Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 12:08 AM EDT

PDB ID	:	5WOB
Title	:	Crystal Structure Analysis of Fab1-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	:	2017-08-01
Resolution	:	3.95 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

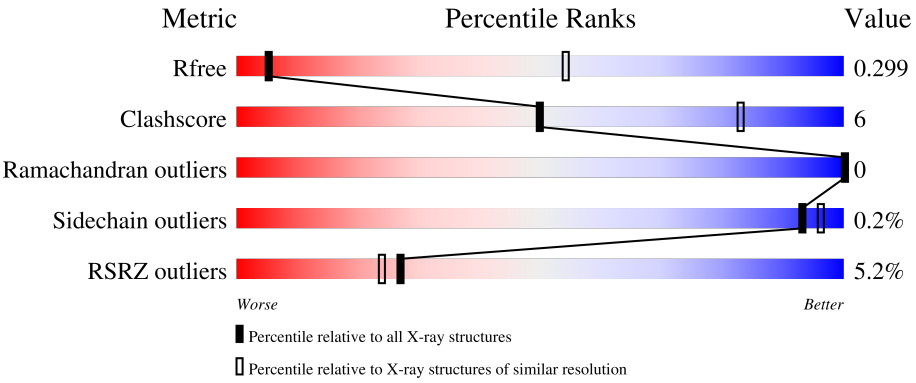
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1025 (4.22-3.70)
Clashscore	141614	1085 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)
RSRZ outliers	127900	1013 (4.28-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	81% 14% 5%
1	B	990	81% 14% .
1	C	990	5% 81% 15% .
1	D	990	6% 80% 16% .
1	E	990	5% 81% 15% 5%

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Mol	Chain	Length	Quality of chain
1	F	990	6% 82% 13% 5%
1	G	990	2% 81% 14% 5%
1	H	990	3% 81% 13% 5%
2	a	20	5% 100%
2	b	20	5% 25% 75%
2	c	20	5% 100%
2	d	20	15% 85%
2	e	20	5% 40% 5% 55%
2	f	20	90% 10%
2	g	20	70% 5% 25%
2	h	20	30% 70%
3	I	263	2% 71% 11% 18%
3	K	263	7% 64% 14% 21%
3	M	263	4% 67% 14% 19%
3	O	263	11% 68% 11% 21%
3	Q	263	12% 65% 11% 24%
3	S	263	5% 66% 16% 18%
3	U	263	8% 61% 14% 24%
3	W	263	5% 64% 13% 22%
4	J	239	2% 67% 15% 17%
4	L	239	7% 62% 11% 26%
4	N	239	6% 71% 13% 16%
4	P	239	9% 67% 10% 23%
4	R	239	10% 63% 11% 26%
4	T	239	10% 68% 15% 17%

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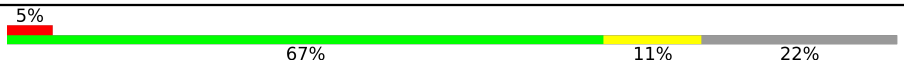
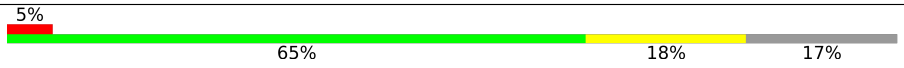
Mol	Chain	Length	Quality of chain
4	V	239	
4	X	239	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 86906 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	947	Total	C	N	O	S	0	0	0
			7758	4997	1302	1437	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	943	Total	C	N	O	S	0	0	0
			7713	4969	1294	1428	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	-	initiating methionine	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	-	initiating methionine	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	ALA	-	expression tag	UNP P14735
B	38	ALA	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ILE	-	expression tag	UNP P14735
B	41	PRO	-	expression tag	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735
C	30	MET	-	initiating methionine	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	-	initiating methionine	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	-	initiating methionine	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	-	initiating methionine	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	-	initiating methionine	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	-	initiating methionine	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 Insulin.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	a	20	Total C N O S 154 95 23 32 4	0	0	0
2	b	5	Total C N O 37 23 6 8	0	0	0
2	c	20	Total C N O S 154 95 23 32 4	0	0	0
2	d	3	Total C N O 19 13 3 3	0	0	0
2	e	9	Total C N O 74 49 11 14	0	0	0
2	f	18	Total C N O S 134 80 21 29 4	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	g	15	Total C N O S 121 76 18 25 2	0	0	0
2	h	6	Total C N O S 43 26 7 9 1	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	I	215	Total C N O S 1632 1041 267 317 7	0	0	0
3	K	207	Total C N O S 1582 1009 259 307 7	0	0	0
3	M	214	Total C N O S 1623 1035 265 316 7	0	0	0
3	O	209	Total C N O S 1587 1011 261 309 6	0	0	0
3	Q	201	Total C N O S 1539 984 252 297 6	0	0	0
3	S	215	Total C N O S 1632 1041 267 317 7	0	0	0
3	U	199	Total C N O S 1518 970 248 293 7	0	0	0
3	W	204	Total C N O S 1546 986 252 302 6	0	0	0

- Molecule 4 is a protein called IDE-bound Fab light chain.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	X	198	Total	C	N	O	S	0	0	0
			1515	949	255	307	4			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

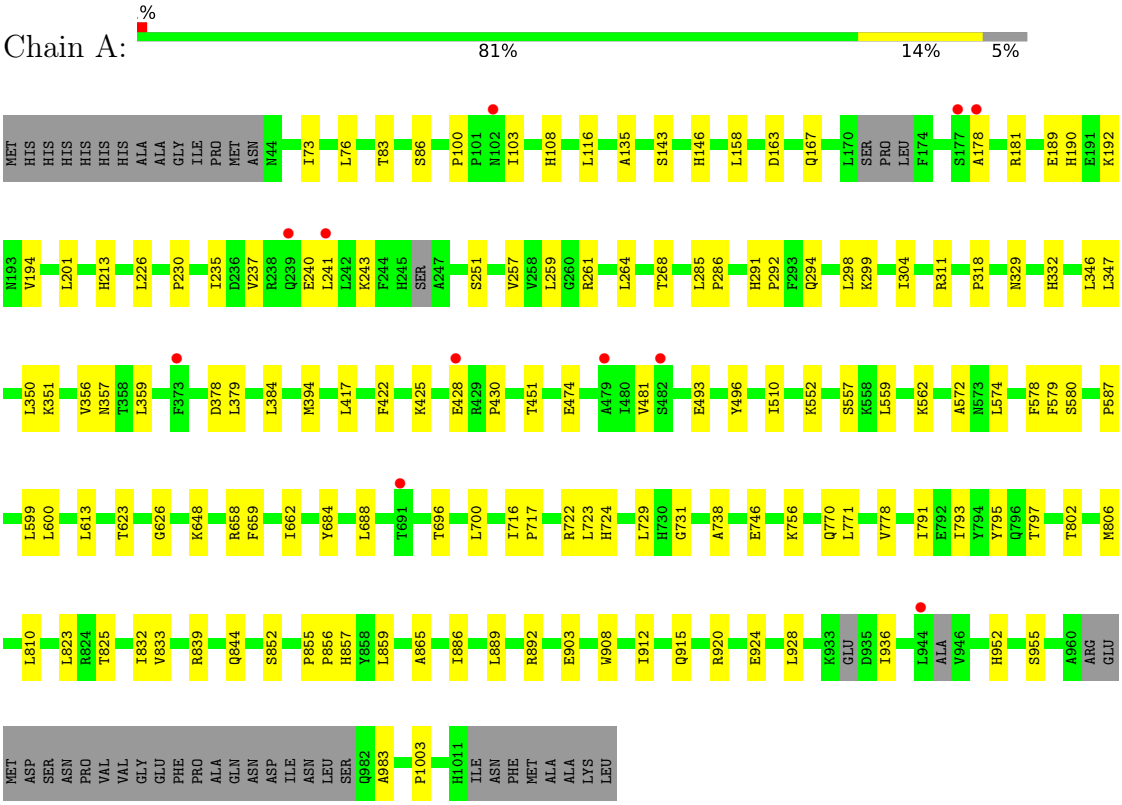
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		
5	C	1	Total	Zn	0	0
			1	1		
5	D	1	Total	Zn	0	0
			1	1		
5	E	1	Total	Zn	0	0
			1	1		
5	F	1	Total	Zn	0	0
			1	1		
5	G	1	Total	Zn	0	0
			1	1		
5	H	1	Total	Zn	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

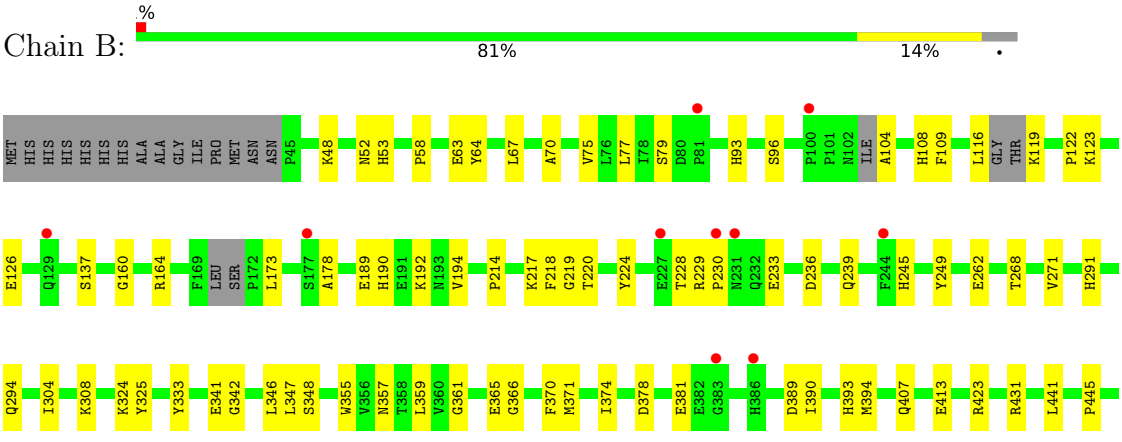
• Molecule 1: Insulin-degrading enzyme

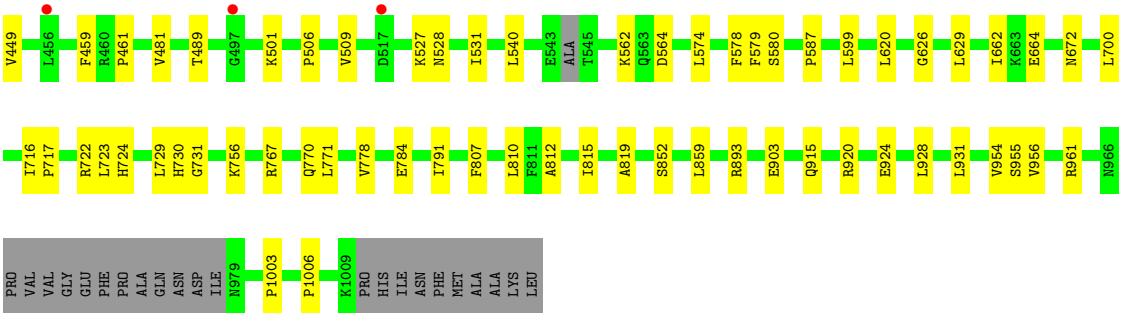
Chain A:



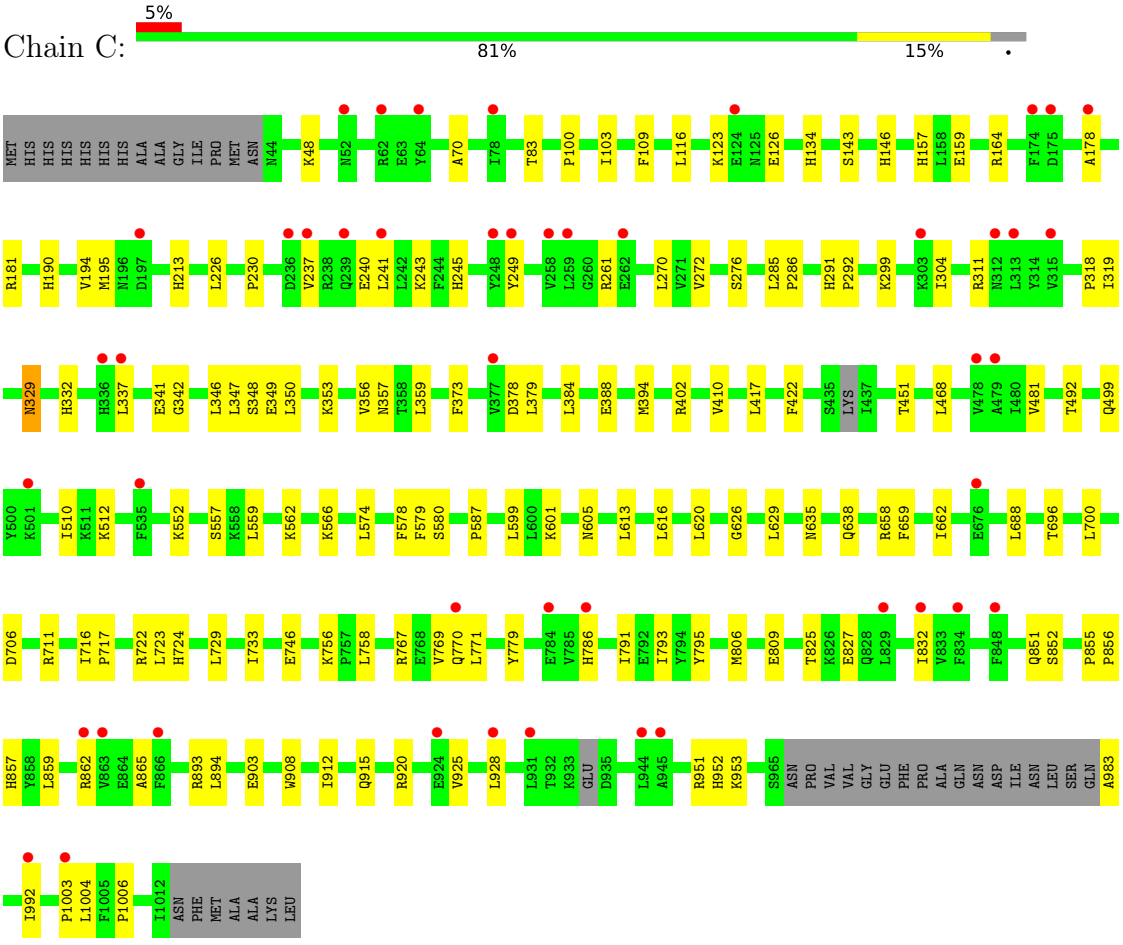
• Molecule 1: Insulin-degrading enzyme

Chain B:

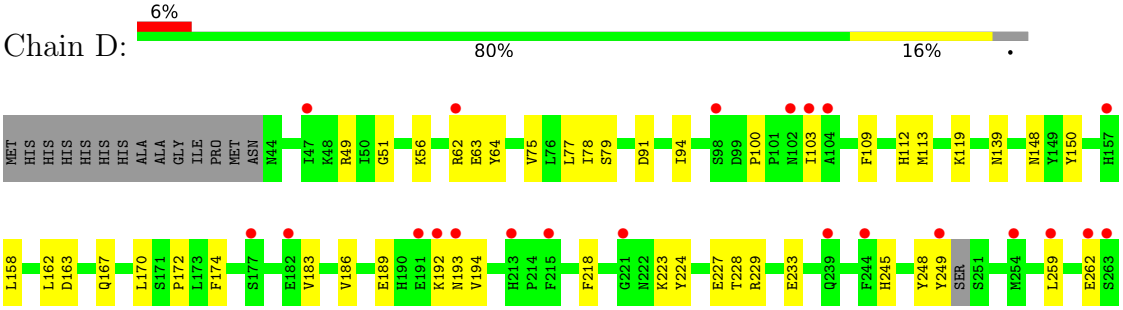


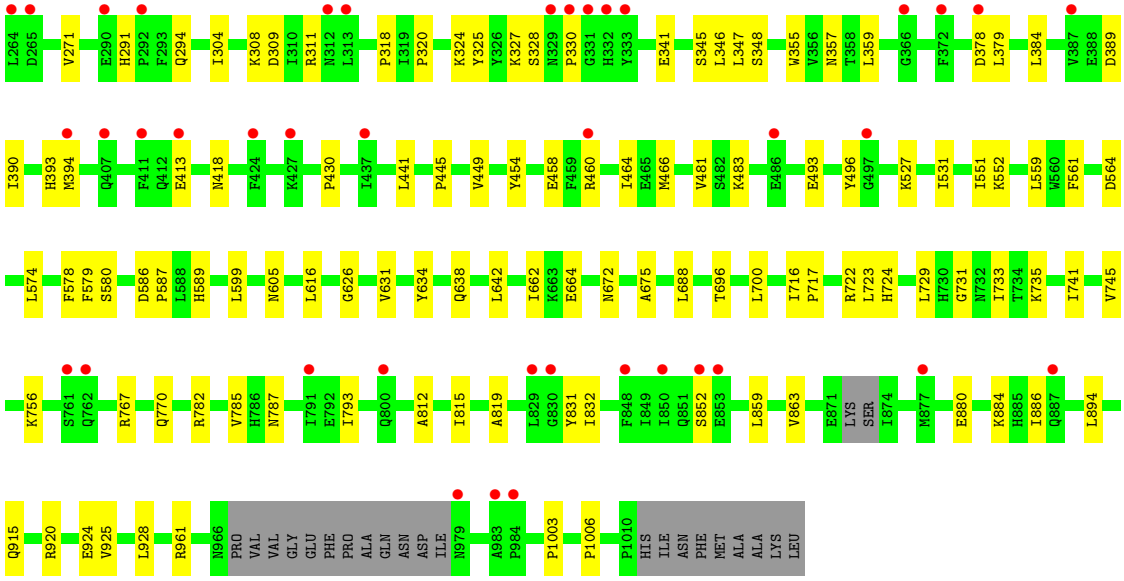


• Molecule 1: Insulin-degrading enzyme



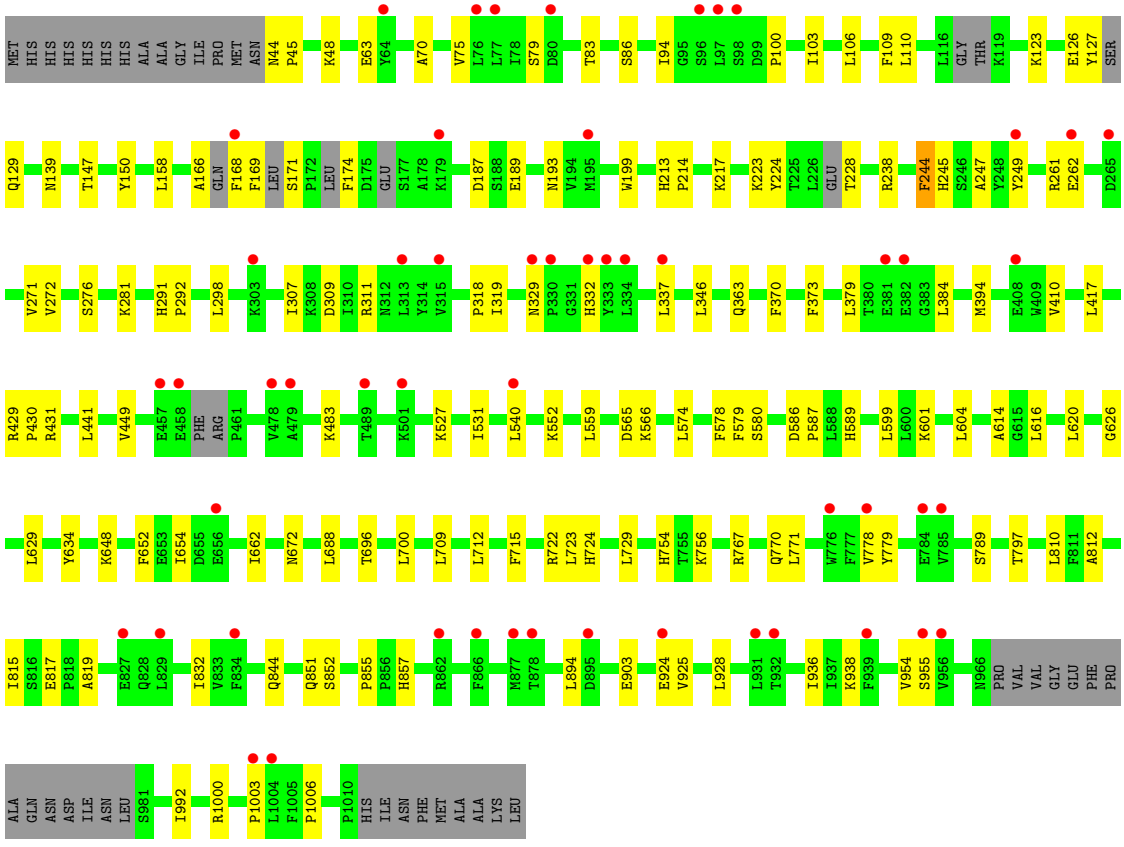
• Molecule 1: Insulin-degrading enzyme





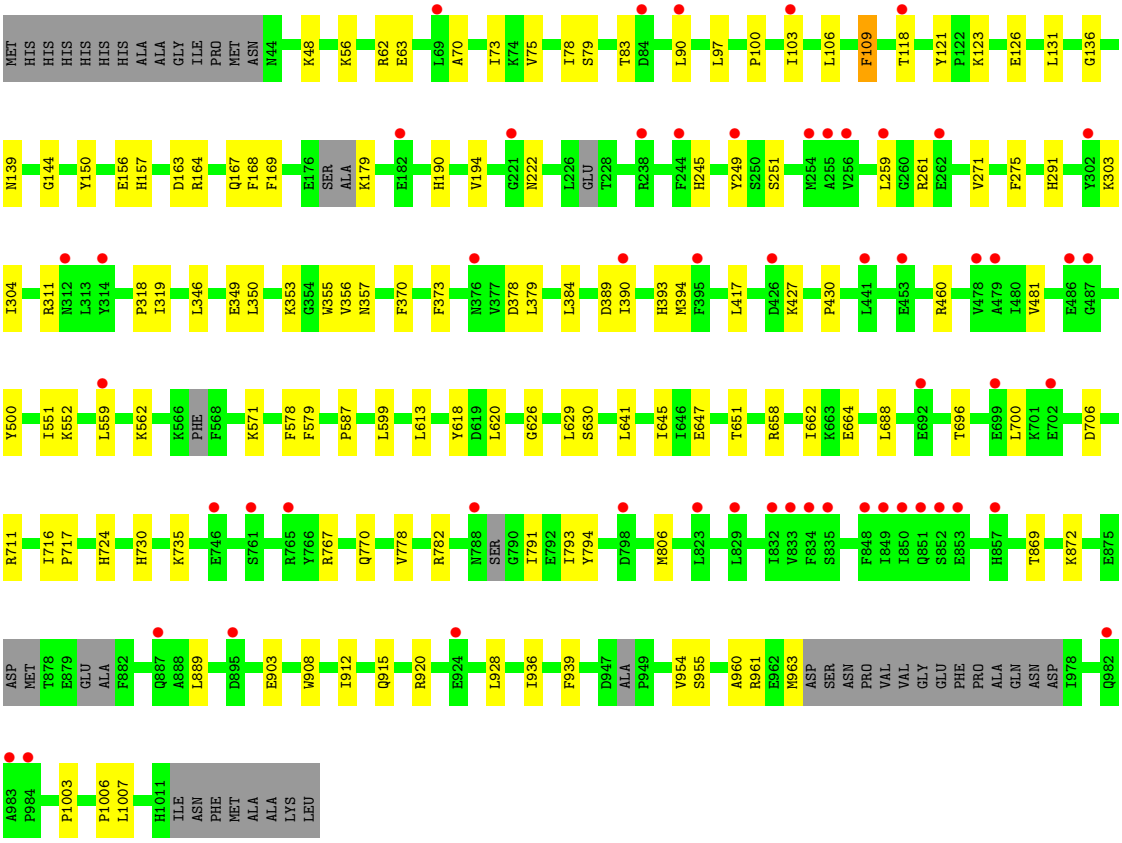
• Molecule 1: Insulin-degrading enzyme

Chain E:



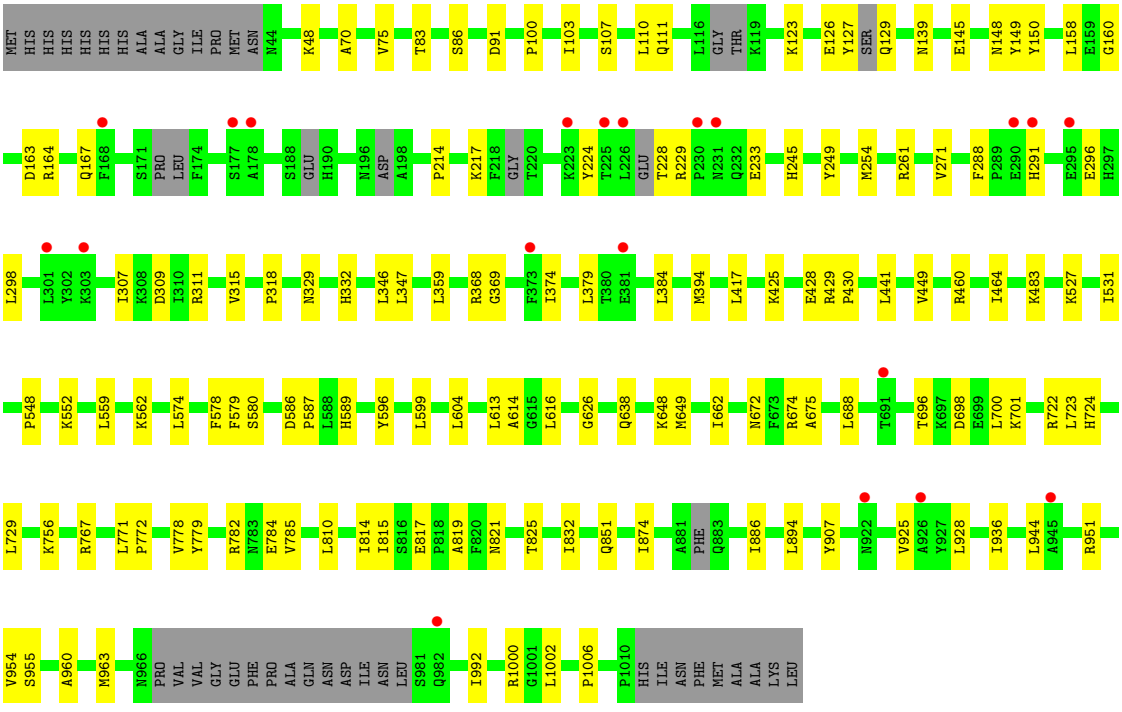
• Molecule 1: Insulin-degrading enzyme

Chain F:



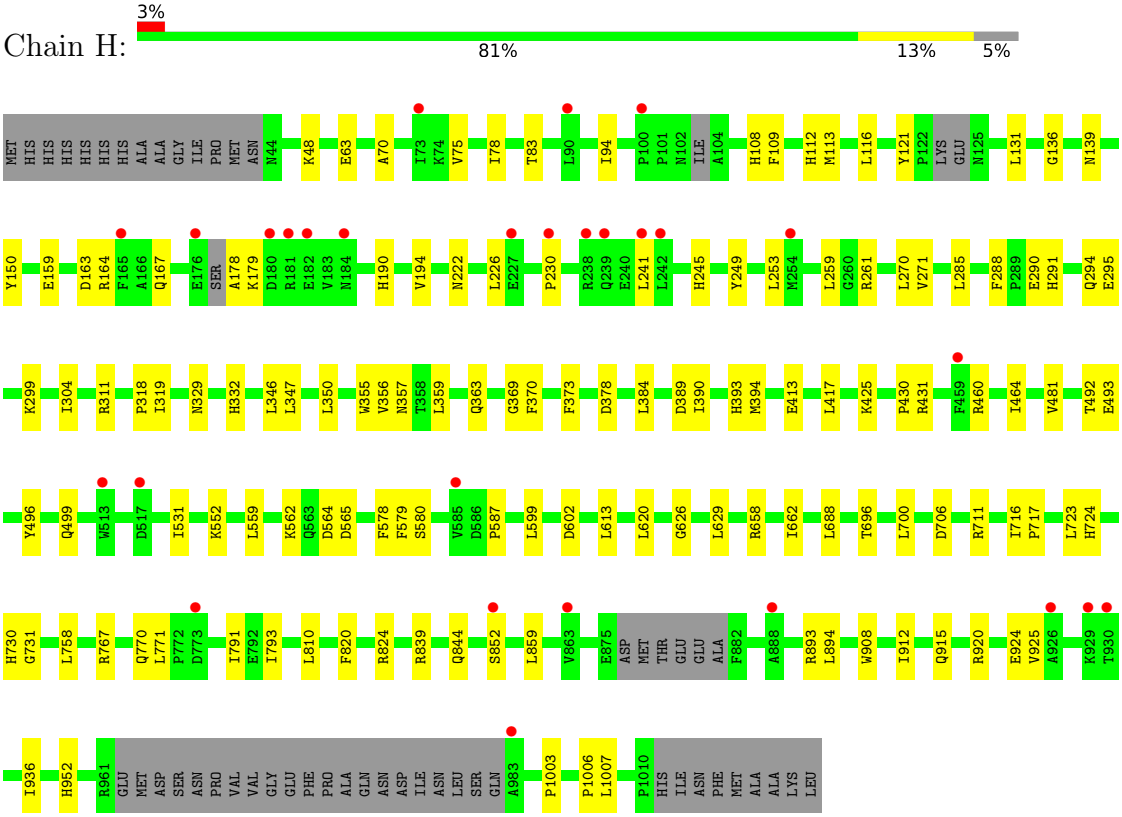
• Molecule 1: Insulin-degrading enzyme

Chain G:



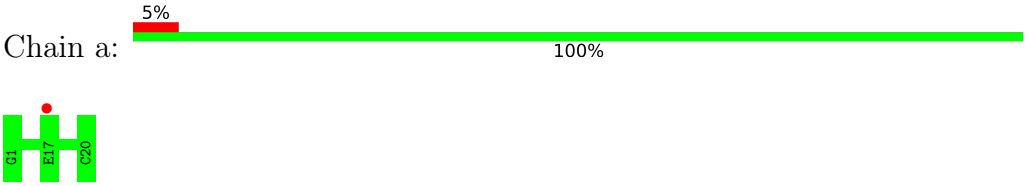
• Molecule 1: Insulin-degrading enzyme

Chain H:



• Molecule 2: Insulin

Chain a:

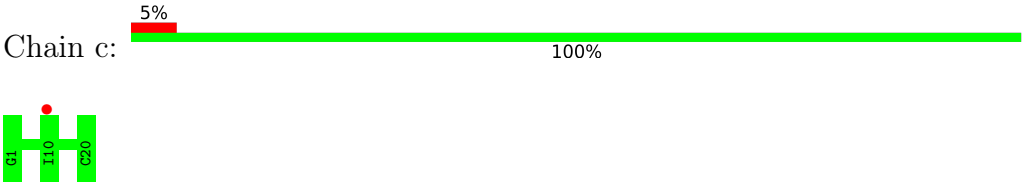


• Molecule 2: Insulin

Chain b:

• Molecule 2: Insulin

Chain c:

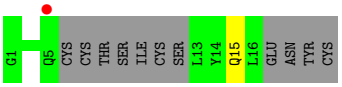


• Molecule 2: Insulin

Chain d:

• Molecule 2: Insulin

Chain e:

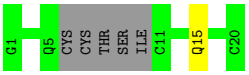


• Molecule 2: Insulin

Chain f:

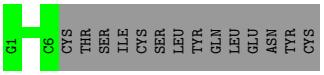
• Molecule 2: Insulin

Chain g:



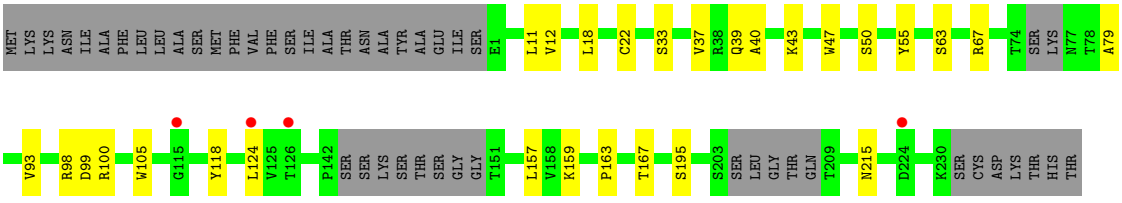
• Molecule 2: Insulin

Chain h:



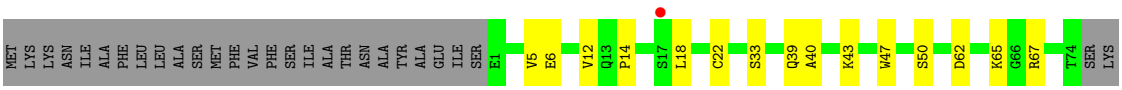
• Molecule 3: IDE-bound Fab heavy chain

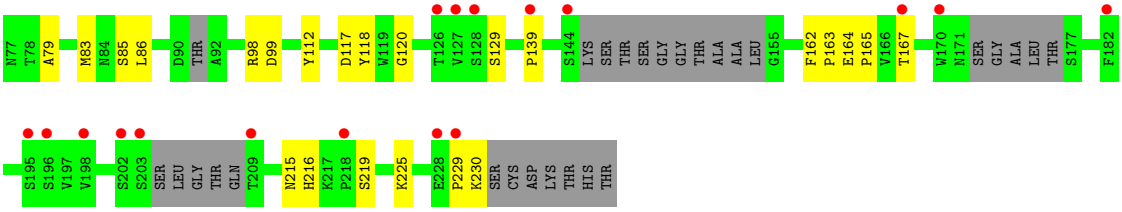
Chain I:



• Molecule 3: IDE-bound Fab heavy chain

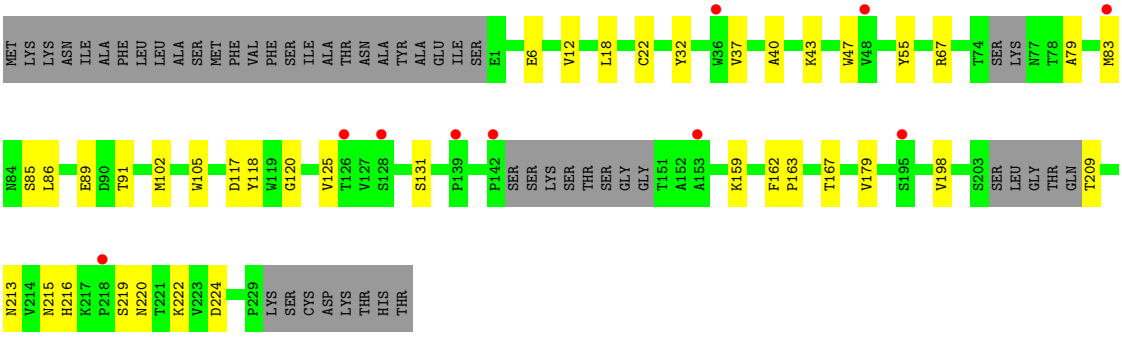
Chain K:





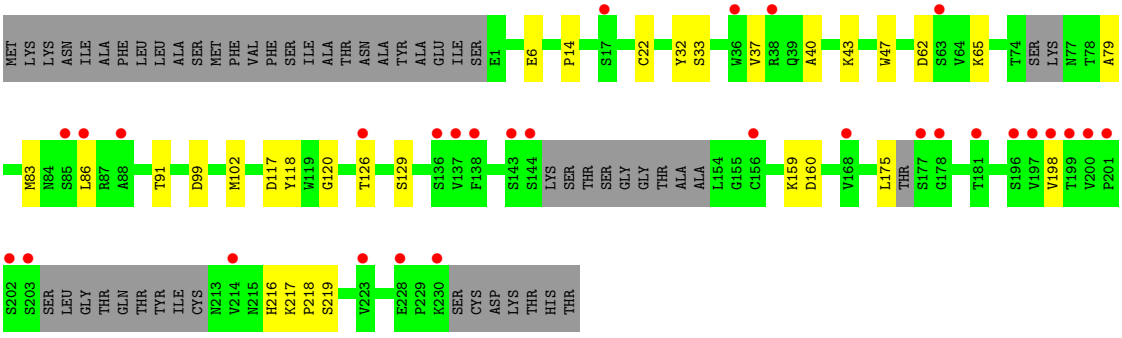
• Molecule 3: IDE-bound Fab heavy chain

Chain M:



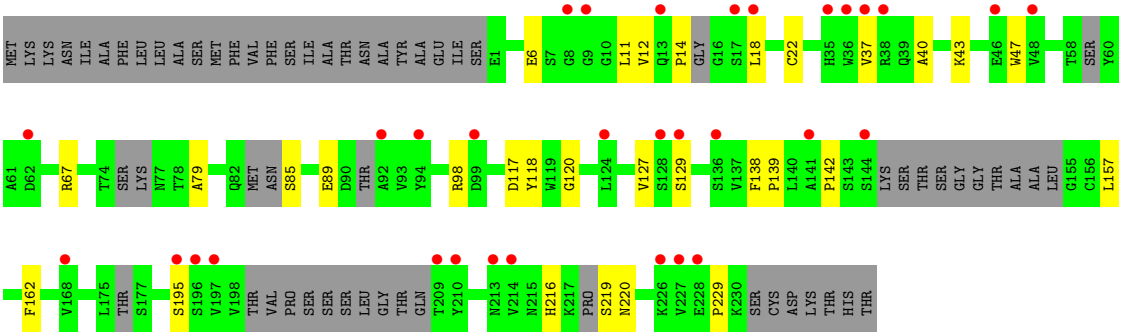
• Molecule 3: IDE-bound Fab heavy chain

Chain O:



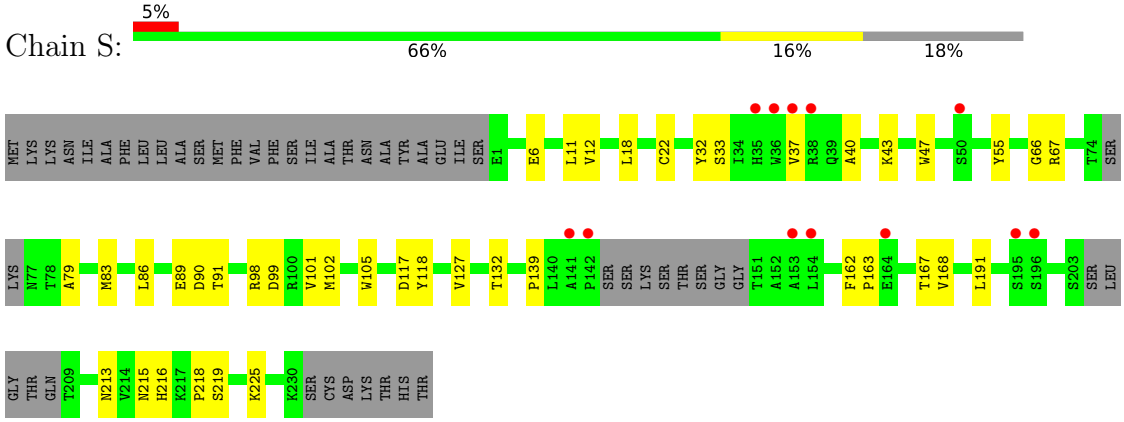
• Molecule 3: IDE-bound Fab heavy chain

Chain Q:



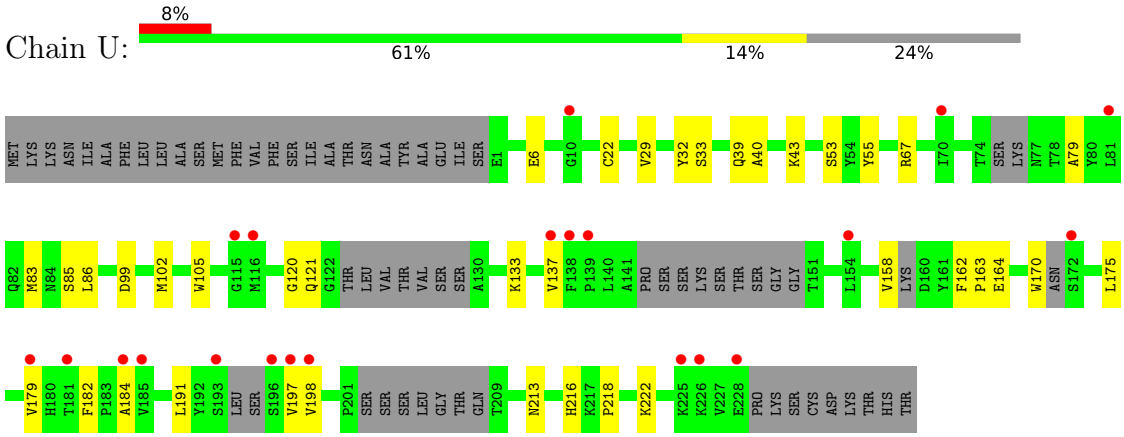
• Molecule 3: IDE-bound Fab heavy chain

Chain S:



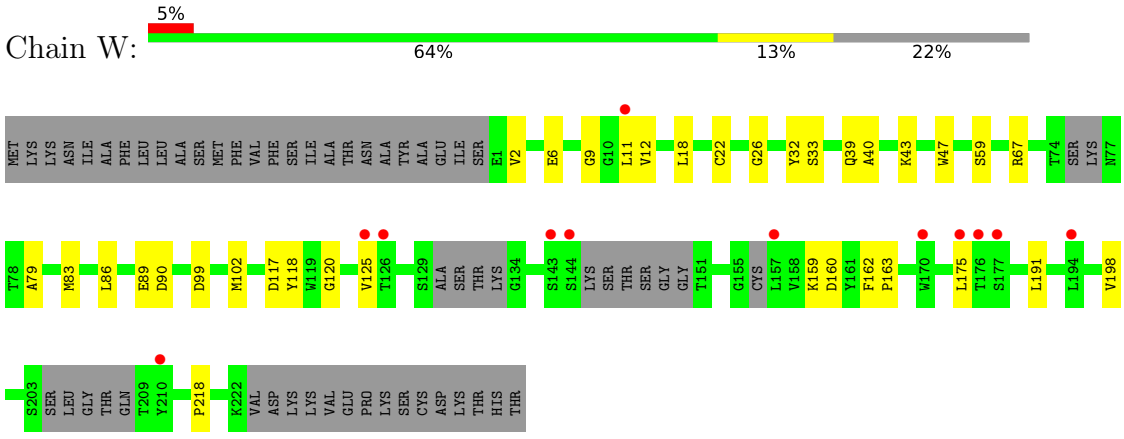
• Molecule 3: IDE-bound Fab heavy chain

Chain U:



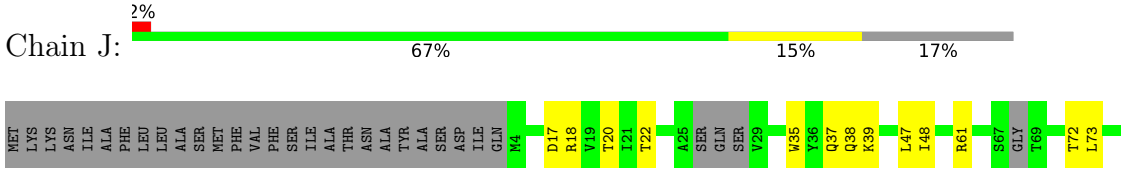
• Molecule 3: IDE-bound Fab heavy chain

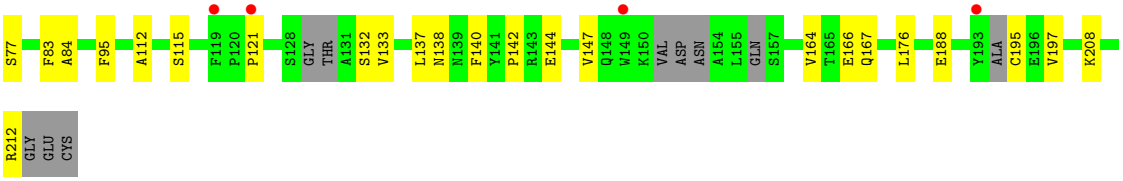
Chain W:



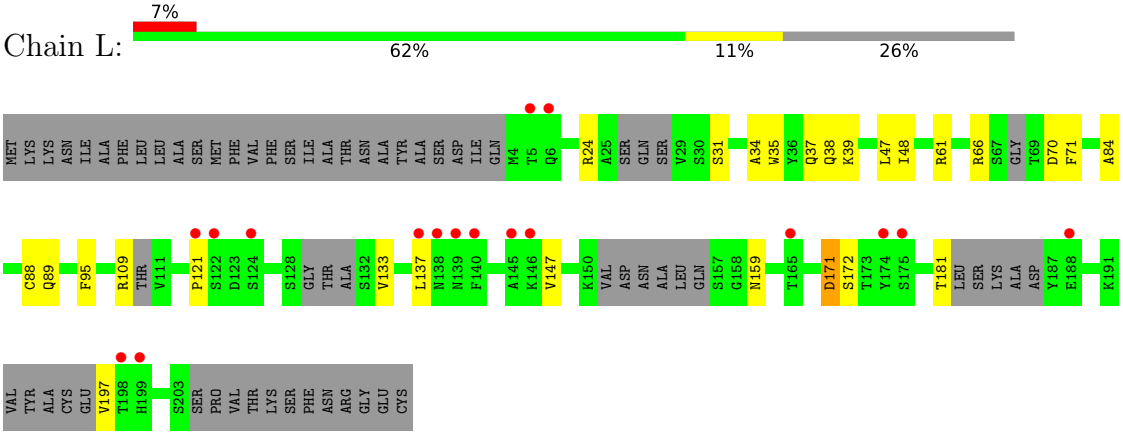
• Molecule 4: IDE-bound Fab light chain

Chain J:

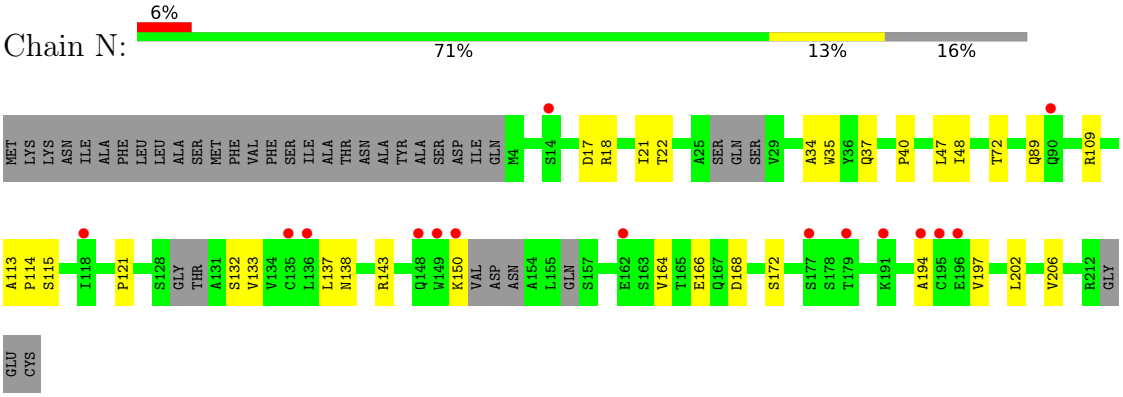




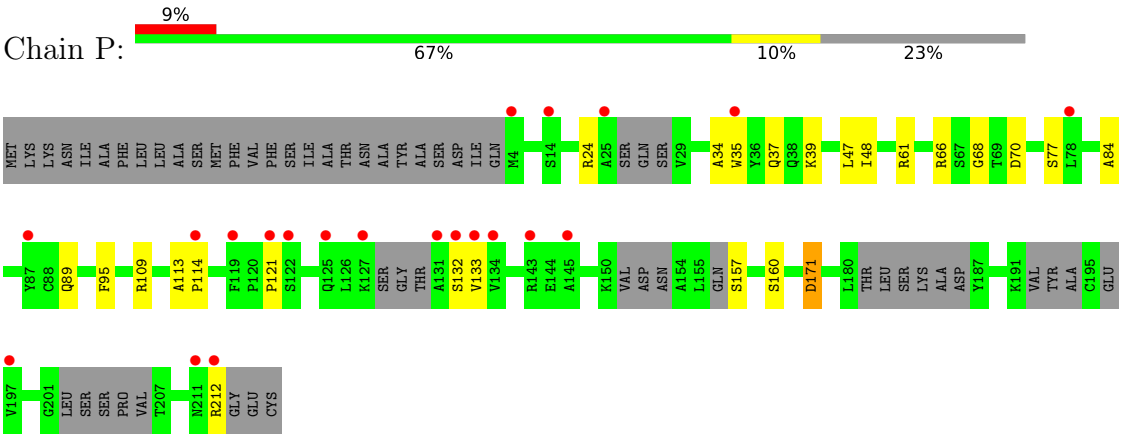
• Molecule 4: IDE-bound Fab light chain



• Molecule 4: IDE-bound Fab light chain

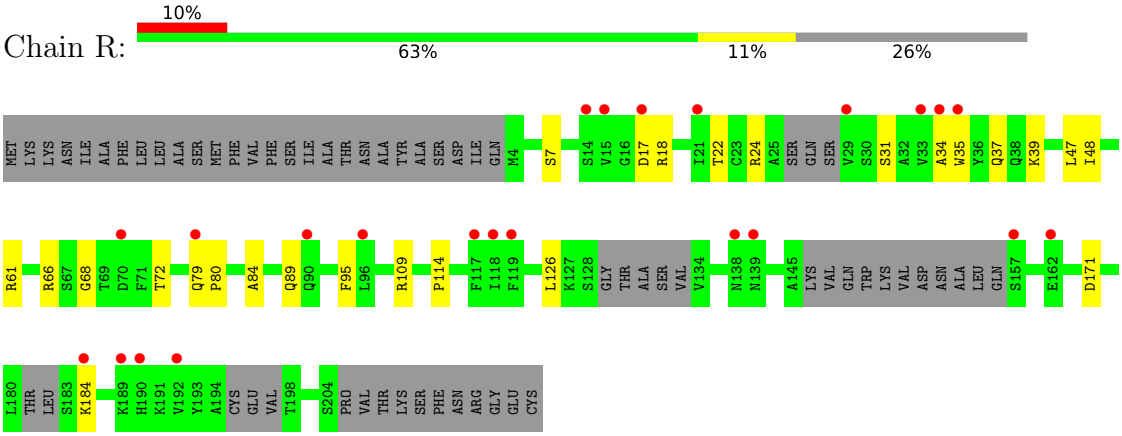


• Molecule 4: IDE-bound Fab light chain



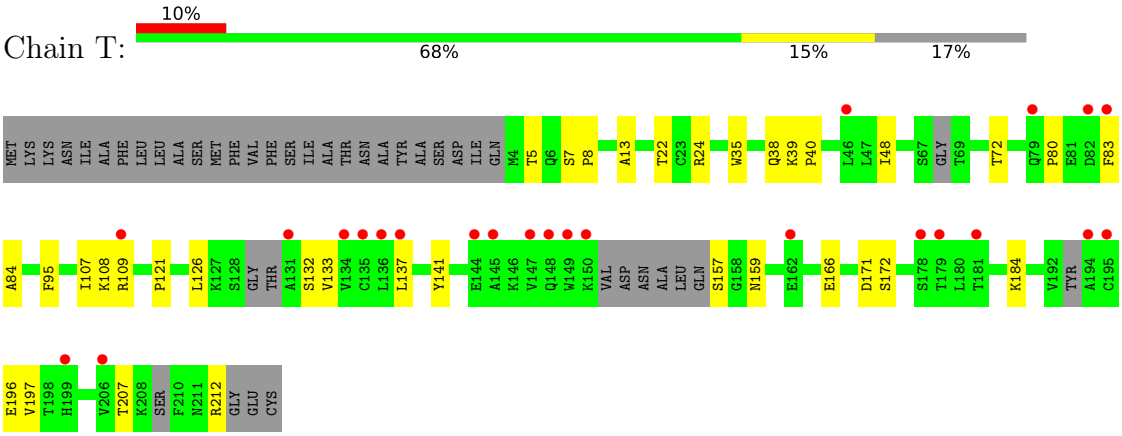
• Molecule 4: IDE-bound Fab light chain

Chain R:



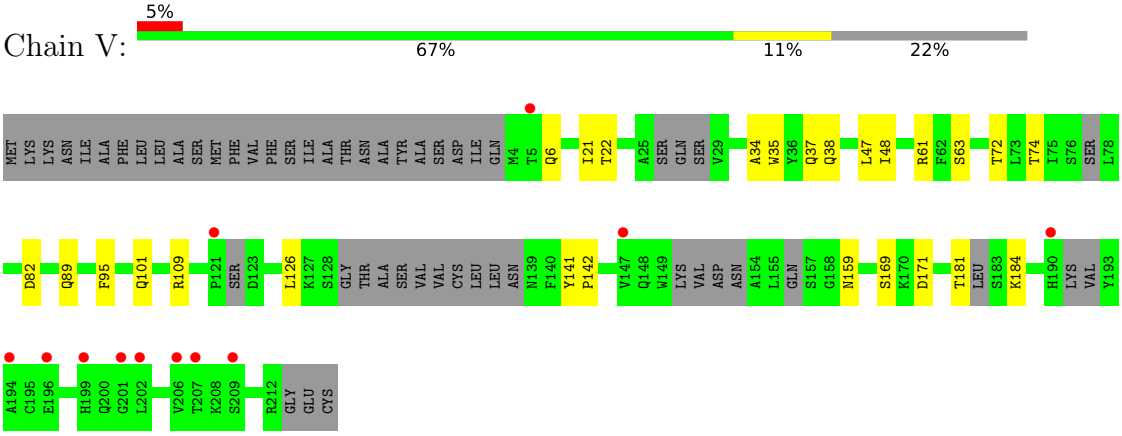
• Molecule 4: IDE-bound Fab light chain

Chain T:



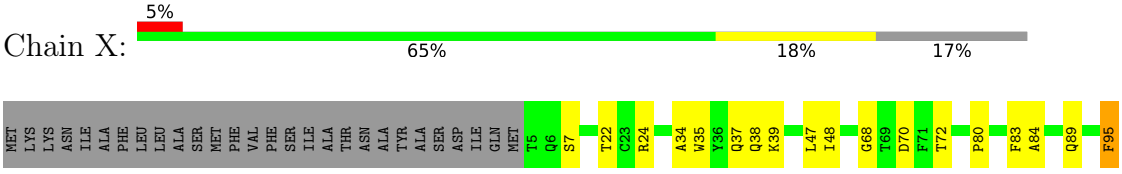
• Molecule 4: IDE-bound Fab light chain

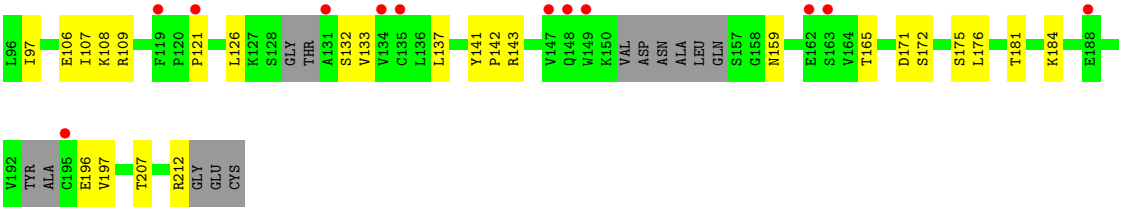
Chain V:



• Molecule 4: IDE-bound Fab light chain

Chain X:




L96
I97
E106
I107
K108
R109
F119
P120
P121
L126
K127
S128
GLY
THR
A131
S132
V133
V134
C135
L136
L137
Y141
P142
R143
V147
Q148
W149
K150
VAL
ASP
ASN
ALA
LEU
GLN
S157
G158
N159
E162
S163
V164
T165
D171
S172
S175
L176
T181
K184
E188
V192
TYR
ALA
C196
E196
V197
T207
R212
GLY
GLU
CYS

4 Data and refinement statistics (i)

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 – 3.95 49.54 – 3.93	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.54-3.95) 93.6 (49.54-3.93)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.243 , 0.291 0.252 , 0.299	Depositor DCC
R_{free} test set	1990 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å^2)	81.3	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 37.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.379 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	86906	wwPDB-VP
Average B, all atoms (Å^2)	111.0	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 27.56 % 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 2.1507e-03.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.24	0/7898	0.39	0/10677
1	B	0.25	0/7947	0.40	0/10739
1	C	0.25	0/7965	0.39	0/10772
1	D	0.25	0/7982	0.39	0/10795
1	E	0.24	0/7898	0.40	0/10670
1	F	0.24	0/7922	0.40	0/10704
1	G	0.24	0/7906	0.40	0/10680
1	H	0.24	0/7853	0.39	0/10618
2	a	0.26	0/155	0.59	0/209
2	b	0.24	0/36	0.44	0/47
2	c	0.32	0/155	0.62	0/209
2	d	0.19	0/18	0.39	0/23
2	e	0.23	0/73	0.53	0/96
2	f	0.26	0/133	0.59	0/177
2	g	0.25	0/121	0.49	0/161
2	h	0.25	0/42	0.50	0/55
3	I	0.24	0/1675	0.44	0/2282
3	K	0.24	0/1623	0.42	0/2206
3	M	0.24	0/1666	0.43	0/2271
3	O	0.24	0/1628	0.42	0/2214
3	Q	0.24	0/1574	0.42	0/2131
3	S	0.24	0/1675	0.43	0/2282
3	U	0.24	0/1555	0.44	0/2111
3	W	0.25	0/1586	0.44	0/2160
4	J	0.24	0/1551	0.41	0/2096
4	L	0.25	0/1380	0.45	0/1862
4	N	0.24	0/1562	0.42	0/2114
4	P	0.24	0/1440	0.42	0/1940
4	R	0.24	0/1375	0.42	0/1858
4	T	0.24	0/1546	0.44	0/2090
4	V	0.24	0/1458	0.42	0/1967
4	X	0.24	0/1545	0.43	0/2092

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.24	0/88943	0.41	0/120308

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7708	0	7652	81	0
1	B	7758	0	7696	83	0
1	C	7772	0	7714	84	0
1	D	7790	0	7728	95	0
1	E	7713	0	7650	86	1
1	F	7735	0	7691	76	0
1	G	7722	0	7667	81	0
1	H	7663	0	7617	77	0
2	a	154	0	145	0	0
2	b	37	0	39	0	0
2	c	154	0	145	0	0
2	d	19	0	25	0	0
2	e	74	0	77	0	0
2	f	134	0	124	0	0
2	g	121	0	113	0	0
2	h	43	0	44	0	0
3	I	1632	0	1575	18	0
3	K	1582	0	1517	22	0
3	M	1623	0	1562	24	0
3	O	1587	0	1530	15	0
3	Q	1539	0	1474	19	0
3	S	1632	0	1575	29	0
3	U	1518	0	1446	24	0
3	W	1546	0	1476	21	0
4	J	1523	0	1495	20	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	1356	0	1327	17	0
4	N	1532	0	1505	19	0
4	P	1416	0	1385	14	0
4	R	1350	0	1311	14	0
4	T	1518	0	1489	20	0
4	V	1432	0	1386	14	0
4	X	1515	0	1485	27	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
All	All	86906	0	85665	958	1

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 (958) 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)
4:T:121:PRO:HB3	4:T:132:SER:H	1.51	0.76
4:R:34:ALA:HB3	4:R:89:GLN:HB3	1.68	0.75
3:I:22:CYS:HB3	3:I:79:ALA:HB3	1.69	0.74
4:L:34:ALA:HB3	4:L:89:GLN:HB3	1.70	0.73
1:F:123:LYS:HB3	1:F:126:GLU:HB2	1.70	0.73
1:G:771:LEU:HD21	1:G:954:VAL:HG23	1.71	0.72
1:H:579:PHE:HB2	1:H:724:HIS:HB3	1.70	0.72
1:C:349:GLU:OE1	1:C:353:LYS:NZ	2.22	0.71
1:E:722:ARG:HG2	1:E:756:LYS:HB2	1.70	0.71
4:R:31:SER:O	4:R:66:ARG:NH1	2.23	0.71
4:X:121:PRO:HB3	4:X:132:SER:H	1.56	0.70
4:T:107:ILE:HG21	4:T:172:SER:HB3	1.73	0.70
1:A:425:LYS:NZ	1:A:428:GLU:OE2	2.18	0.70
1:D:441:LEU:HD23	1:D:449:VAL:HG11	1.75	0.69
4:J:121:PRO:HB3	4:J:132:SER:H	1.57	0.68
4:P:121:PRO:HD3	4:P:133:VAL:HG22	1.76	0.68
1:F:562:LYS:NZ	1:F:903:GLU:OE1	2.23	0.68
3:Q:67:ARG:NH1	3:Q:85:SER:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:147:VAL:HG22	4:J:197:VAL:HG12	1.76	0.68
1:A:562:LYS:NZ	1:A:903:GLU:OE1	2.27	0.68
1:C:579:PHE:HB2	1:C:724:HIS:HB3	1.75	0.68
1:F:889:LEU:HD11	1:F:928:LEU:HD22	1.76	0.68
3:I:11:LEU:HD12	3:I:163:PRO:HG3	1.76	0.67
1:D:341:GLU:OE2	1:D:605:ASN:ND2	2.23	0.67
3:K:22:CYS:HB3	3:K:79:ALA:HB3	1.76	0.67
3:M:22:CYS:HB3	3:M:79:ALA:HB3	1.75	0.67
1:D:722:ARG:HG2	1:D:756:LYS:HB2	1.77	0.67
1:E:565:ASP:OD1	1:E:566:LYS:NZ	2.28	0.67
1:D:189:GLU:O	1:D:193:ASN:ND2	2.28	0.67
1:G:441:LEU:HD23	1:G:449:VAL:HG11	1.77	0.66
1:E:579:PHE:HB2	1:E:724:HIS:HB3	1.77	0.66
3:Q:22:CYS:HB3	3:Q:79:ALA:HB3	1.77	0.66
1:B:245:HIS:O	1:B:249:TYR:HB2	1.96	0.66
4:L:121:PRO:HD3	4:L:133:VAL:HG22	1.78	0.66
1:F:579:PHE:HB2	1:F:724:HIS:HB3	1.76	0.65
1:D:852:SER:HB3	1:D:859:LEU:HD21	1.78	0.65
1:G:579:PHE:HB2	1:G:724:HIS:HB3	1.77	0.65
4:N:137:LEU:HD21	4:N:197:VAL:HG11	1.78	0.65
1:C:116:LEU:HD13	1:C:178:ALA:HB1	1.79	0.65
1:A:201:LEU:HD21	1:A:481:VAL:HG21	1.78	0.65
1:E:441:LEU:HD23	1:E:449:VAL:HG11	1.76	0.65
4:N:121:PRO:HD3	4:N:133:VAL:HG22	1.79	0.65
1:B:137:SER:OG	1:B:431:ARG:NH1	2.30	0.65
1:H:329:ASN:HB3	1:H:332:HIS:HB2	1.79	0.65
1:B:75:VAL:HG11	1:B:271:VAL:HG11	1.78	0.65
1:B:722:ARG:HG2	1:B:756:LYS:HB2	1.79	0.65
3:U:179:VAL:HA	3:U:198:VAL:HG12	1.79	0.65
1:A:579:PHE:HB2	1:A:724:HIS:HB3	1.78	0.64
1:G:722:ARG:HG2	1:G:756:LYS:HB2	1.79	0.64
1:F:767:ARG:NH1	1:F:1006:PRO:HA	2.12	0.64
4:X:121:PRO:HD3	4:X:133:VAL:HG22	1.80	0.64
1:B:341:GLU:HG2	1:B:347:LEU:HD13	1.79	0.64
1:H:389:ASP:O	1:H:393:HIS:ND1	2.30	0.64
3:U:6:GLU:OE2	3:U:120:GLY:HA3	1.97	0.64
3:K:83:MET:HB3	3:K:86:LEU:HD21	1.79	0.64
1:F:311:ARG:HD3	1:F:384:LEU:HD22	1.79	0.64
3:S:163:PRO:O	3:S:216:HIS:NE2	2.29	0.64
1:G:429:ARG:NH1	1:G:430:PRO:HD2	2.13	0.63
3:O:22:CYS:HB3	3:O:79:ALA:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:126:LEU:HD23	4:R:184:LYS:NZ	2.14	0.63
1:A:852:SER:HB3	1:A:859:LEU:HD21	1.80	0.63
1:G:425:LYS:NZ	1:G:428:GLU:OE2	2.17	0.63
3:O:91:THR:HG23	3:O:126:THR:HA	1.80	0.63
4:N:150:LYS:HB2	4:N:194:ALA:HB3	1.81	0.63
1:B:67:LEU:HD21	1:B:268:THR:HG23	1.81	0.63
1:G:129:GLN:HA	1:G:817:GLU:HG2	1.80	0.63
1:B:540:LEU:HB2	1:G:782:ARG:HH21	1.64	0.63
1:D:119:LYS:HE3	1:D:172:PRO:HB3	1.81	0.63
4:L:147:VAL:HG12	4:L:197:VAL:HG12	1.81	0.63
1:A:299:LYS:HD2	1:A:510:ILE:HD13	1.80	0.63
1:D:346:LEU:HD21	1:D:394:MET:HG2	1.81	0.63
4:V:35:TRP:HB2	4:V:48:ILE:HB	1.81	0.63
1:F:460:ARG:NH1	3:S:101:VAL:HB	2.14	0.62
4:N:40:PRO:HG2	4:N:166:GLU:HG2	1.81	0.62
1:B:346:LEU:HD21	1:B:394:MET:HG2	1.81	0.62
3:W:22:CYS:HB3	3:W:79:ALA:HB3	1.79	0.62
1:G:127:TYR:O	1:G:129:GLN:N	2.33	0.62
1:H:109:PHE:HZ	1:H:179:LYS:HG3	1.65	0.62
3:M:83:MET:HB3	3:M:86:LEU:HD21	1.80	0.62
1:F:552:LYS:HB3	1:F:559:LEU:HB3	1.81	0.62
1:F:782:ARG:NH2	1:F:961:ARG:O	2.33	0.61
3:M:222:LYS:NZ	3:U:121:GLN:HB3	2.15	0.61
1:E:429:ARG:NH1	1:E:430:PRO:HD2	2.16	0.61
1:E:709:LEU:HD12	1:E:712:LEU:HD11	1.82	0.61
4:P:34:ALA:HB3	4:P:89:GLN:HB3	1.82	0.61
4:T:39:LYS:HD3	4:T:84:ALA:HB2	1.82	0.61
4:N:34:ALA:HB3	4:N:89:GLN:HB3	1.83	0.61
1:D:767:ARG:NH1	1:D:1006:PRO:HA	2.16	0.61
1:G:674:ARG:NH2	1:G:784:GLU:OE2	2.28	0.61
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.82	0.61
1:F:460:ARG:HH11	3:S:101:VAL:HB	1.66	0.61
1:G:782:ARG:NH1	1:G:784:GLU:HG2	2.16	0.61
1:E:174:PHE:O	1:E:238:ARG:NH1	2.34	0.60
1:F:389:ASP:O	1:F:393:HIS:ND1	2.34	0.60
1:A:578:PHE:O	1:A:626:GLY:HA3	2.01	0.60
1:F:587:PRO:HB3	1:F:700:LEU:HD12	1.82	0.60
1:C:126:GLU:OE2	1:C:164:ARG:NE	2.34	0.60
1:E:1000:ARG:HG2	1:F:1007:LEU:HD12	1.83	0.60
1:H:552:LYS:HB3	1:H:559:LEU:HB3	1.83	0.60
3:S:83:MET:HB3	3:S:86:LEU:HD21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:202:LEU:HD21	4:N:206:VAL:H	1.66	0.60
4:R:61:ARG:NH1	4:R:80:PRO:HG2	2.16	0.60
4:R:109:ARG:NH1	4:R:171:ASP:HA	2.16	0.60
1:E:214:PRO:HA	1:E:217:LYS:HG3	1.83	0.60
3:K:40:ALA:HB3	3:K:43:LYS:HB2	1.84	0.60
1:B:229:ARG:O	1:B:233:GLU:HB2	2.02	0.60
1:F:48:LYS:HB2	1:F:70:ALA:HA	1.84	0.60
1:A:599:LEU:HD23	1:A:662:ILE:HD12	1.83	0.59
3:O:83:MET:HB3	3:O:86:LEU:HD21	1.84	0.59
1:E:166:ALA:O	1:E:168:PHE:N	2.35	0.59
3:W:67:ARG:NH2	3:W:90:ASP:OD2	2.30	0.59
1:E:189:GLU:O	1:E:193:ASN:ND2	2.35	0.59
1:E:604:LEU:HD21	1:E:648:LYS:HG3	1.84	0.59
1:C:852:SER:HB3	1:C:859:LEU:HD21	1.83	0.59
1:B:104:ALA:HB1	1:B:218:PHE:HB3	1.84	0.59
1:G:86:SER:HB3	1:G:158:LEU:HD12	1.82	0.59
1:H:852:SER:HB3	1:H:859:LEU:HD21	1.83	0.59
1:D:782:ARG:NH1	1:E:540:LEU:HD23	2.17	0.59
1:C:337:LEU:HD11	1:C:410:VAL:HG11	1.83	0.59
1:C:492:THR:HG22	1:C:499:GLN:HG2	1.83	0.59
1:C:599:LEU:HD23	1:C:662:ILE:HD12	1.84	0.59
1:D:100:PRO:HG2	1:D:103:ILE:HB	1.84	0.59
1:G:123:LYS:HB3	1:G:126:GLU:HB2	1.84	0.59
4:X:109:ARG:NH1	4:X:171:ASP:O	2.36	0.59
4:X:212:ARG:HA	4:X:212:ARG:HH11	1.66	0.59
1:G:587:PRO:HB3	1:G:700:LEU:HD23	1.84	0.59
1:A:83:THR:O	1:A:261:ARG:NE	2.33	0.59
1:B:852:SER:HB3	1:B:859:LEU:HD21	1.84	0.59
1:E:771:LEU:HD21	1:E:954:VAL:HG23	1.83	0.59
1:E:346:LEU:HD21	1:E:394:MET:HG2	1.83	0.59
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.83	0.58
1:C:100:PRO:HG2	1:C:103:ILE:HB	1.84	0.58
1:C:587:PRO:HB3	1:C:700:LEU:HD23	1.83	0.58
1:C:809:GLU:OE1	1:C:893:ARG:NH1	2.35	0.58
1:E:587:PRO:HB3	1:E:700:LEU:HD23	1.85	0.58
3:M:67:ARG:NH1	3:M:85:SER:O	2.36	0.58
1:D:631:VAL:HG12	1:D:638:GLN:HE21	1.67	0.58
1:G:886:ILE:HG23	1:G:928:LEU:HG	1.85	0.58
1:A:778:VAL:HG22	1:A:955:SER:HB2	1.86	0.58
1:C:915:GLN:OE1	1:C:920:ARG:NH2	2.35	0.58
4:J:137:LEU:HD21	4:J:197:VAL:HG11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:PRO:HA	1:B:217:LYS:HE3	1.86	0.58
3:M:179:VAL:HA	3:M:198:VAL:HG12	1.85	0.58
3:O:159:LYS:NZ	3:O:160:ASP:OD2	2.37	0.58
4:V:109:ARG:NH1	4:V:171:ASP:HA	2.19	0.58
3:S:40:ALA:HB3	3:S:43:LYS:HB2	1.86	0.57
3:U:40:ALA:HB3	3:U:43:LYS:HB2	1.86	0.57
4:P:35:TRP:HB2	4:P:48:ILE:HB	1.85	0.57
1:G:245:HIS:O	1:G:249:TYR:HB2	2.04	0.57
3:U:67:ARG:NH1	3:U:85:SER:O	2.37	0.57
1:C:83:THR:O	1:C:261:ARG:NE	2.34	0.57
1:D:527:LYS:NZ	1:D:531:ILE:HD12	2.19	0.57
1:E:100:PRO:HG2	1:E:103:ILE:HB	1.86	0.57
1:A:802:THR:HG23	1:A:924:GLU:HG2	1.86	0.57
4:J:121:PRO:HD3	4:J:133:VAL:HG22	1.86	0.57
4:X:107:ILE:HG21	4:X:172:SER:HB3	1.85	0.57
3:W:83:MET:HB3	3:W:86:LEU:HD21	1.87	0.57
1:D:561:PHE:HE1	1:D:733:ILE:HG23	1.70	0.57
3:M:209:THR:HG21	4:V:169:SER:HB2	1.87	0.57
4:R:126:LEU:HD23	4:R:184:LYS:HZ3	1.68	0.57
1:H:290:GLU:OE1	1:H:294:GLN:NE2	2.37	0.57
1:H:311:ARG:HD3	1:H:384:LEU:HD22	1.86	0.57
1:H:350:LEU:HB3	1:H:356:VAL:HB	1.87	0.57
3:Q:40:ALA:HB3	3:Q:43:LYS:HB2	1.87	0.57
3:S:67:ARG:NH2	3:S:90:ASP:OD2	2.33	0.57
4:R:66:ARG:HG2	4:R:68:GLY:H	1.69	0.57
1:D:63:GLU:HB2	1:D:79:SER:HB3	1.87	0.56
3:M:37:VAL:HG22	3:M:47:TRP:HA	1.87	0.56
3:W:175:LEU:HD13	3:W:198:VAL:HG21	1.88	0.56
4:L:159:ASN:ND2	4:L:181:THR:O	2.38	0.56
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.87	0.56
1:D:599:LEU:HD23	1:D:662:ILE:HD12	1.87	0.56
1:H:259:LEU:HD23	1:H:430:PRO:HB3	1.87	0.56
1:F:75:VAL:HG11	1:F:271:VAL:HG11	1.87	0.56
1:G:604:LEU:HD21	1:G:648:LYS:HG3	1.88	0.56
3:W:47:TRP:CG	4:X:97:ILE:HB	2.39	0.56
3:I:39:GLN:OE1	4:J:38:GLN:NE2	2.35	0.56
1:E:187:ASP:HB2	1:E:223:LYS:HB2	1.88	0.56
3:O:216:HIS:CE1	3:O:219:SER:H	2.23	0.56
3:W:159:LYS:NZ	3:W:160:ASP:OD2	2.39	0.56
1:B:224:TYR:OH	1:B:229:ARG:NH2	2.37	0.56
4:N:121:PRO:HB3	4:N:132:SER:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:THR:HG21	1:F:168:PHE:HA	1.88	0.56
1:G:599:LEU:HD23	1:G:662:ILE:HD12	1.88	0.56
1:A:86:SER:HB3	1:A:158:LEU:HD12	1.88	0.56
1:A:116:LEU:HD22	1:A:178:ALA:HB1	1.87	0.56
1:B:579:PHE:HB2	1:B:724:HIS:HB3	1.87	0.56
1:C:181:ARG:NH1	1:C:825:THR:O	2.39	0.56
1:C:795:TYR:HE1	1:C:951:ARG:HH12	1.54	0.56
1:F:936:ILE:HA	1:F:939:PHE:HB3	1.89	0.56
4:V:22:THR:HG22	4:V:72:THR:HG22	1.87	0.56
4:X:159:ASN:ND2	4:X:181:THR:O	2.39	0.56
3:U:83:MET:HB3	3:U:86:LEU:HD21	1.88	0.55
1:D:886:ILE:HG23	1:D:928:LEU:HD22	1.87	0.55
3:K:164:GLU:HB2	3:K:165:PRO:HA	1.88	0.55
1:E:83:THR:O	1:E:261:ARG:NE	2.37	0.55
3:Q:6:GLU:OE2	3:Q:120:GLY:HA3	2.07	0.55
1:A:587:PRO:HB3	1:A:700:LEU:HD23	1.88	0.55
1:H:578:PHE:O	1:H:626:GLY:HA3	2.07	0.55
1:F:311:ARG:HB3	1:F:379:LEU:HB2	1.88	0.55
3:Q:98:ARG:NH1	3:Q:118:TYR:HD2	2.05	0.55
3:W:40:ALA:HB3	3:W:43:LYS:HB2	1.88	0.55
1:E:63:GLU:HB2	1:E:79:SER:HB3	1.89	0.55
1:F:346:LEU:HD21	1:F:394:MET:HG2	1.89	0.55
1:D:75:VAL:HG11	1:D:271:VAL:HG11	1.89	0.55
1:D:229:ARG:O	1:D:233:GLU:HB2	2.06	0.55
1:E:601:LYS:HD3	1:E:620:LEU:HB3	1.89	0.55
1:F:770:GLN:HB3	1:F:1003:PRO:HG2	1.88	0.55
1:H:620:LEU:HB2	1:H:629:LEU:HD23	1.88	0.55
4:L:24:ARG:HD3	4:L:70:ASP:HB3	1.90	0.55
1:A:291:HIS:CE1	1:A:318:PRO:HB3	2.42	0.54
1:F:350:LEU:HB3	1:F:356:VAL:HB	1.88	0.54
3:M:222:LYS:HZ1	3:U:121:GLN:HB3	1.72	0.54
4:X:126:LEU:HD23	4:X:184:LYS:NZ	2.23	0.54
1:A:299:LYS:HD3	1:A:474:GLU:HA	1.89	0.54
1:E:778:VAL:HG22	1:E:955:SER:HB2	1.89	0.54
1:F:100:PRO:HG2	1:F:103:ILE:HB	1.89	0.54
1:H:357:ASN:HB2	1:H:378:ASP:OD2	2.07	0.54
3:U:33:SER:HB2	3:U:99:ASP:OD2	2.07	0.54
3:W:12:VAL:HG21	3:W:18:LEU:HG	1.89	0.54
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.89	0.54
1:E:712:LEU:HA	1:E:715:PHE:HB3	1.89	0.54
1:H:109:PHE:O	1:H:113:MET:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:40:ALA:HB3	3:I:43:LYS:HB2	1.89	0.54
1:D:291:HIS:O	1:D:294:GLN:NE2	2.35	0.54
3:W:39:GLN:OE1	4:X:38:GLN:NE2	2.40	0.54
1:A:108:HIS:NE2	1:A:189:GLU:OE2	2.31	0.54
1:B:291:HIS:O	1:B:294:GLN:NE2	2.41	0.54
1:C:722:ARG:HH11	1:C:756:LYS:HE2	1.72	0.54
1:G:562:LYS:NZ	1:G:907:TYR:OH	2.37	0.54
4:X:196:GLU:OE1	4:X:207:THR:OG1	2.23	0.54
1:D:167:GLN:HA	1:D:170:LEU:HD13	1.88	0.54
1:C:578:PHE:O	1:C:626:GLY:HA3	2.08	0.54
1:H:355:TRP:HB3	1:H:390:ILE:HD11	1.90	0.54
1:H:493:GLU:OE1	1:H:496:TYR:N	2.40	0.54
1:A:865:ALA:HB2	1:A:983:ALA:HA	1.89	0.54
1:C:767:ARG:NH1	1:C:1006:PRO:HA	2.22	0.54
1:E:129:GLN:HA	1:E:817:GLU:HG2	1.88	0.54
1:E:150:TYR:HD2	1:E:431:ARG:HG2	1.73	0.54
1:H:116:LEU:HD22	1:H:178:ALA:HB1	1.90	0.54
1:A:572:ALA:HA	1:A:731:GLY:HA3	1.90	0.54
1:E:815:ILE:O	1:E:819:ALA:HB2	2.06	0.54
1:F:599:LEU:HD23	1:F:662:ILE:HD12	1.90	0.54
1:H:291:HIS:CE1	1:H:318:PRO:HB3	2.43	0.54
4:V:126:LEU:HD23	4:V:184:LYS:HG3	1.90	0.54
4:X:39:LYS:HD3	4:X:84:ALA:HB2	1.88	0.54
1:B:915:GLN:OE1	1:B:920:ARG:NH2	2.33	0.53
3:K:62:ASP:HA	3:K:65:LYS:HE2	1.90	0.53
1:C:272:VAL:O	1:C:276:SER:OG	2.26	0.53
1:C:729:LEU:HB3	1:C:733:ILE:HD11	1.89	0.53
1:F:259:LEU:HD23	1:F:430:PRO:HB3	1.90	0.53
1:F:767:ARG:HH12	1:F:1006:PRO:HA	1.72	0.53
1:F:915:GLN:OE1	1:F:920:ARG:NH2	2.38	0.53
1:H:108:HIS:O	1:H:112:HIS:HD2	1.91	0.53
1:B:587:PRO:HB3	1:B:700:LEU:HD23	1.89	0.53
1:C:291:HIS:CE1	1:C:318:PRO:HB3	2.44	0.53
1:C:357:ASN:OD1	1:C:658:ARG:NH2	2.40	0.53
1:E:574:LEU:HD22	1:E:729:LEU:HD22	1.90	0.53
1:G:574:LEU:HD22	1:G:729:LEU:HD22	1.91	0.53
3:I:37:VAL:HG22	3:I:47:TRP:HA	1.90	0.53
1:C:311:ARG:NH1	1:C:379:LEU:O	2.40	0.53
1:D:311:ARG:NH2	1:D:664:GLU:OE2	2.41	0.53
1:D:551:ILE:HB	1:D:735:LYS:HE3	1.90	0.53
1:G:1000:ARG:HG2	1:H:1007:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:133:LYS:HD3	3:U:191:LEU:HD11	1.90	0.53
1:B:771:LEU:HD21	1:B:954:VAL:HG23	1.90	0.53
1:F:620:LEU:HB2	1:F:629:LEU:HD23	1.90	0.53
1:A:889:LEU:HD22	1:A:928:LEU:HG	1.90	0.53
1:C:562:LYS:NZ	1:C:903:GLU:OE1	2.40	0.53
1:C:566:LYS:NZ	1:C:903:GLU:OE1	2.41	0.53
4:T:137:LEU:HD21	4:T:197:VAL:HG11	1.90	0.53
1:A:100:PRO:HG2	1:A:103:ILE:HB	1.91	0.53
1:B:770:GLN:HB3	1:B:1003:PRO:HG2	1.89	0.53
1:G:779:TYR:HB2	1:G:992:ILE:HD12	1.91	0.53
4:T:212:ARG:HA	4:T:212:ARG:HH11	1.74	0.53
4:X:137:LEU:HD21	4:X:197:VAL:HG11	1.91	0.53
1:F:908:TRP:O	1:F:912:ILE:HG12	2.09	0.53
1:B:347:LEU:HD12	1:B:359:LEU:HB3	1.90	0.52
1:B:784:GLU:O	1:B:961:ARG:HG3	2.09	0.52
1:C:402:ARG:NH1	1:C:468:LEU:O	2.42	0.52
3:M:131:SER:O	3:M:162:PHE:CD1	2.62	0.52
1:B:366:GLY:HA3	1:B:370:PHE:O	2.09	0.52
1:D:224:TYR:OH	1:D:229:ARG:NH2	2.43	0.52
4:R:22:THR:HG22	4:R:72:THR:HG22	1.91	0.52
1:G:296:GLU:HB3	4:L:61:ARG:HH11	1.74	0.52
4:P:39:LYS:HD3	4:P:84:ALA:HB2	1.90	0.52
4:P:157:SER:OG	4:P:160:SER:OG	2.24	0.52
1:C:827:GLU:OE2	1:C:862:ARG:NH2	2.38	0.52
1:D:587:PRO:HB3	1:D:700:LEU:HD23	1.90	0.52
1:H:413:GLU:OE2	1:H:531:ILE:HD11	2.10	0.52
1:H:587:PRO:HB3	1:H:700:LEU:HD23	1.91	0.52
1:B:304:ILE:HB	1:B:481:VAL:HG22	1.92	0.52
1:C:706:ASP:O	1:C:711:ARG:NH2	2.43	0.52
1:D:579:PHE:HB2	1:D:724:HIS:HB3	1.92	0.52
4:J:39:LYS:HD3	4:J:84:ALA:HB2	1.92	0.52
3:Q:216:HIS:O	3:Q:220:ASN:HA	2.10	0.52
1:D:112:HIS:HD2	1:D:186:VAL:HG22	1.75	0.52
1:E:75:VAL:HG11	1:E:271:VAL:HG11	1.92	0.52
1:A:791:ILE:HD11	1:A:793:ILE:HD11	1.92	0.52
1:E:48:LYS:HB2	1:E:70:ALA:HA	1.92	0.52
4:J:35:TRP:HB2	4:J:48:ILE:HB	1.92	0.52
1:D:291:HIS:CE1	1:D:318:PRO:HB3	2.45	0.52
1:E:123:LYS:HB3	1:E:126:GLU:HB2	1.92	0.52
1:E:127:TYR:O	1:E:129:GLN:N	2.43	0.52
1:G:596:TYR:OH	1:G:649:MET:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:291:HIS:CE1	1:G:318:PRO:HB3	2.44	0.52
4:V:63:SER:HB2	4:V:74:THR:HB	1.91	0.52
4:X:106:GLU:OE2	4:X:143:ARG:NH1	2.43	0.52
1:D:389:ASP:O	1:D:393:HIS:ND1	2.39	0.51
1:H:562:LYS:O	1:H:730:HIS:HA	2.10	0.51
4:X:80:PRO:HA	4:X:83:PHE:HE2	1.75	0.51
1:B:564:ASP:HB2	1:B:731:GLY:HA2	1.92	0.51
3:K:6:GLU:OE2	3:K:120:GLY:HA3	2.10	0.51
1:A:915:GLN:OE1	1:A:920:ARG:NH2	2.42	0.51
1:C:346:LEU:HD21	1:C:394:MET:HG2	1.93	0.51
1:D:880:GLU:OE2	1:D:884:LYS:HE2	2.10	0.51
4:X:7:SER:HB3	4:X:24:ARG:HH12	1.75	0.51
1:H:599:LEU:HD23	1:H:662:ILE:HD12	1.92	0.51
4:T:121:PRO:HD3	4:T:133:VAL:HG22	1.91	0.51
3:O:33:SER:HB2	3:O:99:ASP:OD2	2.11	0.51
1:E:245:HIS:O	1:E:249:TYR:HB2	2.10	0.51
1:G:139:ASN:HB3	1:G:150:TYR:CE2	2.46	0.51
1:D:915:GLN:OE1	1:D:920:ARG:NH2	2.38	0.51
1:G:288:PHE:O	1:G:369:GLY:HA3	2.11	0.51
4:L:39:LYS:HD3	4:L:84:ALA:HB2	1.92	0.51
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.92	0.51
1:E:832:ILE:HB	1:E:851:GLN:HB3	1.91	0.51
1:G:346:LEU:HD21	1:G:394:MET:HG2	1.92	0.51
3:S:11:LEU:HD12	3:S:163:PRO:HG3	1.92	0.51
4:J:212:ARG:HA	4:J:212:ARG:HH11	1.75	0.51
4:T:196:GLU:OE1	4:T:207:THR:OG1	2.27	0.51
1:C:552:LYS:HB3	1:C:559:LEU:HB3	1.92	0.51
1:D:304:ILE:HB	1:D:481:VAL:HG22	1.92	0.51
1:E:599:LEU:HD13	1:E:654:ILE:HD13	1.93	0.51
3:K:47:TRP:HE1	3:K:50:SER:HG	1.59	0.51
3:W:33:SER:HB2	3:W:99:ASP:OD2	2.11	0.51
1:C:159:GLU:HG3	1:C:270:LEU:HD11	1.93	0.51
3:S:216:HIS:CE1	3:S:219:SER:H	2.29	0.51
4:L:137:LEU:HD21	4:L:197:VAL:HG11	1.92	0.51
4:T:5:THR:OG1	4:T:24:ARG:O	2.28	0.50
1:B:214:PRO:O	1:B:217:LYS:HB2	2.12	0.50
3:U:22:CYS:HB3	3:U:79:ALA:HB3	1.93	0.50
1:B:108:HIS:ND1	1:B:220:THR:HG23	2.26	0.50
1:F:109:PHE:HZ	1:F:179:LYS:HG3	1.76	0.50
3:U:216:HIS:CG	3:U:218:PRO:HD3	2.46	0.50
1:C:706:ASP:HB3	1:C:711:ARG:HH22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:960:ALA:HB3	1:F:963:MET:HG3	1.94	0.50
1:G:229:ARG:NE	1:G:233:GLU:OE2	2.45	0.50
3:O:40:ALA:HB3	3:O:43:LYS:HB2	1.93	0.50
4:T:109:ARG:NH1	4:T:171:ASP:O	2.43	0.50
1:A:552:LYS:HB3	1:A:559:LEU:HB3	1.93	0.50
1:B:48:LYS:HB2	1:B:70:ALA:HA	1.94	0.50
1:F:357:ASN:OD1	1:F:658:ARG:NH2	2.44	0.50
1:G:214:PRO:HA	1:G:217:LYS:HG3	1.93	0.50
1:G:778:VAL:HG22	1:G:955:SER:HB2	1.92	0.50
1:A:329:ASN:HB3	1:A:332:HIS:HB2	1.94	0.50
1:H:460:ARG:NH2	3:W:102:MET:O	2.42	0.50
4:P:121:PRO:HB3	4:P:132:SER:H	1.75	0.50
1:A:346:LEU:HD21	1:A:394:MET:HG2	1.94	0.50
1:G:311:ARG:HD3	1:G:384:LEU:HD22	1.94	0.50
1:G:311:ARG:HB3	1:G:379:LEU:HB2	1.92	0.50
1:A:886:ILE:HG23	1:A:928:LEU:HD13	1.93	0.50
1:D:347:LEU:HD13	1:D:359:LEU:HB2	1.93	0.50
1:B:562:LYS:NZ	1:B:903:GLU:OE2	2.45	0.49
1:C:123:LYS:HB3	1:C:126:GLU:HB2	1.94	0.49
1:C:791:ILE:HD11	1:C:793:ILE:HD11	1.94	0.49
1:E:291:HIS:CD2	1:E:370:PHE:HB2	2.47	0.49
1:H:83:THR:O	1:H:261:ARG:NE	2.40	0.49
1:H:915:GLN:OE1	1:H:920:ARG:NH2	2.44	0.49
4:J:164:VAL:HG22	4:J:176:LEU:HD13	1.94	0.49
4:L:109:ARG:NH1	4:L:171:ASP:HA	2.27	0.49
4:T:109:ARG:HH12	4:T:171:ASP:HA	1.77	0.49
1:A:213:HIS:CE1	1:A:292:PRO:HG3	2.47	0.49
1:C:795:TYR:HE1	1:C:951:ARG:NH1	2.08	0.49
1:D:223:LYS:HG3	1:D:227:GLU:HG2	1.93	0.49
1:G:675:ALA:HA	1:G:785:VAL:HG21	1.94	0.49
1:B:574:LEU:HD22	1:B:729:LEU:HD22	1.93	0.49
1:H:109:PHE:HD2	1:H:241:LEU:HD21	1.77	0.49
4:N:115:SER:HB2	4:N:138:ASN:HB3	1.93	0.49
1:A:135:ALA:HA	1:A:892:ARG:NH1	2.27	0.49
1:E:224:TYR:HA	1:E:228:THR:HB	1.94	0.49
1:E:754:HIS:O	1:E:754:HIS:ND1	2.45	0.49
4:P:109:ARG:NH1	4:P:171:ASP:HA	2.27	0.49
1:D:770:GLN:HB3	1:D:1003:PRO:HG2	1.95	0.49
3:U:29:VAL:O	3:U:53:SER:OG	2.31	0.49
1:A:311:ARG:NH1	1:A:379:LEU:O	2.44	0.49
1:B:562:LYS:O	1:B:730:HIS:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:SER:HB3	1:D:458:GLU:HG3	1.93	0.49
1:F:291:HIS:NE2	1:F:318:PRO:HB3	2.27	0.49
3:Q:14:PRO:HG3	3:Q:127:VAL:HG12	1.94	0.49
3:W:11:LEU:HD12	3:W:163:PRO:HG3	1.94	0.49
1:H:492:THR:HG22	1:H:499:GLN:HG2	1.95	0.49
4:P:157:SER:HG	4:P:160:SER:HG	1.58	0.49
1:B:389:ASP:O	1:B:393:HIS:ND1	2.42	0.49
1:A:688:LEU:HD13	1:A:696:THR:HG22	1.95	0.49
4:N:22:THR:HG22	4:N:72:THR:HG22	1.95	0.49
1:A:417:LEU:HD21	1:A:613:LEU:O	2.13	0.48
1:G:722:ARG:NH2	1:H:706:ASP:OD2	2.44	0.48
4:N:202:LEU:HD11	4:N:206:VAL:HG23	1.94	0.48
1:H:767:ARG:NH1	1:H:1006:PRO:HA	2.27	0.48
3:S:66:GLY:HA3	4:N:202:LEU:HA	1.94	0.48
1:A:351:LYS:HZ2	1:A:658:ARG:HH12	1.62	0.48
1:H:304:ILE:HB	1:H:481:VAL:HG22	1.95	0.48
3:Q:117:ASP:OD1	3:Q:118:TYR:N	2.45	0.48
1:C:48:LYS:HB2	1:C:70:ALA:HA	1.95	0.48
1:C:601:LYS:HD3	1:C:620:LEU:HB3	1.96	0.48
4:J:167:GLN:N	4:J:167:GLN:OE1	2.47	0.48
4:V:21:ILE:O	4:V:72:THR:HA	2.14	0.48
1:B:580:SER:HB2	1:B:723:LEU:HD23	1.95	0.48
1:C:616:LEU:HD11	1:C:638:GLN:HG3	1.95	0.48
1:D:574:LEU:HD22	1:D:729:LEU:HD22	1.95	0.48
3:S:91:THR:HB	3:S:127:VAL:HG22	1.94	0.48
3:K:33:SER:HB2	3:K:99:ASP:OD2	2.14	0.48
1:A:823:LEU:HB2	1:A:833:VAL:HG11	1.96	0.48
1:B:122:PRO:HA	1:B:173:LEU:HD11	1.96	0.48
1:C:417:LEU:HD21	1:C:613:LEU:O	2.14	0.48
1:F:794:TYR:HB3	1:F:954:VAL:HG13	1.95	0.48
3:K:117:ASP:OD1	3:K:118:TYR:N	2.43	0.48
3:S:33:SER:HB2	3:S:99:ASP:OD2	2.14	0.48
1:A:722:ARG:NH1	1:A:756:LYS:HD3	2.28	0.48
1:B:333:TYR:OH	1:B:407:GLN:OE1	2.26	0.48
1:C:347:LEU:HD13	1:C:359:LEU:HB2	1.95	0.48
1:C:350:LEU:HB3	1:C:356:VAL:HB	1.95	0.48
1:C:951:ARG:NH1	1:C:953:LYS:HD2	2.28	0.48
1:D:49:ARG:HH12	1:D:51:GLY:HA2	1.77	0.48
1:G:552:LYS:HB3	1:G:559:LEU:HB3	1.96	0.48
3:S:162:PHE:HB2	3:S:191:LEU:HD22	1.96	0.48
1:E:307:ILE:C	1:E:483:LYS:HZ1	2.18	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:67:ARG:HH12	3:K:86:LEU:HA	1.78	0.48
1:E:767:ARG:NH1	1:E:1006:PRO:HA	2.29	0.48
1:F:311:ARG:NH2	1:F:664:GLU:OE2	2.46	0.48
1:F:869:THR:HG23	1:F:872:LYS:NZ	2.29	0.48
1:H:332:HIS:CE1	1:H:363:GLN:HE21	2.32	0.48
3:Q:142:PRO:HD2	3:Q:229:PRO:HA	1.96	0.48
4:T:22:THR:HG22	4:T:72:THR:HG22	1.96	0.48
1:D:112:HIS:CD2	1:D:186:VAL:HG22	2.49	0.47
1:D:327:LYS:HB2	1:D:458:GLU:OE2	2.14	0.47
1:F:417:LEU:HD21	1:F:613:LEU:O	2.14	0.47
1:G:429:ARG:HH11	1:G:430:PRO:HD2	1.79	0.47
1:H:190:HIS:O	1:H:194:VAL:HG23	2.14	0.47
1:H:894:LEU:HG	1:H:925:VAL:HG21	1.95	0.47
1:B:489:THR:HA	1:B:501:LYS:HB2	1.96	0.47
1:F:303:LYS:O	1:F:500:TYR:HA	2.15	0.47
3:K:216:HIS:CE1	3:K:219:SER:H	2.32	0.47
3:S:22:CYS:HB3	3:S:79:ALA:HB3	1.97	0.47
3:S:163:PRO:HD2	3:S:218:PRO:HB2	1.96	0.47
4:N:143:ARG:HH11	4:N:164:VAL:HG21	1.79	0.47
1:A:76:LEU:HB3	1:A:257:VAL:HG22	1.96	0.47
1:B:578:PHE:O	1:B:626:GLY:HA3	2.14	0.47
1:C:865:ALA:HB2	1:C:983:ALA:HA	1.96	0.47
1:G:311:ARG:NH1	1:G:379:LEU:O	2.47	0.47
1:H:688:LEU:HD13	1:H:696:THR:HG22	1.96	0.47
3:S:117:ASP:OD1	3:S:118:TYR:N	2.45	0.47
3:W:32:TYR:CZ	3:W:102:MET:HG2	2.49	0.47
1:D:328:SER:O	1:D:330:PRO:HD3	2.14	0.47
1:G:298:LEU:HD21	1:G:318:PRO:HG2	1.97	0.47
4:X:37:GLN:HB2	4:X:47:LEU:HD11	1.95	0.47
1:A:143:SER:OG	1:A:146:HIS:HB2	2.15	0.47
1:A:795:TYR:HA	1:A:952:HIS:O	2.14	0.47
1:B:413:GLU:OE2	1:B:531:ILE:HD11	2.15	0.47
1:D:308:LYS:O	1:D:483:LYS:NZ	2.47	0.47
1:F:551:ILE:HB	1:F:735:LYS:HE3	1.96	0.47
3:I:12:VAL:HG11	3:I:18:LEU:HG	1.96	0.47
1:D:224:TYR:HA	1:D:228:THR:HB	1.97	0.47
3:M:89:GLU:OE2	3:M:89:GLU:N	2.46	0.47
3:U:216:HIS:CD2	3:U:218:PRO:HD3	2.49	0.47
1:A:181:ARG:NH1	1:A:825:THR:O	2.48	0.47
1:A:240:GLU:HA	1:A:243:LYS:HG2	1.96	0.47
1:D:64:TYR:HA	1:D:77:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:VAL:HG21	1:D:227:GLU:HB3	1.97	0.47
1:E:586:ASP:OD1	1:E:589:HIS:ND1	2.48	0.47
1:F:83:THR:O	1:F:261:ARG:NE	2.37	0.47
1:F:291:HIS:CE1	1:F:370:PHE:HB2	2.50	0.47
3:M:131:SER:O	3:M:162:PHE:HD1	1.98	0.47
3:S:32:TYR:CZ	3:S:102:MET:HG2	2.50	0.47
3:W:117:ASP:OD1	3:W:118:TYR:N	2.46	0.47
4:R:35:TRP:HB2	4:R:48:ILE:HB	1.95	0.47
1:B:461:PRO:HB2	3:K:112:TYR:CZ	2.50	0.47
1:C:311:ARG:HD3	1:C:384:LEU:HB2	1.96	0.47
1:D:158:LEU:O	1:D:162:LEU:HB2	2.15	0.47
1:D:194:VAL:HA	1:D:496:TYR:HD1	1.80	0.47
1:E:812:ALA:HA	1:E:815:ILE:HG12	1.97	0.47
1:G:111:GLN:HG2	1:G:149:TYR:CE2	2.50	0.47
1:G:698:ASP:HA	1:G:701:LYS:HE2	1.97	0.47
1:C:688:LEU:HD13	1:C:696:THR:HG22	1.95	0.47
1:D:245:HIS:O	1:D:249:TYR:HB2	2.14	0.47
4:N:168:ASP:HB3	4:N:172:SER:H	1.80	0.47
1:B:815:ILE:O	1:B:819:ALA:HB2	2.15	0.47
1:E:578:PHE:O	1:E:626:GLY:HA3	2.14	0.47
1:F:349:GLU:OE1	1:F:353:LYS:HE2	2.16	0.47
1:H:565:ASP:N	1:H:565:ASP:OD1	2.48	0.47
1:H:706:ASP:O	1:H:711:ARG:NH2	2.48	0.47
3:I:159:LYS:HB3	3:I:159:LYS:NZ	2.30	0.47
3:S:89:GLU:N	3:S:89:GLU:OE2	2.47	0.47
3:S:132:THR:HG23	3:S:163:PRO:HD3	1.97	0.47
4:T:13:ALA:O	4:T:108:LYS:N	2.48	0.47
1:A:230:PRO:HB3	1:A:235:ILE:HB	1.97	0.46
1:C:635:ASN:HA	1:C:638:GLN:HB2	1.98	0.46
1:C:724:HIS:HB2	1:C:758:LEU:HD12	1.97	0.46
1:D:357:ASN:HB2	1:D:378:ASP:OD2	2.16	0.46
1:F:139:ASN:HB3	1:F:150:TYR:CZ	2.49	0.46
1:H:417:LEU:HD21	1:H:613:LEU:O	2.15	0.46
1:H:770:GLN:HB3	1:H:1003:PRO:HG2	1.96	0.46
4:J:195:CYS:N	4:J:208:LYS:O	2.48	0.46
4:N:35:TRP:HB2	4:N:48:ILE:HB	1.97	0.46
1:B:262:GLU:OE2	1:B:262:GLU:N	2.46	0.46
1:C:213:HIS:CE1	1:C:292:PRO:HG3	2.50	0.46
1:H:245:HIS:O	1:H:249:TYR:HB2	2.15	0.46
3:Q:216:HIS:ND1	3:Q:219:SER:O	2.45	0.46
1:D:94:ILE:HG13	1:D:248:TYR:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:527:LYS:NZ	1:E:531:ILE:HD12	2.29	0.46
1:G:578:PHE:O	1:G:626:GLY:HA3	2.15	0.46
4:N:17:ASP:OD1	4:N:18:ARG:N	2.45	0.46
1:C:304:ILE:HB	1:C:481:VAL:HG22	1.97	0.46
1:D:616:LEU:HD11	1:D:634:TYR:HB2	1.97	0.46
1:G:91:ASP:HB2	1:G:148:ASN:HD22	1.80	0.46
1:B:190:HIS:O	1:B:194:VAL:HG23	2.14	0.46
1:D:56:LYS:NZ	1:D:62:ARG:O	2.39	0.46
1:E:688:LEU:HD13	1:E:696:THR:HG22	1.97	0.46
1:H:288:PHE:O	1:H:369:GLY:HA3	2.16	0.46
1:H:346:LEU:HD21	1:H:394:MET:HG2	1.96	0.46
1:H:791:ILE:HD11	1:H:793:ILE:HD11	1.97	0.46
4:P:61:ARG:HD2	4:P:77:SER:O	2.15	0.46
1:B:527:LYS:NZ	1:B:531:ILE:HD12	2.30	0.46
1:C:299:LYS:HD2	1:C:510:ILE:HD13	1.97	0.46
1:C:342:GLY:O	1:C:348:SER:OG	2.33	0.46
1:D:262:GLU:OE2	1:D:262:GLU:N	2.47	0.46
1:D:355:TRP:HB3	1:D:390:ILE:HD11	1.98	0.46
1:E:213:HIS:CE1	1:E:292:PRO:HG3	2.50	0.46
1:E:417:LEU:HD11	1:E:614:ALA:HA	1.98	0.46
1:F:578:PHE:O	1:F:626:GLY:HA3	2.16	0.46
1:A:351:LYS:HZ2	1:A:658:ARG:NH1	2.13	0.46
1:B:381:GLU:OE2	1:B:664:GLU:HG3	2.15	0.46
1:C:806:MET:HE3	1:C:928:LEU:HD13	1.97	0.46
1:G:944:LEU:O	1:G:951:ARG:NH2	2.49	0.46
1:B:52:ASN:OD1	1:B:53:HIS:N	2.47	0.46
1:H:810:LEU:HD23	1:H:936:ILE:HD11	1.98	0.46
3:O:6:GLU:OE2	3:O:120:GLY:HA3	2.15	0.46
1:A:311:ARG:HD3	1:A:384:LEU:HD22	1.96	0.46
1:D:341:GLU:HG2	1:D:347:LEU:HD23	1.98	0.46
1:D:831:TYR:CD2	1:D:832:ILE:HG13	2.51	0.46
1:F:806:MET:N	1:F:806:MET:SD	2.88	0.46
4:P:24:ARG:HD3	4:P:70:ASP:HB3	1.98	0.46
1:E:924:GLU:O	1:E:928:LEU:HB2	2.16	0.46
1:G:782:ARG:HH12	1:G:784:GLU:HG2	1.79	0.46
1:H:48:LYS:HB2	1:H:70:ALA:HA	1.98	0.46
4:J:22:THR:HG22	4:J:72:THR:HG22	1.98	0.46
1:B:48:LYS:HE3	1:B:70:ALA:HA	1.97	0.45
1:E:580:SER:HB2	1:E:723:LEU:HD23	1.99	0.45
1:G:767:ARG:NH1	1:G:1006:PRO:HA	2.31	0.45
1:H:580:SER:HB2	1:H:723:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:112:ALA:HB3	4:J:140:PHE:HA	1.97	0.45
1:D:311:ARG:HB3	1:D:379:LEU:HB2	1.98	0.45
1:F:357:ASN:HB2	1:F:378:ASP:OD2	2.17	0.45
1:H:75:VAL:HG11	1:H:271:VAL:HG11	1.97	0.45
4:N:109:ARG:HD3	4:N:172:SER:HB2	1.98	0.45
4:P:212:ARG:HH11	4:P:212:ARG:HA	1.81	0.45
4:X:108:LYS:HA	4:X:141:TYR:OH	2.16	0.45
1:A:580:SER:HB2	1:A:723:LEU:HD23	1.99	0.45
1:B:342:GLY:O	1:B:348:SER:OG	2.32	0.45
1:D:259:LEU:HD22	1:D:430:PRO:HB3	1.98	0.45
1:D:586:ASP:OD1	1:D:589:HIS:ND1	2.49	0.45
1:E:291:HIS:CE1	1:E:318:PRO:HB3	2.50	0.45
3:K:39:GLN:OE1	4:L:38:GLN:NE2	2.49	0.45
4:N:21:ILE:O	4:N:72:THR:HA	2.16	0.45
1:B:893:ARG:NH1	1:B:924:GLU:OE2	2.45	0.45
1:D:460:ARG:O	1:D:464:ILE:HG13	2.16	0.45
1:F:355:TRP:HB3	1:F:390:ILE:HD11	1.98	0.45
1:H:347:LEU:HD13	1:H:359:LEU:HB2	1.99	0.45
4:L:109:ARG:HH12	4:L:171:ASP:HA	1.81	0.45
1:A:259:LEU:HD23	1:A:430:PRO:HB3	1.99	0.45
1:D:91:ASP:HB2	1:D:148:ASN:HD22	1.82	0.45
1:D:831:TYR:HD2	1:D:832:ILE:HG13	1.82	0.45
3:K:12:VAL:HG11	3:K:18:LEU:HG	1.97	0.45
1:B:58:PRO:HG3	1:B:423:ARG:NH1	2.31	0.45
1:B:620:LEU:HB2	1:B:629:LEU:HD13	1.98	0.45
1:D:716:ILE:HB	1:D:717:PRO:HD3	1.99	0.45
1:G:616:LEU:HD11	1:G:638:GLN:HG3	1.98	0.45
1:G:772:PRO:HD3	1:G:1002:LEU:HD22	1.99	0.45
1:C:620:LEU:HB2	1:C:629:LEU:HD23	1.99	0.45
1:C:716:ILE:HB	1:C:717:PRO:HD3	1.98	0.45
1:C:832:ILE:HB	1:C:851:GLN:HB3	1.98	0.45
1:F:62:ARG:HD3	1:F:427:LYS:HE3	1.99	0.45
1:G:163:ASP:O	1:G:167:GLN:HG2	2.17	0.45
1:A:729:LEU:HD12	1:A:738:ALA:HB1	1.99	0.45
1:A:908:TRP:CE2	1:A:912:ILE:HD11	2.52	0.45
1:F:716:ILE:HB	1:F:717:PRO:HD3	1.98	0.45
1:H:253:LEU:HD21	1:H:285:LEU:HG	1.99	0.45
3:M:159:LYS:NZ	3:M:159:LYS:HB3	2.31	0.45
4:X:34:ALA:HB3	4:X:89:GLN:HB3	1.99	0.45
1:A:237:VAL:O	1:A:241:LEU:HG	2.16	0.45
1:B:189:GLU:O	1:B:192:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:578:PHE:O	1:D:626:GLY:HA3	2.17	0.45
1:E:654:ILE:HD12	1:E:712:LEU:HD13	1.99	0.45
1:G:100:PRO:HG2	1:G:103:ILE:HB	1.99	0.45
4:L:31:SER:O	4:L:66:ARG:NH1	2.49	0.45
4:R:39:LYS:HD3	4:R:84:ALA:HB2	1.98	0.45
4:T:35:TRP:HB2	4:T:48:ILE:HB	1.99	0.45
4:X:165:THR:HG22	4:X:175:SER:H	1.81	0.45
1:G:688:LEU:HD13	1:G:696:THR:HG22	1.97	0.45
3:S:37:VAL:HG22	3:S:47:TRP:HA	1.99	0.45
3:W:162:PHE:HB2	3:W:191:LEU:HD22	1.98	0.45
1:B:96:SER:HB2	1:B:219:GLY:HA2	1.98	0.44
1:B:160:GLY:O	1:B:164:ARG:NH1	2.50	0.44
1:B:357:ASN:HB2	1:B:378:ASP:OD2	2.17	0.44
1:D:194:VAL:HA	1:D:496:TYR:CD1	2.51	0.44
1:G:309:ASP:N	1:G:672:ASN:OD1	2.45	0.44
1:G:417:LEU:HD21	1:G:613:LEU:O	2.17	0.44
3:S:167:THR:OG1	3:S:215:ASN:HB3	2.17	0.44
4:T:108:LYS:HA	4:T:141:TYR:OH	2.16	0.44
1:B:355:TRP:HB3	1:B:390:ILE:HD11	1.99	0.44
1:B:459:PHE:CE2	1:B:461:PRO:HG3	2.52	0.44
1:E:94:ILE:O	1:E:147:THR:OG1	2.27	0.44
1:A:351:LYS:NZ	1:A:658:ARG:NH1	2.66	0.44
1:A:600:LEU:HD11	1:A:648:LYS:HB3	1.99	0.44
1:F:163:ASP:O	1:F:167:GLN:HG2	2.17	0.44
3:M:6:GLU:OE2	3:M:120:GLY:HA3	2.17	0.44
3:U:55:TYR:HE2	3:U:105:TRP:HA	1.82	0.44
3:U:170:TRP:HB3	3:U:175:LEU:HD13	1.99	0.44
1:C:580:SER:HB2	1:C:723:LEU:HD23	2.00	0.44
3:S:139:PRO:HD3	3:S:225:LYS:HD3	1.99	0.44
4:J:17:ASP:OD1	4:J:18:ARG:N	2.50	0.44
4:V:37:GLN:HB2	4:V:47:LEU:HD11	1.99	0.44
4:V:159:ASN:ND2	4:V:181:THR:O	2.51	0.44
1:A:350:LEU:HB3	1:A:356:VAL:HB	2.00	0.44
1:A:574:LEU:HD22	1:A:729:LEU:HD22	2.00	0.44
1:C:855:PRO:HB2	1:C:857:HIS:CD2	2.53	0.44
1:E:815:ILE:O	1:E:819:ALA:CB	2.65	0.44
1:F:647:GLU:O	1:F:651:THR:OG1	2.26	0.44
1:F:778:VAL:HG22	1:F:955:SER:HB2	2.00	0.44
4:J:20:THR:HA	4:J:73:LEU:O	2.18	0.44
1:A:357:ASN:HB2	1:A:378:ASP:OD2	2.17	0.44
1:B:445:PRO:O	1:B:449:VAL:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:767:ARG:NH1	1:B:1006:PRO:HA	2.32	0.44
1:H:724:HIS:HB2	1:H:758:LEU:HD12	1.99	0.44
1:H:771:LEU:HB2	1:H:952:HIS:HB3	2.00	0.44
1:A:73:ILE:HG13	1:A:251:SER:HB2	2.00	0.44
1:A:291:HIS:O	1:A:294:GLN:NE2	2.50	0.44
1:C:388:GLU:OE2	1:C:512:LYS:NZ	2.42	0.44
1:C:574:LEU:HD22	1:C:729:LEU:HG	2.00	0.44
1:E:311:ARG:HB3	1:E:379:LEU:HB2	2.00	0.44
3:M:162:PHE:HA	3:M:163:PRO:HA	1.82	0.44
3:Q:12:VAL:HG23	3:Q:127:VAL:HG22	1.99	0.44
3:U:162:PHE:HA	3:U:163:PRO:HA	1.77	0.44
4:R:7:SER:HB3	4:R:24:ARG:HH12	1.83	0.44
4:T:80:PRO:HA	4:T:83:PHE:HE2	1.82	0.44
1:B:308:LYS:HD3	1:B:672:ASN:HB3	2.00	0.44
1:C:134:HIS:HD2	1:C:157:HIS:CE1	2.36	0.44
1:C:779:TYR:HB2	1:C:992:ILE:HD12	1.99	0.44
1:D:309:ASP:N	1:D:672:ASN:OD1	2.44	0.44
1:D:311:ARG:HD3	1:D:384:LEU:HD22	1.99	0.44
1:D:445:PRO:O	1:D:449:VAL:HG13	2.18	0.44
1:E:272:VAL:O	1:E:276:SER:OG	2.33	0.44
1:H:139:ASN:HB3	1:H:150:TYR:CZ	2.53	0.44
3:I:157:LEU:HD13	3:I:195:SER:HB3	2.00	0.44
3:Q:157:LEU:HD13	3:Q:195:SER:HB3	2.00	0.44
1:B:366:GLY:H	1:B:371:MET:HG2	1.83	0.44
1:D:564:ASP:HB2	1:D:731:GLY:HA2	2.00	0.44
1:E:298:LEU:HD21	1:E:318:PRO:HG2	2.00	0.44
1:G:580:SER:HB2	1:G:723:LEU:HD23	2.00	0.44
1:C:143:SER:OG	1:C:146:HIS:HB2	2.18	0.43
1:C:557:SER:OG	1:C:746:GLU:OE1	2.28	0.43
1:F:56:LYS:NZ	1:F:62:ARG:O	2.42	0.43
1:F:190:HIS:O	1:F:194:VAL:HG23	2.18	0.43
1:G:145:GLU:OE2	1:G:368:ARG:N	2.51	0.43
3:K:67:ARG:NH1	3:K:85:SER:O	2.50	0.43
3:U:137:VAL:HG22	3:U:158:VAL:HG22	2.00	0.43
3:U:164:GLU:OE2	3:U:184:ALA:HB3	2.17	0.43
3:W:6:GLU:OE2	3:W:120:GLY:HA3	2.18	0.43
1:A:192:LYS:NZ	1:A:832:ILE:HG13	2.33	0.43
1:A:855:PRO:HB2	1:A:857:HIS:CD2	2.53	0.43
1:D:418:ASN:HB3	1:D:454:TYR:O	2.18	0.43
1:D:782:ARG:HH12	1:E:540:LEU:HD23	1.83	0.43
1:D:924:GLU:O	1:D:928:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:GLU:O	1:F:78:ILE:HA	2.17	0.43
1:G:75:VAL:HG11	1:G:271:VAL:HG11	1.99	0.43
1:G:586:ASP:OD1	1:G:589:HIS:ND1	2.51	0.43
4:X:38:GLN:O	4:X:84:ALA:HB1	2.18	0.43
1:D:345:SER:OG	1:D:348:SER:OG	2.33	0.43
1:G:48:LYS:HB2	1:G:70:ALA:HA	2.01	0.43
1:G:224:TYR:HA	1:G:228:THR:HB	2.00	0.43
1:H:460:ARG:O	1:H:464:ILE:HG13	2.19	0.43
4:J:37:GLN:HB2	4:J:47:LEU:HD11	2.00	0.43
1:B:716:ILE:HB	1:B:717:PRO:HD3	1.99	0.43
1:H:564:ASP:HB2	1:H:731:GLY:HA2	2.00	0.43
3:M:216:HIS:CE1	3:M:219:SER:H	2.37	0.43
1:A:422:PHE:CZ	1:A:451:THR:HG22	2.54	0.43
1:C:240:GLU:HA	1:C:243:LYS:HG2	2.00	0.43
1:C:341:GLU:OE2	1:C:605:ASN:ND2	2.35	0.43
1:E:110:LEU:HD11	1:E:244:PHE:HB3	2.01	0.43
1:A:557:SER:OG	1:A:746:GLU:OE1	2.33	0.43
1:A:770:GLN:HB3	1:A:1003:PRO:HG2	2.00	0.43
1:A:806:MET:SD	1:A:924:GLU:HB3	2.59	0.43
1:B:224:TYR:HA	1:B:228:THR:HB	2.01	0.43
1:B:361:GLY:HA2	1:B:374:ILE:O	2.19	0.43
1:F:688:LEU:HD13	1:F:696:THR:HG22	2.00	0.43
1:G:315:VAL:O	1:G:374:ILE:HA	2.18	0.43
1:H:131:LEU:O	1:H:136:GLY:N	2.42	0.43
1:H:150:TYR:HD1	1:H:431:ARG:HG2	1.82	0.43
1:H:425:LYS:NZ	1:H:425:LYS:HB3	2.33	0.43
3:K:162:PHE:HA	3:K:163:PRO:HA	1.81	0.43
3:Q:89:GLU:N	3:Q:89:GLU:OE2	2.52	0.43
4:L:35:TRP:HB2	4:L:48:ILE:HB	2.01	0.43
4:P:66:ARG:HG2	4:P:68:GLY:H	1.83	0.43
1:A:599:LEU:HD21	1:A:659:PHE:HA	2.01	0.43
1:A:623:THR:OG1	1:A:626:GLY:O	2.28	0.43
1:C:237:VAL:O	1:C:241:LEU:HG	2.19	0.43
1:E:566:LYS:HE3	1:E:903:GLU:OE2	2.18	0.43
1:E:779:TYR:HB2	1:E:992:ILE:HD12	2.01	0.43
1:F:571:LYS:HE3	1:F:571:LYS:HB2	1.90	0.43
3:K:139:PRO:HG3	3:K:225:LYS:HD3	2.01	0.43
3:M:91:THR:HA	3:M:125:VAL:O	2.19	0.43
4:R:79:GLN:HB2	4:R:80:PRO:HD3	2.00	0.43
1:A:797:THR:OG1	1:A:844:GLN:HG3	2.19	0.43
1:D:223:LYS:HG3	1:D:227:GLU:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:812:ALA:HA	1:D:815:ILE:HG12	2.01	0.43
1:E:262:GLU:OE2	1:E:262:GLU:N	2.49	0.43
1:E:938:LYS:HE2	1:E:938:LYS:HB3	1.89	0.43
1:G:139:ASN:ND2	1:G:150:TYR:OH	2.52	0.43
3:S:12:VAL:HG11	3:S:18:LEU:HG	2.01	0.43
4:J:61:ARG:HD2	4:J:77:SER:O	2.19	0.43
4:N:37:GLN:HB2	4:N:47:LEU:HD11	2.00	0.43
1:A:347:LEU:HD13	1:A:359:LEU:HB2	2.00	0.43
1:C:855:PRO:HA	1:C:856:PRO:HD3	1.94	0.43
1:D:163:ASP:O	1:D:167:GLN:HG2	2.19	0.43
1:D:552:LYS:HB3	1:D:559:LEU:HB3	2.01	0.43
1:D:580:SER:HB2	1:D:723:LEU:HD23	2.01	0.43
1:E:311:ARG:HD3	1:E:384:LEU:HD22	2.01	0.43
1:F:131:LEU:O	1:F:136:GLY:N	2.45	0.43
3:U:32:TYR:CZ	3:U:102:MET:HG2	2.53	0.43
3:U:213:ASN:HD22	3:U:222:LYS:NZ	2.16	0.43
4:J:142:PRO:HB2	4:J:144:GLU:OE1	2.19	0.43
4:X:22:THR:HG22	4:X:72:THR:HG22	2.01	0.43
1:A:839:ARG:HG3	1:A:844:GLN:HB3	2.01	0.43
1:B:807:PHE:HE1	1:B:931:LEU:HD22	1.84	0.43
1:E:193:ASN:OD1	1:E:199:TRP:NE1	2.52	0.43
1:F:73:ILE:HG13	1:F:251:SER:HB2	1.99	0.43
1:G:347:LEU:HD23	1:G:359:LEU:HB2	1.99	0.43
1:H:139:ASN:HB3	1:H:150:TYR:CE1	2.54	0.43
3:K:229:PRO:O	3:K:230:LYS:HB2	2.18	0.43
3:M:32:TYR:CZ	3:M:102:MET:HG2	2.54	0.43
3:Q:12:VAL:HG11	3:Q:18:LEU:HG	2.01	0.43
3:U:182:PHE:HE2	3:U:197:VAL:HG22	1.84	0.43
4:L:66:ARG:HH11	4:L:71:PHE:HE1	1.67	0.43
4:V:6:GLN:O	4:V:101:GLN:NE2	2.52	0.43
1:A:163:ASP:O	1:A:167:GLN:HG2	2.18	0.42
1:A:226:LEU:O	1:A:230:PRO:HG2	2.19	0.42
1:B:365:GLU:HA	1:B:371:MET:HG2	2.00	0.42
1:D:894:LEU:HG	1:D:925:VAL:HG21	2.00	0.42
1:E:337:LEU:HD21	1:E:410:VAL:HG11	2.01	0.42
1:E:770:GLN:HB3	1:E:1003:PRO:HG2	2.01	0.42
1:E:855:PRO:HB2	1:E:857:HIS:CD2	2.54	0.42
4:V:61:ARG:NE	4:V:82:ASP:OD2	2.51	0.42
1:B:119:LYS:HE3	1:B:119:LYS:HB2	1.90	0.42
1:C:599:LEU:HD21	1:C:659:PHE:HA	2.01	0.42
1:C:894:LEU:HD11	1:C:925:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:620:LEU:HD13	1:E:629:LEU:HD12	2.01	0.42
1:F:304:ILE:HB	1:F:481:VAL:HG22	2.01	0.42
1:G:894:LEU:HG	1:G:925:VAL:HG21	2.01	0.42
1:B:791:ILE:HA	1:B:956:VAL:O	2.19	0.42
1:D:787:ASN:HA	1:D:961:ARG:HG2	2.01	0.42
1:F:190:HIS:CE1	1:F:222:ASN:HD22	2.37	0.42
1:G:963:MET:HE2	1:G:963:MET:HB3	1.85	0.42
1:H:121:TYR:CD1	1:H:164:ARG:HG3	2.54	0.42
1:H:163:ASP:O	1:H:167:GLN:HG2	2.19	0.42
3:I:100:ARG:NH1	3:I:100:ARG:HB3	2.35	0.42
1:A:264:LEU:O	1:A:268:THR:OG1	2.30	0.42
1:C:226:LEU:O	1:C:230:PRO:HG2	2.19	0.42
1:C:245:HIS:O	1:C:249:TYR:HB2	2.19	0.42
1:D:675:ALA:HA	1:D:785:VAL:HG21	2.01	0.42
1:G:91:ASP:O	1:G:254:MET:HA	2.18	0.42
1:G:548:PRO:HA	1:G:562:LYS:HB2	2.01	0.42
1:G:821:ASN:O	1:G:825:THR:OG1	2.32	0.42
1:G:832:ILE:HB	1:G:851:GLN:HB3	2.01	0.42
1:H:839:ARG:HG3	1:H:844:GLN:HB3	2.01	0.42
3:S:55:TYR:CE2	3:S:105:TRP:HA	2.54	0.42
1:C:285:LEU:HD12	1:C:286:PRO:HD2	2.00	0.42
1:D:527:LYS:HZ3	1:D:531:ILE:HD12	1.85	0.42
1:E:894:LEU:HG	1:E:925:VAL:HG21	2.00	0.42
1:F:90:LEU:HD13	1:F:169:PHE:CE2	2.54	0.42
1:G:160:GLY:O	1:G:164:ARG:NH1	2.53	0.42
1:H:226:LEU:O	1:H:230:PRO:HG2	2.19	0.42
3:K:14:PRO:HD2	3:K:129:SER:HB3	2.00	0.42
3:O:217:LYS:HB2	3:O:218:PRO:HD3	2.01	0.42
1:A:716:ILE:HB	1:A:717:PRO:HD3	2.00	0.42
1:B:236:ASP:HB3	1:B:239:GLN:HB2	2.01	0.42
1:C:422:PHE:CZ	1:C:451:THR:HG22	2.55	0.42
1:D:192:LYS:HB3	1:D:831:TYR:CZ	2.54	0.42
1:E:86:SER:HB3	1:E:158:LEU:HD12	2.01	0.42
3:M:40:ALA:HB3	3:M:43:LYS:HB2	2.00	0.42
4:X:126:LEU:HD23	4:X:184:LYS:HZ3	1.84	0.42
1:B:64:TYR:HA	1:B:77:LEU:O	2.19	0.42
1:C:908:TRP:CE2	1:C:912:ILE:HD11	2.55	0.42
1:D:741:ILE:O	1:D:745:VAL:HG23	2.20	0.42
1:E:44:ASN:N	1:E:45:PRO:HD2	2.34	0.42
3:U:39:GLN:NE2	4:V:38:GLN:OE1	2.44	0.42
3:W:89:GLU:OE2	3:W:89:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:113:ALA:HA	4:P:114:PRO:HD3	1.94	0.42
4:V:34:ALA:HB3	4:V:89:GLN:HB3	2.01	0.42
1:B:116:LEU:HD13	1:B:178:ALA:HB1	2.01	0.42
1:B:506:PRO:HB2	1:B:509:VAL:HG23	2.01	0.42
1:D:320:PRO:HG2	1:D:466:MET:HE1	2.01	0.42
4:R:17:ASP:OD1	4:R:18:ARG:N	2.48	0.42
1:A:86:SER:CB	1:A:158:LEU:HD12	2.50	0.42
1:A:190:HIS:O	1:A:194:VAL:HG23	2.19	0.42
1:C:195:MET:HB2	1:C:786:HIS:CE1	2.55	0.42
1:E:103:ILE:HG21	1:E:106:LEU:HD13	2.01	0.42
1:G:527:LYS:NZ	1:G:531:ILE:HD12	2.35	0.42
3:I:33:SER:HB2	3:I:99:ASP:OD2	2.19	0.42
3:K:5:VAL:O	3:K:22:CYS:HA	2.19	0.42
3:K:167:THR:OG1	3:K:215:ASN:HB3	2.20	0.42
3:O:62:ASP:HA	3:O:65:LYS:HE2	2.02	0.42
3:W:59:SER:HB2	4:X:95:PHE:HB3	2.01	0.42
1:B:63:GLU:HB2	1:B:79:SER:HB3	2.02	0.42
1:B:173:LEU:HD23	1:B:173:LEU:HA	1.87	0.42
1:C:319:ILE:HD13	1:C:373:PHE:HB2	2.02	0.42
1:C:329:ASN:HB3	1:C:332:HIS:HB2	2.00	0.42
1:F:63:GLU:HB2	1:F:79:SER:HB3	2.02	0.42
1:G:417:LEU:HD11	1:G:614:ALA:HA	2.00	0.42
1:H:716:ILE:HB	1:H:717:PRO:HD3	2.01	0.42
3:I:167:THR:OG1	3:I:215:ASN:HB3	2.19	0.42
1:A:493:GLU:OE1	1:A:496:TYR:N	2.38	0.41
1:B:93:HIS:O	1:B:93:HIS:ND1	2.53	0.41
1:B:324:LYS:HE3	1:B:325:TYR:CZ	2.55	0.41
1:D:688:LEU:HD13	1:D:696:THR:HG22	2.02	0.41
1:G:722:ARG:HA	1:G:756:LYS:O	2.20	0.41
1:G:810:LEU:HD22	1:G:936:ILE:HG13	2.02	0.41
3:S:98:ARG:NH1	3:S:118:TYR:HD2	2.18	0.41
4:J:83:PHE:HE2	4:J:166:GLU:HB3	1.84	0.41
1:A:810:LEU:HD22	1:A:936:ILE:HG13	2.02	0.41
1:B:812:ALA:HA	1:B:815:ILE:HG12	2.02	0.41
1:D:413:GLU:OE2	1:D:531:ILE:HD11	2.20	0.41
1:D:793:ILE:HD12	1:D:863:VAL:HG11	2.01	0.41
1:D:815:ILE:O	1:D:819:ALA:HB2	2.20	0.41
1:E:565:ASP:OD1	1:E:565:ASP:N	2.53	0.41
1:E:599:LEU:HD23	1:E:662:ILE:HD12	2.01	0.41
1:F:706:ASP:HB3	1:F:711:ARG:HH22	1.85	0.41
1:G:329:ASN:HB3	1:G:332:HIS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:960:ALA:HB3	1:G:963:MET:HB2	2.01	0.41
3:M:55:TYR:HE2	3:M:105:TRP:HA	1.84	0.41
1:C:341:GLU:HG2	1:C:347:LEU:HD23	2.03	0.41
1:E:139:ASN:HB2	1:E:150:TYR:CE2	2.56	0.41
1:H:295:GLU:OE2	1:H:299:LYS:HE2	2.20	0.41
1:H:893:ARG:NH1	1:H:924:GLU:OE2	2.46	0.41
3:O:32:TYR:CZ	3:O:102:MET:HG2	2.55	0.41
3:Q:14:PRO:HD2	3:Q:129:SER:HB3	2.02	0.41
3:W:9:GLY:HA2	3:W:125:VAL:HG12	2.03	0.41
4:T:38:GLN:O	4:T:84:ALA:HB1	2.21	0.41
4:X:68:GLY:C	4:X:70:ASP:H	2.23	0.41
1:E:810:LEU:HD11	1:E:936:ILE:HG21	2.02	0.41
1:F:319:ILE:HD13	1:F:373:PHE:HB2	2.01	0.41
1:F:791:ILE:HD11	1:F:793:ILE:HD11	2.02	0.41
3:W:2:VAL:HG22	3:W:26:GLY:HA3	2.03	0.41
4:J:115:SER:HB2	4:J:138:ASN:HB3	2.03	0.41
4:P:37:GLN:HB2	4:P:47:LEU:HD11	2.03	0.41
4:T:40:PRO:HG2	4:T:166:GLU:HG2	2.02	0.41
1:C:190:HIS:O	1:C:194:VAL:HG23	2.20	0.41
1:E:319:ILE:HD13	1:E:373:PHE:HB2	2.02	0.41
1:E:652:PHE:CE2	1:E:654:ILE:HG12	2.55	0.41
1:E:797:THR:OG1	1:E:844:GLN:HG3	2.21	0.41
3:O:14:PRO:HD2	3:O:129:SER:HB3	2.03	0.41
4:L:34:ALA:O	4:L:88:CYS:HA	2.21	0.41
4:X:137:LEU:HB2	4:X:176:LEU:HB3	2.03	0.41
1:A:298:LEU:HD21	1:A:318:PRO:HG2	2.03	0.41
1:D:189:GLU:O	1:D:192:LYS:HG2	2.21	0.41
1:F:641:LEU:O	1:F:645:ILE:HG13	2.20	0.41
1:H:190:HIS:CE1	1:H:222:ASN:HD22	2.39	0.41
1:H:908:TRP:O	1:H:912:ILE:HG12	2.19	0.41
3:I:98:ARG:HH11	3:I:118:TYR:HD2	1.68	0.41
3:U:163:PRO:HD2	3:U:218:PRO:HB3	2.02	0.41
4:N:113:ALA:HA	4:N:114:PRO:HD3	1.97	0.41
4:V:141:TYR:HA	4:V:142:PRO:HA	1.91	0.41
1:C:123:LYS:HB2	1:C:123:LYS:HE3	1.71	0.41
1:C:771:LEU:HB2	1:C:952:HIS:HB3	2.01	0.41
1:D:139:ASN:HB3	1:D:150:TYR:CZ	2.55	0.41
1:E:616:LEU:HD11	1:E:634:TYR:HB2	2.03	0.41
1:F:156:GLU:HG3	1:F:157:HIS:ND1	2.36	0.41
1:G:83:THR:O	1:G:261:ARG:NE	2.47	0.41
1:H:159:GLU:HG3	1:H:270:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:602:ASP:OD2	1:H:658:ARG:HD3	2.19	0.41
1:H:820:PHE:CE1	1:H:824:ARG:HD3	2.55	0.41
3:K:98:ARG:NH1	3:K:118:TYR:HD2	2.18	0.41
3:M:117:ASP:OD1	3:M:118:TYR:N	2.52	0.41
3:S:6:GLU:OE1	3:S:6:GLU:N	2.54	0.41
1:D:493:GLU:OE1	1:D:496:TYR:N	2.41	0.41
1:E:329:ASN:HB3	1:E:332:HIS:HB2	2.03	0.41
1:F:271:VAL:O	1:F:275:PHE:HB2	2.21	0.41
1:G:307:ILE:C	1:G:483:LYS:HZ1	2.24	0.41
1:G:460:ARG:O	1:G:464:ILE:HG13	2.20	0.41
3:I:98:ARG:NH1	3:I:118:TYR:CD2	2.89	0.41
3:Q:37:VAL:HG22	3:Q:47:TRP:HA	2.03	0.41
4:L:109:ARG:HD3	4:L:172:SER:HB2	2.01	0.41
1:B:528:ASN:HB3	1:B:531:ILE:HG13	2.02	0.41
1:D:63:GLU:O	1:D:78:ILE:HA	2.20	0.41
1:E:169:PHE:O	1:E:171:SER:N	2.53	0.41
1:F:109:PHE:CZ	1:F:179:LYS:HG3	2.54	0.41
1:F:245:HIS:O	1:F:249:TYR:HB2	2.21	0.41
1:F:618:TYR:HA	1:F:630:SER:O	2.20	0.41
1:G:814:ILE:HG21	1:G:874:ILE:HG12	2.02	0.41
1:G:815:ILE:O	1:G:819:ALA:HB2	2.20	0.41
1:H:319:ILE:HD13	1:H:373:PHE:HB2	2.01	0.41
3:I:55:TYR:CE2	3:I:105:TRP:HA	2.56	0.41
3:M:220:ASN:O	3:U:121:GLN:NE2	2.53	0.41
3:O:117:ASP:OD1	3:O:118:TYR:N	2.52	0.41
3:Q:11:LEU:HD11	3:Q:162:PHE:CE2	2.55	0.41
3:Q:98:ARG:HH11	3:Q:118:TYR:HD2	1.68	0.41
3:Q:138:PHE:HA	3:Q:139:PRO:HD3	1.95	0.41
3:S:162:PHE:HA	3:S:163:PRO:HA	1.82	0.41
3:W:163:PRO:HD2	3:W:218:PRO:HB2	2.03	0.41
4:R:37:GLN:HB2	4:R:47:LEU:HD11	2.01	0.41
4:T:126:LEU:HD23	4:T:184:LYS:NZ	2.35	0.41
1:C:770:GLN:HB3	1:C:1003:PRO:HG2	2.03	0.41
1:D:324:LYS:HE3	1:D:325:TYR:CZ	2.56	0.41
1:D:642:LEU:HD21	1:D:745:VAL:HG22	2.03	0.41
3:M:213:ASN:HD22	3:M:224:ASP:HB3	1.86	0.41
3:O:175:LEU:HD13	3:O:198:VAL:HG21	2.01	0.41
1:A:855:PRO:HA	1:A:856:PRO:HD3	1.94	0.40
1:B:778:VAL:HG22	1:B:955:SER:HB2	2.02	0.40
1:E:247:ALA:HA	1:E:281:LYS:HE3	2.02	0.40
1:E:309:ASP:N	1:E:672:ASN:OD1	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:789:SER:OG	1:E:852:SER:O	2.25	0.40
1:F:103:ILE:HG21	1:F:106:LEU:HD13	2.03	0.40
1:H:767:ARG:HH12	1:H:1006:PRO:HA	1.85	0.40
3:I:47:TRP:NE1	3:I:50:SER:OG	2.49	0.40
3:M:167:THR:OG1	3:M:215:ASN:HB3	2.21	0.40
3:S:12:VAL:HG23	3:S:127:VAL:HG12	2.03	0.40
3:S:132:THR:HG22	3:S:219:SER:HB3	2.02	0.40
4:X:141:TYR:CD1	4:X:142:PRO:HA	2.55	0.40
1:A:285:LEU:HA	1:A:286:PRO:HD3	1.96	0.40
1:A:304:ILE:HB	1:A:481:VAL:HG22	2.02	0.40
1:B:815:ILE:O	1:B:819:ALA:CB	2.68	0.40
1:C:769:VAL:HA	1:C:1004:LEU:HD23	2.02	0.40
1:E:332:HIS:ND1	1:E:363:GLN:OE1	2.54	0.40
1:E:552:LYS:HB3	1:E:559:LEU:HB3	2.03	0.40
1:F:97:LEU:HB2	1:F:144:GLY:O	2.22	0.40
1:H:63:GLU:O	1:H:78:ILE:HA	2.21	0.40
1:H:578:PHE:HA	1:H:724:HIS:O	2.22	0.40
1:D:113:MET:HB3	1:D:174:PHE:CD1	2.57	0.40
1:F:562:LYS:O	1:F:730:HIS:HA	2.22	0.40
1:H:291:HIS:CD2	1:H:370:PHE:HB2	2.56	0.40
3:M:12:VAL:HG11	3:M:18:LEU:HG	2.02	0.40
3:O:37:VAL:HG22	3:O:47:TRP:HA	2.03	0.40
1:A:684:TYR:CZ	1:A:688:LEU:HD11	2.57	0.40
1:B:229:ARG:N	1:B:230:PRO:HD2	2.37	0.40
1:F:139:ASN:HB3	1:F:150:TYR:CE1	2.56	0.40
1:G:107:SER:HA	1:G:110:LEU:HD12	2.03	0.40
1:H:94:ILE:HD12	1:H:94:ILE:HA	1.99	0.40
3:I:98:ARG:NH1	3:I:118:TYR:HD2	2.20	0.40
4:T:7:SER:HA	4:T:8:PRO:HA	1.84	0.40
4:T:157:SER:OG	4:T:159:ASN:OD1	2.39	0.40
4:X:35:TRP:HB2	4:X:48:ILE:HB	2.03	0.40
1:A:771:LEU:HB2	1:A:952:HIS:HB3	2.03	0.40
1:B:810:LEU:HD12	1:B:928:LEU:HD11	2.04	0.40
1:C:357:ASN:HB2	1:C:378:ASP:OD2	2.21	0.40
1:F:121:TYR:CD1	1:F:164:ARG:HG2	2.57	0.40
3:I:63:SER:O	3:I:67:ARG:NH2	2.54	0.40
3:I:93:VAL:HG22	3:I:124:LEU:HD13	2.04	0.40
3:S:168:VAL:HA	3:S:213:ASN:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:LYS:NZ	4:J:188:GLU:O[1_654]	2.08	0.12

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	929/990 (94%)	919 (99%)	10 (1%)	0	100	100
1	B	935/990 (94%)	926 (99%)	9 (1%)	0	100	100
1	C	942/990 (95%)	932 (99%)	10 (1%)	0	100	100
1	D	944/990 (95%)	932 (99%)	12 (1%)	0	100	100
1	E	923/990 (93%)	906 (98%)	17 (2%)	0	100	100
1	F	926/990 (94%)	914 (99%)	12 (1%)	0	100	100
1	G	923/990 (93%)	911 (99%)	12 (1%)	0	100	100
1	H	924/990 (93%)	912 (99%)	12 (1%)	0	100	100
2	a	18/20 (90%)	17 (94%)	1 (6%)	0	100	100
2	b	3/20 (15%)	2 (67%)	1 (33%)	0	100	100
2	c	18/20 (90%)	18 (100%)	0	0	100	100
2	d	1/20 (5%)	0	1 (100%)	0	100	100
2	e	5/20 (25%)	5 (100%)	0	0	100	100
2	f	14/20 (70%)	14 (100%)	0	0	100	100
2	g	11/20 (55%)	10 (91%)	1 (9%)	0	100	100
2	h	4/20 (20%)	3 (75%)	1 (25%)	0	100	100
3	I	207/263 (79%)	200 (97%)	7 (3%)	0	100	100
3	K	195/263 (74%)	189 (97%)	6 (3%)	0	100	100
3	M	206/263 (78%)	195 (95%)	11 (5%)	0	100	100
3	O	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
3	Q	181/263 (69%)	175 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S	207/263 (79%)	201 (97%)	6 (3%)	0	100	100
3	U	183/263 (70%)	174 (95%)	9 (5%)	0	100	100
3	W	192/263 (73%)	186 (97%)	6 (3%)	0	100	100
4	J	184/239 (77%)	175 (95%)	9 (5%)	0	100	100
4	L	160/239 (67%)	156 (98%)	4 (2%)	0	100	100
4	N	190/239 (80%)	183 (96%)	7 (4%)	0	100	100
4	P	167/239 (70%)	162 (97%)	5 (3%)	0	100	100
4	R	165/239 (69%)	160 (97%)	5 (3%)	0	100	100
4	T	186/239 (78%)	179 (96%)	7 (4%)	0	100	100
4	V	168/239 (70%)	167 (99%)	1 (1%)	0	100	100
4	X	190/239 (80%)	183 (96%)	7 (4%)	0	100	100
All	All	10500/12096 (87%)	10299 (98%)	201 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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%)	838 (100%)	0	100	100
1	B	845/879 (96%)	844 (100%)	1 (0%)	93	96
1	C	846/879 (96%)	844 (100%)	2 (0%)	93	96
1	D	848/879 (96%)	846 (100%)	2 (0%)	93	96
1	E	840/879 (96%)	838 (100%)	2 (0%)	93	96
1	F	843/879 (96%)	842 (100%)	1 (0%)	93	96
1	G	841/879 (96%)	841 (100%)	0	100	100
1	H	833/879 (95%)	833 (100%)	0	100	100
2	a	19/19 (100%)	19 (100%)	0	100	100
2	b	4/19 (21%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	c	19/19 (100%)	19 (100%)	0	100 100
2	d	2/19 (10%)	2 (100%)	0	100 100
2	e	8/19 (42%)	7 (88%)	1 (12%)	4 23
2	f	17/19 (90%)	17 (100%)	0	100 100
2	g	14/19 (74%)	13 (93%)	1 (7%)	14 42
2	h	5/19 (26%)	5 (100%)	0	100 100
3	I	180/220 (82%)	180 (100%)	0	100 100
3	K	176/220 (80%)	176 (100%)	0	100 100
3	M	179/220 (81%)	179 (100%)	0	100 100
3	O	176/220 (80%)	176 (100%)	0	100 100
3	Q	169/220 (77%)	169 (100%)	0	100 100
3	S	180/220 (82%)	180 (100%)	0	100 100
3	U	164/220 (74%)	164 (100%)	0	100 100
3	W	170/220 (77%)	170 (100%)	0	100 100
4	J	178/210 (85%)	177 (99%)	1 (1%)	86 91
4	L	159/210 (76%)	157 (99%)	2 (1%)	69 81
4	N	178/210 (85%)	178 (100%)	0	100 100
4	P	164/210 (78%)	162 (99%)	2 (1%)	71 83
4	R	157/210 (75%)	155 (99%)	2 (1%)	69 81
4	T	178/210 (85%)	177 (99%)	1 (1%)	86 91
4	V	165/210 (79%)	164 (99%)	1 (1%)	86 91
4	X	178/210 (85%)	177 (99%)	1 (1%)	86 91
All	All	9573/10624 (90%)	9553 (100%)	20 (0%)	93 96

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	109	PHE
1	C	109	PHE
1	C	329	ASN
1	D	109	PHE
1	D	218	PHE
1	E	109	PHE
1	E	244	PHE

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Mol	Chain	Res	Type
1	F	109	PHE
2	e	15	GLN
2	g	15	GLN
4	J	95	PHE
4	L	95	PHE
4	L	171	ASP
4	P	95	PHE
4	P	171	ASP
4	R	95	PHE
4	R	114	PRO
4	T	95	PHE
4	V	95	PHE
4	X	95	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	HIS
1	A	363	GLN
1	F	190	HIS
1	H	184	ASN
1	H	332	HIS
1	H	363	GLN
2	a	15	GLN
2	e	15	GLN
2	h	5	GLN
4	V	6	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides 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, 95^{th} 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%)	-0.09	11 (1%) 79 70	53, 77, 99, 113	0
1	B	947/990 (95%)	-0.04	13 (1%) 75 66	54, 77, 97, 116	0
1	C	950/990 (95%)	0.21	47 (4%) 29 25	100, 118, 135, 148	0
1	D	952/990 (96%)	0.35	62 (6%) 18 15	116, 136, 150, 161	0
1	E	943/990 (95%)	0.35	53 (5%) 24 21	106, 133, 147, 160	0
1	F	944/990 (95%)	0.29	56 (5%) 22 18	105, 128, 146, 158	0
1	G	943/990 (95%)	0.08	20 (2%) 63 54	66, 88, 106, 131	0
1	H	936/990 (94%)	0.08	28 (2%) 50 39	65, 91, 115, 135	0
2	a	20/20 (100%)	0.13	1 (5%) 28 25	70, 108, 127, 129	0
2	b	5/20 (25%)	0.19	1 (20%) 1 1	74, 83, 103, 114	0
2	c	20/20 (100%)	0.28	1 (5%) 28 25	106, 124, 132, 136	0
2	d	3/20 (15%)	0.03	0 100 100	118, 118, 121, 121	0
2	e	9/20 (45%)	0.60	1 (11%) 5 5	117, 123, 128, 132	0
2	f	18/20 (90%)	0.11	0 100 100	111, 128, 136, 138	0
2	g	15/20 (75%)	0.26	0 100 100	88, 105, 122, 130	0
2	h	6/20 (30%)	0.19	0 100 100	79, 102, 126, 126	0
3	I	215/263 (81%)	0.20	4 (1%) 66 58	73, 103, 126, 140	0
3	K	207/263 (78%)	0.39	18 (8%) 10 9	74, 106, 136, 155	0
3	M	214/263 (81%)	0.30	10 (4%) 31 26	107, 123, 135, 138	0
3	O	209/263 (79%)	0.70	30 (14%) 2 3	128, 153, 170, 180	0
3	Q	201/263 (76%)	0.78	32 (15%) 1 2	140, 156, 170, 177	0
3	S	215/263 (81%)	0.30	12 (5%) 24 21	99, 124, 144, 151	0
3	U	199/263 (75%)	0.49	21 (10%) 6 6	77, 115, 146, 151	0
3	W	204/263 (77%)	0.25	12 (5%) 22 18	82, 106, 138, 155	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
4	J	198/239 (82%)	0.06	4 (2%) 65 56	68, 102, 118, 130	0
4	L	176/239 (73%)	0.40	17 (9%) 7 7	72, 107, 130, 137	0
4	N	200/239 (83%)	0.40	15 (7%) 14 12	104, 125, 135, 145	0
4	P	184/239 (76%)	0.66	21 (11%) 5 5	131, 151, 172, 178	0
4	R	177/239 (74%)	0.75	23 (12%) 3 4	137, 154, 168, 177	0
4	T	198/239 (82%)	0.57	24 (12%) 4 5	108, 136, 154, 160	0
4	V	186/239 (77%)	0.43	12 (6%) 18 15	77, 107, 142, 155	0
4	X	198/239 (82%)	0.33	12 (6%) 21 17	83, 117, 135, 144	0
All	All	10833/12096 (89%)	0.24	561 (5%) 27 24	53, 116, 152, 180	0

All (561) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	852	SER	9.0
4	X	148	GLN	8.3
4	R	79	GLN	5.8
4	X	149	TRP	5.8
3	W	144	SER	5.7
1	E	924	GLU	5.1
1	E	329	ASN	5.1
3	O	196	SER	5.0
3	O	199	THR	5.0
3	U	184	ALA	4.9
3	Q	46	GLU	4.9
3	O	201	PRO	4.9
1	D	829	LEU	4.8
4	P	131	ALA	4.7
4	T	150	LYS	4.6
4	T	148	GLN	4.6
4	T	147	VAL	4.6
4	V	121	PRO	4.6
1	D	262	GLU	4.6
4	N	148	GLN	4.6
1	F	84	ASP	4.5
1	F	853	GLU	4.5
1	H	227	GLU	4.5
1	F	302	TYR	4.5
4	T	145	ALA	4.4
3	Q	38	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	191	GLU	4.3
1	E	784	GLU	4.3
1	F	887	GLN	4.3
1	D	221	GLY	4.2
3	O	200	VAL	4.2
1	G	230	PRO	4.2
3	W	143	SER	4.2
1	D	263	SER	4.1
4	P	119	PHE	4.1
3	Q	36	TRP	4.1
1	H	238	ARG	4.1
4	L	122	SER	4.1
1	C	312	ASN	4.1
3	I	224	ASP	4.0
1	E	334	LEU	4.0
4	N	90	GLN	4.0
4	X	121	PRO	4.0
1	D	761	SER	3.9
1	F	90	LEU	3.9
3	O	197	VAL	3.9
4	P	121	PRO	3.9
1	H	239	GLN	3.9
3	Q	210	TYR	3.9
1	D	215	PHE	3.9
4	L	198	THR	3.8
4	L	175	SER	3.8
1	C	175	ASP	3.8
1	E	479	ALA	3.8
3	Q	228	GLU	3.8
1	D	312	ASN	3.8
3	Q	227	VAL	3.8
3	K	139	PRO	3.8
4	P	122	SER	3.8
3	U	185	VAL	3.8
1	G	373	PHE	3.8
1	F	249	TYR	3.7
1	F	835	SER	3.7
1	E	939	PHE	3.7
3	Q	196	SER	3.7
3	K	203	SER	3.7
4	P	25	ALA	3.7
1	D	265	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	332	HIS	3.7
1	C	501	LYS	3.7
3	K	195	SER	3.6
4	R	190	HIS	3.6
3	K	128	SER	3.6
4	P	14	SER	3.6
3	Q	92	ALA	3.6
1	H	241	LEU	3.6
3	S	142	PRO	3.6
1	H	242	LEU	3.6
3	Q	9	GLY	3.6
1	C	303	LYS	3.6
3	Q	8	GLY	3.6
1	D	332	HIS	3.6
4	N	162	GLU	3.6
3	Q	129	SER	3.5
4	R	33	VAL	3.5
4	X	163	SER	3.5
1	G	178	ALA	3.5
4	T	194	ALA	3.5
1	E	64	TYR	3.5
1	D	103	ILE	3.5
3	U	193	SER	3.5
1	D	407	GLN	3.5
3	Q	18	LEU	3.5
2	e	5	GLN	3.4
4	T	162	GLU	3.4
4	X	147	VAL	3.4
1	F	312	ASN	3.4
4	L	145	ALA	3.4
4	V	207	THR	3.4
1	G	922	ASN	3.4
1	F	829	LEU	3.4
4	N	14	SER	3.4
1	E	330	PRO	3.4
1	C	237	VAL	3.4
1	E	313	LEU	3.4
1	D	333	TYR	3.4
3	O	178	GLY	3.4
3	M	142	PRO	3.4
1	C	931	LEU	3.4
4	N	191	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	850	ILE	3.3
4	R	14	SER	3.3
4	T	136	LEU	3.3
1	G	291	HIS	3.3
1	C	478	VAL	3.3
1	E	829	LEU	3.3
1	D	387	VAL	3.3
1	G	303	LYS	3.3
4	T	109	ARG	3.3
1	E	895	ASP	3.3
1	E	262	GLU	3.3
1	C	248	TYR	3.3
1	D	460	ARG	3.3
4	N	118	ILE	3.3
4	R	162	GLU	3.2
1	B	129	GLN	3.2
4	X	195	CYS	3.2
1	E	501	LYS	3.2
1	D	182	GLU	3.2
3	K	127	VAL	3.2
1	H	176	GLU	3.2
1	D	853	GLU	3.2
1	C	178	ALA	3.2
1	B	497	GLY	3.2
3	O	17	SER	3.2
3	O	144	SER	3.2
1	B	177	SER	3.2
1	C	944	LEU	3.2
3	O	86	LEU	3.2
1	D	192	LYS	3.1
1	F	761	SER	3.1
3	O	181	THR	3.1
3	O	202	SER	3.1
4	T	82	ASP	3.1
1	D	244	PHE	3.1
1	H	181	ARG	3.1
4	N	195	CYS	3.1
1	E	656	GLU	3.1
3	U	228	GLU	3.1
3	Q	226	LYS	3.1
4	N	149	TRP	3.1
1	C	52	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
4	X	131	ALA	3.0
1	D	848	PHE	3.0
3	Q	213	ASN	3.0
4	P	132	SER	3.0
1	F	238	ARG	3.0
3	M	195	SER	3.0
3	Q	13	GLN	3.0
4	T	195	CYS	3.0
1	C	262	GLU	3.0
1	E	489	THR	3.0
1	D	193	ASN	3.0
1	D	329	ASN	3.0
4	L	138	ASN	3.0
1	C	78	ILE	3.0
4	P	134	VAL	3.0
1	C	236	ASP	3.0
4	R	138	ASN	3.0
3	Q	144	SER	3.0
4	L	121	PRO	3.0
1	A	178	ALA	2.9
1	E	955	SER	2.9
3	U	137	VAL	2.9
3	U	154	LEU	2.9
1	C	479	ALA	2.9
1	F	221	GLY	2.9
4	L	188	GLU	2.9
1	G	691	THR	2.9
3	O	177	SER	2.9
3	U	116	MET	2.9
3	Q	37	VAL	2.9
1	B	227	GLU	2.9
1	E	877	MET	2.9
1	B	517	ASP	2.9
1	D	249	TYR	2.9
4	P	35	TRP	2.9
3	Q	99	ASP	2.9
1	H	852	SER	2.9
3	U	181	THR	2.9
1	G	301	LEU	2.9
1	F	262	GLU	2.8
1	C	313	LEU	2.8
1	F	426	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	124	GLU	2.8
1	G	168	PHE	2.8
4	J	193	TYR	2.8
1	F	788	ASN	2.8
3	Q	209	THR	2.8
3	W	126	THR	2.8
3	S	195	SER	2.8
1	H	517	ASP	2.8
3	W	11	LEU	2.8
1	D	852	SER	2.8
1	F	851	GLN	2.8
1	E	458	GLU	2.8
3	Q	62	ASP	2.8
1	E	478	VAL	2.8
3	K	144	SER	2.8
3	K	17	SER	2.8
1	C	924	GLU	2.8
1	D	213	HIS	2.8
4	N	177	SER	2.8
1	F	857	HIS	2.8
3	O	214	VAL	2.8
4	N	179	THR	2.8
1	H	983	ALA	2.8
2	c	10	ILE	2.8
1	D	877	MET	2.8
1	A	479	ALA	2.8
4	X	134	VAL	2.7
1	E	195	MET	2.7
1	D	157	HIS	2.7
1	C	337	LEU	2.7
1	D	424	PHE	2.7
1	D	830	GLY	2.7
1	B	386	HIS	2.7
3	O	136	SER	2.7
1	D	292	PRO	2.7
1	H	184	ASN	2.7
3	U	226	LYS	2.7
1	D	290	GLU	2.7
3	I	126	THR	2.7
4	L	137	LEU	2.7
1	B	383	GLY	2.7
3	O	228	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
4	L	140	PHE	2.7
1	F	765	ARG	2.7
3	U	10	GLY	2.7
1	D	979	ASN	2.7
1	A	177	SER	2.7
1	C	834	PHE	2.7
3	U	139	PRO	2.7
3	W	194	LEU	2.7
4	R	90	GLN	2.7
1	D	427	LYS	2.7
3	S	35	HIS	2.7
1	C	259	LEU	2.6
3	Q	168	VAL	2.6
1	C	945	ALA	2.6
1	G	926	ALA	2.6
1	F	983	ALA	2.6
1	H	459	PHE	2.6
1	F	118	THR	2.6
4	L	174	TYR	2.6
2	a	17	GLU	2.6
3	M	83	MET	2.6
4	R	96	LEU	2.6
3	S	37	VAL	2.6
3	U	225	LYS	2.6
4	P	125	GLN	2.6
3	U	172	SER	2.6
3	U	196	SER	2.6
4	V	209	SER	2.6
1	E	265	ASP	2.6
3	U	115	GLY	2.6
1	D	984	PRO	2.6
4	R	189	LYS	2.6
1	C	829	LEU	2.6
3	M	36	TRP	2.6
4	R	119	PHE	2.6
3	U	81	LEU	2.6
1	F	833	VAL	2.6
3	K	229	PRO	2.6
1	E	866	PHE	2.6
1	E	778	VAL	2.6
1	F	487	GLY	2.6
1	F	69	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	762	GLN	2.6
1	A	691	THR	2.5
3	M	126	THR	2.5
4	V	206	VAL	2.5
3	O	198	VAL	2.5
4	T	144	GLU	2.5
4	X	188	GLU	2.5
1	H	254	MET	2.5
1	E	80	ASP	2.5
1	H	930	THR	2.5
4	L	5	THR	2.5
1	G	226	LEU	2.5
3	O	38	ARG	2.5
1	D	411	PHE	2.5
1	H	929	LYS	2.5
1	E	98	SER	2.5
1	E	1003	PRO	2.5
4	N	196	GLU	2.5
3	M	128	SER	2.5
1	C	239	GLN	2.5
3	U	197	VAL	2.5
4	R	70	ASP	2.5
4	R	34	ALA	2.5
1	H	182	GLU	2.5
1	E	878	THR	2.5
4	V	201	GLY	2.5
1	E	315	VAL	2.5
3	Q	214	VAL	2.5
1	E	931	LEU	2.5
1	H	230	PRO	2.5
4	T	149	TRP	2.5
3	Q	17	SER	2.5
4	X	162	GLU	2.5
1	D	313	LEU	2.5
1	A	373	PHE	2.5
1	C	848	PHE	2.5
1	E	249	TYR	2.5
1	F	453	GLU	2.5
3	Q	136	SER	2.5
4	R	157	SER	2.5
1	E	337	LEU	2.5
1	H	73	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
3	U	138	PHE	2.5
1	C	315	VAL	2.5
4	P	197	VAL	2.5
1	B	81	PRO	2.4
4	V	196	GLU	2.4
1	C	863	VAL	2.4
3	K	228	GLU	2.4
1	D	177	SER	2.4
1	F	982	GLN	2.4
3	K	202	SER	2.4
1	E	408	GLU	2.4
1	F	746	GLU	2.4
1	F	924	GLU	2.4
1	D	850	ILE	2.4
3	K	196	SER	2.4
3	Q	124	LEU	2.4
3	O	168	VAL	2.4
4	N	135	CYS	2.4
1	D	486	GLU	2.4
1	E	382	GLU	2.4
4	T	83	PHE	2.4
1	A	102	ASN	2.4
1	D	98	SER	2.4
1	F	254	MET	2.4
3	O	137	VAL	2.4
1	G	982	GLN	2.4
1	C	241	LEU	2.4
3	W	176	THR	2.4
1	C	174	PHE	2.4
1	D	413	GLU	2.4
1	E	96	SER	2.4
3	O	85	SER	2.4
3	S	153	ALA	2.4
4	R	139	ASN	2.4
1	D	62	ARG	2.4
1	D	264	LEU	2.4
1	H	585	VAL	2.4
3	M	139	PRO	2.4
1	G	381	GLU	2.4
4	J	149	TRP	2.4
1	G	223	LYS	2.4
4	P	4	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	784	GLU	2.4
3	Q	195	SER	2.4
3	K	209	THR	2.4
1	F	702	GLU	2.4
4	X	119	PHE	2.4
1	D	331	GLY	2.4
1	F	441	LEU	2.4
4	T	178	SER	2.4
4	R	117	PHE	2.4
4	N	194	ALA	2.4
4	T	206	VAL	2.4
4	V	5	THR	2.4
4	P	114	PRO	2.3
4	T	79	GLN	2.3
1	B	231	ASN	2.3
3	O	156	CYS	2.3
4	P	133	VAL	2.3
3	Q	94	TYR	2.3
4	L	146	LYS	2.3
1	F	182	GLU	2.3
1	D	983	ALA	2.3
1	E	834	PHE	2.3
1	A	239	GLN	2.3
1	C	197	ASP	2.3
1	F	798	ASP	2.3
4	L	165	THR	2.3
3	K	182	PHE	2.3
4	T	199	HIS	2.3
1	F	895	ASP	2.3
4	N	136	LEU	2.3
1	D	104	ALA	2.3
1	C	258	VAL	2.3
1	C	770	GLN	2.3
3	M	218	PRO	2.3
1	D	372	PHE	2.3
4	L	199	HIS	2.3
1	C	377	VAL	2.3
1	C	928	LEU	2.3
1	G	295	GLU	2.3
4	T	135	CYS	2.3
3	Q	48	VAL	2.3
1	D	330	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
3	M	48	VAL	2.3
1	D	254	MET	2.3
4	R	21	ILE	2.3
1	A	428	GLU	2.3
1	A	241	LEU	2.3
4	L	124	SER	2.3
3	K	126	THR	2.3
1	F	832	ILE	2.3
1	E	333	TYR	2.3
4	R	17	ASP	2.3
1	C	336	HIS	2.3
4	R	35	TRP	2.3
1	F	103	ILE	2.3
1	H	180	ASP	2.3
3	U	70	ILE	2.3
3	W	125	VAL	2.3
3	W	157	LEU	2.3
3	O	88	ALA	2.3
3	O	126	THR	2.3
3	Q	35	HIS	2.3
1	G	290	GLU	2.3
3	O	63	SER	2.3
3	W	170	TRP	2.3
4	V	147	VAL	2.3
1	E	381	GLU	2.2
1	F	692	GLU	2.2
4	N	150	LYS	2.2
1	F	834	PHE	2.2
3	K	218	PRO	2.2
4	V	199	HIS	2.2
4	P	78	LEU	2.2
4	R	29	VAL	2.2
1	D	259	LEU	2.2
4	R	15	VAL	2.2
1	E	862	ARG	2.2
1	D	239	GLN	2.2
1	D	378	ASP	2.2
1	F	559	LEU	2.2
1	C	249	TYR	2.2
1	C	535	PHE	2.2
3	S	196	SER	2.2
1	B	244	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	866	PHE	2.2
1	E	168	PHE	2.2
1	F	486	GLU	2.2
1	C	832	ILE	2.2
1	E	956	VAL	2.2
3	I	115	GLY	2.2
1	H	888	ALA	2.2
2	b	5	GLN	2.2
3	W	177	SER	2.2
4	V	194	ALA	2.2
3	K	170	TRP	2.2
4	P	87	TYR	2.2
1	C	992	ILE	2.2
1	E	827	GLU	2.2
3	Q	128	SER	2.2
4	X	135	CYS	2.2
1	B	100	PRO	2.2
3	W	210	TYR	2.2
1	D	791	ILE	2.2
3	O	143	SER	2.2
3	S	164	GLU	2.2
4	T	134	VAL	2.2
1	E	932	THR	2.2
4	P	211	ASN	2.2
4	P	143	ARG	2.2
1	E	785	VAL	2.2
3	O	138	PHE	2.2
1	A	944	LEU	2.2
1	F	259	LEU	2.2
1	F	390	ILE	2.2
1	H	863	VAL	2.1
1	B	230	PRO	2.1
3	S	141	ALA	2.1
1	B	456	LEU	2.1
1	D	366	GLY	2.1
3	O	230	LYS	2.1
1	H	926	ALA	2.1
1	C	62	ARG	2.1
4	T	137	LEU	2.1
4	V	190	HIS	2.1
4	P	212	ARG	2.1
1	C	1003	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	786	HIS	2.1
1	G	945	ALA	2.1
4	L	6	GLN	2.1
1	C	64	TYR	2.1
1	F	376	ASN	2.1
1	F	848	PHE	2.1
1	D	497	GLY	2.1
3	O	36	TRP	2.1
1	E	97	LEU	2.1
3	Q	141	ALA	2.1
1	H	773	ASP	2.1
1	F	479	ALA	2.1
1	A	482	SER	2.1
1	D	47	ILE	2.1
1	D	102	ASN	2.1
1	H	90	LEU	2.1
3	S	36	TRP	2.1
1	H	165	PHE	2.1
1	D	800	GLN	2.1
1	F	984	PRO	2.1
3	W	175	LEU	2.1
4	L	139	ASN	2.1
1	F	314	TYR	2.1
1	F	478	VAL	2.1
1	F	255	ALA	2.1
1	E	1004	LEU	2.1
3	S	50	SER	2.1
4	J	121	PRO	2.1
1	E	179	LYS	2.1
1	F	849	ILE	2.1
1	G	225	THR	2.1
4	P	127	LYS	2.1
4	T	179	THR	2.1
1	D	437	ILE	2.1
1	F	256	VAL	2.1
3	I	124	LEU	2.1
3	U	198	VAL	2.1
4	R	192	VAL	2.1
3	O	203	SER	2.0
3	S	154	LEU	2.0
1	F	244	PHE	2.0
1	H	513	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	76	LEU	2.0
3	K	198	VAL	2.0
3	O	223	VAL	2.0
3	Q	197	VAL	2.0
4	T	46	LEU	2.0
1	C	676	GLU	2.0
1	F	699	GLU	2.0
4	P	145	ALA	2.0
1	E	457	GLU	2.0
4	J	119	PHE	2.0
1	D	394	MET	2.0
3	M	153	ALA	2.0
4	T	131	ALA	2.0
1	G	177	SER	2.0
1	E	540	LEU	2.0
1	F	395	PHE	2.0
1	F	823	LEU	2.0
4	V	202	LEU	2.0
1	C	862	ARG	2.0
3	K	167	THR	2.0
4	T	181	THR	2.0
1	D	887	GLN	2.0
4	R	118	ILE	2.0
1	E	303	LYS	2.0
1	G	231	ASN	2.0
3	S	38	ARG	2.0
1	E	77	LEU	2.0
1	E	776	TRP	2.0
3	U	179	VAL	2.0
4	R	184	LYS	2.0
1	H	100	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

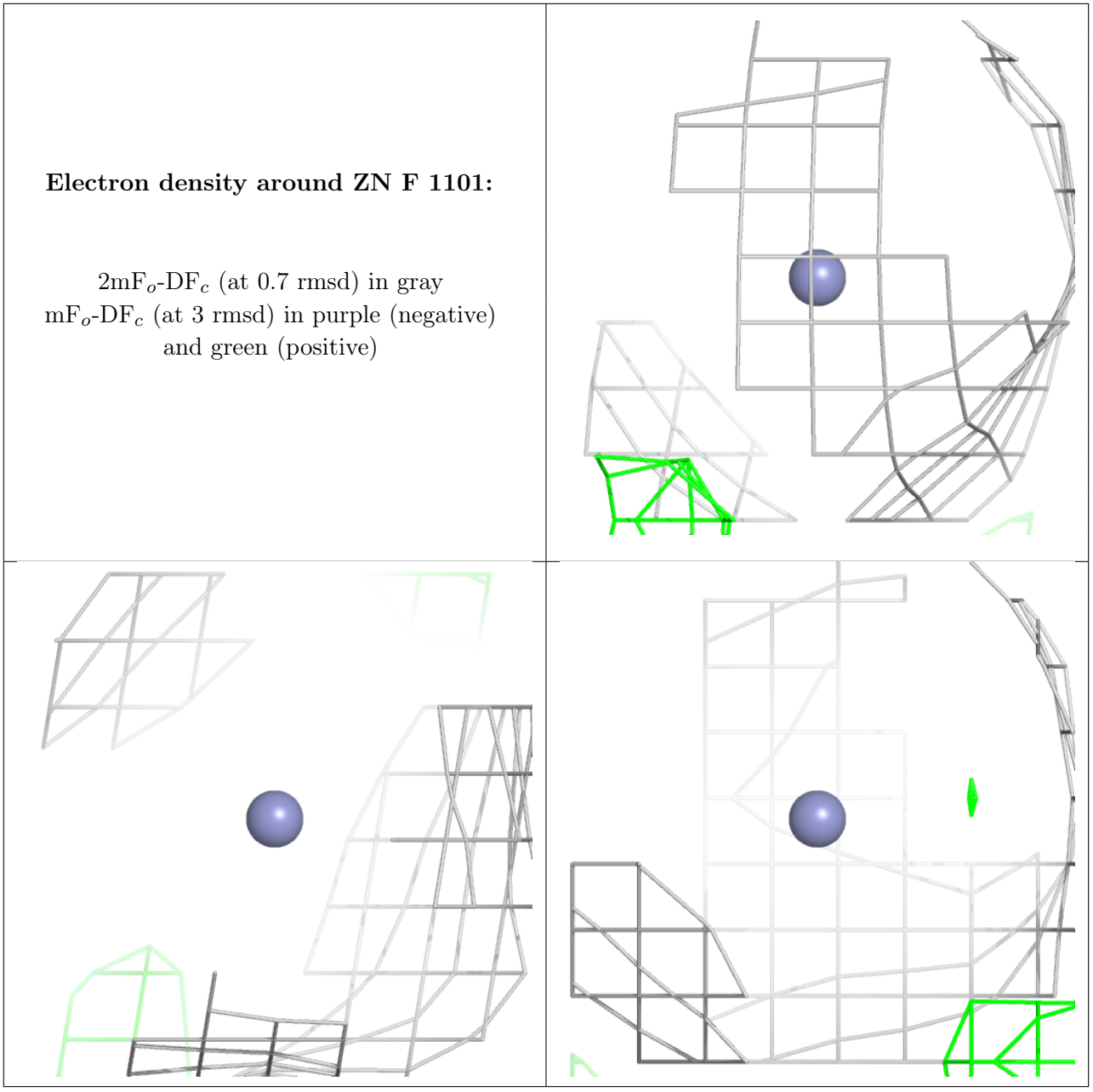
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ZN	F	1101	1/1	0.90	0.11	134,134,134,134	0
5	ZN	D	2001	1/1	0.91	0.10	139,139,139,139	0
5	ZN	C	1101	1/1	0.94	0.12	110,110,110,110	0
5	ZN	E	2001	1/1	0.97	0.04	126,126,126,126	0
5	ZN	H	1101	1/1	0.97	0.15	97,97,97,97	0
5	ZN	B	2001	1/1	0.98	0.16	63,63,63,63	0
5	ZN	A	1101	1/1	0.98	0.17	65,65,65,65	0
5	ZN	G	2001	1/1	0.99	0.17	64,64,64,64	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

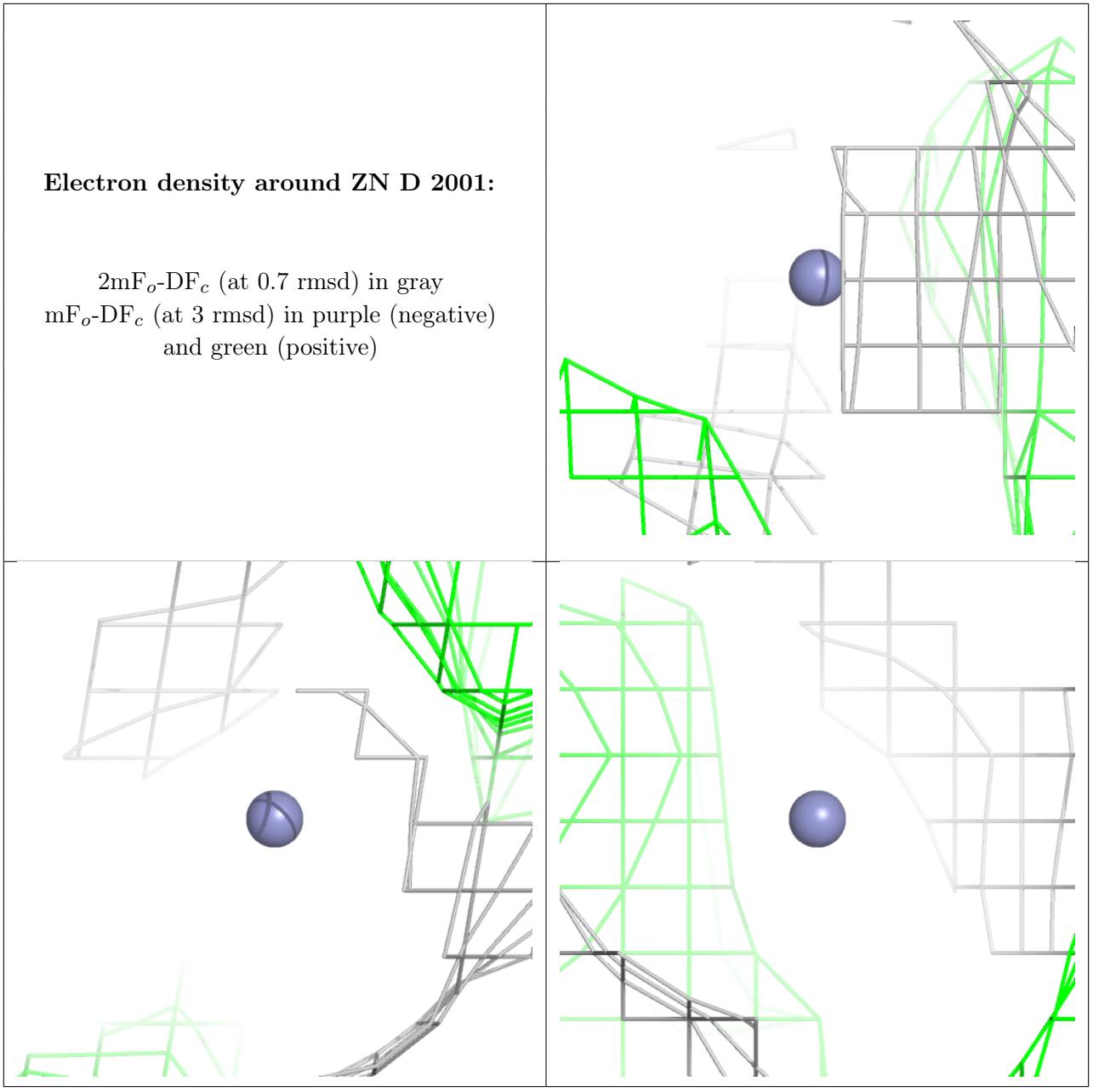
Electron density around ZN F 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



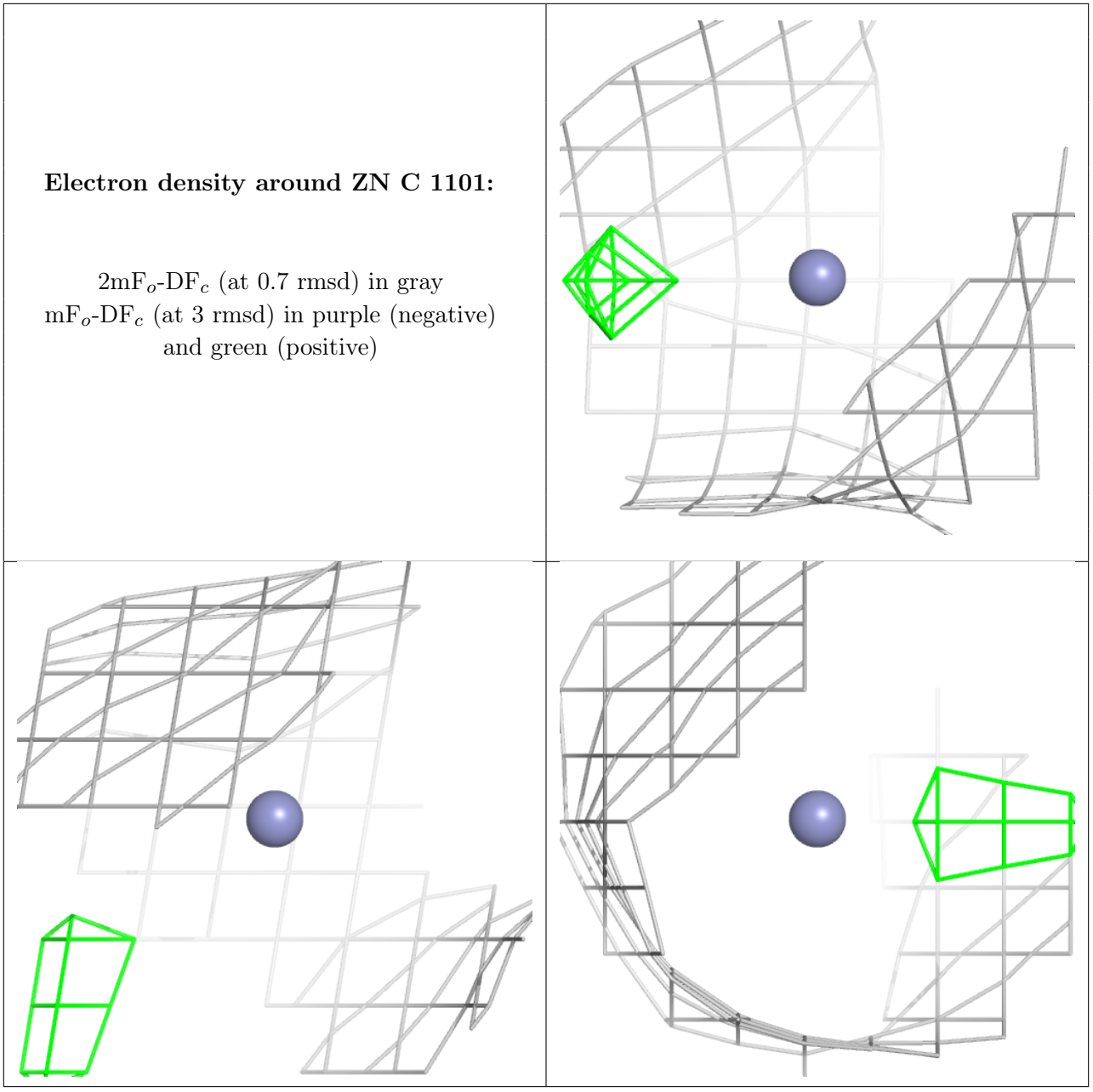
Electron density around ZN D 2001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



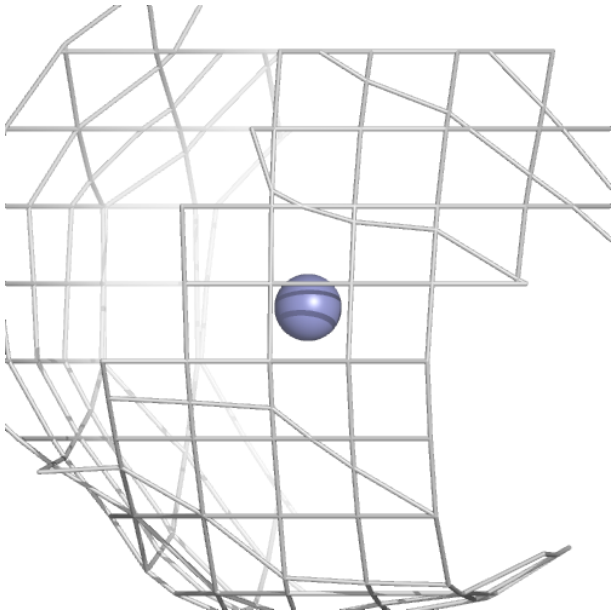
Electron density around ZN C 1101:

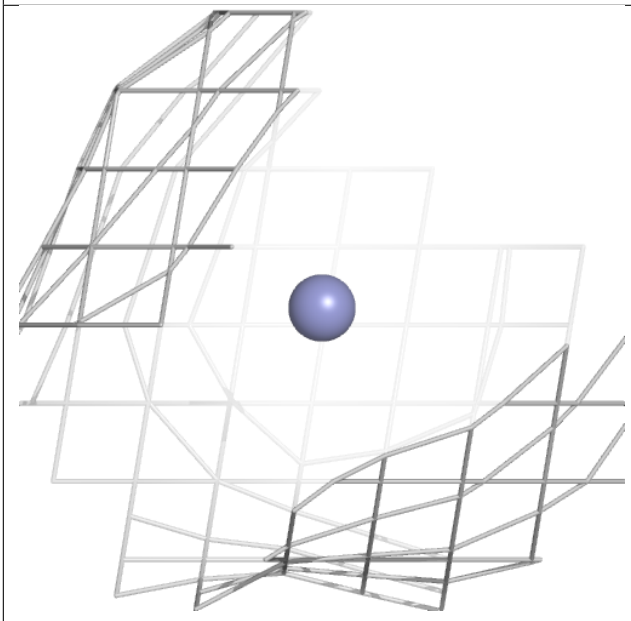
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

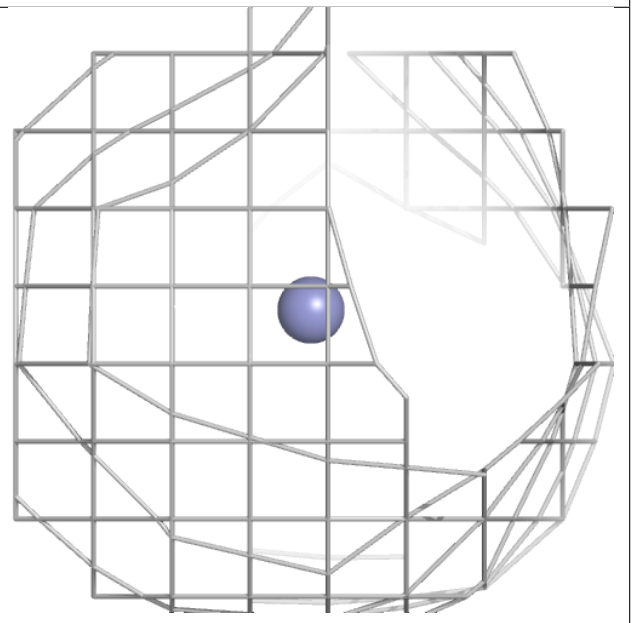


Electron density around ZN E 2001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

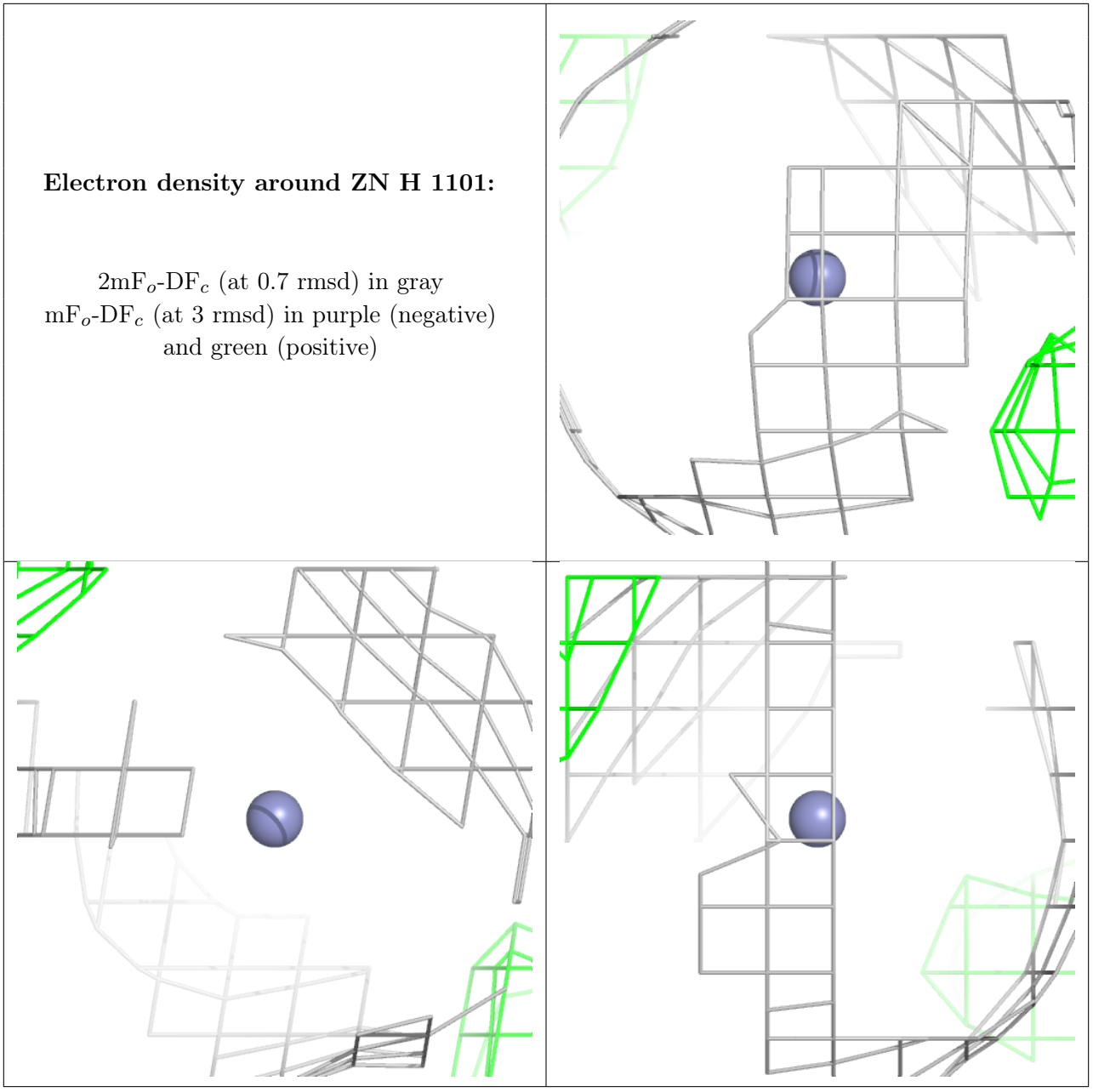






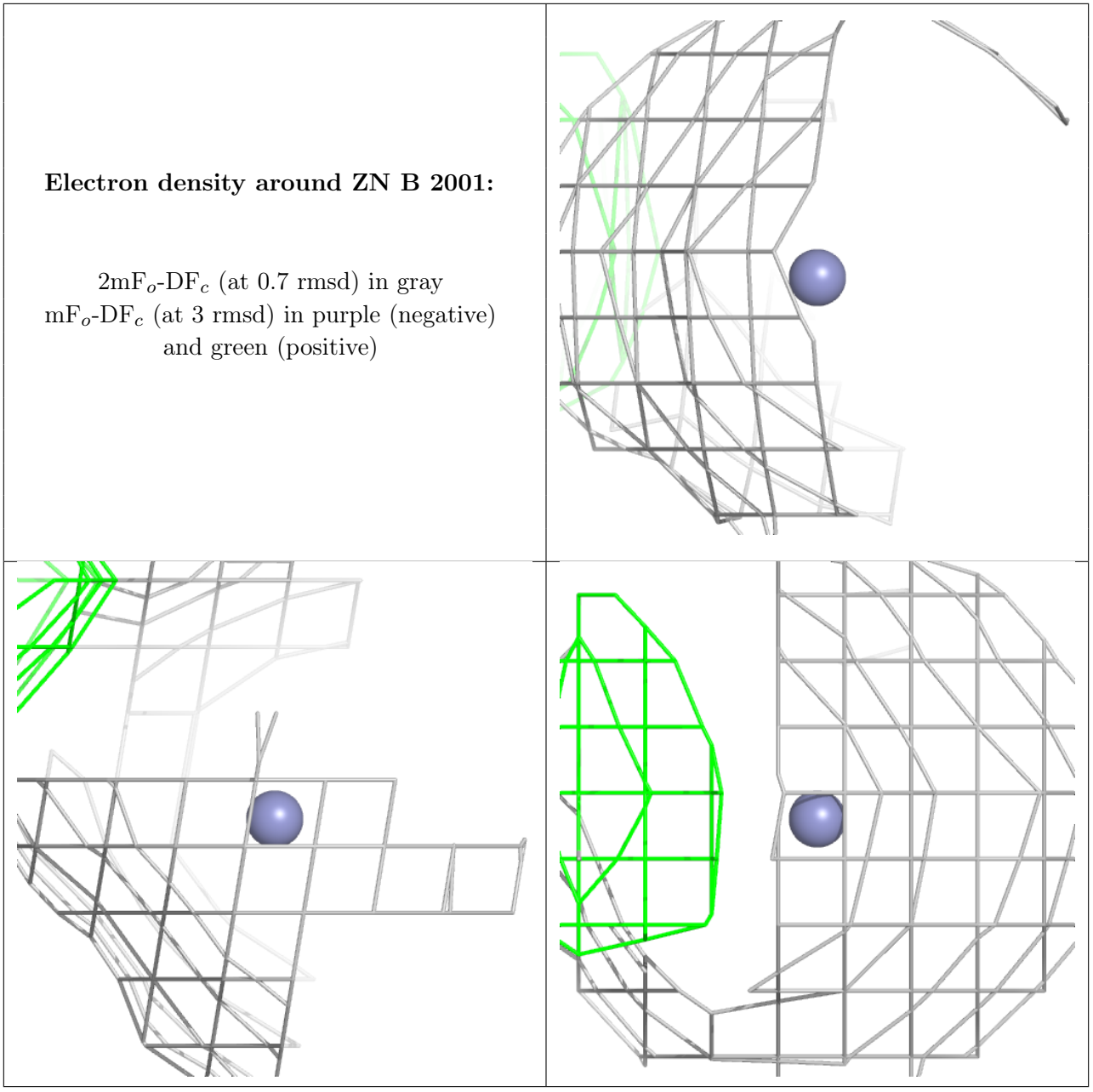
Electron density around ZN H 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



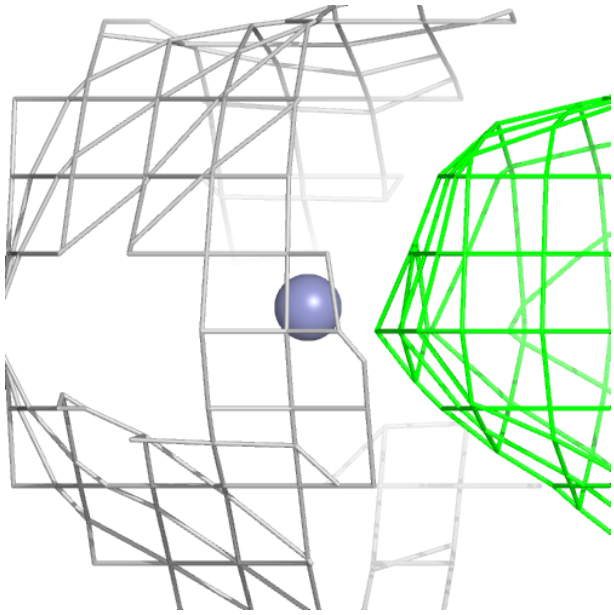
Electron density around ZN B 2001:

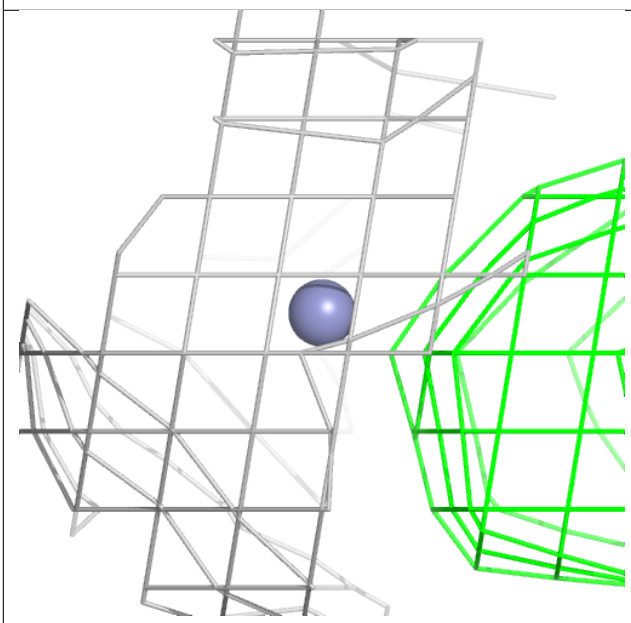
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

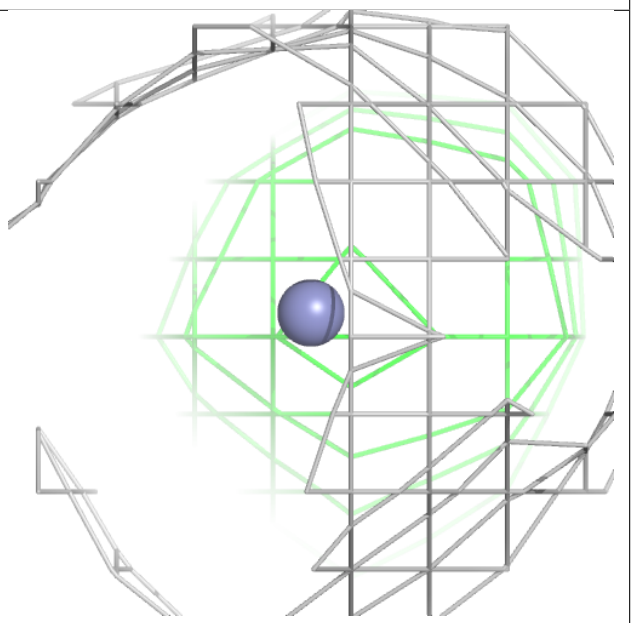


Electron density around ZN A 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

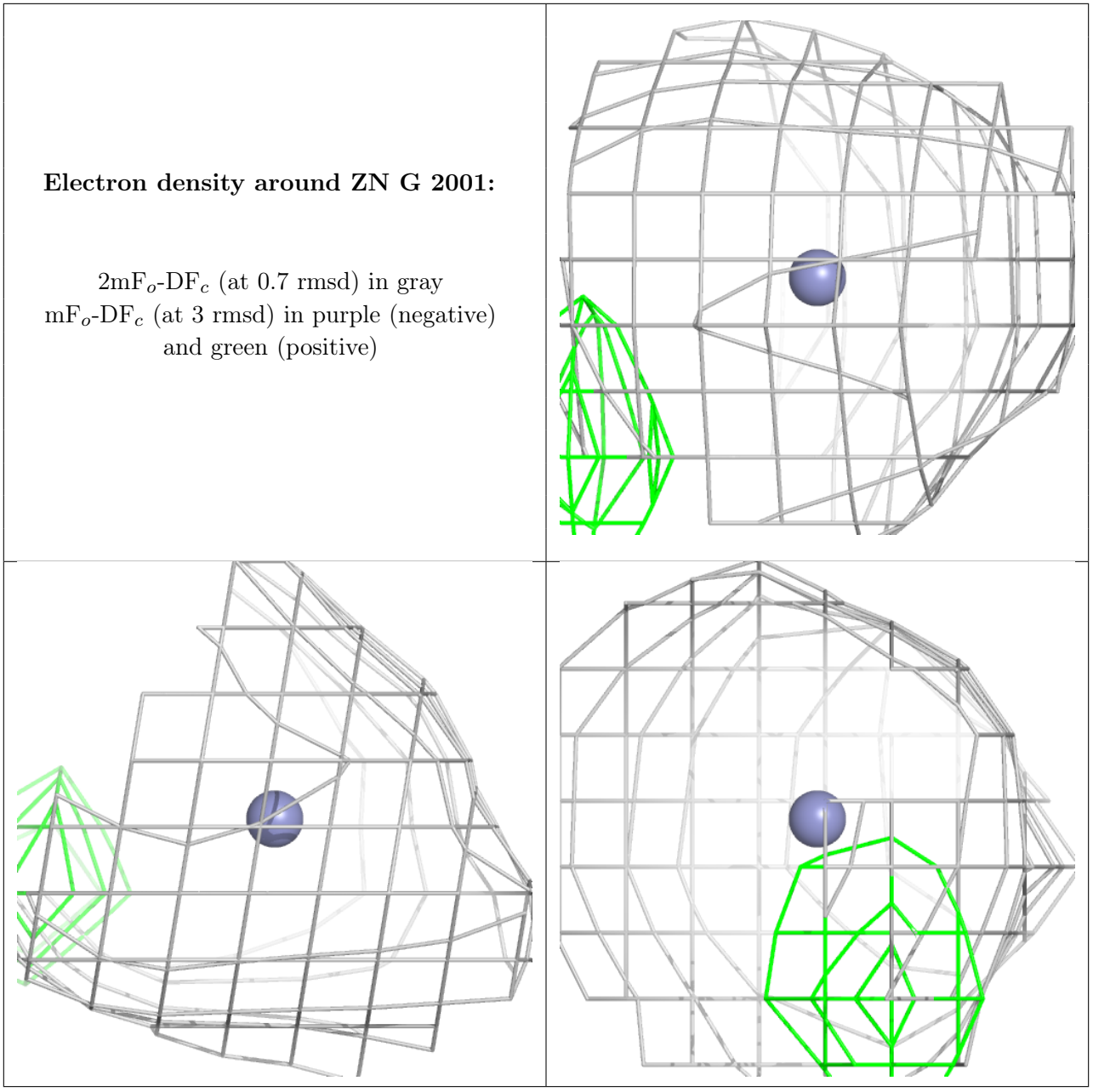






Electron density around ZN G 2001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.