:G:430:PRO:HD2	2.06	0.70
1:G:771:LEU:HD21	1:G:954:VAL:HG23	1.72	0.70
1:E:429:ARG:NH1	1:E:430:PRO:HD2	2.06	0.70
3:R:31:SER:O	3:R:66:ARG:NH1	2.25	0.69
1:F:123:LYS:HB3	1:F:126:GLU:HB2	1.71	0.69
1:F:460:ARG:NH1	2:S:101:VAL:HB	2.07	0.69
1:B:160:GLY:O	1:B:164:ARG:NH1	2.25	0.69
3:R:67:SER:N	3:R:68:GLY:HA2	2.07	0.69
1:H:579:PHE:HB2	1:H:724:HIS:HB3	1.74	0.69
1:B:561:PHE:HE1	1:B:733:ILE:HG23	1.58	0.69
2:S:11:LEU:HD11	2:S:162:PHE:HE2	1.57	0.69
1:F:114:LEU:HD22	1:F:168:PHE:O	1.93	0.68
1:G:886:ILE:HG23	1:G:928:LEU:HD22	1.76	0.68
2:I:22:CYS:HB3	2:I:79:ALA:HB3	1.75	0.68
2:I:11:LEU:HD12	2:I:163:PRO:HG3	1.76	0.67
1:C:123:LYS:HB3	1:C:126:GLU:HB2	1.77	0.67
2:K:22:CYS:HB3	2:K:79:ALA:HB3	1.76	0.67
3:L:34:ALA:HB3	3:L:89:GLN:HB3	1.77	0.67
1:H:329:ASN:HB3	1:H:332:HIS:HB2	1.77	0.67
1:D:189:GLU:O	1:D:193:ASN:ND2	2.28	0.66
1:E:852:SER:HB3	1:E:859:LEU:HD21	1.76	0.66
1:D:441:LEU:HD23	1:D:449:VAL:HG11	1.77	0.66
1:H:389:ASP:O	1:H:393:HIS:ND1	2.27	0.66
1:A:579:PHE:HB2	1:A:724:HIS:HB3	1.76	0.66
2:U:6:GLU:OE2	2:U:120:GLY:HA3	1.95	0.66
1:C:579:PHE:HB2	1:C:724:HIS:HB3	1.76	0.66
2:M:222:LYS:NZ	2:U:121:GLN:HB3	2.11	0.66
1:F:160:GLY:O	1:F:164:ARG:NH1	2.24	0.66
1:H:109:PHE:HZ	1:H:179:LYS:HG3	1.60	0.65
3:R:109:ARG:NH1	3:R:171:ASP:HA	2.10	0.65
1:G:579:PHE:HB2	1:G:724:HIS:HB3	1.77	0.65
2:K:40:ALA:HB3	2:K:43:LYS:HB2	1.79	0.65
1:D:852:SER:HB3	1:D:859:LEU:HD21	1.78	0.65
1:H:852:SER:HB3	1:H:859:LEU:HD21	1.79	0.65
1:E:579:PHE:HB2	1:E:724:HIS:HB3	1.77	0.65
2:Q:22:CYS:HB3	2:Q:79:ALA:HB3	1.78	0.65
1:F:389:ASP:O	1:F:393:HIS:ND1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:LYS:NZ	1:A:903:GLU:OE1	2.29	0.65
3:P:121:PRO:HD3	3:P:133:VAL:HG22	1.78	0.65
3:P:108:LYS:HZ2	3:P:108:LYS:HB3	1.62	0.64
2:U:22:CYS:HB3	2:U:79:ALA:HB3	1.78	0.64
1:D:604:LEU:HD21	1:D:648:LYS:HG3	1.79	0.64
1:D:203:GLN:NE2	1:D:218:PHE:O	2.27	0.64
1:E:771:LEU:HD21	1:E:954:VAL:HG23	1.78	0.64
2:O:22:CYS:HB3	2:O:79:ALA:HB3	1.79	0.64
2:U:40:ALA:HB3	2:U:43:LYS:HB2	1.80	0.64
3:N:150:LYS:HB2	3:N:194:ALA:HB3	1.81	0.64
1:A:291:HIS:HD2	1:A:293:PHE:H	1.46	0.63
3:T:107:ILE:HG21	3:T:172:SER:HB3	1.80	0.63
2:S:67:ARG:NH2	2:S:90:ASP:OD2	2.28	0.63
1:A:123:LYS:HB3	1:A:126:GLU:HB2	1.80	0.63
1:B:771:LEU:HD21	1:B:954:VAL:HG23	1.80	0.63
1:E:441:LEU:HD23	1:E:449:VAL:HG11	1.81	0.63
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.79	0.63
3:R:66:ARG:HG2	3:R:68:GLY:HA3	1.81	0.63
3:N:137:LEU:HD21	3:N:197:VAL:HG11	1.80	0.63
1:B:224:TYR:HA	1:B:228:THR:HB	1.81	0.62
1:E:189:GLU:O	1:E:193:ASN:ND2	2.32	0.62
1:F:552:LYS:HB3	1:F:559:LEU:HB3	1.80	0.62
1:B:565:ASP:O	1:B:568:PHE:CZ	2.52	0.62
1:E:166:ALA:O	1:E:168:PHE:N	2.31	0.62
1:E:616:LEU:HD21	1:E:638:GLN:HG3	1.81	0.62
2:M:22:CYS:HB3	2:M:79:ALA:HB3	1.79	0.62
3:N:92:SER:HB2	3:N:93:PRO:HD2	1.81	0.62
1:F:852:SER:HB3	1:F:859:LEU:HD21	1.82	0.62
3:V:22:THR:HG22	3:V:72:THR:HG22	1.81	0.62
1:G:429:ARG:HH11	1:G:430:PRO:HD2	1.64	0.62
1:H:552:LYS:HB3	1:H:559:LEU:HB3	1.80	0.62
2:S:11:LEU:HD12	2:S:163:PRO:HG3	1.80	0.62
2:S:40:ALA:HB3	2:S:43:LYS:HB2	1.82	0.62
1:C:635:ASN:HA	1:C:638:GLN:HB2	1.81	0.62
1:F:782:ARG:NH2	1:F:961:ARG:O	2.32	0.62
1:F:562:LYS:NZ	1:F:903:GLU:OE1	2.33	0.62
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.80	0.62
1:G:441:LEU:HD23	1:G:449:VAL:HG11	1.82	0.62
3:L:121:PRO:HD3	3:L:133:VAL:HG22	1.81	0.62
1:D:889:LEU:HD13	1:D:928:LEU:HD11	1.82	0.61
1:A:299:LYS:HD2	1:A:510:ILE:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:886:ILE:HG23	1:B:928:LEU:HD22	1.82	0.61
1:C:100:PRO:HG2	1:C:103:ILE:HB	1.82	0.61
1:F:767:ARG:NH1	1:F:1006:PRO:HA	2.16	0.61
3:R:61:ARG:NH1	3:R:80:PRO:HG2	2.15	0.61
3:X:107:ILE:HG21	3:X:172:SER:HB3	1.82	0.61
1:D:620:LEU:HD13	1:D:629:LEU:HG	1.83	0.61
3:R:22:THR:HG22	3:R:72:THR:HG22	1.81	0.61
1:C:126:GLU:OE2	1:C:164:ARG:NE	2.32	0.61
1:A:83:THR:O	1:A:261:ARG:NE	2.32	0.61
1:B:852:SER:HB3	1:B:859:LEU:HD21	1.81	0.61
1:A:852:SER:HB3	1:A:859:LEU:HD21	1.83	0.61
1:E:1000:ARG:HG2	1:F:1007:LEU:HD12	1.82	0.61
1:G:311:ARG:HB3	1:G:379:LEU:HB2	1.83	0.60
3:N:22:THR:HG22	3:N:72:THR:HG22	1.84	0.60
1:E:100:PRO:HG2	1:E:103:ILE:HB	1.83	0.60
3:X:212:ARG:HA	3:X:212:ARG:HH11	1.65	0.60
3:V:35:TRP:HB2	3:V:48:ILE:HB	1.82	0.60
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.82	0.60
1:G:562:LYS:NZ	1:G:907:TYR:OH	2.34	0.60
1:E:604:LEU:HD21	1:E:648:LYS:HG3	1.84	0.60
1:G:604:LEU:HD21	1:G:648:LYS:HG3	1.84	0.60
1:F:100:PRO:HG2	1:F:103:ILE:HB	1.82	0.60
2:W:67:ARG:NH2	2:W:90:ASP:OD2	2.30	0.60
1:A:635:ASN:HA	1:A:638:GLN:HB2	1.84	0.60
2:M:209:THR:HG21	3:V:169:SER:HB2	1.84	0.60
3:J:22:THR:HG22	3:J:72:THR:HG22	1.83	0.60
3:T:121:PRO:HB3	3:T:132:SER:H	1.67	0.60
2:O:91:THR:HB	2:O:127:VAL:H	1.66	0.60
3:P:35:TRP:HB2	3:P:48:ILE:HB	1.83	0.59
2:S:83:MET:HB3	2:S:86:LEU:HD21	1.83	0.59
3:V:109:ARG:NH1	3:V:171:ASP:HA	2.18	0.59
3:J:121:PRO:HD3	3:J:133:VAL:HG22	1.83	0.59
3:N:121:PRO:HD3	3:N:133:VAL:HG22	1.84	0.59
1:D:291:HIS:O	1:D:294:GLN:NE2	2.32	0.59
1:D:346:LEU:HD21	1:D:394:MET:HG2	1.83	0.59
1:B:346:LEU:HD21	1:B:394:MET:HG2	1.84	0.59
1:F:109:PHE:HZ	1:F:179:LYS:HG3	1.67	0.59
3:X:121:PRO:HD3	3:X:133:VAL:HG22	1.85	0.59
2:S:162:PHE:CG	2:S:163:PRO:CA	2.84	0.59
1:F:579:PHE:HB2	1:F:724:HIS:HB3	1.84	0.59
1:B:540:LEU:HB2	1:G:782:ARG:HH21	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:886:ILE:HG23	1:E:928:LEU:HD22	1.84	0.59
1:H:311:ARG:HD3	1:H:384:LEU:HD22	1.83	0.59
2:Q:6:GLU:OE2	2:Q:120:GLY:HA3	2.03	0.58
1:F:311:ARG:HD3	1:F:384:LEU:HD22	1.84	0.58
1:D:100:PRO:HG2	1:D:103:ILE:HB	1.85	0.58
1:G:417:LEU:HD11	1:G:614:ALA:HA	1.84	0.58
3:J:137:LEU:HD21	3:J:197:VAL:HG11	1.85	0.58
1:H:324:LYS:HB3	1:H:324:LYS:NZ	2.19	0.58
1:A:620:LEU:HD13	1:A:629:LEU:HG	1.84	0.58
1:G:127:TYR:O	1:G:129:GLN:N	2.36	0.58
1:D:311:ARG:NH2	1:D:664:GLU:OE2	2.36	0.58
3:V:108:LYS:HB3	3:V:108:LYS:NZ	2.18	0.58
2:Q:40:ALA:HB3	2:Q:43:LYS:HB2	1.86	0.58
1:B:579:PHE:HB2	1:B:724:HIS:HB3	1.84	0.58
2:M:83:MET:HB3	2:M:86:LEU:HD21	1.85	0.58
1:F:311:ARG:HB3	1:F:379:LEU:HB2	1.84	0.58
1:G:123:LYS:HB3	1:G:126:GLU:HB2	1.86	0.58
1:C:349:GLU:OE1	1:C:353:LYS:NZ	2.37	0.58
1:D:120:LYS:O	1:D:121:TYR:CG	2.55	0.58
1:F:720:LEU:HD12	1:F:723:LEU:HD11	1.85	0.58
2:W:40:ALA:HB3	2:W:43:LYS:HB2	1.86	0.58
1:G:616:LEU:HD21	1:G:638:GLN:HG3	1.86	0.58
2:K:83:MET:HB3	2:K:86:LEU:HD21	1.84	0.58
1:H:616:LEU:HD21	1:H:638:GLN:HG2	1.84	0.58
1:D:328:SER:OG	1:D:460:ARG:HG3	2.04	0.58
3:L:24:ARG:HD3	3:L:70:ASP:HB3	1.86	0.58
3:X:159:ASN:ND2	3:X:181:THR:O	2.37	0.58
2:O:40:ALA:HB3	2:O:43:LYS:HB2	1.86	0.58
1:F:117:GLY:O	1:F:118:THR:HG23	2.04	0.57
1:D:782:ARG:NH1	1:E:540:LEU:HD23	2.19	0.57
1:A:720:LEU:HD12	1:A:723:LEU:HD11	1.86	0.57
3:T:22:THR:HG22	3:T:72:THR:HG22	1.85	0.57
1:F:62:ARG:HD3	1:F:427:LYS:HE3	1.87	0.57
1:C:827:GLU:OE2	1:C:862:ARG:NH2	2.35	0.57
1:G:852:SER:HB3	1:G:859:LEU:HD21	1.85	0.57
1:C:83:THR:O	1:C:261:ARG:NE	2.34	0.57
1:G:889:LEU:HD13	1:G:928:LEU:HD11	1.86	0.57
1:D:886:ILE:HG23	1:D:928:LEU:HD22	1.84	0.57
3:L:137:LEU:HD21	3:L:197:VAL:HG11	1.86	0.57
1:G:782:ARG:NH1	1:G:784:GLU:HG2	2.19	0.57
1:D:179:LYS:HB3	1:D:179:LYS:NZ	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:795:TYR:HE1	1:C:951:ARG:HH12	1.51	0.57
1:C:324:LYS:NZ	1:C:324:LYS:HB3	2.19	0.57
1:C:599:LEU:HD23	1:C:662:ILE:HD12	1.86	0.57
1:C:809:GLU:OE1	1:C:893:ARG:NH1	2.36	0.57
2:Q:98:ARG:NH1	2:Q:118:TYR:HD2	2.02	0.57
1:F:770:GLN:HB3	1:F:1003:PRO:HG2	1.86	0.57
1:B:137:SER:OG	1:B:431:ARG:NH1	2.39	0.56
1:C:886:ILE:HG23	1:C:928:LEU:HD13	1.88	0.56
1:A:100:PRO:HG2	1:A:103:ILE:HB	1.87	0.56
2:M:222:LYS:HZ1	2:U:121:GLN:HB3	1.69	0.56
2:O:83:MET:HB3	2:O:86:LEU:HD21	1.87	0.56
1:F:192:LYS:HZ1	1:F:832:ILE:HG13	1.70	0.56
1:E:620:LEU:HD13	1:E:629:LEU:HG	1.86	0.56
3:T:109:ARG:NH1	3:T:171:ASP:O	2.39	0.56
3:X:121:PRO:HB3	3:X:132:SER:H	1.71	0.56
2:W:83:MET:HB3	2:W:86:LEU:HD21	1.86	0.56
3:X:109:ARG:NH1	3:X:171:ASP:O	2.38	0.56
1:H:915:GLN:OE1	1:H:920:ARG:NH2	2.39	0.56
1:A:599:LEU:HD23	1:A:662:ILE:HD12	1.88	0.56
3:T:5:THR:OG1	3:T:24:ARG:O	2.23	0.56
3:X:22:THR:HG22	3:X:72:THR:HG22	1.88	0.56
1:H:116:LEU:HD22	1:H:178:ALA:HB1	1.88	0.56
2:U:83:MET:HB3	2:U:86:LEU:HD21	1.87	0.56
1:B:460:ARG:HH21	2:K:101:VAL:HB	1.71	0.56
1:C:492:THR:HG22	1:C:499:GLN:HG2	1.87	0.55
3:L:159:ASN:ND2	3:L:181:THR:O	2.39	0.55
1:E:778:VAL:HG22	1:E:955:SER:HB2	1.88	0.55
1:E:63:GLU:HB2	1:E:79:SER:HB3	1.88	0.55
1:H:109:PHE:HD2	1:H:241:LEU:HD21	1.72	0.55
2:M:12:VAL:HG23	2:M:127:VAL:HG13	1.88	0.55
1:E:346:LEU:HD21	1:E:394:MET:HG2	1.88	0.55
1:C:311:ARG:NH1	1:C:379:LEU:O	2.35	0.55
1:D:389:ASP:O	1:D:393:HIS:ND1	2.36	0.55
2:Q:67:ARG:NH1	2:Q:85:SER:O	2.40	0.55
1:B:285:LEU:HD23	1:B:286:PRO:HD2	1.87	0.55
1:D:527:LYS:NZ	1:D:531:ILE:HD12	2.21	0.55
3:T:39:LYS:HD3	3:T:84:ALA:HB2	1.89	0.55
1:H:350:LEU:HB3	1:H:356:VAL:HB	1.89	0.55
1:E:83:THR:O	1:E:261:ARG:NE	2.38	0.55
3:J:195:CYS:N	3:J:208:LYS:O	2.39	0.55
1:H:722:ARG:HD2	1:H:756:LYS:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:39:GLN:OE1	3:X:38:GLN:NE2	2.39	0.55
3:X:39:LYS:HD3	3:X:84:ALA:HB2	1.88	0.55
1:F:460:ARG:HH11	2:S:101:VAL:HB	1.71	0.55
1:F:48:LYS:HB2	1:F:70:ALA:HA	1.87	0.55
3:X:80:PRO:HA	3:X:83:PHE:HE2	1.72	0.55
2:U:222:LYS:NZ	2:U:222:LYS:HB2	2.21	0.55
1:D:119:LYS:HE3	1:D:172:PRO:HB3	1.89	0.55
1:E:889:LEU:HD13	1:E:928:LEU:HD11	1.88	0.55
1:C:852:SER:HB3	1:C:859:LEU:HD21	1.88	0.55
1:E:127:TYR:O	1:E:129:GLN:N	2.40	0.55
1:A:116:LEU:HD22	1:A:178:ALA:HB1	1.87	0.55
2:I:40:ALA:HB3	2:I:43:LYS:HB2	1.88	0.54
3:P:108:LYS:NZ	3:P:108:LYS:HB3	2.22	0.54
1:H:357:ASN:HB2	1:H:378:ASP:OD2	2.07	0.54
1:B:304:ILE:HB	1:B:481:VAL:HG22	1.89	0.54
2:W:22:CYS:HB3	2:W:79:ALA:HB3	1.89	0.54
3:R:126:LEU:HD23	3:R:184:LYS:NZ	2.22	0.54
2:S:132:THR:HG23	2:S:163:PRO:HD3	1.89	0.54
3:T:121:PRO:HD3	3:T:133:VAL:HG22	1.89	0.54
2:S:166:VAL:HG12	2:S:216:HIS:CD2	2.42	0.54
1:A:108:HIS:NE2	1:A:189:GLU:OE2	2.39	0.54
1:G:675:ALA:HA	1:G:785:VAL:HG21	1.90	0.54
3:N:143:ARG:HH11	3:N:164:VAL:HG21	1.72	0.54
1:H:620:LEU:HB2	1:H:629:LEU:HD23	1.90	0.54
1:G:778:VAL:HG22	1:G:955:SER:HB2	1.88	0.54
3:L:39:LYS:HD3	3:L:84:ALA:HB2	1.89	0.54
1:D:880:GLU:OE2	1:D:884:LYS:HE2	2.07	0.54
1:F:324:LYS:HB3	1:F:324:LYS:NZ	2.23	0.54
3:P:34:ALA:HB3	3:P:89:GLN:HB3	1.90	0.54
1:E:187:ASP:HB2	1:E:223:LYS:HB2	1.90	0.54
1:D:405:GLY:O	1:D:407:GLN:NE2	2.41	0.54
1:H:886:ILE:HG23	1:H:928:LEU:HD13	1.90	0.54
1:F:599:LEU:HD23	1:F:662:ILE:HD12	1.90	0.54
1:F:114:LEU:HD12	1:F:149:TYR:OH	2.08	0.54
1:A:299:LYS:HD3	1:A:474:GLU:HA	1.90	0.54
1:C:347:LEU:HD13	1:C:359:LEU:HB2	1.89	0.54
1:E:139:ASN:OD1	1:E:140:ALA:N	2.41	0.53
2:W:11:LEU:HD12	2:W:163:PRO:HG3	1.90	0.53
3:L:31:SER:O	3:L:66:ARG:NH1	2.41	0.53
1:E:722:ARG:HG2	1:E:756:LYS:HB2	1.88	0.53
3:N:182:LEU:HD13	3:N:187:TYR:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:564:ASP:HB2	1:H:731:GLY:HA2	1.90	0.53
1:A:123:LYS:HD3	1:A:124:GLU:H	1.72	0.53
1:C:552:LYS:HB3	1:C:559:LEU:HB3	1.88	0.53
1:F:587:PRO:HB3	1:F:700:LEU:HD12	1.90	0.53
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.90	0.53
2:M:175:LEU:HD13	2:M:176:THR:H	1.73	0.53
1:G:574:LEU:HD22	1:G:729:LEU:HD22	1.91	0.53
1:B:620:LEU:HD13	1:B:629:LEU:HG	1.90	0.53
3:X:137:LEU:HD21	3:X:197:VAL:HG11	1.90	0.53
1:H:99:ASP:OD1	1:H:107:SER:OG	2.27	0.53
1:D:112:HIS:HD2	1:D:186:VAL:HG22	1.73	0.53
2:K:62:ASP:HA	2:K:65:LYS:HE2	1.91	0.53
2:S:162:PHE:CD2	2:S:163:PRO:CB	2.90	0.53
1:D:915:GLN:OE1	1:D:920:ARG:NH2	2.36	0.53
3:L:109:ARG:NH1	3:L:171:ASP:HA	2.23	0.53
1:F:346:LEU:HD21	1:F:394:MET:HG2	1.91	0.53
3:L:108:LYS:NZ	3:L:108:LYS:HB3	2.24	0.53
1:F:349:GLU:OE1	1:F:353:LYS:NZ	2.29	0.53
1:D:599:LEU:HD23	1:D:662:ILE:HD12	1.91	0.53
2:S:167:THR:OG1	2:S:215:ASN:HB3	2.09	0.53
1:B:52:ASN:OD1	1:B:53:HIS:N	2.40	0.53
1:G:129:GLN:HA	1:G:817:GLU:HG2	1.91	0.53
1:E:586:ASP:OD1	1:E:589:HIS:ND1	2.42	0.53
1:F:767:ARG:HH12	1:F:1006:PRO:HA	1.74	0.53
3:X:182:LEU:HD13	3:X:187:TYR:HB2	1.90	0.53
1:B:580:SER:HB2	1:B:723:LEU:HD23	1.91	0.53
1:H:113:MET:HG3	1:H:174:PHE:HD1	1.74	0.52
1:F:620:LEU:HB2	1:F:629:LEU:HD23	1.90	0.52
3:P:109:ARG:NH1	3:P:171:ASP:HA	2.24	0.52
1:H:894:LEU:HG	1:H:925:VAL:HG21	1.91	0.52
1:B:179:LYS:NZ	1:B:179:LYS:HB3	2.22	0.52
3:P:39:LYS:HD3	3:P:84:ALA:HB2	1.90	0.52
1:B:122:PRO:HA	1:B:173:LEU:HD11	1.91	0.52
1:G:944:LEU:O	1:G:951:ARG:NH2	2.42	0.52
1:G:289:PRO:HA	1:G:369:GLY:HA3	1.91	0.52
1:D:245:HIS:O	1:D:249:TYR:HB2	2.09	0.52
1:C:350:LEU:HB3	1:C:356:VAL:HB	1.90	0.52
1:E:565:ASP:O	1:E:568:PHE:CZ	2.62	0.52
3:V:197:VAL:HG23	3:V:206:VAL:HB	1.91	0.52
2:U:33:SER:HB2	2:U:99:ASP:OD2	2.09	0.52
3:T:135:CYS:HB3	3:T:178:SER:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:6:GLU:OE2	2:K:120:GLY:HA3	2.10	0.52
1:B:893:ARG:NH1	1:B:924:GLU:OE2	2.39	0.52
3:J:35:TRP:HB2	3:J:48:ILE:HB	1.90	0.52
1:A:886:ILE:HG23	1:A:928:LEU:HD13	1.91	0.52
3:T:196:GLU:OE1	3:T:207:THR:OG1	2.27	0.52
1:E:179:LYS:NZ	1:E:179:LYS:HB3	2.23	0.52
1:C:616:LEU:HD21	1:C:638:GLN:HG3	1.90	0.52
1:E:601:LYS:HD3	1:E:620:LEU:HB3	1.92	0.52
1:E:542:LYS:HB2	1:E:542:LYS:HZ2	1.75	0.52
3:R:35:TRP:HB2	3:R:48:ILE:HB	1.90	0.52
3:V:63:SER:HB2	3:V:74:THR:HB	1.91	0.52
2:K:117:ASP:OD1	2:K:118:TYR:N	2.43	0.52
2:O:216:HIS:CE1	2:O:219:SER:H	2.28	0.52
1:G:346:LEU:HD21	1:G:394:MET:HG2	1.91	0.52
2:S:170:TRP:HB2	2:S:175:LEU:HB2	1.92	0.52
1:G:599:LEU:HD23	1:G:662:ILE:HD12	1.91	0.52
1:C:795:TYR:HE1	1:C:951:ARG:NH1	2.06	0.52
1:B:176:GLU:CD	1:B:179:LYS:HZ1	2.13	0.52
1:G:587:PRO:HB3	1:G:700:LEU:HD23	1.91	0.52
3:X:196:GLU:OE1	3:X:207:THR:OG1	2.24	0.52
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.92	0.52
1:B:291:HIS:O	1:B:294:GLN:NE2	2.43	0.52
3:N:14:SER:HG	3:N:108:LYS:HZ3	1.53	0.52
3:N:115:SER:HB2	3:N:138:ASN:HB3	1.91	0.52
1:G:425:LYS:NZ	1:G:428:GLU:OE2	2.24	0.52
1:H:304:ILE:HB	1:H:481:VAL:HG22	1.92	0.52
1:H:756:LYS:NZ	1:H:756:LYS:HB3	2.25	0.51
1:E:574:LEU:HD22	1:E:729:LEU:HD22	1.91	0.51
2:U:216:HIS:CG	2:U:218:PRO:HD3	2.45	0.51
1:B:574:LEU:HD22	1:B:729:LEU:HD22	1.92	0.51
1:G:620:LEU:HD13	1:G:629:LEU:HG	1.92	0.51
1:D:229:ARG:NE	1:D:233:GLU:OE2	2.44	0.51
3:R:108:LYS:NZ	3:R:108:LYS:HB3	2.24	0.51
2:W:159:LYS:HB3	2:W:159:LYS:NZ	2.25	0.51
1:D:579:PHE:HB2	1:D:724:HIS:HB3	1.93	0.51
3:X:35:TRP:HB2	3:X:48:ILE:HB	1.91	0.51
1:F:915:GLN:OE1	1:F:920:ARG:NH2	2.41	0.51
2:I:37:VAL:HG22	2:I:47:TRP:HA	1.92	0.51
3:N:50:SER:OG	3:N:53:SER:OG	2.28	0.51
1:H:290:GLU:OE1	1:H:294:GLN:NE2	2.44	0.51
3:V:143:ARG:NE	3:V:143:ARG:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:108:LYS:HZ2	3:R:108:LYS:HB3	1.76	0.51
1:E:311:ARG:HB3	1:E:379:LEU:HB2	1.92	0.51
1:A:616:LEU:HD21	1:A:638:GLN:HG3	1.92	0.51
1:H:108:HIS:O	1:H:112:HIS:HD2	1.94	0.51
1:E:429:ARG:HH11	1:E:430:PRO:HD2	1.73	0.51
3:P:157:SER:OG	3:P:160:SER:OG	2.29	0.51
1:F:304:ILE:HB	1:F:481:VAL:HG22	1.93	0.51
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.92	0.51
1:D:341:GLU:OE2	1:D:605:ASN:ND2	2.35	0.51
1:E:139:ASN:HB3	1:E:150:TYR:CE2	2.46	0.51
3:T:137:LEU:HD21	3:T:197:VAL:HG11	1.91	0.51
1:D:551:ILE:HB	1:D:735:LYS:HE3	1.92	0.50
1:E:75:VAL:HG11	1:E:271:VAL:HG11	1.92	0.50
3:V:126:LEU:HD23	3:V:184:LYS:HG3	1.93	0.50
1:E:291:HIS:CD2	1:E:370:PHE:HB2	2.46	0.50
2:O:230:LYS:NZ	2:O:230:LYS:HB2	2.26	0.50
1:E:169:PHE:O	1:E:171:SER:N	2.43	0.50
1:F:75:VAL:HG11	1:F:271:VAL:HG11	1.93	0.50
3:J:212:ARG:HH11	3:J:212:ARG:HA	1.76	0.50
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.93	0.50
1:C:159:GLU:HG3	1:C:270:LEU:HD11	1.93	0.50
2:I:230:LYS:HB2	2:I:230:LYS:NZ	2.27	0.50
1:F:889:LEU:HD22	1:F:928:LEU:HG	1.93	0.50
1:C:706:ASP:O	1:C:711:ARG:NH2	2.44	0.50
2:O:159:LYS:NZ	2:O:159:LYS:HB3	2.26	0.50
1:H:493:GLU:OE1	1:H:496:TYR:N	2.43	0.50
1:C:346:LEU:HD21	1:C:394:MET:HG2	1.92	0.50
1:A:240:GLU:HA	1:A:243:LYS:HG2	1.93	0.50
1:G:291:HIS:CD2	1:G:370:PHE:HB2	2.46	0.50
1:C:601:LYS:HD3	1:C:620:LEU:HB3	1.94	0.50
1:G:100:PRO:HG2	1:G:103:ILE:HB	1.93	0.50
1:G:311:ARG:NH1	1:G:379:LEU:O	2.43	0.50
1:A:580:SER:HB2	1:A:723:LEU:HD23	1.94	0.50
1:E:48:LYS:HB2	1:E:70:ALA:HA	1.94	0.50
1:E:566:LYS:HE3	1:E:903:GLU:OE2	2.12	0.50
1:B:561:PHE:CE1	1:B:733:ILE:HG23	2.43	0.50
1:G:139:ASN:OD1	1:G:140:ALA:N	2.43	0.50
3:V:159:ASN:ND2	3:V:181:THR:O	2.45	0.50
3:N:109:ARG:HD3	3:N:172:SER:HB2	1.94	0.50
1:D:580:SER:HB2	1:D:723:LEU:HD23	1.93	0.50
1:E:587:PRO:HB3	1:E:700:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:17:ASP:OD1	3:N:18:ARG:N	2.45	0.49
1:F:894:LEU:HG	1:F:925:VAL:HG21	1.94	0.49
2:Q:230:LYS:NZ	2:Q:230:LYS:HB2	2.27	0.49
1:D:574:LEU:HD22	1:D:729:LEU:HD22	1.94	0.49
1:C:951:ARG:NH1	1:C:953:LYS:HD2	2.26	0.49
1:E:580:SER:HB2	1:E:723:LEU:HD23	1.93	0.49
1:E:159:GLU:HG3	1:E:270:LEU:HD21	1.94	0.49
3:R:39:LYS:HD3	3:R:84:ALA:HB2	1.94	0.49
1:A:865:ALA:HB2	1:A:983:ALA:HA	1.93	0.49
3:T:212:ARG:HH11	3:T:212:ARG:HA	1.77	0.49
1:B:564:ASP:HB2	1:B:731:GLY:HA2	1.95	0.49
2:O:6:GLU:OE2	2:O:120:GLY:HA3	2.12	0.49
1:B:768:GLU:OE2	1:B:796:GLN:NE2	2.45	0.49
1:C:319:ILE:HD13	1:C:373:PHE:HB2	1.94	0.49
1:D:870:MET:O	1:D:874:ILE:N	2.45	0.49
1:F:756:LYS:HB3	1:F:756:LYS:NZ	2.27	0.49
1:F:311:ARG:NH2	1:F:664:GLU:OE2	2.45	0.49
1:C:566:LYS:NZ	1:C:903:GLU:OE1	2.45	0.49
1:G:1000:ARG:HG2	1:H:1007:LEU:HD12	1.94	0.49
1:A:123:LYS:HD3	1:A:124:GLU:N	2.28	0.49
1:B:109:PHE:CZ	1:B:179:LYS:HG3	2.47	0.49
1:G:160:GLY:O	1:G:164:ARG:NH1	2.46	0.49
1:B:214:PRO:HA	1:B:217:LYS:HE3	1.94	0.49
1:C:720:LEU:HD12	1:C:723:LEU:HD11	1.94	0.49
2:W:175:LEU:HD13	2:W:198:VAL:HG21	1.95	0.49
3:L:109:ARG:HH12	3:L:171:ASP:HA	1.77	0.49
1:C:915:GLN:OE1	1:C:920:ARG:NH2	2.38	0.49
1:G:91:ASP:HB2	1:G:148:ASN:HD22	1.77	0.49
1:F:350:LEU:HB3	1:F:356:VAL:HB	1.92	0.49
1:C:402:ARG:NH1	1:C:468:LEU:O	2.45	0.49
1:G:596:TYR:OH	1:G:649:MET:O	2.30	0.49
2:M:40:ALA:HB3	2:M:43:LYS:HB2	1.95	0.49
1:H:580:SER:HB2	1:H:723:LEU:HD23	1.95	0.49
1:A:778:VAL:HG22	1:A:955:SER:HB2	1.95	0.49
2:W:47:TRP:CG	3:X:97:ILE:HB	2.47	0.49
1:F:960:ALA:HB3	1:F:963:MET:HG3	1.95	0.49
1:C:756:LYS:NZ	1:C:756:LYS:HB3	2.28	0.49
1:B:733:ILE:HG13	1:B:734:THR:H	1.78	0.49
1:H:599:LEU:HD23	1:H:662:ILE:HD12	1.95	0.49
1:D:304:ILE:HB	1:D:481:VAL:HG22	1.94	0.49
1:C:580:SER:HB2	1:C:723:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:806:MET:O	1:E:810:LEU:HB2	2.13	0.48
1:C:587:PRO:HB3	1:C:700:LEU:HD23	1.94	0.48
2:Q:142:PRO:HD2	2:Q:229:PRO:HA	1.95	0.48
1:B:224:TYR:O	1:B:229:ARG:HB2	2.13	0.48
1:F:580:SER:HB2	1:F:723:LEU:HD23	1.94	0.48
1:G:405:GLY:O	1:G:407:GLN:NE2	2.46	0.48
2:M:216:HIS:CE1	2:M:219:SER:H	2.30	0.48
2:W:6:GLU:OE2	2:W:120:GLY:HA3	2.13	0.48
3:V:61:ARG:NE	3:V:82:ASP:OD2	2.44	0.48
1:C:865:ALA:HB2	1:C:983:ALA:HA	1.95	0.48
1:E:417:LEU:HD11	1:E:614:ALA:HA	1.96	0.48
2:O:33:SER:HB2	2:O:99:ASP:OD2	2.13	0.48
1:B:770:GLN:HB3	1:B:1003:PRO:HG2	1.93	0.48
2:S:159:LYS:NZ	2:S:159:LYS:HB3	2.28	0.48
1:C:722:ARG:HD2	1:C:756:LYS:HB2	1.94	0.48
1:F:616:LEU:HD21	1:F:638:GLN:HG2	1.95	0.48
3:N:31:SER:O	3:N:66:ARG:NH2	2.46	0.48
1:A:213:HIS:CE1	1:A:292:PRO:HG3	2.49	0.48
1:D:167:GLN:HA	1:D:170:LEU:HD13	1.94	0.48
1:E:789:SER:OG	1:E:852:SER:O	2.24	0.48
2:Q:117:ASP:OD1	2:Q:118:TYR:N	2.44	0.48
3:X:165:THR:HG22	3:X:175:SER:H	1.77	0.48
1:D:770:GLN:HB3	1:D:1003:PRO:HG2	1.95	0.48
3:P:59:PRO:HB2	3:P:61:ARG:HG2	1.95	0.48
1:D:586:ASP:OD1	1:D:589:HIS:ND1	2.45	0.48
3:T:13:ALA:O	3:T:108:LYS:N	2.45	0.48
3:J:182:LEU:HD13	3:J:187:TYR:HB2	1.95	0.48
2:S:11:LEU:CD1	2:S:162:PHE:HE2	2.25	0.48
3:X:135:CYS:HB3	3:X:178:SER:HB3	1.96	0.48
1:E:298:LEU:HD21	1:E:318:PRO:HG2	1.95	0.48
1:G:580:SER:HB2	1:G:723:LEU:HD23	1.95	0.48
1:E:71:ASN:ND2	1:E:275:PHE:O	2.43	0.48
3:X:50:SER:OG	3:X:53:SER:OG	2.28	0.48
2:K:139:PRO:HG3	2:K:225:LYS:HD3	1.95	0.48
1:C:357:ASN:OD1	1:C:658:ARG:NH2	2.45	0.48
3:J:167:GLN:OE1	3:J:167:GLN:N	2.46	0.48
2:K:159:LYS:NZ	2:K:159:LYS:HB3	2.28	0.48
1:C:706:ASP:HB3	1:C:711:ARG:HH22	1.77	0.48
1:A:574:LEU:HD22	1:A:729:LEU:HD22	1.96	0.48
1:B:381:GLU:OE2	1:B:664:GLU:HG3	2.13	0.48
2:K:12:VAL:HG11	2:K:18:LEU:HG	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:831:TYR:CD2	1:D:832:ILE:HG13	2.49	0.48
1:C:374:ILE:HD12	1:C:376:ASN:HD21	1.78	0.48
3:T:28:SER:HB2	3:T:29:VAL:HA	1.96	0.48
3:T:50:SER:OG	3:T:53:SER:OG	2.29	0.48
1:D:631:VAL:HG12	1:D:638:GLN:HE21	1.78	0.48
1:C:213:HIS:CE1	1:C:292:PRO:HG3	2.49	0.48
1:D:357:ASN:HB2	1:D:378:ASP:OD2	2.14	0.48
1:D:557:SER:OG	1:D:746:GLU:OE1	2.21	0.48
1:E:213:HIS:CE1	1:E:292:PRO:HG3	2.48	0.48
3:V:37:GLN:HB2	3:V:47:LEU:HD11	1.96	0.48
3:N:135:CYS:HB3	3:N:178:SER:HB3	1.96	0.47
3:T:182:LEU:HD13	3:T:187:TYR:HB2	1.95	0.47
3:N:37:GLN:O	3:N:45:LYS:N	2.35	0.47
1:F:240:GLU:HA	1:F:243:LYS:HG2	1.96	0.47
2:I:216:HIS:CE1	2:I:219:SER:H	2.32	0.47
1:F:551:ILE:HB	1:F:735:LYS:HE3	1.96	0.47
1:A:350:LEU:HB3	1:A:356:VAL:HB	1.96	0.47
1:D:894:LEU:HG	1:D:925:VAL:HG21	1.95	0.47
2:S:117:ASP:OD1	2:S:118:TYR:N	2.45	0.47
2:U:133:LYS:HD3	2:U:191:LEU:HD11	1.95	0.47
1:D:309:ASP:N	1:D:672:ASN:OD1	2.43	0.47
1:H:587:PRO:HB3	1:H:700:LEU:HD12	1.95	0.47
1:D:194:VAL:HA	1:D:496:TYR:HD1	1.79	0.47
1:B:778:VAL:HG22	1:B:955:SER:HB2	1.95	0.47
1:G:821:ASN:O	1:G:825:THR:OG1	2.27	0.47
2:M:37:VAL:HG22	2:M:47:TRP:HA	1.96	0.47
1:C:779:TYR:HB2	1:C:992:ILE:HD12	1.97	0.47
1:B:75:VAL:HG11	1:B:271:VAL:HG11	1.96	0.47
1:B:459:PHE:CE2	1:B:461:PRO:HG3	2.49	0.47
2:S:89:GLU:OE2	2:S:89:GLU:N	2.47	0.47
1:E:507:ASP:O	1:E:507:ASP:OD1	2.31	0.47
1:H:311:ARG:HB3	1:H:379:LEU:HB2	1.96	0.47
1:D:561:PHE:HE1	1:D:733:ILE:HG23	1.79	0.47
1:A:791:ILE:HD11	1:A:793:ILE:HD11	1.95	0.47
1:C:945:ALA:HB3	1:C:948:ALA:HB2	1.95	0.47
1:F:357:ASN:HB2	1:F:378:ASP:OD2	2.15	0.47
1:G:71:ASN:ND2	1:G:275:PHE:O	2.44	0.47
1:H:291:HIS:CE1	1:H:318:PRO:HB3	2.50	0.47
3:R:22:THR:OG1	3:R:24:ARG:NH1	2.48	0.47
1:D:311:ARG:HB3	1:D:379:LEU:HB2	1.96	0.47
3:T:108:LYS:HA	3:T:141:TYR:OH	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:862:ARG:HH12	1:G:981:SER:N	2.13	0.47
1:F:806:MET:O	1:F:810:LEU:HB2	2.15	0.47
1:G:722:ARG:HG2	1:G:756:LYS:HB2	1.95	0.47
3:R:37:GLN:HB2	3:R:47:LEU:HD11	1.97	0.47
1:D:75:VAL:HG11	1:D:271:VAL:HG11	1.97	0.47
2:K:161:TYR:HE2	2:K:164:GLU:HG2	1.79	0.47
1:G:311:ARG:HD3	1:G:384:LEU:HD22	1.96	0.47
2:U:137:VAL:HG22	2:U:158:VAL:HG22	1.96	0.47
1:G:347:LEU:HD23	1:G:359:LEU:HB2	1.95	0.47
1:C:174:PHE:HD2	1:C:242:LEU:HD22	1.80	0.47
3:N:35:TRP:HB2	3:N:48:ILE:HB	1.95	0.47
2:U:29:VAL:O	2:U:53:SER:OG	2.33	0.47
1:B:109:PHE:HZ	1:B:179:LYS:HG3	1.79	0.47
2:O:37:VAL:HG22	2:O:47:TRP:HA	1.97	0.47
1:A:347:LEU:HD13	1:A:359:LEU:HB2	1.97	0.47
3:T:157:SER:OG	3:T:159:ASN:OD1	2.33	0.47
1:D:787:ASN:HA	1:D:961:ARG:HG2	1.97	0.47
1:C:253:LEU:HD22	1:C:285:LEU:HD23	1.95	0.47
1:A:319:ILE:HD13	1:A:373:PHE:HB2	1.95	0.47
1:D:237:VAL:HA	1:D:239:GLN:HB3	1.96	0.47
1:G:75:VAL:HG11	1:G:271:VAL:HG11	1.97	0.47
1:H:810:LEU:HG	1:H:928:LEU:HD21	1.97	0.47
1:E:894:LEU:HG	1:E:925:VAL:HG21	1.96	0.47
1:E:307:ILE:C	1:E:483:LYS:HZ1	2.19	0.47
1:E:94:ILE:O	1:E:147:THR:OG1	2.23	0.47
2:M:89:GLU:N	2:M:89:GLU:OE2	2.47	0.47
1:C:599:LEU:HD21	1:C:659:PHE:HA	1.97	0.46
3:X:38:GLN:O	3:X:84:ALA:HB1	2.15	0.46
1:A:908:TRP:CE2	1:A:912:ILE:HD11	2.50	0.46
3:T:113:ALA:HA	3:T:114:PRO:HD3	1.81	0.46
2:W:59:SER:HB2	3:X:95:PHE:HB3	1.97	0.46
2:S:230:LYS:HB2	2:S:230:LYS:NZ	2.29	0.46
2:M:159:LYS:HB3	2:M:159:LYS:NZ	2.30	0.46
1:B:732:ASN:O	1:B:733:ILE:HB	2.15	0.46
1:H:329:ASN:ND2	1:H:456:LEU:HD21	2.30	0.46
1:F:56:LYS:NZ	1:F:62:ARG:O	2.40	0.46
1:B:179:LYS:HB3	1:B:179:LYS:HZ2	1.80	0.46
1:G:688:LEU:HD13	1:G:696:THR:HG22	1.96	0.46
2:S:158:VAL:HG12	2:S:161:TYR:CD2	2.50	0.46
2:Q:159:LYS:HB3	2:Q:159:LYS:NZ	2.29	0.46
1:H:402:ARG:NH1	1:H:468:LEU:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:HIS:O	1:B:249:TYR:HB2	2.16	0.46
1:H:253:LEU:HD21	1:H:285:LEU:HG	1.97	0.46
2:K:230:LYS:HB2	2:K:230:LYS:NZ	2.29	0.46
1:D:194:VAL:HA	1:D:496:TYR:CD1	2.50	0.46
3:N:34:ALA:HB3	3:N:89:GLN:HB3	1.97	0.46
3:X:108:LYS:HA	3:X:141:TYR:OH	2.15	0.46
2:K:161:TYR:OH	2:K:164:GLU:OE2	2.33	0.46
1:D:564:ASP:HB2	1:D:731:GLY:HA2	1.98	0.46
1:F:716:ILE:HB	1:F:717:PRO:HD3	1.97	0.46
1:F:908:TRP:O	1:F:912:ILE:HG12	2.16	0.46
1:D:308:LYS:O	1:D:483:LYS:NZ	2.48	0.46
2:I:12:VAL:HG11	2:I:18:LEU:HG	1.97	0.46
1:D:587:PRO:HB3	1:D:700:LEU:HD23	1.97	0.46
1:H:109:PHE:O	1:H:113:MET:HB2	2.15	0.46
1:F:109:PHE:CZ	1:F:179:LYS:HG3	2.50	0.46
1:D:94:ILE:HG13	1:D:248:TYR:HB3	1.97	0.46
3:T:4:MET:HG3	3:T:26:SER:HB3	1.96	0.46
3:P:22:THR:HG22	3:P:72:THR:HG22	1.98	0.46
2:I:159:LYS:NZ	2:I:159:LYS:HB3	2.31	0.46
1:E:635:ASN:HA	1:E:638:GLN:HB2	1.96	0.46
3:T:40:PRO:HG2	3:T:166:GLU:HG2	1.96	0.46
1:H:706:ASP:O	1:H:711:ARG:NH2	2.49	0.46
3:J:61:ARG:HD2	3:J:77:SER:O	2.15	0.46
1:A:915:GLN:OE1	1:A:920:ARG:NH2	2.45	0.46
2:Q:171:ASN:HB2	2:Q:174:ALA:HB3	1.97	0.46
3:T:80:PRO:HA	3:T:83:PHE:HE2	1.80	0.46
1:D:767:ARG:NH1	1:D:1006:PRO:HA	2.31	0.46
3:J:112:ALA:HB3	3:J:140:PHE:HA	1.97	0.46
3:N:40:PRO:HG2	3:N:166:GLU:HG2	1.97	0.46
1:G:309:ASP:N	1:G:672:ASN:OD1	2.44	0.46
1:G:806:MET:O	1:G:810:LEU:HB2	2.16	0.46
1:C:299:LYS:HD2	1:C:510:ILE:HD13	1.98	0.46
2:K:216:HIS:CE1	2:K:219:SER:H	2.33	0.46
3:T:35:TRP:HB2	3:T:48:ILE:HB	1.97	0.46
1:F:83:THR:O	1:F:261:ARG:NE	2.38	0.46
1:E:754:HIS:ND1	1:E:754:HIS:O	2.49	0.46
1:C:557:SER:OG	1:C:746:GLU:OE1	2.27	0.46
1:E:174:PHE:O	1:E:238:ARG:NH1	2.49	0.46
1:G:245:HIS:O	1:G:249:TYR:HB2	2.16	0.46
1:F:319:ILE:HD13	1:F:373:PHE:HB2	1.97	0.46
1:E:224:TYR:HA	1:E:228:THR:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:HD21	1:A:394:MET:HG2	1.98	0.46
1:A:587:PRO:HB3	1:A:700:LEU:HD23	1.97	0.46
1:B:425:LYS:HB3	1:B:425:LYS:NZ	2.31	0.46
2:U:50:SER:HB2	2:U:59:SER:HB3	1.97	0.46
3:R:126:LEU:HD23	3:R:184:LYS:HZ3	1.79	0.45
1:F:886:ILE:HG23	1:F:928:LEU:HD13	1.98	0.45
1:C:864:GLU:HG2	1:C:986:LEU:HD21	1.98	0.45
1:A:716:ILE:HB	1:A:717:PRO:HD3	1.98	0.45
1:C:791:ILE:HD11	1:C:793:ILE:HD11	1.97	0.45
3:T:38:GLN:O	3:T:84:ALA:HB1	2.16	0.45
3:P:61:ARG:HD2	3:P:77:SER:O	2.17	0.45
1:A:688:LEU:HD13	1:A:696:THR:HG22	1.98	0.45
1:B:94:ILE:HG13	1:B:248:TYR:HB3	1.97	0.45
1:A:304:ILE:HB	1:A:481:VAL:HG22	1.97	0.45
1:F:460:ARG:HH12	2:S:102:MET:H	1.64	0.45
2:M:140:LEU:HB3	3:N:119:PHE:CD1	2.52	0.45
1:C:688:LEU:HD13	1:C:696:THR:HG22	1.97	0.45
1:B:562:LYS:NZ	1:B:903:GLU:OE2	2.47	0.45
1:D:56:LYS:NZ	1:D:62:ARG:O	2.40	0.45
1:E:557:SER:OG	1:E:746:GLU:OE1	2.23	0.45
2:K:33:SER:HB2	2:K:99:ASP:OD2	2.16	0.45
1:G:586:ASP:OD1	1:G:589:HIS:ND1	2.50	0.45
1:D:139:ASN:HB3	1:D:150:TYR:CZ	2.51	0.45
1:F:869:THR:O	1:F:872:LYS:HG3	2.17	0.45
1:G:139:ASN:HB3	1:G:150:TYR:CE2	2.51	0.45
2:S:161:TYR:CE2	2:S:194:LEU:HD22	2.51	0.45
2:K:47:TRP:HE1	2:K:50:SER:HG	1.63	0.45
2:K:93:VAL:HG22	2:K:124:LEU:HB2	1.99	0.45
1:B:194:VAL:HA	1:B:496:TYR:CD1	2.52	0.45
1:H:770:GLN:HB3	1:H:1003:PRO:HG2	1.97	0.45
1:D:120:LYS:O	1:D:121:TYR:CD1	2.70	0.45
1:G:698:ASP:HA	1:G:701:LYS:HE2	1.98	0.45
1:G:779:TYR:HB2	1:G:992:ILE:HD12	1.98	0.45
1:G:578:PHE:O	1:G:626:GLY:HA3	2.17	0.45
1:H:346:LEU:HD21	1:H:394:MET:HG2	1.97	0.45
1:E:100:PRO:HA	1:E:101:PRO:HD3	1.87	0.45
2:M:175:LEU:HD22	2:M:175:LEU:HA	1.83	0.45
1:C:855:PRO:HA	1:C:856:PRO:HD3	1.84	0.45
1:B:806:MET:O	1:B:810:LEU:HB2	2.17	0.45
3:R:36:TYR:HE1	3:R:89:GLN:HE21	1.62	0.45
1:E:832:ILE:HB	1:E:851:GLN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ASP:O	1:B:393:HIS:ND1	2.42	0.45
1:H:565:ASP:OD1	1:H:565:ASP:N	2.50	0.45
1:E:150:TYR:HD2	1:E:431:ARG:HG2	1.82	0.45
3:N:31:SER:HB2	3:N:66:ARG:HH22	1.82	0.45
1:C:388:GLU:OE2	1:C:512:LYS:NZ	2.40	0.45
1:G:214:PRO:HA	1:G:217:LYS:HG3	1.99	0.45
1:G:285:LEU:HD23	1:G:286:PRO:HD2	1.99	0.45
1:G:557:SER:OG	1:G:746:GLU:OE1	2.25	0.45
2:M:67:ARG:NH1	2:M:85:SER:O	2.50	0.45
2:U:55:TYR:HE2	2:U:105:TRP:HA	1.81	0.45
2:S:32:TYR:CZ	2:S:102:MET:HG2	2.52	0.45
1:D:852:SER:OG	1:D:853:GLU:N	2.50	0.45
1:A:311:ARG:NH1	1:A:379:LEU:O	2.49	0.45
1:C:100:PRO:HA	1:C:101:PRO:HD3	1.86	0.45
2:Q:141:ALA:HA	2:Q:142:PRO:HD3	1.87	0.45
1:B:587:PRO:HB3	1:B:700:LEU:HD23	1.97	0.45
1:C:304:ILE:HB	1:C:481:VAL:HG22	1.99	0.45
1:E:855:PRO:HA	1:E:856:PRO:HD3	1.86	0.45
1:E:779:TYR:HB2	1:E:992:ILE:HD12	1.98	0.45
1:F:810:LEU:HG	1:F:928:LEU:HD21	1.99	0.44
1:D:771:LEU:HD21	1:D:954:VAL:HG23	1.98	0.44
1:D:864:GLU:HG2	1:D:986:LEU:HD21	1.98	0.44
1:H:465:GLU:OE2	2:W:110:TYR:HD2	2.00	0.44
3:R:61:ARG:CZ	3:R:80:PRO:HG2	2.47	0.44
1:H:806:MET:O	1:H:810:LEU:HB2	2.16	0.44
3:P:66:ARG:HG2	3:P:68:GLY:H	1.82	0.44
1:H:259:LEU:HD23	1:H:430:PRO:HB3	1.99	0.44
1:C:894:LEU:HD11	1:C:925:VAL:HG11	2.00	0.44
2:U:162:PHE:HA	2:U:163:PRO:HA	1.63	0.44
1:B:355:TRP:HB3	1:B:390:ILE:HD11	1.99	0.44
3:N:40:PRO:HA	3:N:41:GLY:HA2	1.48	0.44
1:G:94:ILE:HG13	1:G:248:TYR:HB3	1.99	0.44
3:V:39:LYS:HD3	3:V:84:ALA:HB2	1.99	0.44
2:W:117:ASP:OD1	2:W:118:TYR:N	2.49	0.44
3:X:92:SER:HB2	3:X:93:PRO:HD2	1.99	0.44
2:Q:98:ARG:HH11	2:Q:118:TYR:HD2	1.64	0.44
3:J:39:LYS:HD3	3:J:84:ALA:HB2	2.00	0.44
3:J:138:ASN:O	3:J:139:ASN:ND2	2.50	0.44
1:D:793:ILE:HD12	1:D:863:VAL:HG11	1.99	0.44
1:A:468:LEU:HD23	1:A:471:LEU:HD12	2.00	0.44
1:B:557:SER:OG	1:B:746:GLU:OE1	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ARG:HD3	1:A:384:LEU:HD22	1.98	0.44
1:F:564:ASP:HB2	1:F:731:GLY:HA2	1.98	0.44
1:B:716:ILE:HB	1:B:717:PRO:HD3	1.99	0.44
1:E:214:PRO:HA	1:E:217:LYS:HG3	1.98	0.44
1:F:73:ILE:HG13	1:F:251:SER:HB2	1.99	0.44
1:B:49:ARG:NH2	1:B:68:GLU:OE1	2.49	0.44
1:F:722:ARG:HD2	1:F:756:LYS:HB2	2.00	0.44
2:K:37:VAL:HG22	2:K:47:TRP:HA	2.00	0.44
1:B:100:PRO:HA	1:B:101:PRO:HD3	1.90	0.44
1:B:528:ASN:HB3	1:B:531:ILE:HG13	1.99	0.44
3:L:113:ALA:HA	3:L:114:PRO:HD3	1.84	0.44
2:U:182:PHE:CD1	3:V:165:THR:HB	2.53	0.44
1:A:572:ALA:HA	1:A:731:GLY:HA3	1.99	0.44
3:P:108:LYS:HZ2	3:P:108:LYS:CB	2.29	0.44
1:G:635:ASN:HA	1:G:638:GLN:HB2	1.99	0.44
1:A:729:LEU:HD12	1:A:738:ALA:HB1	2.00	0.44
2:S:141:ALA:HA	2:S:142:PRO:HD3	1.83	0.44
3:P:24:ARG:HD3	3:P:70:ASP:HB3	1.98	0.44
3:R:6:GLN:HB3	3:R:101:GLN:HE22	1.82	0.44
1:D:179:LYS:HB3	1:D:179:LYS:HZ2	1.82	0.44
1:C:580:SER:HA	1:C:581:PRO:HD3	1.89	0.44
1:F:90:LEU:HD13	1:F:169:PHE:CE2	2.52	0.44
1:C:832:ILE:HB	1:C:851:GLN:HB3	1.99	0.44
1:H:245:HIS:O	1:H:249:TYR:HB2	2.18	0.44
1:G:296:GLU:HB3	3:L:61:ARG:HH11	1.82	0.44
1:G:109:PHE:HZ	1:G:179:LYS:HG3	1.83	0.44
1:B:119:LYS:HB2	1:B:119:LYS:HE3	1.85	0.44
3:P:212:ARG:HH11	3:P:212:ARG:HA	1.83	0.44
1:B:527:LYS:NZ	1:B:531:ILE:HD12	2.33	0.44
1:A:230:PRO:HB3	1:A:235:ILE:HB	2.00	0.44
1:C:461:PRO:HD2	2:M:114:TYR:OH	2.18	0.44
3:J:17:ASP:OD1	3:J:18:ARG:N	2.49	0.44
1:D:806:MET:O	1:D:810:LEU:HB2	2.18	0.44
2:M:6:GLU:OE2	2:M:120:GLY:HA3	2.18	0.44
2:I:162:PHE:HA	2:I:163:PRO:HA	1.77	0.43
1:D:100:PRO:HA	1:D:101:PRO:HD3	1.87	0.43
3:P:168:ASP:OD2	3:P:171:ASP:OD2	2.36	0.43
1:B:176:GLU:HA	1:B:179:LYS:NZ	2.33	0.43
2:I:100:ARG:HA	2:I:117:ASP:OD2	2.18	0.43
1:B:324:LYS:HE3	1:B:325:TYR:CZ	2.52	0.43
1:G:389:ASP:O	1:G:393:HIS:ND1	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:965:SER:HA	1:G:966:ASN:HA	1.69	0.43
1:F:156:GLU:HG3	1:F:157:HIS:ND1	2.33	0.43
1:H:791:ILE:HD11	1:H:793:ILE:HD11	1.99	0.43
1:H:240:GLU:HA	1:H:243:LYS:HG2	2.00	0.43
1:H:88:ALA:HB3	1:H:151:PHE:CE1	2.53	0.43
1:D:63:GLU:HB2	1:D:79:SER:HB3	2.00	0.43
3:R:113:ALA:HA	3:R:114:PRO:HD3	1.81	0.43
1:C:716:ILE:HB	1:C:717:PRO:HD3	1.98	0.43
3:R:34:ALA:HB3	3:R:89:GLN:HB3	2.01	0.43
3:X:37:GLN:HB2	3:X:47:LEU:HD11	1.99	0.43
3:T:37:GLN:O	3:T:45:LYS:N	2.38	0.43
1:A:802:THR:HG23	1:A:924:GLU:HG2	2.00	0.43
1:D:552:LYS:HB3	1:D:559:LEU:HB3	2.01	0.43
1:H:602:ASP:OD2	1:H:658:ARG:HD3	2.18	0.43
3:P:79:GLN:HB2	3:P:82:ASP:OD2	2.18	0.43
1:E:578:PHE:O	1:E:626:GLY:HA3	2.17	0.43
3:L:92:SER:OG	3:L:96:LEU:HB2	2.18	0.43
1:F:557:SER:OG	1:F:746:GLU:OE1	2.26	0.43
1:C:724:HIS:HB2	1:C:758:LEU:HD12	1.99	0.43
1:B:93:HIS:CD2	1:B:285:LEU:HD21	2.53	0.43
1:C:240:GLU:HA	1:C:243:LYS:HG2	2.00	0.43
1:C:245:HIS:O	1:C:249:TYR:HB2	2.18	0.43
1:G:357:ASN:HB2	1:G:378:ASP:OD2	2.19	0.43
1:B:915:GLN:OE1	1:B:920:ARG:NH2	2.38	0.43
1:C:806:MET:O	1:C:810:LEU:HB2	2.19	0.43
1:G:111:GLN:HG2	1:G:149:TYR:CE2	2.54	0.43
1:H:852:SER:OG	1:H:853:GLU:N	2.51	0.43
1:F:357:ASN:OD1	1:F:658:ARG:NH2	2.52	0.43
1:B:810:LEU:HD12	1:B:931:LEU:HD23	2.00	0.43
1:H:492:THR:HG22	1:H:499:GLN:HG2	2.00	0.43
1:E:552:LYS:HB3	1:E:559:LEU:HB3	2.00	0.43
2:I:98:ARG:HH11	2:I:118:TYR:HD2	1.66	0.43
1:H:413:GLU:OE2	1:H:531:ILE:HD11	2.19	0.43
2:U:161:TYR:OH	2:U:164:GLU:OE2	2.28	0.43
2:O:187:GLN:HA	3:P:161:GLN:NE2	2.34	0.43
3:X:141:TYR:CD1	3:X:142:PRO:HA	2.54	0.43
1:G:229:ARG:NE	1:G:233:GLU:OE2	2.52	0.43
1:D:49:ARG:HH12	1:D:51:GLY:HA2	1.83	0.43
2:I:23:ALA:HA	2:I:78:THR:HG23	2.01	0.43
1:A:158:LEU:HD22	1:A:162:LEU:HD12	2.01	0.43
2:W:12:VAL:HG11	2:W:18:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:986:LEU:HA	1:B:987:PRO:HD3	1.89	0.43
2:Q:14:PRO:HG3	2:Q:127:VAL:HG12	1.99	0.43
3:X:113:ALA:HA	3:X:114:PRO:HD3	1.82	0.43
2:W:33:SER:HB2	2:W:99:ASP:OD2	2.18	0.43
1:F:688:LEU:HD13	1:F:696:THR:HG22	2.00	0.43
1:D:565:ASP:OD1	1:D:565:ASP:N	2.48	0.43
3:V:70:ASP:OD1	3:V:70:ASP:N	2.49	0.43
1:A:332:HIS:CE1	1:A:363:GLN:HE21	2.37	0.43
1:H:460:ARG:NH2	2:W:102:MET:O	2.49	0.43
1:H:355:TRP:HB3	1:H:390:ILE:HD11	2.01	0.43
3:V:34:ALA:HB3	3:V:89:GLN:HB3	2.00	0.43
1:C:908:TRP:CE2	1:C:912:ILE:HD11	2.54	0.43
1:B:852:SER:OG	1:B:853:GLU:N	2.51	0.43
3:T:141:TYR:CD1	3:T:142:PRO:HA	2.54	0.43
2:S:158:VAL:HG12	2:S:161:TYR:HD2	1.83	0.43
3:P:37:GLN:HB2	3:P:47:LEU:HD11	2.00	0.43
1:F:93:HIS:CD2	1:F:285:LEU:HD21	2.54	0.43
2:K:167:THR:OG1	2:K:215:ASN:HB3	2.19	0.43
1:H:319:ILE:HD13	1:H:373:PHE:HB2	2.01	0.43
2:U:32:TYR:CZ	2:U:102:MET:HG2	2.54	0.43
3:P:17:ASP:OD1	3:P:18:ARG:N	2.48	0.43
1:A:174:PHE:HD2	1:A:242:LEU:HD22	1.84	0.43
1:C:48:LYS:HB2	1:C:70:ALA:HA	2.01	0.43
1:E:123:LYS:HB3	1:E:126:GLU:HB2	1.99	0.43
1:A:771:LEU:HB2	1:A:952:HIS:HB3	2.01	0.43
1:B:489:THR:HA	1:B:501:LYS:HB2	2.00	0.43
3:T:196:GLU:OE2	3:T:205:PRO:HB3	2.19	0.42
1:C:986:LEU:HA	1:C:987:PRO:HD3	1.92	0.42
1:D:355:TRP:HB3	1:D:390:ILE:HD11	2.01	0.42
1:E:908:TRP:CZ2	1:E:912:ILE:HD11	2.53	0.42
1:E:309:ASP:N	1:E:672:ASN:OD1	2.46	0.42
1:C:578:PHE:O	1:C:626:GLY:HA3	2.19	0.42
1:E:332:HIS:ND1	1:E:363:GLN:OE1	2.52	0.42
1:H:200:ARG:O	1:H:204:LEU:HB2	2.19	0.42
1:E:565:ASP:O	1:E:568:PHE:CE2	2.71	0.42
3:X:137:LEU:HB2	3:X:176:LEU:HB3	2.02	0.42
2:K:164:GLU:OE2	2:K:184:ALA:HB2	2.19	0.42
1:F:90:LEU:HG	1:F:256:VAL:HG12	2.01	0.42
1:G:894:LEU:HG	1:G:925:VAL:HG21	2.01	0.42
1:E:599:LEU:HD23	1:E:662:ILE:HD12	2.00	0.42
3:X:68:GLY:HA2	3:X:69:THR:HA	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:552:LYS:HB3	1:G:559:LEU:HB3	2.01	0.42
1:D:324:LYS:HE3	1:D:325:TYR:CZ	2.54	0.42
1:H:75:VAL:HG11	1:H:271:VAL:HG11	2.02	0.42
1:D:88:ALA:HB3	1:D:151:PHE:CE1	2.54	0.42
1:D:716:ILE:HB	1:D:717:PRO:HD3	2.00	0.42
2:Q:89:GLU:N	2:Q:89:GLU:OE2	2.52	0.42
1:C:123:LYS:HB2	1:C:123:LYS:HE3	1.47	0.42
1:A:291:HIS:O	1:A:294:GLN:NE2	2.52	0.42
3:N:137:LEU:HB2	3:N:176:LEU:HB3	2.01	0.42
1:D:176:GLU:HA	1:D:179:LYS:NZ	2.34	0.42
2:K:141:ALA:HA	2:K:142:PRO:HD3	1.87	0.42
1:B:67:LEU:HD21	1:B:268:THR:HG23	2.02	0.42
1:C:769:VAL:HA	1:C:1004:LEU:HD23	2.00	0.42
3:R:79:GLN:HB2	3:R:80:PRO:HD3	2.00	0.42
1:G:722:ARG:NH2	1:H:706:ASP:OD2	2.50	0.42
1:B:48:LYS:HE3	1:B:70:ALA:HA	2.01	0.42
1:A:604:LEU:HD21	1:A:648:LYS:HG3	2.01	0.42
2:M:32:TYR:CZ	2:M:102:MET:HG2	2.54	0.42
2:Q:168:VAL:HG22	2:Q:214:VAL:HG22	2.00	0.42
1:A:894:LEU:HG	1:A:925:VAL:HG21	2.01	0.42
1:B:446:LEU:H	1:B:446:LEU:HD22	1.84	0.42
3:V:108:LYS:HB3	3:V:108:LYS:HZ3	1.85	0.42
1:D:189:GLU:O	1:D:192:LYS:HG2	2.20	0.42
1:B:461:PRO:HB2	2:K:112:TYR:CZ	2.55	0.42
2:U:100:ARG:HA	2:U:117:ASP:OD2	2.18	0.42
1:A:298:LEU:HD21	1:A:318:PRO:HG2	2.02	0.42
1:H:83:THR:O	1:H:261:ARG:NE	2.39	0.42
1:C:111:GLN:HG2	1:C:149:TYR:CE2	2.54	0.42
1:C:771:LEU:HB2	1:C:952:HIS:HB3	2.01	0.42
2:M:162:PHE:HA	2:M:163:PRO:HA	1.81	0.42
2:Q:12:VAL:HG11	2:Q:18:LEU:HG	2.01	0.42
1:A:460:ARG:HA	1:A:461:PRO:HD3	1.77	0.42
1:H:647:GLU:O	1:H:651:THR:OG1	2.32	0.42
1:H:250:SER:HB3	1:H:283:VAL:HG12	2.01	0.42
1:H:139:ASN:OD1	1:H:140:ALA:N	2.47	0.42
3:X:126:LEU:HD23	3:X:184:LYS:NZ	2.34	0.42
1:A:160:GLY:O	1:A:164:ARG:NH1	2.52	0.42
2:Q:216:HIS:ND1	2:Q:219:SER:O	2.42	0.42
1:E:688:LEU:HD13	1:E:696:THR:HG22	2.00	0.42
1:C:311:ARG:HD3	1:C:384:LEU:HB2	2.01	0.42
1:H:429:ARG:HA	1:H:430:PRO:HD3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:PHE:O	1:A:168:PHE:HB2	2.20	0.42
1:D:855:PRO:HA	1:D:856:PRO:HD3	1.86	0.42
2:O:140:LEU:HB3	3:P:119:PHE:CD1	2.55	0.42
1:A:806:MET:O	1:A:810:LEU:HB2	2.19	0.42
1:D:506:PRO:HB2	1:D:509:VAL:HG23	2.01	0.42
1:G:306:PRO:C	1:G:483:LYS:HZ2	2.23	0.42
3:N:204:SER:HA	3:N:205:PRO:HD3	1.94	0.42
2:S:6:GLU:OE1	2:S:6:GLU:N	2.53	0.42
1:C:88:ALA:HB3	1:C:151:PHE:CE1	2.55	0.42
1:F:63:GLU:HB2	1:F:79:SER:HB3	2.02	0.42
1:B:894:LEU:HG	1:B:925:VAL:HG21	2.02	0.42
1:C:181:ARG:NH1	1:C:825:THR:O	2.52	0.42
1:D:623:THR:HG23	1:D:625:TYR:H	1.83	0.42
3:L:108:LYS:HB3	3:L:108:LYS:HZ2	1.85	0.42
1:G:229:ARG:HB3	1:G:230:PRO:HD3	2.01	0.42
1:D:623:THR:CG2	1:D:625:TYR:H	2.33	0.42
1:F:96:SER:O	1:F:217:LYS:HD2	2.19	0.42
3:J:204:SER:HA	3:J:205:PRO:HD3	1.93	0.42
3:J:142:PRO:HB2	3:J:144:GLU:HG2	2.01	0.42
1:G:1009:LYS:HA	1:G:1010:PRO:HD3	1.94	0.42
1:H:110:LEU:O	1:H:114:LEU:HG	2.20	0.42
2:K:67:ARG:HH12	2:K:86:LEU:HA	1.85	0.42
1:D:831:TYR:HD2	1:D:832:ILE:HG13	1.83	0.42
1:H:139:ASN:HB3	1:H:150:TYR:CE1	2.55	0.42
1:H:771:LEU:HB2	1:H:952:HIS:HB3	2.02	0.42
1:F:259:LEU:HD23	1:F:430:PRO:HB3	2.01	0.42
1:F:706:ASP:HB3	1:F:711:ARG:HH22	1.85	0.42
2:I:157:LEU:HD13	2:I:195:SER:HB3	2.02	0.42
1:G:76:LEU:HB3	1:G:257:VAL:HG22	2.01	0.42
1:C:675:ALA:HA	1:C:785:VAL:HG21	2.02	0.42
1:H:716:ILE:HB	1:H:717:PRO:HD3	2.01	0.42
1:H:893:ARG:NH1	1:H:924:GLU:OE2	2.46	0.42
1:D:418:ASN:HB3	1:D:454:TYR:O	2.20	0.42
1:A:80:ASP:O	1:A:83:THR:HG22	2.20	0.41
1:C:80:ASP:O	1:C:83:THR:HG22	2.20	0.41
1:C:944:LEU:O	1:C:951:ARG:NH2	2.52	0.41
3:J:187:TYR:O	3:J:193:TYR:OH	2.36	0.41
2:M:11:LEU:HD12	2:M:163:PRO:HG3	2.01	0.41
3:P:137:LEU:HD21	3:P:197:VAL:HG11	2.02	0.41
2:I:83:MET:HB3	2:I:86:LEU:HD21	2.02	0.41
2:S:33:SER:HB2	2:S:99:ASP:OD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:100:ARG:HA	2:M:117:ASP:OD2	2.20	0.41
1:B:646:ILE:O	1:B:649:MET:HG2	2.19	0.41
3:R:66:ARG:HG2	3:R:68:GLY:CA	2.47	0.41
3:R:168:ASP:OD2	3:R:171:ASP:OD2	2.37	0.41
1:D:782:ARG:HH12	1:E:540:LEU:HD23	1.85	0.41
1:H:580:SER:HA	1:H:581:PRO:HD3	1.90	0.41
1:C:93:HIS:CG	1:C:285:LEU:HD21	2.55	0.41
1:F:80:ASP:O	1:F:83:THR:HG22	2.20	0.41
1:F:245:HIS:O	1:F:249:TYR:HB2	2.20	0.41
1:A:425:LYS:NZ	1:A:428:GLU:OE2	2.31	0.41
2:Q:138:PHE:HA	2:Q:139:PRO:HD3	1.87	0.41
1:D:218:PHE:N	1:D:219:GLY:HA2	2.36	0.41
1:F:192:LYS:NZ	1:F:832:ILE:HG13	2.36	0.41
2:W:37:VAL:HG22	2:W:47:TRP:HA	2.02	0.41
1:E:294:GLN:O	1:E:298:LEU:HG	2.20	0.41
1:C:242:LEU:HA	1:C:242:LEU:HD13	1.93	0.41
2:I:100:ARG:HB3	2:I:100:ARG:NH1	2.36	0.41
1:B:874:ILE:O	1:B:933:LYS:HE3	2.20	0.41
1:C:778:VAL:HG22	1:C:955:SER:HB2	2.03	0.41
1:G:772:PRO:HD3	1:G:1002:LEU:HD22	2.02	0.41
1:C:337:LEU:HD23	1:C:401:LEU:HD22	2.03	0.41
1:B:116:LEU:HD13	1:B:178:ALA:HB1	2.02	0.41
1:B:58:PRO:HG3	1:B:423:ARG:NH1	2.35	0.41
1:C:852:SER:OG	1:C:853:GLU:N	2.53	0.41
2:U:59:SER:HB2	3:V:95:PHE:HB3	2.02	0.41
1:G:959:LEU:CD1	1:G:965:SER:HB3	2.50	0.41
3:X:126:LEU:HD23	3:X:184:LYS:HG3	2.02	0.41
2:Q:216:HIS:O	2:Q:220:ASN:HA	2.21	0.41
1:F:538:LEU:HA	1:F:539:PRO:HD3	1.94	0.41
1:D:1009:LYS:HA	1:D:1010:PRO:HD3	1.95	0.41
1:G:528:ASN:HB3	1:G:531:ILE:HG13	2.01	0.41
1:C:195:MET:HB2	1:C:786:HIS:CE1	2.55	0.41
1:A:422:PHE:CZ	1:A:451:THR:HG22	2.55	0.41
1:G:187:ASP:HB2	1:G:223:LYS:HB2	2.02	0.41
1:A:770:GLN:HB3	1:A:1003:PRO:HG2	2.03	0.41
1:F:794:TYR:HB3	1:F:954:VAL:HG13	2.02	0.41
1:F:179:LYS:NZ	1:F:180:ASP:OD1	2.48	0.41
1:G:795:TYR:HE1	1:G:951:ARG:HH12	1.68	0.41
2:I:47:TRP:NE1	2:I:49:ALA:O	2.54	0.41
1:C:620:LEU:HB2	1:C:629:LEU:HD23	2.01	0.41
1:D:238:ARG:N	1:D:239:GLN:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:586:ASP:OD1	1:C:589:HIS:ND1	2.53	0.41
3:V:113:ALA:HA	3:V:114:PRO:HD3	1.82	0.41
2:W:91:THR:HB	2:W:127:VAL:H	1.85	0.41
2:S:139:PRO:HD3	2:S:225:LYS:HD3	2.02	0.41
1:E:245:HIS:O	1:E:249:TYR:HB2	2.21	0.41
1:D:294:GLN:O	1:D:298:LEU:HG	2.21	0.41
3:L:159:ASN:N	3:L:159:ASN:OD1	2.53	0.41
3:T:39:LYS:HA	3:T:40:PRO:HD3	1.95	0.41
1:H:190:HIS:CE1	1:H:222:ASN:HD22	2.38	0.41
1:C:493:GLU:OE1	1:C:496:TYR:N	2.45	0.41
1:G:814:ILE:HG21	1:G:874:ILE:HG12	2.02	0.41
1:F:294:GLN:O	1:F:298:LEU:HG	2.21	0.41
1:F:309:ASP:N	1:F:672:ASN:OD1	2.43	0.41
1:G:542:LYS:HB2	1:G:542:LYS:NZ	2.35	0.41
1:B:262:GLU:N	1:B:262:GLU:OE2	2.51	0.41
2:S:162:PHE:CE1	2:S:192:TYR:HE1	2.39	0.41
1:D:311:ARG:HD3	1:D:384:LEU:HD22	2.02	0.41
2:W:162:PHE:HA	2:W:163:PRO:HA	1.82	0.41
2:M:11:LEU:HG	2:M:126:THR:HG23	2.03	0.41
1:G:321:ASP:OD2	1:G:323:GLN:HB3	2.20	0.41
3:R:17:ASP:OD1	3:R:18:ARG:N	2.48	0.41
1:G:90:LEU:HD13	1:G:169:PHE:CE1	2.55	0.41
3:J:113:ALA:HA	3:J:114:PRO:HD3	1.85	0.41
1:E:389:ASP:O	1:E:393:HIS:ND1	2.43	0.41
3:N:202:LEU:HA	2:S:66:GLY:HA3	2.03	0.41
2:K:162:PHE:HA	2:K:163:PRO:HA	1.84	0.41
2:W:89:GLU:N	2:W:89:GLU:OE2	2.53	0.41
1:H:724:HIS:HB2	1:H:758:LEU:HD12	2.02	0.41
1:A:908:TRP:O	1:A:912:ILE:HG12	2.21	0.41
1:F:99:ASP:O	1:F:217:LYS:NZ	2.53	0.41
3:V:68:GLY:HA2	3:V:69:THR:HA	1.66	0.41
3:P:14:SER:O	3:P:78:LEU:HD23	2.21	0.41
1:F:855:PRO:HA	1:F:856:PRO:HD3	1.90	0.41
1:H:48:LYS:HB2	1:H:70:ALA:HA	2.03	0.41
1:G:938:LYS:HE2	1:G:938:LYS:HB3	1.84	0.41
1:F:192:LYS:HZ1	1:F:831:TYR:HD2	1.68	0.41
2:O:135:PRO:HG3	2:O:216:HIS:HB2	2.02	0.41
1:F:908:TRP:CE2	1:F:912:ILE:HD11	2.56	0.41
1:G:286:PRO:HA	1:G:287:GLU:HA	1.63	0.41
1:C:894:LEU:HG	1:C:925:VAL:HG21	2.02	0.41
1:G:90:LEU:HD22	1:G:169:PHE:HZ	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:PHE:CZ	1:C:451:THR:HG22	2.56	0.41
2:M:157:LEU:HD13	2:M:195:SER:HB3	2.01	0.41
1:H:100:PRO:HA	1:H:101:PRO:HD3	1.88	0.41
1:A:493:GLU:OE1	1:A:496:TYR:N	2.41	0.41
1:G:960:ALA:HB3	1:G:963:MET:HB2	2.01	0.41
1:A:675:ALA:HA	1:A:785:VAL:HG21	2.02	0.41
1:D:285:LEU:HA	1:D:286:PRO:HD3	1.90	0.41
1:G:210:ASN:HA	1:G:211:PRO:HD3	1.93	0.41
1:C:139:ASN:OD1	1:C:140:ALA:N	2.49	0.41
1:F:291:HIS:HD2	1:F:293:PHE:H	1.68	0.41
3:P:92:SER:OG	3:P:96:LEU:HB2	2.21	0.41
1:C:190:HIS:O	1:C:194:VAL:HG23	2.21	0.41
1:B:320:PRO:HD3	1:B:470:LYS:HZ3	1.86	0.41
1:H:425:LYS:NZ	1:H:425:LYS:HB3	2.36	0.41
1:H:113:MET:HG3	1:H:174:PHE:CD1	2.53	0.41
1:G:307:ILE:C	1:G:483:LYS:HZ1	2.24	0.41
1:H:776:TRP:HA	1:H:953:LYS:O	2.21	0.41
1:F:451:THR:HB	1:F:455:LEU:HD13	2.03	0.41
1:C:99:ASP:O	1:C:217:LYS:NZ	2.40	0.41
2:M:182:PHE:HA	2:M:183:PRO:HD3	1.98	0.41
3:T:165:THR:HG22	3:T:175:SER:H	1.85	0.41
1:C:545:THR:HA	1:C:546:PRO:HD3	1.94	0.41
1:D:542:LYS:HB2	1:D:542:LYS:NZ	2.36	0.41
1:H:93:HIS:ND1	1:H:93:HIS:O	2.54	0.41
1:E:938:LYS:HB3	1:E:938:LYS:HE2	1.87	0.41
2:W:162:PHE:HB2	2:W:191:LEU:HD22	2.03	0.40
3:R:35:TRP:CD2	3:R:73:LEU:HB2	2.56	0.40
3:T:14:SER:OG	3:T:108:LYS:NZ	2.26	0.40
1:H:222:ASN:O	1:H:226:LEU:HB2	2.21	0.40
1:C:574:LEU:HD22	1:C:729:LEU:HG	2.04	0.40
2:W:153:ALA:HB2	2:W:199:THR:HG22	2.02	0.40
1:B:97:LEU:HB2	1:B:144:GLY:O	2.21	0.40
1:B:604:LEU:HG	1:B:648:LYS:HG2	2.02	0.40
1:B:281:LYS:HB2	1:B:283:VAL:HG23	2.03	0.40
1:E:137:SER:OG	1:E:152:ASP:OD1	2.29	0.40
1:F:571:LYS:HB2	1:F:571:LYS:HE3	1.86	0.40
2:K:138:PHE:HA	2:K:139:PRO:HD3	1.86	0.40
1:G:109:PHE:CZ	1:G:179:LYS:HG3	2.56	0.40
2:U:164:GLU:HA	2:U:165:PRO:HA	1.66	0.40
1:F:291:HIS:CE1	1:F:370:PHE:HB2	2.56	0.40
3:J:50:SER:OG	3:J:53:SER:OG	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:30:SER:HB2	3:T:90:GLN:NE2	2.37	0.40
1:C:460:ARG:HH11	1:C:463:LEU:HD11	1.86	0.40
1:A:706:ASP:HB3	1:A:711:ARG:HH22	1.86	0.40
1:H:562:LYS:O	1:H:730:HIS:HA	2.21	0.40
1:F:88:ALA:HB3	1:F:151:PHE:CE1	2.56	0.40
1:F:118:THR:HG21	1:F:168:PHE:HA	2.02	0.40
1:C:324:LYS:HD3	2:M:103:TYR:CZ	2.56	0.40
1:E:306:PRO:C	1:E:483:LYS:HZ2	2.23	0.40
1:D:765:ARG:NH2	1:D:912:ILE:O	2.55	0.40
1:A:195:MET:HB2	1:A:786:HIS:CE1	2.56	0.40
1:H:908:TRP:O	1:H:912:ILE:HG12	2.21	0.40
1:E:528:ASN:HB3	1:E:531:ILE:HG13	2.02	0.40
1:D:445:PRO:O	1:D:449:VAL:HG13	2.21	0.40
1:G:729:LEU:HD12	1:G:738:ALA:HB1	2.04	0.40
1:D:874:ILE:O	1:D:877:MET:HG2	2.22	0.40
2:I:98:ARG:NH1	2:I:118:TYR:CD2	2.90	0.40
1:E:815:ILE:HA	1:E:870:MET:HE2	2.04	0.40
1:H:156:GLU:HG3	1:H:157:HIS:ND1	2.36	0.40
1:H:159:GLU:HG3	1:H:270:LEU:HD11	2.03	0.40
2:O:175:LEU:HD13	2:O:198:VAL:HG21	2.02	0.40
1:F:97:LEU:HB2	1:F:144:GLY:O	2.21	0.40
1:G:83:THR:O	1:G:261:ARG:NE	2.48	0.40
1:F:460:ARG:HD2	1:F:463:LEU:HG	2.02	0.40
1:H:109:PHE:CD2	1:H:241:LEU:HD21	2.54	0.40
1:E:80:ASP:O	1:E:83:THR:HG22	2.21	0.40
3:T:204:SER:HA	3:T:205:PRO:HD3	1.95	0.40
2:M:47:TRP:NE1	2:M:49:ALA:O	2.54	0.40
3:L:59:PRO:HB2	3:L:61:ARG:HG2	2.04	0.40
1:F:285:LEU:HA	1:F:286:PRO:HD3	1.92	0.40
1:E:683:MET:HA	1:E:792:GLU:OE2	2.21	0.40
3:L:30:SER:HB3	3:L:90:GLN:NE2	2.37	0.40
1:H:94:ILE:HA	1:H:94:ILE:HD12	1.98	0.40

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	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	LEU
1	A	111	GLN
1	A	129	GLN
1	A	158	LEU
1	A	192	LYS
1	A	201	LEU
1	A	242	LEU
1	A	285	LEU
1	A	337	LEU
1	A	507	ASP

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Mol	Chain	Res	Type
1	A	616	LEU
1	A	629	LEU
1	A	642	LEU
1	A	712	LEU
1	A	810	LEU
1	A	823	LEU
1	A	889	LEU
1	B	53	HIS
1	B	67	LEU
1	B	76	LEU
1	B	158	LEU
1	B	229	ARG
1	B	238	ARG
1	B	285	LEU
1	B	308	LYS
1	B	347	LEU
1	B	460	ARG
1	B	524	LEU
1	B	542	LYS
1	B	616	LEU
1	B	629	LEU
1	B	642	LEU
1	B	712	LEU
1	B	733	ILE
1	B	810	LEU
1	B	846	LEU
1	B	931	LEU
1	C	67	LEU
1	C	111	GLN
1	C	158	LEU
1	C	201	LEU
1	C	242	LEU
1	C	285	LEU
1	C	324	LYS
1	C	329	ASN
1	C	337	LEU
1	C	616	LEU
1	C	642	LEU
1	C	712	LEU
1	C	720	LEU
1	C	733	ILE
1	C	798	ASP

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Mol	Chain	Res	Type
1	C	810	LEU
1	C	846	LEU
1	C	963	MET
1	D	53	HIS
1	D	158	LEU
1	D	201	LEU
1	D	218	PHE
1	D	239	GLN
1	D	281	LYS
1	D	287	GLU
1	D	347	LEU
1	D	460	ARG
1	D	542	LYS
1	D	616	LEU
1	D	623	THR
1	D	629	LEU
1	D	642	LEU
1	D	712	LEU
1	D	810	LEU
1	D	846	LEU
1	D	889	LEU
1	E	111	GLN
1	E	158	LEU
1	E	201	LEU
1	E	244	PHE
1	E	270	LEU
1	E	281	LYS
1	E	287	GLU
1	E	337	LEU
1	E	360	VAL
1	E	488	LYS
1	E	542	LYS
1	E	616	LEU
1	E	629	LEU
1	E	642	LEU
1	E	712	LEU
1	E	810	LEU
1	E	846	LEU
1	E	889	LEU
1	E	933	LYS
1	E	986	LEU
1	F	67	LEU

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Mol	Chain	Res	Type
1	F	94	ILE
1	F	112	HIS
1	F	158	LEU
1	F	201	LEU
1	F	204	LEU
1	F	285	LEU
1	F	324	LYS
1	F	337	LEU
1	F	404	GLU
1	F	488	LYS
1	F	616	LEU
1	F	642	LEU
1	F	712	LEU
1	F	720	LEU
1	F	733	ILE
1	F	756	LYS
1	F	810	LEU
1	F	827	GLU
1	F	846	LEU
1	F	862	ARG
1	F	872	LYS
1	G	56	LYS
1	G	158	LEU
1	G	270	LEU
1	G	285	LEU
1	G	542	LYS
1	G	616	LEU
1	G	629	LEU
1	G	642	LEU
1	G	712	LEU
1	G	810	LEU
1	G	823	LEU
1	G	846	LEU
1	G	859	LEU
1	G	884	LYS
1	G	889	LEU
1	G	928	LEU
1	G	933	LYS
1	H	67	LEU
1	H	107	SER
1	H	125	ASN
1	H	158	LEU

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Mol	Chain	Res	Type
1	H	192	LYS
1	H	201	LEU
1	H	204	LEU
1	H	226	LEU
1	H	324	LYS
1	H	337	LEU
1	H	460	ARG
1	H	616	LEU
1	H	642	LEU
1	H	712	LEU
1	H	733	ILE
1	H	756	LYS
1	H	810	LEU
1	H	846	LEU
2	I	91	THR
2	I	126	THR
2	I	211	ILE
3	J	33	VAL
3	J	92	SER
3	J	95	PHE
3	J	144	GLU
3	J	182	LEU
2	K	126	THR
2	K	164	GLU
2	K	209	THR
3	L	63	SER
3	L	95	PHE
3	L	108	LYS
3	L	143	ARG
3	L	144	GLU
3	L	171	ASP
2	M	81	LEU
2	M	91	THR
2	M	126	THR
2	M	127	VAL
2	M	129	SER
2	M	175	LEU
2	M	198	VAL
2	M	211	ILE
3	N	33	VAL
3	N	66	ARG
3	N	95	PHE

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Mol	Chain	Res	Type
3	N	108	LYS
3	N	144	GLU
3	N	182	LEU
2	O	91	THR
2	O	126	THR
3	P	95	PHE
3	P	108	LYS
3	P	143	ARG
3	P	144	GLU
3	P	171	ASP
2	Q	126	THR
2	Q	213	ASN
3	R	24	ARG
3	R	67	SER
3	R	69	THR
3	R	78	LEU
3	R	89	GLN
3	R	95	PHE
3	R	108	LYS
3	R	143	ARG
3	R	144	GLU
2	S	91	THR
2	S	126	THR
2	S	127	VAL
2	S	175	LEU
2	S	211	ILE
2	S	216	HIS
3	T	29	VAL
3	T	95	PHE
3	T	98	THR
3	T	108	LYS
3	T	143	ARG
3	T	144	GLU
3	T	171	ASP
3	T	182	LEU
2	U	2	VAL
2	U	91	THR
2	U	175	LEU
2	U	198	VAL
2	U	209	THR
2	U	222	LYS
3	V	33	VAL

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Mol	Chain	Res	Type
3	V	67	SER
3	V	69	THR
3	V	95	PHE
3	V	108	LYS
3	V	143	ARG
3	V	144	GLU
3	V	197	VAL
2	W	91	THR
2	W	126	THR
3	X	24	ARG
3	X	29	VAL
3	X	69	THR
3	X	70	ASP
3	X	95	PHE
3	X	98	THR
3	X	108	LYS
3	X	143	ARG
3	X	144	GLU
3	X	182	LEU
4	a	3	VAL
4	a	14	TYR
4	a	15	GLN
4	b	2	ILE
4	c	14	TYR
4	d	2	ILE
4	d	4	GLU
4	e	3	VAL
4	f	3	VAL
4	g	14	TYR
4	h	3	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	HIS
1	A	332	HIS
1	A	786	HIS
1	E	203	GLN
1	E	442	HIS
1	H	190	HIS
1	H	329	ASN
1	H	332	HIS

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Mol	Chain	Res	Type
1	H	363	GLN
3	J	139	ASN
3	P	139	ASN
3	R	139	ASN
3	X	139	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

All (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
2	Q	38	ARG	5.6
1	E	924	GLU	5.1
3	X	149	TRP	5.1
1	F	853	GLU	5.0
1	E	479	ALA	4.9
2	O	201	PRO	4.9
2	O	200	VAL	4.9
3	P	131	ALA	4.8
3	T	148	GLN	4.8
1	D	312	ASN	4.8
2	O	196	SER	4.7
2	Q	46	GLU	4.7
3	N	148	GLN	4.7
2	U	184	ALA	4.6
3	T	147	VAL	4.6
1	F	302	TYR	4.6
1	D	829	LEU	4.6
2	W	144	SER	4.6
3	T	150	LYS	4.6
1	F	84	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	263	SER	4.5
1	D	761	SER	4.5
3	V	121	PRO	4.4
2	Q	196	SER	4.4
1	C	175	ASP	4.4
3	P	134	VAL	4.3
1	D	215	PHE	4.3
1	C	312	ASN	4.3
1	E	334	LEU	4.3
2	Q	210	TYR	4.2
3	P	132	SER	4.2
3	P	14	SER	4.2
1	H	176	GLU	4.2
2	Q	36	TRP	4.2
2	Q	8	GLY	4.1
1	H	227	GLU	4.1
2	Q	92	ALA	4.1
1	G	373	PHE	4.1
2	O	144	SER	4.0
3	P	25	ALA	4.0
3	N	162	GLU	4.0
3	T	145	ALA	4.0
1	F	249	TYR	3.9
1	E	330	PRO	3.9
3	T	136	LEU	3.9
1	E	262	GLU	3.9
3	R	190	HIS	3.9
1	E	332	HIS	3.9
1	D	221	GLY	3.9
3	L	198	THR	3.9
3	L	122	SER	3.8
3	X	131	ALA	3.8
2	Q	209	THR	3.8
1	D	333	TYR	3.8
1	H	238	ARG	3.8
3	L	175	SER	3.8
1	D	983	ALA	3.8
3	P	119	PHE	3.8
2	O	197	VAL	3.8
1	D	265	ASP	3.7
1	E	895	ASP	3.7
2	I	224	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	407	GLN	3.7
1	D	239	GLN	3.6
1	E	313	LEU	3.6
1	B	497	GLY	3.6
3	T	195	CYS	3.6
1	E	489	THR	3.6
1	G	922	ASN	3.6
3	R	33	VAL	3.5
1	E	329	ASN	3.5
2	Q	213	ASN	3.5
1	C	501	LYS	3.5
1	B	177	SER	3.5
1	D	154	SER	3.5
1	E	64	TYR	3.5
1	D	387	VAL	3.5
1	D	103	ILE	3.5
1	E	939	PHE	3.5
2	Q	228	GLU	3.5
3	X	121	PRO	3.5
2	Q	9	GLY	3.4
1	G	178	ALA	3.4
2	Q	227	VAL	3.4
2	Q	129	SER	3.4
2	Q	144	SER	3.4
1	F	312	ASN	3.4
1	B	517	ASP	3.4
1	H	180	ASP	3.4
1	D	984	PRO	3.4
3	N	195	CYS	3.4
1	D	191	GLU	3.4
1	F	850	ILE	3.4
2	W	11	LEU	3.4
1	H	241	LEU	3.4
3	N	90	GLN	3.4
2	M	142	PRO	3.3
2	K	195	SER	3.3
1	D	979	ASN	3.3
1	H	242	LEU	3.3
1	H	181	ARG	3.3
2	S	142	PRO	3.3
1	E	829	LEU	3.3
1	F	90	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	M	153	ALA	3.3
1	D	182	GLU	3.3
1	G	230	PRO	3.3
1	E	784	GLU	3.3
1	C	236	ASP	3.3
1	D	290	GLU	3.3
1	F	761	SER	3.3
3	P	87	TYR	3.2
3	P	133	VAL	3.2
1	G	291	HIS	3.2
3	R	138	ASN	3.2
2	Q	37	VAL	3.2
2	O	181	THR	3.2
1	D	424	PHE	3.2
1	D	853	GLU	3.2
1	C	124	GLU	3.2
1	C	313	LEU	3.2
3	X	195	CYS	3.2
3	T	162	GLU	3.1
2	M	195	SER	3.1
1	C	197	ASP	3.1
1	F	835	SER	3.1
3	N	14	SER	3.1
1	C	178	ALA	3.1
1	E	877	MET	3.1
2	Q	195	SER	3.1
1	F	887	GLN	3.0
1	C	478	VAL	3.0
2	U	185	VAL	3.0
1	D	877	MET	3.0
1	D	213	HIS	3.0
1	D	852	SER	3.0
1	C	931	LEU	3.0
1	D	848	PHE	3.0
1	F	238	ARG	3.0
2	O	198	VAL	3.0
2	U	137	VAL	3.0
1	E	80	ASP	3.0
1	C	52	ASN	3.0
1	E	478	VAL	3.0
1	F	692	GLU	3.0
1	F	441	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
3	V	206	VAL	3.0
3	P	35	TRP	2.9
2	O	143	SER	2.9
3	T	82	ASP	2.9
1	A	428	GLU	2.9
3	P	122	SER	2.9
3	R	193	TYR	2.9
3	T	206	VAL	2.9
3	X	163	SER	2.9
1	H	230	PRO	2.9
1	C	303	LYS	2.9
3	X	147	VAL	2.9
1	E	195	MET	2.9
1	E	458	GLU	2.9
2	M	126	THR	2.9
1	C	78	ILE	2.9
1	F	765	ARG	2.9
2	M	218	PRO	2.9
1	H	239	GLN	2.9
2	S	195	SER	2.9
3	R	117	PHE	2.9
1	H	585	VAL	2.9
3	N	177	SER	2.9
2	Q	13	GLN	2.9
3	R	14	SER	2.9
1	B	81	PRO	2.8
1	G	301	LEU	2.8
1	H	852	SER	2.8
3	R	21	ILE	2.8
1	D	177	SER	2.8
1	E	656	GLU	2.8
3	R	162	GLU	2.8
1	C	248	TYR	2.8
1	C	239	GLN	2.8
3	P	197	VAL	2.8
1	B	386	HIS	2.8
1	F	118	THR	2.8
3	R	119	PHE	2.8
1	F	983	ALA	2.8
2	S	35	HIS	2.8
2	O	88	ALA	2.8
3	T	194	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	332	HIS	2.8
1	A	373	PHE	2.8
1	D	411	PHE	2.8
3	N	191	LYS	2.8
2	I	126	THR	2.8
2	K	127	VAL	2.8
1	F	702	GLU	2.8
3	R	25	ALA	2.8
3	R	194	ALA	2.8
2	U	181	THR	2.8
1	F	788	ASN	2.8
2	K	128	SER	2.8
1	C	770	GLN	2.8
1	G	303	LYS	2.8
3	R	96	LEU	2.7
2	Q	99	ASP	2.7
2	Q	18	LEU	2.7
1	C	337	LEU	2.7
1	G	926	ALA	2.7
3	N	194	ALA	2.7
2	W	143	SER	2.7
1	G	168	PHE	2.7
1	G	177	SER	2.7
1	F	829	LEU	2.7
3	V	207	THR	2.7
2	O	63	SER	2.7
1	A	178	ALA	2.7
2	O	202	SER	2.7
1	D	1010	PRO	2.7
3	R	192	VAL	2.7
1	A	482	SER	2.7
2	O	38	ARG	2.7
1	E	197	ASP	2.7
3	P	121	PRO	2.7
1	C	535	PHE	2.7
1	D	193	ASN	2.7
1	D	413	GLU	2.7
2	U	92	ALA	2.7
1	H	517	ASP	2.7
1	C	262	GLU	2.6
2	W	210	TYR	2.6
3	R	90	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
2	O	228	GLU	2.6
2	Q	48	VAL	2.6
3	X	135	CYS	2.6
1	D	62	ARG	2.6
3	N	135	CYS	2.6
2	U	193	SER	2.6
3	L	145	ALA	2.6
2	W	170	TRP	2.6
1	D	313	LEU	2.6
3	T	137	LEU	2.6
1	F	746	GLU	2.6
2	S	196	SER	2.6
1	E	168	PHE	2.6
1	A	177	SER	2.6
1	E	866	PHE	2.6
1	C	944	LEU	2.6
1	D	850	ILE	2.6
1	D	329	ASN	2.6
1	G	381	GLU	2.6
3	L	5	THR	2.6
1	E	501	LYS	2.6
2	W	158	VAL	2.6
1	G	982	GLN	2.6
1	H	178	ALA	2.6
1	F	453	GLU	2.6
2	K	17	SER	2.6
1	D	759	LEU	2.6
1	F	699	GLU	2.6
1	E	315	VAL	2.6
1	E	408	GLU	2.6
1	E	878	THR	2.6
2	O	17	SER	2.6
3	R	139	ASN	2.6
2	W	126	THR	2.5
1	E	98	SER	2.5
1	F	182	GLU	2.5
2	M	83	MET	2.5
3	R	15	VAL	2.5
3	P	78	LEU	2.5
1	D	292	PRO	2.5
1	C	479	ALA	2.5
2	U	81	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	895	ASP	2.5
3	N	118	ILE	2.5
1	C	784	GLU	2.5
1	D	762	GLN	2.5
1	D	104	ALA	2.5
1	G	295	GLU	2.5
1	C	862	ARG	2.5
2	U	70	ILE	2.5
1	B	244	PHE	2.5
2	O	214	VAL	2.5
3	L	121	PRO	2.5
3	T	79	GLN	2.5
1	E	249	TYR	2.5
3	L	138	ASN	2.5
1	D	178	ALA	2.5
3	V	17	ASP	2.5
1	E	570	PRO	2.5
1	F	984	PRO	2.5
3	N	149	TRP	2.5
3	P	136	LEU	2.5
1	C	866	PHE	2.5
2	M	99	ASP	2.5
1	D	449	VAL	2.5
2	S	37	VAL	2.5
2	U	226	LYS	2.5
1	E	179	LYS	2.5
1	C	991	VAL	2.5
3	P	15	VAL	2.5
3	X	188	GLU	2.5
1	C	834	PHE	2.5
1	D	378	ASP	2.5
1	H	458	GLU	2.5
3	L	188	GLU	2.5
1	D	192	LYS	2.5
2	W	194	LEU	2.5
1	C	992	ILE	2.5
3	P	135	CYS	2.5
1	C	241	LEU	2.4
1	D	460	ARG	2.4
1	D	249	TYR	2.4
1	F	851	GLN	2.4
2	Q	226	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	798	ASP	2.4
1	G	249	TYR	2.4
2	W	157	LEU	2.4
3	R	34	ALA	2.4
2	O	230	LYS	2.4
1	B	227	GLU	2.4
1	C	924	GLU	2.4
1	E	296	GLU	2.4
1	H	434	THR	2.4
1	E	862	ARG	2.4
2	K	230	LYS	2.4
3	P	4	MET	2.4
3	X	134	VAL	2.4
2	S	135	PRO	2.4
1	F	857	HIS	2.4
2	M	38	ARG	2.4
1	C	776	TRP	2.4
3	N	196	GLU	2.4
4	g	13	LEU	2.4
1	F	479	ALA	2.4
1	D	830	GLY	2.4
1	F	863	VAL	2.4
1	G	428	GLU	2.4
2	Q	35	HIS	2.4
2	W	184	ALA	2.4
3	X	119	PHE	2.4
1	C	863	VAL	2.4
3	V	5	THR	2.4
3	R	47	LEU	2.4
2	Q	62	ASP	2.4
2	U	38	ARG	2.4
2	U	225	LYS	2.4
1	C	829	LEU	2.4
3	N	150	LYS	2.4
3	P	125	GLN	2.4
2	Q	128	SER	2.4
1	F	83	THR	2.4
3	L	174	TYR	2.4
3	T	46	LEU	2.4
2	K	144	SER	2.4
1	H	459	PHE	2.4
3	T	83	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
3	X	83	PHE	2.4
1	C	237	VAL	2.4
2	M	48	VAL	2.4
1	A	700	LEU	2.3
1	E	337	LEU	2.3
1	E	955	SER	2.3
3	L	137	LEU	2.3
3	T	196	GLU	2.3
1	B	129	GLN	2.3
1	E	854	LYS	2.3
2	K	106	SER	2.3
1	D	334	LEU	2.3
3	J	193	TYR	2.3
3	T	149	TRP	2.3
1	E	706	ASP	2.3
3	R	70	ASP	2.3
1	D	792	GLU	2.3
1	D	444	TYR	2.3
1	F	255	ALA	2.3
1	H	983	ALA	2.3
2	U	172	SER	2.3
1	C	174	PHE	2.3
1	C	259	LEU	2.3
1	D	220	THR	2.3
1	G	226	LEU	2.3
1	E	333	TYR	2.3
3	T	118	ILE	2.3
1	A	479	ALA	2.3
1	C	853	GLU	2.3
1	D	331	GLY	2.3
1	E	834	PHE	2.3
2	M	36	TRP	2.3
1	E	303	LYS	2.3
1	A	241	LEU	2.3
2	S	141	ALA	2.3
3	V	196	GLU	2.3
1	H	513	TRP	2.3
2	U	116	MET	2.3
1	D	259	LEU	2.3
3	P	114	PRO	2.3
3	L	6	GLN	2.3
1	D	497	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	U	10	GLY	2.3
2	U	138	PHE	2.3
1	C	377	VAL	2.3
1	F	262	GLU	2.3
1	F	221	GLY	2.3
1	H	231	ASN	2.2
1	H	482	SER	2.2
2	O	172	SER	2.2
1	H	175	ASP	2.2
1	D	300	GLN	2.2
1	A	239	GLN	2.2
2	M	139	PRO	2.2
2	I	10	GLY	2.2
1	D	330	PRO	2.2
1	F	478	VAL	2.2
3	R	116	VAL	2.2
2	S	154	LEU	2.2
2	U	228	GLU	2.2
3	X	162	GLU	2.2
1	F	426	ASP	2.2
1	H	930	THR	2.2
1	D	427	LYS	2.2
1	F	378	ASP	2.2
3	R	189	LYS	2.2
1	H	182	GLU	2.2
2	K	218	PRO	2.2
2	Q	159	LYS	2.2
1	E	516	ALA	2.2
1	G	945	ALA	2.2
2	O	86	LEU	2.2
3	R	17	ASP	2.2
1	C	848	PHE	2.2
1	D	372	PHE	2.2
1	G	254	MET	2.2
1	F	1009	LYS	2.2
1	G	223	LYS	2.2
1	F	487	GLY	2.2
3	L	23	CYS	2.2
1	D	463	LEU	2.2
1	D	791	ILE	2.2
1	E	931	LEU	2.2
2	K	167	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	785	VAL	2.2
3	R	38	GLN	2.2
2	W	125	VAL	2.2
3	V	147	VAL	2.2
1	G	175	ASP	2.2
1	D	981	SER	2.2
2	U	115	GLY	2.2
1	E	457	GLU	2.2
2	O	223	VAL	2.2
1	C	397	TYR	2.2
1	D	98	SER	2.2
1	F	924	GLU	2.2
1	D	823	LEU	2.2
1	H	73	ILE	2.2
1	B	309	ASP	2.2
1	C	536	GLU	2.2
1	D	954	VAL	2.2
1	D	1009	LYS	2.2
1	E	96	SER	2.2
1	H	863	VAL	2.2
3	J	131	ALA	2.2
1	E	846	LEU	2.1
1	F	832	ILE	2.1
2	I	124	LEU	2.1
3	T	109	ARG	2.1
3	T	199	HIS	2.1
1	H	929	LYS	2.1
1	B	888	ALA	2.1
1	A	944	LEU	2.1
1	E	97	LEU	2.1
1	F	823	LEU	2.1
1	C	62	ARG	2.1
1	F	486	GLU	2.1
2	O	156	CYS	2.1
1	H	90	LEU	2.1
2	M	128	SER	2.1
2	K	126	THR	2.1
2	M	141	ALA	2.1
1	A	389	ASP	2.1
2	K	139	PRO	2.1
1	C	592	MET	2.1
2	U	154	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	R	118	ILE	2.1
1	D	957	HIS	2.1
1	F	256	VAL	2.1
2	M	152	ALA	2.1
2	M	37	VAL	2.1
1	D	157	HIS	2.1
1	H	835	SER	2.1
3	T	178	SER	2.1
1	F	103	ILE	2.1
1	H	184	ASN	2.1
2	S	36	TRP	2.1
1	D	244	PHE	2.1
2	O	98	ARG	2.1
1	F	376	ASN	2.1
2	O	178	GLY	2.1
3	V	201	GLY	2.1
1	H	926	ALA	2.1
1	D	254	MET	2.1
2	Q	168	VAL	2.1
2	U	139	PRO	2.1
1	D	264	LEU	2.1
2	K	182	PHE	2.1
2	Q	143	SER	2.1
3	V	14	SER	2.1
3	X	164	VAL	2.1
1	A	771	LEU	2.1
1	D	203	GLN	2.1
2	K	203	SER	2.1
3	R	35	TRP	2.1
3	P	191	LYS	2.1
2	U	88	ALA	2.1
2	O	46	GLU	2.1
2	U	224	ASP	2.1
2	O	218	PRO	2.1
2	K	170	TRP	2.1
2	Q	69	THR	2.1
2	Q	181	THR	2.1
1	C	249	TYR	2.1
1	C	334	LEU	2.1
1	C	336	HIS	2.1
1	D	64	TYR	2.1
2	U	63	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	R	16	GLY	2.1
1	B	983	ALA	2.1
1	D	760	PRO	2.1
3	R	125	GLN	2.1
1	F	121	TYR	2.0
2	Q	94	TYR	2.0
1	D	620	LEU	2.0
1	G	444	TYR	2.0
1	C	258	VAL	2.0
1	A	222	ASN	2.0
1	E	517	ASP	2.0
1	A	691	THR	2.0
1	H	582	PHE	2.0
3	N	33	VAL	2.0
3	N	147	VAL	2.0
1	C	614	ALA	2.0
2	O	136	SER	2.0
3	L	163	SER	2.0
1	F	64	TYR	2.0
1	F	390	ILE	2.0
1	G	374	ILE	2.0
1	B	82	THR	2.0
1	B	230	PRO	2.0
1	D	214	PRO	2.0
1	D	437	ILE	2.0
1	A	102	ASN	2.0
2	O	180	HIS	2.0
2	U	183	PRO	2.0
1	C	64	TYR	2.0
1	A	895	ASP	2.0
3	V	190	HIS	2.0

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 [i](#)

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(Å 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.