Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:09 PM GMT

PDB ID	:	3QAZ
Title	:	IL-2 mutant D10 ternary complex
Authors	:	Levin, A.M.; Bates, D.L.; Ring, A.M.; Lin, J.T.; Su, L.; Krieg, C.; Bowman, G.R.; Novick, P.; Pande, V.S.; Khort, H.E.; Boyman, O.; Gathman, C.G.; Garcia, K.C.
Deposited on	:	2011-01-12
Resolution	:	3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

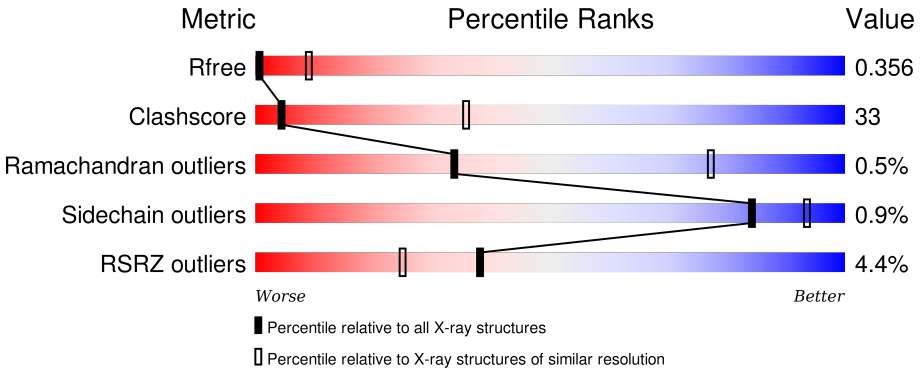
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	136	45% 43% • 11%
1	D	136	41% 48% 11%
1	G	136	38% 48% • 11%
1	J	136	35% 51% • 11%
1	M	136	44% 44% • 11%

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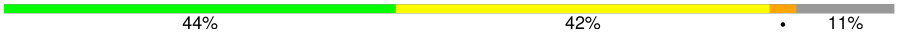
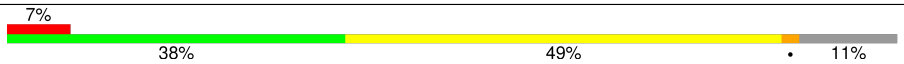
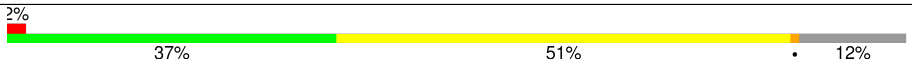
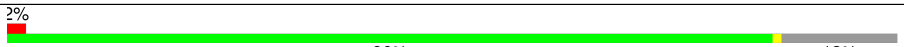
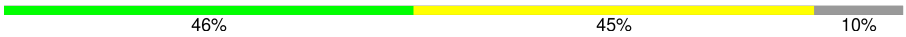
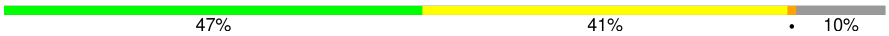
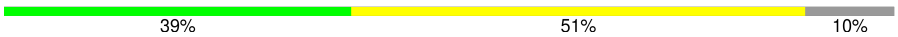
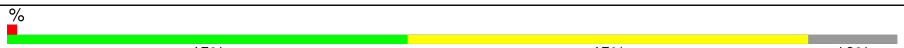
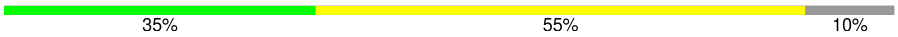
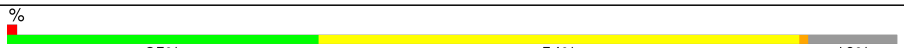
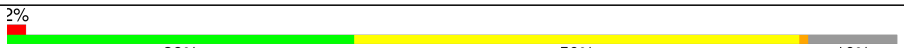
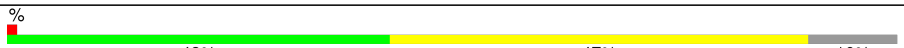
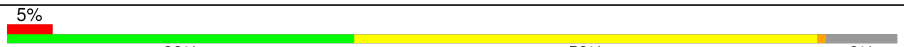
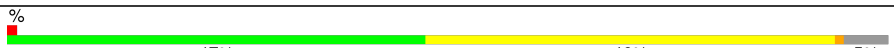
Mol	Chain	Length	Quality of chain
1	P	136	
1	S	136	
1	V	136	
1	Y	136	
1	b	136	
1	e	136	
1	h	136	
2	B	217	
2	E	217	
2	H	217	
2	K	217	
2	N	217	
2	Q	217	
2	T	217	
2	W	217	
2	Z	217	
2	c	217	
2	f	217	
2	i	217	
3	C	202	
3	F	202	
3	I	202	
3	L	202	
3	O	202	
3	R	202	

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Mol	Chain	Length	Quality of chain
3	U	202	11% 46% 48% 5%
3	X	202	19% 48% 46% 5%
3	a	202	15% 95% 5%
3	d	202	13% 94% 5%
3	g	202	12% 94% 5%
3	j	202	13% 94% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	K	215	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 51562 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 Interleukin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	D	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	G	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	J	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	M	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	P	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	S	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	V	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	Y	120	Total	C	N	O	S	0	0	0
			991	643	161	180	7			
1	b	119	Total	C	N	O	S	0	0	0
			983	637	160	179	7			
1	e	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			
1	h	121	Total	C	N	O	S	0	0	0
			998	647	162	182	7			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	EXPRESSION TAG	UNP P60568
A	-1	ASP	-	EXPRESSION TAG	UNP P60568
A	0	PRO	-	EXPRESSION TAG	UNP P60568
A	74	HIS	GLN	ENGINEERED MUTATION	UNP P60568
A	80	PHE	LEU	ENGINEERED MUTATION	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
A	81	ASP	ARG	ENGINEERED MUTATION	UNP P60568
A	85	VAL	LEU	ENGINEERED MUTATION	UNP P60568
A	86	VAL	ILE	ENGINEERED MUTATION	UNP P60568
A	92	PHE	ILE	ENGINEERED MUTATION	UNP P60568
D	-2	ALA	-	EXPRESSION TAG	UNP P60568
D	-1	ASP	-	EXPRESSION TAG	UNP P60568
D	0	PRO	-	EXPRESSION TAG	UNP P60568
D	74	HIS	GLN	ENGINEERED MUTATION	UNP P60568
D	80	PHE	LEU	ENGINEERED MUTATION	UNP P60568
D	81	ASP	ARG	ENGINEERED MUTATION	UNP P60568
D	85	VAL	LEU	ENGINEERED MUTATION	UNP P60568
D	86	VAL	ILE	ENGINEERED MUTATION	UNP P60568
D	92	PHE	ILE	ENGINEERED MUTATION	UNP P60568
G	-2	ALA	-	EXPRESSION TAG	UNP P60568
G	-1	ASP	-	EXPRESSION TAG	UNP P60568
G	0	PRO	-	EXPRESSION TAG	UNP P60568
G	74	HIS	GLN	ENGINEERED MUTATION	UNP P60568
G	80	PHE	LEU	ENGINEERED MUTATION	UNP P60568
G	81	ASP	ARG	ENGINEERED MUTATION	UNP P60568
G	85	VAL	LEU	ENGINEERED MUTATION	UNP P60568
G	86	VAL	ILE	ENGINEERED MUTATION	UNP P60568
G	92	PHE	ILE	ENGINEERED MUTATION	UNP P60568
J	-2	ALA	-	EXPRESSION TAG	UNP P60568
J	-1	ASP	-	EXPRESSION TAG	UNP P60568
J	0	PRO	-	EXPRESSION TAG	UNP P60568
J	74	HIS	GLN	ENGINEERED MUTATION	UNP P60568
J	80	PHE	LEU	ENGINEERED MUTATION	UNP P60568
J	81	ASP	ARG	ENGINEERED MUTATION	UNP P60568
J	85	VAL	LEU	ENGINEERED MUTATION	UNP P60568
J	86	VAL	ILE	ENGINEERED MUTATION	UNP P60568
J	92	PHE	ILE	ENGINEERED MUTATION	UNP P60568
M	-2	ALA	-	EXPRESSION TAG	UNP P60568
M	-1	ASP	-	EXPRESSION TAG	UNP P60568
M	0	PRO	-	EXPRESSION TAG	UNP P60568
M	74	HIS	GLN	ENGINEERED MUTATION	UNP P60568
M	80	PHE	LEU	ENGINEERED MUTATION	UNP P60568
M	81	ASP	ARG	ENGINEERED MUTATION	UNP P60568
M	85	VAL	LEU	ENGINEERED MUTATION	UNP P60568
M	86	VAL	ILE	ENGINEERED MUTATION	UNP P60568
M	92	PHE	ILE	ENGINEERED MUTATION	UNP P60568
P	-2	ALA	-	EXPRESSION TAG	UNP P60568
P	-1	ASP	-	EXPRESSION TAG	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
P	0	PRO	-	EXPRESSION TAG	UNP P60568
P	74	HIS	GLN	ENGINEERED MUTATION	UNP P60568
P	80	PHE	LEU	ENGINEERED MUTATION	UNP P60568
P	81	ASP	ARG	ENGINEERED MUTATION	UNP P60568
P	85	VAL	LEU	ENGINEERED MUTATION	UNP P60568
P	86	VAL	ILE	ENGINEERED MUTATION	UNP P60568
P	92	PHE	ILE	ENGINEERED MUTATION	UNP P60568
S	-2	ALA	-	EXPRESSION TAG	UNP P60568
S	-1	ASP	-	EXPRESSION TAG	UNP P60568
S	0	PRO	-	EXPRESSION TAG	UNP P60568
S	74	HIS	GLN	ENGINEERED MUTATION	UNP P60568
S	80	PHE	LEU	ENGINEERED MUTATION	UNP P60568
S	81	ASP	ARG	ENGINEERED MUTATION	UNP P60568
S	85	VAL	LEU	ENGINEERED MUTATION	UNP P60568
S	86	VAL	ILE	ENGINEERED MUTATION	UNP P60568
S	92	PHE	ILE	ENGINEERED MUTATION	UNP P60568
V	-2	ALA	-	EXPRESSION TAG	UNP P60568
V	-1	ASP	-	EXPRESSION TAG	UNP P60568
V	0	PRO	-	EXPRESSION TAG	UNP P60568
V	74	HIS	GLN	ENGINEERED MUTATION	UNP P60568
V	80	PHE	LEU	ENGINEERED MUTATION	UNP P60568
V	81	ASP	ARG	ENGINEERED MUTATION	UNP P60568
V	85	VAL	LEU	ENGINEERED MUTATION	UNP P60568
V	86	VAL	ILE	ENGINEERED MUTATION	UNP P60568
V	92	PHE	ILE	ENGINEERED MUTATION	UNP P60568
Y	-2	ALA	-	EXPRESSION TAG	UNP P60568
Y	-1	ASP	-	EXPRESSION TAG	UNP P60568
Y	0	PRO	-	EXPRESSION TAG	UNP P60568
Y	74	HIS	GLN	ENGINEERED MUTATION	UNP P60568
Y	80	PHE	LEU	ENGINEERED MUTATION	UNP P60568
Y	81	ASP	ARG	ENGINEERED MUTATION	UNP P60568
Y	85	VAL	LEU	ENGINEERED MUTATION	UNP P60568
Y	86	VAL	ILE	ENGINEERED MUTATION	UNP P60568
Y	92	PHE	ILE	ENGINEERED MUTATION	UNP P60568
b	-2	ALA	-	EXPRESSION TAG	UNP P60568
b	-1	ASP	-	EXPRESSION TAG	UNP P60568
b	0	PRO	-	EXPRESSION TAG	UNP P60568
b	74	HIS	GLN	ENGINEERED MUTATION	UNP P60568
b	80	PHE	LEU	ENGINEERED MUTATION	UNP P60568
b	81	ASP	ARG	ENGINEERED MUTATION	UNP P60568
b	85	VAL	LEU	ENGINEERED MUTATION	UNP P60568
b	86	VAL	ILE	ENGINEERED MUTATION	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
b	92	PHE	ILE	ENGINEERED MUTATION	UNP P60568
e	-2	ALA	-	EXPRESSION TAG	UNP P60568
e	-1	ASP	-	EXPRESSION TAG	UNP P60568
e	0	PRO	-	EXPRESSION TAG	UNP P60568
e	74	HIS	GLN	ENGINEERED MUTATION	UNP P60568
e	80	PHE	LEU	ENGINEERED MUTATION	UNP P60568
e	81	ASP	ARG	ENGINEERED MUTATION	UNP P60568
e	85	VAL	LEU	ENGINEERED MUTATION	UNP P60568
e	86	VAL	ILE	ENGINEERED MUTATION	UNP P60568
e	92	PHE	ILE	ENGINEERED MUTATION	UNP P60568
h	-2	ALA	-	EXPRESSION TAG	UNP P60568
h	-1	ASP	-	EXPRESSION TAG	UNP P60568
h	0	PRO	-	EXPRESSION TAG	UNP P60568
h	74	HIS	GLN	ENGINEERED MUTATION	UNP P60568
h	80	PHE	LEU	ENGINEERED MUTATION	UNP P60568
h	81	ASP	ARG	ENGINEERED MUTATION	UNP P60568
h	85	VAL	LEU	ENGINEERED MUTATION	UNP P60568
h	86	VAL	ILE	ENGINEERED MUTATION	UNP P60568
h	92	PHE	ILE	ENGINEERED MUTATION	UNP P60568

- Molecule 2 is a protein called Interleukin-2 receptor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total	C	N	O	S	0	0	0
			1612	1031	285	286	10			
2	E	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			
2	H	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			
2	K	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			
2	N	195	Total	C	N	O	S	0	0	0
			1612	1031	285	286	10			
2	Q	195	Total	C	N	O	S	0	0	0
			1612	1031	285	286	10			
2	T	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			
2	W	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			
2	Z	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			
2	c	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	f	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			
2	i	196	Total	C	N	O	S	0	0	0
			1618	1034	286	288	10			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	ASP	SER	ENGINEERED MUTATION	UNP P14784
B	0	PRO	ALA	ENGINEERED MUTATION	UNP P14784
B	3	GLN	ASN	ENGINEERED MUTATION	UNP P14784
B	17	GLN	ASN	ENGINEERED MUTATION	UNP P14784
B	45	GLN	ASN	ENGINEERED MUTATION	UNP P14784
E	-1	ASP	SER	ENGINEERED MUTATION	UNP P14784
E	0	PRO	ALA	ENGINEERED MUTATION	UNP P14784
E	3	GLN	ASN	ENGINEERED MUTATION	UNP P14784
E	17	GLN	ASN	ENGINEERED MUTATION	UNP P14784
E	45	GLN	ASN	ENGINEERED MUTATION	UNP P14784
H	-1	ASP	SER	ENGINEERED MUTATION	UNP P14784
H	0	PRO	ALA	ENGINEERED MUTATION	UNP P14784
H	3	GLN	ASN	ENGINEERED MUTATION	UNP P14784
H	17	GLN	ASN	ENGINEERED MUTATION	UNP P14784
H	45	GLN	ASN	ENGINEERED MUTATION	UNP P14784
K	-1	ASP	SER	ENGINEERED MUTATION	UNP P14784
K	0	PRO	ALA	ENGINEERED MUTATION	UNP P14784
K	3	GLN	ASN	ENGINEERED MUTATION	UNP P14784
K	17	GLN	ASN	ENGINEERED MUTATION	UNP P14784
K	45	GLN	ASN	ENGINEERED MUTATION	UNP P14784
N	-1	ASP	SER	ENGINEERED MUTATION	UNP P14784
N	0	PRO	ALA	ENGINEERED MUTATION	UNP P14784
N	3	GLN	ASN	ENGINEERED MUTATION	UNP P14784
N	17	GLN	ASN	ENGINEERED MUTATION	UNP P14784
N	45	GLN	ASN	ENGINEERED MUTATION	UNP P14784
Q	-1	ASP	SER	ENGINEERED MUTATION	UNP P14784
Q	0	PRO	ALA	ENGINEERED MUTATION	UNP P14784
Q	3	GLN	ASN	ENGINEERED MUTATION	UNP P14784
Q	17	GLN	ASN	ENGINEERED MUTATION	UNP P14784
Q	45	GLN	ASN	ENGINEERED MUTATION	UNP P14784
T	-1	ASP	SER	ENGINEERED MUTATION	UNP P14784
T	0	PRO	ALA	ENGINEERED MUTATION	UNP P14784
T	3	GLN	ASN	ENGINEERED MUTATION	UNP P14784
T	17	GLN	ASN	ENGINEERED MUTATION	UNP P14784

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Chain	Residue	Modelled	Actual	Comment	Reference
T	45	GLN	ASN	ENGINEERED MUTATION	UNP P14784
W	-1	ASP	SER	ENGINEERED MUTATION	UNP P14784
W	0	PRO	ALA	ENGINEERED MUTATION	UNP P14784
W	3	GLN	ASN	ENGINEERED MUTATION	UNP P14784
W	17	GLN	ASN	ENGINEERED MUTATION	UNP P14784
W	45	GLN	ASN	ENGINEERED MUTATION	UNP P14784
Z	-1	ASP	SER	ENGINEERED MUTATION	UNP P14784
Z	0	PRO	ALA	ENGINEERED MUTATION	UNP P14784
Z	3	GLN	ASN	ENGINEERED MUTATION	UNP P14784
Z	17	GLN	ASN	ENGINEERED MUTATION	UNP P14784
Z	45	GLN	ASN	ENGINEERED MUTATION	UNP P14784
c	-1	ASP	SER	ENGINEERED MUTATION	UNP P14784
c	0	PRO	ALA	ENGINEERED MUTATION	UNP P14784
c	3	GLN	ASN	ENGINEERED MUTATION	UNP P14784
c	17	GLN	ASN	ENGINEERED MUTATION	UNP P14784
c	45	GLN	ASN	ENGINEERED MUTATION	UNP P14784
f	-1	ASP	SER	ENGINEERED MUTATION	UNP P14784
f	0	PRO	ALA	ENGINEERED MUTATION	UNP P14784
f	3	GLN	ASN	ENGINEERED MUTATION	UNP P14784
f	17	GLN	ASN	ENGINEERED MUTATION	UNP P14784
f	45	GLN	ASN	ENGINEERED MUTATION	UNP P14784
i	-1	ASP	SER	ENGINEERED MUTATION	UNP P14784
i	0	PRO	ALA	ENGINEERED MUTATION	UNP P14784
i	3	GLN	ASN	ENGINEERED MUTATION	UNP P14784
i	17	GLN	ASN	ENGINEERED MUTATION	UNP P14784
i	45	GLN	ASN	ENGINEERED MUTATION	UNP P14784

- Molecule 3 is a protein called Cytokine receptor common subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	188	Total	C	N	O	S	0	0	0
			1605	1022	286	289	8			
3	F	186	Total	C	N	O	S	0	0	0
			1592	1014	284	286	8			
3	I	188	Total	C	N	O	S	0	0	0
			1605	1022	286	289	8			
3	L	191	Total	C	N	O	S	0	0	0
			1630	1037	290	295	8			
3	O	191	Total	C	N	O	S	0	0	0
			1630	1037	290	295	8			
3	R	188	Total	C	N	O	S	0	0	0
			1612	1028	287	289	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	U	191	Total	C	N	O	S	0	0	0
			1630	1037	290	295	8			
3	X	191	Total	C	N	O	S	0	0	0
			1630	1037	290	295	8			
3	a	191	Total	C	N	O	S	0	0	0
			1630	1037	290	295	8			
3	d	191	Total	C	N	O	S	0	0	0
			1630	1037	290	295	8			
3	g	191	Total	C	N	O	S	0	0	0
			1630	1037	290	295	8			
3	j	191	Total	C	N	O	S	0	0	0
			1630	1037	290	295	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	31	ALA	-	EXPRESSION TAG	UNP P31785
C	32	ASP	-	EXPRESSION TAG	UNP P31785
C	33	PRO	-	EXPRESSION TAG	UNP P31785
C	53	GLN	ASN	ENGINEERED MUTATION	UNP P31785
F	31	ALA	-	EXPRESSION TAG	UNP P31785
F	32	ASP	-	EXPRESSION TAG	UNP P31785
F	33	PRO	-	EXPRESSION TAG	UNP P31785
F	53	GLN	ASN	ENGINEERED MUTATION	UNP P31785
I	31	ALA	-	EXPRESSION TAG	UNP P31785
I	32	ASP	-	EXPRESSION TAG	UNP P31785
I	33	PRO	-	EXPRESSION TAG	UNP P31785
I	53	GLN	ASN	ENGINEERED MUTATION	UNP P31785
L	31	ALA	-	EXPRESSION TAG	UNP P31785
L	32	ASP	-	EXPRESSION TAG	UNP P31785
L	33	PRO	-	EXPRESSION TAG	UNP P31785
L	53	GLN	ASN	ENGINEERED MUTATION	UNP P31785
O	31	ALA	-	EXPRESSION TAG	UNP P31785
O	32	ASP	-	EXPRESSION TAG	UNP P31785
O	33	PRO	-	EXPRESSION TAG	UNP P31785
O	53	GLN	ASN	ENGINEERED MUTATION	UNP P31785
R	31	ALA	-	EXPRESSION TAG	UNP P31785
R	32	ASP	-	EXPRESSION TAG	UNP P31785
R	33	PRO	-	EXPRESSION TAG	UNP P31785
R	53	GLN	ASN	ENGINEERED MUTATION	UNP P31785
U	31	ALA	-	EXPRESSION TAG	UNP P31785
U	32	ASP	-	EXPRESSION TAG	UNP P31785
U	33	PRO	-	EXPRESSION TAG	UNP P31785

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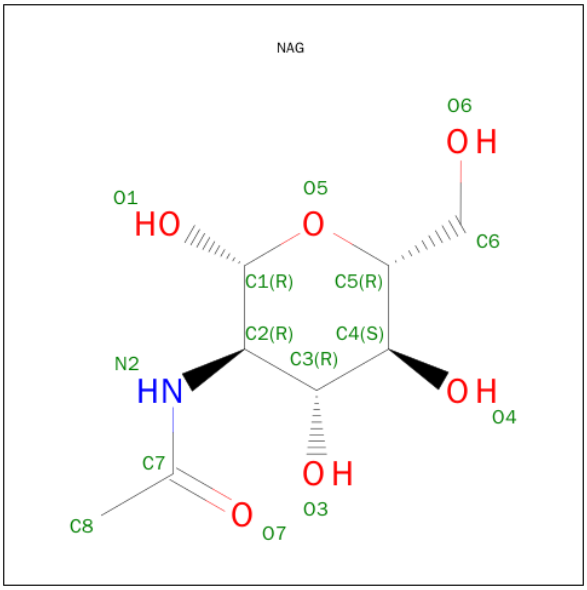
Chain	Residue	Modelled	Actual	Comment	Reference
U	53	GLN	ASN	ENGINEERED MUTATION	UNP P31785
X	31	ALA	-	EXPRESSION TAG	UNP P31785
X	32	ASP	-	EXPRESSION TAG	UNP P31785
X	33	PRO	-	EXPRESSION TAG	UNP P31785
X	53	GLN	ASN	ENGINEERED MUTATION	UNP P31785
a	31	ALA	-	EXPRESSION TAG	UNP P31785
a	32	ASP	-	EXPRESSION TAG	UNP P31785
a	33	PRO	-	EXPRESSION TAG	UNP P31785
a	53	GLN	ASN	ENGINEERED MUTATION	UNP P31785
d	31	ALA	-	EXPRESSION TAG	UNP P31785
d	32	ASP	-	EXPRESSION TAG	UNP P31785
d	33	PRO	-	EXPRESSION TAG	UNP P31785
d	53	GLN	ASN	ENGINEERED MUTATION	UNP P31785
g	31	ALA	-	EXPRESSION TAG	UNP P31785
g	32	ASP	-	EXPRESSION TAG	UNP P31785
g	33	PRO	-	EXPRESSION TAG	UNP P31785
g	53	GLN	ASN	ENGINEERED MUTATION	UNP P31785
j	31	ALA	-	EXPRESSION TAG	UNP P31785
j	32	ASP	-	EXPRESSION TAG	UNP P31785
j	33	PRO	-	EXPRESSION TAG	UNP P31785
j	53	GLN	ASN	ENGINEERED MUTATION	UNP P31785

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	K	1	Total	C	N	O	0	0
			14	8	1	5		
4	K	1	Total	C	N	O	0	0
			14	8	1	5		
4	L	1	Total	C	N	O	0	0
			14	8	1	5		
4	L	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	L	1	Total	C	N	O	0	0
			14	8	1	5		
4	L	1	Total	C	N	O	0	0
			14	8	1	5		
4	N	1	Total	C	N	O	0	0
			14	8	1	5		
4	O	1	Total	C	N	O	0	0
			14	8	1	5		
4	O	1	Total	C	N	O	0	0
			14	8	1	5		
4	O	1	Total	C	N	O	0	0
			14	8	1	5		
4	O	1	Total	C	N	O	0	0
			14	8	1	5		
4	O	1	Total	C	N	O	0	0
			14	8	1	5		
4	Q	1	Total	C	N	O	0	0
			14	8	1	5		
4	R	1	Total	C	N	O	0	0
			14	8	1	5		
4	R	1	Total	C	N	O	0	0
			14	8	1	5		
4	R	1	Total	C	N	O	0	0
			14	8	1	5		
4	R	1	Total	C	N	O	0	0
			14	8	1	5		
4	R	1	Total	C	N	O	0	0
			14	8	1	5		
4	T	1	Total	C	N	O	0	0
			14	8	1	5		
4	U	1	Total	C	N	O	0	0
			14	8	1	5		
4	U	1	Total	C	N	O	0	0
			14	8	1	5		
4	W	1	Total	C	N	O	0	0
			14	8	1	5		
4	X	1	Total	C	N	O	0	0
			14	8	1	5		
4	X	1	Total	C	N	O	0	0
			14	8	1	5		
4	Z	1	Total	C	N	O	0	0
			14	8	1	5		

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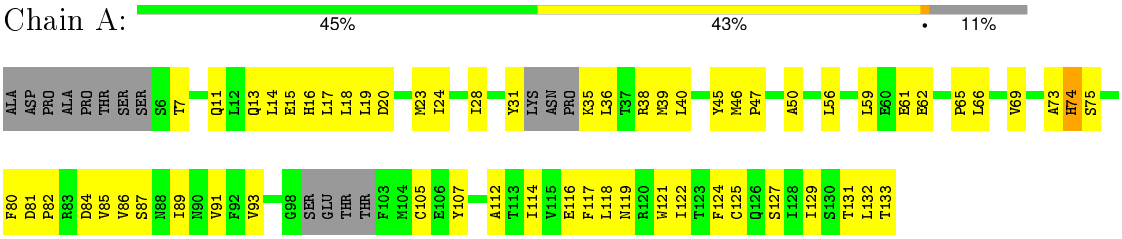
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	a	1	Total	C	N	O	0	0
			14	8	1	5		
4	a	1	Total	C	N	O	0	0
			14	8	1	5		
4	c	1	Total	C	N	O	0	0
			14	8	1	5		
4	c	1	Total	C	N	O	0	0
			14	8	1	5		
4	d	1	Total	C	N	O	0	0
			14	8	1	5		
4	f	1	Total	C	N	O	0	0
			14	8	1	5		
4	g	1	Total	C	N	O	0	0
			14	8	1	5		
4	g	1	Total	C	N	O	0	0
			14	8	1	5		
4	i	1	Total	C	N	O	0	0
			14	8	1	5		
4	i	1	Total	C	N	O	0	0
			14	8	1	5		
4	j	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots (i)

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

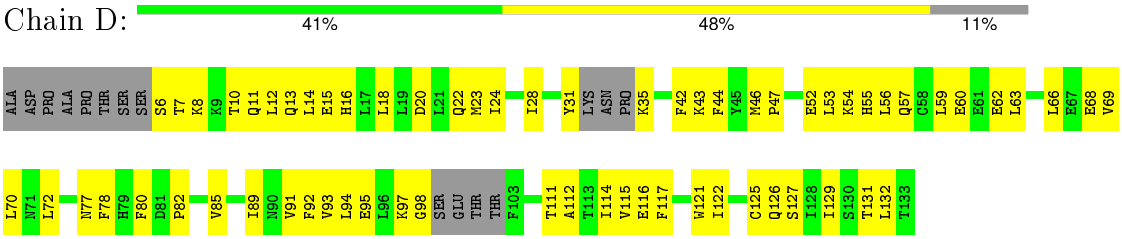
- Molecule 1: Interleukin-2

Chain A:



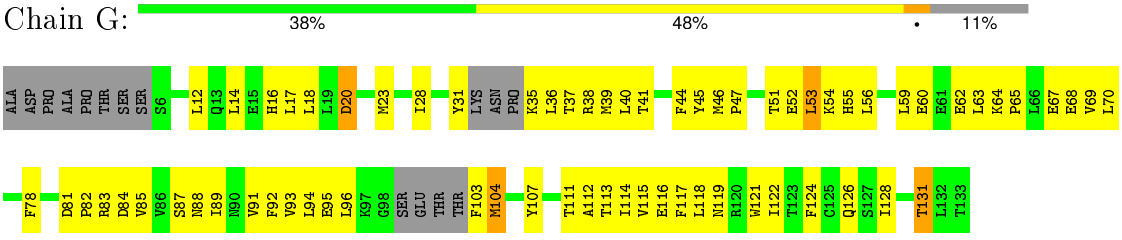
- Molecule 1: Interleukin-2

Chain D:



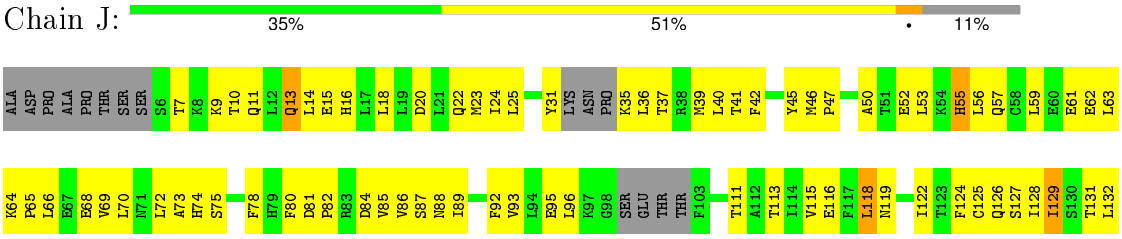
- Molecule 1: Interleukin-2

Chain G:



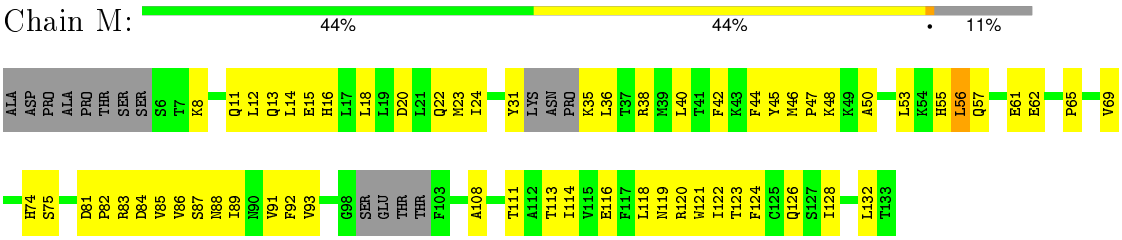
- Molecule 1: Interleukin-2

Chain J:



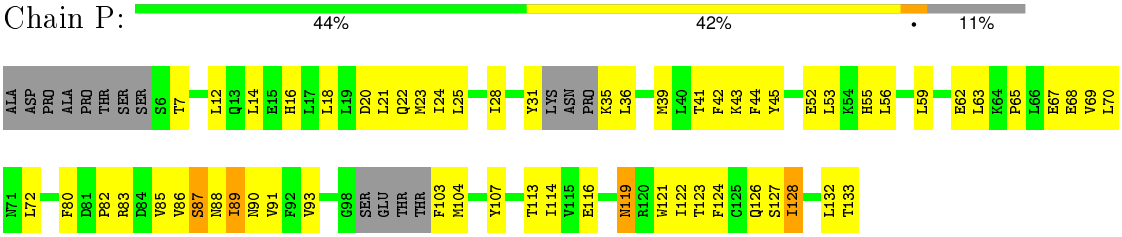
- Molecule 1: Interleukin-2

Chain M:



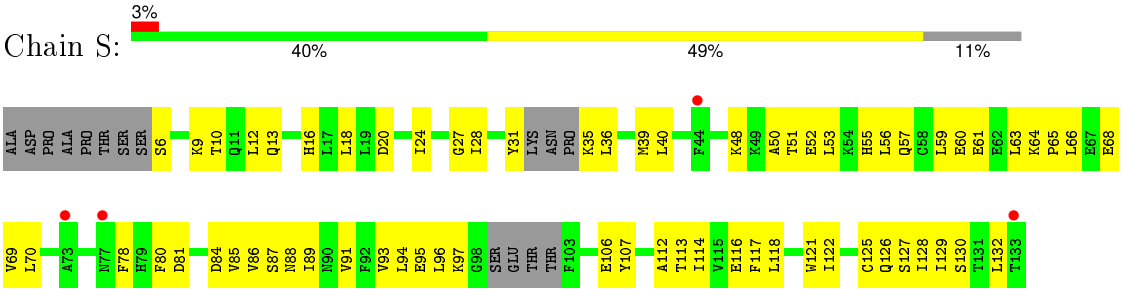
- Molecule 1: Interleukin-2

Chain P:



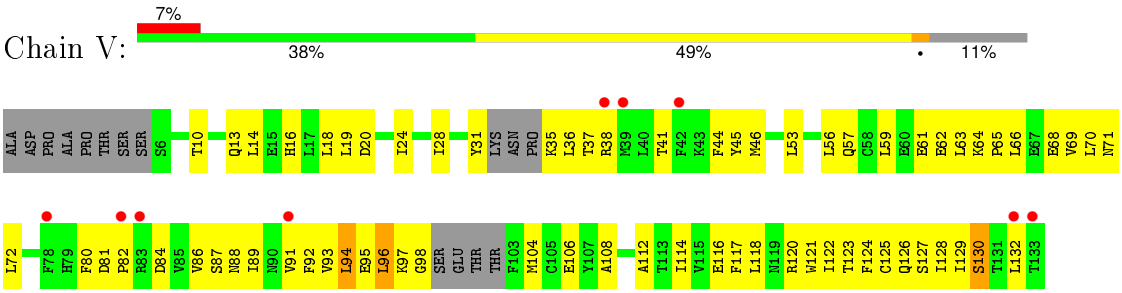
- Molecule 1: Interleukin-2

Chain S:



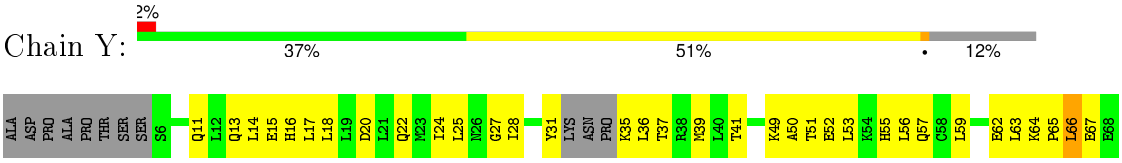
- Molecule 1: Interleukin-2

Chain V:



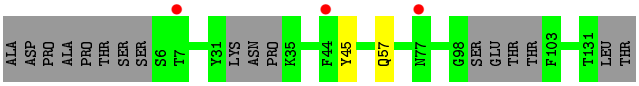
- Molecule 1: Interleukin-2

Chain Y:



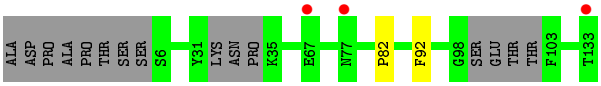
• Molecule 1: Interleukin-2

Chain b:



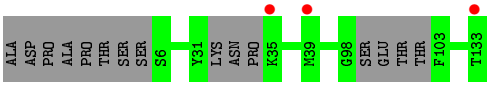
• Molecule 1: Interleukin-2

Chain e:



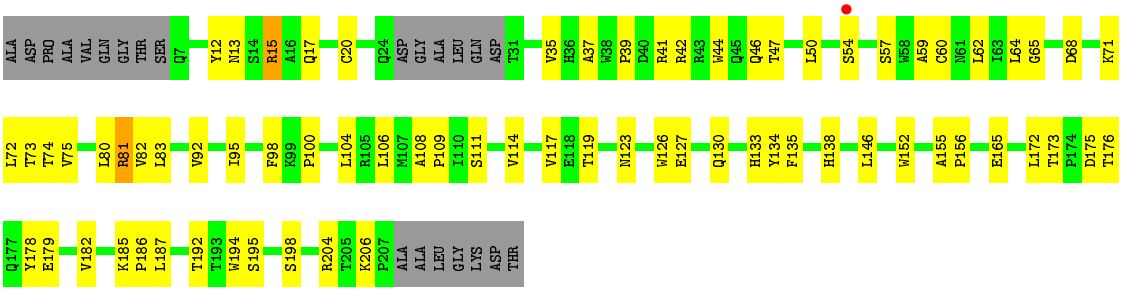
• Molecule 1: Interleukin-2

Chain h:



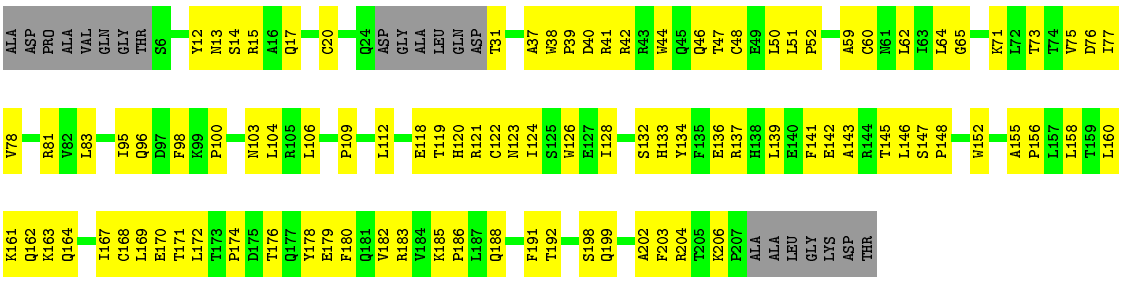
• Molecule 2: Interleukin-2 receptor subunit beta

Chain B:



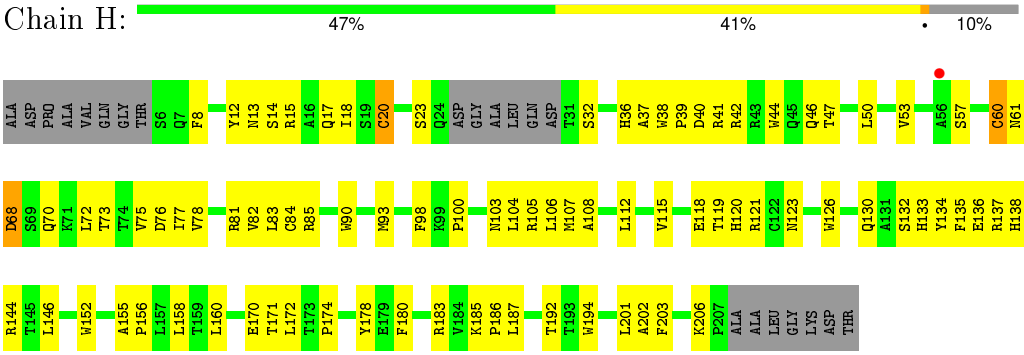
• Molecule 2: Interleukin-2 receptor subunit beta

Chain E:



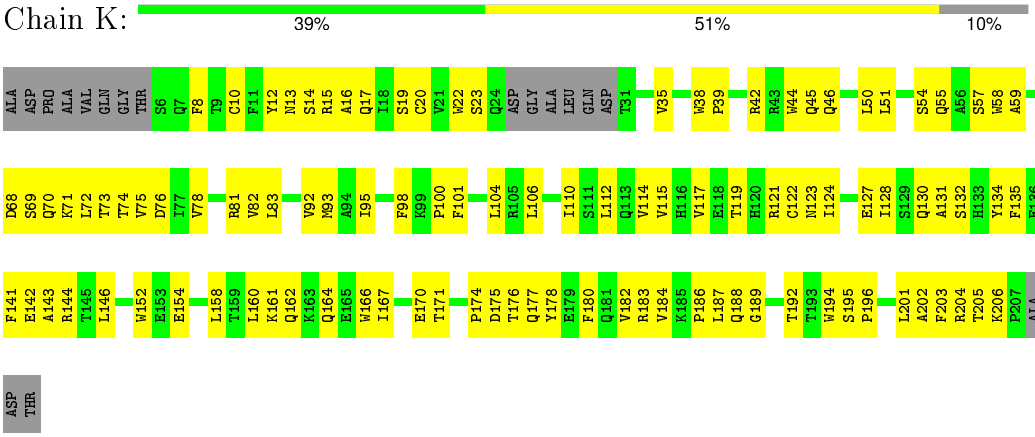
• Molecule 2: Interleukin-2 receptor subunit beta

Chain H:



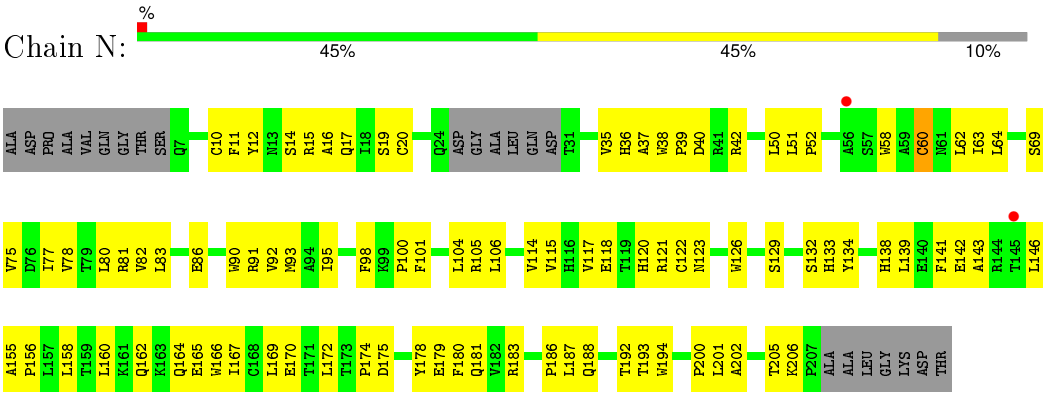
• Molecule 2: Interleukin-2 receptor subunit beta

Chain K:



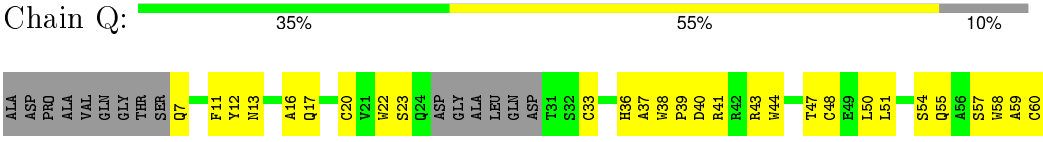
• Molecule 2: Interleukin-2 receptor subunit beta

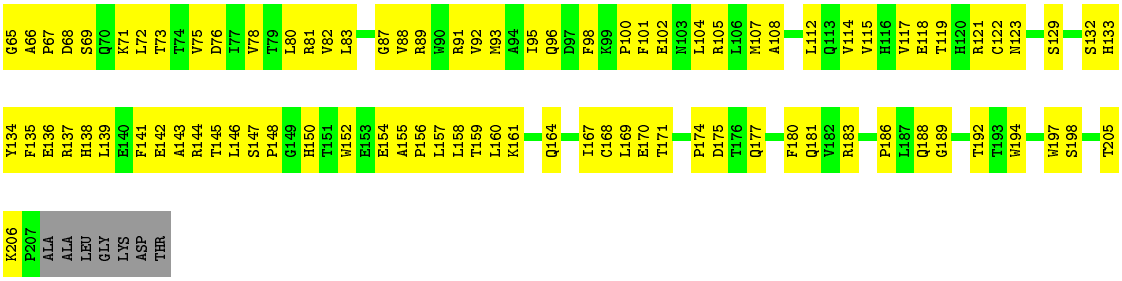
Chain N:



• Molecule 2: Interleukin-2 receptor subunit beta

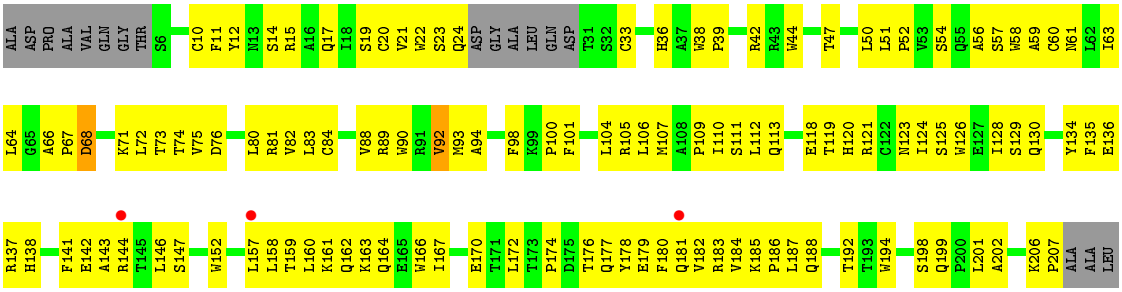
Chain Q:





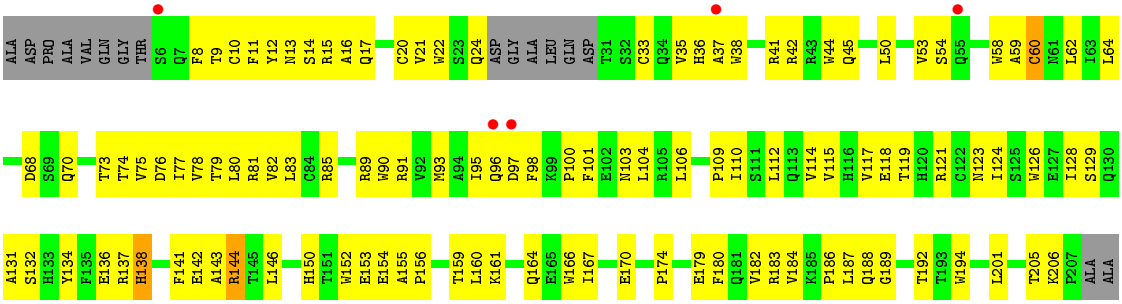
• Molecule 2: Interleukin-2 receptor subunit beta

Chain T:



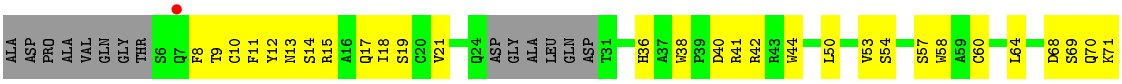
• Molecule 2: Interleukin-2 receptor subunit beta

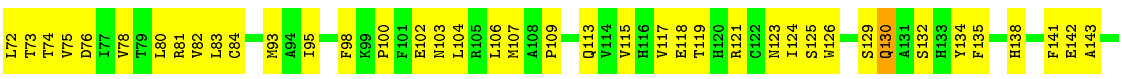
Chain W:

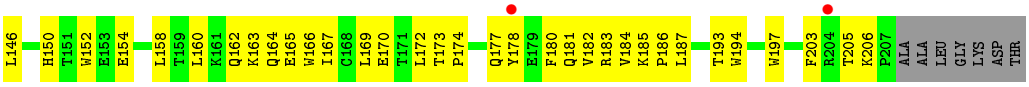


• Molecule 2: Interleukin-2 receptor subunit beta

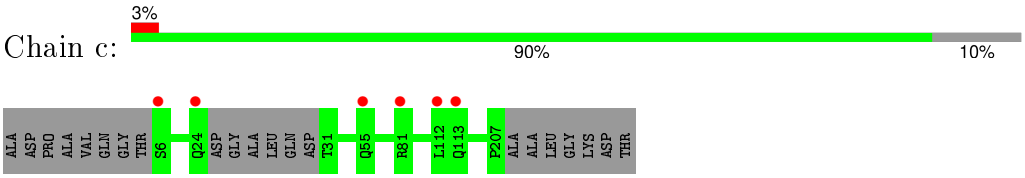
Chain Z:



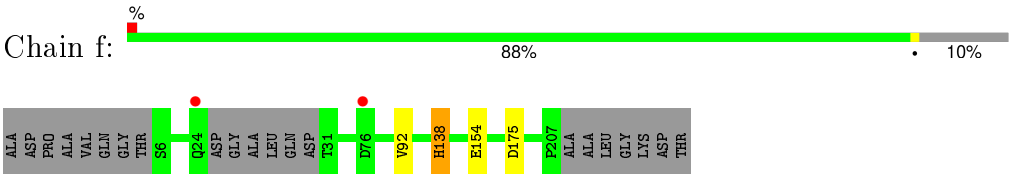




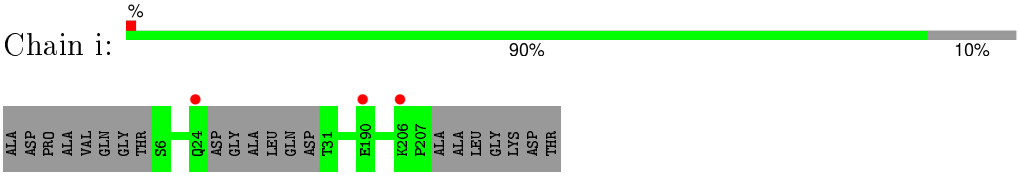
• Molecule 2: Interleukin-2 receptor subunit beta



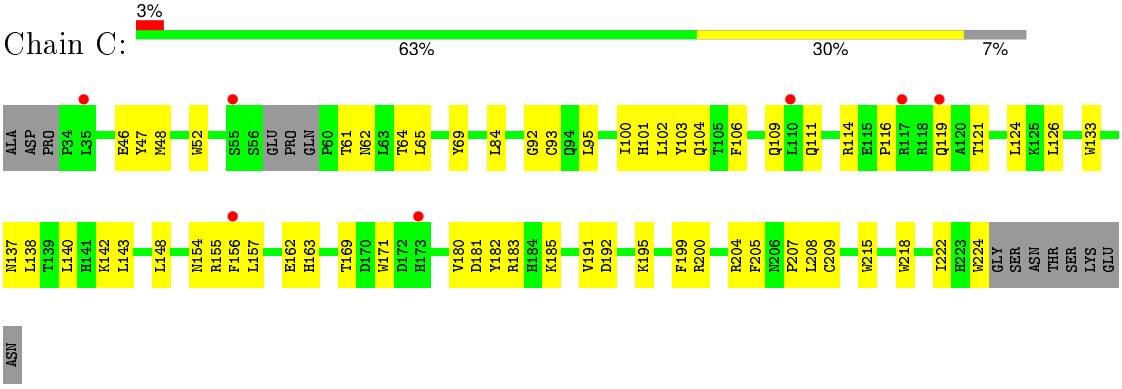
• Molecule 2: Interleukin-2 receptor subunit beta



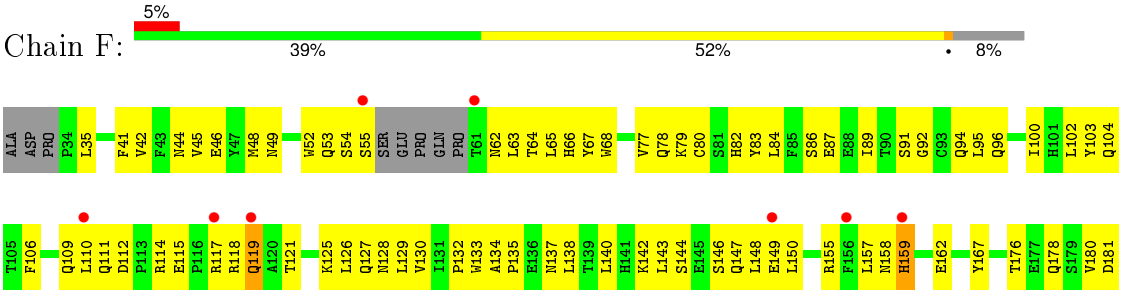
• Molecule 2: Interleukin-2 receptor subunit beta



• Molecule 3: Cytokine receptor common subunit gamma

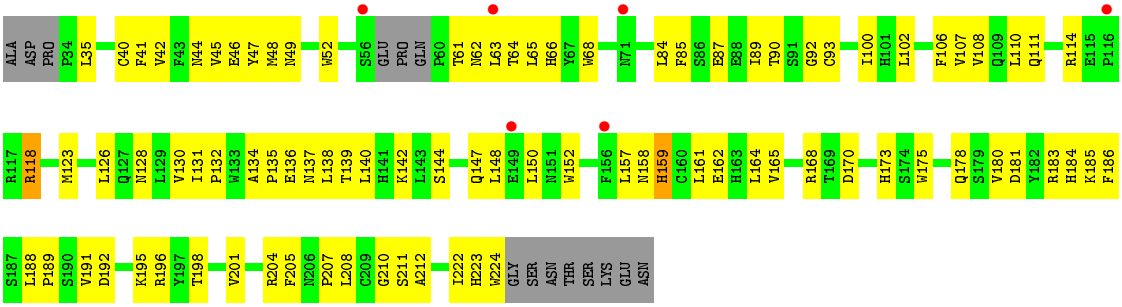


• Molecule 3: Cytokine receptor common subunit gamma



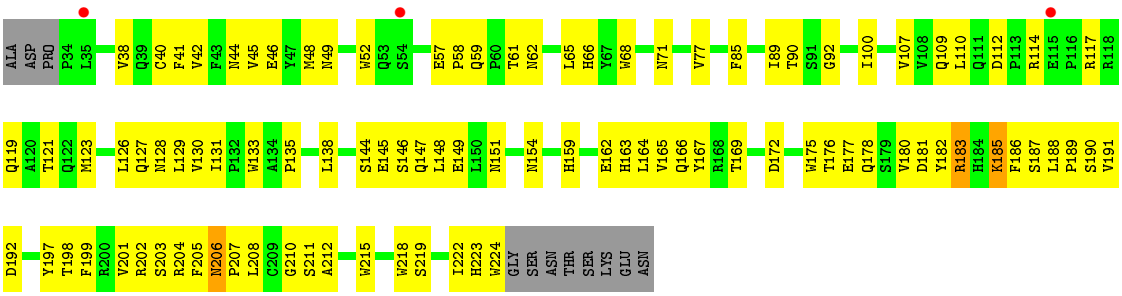
• Molecule 3: Cytokine receptor common subunit gamma

Chain I:



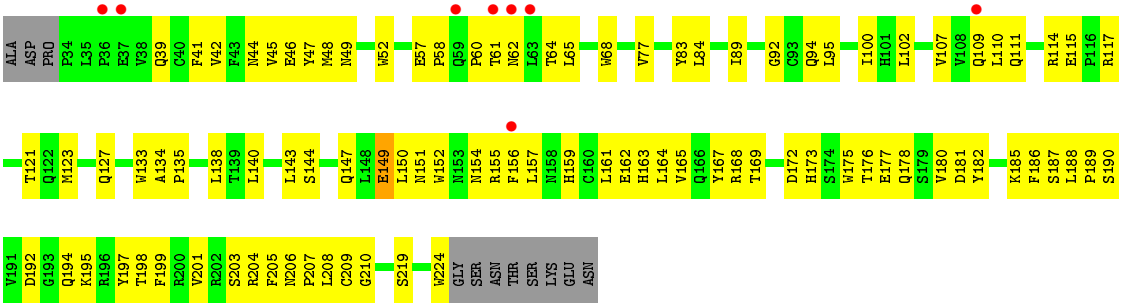
• Molecule 3: Cytokine receptor common subunit gamma

Chain L:



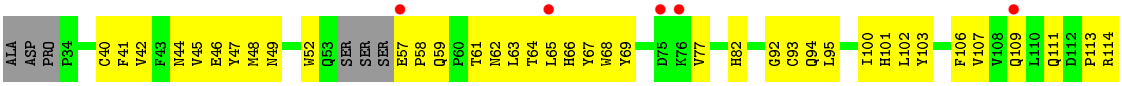
• Molecule 3: Cytokine receptor common subunit gamma

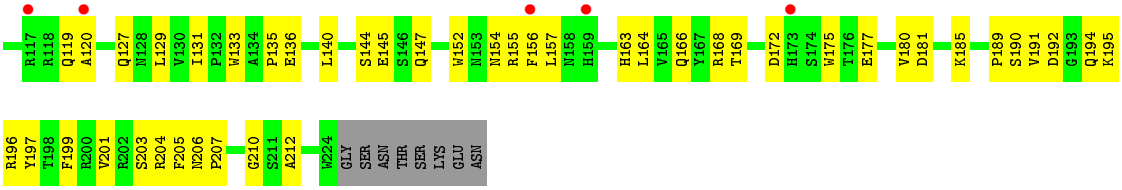
Chain O:



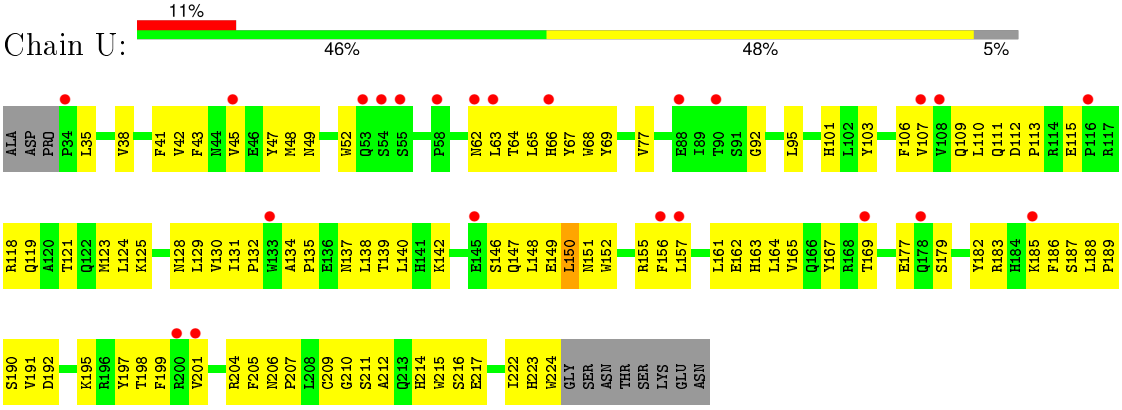
• Molecule 3: Cytokine receptor common subunit gamma

Chain R:

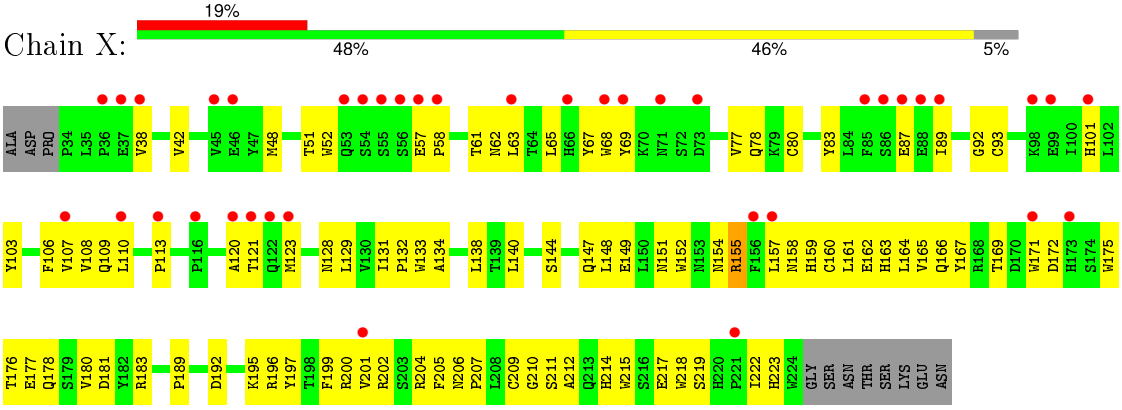




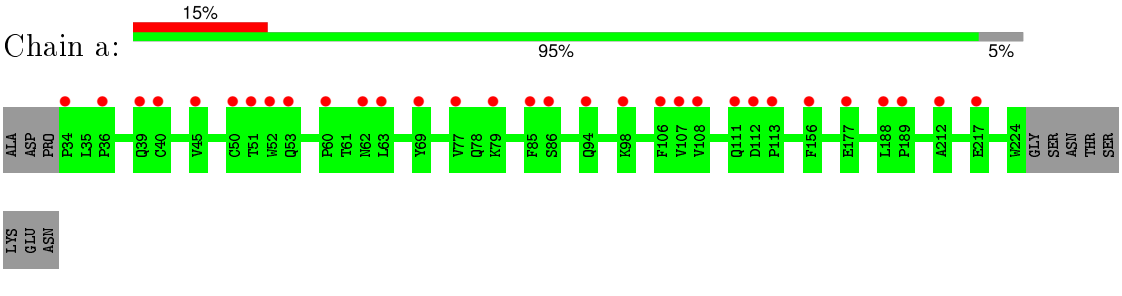
• Molecule 3: Cytokine receptor common subunit gamma



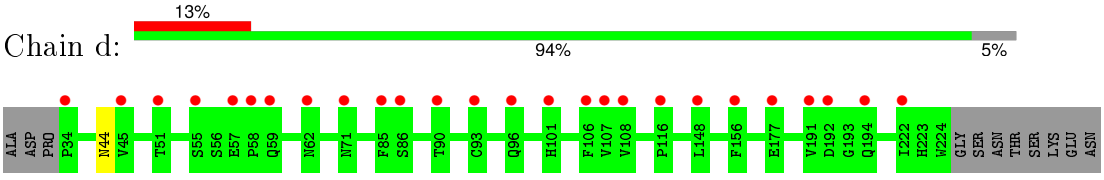
• Molecule 3: Cytokine receptor common subunit gamma



• Molecule 3: Cytokine receptor common subunit gamma

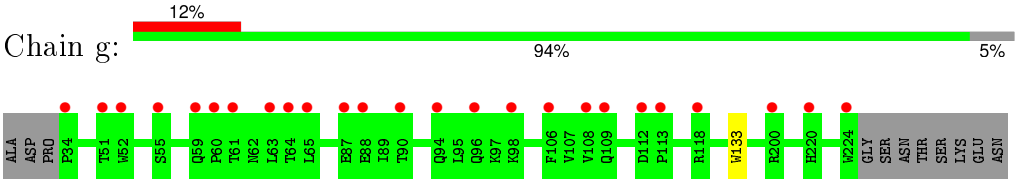


• Molecule 3: Cytokine receptor common subunit gamma



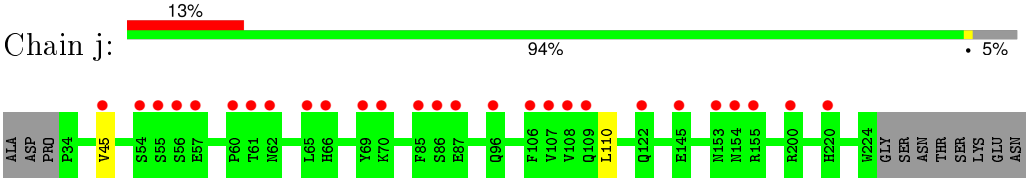
• Molecule 3: Cytokine receptor common subunit gamma

Chain g:



• Molecule 3: Cytokine receptor common subunit gamma

Chain j:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	118.23Å 118.10Å 236.12Å 99.86° 99.86° 99.74°	Depositor
Resolution (Å)	52.19 – 3.80 52.19 – 3.80	Depositor EDS
% Data completeness (in resolution range)	93.2 (52.19-3.80) 89.7 (52.19-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_621)	Depositor
R, R_{free}	0.291 , 0.344 0.299 , 0.356	Depositor DCC
R_{free} test set	1881 reflections (1.70%)	DCC
Wilson B-factor (Å^2)	82.1	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 83.9	EDS
Estimated twinning fraction	0.036 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 112706 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	51562	wwPDB-VP
Average B, all atoms (Å^2)	99.0	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 73.68 % 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 1.7576e-06.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.33	0/1015	0.52	0/1367
1	D	0.36	0/1015	0.57	0/1367
1	G	0.36	0/1015	0.53	0/1367
1	J	0.36	0/1015	0.56	0/1367
1	M	0.31	0/1015	0.51	0/1367
1	P	0.36	0/1015	0.53	0/1367
1	S	0.32	0/1015	0.51	0/1367
1	V	0.38	0/1015	0.60	1/1367 (0.1%)
1	Y	0.34	0/1008	0.53	0/1357
1	b	0.38	0/1000	0.57	0/1346
1	e	0.45	0/1015	0.65	0/1367
1	h	0.34	0/1015	0.53	0/1367
2	B	0.35	0/1660	0.55	0/2264
2	E	0.34	0/1666	0.57	0/2272
2	H	0.34	0/1666	0.54	0/2272
2	K	0.38	0/1666	0.60	0/2272
2	N	0.32	0/1660	0.54	0/2264
2	Q	0.37	0/1660	0.57	0/2264
2	T	0.33	0/1666	0.54	0/2272
2	W	0.36	0/1666	0.57	0/2272
2	Z	0.34	0/1666	0.56	0/2272
2	c	0.35	0/1666	0.53	0/2272
2	f	0.37	0/1666	0.56	0/2272
2	i	0.33	0/1666	0.54	0/2272
3	C	0.34	0/1658	0.53	0/2254
3	F	0.34	0/1644	0.59	0/2235
3	I	0.31	0/1658	0.53	0/2254
3	L	0.39	0/1685	0.62	1/2294 (0.0%)
3	O	0.32	0/1685	0.55	0/2294
3	R	0.31	0/1666	0.53	0/2267
3	U	0.26	0/1685	0.47	0/2294
3	X	0.26	0/1685	0.47	0/2294

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
3	a	0.27	0/1685	0.47	0/2294
3	d	0.26	0/1685	0.47	0/2294
3	g	0.26	0/1685	0.48	0/2294
3	j	0.29	0/1685	0.49	0/2294
All	All	0.34	0/52238	0.54	2/70975 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	208	LEU	CB-CG-CD2	-6.00	100.79	111.00
1	V	96	LEU	CA-CB-CG	-5.37	102.95	115.30

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	998	0	1015	60	0
1	D	998	0	1015	98	0
1	G	998	0	1015	70	0
1	J	998	0	1015	79	0
1	M	998	0	1015	58	0
1	P	998	0	1015	63	1
1	S	998	0	1015	69	0
1	V	998	0	1015	92	0
1	Y	991	0	1008	70	0
1	b	983	0	997	0	2
1	e	998	0	1015	0	0
1	h	998	0	1015	0	0
2	B	1612	0	1565	60	0
2	E	1618	0	1570	123	1
2	H	1618	0	1570	101	0
2	K	1618	0	1570	146	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	1612	0	1565	112	0
2	Q	1612	0	1565	113	1
2	T	1618	0	1570	156	0
2	W	1618	0	1570	155	0
2	Z	1618	0	1570	108	0
2	c	1618	0	1570	0	0
2	f	1618	0	1570	0	1
2	i	1618	0	1570	0	0
3	C	1605	0	1512	52	0
3	F	1592	0	1499	147	0
3	I	1605	0	1512	88	2
3	L	1630	0	1533	106	0
3	O	1630	0	1533	103	0
3	R	1612	0	1517	76	0
3	U	1630	0	1533	103	0
3	X	1630	0	1533	101	0
3	a	1630	0	1533	0	0
3	d	1630	0	1533	0	0
3	g	1630	0	1533	0	0
3	j	1630	0	1533	0	0
4	B	14	0	13	3	0
4	C	70	0	65	11	0
4	E	14	0	13	6	0
4	F	70	0	65	10	0
4	H	14	0	13	5	0
4	I	70	0	65	4	0
4	K	28	0	26	7	0
4	L	56	0	52	6	0
4	N	14	0	13	5	0
4	O	70	0	65	9	0
4	Q	14	0	13	4	0
4	R	70	0	65	6	0
4	T	14	0	13	5	0
4	U	28	0	26	7	0
4	W	14	0	13	5	0
4	X	28	0	26	6	0
4	Z	14	0	13	3	0
4	a	28	0	26	0	0
4	c	28	0	26	0	0
4	d	14	0	13	0	0
4	f	14	0	13	0	0
4	g	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	i	28	0	26	0	0
4	j	14	0	13	0	0
All	All	51562	0	49986	2335	4

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 33.

All (2335) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:15:GLU:HG2	1:J:129:ILE:HD11	1.25	1.16
2:W:15:ARG:NE	2:W:131:ALA:O	1.79	1.15
3:F:206:ASN:OD1	3:F:210:GLY:O	1.70	1.10
2:W:110:ILE:HG12	2:W:129:SER:HB2	1.36	1.07
2:T:123:ASN:HD21	4:T:215:NAG:C1	1.72	1.03
1:V:81:ASP:HB3	1:V:84:ASP:HB2	1.41	1.02
2:K:54:SER:HB3	2:K:57:SER:HB2	1.42	1.01
2:Q:115:VAL:HG11	4:Q:215:NAG:H62	1.42	1.00
3:I:204:ARG:N	3:O:114:ARG:O	88.94	1.00
1:D:42:PHE:HE1	1:D:72:LEU:HD11	1.24	0.99
1:J:53:LEU:HD11	1:J:96:LEU:HB3	1.46	0.97
2:Z:138:HIS:HB3	2:Z:187:LEU:HD12	1.46	0.97
2:E:162:GLN:NE2	3:F:187:SER:H	1.61	0.96
1:M:31:TYR:HH	1:M:35:LYS:N	1.62	0.96
3:R:52:TRP:CZ3	3:R:92:GLY:HA2	2.01	0.96
2:Z:15:ARG:HD2	2:Z:130:GLN:HB3	1.48	0.96
3:O:57:GLU:HG2	3:O:58:PRO:HD2	1.45	0.95
1:Y:89:ILE:O	1:Y:93:VAL:HG23	1.65	0.95
2:B:114:VAL:HG11	2:B:117:VAL:HG23	1.47	0.95
2:Z:98:PHE:HE2	2:Z:100:PRO:HA	1.32	0.95
2:Z:13:ASN:ND2	2:Z:17:GLN:HB2	1.82	0.94
3:L:52:TRP:CZ3	3:L:92:GLY:HA2	2.03	0.94
1:J:16:HIS:CE1	2:K:134:TYR:HB3	2.02	0.94
2:T:109:PRO:HG3	2:T:184:VAL:HG23	1.48	0.94
2:K:123:ASN:HD21	4:K:215:NAG:C1	1.79	0.93
3:X:164:LEU:HD11	3:X:177:GLU:HB2	1.51	0.93
1:Y:81:ASP:HB3	1:Y:84:ASP:HB2	1.51	0.93
1:D:42:PHE:CE1	1:D:72:LEU:HD11	2.04	0.93
2:E:81:ARG:HG2	2:E:95:ILE:HG22	1.51	0.93
2:K:138:HIS:C	2:K:187:LEU:HG	1.89	0.92
3:O:169:THR:H	3:O:172:ASP:HB2	1.31	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:119:THR:HB	2:W:174:PRO:HG3	1.52	0.91
3:L:188:LEU:HD22	3:L:199:PHE:HE2	1.37	0.90
3:F:52:TRP:CZ3	3:F:92:GLY:HA2	2.07	0.90
3:F:62:ASN:HD21	4:F:300:NAG:C1	1.85	0.89
2:N:123:ASN:HD21	4:N:215:NAG:C1	1.85	0.89
2:Z:106:LEU:HD11	2:Z:186:PRO:HG3	1.54	0.89
1:S:89:ILE:O	1:S:93:VAL:HG23	1.73	0.89
2:W:110:ILE:CG1	2:W:129:SER:HB2	2.02	0.89
2:W:123:ASN:HD21	4:W:215:NAG:C1	1.86	0.88
3:I:107:VAL:HG22	3:I:123:MET:HG2	1.55	0.88
2:E:83:LEU:HD11	2:T:38:TRP:HH2	1.38	0.88
3:F:206:ASN:OD1	3:F:211:SER:HA	1.73	0.88
3:L:169:THR:H	3:L:172:ASP:HB2	1.39	0.88
2:K:146:LEU:HB2	2:K:152:TRP:CH2	2.09	0.88
3:F:137:ASN:ND2	4:F:400:NAG:C1	2.38	0.87
2:E:65:GLY:HA3	2:E:71:LYS:HE3	1.57	0.86
2:T:66:ALA:HB1	2:T:67:PRO:HD2	1.58	0.86
3:L:144:SER:HB3	3:L:147:GLN:HB2	1.57	0.86
1:J:125:CYS:O	1:J:129:ILE:HG22	1.75	0.86
3:L:62:ASN:HD21	4:L:300:NAG:C1	1.88	0.86
1:D:60:GLU:HA	1:D:63:LEU:HD12	1.58	0.86
1:J:15:GLU:HG2	1:J:129:ILE:CD1	2.07	0.85
3:F:137:ASN:ND2	4:F:400:NAG:O5	2.10	0.85
2:H:123:ASN:HD21	4:H:215:NAG:C1	1.89	0.85
2:Z:167:ILE:HG21	2:Z:180:PHE:CZ	2.12	0.84
3:F:137:ASN:HD21	4:F:400:NAG:C1	1.90	0.84
2:Z:98:PHE:CE2	2:Z:100:PRO:HA	2.11	0.84
3:I:62:ASN:HD21	4:I:300:NAG:C1	1.89	0.84
2:W:36:HIS:HD1	2:W:38:TRP:HE1	1.24	0.84
3:X:52:TRP:HZ3	3:X:65:LEU:HD12	1.43	0.84
2:K:146:LEU:HD13	2:K:152:TRP:CD2	2.11	0.84
2:W:98:PHE:CE2	2:W:100:PRO:HA	2.11	0.84
3:O:84:LEU:HD21	4:O:234:NAG:H62	1.60	0.83
1:D:11:GLN:HA	1:D:14:LEU:HD12	1.59	0.83
3:F:206:ASN:OD1	3:F:207:PRO:HA	1.78	0.83
3:U:204:ARG:HD3	3:U:212:ALA:O	1.79	0.83
3:F:109:GLN:HG3	3:F:121:THR:HG22	1.61	0.83
3:R:62:ASN:HD21	4:R:300:NAG:C1	1.91	0.83
1:M:56:LEU:HB3	1:M:93:VAL:HG13	1.60	0.83
1:J:14:LEU:HD23	1:J:129:ILE:HB	1.58	0.83
3:X:38:VAL:HG22	3:X:52:TRP:HB3	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:ASN:HD21	4:C:300:NAG:C1	1.90	0.82
2:E:162:GLN:HE22	3:F:187:SER:N	1.75	0.82
2:Q:17:GLN:HG3	2:Q:63:ILE:HD13	1.60	0.82
2:E:162:GLN:HE22	3:F:187:SER:CA	1.92	0.82
2:Q:12:TYR:OH	2:Q:72:LEU:HB2	1.79	0.82
3:L:204:ARG:HD3	3:L:212:ALA:O	1.80	0.82
2:H:18:ILE:HB	2:H:62:LEU:HB2	1.60	0.82
1:P:31:TYR:HH	1:P:35:LYS:N	1.78	0.82
1:J:31:TYR:OH	1:J:35:LYS:HB3	1.80	0.81
3:C:137:ASN:HD21	4:C:400:NAG:C1	1.93	0.81
2:K:170:GLU:HB2	3:L:190:SER:HB3	1.62	0.81
2:N:175:ASP:H	2:N:205:THR:HB	1.44	0.81
2:K:81:ARG:CD	2:K:95:ILE:HG22	2.11	0.81
3:C:109:GLN:HG3	3:C:121:THR:HG22	1.63	0.81
1:S:81:ASP:HB3	1:S:84:ASP:HB2	1.63	0.81
3:I:181:ASP:OD2	3:I:183:ARG:HD3	1.81	0.81
2:B:35:VAL:HG22	2:B:82:VAL:HG22	1.63	0.80
2:T:158:LEU:HD22	3:U:189:PRO:HB2	1.63	0.80
2:E:162:GLN:NE2	3:F:187:SER:N	2.27	0.80
2:Q:95:ILE:HG12	2:Q:96:GLN:N	1.95	0.80
2:K:146:LEU:HD22	2:K:152:TRP:CE2	2.16	0.80
1:V:92:PHE:CZ	2:W:73:THR:HB	2.17	0.80
3:X:158:ASN:O	3:X:159:HIS:HB2	1.80	0.80
3:C:84:LEU:HD22	4:C:234:NAG:H62	1.62	0.80
2:K:15:ARG:HD2	2:K:68:ASP:O	1.81	0.79
1:V:120:ARG:O	1:V:123:THR:HB	1.82	0.79
1:V:66:LEU:CD1	1:V:114:ILE:HD11	2.13	0.79
3:L:188:LEU:HD22	3:L:199:PHE:CE2	2.18	0.79
1:V:63:LEU:HD11	1:V:86:VAL:HB	1.65	0.79
2:Z:119:THR:HB	2:Z:174:PRO:HG3	1.65	0.79
2:Z:12:TYR:CE2	2:Z:14:SER:HA	2.18	0.78
3:R:156:PHE:HD2	3:R:157:LEU:HG	1.48	0.78
2:N:50:LEU:HD22	2:N:58:TRP:HB3	1.65	0.78
1:D:69:VAL:HG11	1:D:114:ILE:HD12	1.66	0.78
2:E:162:GLN:CD	3:F:187:SER:H	1.85	0.78
3:U:107:VAL:HG22	3:U:123:MET:HG2	1.66	0.78
2:B:15:ARG:HG3	2:B:68:ASP:HA	1.64	0.78
1:Y:125:CYS:O	1:Y:129:ILE:HG13	1.83	0.78
1:V:68:GLU:O	1:V:72:LEU:HD23	1.84	0.77
3:X:132:PRO:HB3	3:X:161:LEU:HD21	1.66	0.77
2:W:110:ILE:CD1	2:W:129:SER:HB2	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:83:LEU:HD11	2:T:38:TRP:CH2	2.18	0.77
2:N:101:PHE:HA	2:N:104:LEU:HD21	1.65	0.77
3:R:156:PHE:CD2	3:R:157:LEU:HG	2.20	0.77
2:E:13:ASN:O	2:E:14:SER:HB3	1.84	0.77
3:X:165:VAL:HG22	3:X:201:VAL:HG22	1.63	0.77
3:U:148:LEU:HD21	3:U:191:VAL:HG11	1.66	0.77
2:K:167:ILE:HG21	2:K:180:PHE:CZ	2.20	0.77
1:D:31:TYR:OH	1:D:35:LYS:HB2	1.85	0.77
3:O:165:VAL:HG22	3:O:178:GLN:O	1.84	0.77
1:V:97:LYS:HG3	1:V:98:GLY:H	1.47	0.77
2:T:138:HIS:CE1	3:U:182:TYR:CE2	2.73	0.76
2:Z:185:LYS:HB2	2:Z:194:TRP:CE3	2.20	0.76
2:K:14:SER:HG	2:K:135:PHE:HE2	1.33	0.76
2:B:50:LEU:HD23	2:B:60:CYS:HB2	1.68	0.76
2:Q:44:TRP:HH2	2:Q:64:LEU:HD13	1.50	0.76
3:L:109:GLN:HG3	3:L:121:THR:HG22	1.66	0.76
3:O:52:TRP:CZ3	3:O:92:GLY:HA2	2.20	0.76
3:U:52:TRP:CZ3	3:U:92:GLY:HA2	2.20	0.76
2:H:50:LEU:HD23	2:H:60:CYS:HB2	1.68	0.76
3:R:163:HIS:ND1	3:R:203:SER:HB3	2.00	0.76
1:V:124:PHE:O	1:V:128:ILE:HG12	1.86	0.76
1:D:31:TYR:OH	1:D:35:LYS:HE3	1.86	0.75
2:T:119:THR:HB	2:T:174:PRO:HG3	1.67	0.75
2:T:50:LEU:HD22	2:T:58:TRP:HB3	1.68	0.75
2:Z:73:THR:HG22	2:Z:76:ASP:OD1	1.85	0.75
3:F:183:ARG:HD3	3:F:185:LYS:HE2	1.67	0.75
2:B:13:ASN:ND2	2:B:17:GLN:HB3	2.00	0.75
2:Z:82:VAL:O	2:Z:83:LEU:HD23	1.87	0.75
1:M:16:HIS:HD1	2:N:134:TYR:HB3	1.51	0.75
1:J:66:LEU:O	1:J:70:LEU:HD12	1.86	0.75
3:F:204:ARG:HH21	3:F:213:GLN:HA	1.50	0.75
2:W:115:VAL:HB	2:W:123:ASN:HD22	1.52	0.75
2:E:164:GLN:HE21	3:F:178:GLN:HG2	1.52	0.75
2:Z:143:ALA:HB3	2:Z:158:LEU:HB2	1.69	0.74
2:W:161:LYS:O	3:X:183:ARG:NH2	2.19	0.74
1:J:9:LYS:O	1:J:13:GLN:HG3	1.86	0.74
2:K:139:LEU:O	2:K:187:LEU:HD21	1.88	0.74
2:K:138:HIS:O	2:K:187:LEU:HG	1.85	0.74
2:N:118:GLU:O	2:N:205:THR:HG23	1.88	0.74
2:K:137:ARG:O	3:L:181:ASP:HB3	1.87	0.74
3:C:207:PRO:CG	3:F:117:ARG:HH21	32.33	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:69:VAL:O	1:V:72:LEU:HB2	1.87	0.74
3:X:197:TYR:O	3:X:223:HIS:HA	1.88	0.74
1:D:24:ILE:HA	1:D:80:PHE:HE2	1.53	0.74
2:K:146:LEU:HD22	2:K:152:TRP:CZ2	2.22	0.74
3:R:154:ASN:HD21	3:R:163:HIS:HE1	1.33	0.74
1:D:16:HIS:HB3	2:E:134:TYR:CD2	2.22	0.74
3:U:52:TRP:HZ3	3:U:65:LEU:HD12	1.53	0.74
1:D:11:GLN:HG3	1:D:129:ILE:HG23	1.70	0.73
1:J:63:LEU:CD2	1:J:66:LEU:HD23	2.18	0.73
3:F:68:TRP:HH2	3:F:109:GLN:NE2	1.85	0.73
2:K:143:ALA:HB1	2:K:180:PHE:CE1	2.23	0.73
1:J:88:ASN:ND2	2:K:42:ARG:HH22	1.85	0.73
1:A:74:HIS:CG	1:A:75:SER:H	2.05	0.73
1:P:44:PHE:CZ	1:P:69:VAL:HG21	2.22	0.73
1:V:28:ILE:O	1:V:36:LEU:HD11	1.87	0.73
2:E:137:ARG:HB3	3:F:181:ASP:HB3	1.70	0.73
2:E:119:THR:HB	2:E:174:PRO:HG3	1.69	0.73
1:D:18:LEU:HD11	1:D:122:ILE:HG23	1.71	0.73
2:W:82:VAL:HB	2:W:93:MET:HB2	1.71	0.73
2:N:123:ASN:ND2	4:N:215:NAG:C1	2.51	0.73
2:K:121:ARG:HG2	2:K:170:GLU:OE1	1.88	0.73
2:T:172:LEU:HD22	2:T:178:TYR:CZ	2.23	0.73
2:N:69:SER:HB2	2:N:71:LYS:HE2	1.68	0.73
3:I:181:ASP:OD1	3:I:183:ARG:HD2	1.89	0.73
2:Q:144:ARG:HH11	2:Q:152:TRP:HB3	1.52	0.73
2:W:13:ASN:HD21	2:W:16:ALA:H	1.34	0.73
2:T:109:PRO:HG3	2:T:184:VAL:CG2	2.18	0.73
2:K:138:HIS:CA	2:K:187:LEU:HD12	2.19	0.73
3:O:135:PRO:HG2	3:O:201:VAL:HG12	1.70	0.73
3:U:192:ASP:OD2	3:U:195:LYS:HE3	1.88	0.73
3:C:84:LEU:CD2	4:C:234:NAG:H62	2.19	0.73
2:Q:115:VAL:CG1	4:Q:215:NAG:H62	2.18	0.72
3:X:181:ASP:OD1	3:X:183:ARG:NH1	2.22	0.72
1:D:125:CYS:O	1:D:129:ILE:HG13	1.89	0.72
3:F:204:ARG:HG3	3:F:214:HIS:O	1.89	0.72
1:M:16:HIS:ND1	2:N:134:TYR:HB3	2.04	0.72
1:Y:16:HIS:CE1	2:Z:134:TYR:HB3	2.24	0.72
3:C:207:PRO:HG2	3:F:117:ARG:HH21	32.69	0.72
3:F:52:TRP:NE1	3:F:63:LEU:HD12	2.05	0.72
2:B:114:VAL:CG1	2:B:117:VAL:HG23	2.20	0.72
1:V:95:GLU:HG3	2:W:41:ARG:HH12	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:104:LEU:O	2:K:192:THR:HG23	1.89	0.72
1:G:45:TYR:CE1	1:G:111:THR:HG22	2.24	0.72
2:W:109:PRO:HG3	2:W:184:VAL:HG23	1.69	0.72
2:E:128:ILE:O	2:E:128:ILE:HD12	1.89	0.72
3:I:138:LEU:HD12	3:I:138:LEU:H	1.54	0.71
2:Q:174:PRO:HA	2:Q:205:THR:HG21	1.72	0.71
1:M:35:LYS:HD2	1:M:38:ARG:HH21	1.54	0.71
3:F:52:TRP:HE1	3:F:63:LEU:HD12	1.55	0.71
1:G:31:TYR:HH	1:G:35:LYS:N	1.87	0.71
3:O:62:ASN:ND2	4:O:300:NAG:H83	2.05	0.71
3:U:147:GLN:HG2	3:U:189:PRO:O	1.90	0.71
1:D:11:GLN:HB2	1:D:132:LEU:HD22	1.70	0.71
2:B:123:ASN:HD21	4:B:215:NAG:C1	2.02	0.71
3:R:154:ASN:HD21	3:R:163:HIS:CE1	2.09	0.71
2:K:161:LYS:HZ3	3:L:185:LYS:HD3	1.56	0.71
3:R:48:MET:HB2	3:R:100:ILE:HD11	1.72	0.71
2:T:183:ARG:HD2	2:T:194:TRP:HB3	1.71	0.71
3:X:140:LEU:HG	3:X:222:ILE:HD11	1.73	0.71
1:M:62:GLU:O	1:M:65:PRO:HG2	1.91	0.70
2:W:189:GLY:HA3	2:W:192:THR:OG1	1.91	0.70
2:T:138:HIS:CE1	3:U:182:TYR:CD2	2.79	0.70
3:I:47:TYR:HE1	3:I:49:ASN:HD21	1.38	0.70
1:P:56:LEU:HB3	1:P:93:VAL:HG13	1.73	0.70
1:G:37:THR:O	1:G:41:THR:HG23	1.91	0.70
3:U:164:LEU:HD11	3:U:177:GLU:HB2	1.72	0.70
3:F:62:ASN:CG	4:F:300:NAG:H83	2.11	0.70
2:W:110:ILE:HG12	2:W:129:SER:CB	2.19	0.70
3:O:42:VAL:HG22	3:O:100:ILE:HD13	1.73	0.70
1:G:44:PHE:HE2	1:G:114:ILE:HB	1.56	0.70
1:D:7:THR:HG22	1:D:132:LEU:HD11	1.72	0.70
3:I:168:ARG:HG2	3:I:175:TRP:CZ3	2.26	0.70
2:E:112:LEU:HG	2:E:126:TRP:HB3	1.74	0.70
3:U:188:LEU:HD11	3:U:199:PHE:HE1	1.55	0.70
1:D:66:LEU:O	1:D:70:LEU:HD12	1.92	0.70
3:O:154:ASN:HD21	3:O:163:HIS:CE1	2.09	0.70
2:W:78:VAL:HG23	2:W:100:PRO:HG3	1.72	0.70
1:J:126:GLN:OE1	3:L:210:GLY:HA2	1.92	0.70
2:Q:160:LEU:HD13	2:Q:164:GLN:HB3	1.72	0.70
2:Q:33:CYS:HB3	2:Q:50:LEU:HD12	1.74	0.70
1:Y:128:ILE:O	1:Y:132:LEU:HG	1.91	0.69
2:T:98:PHE:CE2	2:T:100:PRO:HA	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:146:LEU:HD23	2:T:179:GLU:HB2	1.74	0.69
2:Z:123:ASN:HD21	4:Z:215:NAG:C1	2.05	0.69
2:W:12:TYR:CE2	2:W:14:SER:HA	2.27	0.69
3:U:62:ASN:ND2	4:U:300:NAG:H83	2.07	0.69
3:X:68:TRP:HB3	3:X:77:VAL:HA	1.74	0.69
2:Q:44:TRP:CH2	2:Q:64:LEU:HD13	2.26	0.69
3:U:68:TRP:HE3	3:U:77:VAL:HG13	1.57	0.69
3:L:57:GLU:CG	3:L:58:PRO:HD2	2.21	0.69
2:N:12:TYR:CE2	2:N:14:SER:HA	2.28	0.69
2:W:13:ASN:O	2:W:14:SER:OG	2.09	0.69
1:D:122:ILE:O	1:D:126:GLN:HG3	1.93	0.69
3:U:161:LEU:HD23	3:U:205:PHE:HA	1.74	0.69
1:V:69:VAL:HA	1:V:72:LEU:HD23	1.74	0.69
3:O:107:VAL:HG22	3:O:123:MET:HG2	1.73	0.69
2:T:159:THR:HG21	2:T:161:LYS:HE3	1.75	0.69
3:R:57:GLU:HB3	3:R:58:PRO:HD2	1.75	0.69
1:M:122:ILE:O	1:M:126:GLN:HG3	1.93	0.69
2:Z:104:LEU:HD22	2:Z:135:PHE:HZ	1.58	0.69
2:W:35:VAL:HG23	2:W:50:LEU:HD11	1.73	0.69
1:S:125:CYS:O	1:S:129:ILE:HG13	1.93	0.69
1:M:16:HIS:HD1	2:N:134:TYR:HD2	1.42	0.68
2:Q:146:LEU:HD22	2:Q:152:TRP:CE2	2.28	0.68
1:V:16:HIS:CE1	2:W:134:TYR:HB3	2.28	0.68
3:F:188:LEU:HD21	3:F:191:VAL:HG12	1.74	0.68
2:Q:17:GLN:CG	2:Q:63:ILE:HD13	2.23	0.68
1:J:36:LEU:O	1:J:40:LEU:HG	1.92	0.68
3:O:109:GLN:HG3	3:O:121:THR:HG22	1.76	0.68
2:E:123:ASN:HD21	4:E:215:NAG:C1	2.06	0.68
1:G:122:ILE:O	1:G:126:GLN:HG3	1.94	0.68
2:N:143:ALA:HB1	2:N:180:PHE:CE1	2.28	0.68
1:D:95:GLU:CD	2:E:41:ARG:HH12	1.97	0.68
3:L:188:LEU:HD12	3:L:189:PRO:HD2	1.76	0.68
1:A:16:HIS:CE1	2:B:134:TYR:HB3	2.29	0.68
3:X:154:ASN:HD21	3:X:163:HIS:CE1	2.10	0.68
2:T:82:VAL:HG13	2:T:93:MET:HB2	1.75	0.68
3:X:128:ASN:O	3:X:129:LEU:HD23	1.94	0.68
1:M:87:SER:O	1:M:91:VAL:HG23	1.94	0.68
3:F:45:VAL:HG12	3:F:45:VAL:O	1.93	0.68
1:S:127:SER:HA	3:U:103:TYR:CD1	2.29	0.68
2:T:136:GLU:OE2	3:U:207:PRO:HG3	1.93	0.68
3:U:128:ASN:O	3:U:212:ALA:HA	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:138:HIS:HB3	2:K:187:LEU:HD12	1.74	0.67
3:O:169:THR:N	3:O:172:ASP:HB2	2.07	0.67
2:T:36:HIS:CD2	2:T:47:THR:HG22	2.28	0.67
3:O:57:GLU:HG2	3:O:58:PRO:CD	2.23	0.67
1:J:45:TYR:HE1	1:J:111:THR:HG22	1.58	0.67
1:V:31:TYR:HH	1:V:35:LYS:N	1.92	0.67
2:W:76:ASP:O	2:W:100:PRO:HD2	1.93	0.67
2:Z:123:ASN:ND2	4:Z:215:NAG:C1	2.58	0.67
2:N:17:GLN:HG2	2:N:63:ILE:HD13	1.76	0.67
1:G:112:ALA:HB1	1:G:116:GLU:HB2	1.77	0.67
2:W:119:THR:HG22	2:W:206:LYS:O	1.93	0.67
2:Q:98:PHE:CE2	2:Q:100:PRO:HA	2.29	0.67
1:V:95:GLU:CG	2:W:41:ARG:HH12	2.08	0.67
1:P:52:GLU:O	1:P:55:HIS:HB2	1.95	0.67
2:Q:117:VAL:HG12	2:Q:122:CYS:SG	2.35	0.67
2:K:115:VAL:HG11	4:K:215:NAG:H62	1.76	0.67
1:S:59:LEU:HD13	1:S:121:TRP:CD1	2.28	0.67
1:J:124:PHE:O	1:J:127:SER:HB3	1.95	0.67
3:R:206:ASN:OD1	3:R:207:PRO:HA	1.95	0.67
2:T:142:GLU:OE1	2:T:183:ARG:NH2	2.28	0.67
3:U:135:PRO:HG2	3:U:201:VAL:O	1.94	0.67
2:B:73:THR:HG22	2:B:74:THR:N	2.10	0.67
1:D:62:GLU:HG3	1:D:117:PHE:HE1	1.60	0.67
3:F:48:MET:CB	3:F:100:ILE:HD11	2.25	0.66
3:X:154:ASN:HD21	3:X:163:HIS:HE1	1.41	0.66
3:L:206:ASN:HB3	3:L:212:ALA:H	1.60	0.66
2:Q:104:LEU:O	2:Q:192:THR:HG23	1.96	0.66
1:D:10:THR:O	1:D:14:LEU:HD12	1.94	0.66
2:B:68:ASP:OD1	2:B:130:GLN:HG2	1.95	0.66
3:F:102:LEU:HD22	3:F:127:GLN:HA	1.76	0.66
2:H:73:THR:HG22	2:H:75:VAL:H	1.60	0.66
1:S:114:ILE:O	1:S:118:LEU:HG	1.95	0.66
3:R:47:TYR:HE1	3:R:49:ASN:ND2	1.94	0.66
3:X:138:LEU:H	3:X:138:LEU:HD12	1.59	0.66
1:A:31:TYR:HE2	1:A:36:LEU:N	1.92	0.66
2:K:146:LEU:HB2	2:K:152:TRP:CZ3	2.29	0.66
3:O:41:PHE:O	3:O:48:MET:HG3	1.96	0.66
3:C:181:ASP:OD2	3:C:183:ARG:HD3	1.96	0.66
2:Q:170:GLU:HB2	3:R:190:SER:HB3	1.77	0.66
3:F:206:ASN:CG	3:F:207:PRO:HA	2.16	0.66
3:U:188:LEU:HD11	3:U:199:PHE:CE1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:16:HIS:CE1	2:N:134:TYR:HB3	2.31	0.66
1:J:45:TYR:CE1	1:J:111:THR:HG22	2.30	0.66
2:B:108:ALA:HB1	2:B:198:SER:HA	1.78	0.66
2:W:15:ARG:HD3	2:W:68:ASP:O	1.97	0.65
1:J:63:LEU:HD23	1:J:66:LEU:HD23	1.78	0.65
1:D:16:HIS:ND1	2:E:134:TYR:HD2	1.93	0.65
2:W:21:VAL:HA	2:W:58:TRP:O	1.95	0.65
2:Z:15:ARG:HD2	2:Z:130:GLN:CB	2.26	0.65
1:A:20:ASP:HB2	1:A:23:MET:HE2	1.76	0.65
3:L:166:GLN:HG2	3:L:177:GLU:HB3	1.77	0.65
3:F:140:LEU:HD23	3:F:150:LEU:HD13	1.78	0.65
3:I:135:PRO:HG2	3:I:201:VAL:HG12	1.79	0.65
2:K:71:LYS:O	2:K:72:LEU:HD23	1.95	0.65
1:V:128:ILE:O	1:V:132:LEU:HG	1.96	0.65
1:A:62:GLU:O	1:A:65:PRO:HG2	1.97	0.65
1:Y:20:ASP:OD1	1:Y:85:VAL:HG23	1.97	0.65
2:W:98:PHE:O	2:W:100:PRO:HD3	1.96	0.65
2:K:13:ASN:HD21	2:K:16:ALA:H	1.45	0.65
1:M:18:LEU:O	1:M:22:GLN:HG3	1.97	0.65
2:K:128:ILE:HD12	2:K:131:ALA:HB3	1.78	0.65
2:Z:69:SER:OG	2:Z:71:LYS:HE2	1.96	0.65
2:W:15:ARG:CZ	2:W:131:ALA:O	2.45	0.65
2:W:138:HIS:HB3	2:W:187:LEU:HD12	1.78	0.65
3:C:140:LEU:HD22	3:C:148:LEU:HD23	1.78	0.65
2:T:123:ASN:ND2	4:T:215:NAG:C1	2.53	0.65
2:K:138:HIS:HA	2:K:187:LEU:HD12	1.77	0.65
2:Q:114:VAL:HG11	2:Q:117:VAL:HG13	1.79	0.65
3:X:107:VAL:HG22	3:X:123:MET:HG2	1.77	0.65
2:Q:36:HIS:HD2	2:Q:83:LEU:HG	1.61	0.65
2:B:12:TYR:CD2	2:B:100:PRO:HB3	2.32	0.65
2:B:41:ARG:O	2:B:42:ARG:HD3	1.97	0.65
3:L:57:GLU:HG2	3:L:58:PRO:HD2	1.76	0.65
2:Q:20:CYS:O	2:Q:59:ALA:HA	1.96	0.65
2:E:38:TRP:HH2	2:T:83:LEU:HD21	1.62	0.65
2:K:144:ARG:HD3	2:K:152:TRP:HE3	1.61	0.65
2:N:175:ASP:N	2:N:205:THR:HB	2.11	0.65
1:V:59:LEU:HB2	1:V:121:TRP:CE2	2.32	0.65
3:R:169:THR:H	3:R:172:ASP:HB2	1.62	0.65
1:D:24:ILE:HA	1:D:80:PHE:CE2	2.32	0.64
3:F:112:ASP:OD1	3:F:114:ARG:HG3	1.97	0.64
3:I:52:TRP:HZ3	3:I:65:LEU:HD12	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:20:ASP:O	1:P:24:ILE:HD12	1.95	0.64
1:G:12:LEU:O	1:G:12:LEU:HD23	1.96	0.64
1:D:132:LEU:O	1:D:132:LEU:HD23	1.97	0.64
2:H:123:ASN:ND2	4:H:215:NAG:C1	2.60	0.64
3:L:191:VAL:HG12	3:L:197:TYR:CZ	2.32	0.64
3:L:191:VAL:HB	3:L:197:TYR:CE1	2.32	0.64
3:L:164:LEU:HD11	3:L:177:GLU:HB2	1.79	0.64
1:M:13:GLN:NE2	2:N:75:VAL:HG12	2.13	0.64
2:K:123:ASN:ND2	4:K:215:NAG:C1	2.59	0.64
1:V:93:VAL:O	1:V:96:LEU:N	2.26	0.64
1:S:70:LEU:HD22	1:S:78:PHE:CE2	2.32	0.64
2:K:146:LEU:HD13	2:K:152:TRP:CE3	2.33	0.64
2:H:119:THR:HG22	2:H:206:LYS:O	1.96	0.64
1:J:52:GLU:O	1:J:55:HIS:HB2	1.97	0.64
2:N:104:LEU:O	2:N:192:THR:HG23	1.96	0.64
2:Q:54:SER:HB3	2:Q:57:SER:HB2	1.79	0.64
3:F:87:GLU:O	3:F:89:ILE:HG13	1.97	0.64
3:F:204:ARG:NH2	3:F:213:GLN:HA	2.11	0.64
1:P:122:ILE:O	1:P:126:GLN:HG3	1.97	0.64
3:R:47:TYR:HE1	3:R:49:ASN:HD21	1.44	0.64
2:N:158:LEU:HA	3:O:147:GLN:NE2	2.12	0.64
1:Y:97:LYS:HG3	1:Y:98:GLY:H	1.63	0.64
3:R:157:LEU:HD13	3:R:205:PHE:HE1	1.63	0.64
1:V:10:THR:HA	1:V:13:GLN:OE1	1.98	0.64
1:D:16:HIS:HB3	2:E:134:TYR:CE2	2.33	0.64
2:W:188:GLN:HG2	2:W:189:GLY:N	2.12	0.64
2:T:185:LYS:HB2	2:T:194:TRP:CE3	2.32	0.64
1:A:31:TYR:HH	1:A:35:LYS:N	1.95	0.64
1:J:86:VAL:HA	1:J:89:ILE:HD12	1.80	0.64
2:N:69:SER:CB	2:N:71:LYS:HE2	2.28	0.63
2:N:139:LEU:HD23	2:N:186:PRO:HA	1.80	0.63
3:L:188:LEU:CD2	3:L:199:PHE:CE2	2.80	0.63
3:X:169:THR:HG22	3:X:172:ASP:OD2	1.98	0.63
2:K:114:VAL:CG1	2:K:117:VAL:HG13	2.27	0.63
2:E:38:TRP:CE3	2:T:81:ARG:NH1	2.67	0.63
3:I:165:VAL:HG11	3:I:186:PHE:CD2	2.33	0.63
2:Q:118:GLU:OE1	2:Q:121:ARG:HD3	1.98	0.63
1:P:25:LEU:HD22	1:P:122:ILE:HD12	1.80	0.63
2:N:158:LEU:HA	3:O:147:GLN:HE22	1.64	0.63
1:G:56:LEU:HD13	1:G:124:PHE:CE2	2.34	0.63
2:Z:126:TRP:NE1	2:Z:165:GLU:HA	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:72:LEU:CD1	2:Q:78:VAL:HG21	2.28	0.63
1:Y:97:LYS:HG3	1:Y:98:GLY:N	2.13	0.63
2:Z:169:LEU:HB3	2:Z:172:LEU:HD21	1.80	0.63
1:A:114:ILE:O	1:A:117:PHE:HB3	1.99	0.63
3:U:42:VAL:HG22	3:U:48:MET:HB2	1.79	0.63
1:D:91:VAL:HG13	2:E:41:ARG:HD2	1.80	0.63
2:Z:121:ARG:HG2	2:Z:170:GLU:OE2	1.98	0.63
1:S:127:SER:HA	3:U:103:TYR:CE1	2.34	0.63
3:I:44:ASN:HB3	3:I:46:GLU:HG3	1.80	0.63
1:V:125:CYS:O	1:V:129:ILE:HG13	1.99	0.63
1:A:46:MET:HB3	1:A:47:PRO:HD2	1.81	0.63
2:E:172:LEU:HD22	2:E:178:TYR:CZ	2.34	0.63
1:S:70:LEU:HD22	1:S:78:PHE:HE2	1.63	0.63
3:I:65:LEU:HD23	3:I:66:HIS:N	2.14	0.63
1:V:24:ILE:O	1:V:28:ILE:HG13	1.99	0.63
2:N:146:LEU:HD22	2:N:152:TRP:CE2	2.34	0.63
1:G:89:ILE:O	1:G:93:VAL:HG23	1.98	0.63
2:N:162:GLN:N	2:N:162:GLN:OE1	2.32	0.63
2:K:44:TRP:CZ3	2:K:64:LEU:HD22	2.34	0.63
1:A:125:CYS:O	1:A:129:ILE:HG13	1.98	0.63
1:P:44:PHE:HE2	1:P:114:ILE:HB	1.64	0.62
2:N:181:GLN:HE21	2:N:200:PRO:HD3	1.64	0.62
2:T:74:THR:HA	2:T:101:PHE:HB2	1.81	0.62
3:R:206:ASN:HA	3:R:210:GLY:O	1.99	0.62
2:K:106:LEU:HD22	2:K:186:PRO:HD3	1.81	0.62
3:U:169:THR:HG22	3:U:197:TYR:CE2	2.33	0.62
1:D:56:LEU:HG	1:D:93:VAL:HG13	1.80	0.62
3:F:180:VAL:HG12	3:F:181:ASP:O	1.98	0.62
1:A:18:LEU:HD11	1:A:122:ILE:HG23	1.82	0.62
2:N:17:GLN:HA	2:N:62:LEU:O	1.99	0.62
3:F:140:LEU:CD1	3:F:224:TRP:HB2	2.29	0.62
2:W:188:GLN:HG2	2:W:189:GLY:H	1.64	0.62
2:E:168:CYS:HB2	4:E:215:NAG:H82	1.81	0.62
1:M:123:THR:HA	1:M:126:GLN:HG3	1.80	0.62
2:N:83:LEU:HD22	2:N:92:VAL:HA	1.81	0.62
1:V:117:PHE:CE1	1:V:121:TRP:CD1	2.88	0.62
3:X:63:LEU:HB3	3:X:110:LEU:HD11	1.81	0.62
3:R:59:GLN:OE1	3:R:114:ARG:NH2	2.33	0.62
2:E:73:THR:O	2:E:76:ASP:HB2	1.99	0.62
2:W:85:ARG:HD3	2:W:90:TRP:CE2	2.34	0.62
3:C:64:THR:OG1	3:C:111:GLN:HB3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:40:ASP:OD2	2:N:77:ILE:HB	1.99	0.62
2:W:82:VAL:O	2:W:83:LEU:HD23	1.99	0.62
1:A:35:LYS:HD2	1:A:38:ARG:HH21	1.64	0.62
2:T:73:THR:HG22	2:T:76:ASP:OD1	2.00	0.62
2:B:106:LEU:HD11	2:B:186:PRO:HG3	1.82	0.62
3:O:64:THR:OG1	3:O:111:GLN:HB3	2.00	0.62
1:V:18:LEU:HD11	1:V:122:ILE:HG23	1.82	0.62
3:F:48:MET:HB3	3:F:100:ILE:HD11	1.82	0.62
2:B:81:ARG:NH1	2:B:95:ILE:HD12	2.14	0.62
2:K:141:PHE:CE2	2:K:184:VAL:HB	2.34	0.62
3:O:138:LEU:H	3:O:138:LEU:HD12	1.65	0.62
3:I:162:GLU:OE2	3:I:204:ARG:HD2	1.99	0.61
2:H:13:ASN:HB2	2:H:17:GLN:HB3	1.82	0.61
2:T:146:LEU:HB3	2:T:179:GLU:HB2	1.81	0.61
2:K:117:VAL:HG12	2:K:122:CYS:SG	2.39	0.61
2:Q:41:ARG:NH1	2:Q:75:VAL:O	2.33	0.61
2:E:137:ARG:HG2	2:E:137:ARG:HH11	1.66	0.61
2:Z:53:VAL:HG12	2:Z:54:SER:N	2.15	0.61
1:D:11:GLN:O	1:D:11:GLN:HG2	2.00	0.61
2:T:39:PRO:HB2	2:T:42:ARG:HB2	1.83	0.61
1:V:69:VAL:CA	1:V:72:LEU:HD23	2.30	0.61
1:P:22:GLN:HG2	1:P:122:ILE:HD13	1.81	0.61
2:B:104:LEU:O	2:B:192:THR:HG23	1.99	0.61
1:D:60:GLU:HA	1:D:63:LEU:CD1	2.28	0.61
3:F:204:ARG:HD2	3:F:215:TRP:CE2	2.34	0.61
3:L:148:LEU:HD11	3:L:188:LEU:HD23	1.82	0.61
1:G:60:GLU:OE2	1:G:94:LEU:HD21	2.01	0.61
3:U:125:LYS:O	3:U:128:ASN:HB2	1.99	0.61
1:V:117:PHE:HE1	1:V:121:TRP:CD1	2.19	0.61
3:X:65:LEU:HD13	3:X:93:CYS:HB3	1.81	0.61
2:T:143:ALA:HB1	2:T:180:PHE:CE1	2.36	0.61
1:V:56:LEU:O	1:V:59:LEU:N	2.34	0.61
1:P:85:VAL:O	1:P:89:ILE:HG13	2.00	0.61
1:P:36:LEU:HD12	1:P:39:MET:HB3	1.81	0.61
3:I:165:VAL:HG11	3:I:186:PHE:CE2	2.36	0.61
3:L:182:TYR:CE1	3:L:183:ARG:HD3	2.35	0.61
2:T:110:ILE:HD12	2:T:111:SER:OG	1.99	0.61
1:Y:52:GLU:O	1:Y:55:HIS:HB2	2.00	0.61
2:B:204:ARG:HD3	1:D:43:LYS:O	2.00	0.61
4:T:215:NAG:H61	4:U:233:NAG:H82	1.81	0.61
2:K:140:GLU:HG3	2:K:187:LEU:HD21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:186:PRO:HD2	2:E:192:THR:HG21	1.83	0.61
1:S:40:LEU:HD23	1:S:113:THR:HB	1.81	0.61
2:W:115:VAL:CB	2:W:123:ASN:HD22	2.13	0.61
2:K:144:ARG:HH11	2:K:152:TRP:HB3	1.66	0.61
3:I:47:TYR:HE1	3:I:49:ASN:ND2	1.99	0.61
2:T:44:TRP:CH2	2:T:64:LEU:HD13	2.36	0.61
2:Z:13:ASN:HD22	2:Z:17:GLN:HB2	1.64	0.60
3:I:138:LEU:HB2	3:I:222:ILE:HG21	1.83	0.60
2:Q:132:SER:OG	2:Q:134:TYR:HD1	1.83	0.60
2:E:198:SER:O	2:E:199:GLN:C	2.38	0.60
1:Y:91:VAL:HG13	2:Z:41:ARG:HD3	1.83	0.60
3:C:137:ASN:ND2	4:C:400:NAG:C1	2.64	0.60
2:K:161:LYS:NZ	3:L:149:GLU:OE2	2.33	0.60
1:P:18:LEU:HD11	1:P:122:ILE:HG23	1.82	0.60
2:W:137:ARG:NH2	3:X:162:GLU:OE1	2.34	0.60
1:P:62:GLU:O	1:P:65:PRO:HG2	2.01	0.60
1:M:42:PHE:CD2	1:M:69:VAL:HG22	2.36	0.60
2:W:14:SER:HB3	2:W:104:LEU:HD22	1.83	0.60
2:N:120:HIS:CE1	2:N:174:PRO:HG3	2.35	0.60
2:Q:142:GLU:HG3	2:Q:194:TRP:CZ2	2.36	0.60
2:W:53:VAL:HG12	2:W:54:SER:N	2.17	0.60
2:E:109:PRO:HG2	2:E:182:VAL:HG13	1.82	0.60
1:D:16:HIS:ND1	2:E:134:TYR:CD2	2.69	0.60
2:W:141:PHE:CE2	2:W:184:VAL:HG22	2.36	0.60
3:X:140:LEU:HD11	3:X:199:PHE:HD1	1.65	0.60
3:O:46:GLU:CD	3:O:133:TRP:HE1	2.05	0.60
3:L:41:PHE:O	3:L:48:MET:HG3	2.01	0.60
2:Z:117:VAL:O	2:Z:118:GLU:HG3	2.02	0.60
3:U:148:LEU:HD11	3:U:188:LEU:HD12	1.83	0.60
3:C:200:ARG:HG3	3:C:218:TRP:CE3	2.37	0.60
1:P:24:ILE:HG23	1:P:70:LEU:HD21	1.83	0.60
1:Y:14:LEU:HD11	1:Y:53:LEU:HD21	1.82	0.60
2:E:152:TRP:O	2:E:155:ALA:HB3	2.01	0.60
1:D:59:LEU:HD13	1:D:121:TRP:CD1	2.35	0.60
3:F:82:HIS:ND1	3:F:94:GLN:HB3	2.17	0.60
2:W:78:VAL:O	2:W:80:LEU:CD1	2.50	0.60
3:U:142:LYS:HA	3:U:148:LEU:HA	1.83	0.60
1:M:12:LEU:O	1:M:16:HIS:HD2	1.85	0.60
2:E:123:ASN:HD21	4:E:215:NAG:C2	2.14	0.60
2:Z:129:SER:O	2:Z:130:GLN:C	2.37	0.60
2:W:80:LEU:HD13	2:W:98:PHE:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:164:GLN:NE2	3:F:178:GLN:HG2	2.16	0.60
2:Z:54:SER:H	2:Z:57:SER:HB2	1.65	0.60
1:S:10:THR:HA	1:S:13:GLN:HE21	1.66	0.60
1:Y:67:GLU:O	1:Y:71:ASN:ND2	2.35	0.60
3:L:44:ASN:HB3	3:L:46:GLU:HG3	1.83	0.60
2:N:83:LEU:CD2	2:N:92:VAL:HA	2.32	0.60
1:D:18:LEU:CD1	1:D:122:ILE:HG23	2.32	0.59
2:E:137:ARG:CB	3:F:181:ASP:HB3	2.32	0.59
2:W:98:PHE:HE2	2:W:100:PRO:HA	1.62	0.59
2:B:123:ASN:ND2	4:B:215:NAG:C1	2.65	0.59
1:D:16:HIS:CG	2:E:134:TYR:HD2	2.20	0.59
1:J:56:LEU:HB3	1:J:93:VAL:HG13	1.83	0.59
3:U:62:ASN:HD21	4:U:300:NAG:C1	2.14	0.59
3:O:44:ASN:HB3	3:O:46:GLU:HG3	1.83	0.59
2:Z:117:VAL:HG23	2:Z:206:LYS:HE2	1.83	0.59
2:E:164:GLN:HE21	3:F:178:GLN:CG	2.16	0.59
1:D:24:ILE:HG23	1:D:70:LEU:HD21	1.85	0.59
1:S:85:VAL:O	1:S:89:ILE:HG13	2.02	0.59
2:Q:71:LYS:O	2:Q:72:LEU:HD23	2.03	0.59
3:U:52:TRP:CZ3	3:U:65:LEU:HD12	2.37	0.59
2:Q:101:PHE:CD2	2:Q:104:LEU:HD11	2.38	0.59
3:C:207:PRO:HG2	3:F:117:ARG:NH2	32.64	0.59
3:U:65:LEU:HD23	3:U:66:HIS:N	2.17	0.59
1:S:117:PHE:CE1	1:S:121:TRP:CD1	2.91	0.59
2:W:118:GLU:O	2:W:205:THR:HB	2.02	0.59
1:G:62:GLU:O	1:G:65:PRO:HG2	2.03	0.59
2:E:47:THR:HG22	2:E:48:CYS:N	2.17	0.59
2:E:179:GLU:HG2	2:E:202:ALA:HB2	1.85	0.59
3:X:202:ARG:HG3	3:X:215:TRP:CE3	2.37	0.59
1:D:14:LEU:HD21	1:D:53:LEU:HD21	1.83	0.59
1:D:56:LEU:O	1:D:59:LEU:HB3	2.02	0.59
3:F:46:GLU:CD	3:F:133:TRP:HE1	2.06	0.59
2:T:128:ILE:HG22	2:T:184:VAL:HG21	1.84	0.59
2:T:109:PRO:CG	2:T:184:VAL:HG23	2.28	0.59
2:K:138:HIS:CB	2:K:187:LEU:HD12	2.31	0.59
3:R:180:VAL:HG11	3:R:185:LYS:O	2.02	0.59
3:C:138:LEU:HB3	3:C:222:ILE:HD13	1.83	0.59
3:R:145:GLU:OE1	3:R:145:GLU:HA	2.02	0.59
2:H:13:ASN:ND2	2:H:130:GLN:NE2	2.51	0.59
2:K:15:ARG:HH11	2:K:70:GLN:HB2	1.66	0.59
2:W:109:PRO:HG3	2:W:184:VAL:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:132:SER:OG	2:W:134:TYR:HD1	1.86	0.59
1:V:118:LEU:O	1:V:122:ILE:HG13	2.02	0.59
1:S:12:LEU:HD11	2:T:188:GLN:HG3	1.85	0.59
1:S:112:ALA:HB1	1:S:116:GLU:HB2	1.84	0.59
1:A:85:VAL:HG13	1:A:86:VAL:H	1.65	0.59
1:V:86:VAL:HG12	1:V:89:ILE:HD12	1.85	0.59
2:B:123:ASN:HD21	4:B:215:NAG:C2	2.15	0.59
2:Q:132:SER:HG	2:Q:134:TYR:HD1	1.51	0.59
2:N:106:LEU:HD11	2:N:186:PRO:HG3	1.83	0.59
2:W:80:LEU:HD13	2:W:98:PHE:CB	2.33	0.59
2:K:73:THR:O	2:K:76:ASP:HB2	2.03	0.59
2:Z:14:SER:O	2:Z:132:SER:HB2	2.03	0.59
3:O:150:LEU:HD22	3:O:152:TRP:CE3	2.38	0.59
2:T:39:PRO:HG2	2:T:42:ARG:HB2	1.85	0.59
2:K:144:ARG:CD	2:K:152:TRP:HE3	2.16	0.59
2:Q:12:TYR:CZ	2:Q:72:LEU:HB2	2.38	0.59
2:K:14:SER:OG	2:K:135:PHE:HE2	1.85	0.59
2:Q:138:HIS:O	2:Q:139:LEU:HG	2.03	0.59
2:N:160:LEU:HD13	2:N:164:GLN:HB3	1.85	0.58
1:A:74:HIS:CG	1:A:75:SER:N	2.71	0.58
2:W:128:ILE:HG13	2:W:128:ILE:O	2.02	0.58
2:W:83:LEU:HB3	2:W:90:TRP:CE3	2.38	0.58
2:T:141:PHE:CD2	2:T:184:VAL:HG22	2.38	0.58
3:I:52:TRP:CZ3	3:I:92:GLY:HA2	2.38	0.58
2:T:112:LEU:HA	2:T:125:SER:O	2.03	0.58
1:V:45:TYR:CD2	1:V:62:GLU:HG3	2.38	0.58
2:Q:123:ASN:HD21	4:Q:215:NAG:C1	2.16	0.58
3:L:62:ASN:HD21	4:L:300:NAG:C2	2.16	0.58
2:H:82:VAL:C	2:H:83:LEU:HD12	2.22	0.58
2:W:138:HIS:HB3	2:W:187:LEU:CD1	2.32	0.58
2:B:54:SER:HB3	2:B:57:SER:HB3	1.85	0.58
2:H:201:LEU:HD12	2:H:202:ALA:N	2.19	0.58
3:F:127:GLN:HG2	3:F:128:ASN:OD1	2.03	0.58
3:F:205:PHE:CE2	3:F:209:CYS:O	2.57	0.58
1:Y:13:GLN:NE2	2:Z:75:VAL:HG12	2.18	0.58
2:W:167:ILE:HG21	2:W:180:PHE:CZ	2.38	0.58
1:Y:37:THR:O	1:Y:41:THR:HG23	2.02	0.58
3:L:126:LEU:O	3:L:128:ASN:N	2.36	0.58
3:I:106:PHE:CE2	3:I:108:VAL:HG13	2.38	0.58
2:W:118:GLU:OE1	2:W:121:ARG:HB2	2.03	0.58
3:O:147:GLN:HG2	3:O:189:PRO:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:37:ALA:HA	2:Q:80:LEU:HD23	1.85	0.58
1:D:24:ILE:HD11	1:D:85:VAL:CG2	2.34	0.58
3:O:154:ASN:ND2	3:O:163:HIS:CE1	2.72	0.58
2:Q:83:LEU:CD2	2:Q:92:VAL:HG22	2.34	0.58
1:G:95:GLU:O	1:G:95:GLU:HG3	2.03	0.58
2:E:38:TRP:CH2	2:T:83:LEU:HD11	2.39	0.58
1:S:31:TYR:HE2	1:S:35:LYS:N	2.01	0.58
3:U:52:TRP:CE3	3:U:110:LEU:HD21	2.38	0.58
2:T:98:PHE:O	2:T:100:PRO:HD3	2.03	0.58
3:R:68:TRP:CE3	3:R:77:VAL:HG13	2.39	0.58
2:B:172:LEU:HD22	2:B:178:TYR:CZ	2.39	0.58
3:F:148:LEU:HG	3:F:191:VAL:HG11	1.86	0.58
3:F:41:PHE:O	3:F:48:MET:HG3	2.04	0.58
2:H:12:TYR:CD1	2:H:13:ASN:N	2.72	0.58
2:E:64:LEU:HD23	2:E:64:LEU:N	2.18	0.58
2:N:167:ILE:HG21	2:N:180:PHE:CZ	2.39	0.58
2:B:106:LEU:O	2:B:195:SER:HB2	2.04	0.58
3:X:166:GLN:HB3	3:X:175:TRP:CE3	2.39	0.58
2:H:146:LEU:HD13	2:H:152:TRP:CD2	2.38	0.58
2:H:146:LEU:HD22	2:H:152:TRP:CZ2	2.39	0.58
1:S:95:GLU:HG3	1:S:95:GLU:O	2.02	0.58
1:D:44:PHE:CZ	1:D:69:VAL:HG21	2.39	0.58
2:H:187:LEU:HD11	3:I:183:ARG:NE	2.18	0.58
2:Q:72:LEU:HD11	2:Q:78:VAL:HG21	1.84	0.58
3:U:62:ASN:O	3:U:113:PRO:HD3	2.04	0.58
1:M:15:GLU:OE2	3:O:208:LEU:HD22	2.03	0.58
3:I:204:ARG:HB3	3:O:115:GLU:HA	90.51	0.57
2:K:44:TRP:HH2	2:K:72:LEU:HD21	1.69	0.57
3:O:61:THR:HG22	3:O:62:ASN:N	2.19	0.57
2:W:136:GLU:OE2	3:X:207:PRO:HG3	2.04	0.57
3:O:206:ASN:HA	3:O:210:GLY:O	2.03	0.57
1:M:20:ASP:OD1	1:M:23:MET:HE2	2.04	0.57
3:F:106:PHE:CD2	3:F:126:LEU:HD21	2.39	0.57
2:B:15:ARG:HG2	2:B:130:GLN:HB3	1.86	0.57
3:C:52:TRP:CZ3	3:C:92:GLY:HA2	2.39	0.57
2:Q:51:LEU:O	2:Q:58:TRP:HA	2.04	0.57
3:R:192:ASP:HB3	3:R:195:LYS:HD2	1.84	0.57
2:K:124:ILE:HD11	2:K:203:PHE:CE2	2.39	0.57
3:L:206:ASN:HB2	3:L:207:PRO:HA	1.86	0.57
4:K:215:NAG:H4	4:K:216:NAG:C1	2.33	0.57
3:R:41:PHE:HD2	3:R:131:ILE:HD11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:103:ASN:OD1	2:E:191:PHE:HB2	2.04	0.57
1:S:64:LYS:N	1:S:65:PRO:HD2	2.19	0.57
2:W:123:ASN:ND2	4:W:215:NAG:C1	2.64	0.57
2:Z:106:LEU:HD11	2:Z:186:PRO:CG	2.32	0.57
2:H:46:GLN:OE1	2:W:89:ARG:HA	2.04	0.57
1:A:45:TYR:HB3	1:A:107:TYR:HD1	1.69	0.57
2:N:139:LEU:HD23	2:N:186:PRO:CA	2.35	0.57
1:Y:53:LEU:HD13	1:Y:96:LEU:HB3	1.86	0.57
1:Y:67:GLU:OE2	1:Y:83:ARG:HG3	2.04	0.57
3:I:204:ARG:NH1	3:O:117:ARG:HG3	96.51	0.57
2:N:205:THR:HG22	2:N:206:LYS:N	2.19	0.57
1:M:13:GLN:HG2	2:N:75:VAL:CG1	2.35	0.57
3:O:102:LEU:HD22	3:O:127:GLN:HA	1.86	0.57
1:D:7:THR:HG23	1:D:10:THR:HB	1.86	0.57
2:H:119:THR:HB	2:H:174:PRO:HG3	1.87	0.57
2:W:36:HIS:HB3	2:W:38:TRP:NE1	2.20	0.57
2:K:106:LEU:O	2:K:195:SER:HB2	2.05	0.57
3:I:128:ASN:C	3:I:212:ALA:HB2	2.25	0.57
2:K:13:ASN:O	2:K:14:SER:CB	2.53	0.57
3:F:167:TYR:CZ	3:F:176:THR:HG21	2.40	0.57
3:F:205:PHE:HE2	3:F:209:CYS:O	1.88	0.57
1:Y:24:ILE:HD11	1:Y:89:ILE:HD11	1.87	0.57
2:H:50:LEU:CD2	2:H:60:CYS:HB2	2.35	0.57
1:S:87:SER:O	1:S:91:VAL:HG23	2.05	0.57
2:K:69:SER:HB2	2:K:71:LYS:HE2	1.86	0.57
3:O:52:TRP:CH2	3:O:92:GLY:HA2	2.40	0.57
1:J:62:GLU:OE2	1:J:62:GLU:HA	2.04	0.57
1:J:78:PHE:CD2	1:J:80:PHE:CZ	2.92	0.57
1:A:24:ILE:O	1:A:28:ILE:HG13	2.04	0.57
2:K:112:LEU:O	2:K:201:LEU:HD22	2.04	0.57
2:E:14:SER:O	2:E:132:SER:HB2	2.05	0.56
1:D:18:LEU:O	1:D:22:GLN:HG3	2.04	0.56
2:E:41:ARG:O	2:E:42:ARG:HD3	2.05	0.56
1:V:93:VAL:HG23	1:V:94:LEU:N	2.19	0.56
2:Z:185:LYS:HD2	2:Z:193:THR:HA	1.87	0.56
1:D:20:ASP:OD1	1:D:23:MET:HE1	2.05	0.56
3:L:62:ASN:ND2	4:L:300:NAG:C1	2.65	0.56
3:X:52:TRP:CZ3	3:X:65:LEU:HD12	2.32	0.56
2:K:81:ARG:HD3	2:K:95:ILE:HG22	1.86	0.56
2:H:106:LEU:HD11	2:H:186:PRO:HG3	1.87	0.56
1:Y:28:ILE:HG12	1:Y:78:PHE:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:CD1	1:A:89:ILE:HG23	2.36	0.56
1:J:16:HIS:ND1	2:K:134:TYR:HB3	2.20	0.56
4:W:215:NAG:H83	3:X:176:THR:HG21	1.87	0.56
2:Q:13:ASN:ND2	2:Q:17:GLN:HB3	2.19	0.56
2:H:144:ARG:HH11	2:H:152:TRP:HB3	1.71	0.56
1:Y:117:PHE:CE1	1:Y:121:TRP:CD1	2.94	0.56
3:R:65:LEU:HD23	3:R:66:HIS:N	2.20	0.56
1:A:87:SER:O	1:A:91:VAL:HG23	2.05	0.56
2:K:175:ASP:N	2:K:205:THR:HB	2.20	0.56
1:J:126:GLN:HA	1:J:129:ILE:CG2	2.36	0.56
3:F:188:LEU:CD2	3:F:191:VAL:HG12	2.35	0.56
1:M:35:LYS:HD2	1:M:38:ARG:NH2	2.21	0.56
2:W:77:ILE:HA	2:W:100:PRO:HD3	1.87	0.56
2:H:172:LEU:HD22	2:H:178:TYR:CE1	2.40	0.56
3:X:157:LEU:HD13	3:X:160:CYS:HB2	1.87	0.56
2:Q:37:ALA:HB2	2:Q:62:LEU:HD13	1.88	0.56
1:Y:28:ILE:HG12	1:Y:78:PHE:HZ	1.69	0.56
2:W:164:GLN:NE2	3:X:178:GLN:HG2	2.20	0.56
3:I:181:ASP:CG	3:I:183:ARG:HH11	2.09	0.56
1:V:117:PHE:CE1	1:V:121:TRP:HD1	2.23	0.56
3:O:52:TRP:HZ3	3:O:65:LEU:HD12	1.68	0.56
1:J:84:ASP:O	1:J:87:SER:HB2	2.05	0.56
3:I:158:ASN:O	3:I:159:HIS:HB3	2.04	0.56
1:P:7:THR:HG23	1:P:132:LEU:HD13	1.87	0.56
3:R:164:LEU:HD11	3:R:177:GLU:HB2	1.88	0.56
3:U:155:ARG:O	3:U:156:PHE:CD2	2.59	0.56
1:S:28:ILE:O	1:S:36:LEU:HD11	2.06	0.56
2:H:37:ALA:HB2	2:H:62:LEU:CD1	2.35	0.56
2:T:143:ALA:HB3	2:T:158:LEU:HB2	1.87	0.56
1:D:16:HIS:HB3	2:E:134:TYR:HD2	1.67	0.56
1:M:85:VAL:O	1:M:89:ILE:HG13	2.05	0.56
3:C:48:MET:CE	3:C:95:LEU:HD12	2.36	0.56
1:S:28:ILE:HG23	1:S:36:LEU:HD11	1.88	0.56
2:T:51:LEU:O	2:T:58:TRP:HA	2.05	0.56
3:U:169:THR:HG22	3:U:197:TYR:HE2	1.71	0.56
1:D:57:GLN:HB2	1:D:97:LYS:HD3	1.88	0.56
3:I:137:ASN:O	3:I:139:THR:HG23	2.05	0.56
3:F:205:PHE:CZ	3:F:209:CYS:HB2	2.40	0.56
2:E:162:GLN:OE1	2:E:162:GLN:N	2.38	0.56
2:N:162:GLN:HE21	2:N:164:GLN:NE2	2.03	0.56
2:Z:73:THR:HG23	2:Z:75:VAL:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:195:SER:HB2	2:K:196:PRO:HD2	1.88	0.56
1:S:31:TYR:HB3	1:S:36:LEU:HD13	1.88	0.56
1:S:24:ILE:HD11	1:S:89:ILE:HD11	1.88	0.56
2:N:164:GLN:HG2	2:N:166:TRP:O	2.06	0.56
3:C:140:LEU:HD13	3:C:224:TRP:HB2	1.88	0.56
2:W:164:GLN:HE21	3:X:178:GLN:HG2	1.71	0.56
2:W:11:PHE:HA	2:W:103:ASN:HB3	1.88	0.56
2:Z:74:THR:HG23	2:Z:75:VAL:HG13	1.88	0.56
3:R:44:ASN:HB3	3:R:46:GLU:HG3	1.87	0.56
3:L:68:TRP:HE3	3:L:77:VAL:HG13	1.71	0.56
1:A:36:LEU:HD13	1:A:39:MET:HE3	1.87	0.55
3:X:165:VAL:HG22	3:X:201:VAL:CG2	2.36	0.55
1:V:68:GLU:O	1:V:72:LEU:CD2	2.52	0.55
3:O:62:ASN:HD21	4:O:300:NAG:C2	2.19	0.55
2:N:146:LEU:HD13	2:N:152:TRP:CG	2.40	0.55
1:G:53:LEU:HD22	1:G:96:LEU:HD22	1.88	0.55
2:T:106:LEU:HD12	2:T:184:VAL:HG12	1.87	0.55
2:Z:160:LEU:HD13	2:Z:164:GLN:HB3	1.89	0.55
1:S:117:PHE:CE1	1:S:121:TRP:HD1	2.24	0.55
1:S:69:VAL:HG11	1:S:114:ILE:HD12	1.89	0.55
2:T:112:LEU:HD12	2:T:112:LEU:N	2.20	0.55
1:Y:22:GLN:HG2	1:Y:122:ILE:HD13	1.86	0.55
3:X:133:TRP:HB3	3:X:155:ARG:HG3	1.88	0.55
3:U:109:GLN:HE21	3:U:121:THR:HG22	1.71	0.55
2:E:50:LEU:HD23	2:E:60:CYS:HB2	1.87	0.55
1:D:11:GLN:CB	1:D:132:LEU:HD22	2.36	0.55
1:D:85:VAL:O	1:D:89:ILE:HG13	2.06	0.55
3:I:128:ASN:OD1	3:I:211:SER:HB2	2.06	0.55
3:I:62:ASN:HD21	4:I:300:NAG:C2	2.18	0.55
1:S:28:ILE:O	1:S:28:ILE:HG22	2.06	0.55
2:H:20:CYS:HB2	2:H:60:CYS:O	2.06	0.55
4:H:215:NAG:O4	4:I:233:NAG:C1	2.55	0.55
2:K:143:ALA:HB1	2:K:180:PHE:CZ	2.42	0.55
2:K:114:VAL:HG13	2:K:117:VAL:HG13	1.86	0.55
1:Y:31:TYR:OH	1:Y:35:LYS:HE3	2.07	0.55
2:K:183:ARG:HG3	2:K:194:TRP:CE3	2.40	0.55
2:T:170:GLU:H	3:U:190:SER:HB3	1.70	0.55
2:B:175:ASP:OD1	2:B:204:ARG:NH2	2.38	0.55
3:I:65:LEU:HD13	3:I:93:CYS:HB3	1.87	0.55
2:W:44:TRP:CH2	2:W:64:LEU:HD13	2.41	0.55
3:U:140:LEU:HD12	3:U:222:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:183:ARG:HG2	2:Q:197:TRP:CZ3	2.41	0.55
1:A:17:LEU:HD11	1:A:89:ILE:HG23	1.88	0.55
1:A:31:TYR:OH	1:A:35:LYS:HB2	2.07	0.55
1:V:112:ALA:HB1	1:V:116:GLU:HB2	1.87	0.55
2:Z:118:GLU:OE1	2:Z:121:ARG:HB2	2.07	0.55
3:X:161:LEU:HD12	3:X:205:PHE:HA	1.88	0.55
3:C:148:LEU:HD13	3:C:191:VAL:HG21	1.89	0.55
3:R:204:ARG:HD2	3:R:212:ALA:O	2.06	0.55
3:R:135:PRO:HG2	3:R:201:VAL:HG12	1.89	0.55
2:E:38:TRP:CH2	2:T:83:LEU:HD21	2.42	0.55
3:F:159:HIS:O	3:F:159:HIS:CD2	2.59	0.55
1:A:35:LYS:HB2	1:A:35:LYS:NZ	2.22	0.55
1:S:56:LEU:HD22	1:S:93:VAL:HG13	1.87	0.55
1:G:45:TYR:HB3	1:G:107:TYR:HD1	1.72	0.55
2:T:39:PRO:CB	2:T:42:ARG:HB2	2.37	0.55
2:W:50:LEU:HD23	2:W:60:CYS:HB2	1.89	0.55
3:O:64:THR:HG22	3:O:83:TYR:OH	2.06	0.55
2:T:144:ARG:HD3	2:T:157:LEU:HD23	1.89	0.55
2:H:15:ARG:HH11	2:H:70:GLN:HB2	1.71	0.55
2:H:36:HIS:HE1	2:W:36:HIS:HE1	1.55	0.55
3:C:162:GLU:OE2	3:C:204:ARG:HD2	2.07	0.55
1:P:16:HIS:ND1	2:Q:134:TYR:CD2	2.75	0.55
1:A:69:VAL:HG11	1:A:114:ILE:HD12	1.88	0.55
2:T:141:PHE:HE1	2:T:163:LYS:HA	1.70	0.55
4:K:215:NAG:O4	4:K:216:NAG:C7	2.54	0.55
1:J:35:LYS:NZ	1:J:73:ALA:HA	2.21	0.55
2:K:16:ALA:HB1	2:K:65:GLY:H	1.72	0.55
2:E:178:TYR:HB2	2:E:203:PHE:CZ	2.41	0.55
2:E:104:LEU:HB2	2:E:192:THR:OG1	2.06	0.55
2:Q:143:ALA:HB1	2:Q:180:PHE:CE1	2.41	0.55
1:Y:112:ALA:HB1	1:Y:116:GLU:HB2	1.88	0.55
3:L:145:GLU:OE1	3:L:145:GLU:HA	2.06	0.55
4:W:215:NAG:H61	4:X:233:NAG:H82	1.89	0.55
2:W:36:HIS:HB3	2:W:38:TRP:CD1	2.41	0.55
3:U:68:TRP:HB3	3:U:77:VAL:HA	1.88	0.55
2:E:104:LEU:HD12	2:E:188:GLN:O	2.07	0.55
3:O:150:LEU:HD23	3:O:151:ASN:N	2.22	0.55
2:T:113:GLN:O	2:T:124:ILE:HG23	2.07	0.55
1:V:45:TYR:HD2	1:V:62:GLU:HG3	1.71	0.55
3:O:68:TRP:HE3	3:O:77:VAL:HG13	1.71	0.55
3:O:157:LEU:HD13	3:O:205:PHE:CD1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:23:MET:HE1	2:Q:133:HIS:CE1	2.42	0.55
2:E:38:TRP:CZ2	2:T:83:LEU:HD11	2.42	0.55
1:G:23:MET:SD	2:H:133:HIS:CE1	3.00	0.55
2:Q:95:ILE:HG12	2:Q:96:GLN:H	1.67	0.55
3:X:152:TRP:HE1	3:X:163:HIS:CE1	2.25	0.55
2:W:146:LEU:HD22	2:W:152:TRP:CE2	2.41	0.55
2:E:123:ASN:ND2	4:E:215:NAG:C1	2.70	0.54
2:H:13:ASN:HD21	2:H:130:GLN:NE2	2.04	0.54
2:T:88:VAL:HG23	2:T:89:ARG:H	1.72	0.54
3:O:62:ASN:HD21	4:O:300:NAG:C1	2.20	0.54
3:X:106:PHE:HE2	3:X:108:VAL:CG2	2.20	0.54
3:F:207:PRO:HA	3:F:210:GLY:O	2.08	0.54
1:S:9:LYS:O	1:S:13:GLN:HG3	2.08	0.54
3:L:130:VAL:HB	3:L:205:PHE:CD2	2.42	0.54
1:D:11:GLN:CG	1:D:129:ILE:HG23	2.36	0.54
3:F:68:TRP:CH2	3:F:109:GLN:NE2	2.73	0.54
2:T:88:VAL:HG23	2:T:89:ARG:N	2.23	0.54
1:A:7:THR:HG23	1:A:132:LEU:HD13	1.89	0.54
2:K:13:ASN:ND2	2:K:17:GLN:HB2	2.23	0.54
2:K:44:TRP:CH2	2:K:72:LEU:HD21	2.42	0.54
3:U:186:PHE:CE2	3:U:187:SER:O	2.61	0.54
1:D:28:ILE:CD1	1:D:114:ILE:HD13	2.36	0.54
3:F:64:THR:OG1	3:F:111:GLN:HB3	2.07	0.54
1:G:92:PHE:CZ	2:H:73:THR:HG23	2.42	0.54
2:T:158:LEU:HD13	2:T:167:ILE:HD11	1.89	0.54
2:W:146:LEU:HD23	2:W:179:GLU:OE1	2.07	0.54
2:W:8:PHE:CE1	2:W:82:VAL:HG22	2.42	0.54
2:W:80:LEU:CD1	2:W:98:PHE:HB3	2.37	0.54
2:Q:81:ARG:NH1	2:Q:95:ILE:HB	2.23	0.54
3:R:45:VAL:HG21	3:R:157:LEU:HD11	1.90	0.54
1:P:88:ASN:HD22	1:P:88:ASN:N	2.05	0.54
1:G:56:LEU:HD13	1:G:124:PHE:HE2	1.72	0.54
1:P:45:TYR:HB3	1:P:107:TYR:HD1	1.72	0.54
2:B:126:TRP:NE1	2:B:165:GLU:HA	2.22	0.54
1:A:61:GLU:OE2	1:A:105:CYS:HB3	2.08	0.54
1:V:46:MET:HB2	1:V:108:ALA:HB3	1.90	0.54
1:V:56:LEU:O	1:V:57:GLN:C	2.45	0.54
3:X:132:PRO:CB	3:X:161:LEU:HD21	2.36	0.54
2:K:137:ARG:NH2	3:L:162:GLU:OE1	2.40	0.54
1:V:35:LYS:HD2	1:V:38:ARG:HH21	1.73	0.54
3:O:39:GLN:HB2	3:O:41:PHE:HE1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:144:SER:HB3	3:R:147:GLN:HB2	1.89	0.54
1:D:11:GLN:O	1:D:15:GLU:HB2	2.07	0.54
3:I:198:THR:HG1	3:I:223:HIS:CE1	2.26	0.54
3:U:132:PRO:O	3:U:216:SER:HB2	2.07	0.54
1:V:44:PHE:CZ	1:V:114:ILE:HD12	2.43	0.54
2:N:141:PHE:HB2	2:N:160:LEU:HB2	1.89	0.54
2:Q:54:SER:OG	2:Q:55:GLN:N	2.41	0.54
3:O:157:LEU:HD13	3:O:205:PHE:CE1	2.42	0.54
2:Z:146:LEU:HD22	2:Z:152:TRP:CE2	2.43	0.54
3:C:169:THR:C	3:C:171:TRP:H	2.12	0.54
1:D:69:VAL:CG1	1:D:114:ILE:HD12	2.35	0.54
2:T:142:GLU:O	2:T:182:VAL:HG23	2.07	0.54
2:N:132:SER:OG	2:N:134:TYR:HD1	1.90	0.54
1:M:24:ILE:HG22	1:M:118:LEU:HD11	1.88	0.54
2:Z:143:ALA:O	2:Z:158:LEU:HG	2.08	0.54
1:D:11:GLN:HA	1:D:14:LEU:CD1	2.33	0.54
2:K:115:VAL:CG1	4:K:215:NAG:H62	2.36	0.54
3:U:204:ARG:HH21	3:U:215:TRP:HE1	1.56	0.54
2:T:73:THR:HA	2:T:101:PHE:HE1	1.73	0.54
2:Z:82:VAL:C	2:Z:83:LEU:HD23	2.27	0.54
3:X:62:ASN:O	3:X:113:PRO:HD3	2.08	0.54
1:J:122:ILE:O	1:J:126:GLN:HG3	2.07	0.54
3:I:180:VAL:HG11	3:I:185:LYS:O	2.07	0.54
3:I:192:ASP:OD2	3:I:195:LYS:HE3	2.07	0.54
1:Y:91:VAL:HG13	2:Z:41:ARG:CD	2.37	0.54
3:U:205:PHE:O	3:U:212:ALA:HB3	2.07	0.54
3:X:205:PHE:CZ	3:X:209:CYS:HB2	2.42	0.54
3:L:166:GLN:HA	3:L:176:THR:O	2.07	0.54
3:I:164:LEU:HD12	3:I:178:GLN:O	2.07	0.54
1:M:82:PRO:O	1:M:86:VAL:HG23	2.07	0.54
2:E:31:THR:O	2:E:31:THR:HG22	2.08	0.54
2:Q:66:ALA:HB1	2:Q:67:PRO:HD2	1.89	0.54
2:H:83:LEU:HD23	2:H:90:TRP:HB3	1.89	0.53
2:Q:146:LEU:HD22	2:Q:152:TRP:CZ2	2.43	0.53
1:Y:50:ALA:HA	1:Y:55:HIS:ND1	2.24	0.53
3:F:204:ARG:HB2	3:F:215:TRP:CE3	2.43	0.53
2:W:50:LEU:HD22	2:W:58:TRP:HB3	1.90	0.53
3:C:62:ASN:ND2	4:C:300:NAG:H83	2.23	0.53
1:D:131:THR:CG2	1:D:131:THR:O	2.57	0.53
2:H:15:ARG:NH1	2:H:70:GLN:HB2	2.22	0.53
3:O:84:LEU:HD21	4:O:234:NAG:C6	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:129:ILE:O	1:V:132:LEU:HB2	2.08	0.53
2:H:146:LEU:HD22	2:H:152:TRP:CE2	2.44	0.53
1:Y:31:TYR:HB3	1:Y:36:LEU:HD13	1.89	0.53
2:Q:150:HIS:HB3	2:Q:154:GLU:OE1	2.08	0.53
3:F:94:GLN:HE21	3:F:96:GLN:NE2	2.07	0.53
2:W:73:THR:OG1	2:W:75:VAL:HG22	2.08	0.53
1:V:68:GLU:C	1:V:71:ASN:H	2.11	0.53
1:M:16:HIS:HD1	2:N:134:TYR:CB	2.19	0.53
1:Y:28:ILE:HG22	1:Y:28:ILE:O	2.08	0.53
2:Q:11:PHE:HD1	2:Q:105:ARG:HD3	1.73	0.53
3:X:144:SER:HB3	3:X:147:GLN:HG3	1.91	0.53
3:F:183:ARG:HD3	3:F:185:LYS:CE	2.37	0.53
3:U:62:ASN:HD21	4:U:300:NAG:H83	1.72	0.53
2:N:146:LEU:HD13	2:N:152:TRP:CD2	2.43	0.53
2:N:146:LEU:HD22	2:N:152:TRP:NE1	2.23	0.53
1:S:112:ALA:HB1	1:S:116:GLU:CB	2.38	0.53
2:H:160:LEU:HD21	3:I:189:PRO:HG3	1.90	0.53
1:Y:120:ARG:O	1:Y:123:THR:HB	2.09	0.53
3:L:148:LEU:HD12	3:L:188:LEU:HB3	1.90	0.53
1:G:45:TYR:HE1	1:G:111:THR:HG22	1.69	0.53
2:H:36:HIS:CE1	2:W:36:HIS:HE1	2.26	0.53
2:T:44:TRP:HH2	2:T:72:LEU:HD21	1.74	0.53
3:I:140:LEU:HD22	3:I:148:LEU:HD13	1.90	0.53
3:R:64:THR:OG1	3:R:111:GLN:HB3	2.09	0.53
3:L:192:ASP:N	3:L:197:TYR:OH	2.33	0.53
1:V:28:ILE:O	1:V:28:ILE:HG22	2.09	0.53
3:U:164:LEU:HD12	3:U:165:VAL:N	2.24	0.53
3:O:144:SER:HB3	3:O:147:GLN:HB2	1.90	0.53
3:I:158:ASN:O	3:I:159:HIS:CB	2.55	0.53
2:Q:87:GLY:O	2:Q:89:ARG:N	2.42	0.53
3:C:154:ASN:HD21	3:C:163:HIS:HE1	1.54	0.53
3:X:65:LEU:HD13	3:X:93:CYS:CB	2.37	0.53
3:R:100:ILE:HG22	3:R:100:ILE:O	2.07	0.53
3:U:165:VAL:HG13	3:U:201:VAL:HG22	1.91	0.53
1:J:25:LEU:HD21	1:J:119:ASN:OD1	2.08	0.53
3:L:206:ASN:HB2	3:L:211:SER:HA	1.91	0.53
2:Z:42:ARG:HB3	2:Z:44:TRP:NE1	2.24	0.53
1:Y:28:ILE:O	1:Y:36:LEU:HD11	2.08	0.53
3:F:53:GLN:HE21	3:F:55:SER:HB3	1.73	0.53
2:H:183:ARG:HG3	2:H:194:TRP:CE3	2.43	0.53
3:L:202:ARG:HD2	3:L:215:TRP:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:44:TRP:HH2	2:Z:72:LEU:HD21	1.74	0.53
1:G:18:LEU:HD11	1:G:122:ILE:HG23	1.91	0.53
1:J:10:THR:HA	1:J:13:GLN:OE1	2.08	0.53
2:N:146:LEU:HB3	2:N:179:GLU:HB2	1.90	0.53
3:O:138:LEU:H	3:O:138:LEU:CD1	2.21	0.53
2:H:185:LYS:HB2	2:H:194:TRP:CE3	2.44	0.53
2:W:85:ARG:HD3	2:W:90:TRP:CZ2	2.44	0.52
3:R:62:ASN:ND2	4:R:300:NAG:C1	2.69	0.52
2:H:44:TRP:CH2	2:H:64:LEU:HD13	2.45	0.52
2:N:78:VAL:O	2:N:98:PHE:HB3	2.09	0.52
3:X:128:ASN:C	3:X:129:LEU:HD23	2.29	0.52
3:X:109:GLN:HA	3:X:120:ALA:O	2.10	0.52
1:A:62:GLU:HA	1:A:62:GLU:OE2	2.10	0.52
2:Z:41:ARG:O	2:Z:42:ARG:HD3	2.09	0.52
4:C:234:NAG:O7	4:C:234:NAG:H3	2.08	0.52
2:N:71:LYS:O	2:N:72:LEU:HD23	2.08	0.52
2:H:135:PHE:CE1	2:H:186:PRO:HB3	2.44	0.52
2:Z:141:PHE:HA	2:Z:183:ARG:O	2.08	0.52
2:Z:21:VAL:HA	2:Z:58:TRP:O	2.09	0.52
2:E:139:LEU:HB2	2:E:163:LYS:HB2	1.91	0.52
1:D:24:ILE:HD11	1:D:85:VAL:HG21	1.91	0.52
1:A:85:VAL:O	1:A:89:ILE:HG13	2.10	0.52
1:A:85:VAL:HG13	1:A:86:VAL:N	2.23	0.52
3:U:204:ARG:HB2	3:U:215:TRP:CE3	2.44	0.52
3:X:204:ARG:HG2	3:X:205:PHE:N	2.25	0.52
2:E:124:ILE:HG21	2:E:180:PHE:CD2	2.45	0.52
3:X:68:TRP:HE3	3:X:77:VAL:HG13	1.73	0.52
1:Y:69:VAL:HG11	1:Y:114:ILE:HD12	1.91	0.52
1:Y:28:ILE:HD11	1:Y:70:LEU:CD2	2.39	0.52
1:P:63:LEU:HD13	1:P:90:ASN:HB2	1.91	0.52
1:A:31:TYR:HD2	1:A:36:LEU:HB2	1.74	0.52
2:N:162:GLN:HG3	3:O:178:GLN:HE21	1.74	0.52
2:Z:8:PHE:CE1	2:Z:82:VAL:HG22	2.44	0.52
1:J:88:ASN:HD21	2:K:42:ARG:HH22	1.52	0.52
2:Z:160:LEU:CD1	2:Z:164:GLN:HB3	2.39	0.52
2:N:17:GLN:HE21	2:N:63:ILE:HD11	1.74	0.52
2:E:172:LEU:HD22	2:E:178:TYR:CE1	2.45	0.52
1:Y:117:PHE:HE1	1:Y:121:TRP:NE1	2.06	0.52
3:X:192:ASP:OD2	3:X:195:LYS:HG3	2.10	0.52
3:R:67:TYR:HB2	3:R:106:PHE:CZ	2.44	0.52
2:E:162:GLN:HE22	3:F:187:SER:CB	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:107:MET:HB2	2:Z:129:SER:HB3	1.91	0.52
2:Z:15:ARG:HD3	2:Z:68:ASP:O	2.09	0.52
2:B:50:LEU:CD2	2:B:60:CYS:HB2	2.38	0.52
2:K:142:GLU:HA	2:K:158:LEU:O	2.10	0.52
1:S:28:ILE:HG12	1:S:78:PHE:HZ	1.73	0.52
2:K:101:PHE:HA	2:K:104:LEU:HD21	1.91	0.52
2:N:143:ALA:HB1	2:N:180:PHE:HE1	1.73	0.52
2:K:162:GLN:OE1	2:K:162:GLN:N	2.43	0.52
2:E:42:ARG:NH2	2:E:76:ASP:OD1	2.38	0.52
2:T:166:TRP:NE1	4:T:215:NAG:H3	2.25	0.52
2:K:54:SER:OG	2:K:55:GLN:N	2.43	0.52
3:U:123:MET:O	3:U:124:LEU:HD23	2.09	0.52
2:Q:144:ARG:NH1	2:Q:152:TRP:HB3	2.23	0.52
1:P:82:PRO:O	1:P:86:VAL:HG23	2.10	0.52
2:T:52:PRO:HA	2:T:57:SER:O	2.10	0.52
3:C:133:TRP:HB2	3:C:155:ARG:HG3	1.91	0.52
2:K:142:GLU:O	2:K:182:VAL:HA	2.10	0.52
1:J:46:MET:HB3	1:J:47:PRO:HD2	1.89	0.52
2:T:22:TRP:CZ2	2:T:24:GLN:HB2	2.44	0.52
1:S:65:PRO:O	1:S:68:GLU:N	2.42	0.52
3:R:69:TYR:CE1	3:R:101:HIS:HD2	2.27	0.52
3:O:162:GLU:OE2	3:O:204:ARG:HD2	2.09	0.52
2:W:74:THR:HA	2:W:101:PHE:CD1	2.44	0.52
3:L:198:THR:HG23	3:L:223:HIS:CE1	2.44	0.52
2:Q:16:ALA:HB1	2:Q:65:GLY:N	2.25	0.52
3:F:49:ASN:ND2	4:F:234:NAG:C1	2.73	0.52
1:Y:64:LYS:N	1:Y:65:PRO:HD2	2.24	0.52
1:G:84:ASP:O	1:G:87:SER:HB2	2.10	0.52
2:Q:98:PHE:CZ	2:Q:100:PRO:HA	2.44	0.52
1:Y:17:LEU:HD23	1:Y:125:CYS:SG	2.49	0.52
3:U:68:TRP:CE3	3:U:77:VAL:HG13	2.41	0.52
1:Y:63:LEU:O	1:Y:66:LEU:HB3	2.09	0.52
2:T:137:ARG:NH2	3:U:162:GLU:OE1	2.38	0.52
2:Z:124:ILE:HD11	2:Z:203:PHE:CE2	2.44	0.52
3:F:102:LEU:HD23	3:F:126:LEU:HB3	1.92	0.52
3:I:68:TRP:CZ2	3:I:107:VAL:HG11	2.45	0.52
1:S:40:LEU:O	1:S:113:THR:HG22	2.10	0.52
2:Q:101:PHE:HD2	2:Q:104:LEU:HD11	1.72	0.52
1:Y:15:GLU:O	1:Y:18:LEU:HB3	2.09	0.52
1:J:74:HIS:CG	1:J:75:SER:N	2.78	0.52
1:S:94:LEU:HD23	1:S:97:LYS:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:THR:CG2	1:D:132:LEU:HD11	2.40	0.52
3:F:102:LEU:C	3:F:104:GLN:H	2.12	0.52
2:Z:12:TYR:O	2:Z:104:LEU:HA	2.10	0.52
1:P:21:LEU:HA	1:P:24:ILE:HD13	1.92	0.52
2:T:112:LEU:HD12	2:T:112:LEU:H	1.75	0.52
2:T:54:SER:H	2:T:57:SER:HB2	1.74	0.52
1:D:131:THR:HG22	1:D:131:THR:O	2.09	0.51
3:R:61:THR:HG22	3:R:62:ASN:N	2.25	0.51
2:H:72:LEU:HD13	2:H:100:PRO:CG	2.40	0.51
1:S:84:ASP:O	1:S:87:SER:HB2	2.10	0.51
2:B:39:PRO:HD2	2:B:44:TRP:O	2.10	0.51
2:Q:118:GLU:O	2:Q:205:THR:HG23	2.10	0.51
3:O:60:PRO:HB3	3:O:89:ILE:HD11	1.91	0.51
1:V:19:LEU:CD2	2:W:136:GLU:HB2	2.39	0.51
1:P:42:PHE:CE1	1:P:72:LEU:HD11	2.44	0.51
1:M:113:THR:HG23	1:M:116:GLU:OE1	2.10	0.51
4:C:300:NAG:H82	2:Z:113:GLN:OE1	2.10	0.51
4:T:215:NAG:H61	4:U:233:NAG:C8	2.41	0.51
3:I:150:LEU:O	3:I:185:LYS:HA	2.10	0.51
2:H:115:VAL:HG11	4:H:215:NAG:O5	2.10	0.51
2:H:178:TYR:HB2	2:H:203:PHE:CE1	2.45	0.51
2:K:13:ASN:O	2:K:14:SER:HB3	2.09	0.51
2:B:12:TYR:CD2	2:B:100:PRO:CB	2.93	0.51
2:B:72:LEU:HD13	2:B:100:PRO:CG	2.39	0.51
1:A:11:GLN:NE2	1:A:133:THR:OG1	2.39	0.51
2:E:51:LEU:HB3	2:E:52:PRO:HD2	1.91	0.51
2:Z:177:GLN:O	2:Z:178:TYR:CD2	2.64	0.51
1:S:50:ALA:HA	1:S:55:HIS:ND1	2.25	0.51
2:E:119:THR:HG22	2:E:206:LYS:O	2.10	0.51
1:D:66:LEU:CD1	1:D:70:LEU:HD11	2.39	0.51
2:T:92:VAL:O	2:T:92:VAL:HG12	2.10	0.51
2:T:141:PHE:CE2	2:T:184:VAL:HG22	2.46	0.51
2:E:44:TRP:CH2	2:E:64:LEU:HD13	2.46	0.51
1:J:24:ILE:HG23	1:J:70:LEU:HD21	1.92	0.51
3:U:68:TRP:CE3	3:U:77:VAL:HG22	2.45	0.51
2:K:141:PHE:HB2	2:K:160:LEU:HB2	1.92	0.51
2:Q:142:GLU:OE1	2:Q:157:LEU:HD13	2.09	0.51
2:T:54:SER:HB3	2:T:57:SER:HB2	1.93	0.51
1:G:81:ASP:OD1	1:G:82:PRO:HD2	2.10	0.51
2:W:13:ASN:ND2	2:W:16:ALA:H	2.05	0.51
1:D:43:LYS:HB3	1:D:111:THR:OG1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:71:LYS:O	2:Z:72:LEU:HD23	2.09	0.51
1:M:122:ILE:O	1:M:126:GLN:CG	2.58	0.51
1:D:97:LYS:HG3	1:D:98:GLY:H	1.76	0.51
3:O:205:PHE:CZ	3:O:209:CYS:HB2	2.45	0.51
3:X:67:TYR:CE1	3:X:78:GLN:HB2	2.46	0.51
1:J:18:LEU:HD22	1:J:126:GLN:HG2	1.92	0.51
1:J:35:LYS:HZ3	1:J:73:ALA:HA	1.76	0.51
3:U:140:LEU:HD11	3:U:199:PHE:CD2	2.46	0.51
1:J:62:GLU:O	1:J:65:PRO:HG2	2.10	0.51
3:U:42:VAL:O	3:U:130:VAL:HA	2.10	0.51
2:T:12:TYR:CE2	2:T:14:SER:HA	2.45	0.51
2:B:109:PRO:HG2	2:B:182:VAL:HG13	1.92	0.51
3:F:167:TYR:CD1	3:F:167:TYR:C	2.84	0.51
3:U:204:ARG:HG2	3:U:205:PHE:N	2.26	0.51
2:W:33:CYS:O	2:W:50:LEU:HB2	2.11	0.51
2:Z:142:GLU:O	2:Z:182:VAL:HA	2.10	0.51
2:E:13:ASN:OD1	2:E:13:ASN:O	2.29	0.51
2:Q:115:VAL:HG11	4:Q:215:NAG:C6	2.28	0.51
2:K:73:THR:HG22	2:K:75:VAL:H	1.74	0.51
1:M:16:HIS:ND1	2:N:134:TYR:HD2	2.06	0.51
2:E:12:TYR:CD2	2:E:100:PRO:HB3	2.46	0.51
1:S:28:ILE:HG12	1:S:78:PHE:CZ	2.46	0.51
2:H:46:GLN:HG3	2:H:62:LEU:HD22	1.92	0.51
1:V:24:ILE:HG23	1:V:80:PHE:CZ	2.45	0.51
1:P:67:GLU:OE2	1:P:83:ARG:HA	2.11	0.51
1:G:59:LEU:HD13	1:G:121:TRP:CG	2.46	0.51
3:X:154:ASN:ND2	3:X:163:HIS:HE1	2.08	0.51
3:R:136:GLU:OE2	3:R:155:ARG:HD3	2.11	0.51
1:D:12:LEU:O	1:D:12:LEU:HD23	2.10	0.51
3:X:38:VAL:HG13	3:X:51:THR:O	2.10	0.51
3:L:182:TYR:CD1	3:L:183:ARG:HD3	2.46	0.51
2:T:112:LEU:HG	2:T:126:TRP:HB3	1.93	0.51
2:H:139:LEU:HD23	2:H:186:PRO:HA	1.93	0.51
2:N:10:CYS:HA	2:N:19:SER:O	2.11	0.51
2:H:12:TYR:HD1	2:H:13:ASN:H	1.59	0.51
3:F:162:GLU:OE2	3:F:204:ARG:HD3	2.10	0.51
3:L:188:LEU:CD2	3:L:199:PHE:CZ	2.94	0.51
1:V:97:LYS:HG3	1:V:98:GLY:N	2.20	0.51
3:F:140:LEU:HD13	3:F:224:TRP:HB2	1.92	0.51
2:N:83:LEU:HD21	2:N:92:VAL:HG22	1.93	0.51
2:Q:7:GLN:O	2:Q:22:TRP:HD1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:46:MET:HB3	1:M:47:PRO:HD2	1.92	0.51
2:H:39:PRO:HG3	2:H:44:TRP:CZ3	2.46	0.50
2:K:74:THR:N	2:K:101:PHE:CD1	2.78	0.50
1:G:103:PHE:CD1	1:G:104:MET:N	2.79	0.50
2:B:73:THR:CG2	2:B:74:THR:N	2.74	0.50
2:N:181:GLN:HE21	2:N:200:PRO:CD	2.24	0.50
3:O:64:THR:HA	3:O:83:TYR:OH	2.11	0.50
2:W:146:LEU:HB3	2:W:179:GLU:HB2	1.92	0.50
1:J:74:HIS:CD2	1:J:75:SER:H	2.29	0.50
3:U:152:TRP:HZ2	3:U:163:HIS:CD2	2.29	0.50
2:W:95:ILE:HG12	2:W:96:GLN:N	2.25	0.50
3:F:48:MET:HB2	3:F:100:ILE:HD11	1.93	0.50
3:U:204:ARG:HG3	3:U:214:HIS:O	2.12	0.50
2:T:167:ILE:HG21	2:T:180:PHE:CE1	2.46	0.50
2:K:162:GLN:NE2	2:K:164:GLN:OE1	2.44	0.50
3:R:65:LEU:HD23	3:R:65:LEU:C	2.31	0.50
2:H:141:PHE:HA	2:H:183:ARG:O	2.11	0.50
1:D:46:MET:HB3	1:D:47:PRO:HD2	1.92	0.50
3:O:175:TRP:HE1	1:V:106:GLU:HG3	1.76	0.50
2:B:146:LEU:HB2	2:B:152:TRP:CH2	2.46	0.50
2:W:106:LEU:HD12	2:W:106:LEU:N	2.27	0.50
2:K:78:VAL:O	2:K:98:PHE:HB3	2.11	0.50
3:L:89:ILE:HG22	3:L:90:THR:N	2.26	0.50
1:D:112:ALA:HB1	1:D:116:GLU:HB2	1.92	0.50
1:G:18:LEU:CD2	3:I:208:LEU:HA	2.41	0.50
1:V:127:SER:O	1:V:130:SER:HB3	2.12	0.50
1:A:23:MET:SD	1:A:80:PHE:HB3	2.50	0.50
2:W:141:PHE:HA	2:W:183:ARG:O	2.11	0.50
2:T:159:THR:HG22	2:T:161:LYS:HG3	1.92	0.50
3:L:129:LEU:O	3:L:131:ILE:HG12	2.12	0.50
1:Y:69:VAL:O	1:Y:72:LEU:HG	2.11	0.50
2:W:106:LEU:HD13	2:W:186:PRO:HD3	1.93	0.50
2:Q:112:LEU:HD21	2:Q:198:SER:OG	2.11	0.50
1:S:48:LYS:HB2	1:S:106:GLU:O	2.11	0.50
1:M:45:TYR:CE1	1:M:111:THR:HG22	2.46	0.50
1:Y:103:PHE:CG	1:Y:104:MET:N	2.79	0.50
1:D:11:GLN:CA	1:D:14:LEU:HD12	2.36	0.50
1:G:31:TYR:CE2	1:G:36:LEU:HB2	2.47	0.50
2:W:36:HIS:CG	2:W:38:TRP:HE1	2.30	0.50
1:V:91:VAL:HG12	2:W:75:VAL:CG2	2.42	0.50
3:O:150:LEU:HD22	3:O:152:TRP:HE3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:11:GLN:O	1:Y:15:GLU:HG3	2.11	0.50
2:K:39:PRO:HA	2:K:78:VAL:HA	1.94	0.50
3:R:191:VAL:HG23	3:R:197:TYR:CE1	2.46	0.50
1:D:78:PHE:HD2	1:D:80:PHE:CE1	2.29	0.50
1:G:52:GLU:H	1:G:55:HIS:CE1	2.30	0.50
2:Z:8:PHE:CE1	2:Z:82:VAL:CG2	2.95	0.50
2:W:141:PHE:CD2	2:W:184:VAL:HG22	2.47	0.50
3:L:85:PHE:HA	3:L:89:ILE:O	2.11	0.50
3:O:188:LEU:HD22	3:O:199:PHE:HE2	1.77	0.50
1:D:23:MET:HE3	1:D:80:PHE:HB3	1.93	0.50
3:C:46:GLU:CD	3:C:133:TRP:HE1	2.15	0.50
1:V:93:VAL:HG23	1:V:94:LEU:H	1.77	0.50
2:E:143:ALA:HB3	2:E:158:LEU:HD12	1.94	0.50
2:T:44:TRP:HH2	2:T:64:LEU:HD13	1.75	0.50
1:P:132:LEU:O	1:P:133:THR:CB	2.60	0.50
2:T:162:GLN:HE21	2:T:164:GLN:NE2	2.09	0.50
2:T:107:MET:HB2	2:T:129:SER:HB3	1.93	0.50
3:C:46:GLU:OE2	3:C:156:PHE:CE1	2.65	0.50
2:E:81:ARG:CG	2:E:95:ILE:HG22	2.34	0.50
2:K:138:HIS:CA	2:K:187:LEU:CD1	2.90	0.50
2:N:115:VAL:HG11	4:N:215:NAG:H62	1.94	0.50
3:U:148:LEU:CD2	3:U:191:VAL:HG11	2.37	0.50
2:Z:115:VAL:HG11	4:Z:215:NAG:O5	2.11	0.50
1:G:53:LEU:CD2	1:G:96:LEU:HD22	2.42	0.50
1:S:48:LYS:HD3	1:S:107:TYR:O	2.11	0.50
1:D:24:ILE:O	1:D:28:ILE:HG13	2.12	0.50
1:D:68:GLU:OE2	1:D:68:GLU:HA	2.12	0.50
2:E:39:PRO:HB2	2:E:42:ARG:HB2	1.94	0.50
1:A:36:LEU:HA	1:A:39:MET:HB3	1.93	0.50
2:E:161:LYS:H	3:F:187:SER:CB	2.23	0.50
2:H:120:HIS:CD2	2:H:174:PRO:HD3	2.46	0.50
3:R:62:ASN:HD21	4:R:300:NAG:C2	2.25	0.50
2:K:162:GLN:NE2	3:L:186:PHE:CE1	2.80	0.50
2:N:201:LEU:HD12	2:N:202:ALA:H	1.77	0.50
3:O:143:LEU:HD23	3:O:149:GLU:HB3	1.94	0.50
3:U:138:LEU:H	3:U:138:LEU:HD12	1.77	0.50
3:F:167:TYR:OH	3:F:176:THR:HG21	2.11	0.50
1:V:57:GLN:HG3	1:V:61:GLU:OE2	2.11	0.50
2:K:128:ILE:HD12	2:K:131:ALA:CB	2.41	0.50
1:G:14:LEU:HD13	1:G:128:ILE:HB	1.93	0.50
1:D:89:ILE:O	1:D:92:PHE:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:VAL:HG12	2:E:75:VAL:CG2	2.42	0.49
3:F:158:ASN:O	3:F:159:HIS:CB	2.60	0.49
3:F:67:TYR:CD1	3:F:67:TYR:C	2.86	0.49
3:F:138:LEU:HD21	3:F:219:SER:OG	2.12	0.49
3:L:109:GLN:HE21	3:L:121:THR:CG2	2.25	0.49
1:J:88:ASN:ND2	2:K:42:ARG:NH2	2.57	0.49
2:Q:136:GLU:HG3	2:Q:137:ARG:N	2.27	0.49
3:R:147:GLN:HG2	3:R:189:PRO:O	2.12	0.49
2:Z:81:ARG:HE	2:Z:95:ILE:HD12	1.77	0.49
2:W:37:ALA:HB2	2:W:62:LEU:HD22	1.94	0.49
1:G:131:THR:HG22	1:G:131:THR:O	2.11	0.49
1:M:36:LEU:O	1:M:36:LEU:HD12	2.12	0.49
2:Z:126:TRP:HZ3	2:Z:167:ILE:HG22	1.77	0.49
1:G:60:GLU:HB2	1:G:93:VAL:HG11	1.93	0.49
1:G:85:VAL:O	1:G:89:ILE:HG13	2.12	0.49
2:E:44:TRP:HH2	2:E:64:LEU:HD13	1.76	0.49
1:V:46:MET:HE3	1:V:120:ARG:HG2	1.95	0.49
3:U:38:VAL:HG21	3:U:110:LEU:HD13	1.93	0.49
2:E:143:ALA:HB1	2:E:180:PHE:CE1	2.47	0.49
3:U:69:TYR:CE1	3:U:101:HIS:ND1	2.80	0.49
1:P:113:THR:OG1	1:P:116:GLU:HG3	2.12	0.49
2:Z:10:CYS:HA	2:Z:19:SER:O	2.11	0.49
1:J:126:GLN:CD	3:L:210:GLY:HA2	2.32	0.49
2:E:171:THR:O	2:E:171:THR:HG22	2.13	0.49
2:E:161:LYS:N	3:F:187:SER:OG	2.34	0.49
1:V:91:VAL:HG12	2:W:75:VAL:HG21	1.94	0.49
1:V:46:MET:SD	1:V:112:ALA:HB3	2.52	0.49
1:D:16:HIS:CB	2:E:134:TYR:HD2	2.26	0.49
1:J:65:PRO:HA	1:J:68:GLU:HB2	1.93	0.49
2:Z:109:PRO:HG3	2:Z:184:VAL:CG2	2.42	0.49
2:B:173:THR:HB	2:B:176:THR:OG1	2.12	0.49
2:W:13:ASN:CG	2:W:17:GLN:H	2.15	0.49
2:E:167:ILE:HD11	3:F:189:PRO:CB	2.43	0.49
1:D:60:GLU:CA	1:D:63:LEU:HD12	2.36	0.49
3:F:103:TYR:OH	3:F:209:CYS:HB3	2.13	0.49
2:T:83:LEU:HB3	2:T:90:TRP:HB3	1.93	0.49
3:F:204:ARG:HB2	3:F:215:TRP:CD2	2.47	0.49
2:Z:40:ASP:OD2	2:Z:41:ARG:NH1	2.45	0.49
1:S:28:ILE:CG2	1:S:28:ILE:O	2.61	0.49
2:T:66:ALA:O	2:T:67:PRO:C	2.50	0.49
1:V:87:SER:O	1:V:91:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:157:LEU:CD1	3:X:161:LEU:HD13	2.42	0.49
2:H:23:SER:HB3	2:H:57:SER:OG	2.12	0.49
2:Q:205:THR:HG22	2:Q:206:LYS:N	2.26	0.49
2:W:143:ALA:HB1	2:W:180:PHE:CE1	2.47	0.49
2:Q:158:LEU:HD23	3:R:147:GLN:NE2	2.27	0.49
3:U:134:ALA:HB2	3:U:217:GLU:O	2.12	0.49
2:T:176:THR:HG22	2:T:177:GLN:O	2.12	0.49
3:F:144:SER:OG	3:F:147:GLN:HG3	2.13	0.49
2:T:23:SER:HB2	2:T:56:ALA:O	2.12	0.49
3:F:68:TRP:CE3	3:F:77:VAL:HG13	2.48	0.49
3:F:80:CYS:HB3	3:F:83:TYR:CE1	2.48	0.49
2:W:78:VAL:CG2	2:W:100:PRO:HG3	2.42	0.49
1:J:47:PRO:CG	1:J:50:ALA:HB2	2.43	0.49
3:U:67:TYR:HE2	3:U:95:LEU:HD21	1.75	0.49
2:K:8:PHE:CE1	2:K:82:VAL:CG2	2.95	0.49
1:G:28:ILE:HD11	1:G:70:LEU:HD21	1.94	0.49
1:M:50:ALA:HB3	1:M:120:ARG:NH2	2.27	0.49
2:H:138:HIS:HB2	2:H:187:LEU:HG	1.95	0.49
3:I:110:LEU:C	3:I:110:LEU:HD23	2.33	0.49
1:G:114:ILE:O	1:G:118:LEU:HD12	2.11	0.49
2:K:162:GLN:HG3	3:L:178:GLN:HE21	1.76	0.49
3:L:166:GLN:NE2	3:L:218:TRP:CH2	2.81	0.49
2:Q:23:SER:HB3	2:Q:57:SER:OG	2.13	0.49
3:L:44:ASN:ND2	3:L:133:TRP:CD1	2.80	0.49
2:K:201:LEU:HD12	2:K:202:ALA:H	1.77	0.49
3:R:82:HIS:HD2	3:R:94:GLN:HB3	1.77	0.49
2:E:118:GLU:OE1	2:E:121:ARG:HD3	2.10	0.49
3:C:192:ASP:OD2	3:C:195:LYS:HE3	2.12	0.49
1:D:89:ILE:O	1:D:93:VAL:HG23	2.13	0.49
3:I:204:ARG:HG2	3:I:205:PHE:N	2.27	0.49
1:G:64:LYS:O	1:G:68:GLU:HG2	2.12	0.49
3:X:157:LEU:HD12	3:X:157:LEU:O	2.12	0.49
3:O:45:VAL:HG12	3:O:45:VAL:O	2.12	0.49
1:V:18:LEU:CD1	1:V:122:ILE:HG23	2.42	0.49
1:Y:18:LEU:CD1	1:Y:122:ILE:HG23	2.43	0.49
3:F:65:LEU:HD23	3:F:66:HIS:N	2.28	0.49
2:H:171:THR:O	2:H:171:THR:HG22	2.12	0.49
1:A:31:TYR:CD2	1:A:36:LEU:HB2	2.48	0.49
2:H:40:ASP:OD1	2:H:41:ARG:N	2.46	0.49
3:U:106:PHE:O	3:U:124:LEU:N	2.46	0.49
2:B:72:LEU:HD13	2:B:100:PRO:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:192:ASP:OD1	3:R:195:LYS:HG3	2.12	0.49
1:P:41:THR:O	1:P:43:LYS:HG3	2.12	0.49
1:A:81:ASP:HB3	1:A:84:ASP:HB2	1.95	0.49
2:W:79:THR:HA	2:W:97:ASP:HA	1.93	0.49
2:Q:91:ARG:HG2	2:Q:93:MET:HE1	1.94	0.49
2:T:181:GLN:HG2	2:T:198:SER:O	2.13	0.49
2:B:81:ARG:HH11	2:B:95:ILE:HD12	1.76	0.49
2:Z:102:GLU:C	2:Z:103:ASN:HD22	2.16	0.49
2:K:101:PHE:HD2	2:K:188:GLN:OE1	1.96	0.49
1:P:20:ASP:OD2	2:Q:134:TYR:OH	2.18	0.49
3:R:136:GLU:CD	3:R:155:ARG:HD3	2.33	0.49
3:I:85:PHE:CE2	3:I:90:THR:HG22	2.48	0.49
3:L:65:LEU:HD23	3:L:66:HIS:N	2.27	0.49
3:O:192:ASP:OD1	3:O:195:LYS:HG3	2.12	0.49
1:G:62:GLU:OE2	1:G:62:GLU:HA	2.12	0.49
1:S:81:ASP:CB	1:S:84:ASP:HB2	2.40	0.49
2:K:201:LEU:HD12	2:K:202:ALA:N	2.27	0.49
1:A:59:LEU:HD13	1:A:121:TRP:CG	2.47	0.49
3:I:102:LEU:HD23	3:I:126:LEU:HB3	1.94	0.49
1:J:69:VAL:O	1:J:72:LEU:HG	2.12	0.49
2:Q:145:THR:OG1	2:Q:169:LEU:HD13	2.12	0.49
1:D:59:LEU:HD13	1:D:121:TRP:CG	2.47	0.48
2:Z:78:VAL:O	2:Z:98:PHE:HB3	2.12	0.48
1:G:78:PHE:CD1	1:G:78:PHE:N	2.80	0.48
2:E:47:THR:CG2	2:E:48:CYS:N	2.76	0.48
2:H:8:PHE:CE1	2:H:82:VAL:HG21	2.48	0.48
1:P:89:ILE:O	1:P:93:VAL:HG23	2.13	0.48
2:E:98:PHE:O	2:E:100:PRO:HD3	2.12	0.48
2:W:78:VAL:O	2:W:80:LEU:HD12	2.11	0.48
1:Y:92:PHE:CZ	2:Z:73:THR:OG1	2.63	0.48
1:V:24:ILE:CG2	1:V:70:LEU:HD11	2.43	0.48
1:G:14:LEU:CD1	1:G:128:ILE:HB	2.43	0.48
1:M:14:LEU:HD11	1:M:128:ILE:HG21	1.95	0.48
3:U:45:VAL:CG2	3:U:157:LEU:HD11	2.43	0.48
1:S:128:ILE:O	1:S:132:LEU:HD23	2.14	0.48
1:D:53:LEU:O	1:D:56:LEU:HB2	2.13	0.48
3:I:63:LEU:HD13	3:I:110:LEU:HD21	1.95	0.48
3:U:167:TYR:HB3	3:U:199:PHE:CD1	2.48	0.48
2:B:98:PHE:CE2	2:B:100:PRO:HA	2.48	0.48
2:Q:114:VAL:CG1	2:Q:117:VAL:HG13	2.42	0.48
2:T:44:TRP:CH2	2:T:72:LEU:HD21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:6:SER:HA	1:S:9:LYS:HE2	1.95	0.48
3:O:143:LEU:CD2	3:O:149:GLU:HB3	2.43	0.48
3:L:154:ASN:HD21	3:L:163:HIS:CE1	2.31	0.48
2:K:23:SER:HB3	2:K:57:SER:OG	2.14	0.48
3:X:201:VAL:O	3:X:219:SER:HB3	2.14	0.48
2:H:83:LEU:HD21	2:W:38:TRP:CH2	2.49	0.48
2:T:74:THR:N	2:T:101:PHE:CD1	2.81	0.48
1:V:92:PHE:O	1:V:96:LEU:HD13	2.13	0.48
2:N:15:ARG:NH1	2:N:70:GLN:OE1	2.42	0.48
2:E:103:ASN:OD1	2:E:191:PHE:CB	2.60	0.48
3:I:48:MET:HB2	3:I:100:ILE:HD11	1.95	0.48
2:K:183:ARG:HD2	2:K:194:TRP:HB3	1.96	0.48
2:T:198:SER:O	2:T:199:GLN:C	2.52	0.48
2:Q:167:ILE:HG12	2:Q:168:CYS:N	2.28	0.48
2:T:118:GLU:HA	2:T:206:LYS:HD2	1.94	0.48
2:W:118:GLU:C	2:W:206:LYS:HB2	2.33	0.48
3:L:169:THR:N	3:L:172:ASP:HB2	2.19	0.48
2:E:146:LEU:HD22	2:E:152:TRP:CE2	2.48	0.48
1:Y:49:LYS:HE2	1:Y:49:LYS:HB3	1.68	0.48
1:J:126:GLN:HA	1:J:129:ILE:HG22	1.95	0.48
3:F:128:ASN:CG	3:F:211:SER:HB2	2.33	0.48
1:Y:87:SER:O	1:Y:91:VAL:HG23	2.14	0.48
2:W:115:VAL:HG21	2:W:123:ASN:ND2	2.28	0.48
2:Q:95:ILE:CG1	2:Q:96:GLN:N	2.72	0.48
2:T:71:LYS:O	2:T:72:LEU:HD23	2.13	0.48
2:B:146:LEU:HB3	2:B:179:GLU:HB2	1.95	0.48
1:P:103:PHE:CG	1:P:104:MET:N	2.81	0.48
3:O:155:ARG:HG3	3:O:156:PHE:CD2	2.49	0.48
2:N:114:VAL:CG1	2:N:117:VAL:HG13	2.44	0.48
2:Z:146:LEU:HD22	2:Z:152:TRP:NE1	2.29	0.48
2:Z:9:THR:HG22	2:Z:11:PHE:HE1	1.77	0.48
1:S:28:ILE:HD13	1:S:39:MET:HE2	1.95	0.48
3:X:160:CYS:HB3	3:X:205:PHE:CE1	2.48	0.48
3:U:52:TRP:CH2	3:U:92:GLY:HA2	2.48	0.48
2:T:33:CYS:O	2:T:50:LEU:HB2	2.14	0.48
1:J:64:LYS:N	1:J:65:PRO:HD2	2.28	0.48
3:L:40:CYS:O	3:L:41:PHE:CG	2.66	0.48
2:Z:166:TRP:C	2:Z:166:TRP:CE3	2.87	0.48
3:O:110:LEU:HA	3:O:110:LEU:HD23	1.58	0.48
1:P:80:PHE:CD1	1:P:80:PHE:O	2.67	0.48
1:D:52:GLU:OE1	1:D:54:LYS:HE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:24:ILE:HD11	1:J:85:VAL:HG21	1.94	0.48
2:Q:83:LEU:HD22	2:Q:92:VAL:HG22	1.96	0.48
2:N:181:GLN:NE2	2:N:200:PRO:HD3	2.26	0.48
2:W:136:GLU:HG2	2:W:137:ARG:N	2.29	0.48
1:S:18:LEU:HD11	1:S:122:ILE:HG23	1.95	0.48
3:O:198:THR:HG21	1:V:104:MET:CE	2.44	0.48
2:B:46:GLN:HG3	2:B:47:THR:N	2.28	0.48
1:J:18:LEU:HD21	1:J:126:GLN:HE21	1.78	0.48
1:J:25:LEU:HD11	1:J:115:VAL:HG13	1.96	0.48
1:G:45:TYR:HE1	1:G:111:THR:CG2	2.26	0.48
1:M:16:HIS:ND1	2:N:134:TYR:CD2	2.77	0.48
2:K:176:THR:HG22	2:K:177:GLN:N	2.29	0.48
3:F:110:LEU:C	3:F:110:LEU:HD23	2.33	0.48
1:S:27:GLY:O	1:S:78:PHE:HE1	1.97	0.48
3:O:164:LEU:HD11	3:O:177:GLU:HB2	1.96	0.48
2:K:12:TYR:CD1	2:K:13:ASN:N	2.82	0.48
1:V:20:ASP:OD2	2:W:134:TYR:CE2	2.67	0.48
1:P:24:ILE:HD12	1:P:24:ILE:H	1.79	0.48
1:P:65:PRO:O	1:P:68:GLU:HB2	2.13	0.48
3:O:102:LEU:HD22	3:O:127:GLN:CA	2.44	0.48
3:R:166:GLN:HG2	3:R:177:GLU:HB3	1.95	0.48
1:Y:18:LEU:HD11	1:Y:22:GLN:NE2	2.28	0.48
2:K:50:LEU:HD22	2:K:58:TRP:HB3	1.95	0.48
1:M:74:HIS:CG	1:M:75:SER:N	2.81	0.48
2:E:161:LYS:HB2	3:F:187:SER:OG	2.14	0.47
1:G:20:ASP:OD2	2:H:134:TYR:OH	2.22	0.47
1:G:39:MET:HG3	1:G:69:VAL:HG13	1.96	0.47
2:H:39:PRO:HA	2:H:78:VAL:HA	1.95	0.47
1:Y:57:GLN:CD	1:Y:97:LYS:HZ2	2.17	0.47
1:J:11:GLN:HB2	1:J:132:LEU:HD13	1.95	0.47
3:R:69:TYR:CE1	3:R:101:HIS:CD2	3.02	0.47
2:K:51:LEU:C	2:K:58:TRP:HD1	2.16	0.47
3:U:137:ASN:O	3:U:139:THR:HG23	2.14	0.47
1:S:60:GLU:O	1:S:63:LEU:HB2	2.14	0.47
1:P:28:ILE:HG22	1:P:28:ILE:O	2.14	0.47
3:F:146:SER:O	3:F:191:VAL:HG22	2.14	0.47
2:K:139:LEU:N	2:K:187:LEU:HG	2.28	0.47
1:V:95:GLU:CG	2:W:41:ARG:NH1	2.77	0.47
1:J:24:ILE:CG2	1:J:118:LEU:HD11	2.44	0.47
3:X:68:TRP:CE3	3:X:77:VAL:HG13	2.48	0.47
3:R:169:THR:HA	3:R:196:ARG:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:56:LEU:HD23	1:Y:121:TRP:HZ3	1.79	0.47
3:R:65:LEU:HD13	3:R:93:CYS:HB3	1.96	0.47
3:L:135:PRO:HG2	3:L:201:VAL:HG12	1.95	0.47
2:K:83:LEU:HD21	2:K:92:VAL:HG22	1.96	0.47
3:O:168:ARG:HB2	3:O:172:ASP:HB3	1.95	0.47
2:T:98:PHE:HE2	2:T:100:PRO:HA	1.77	0.47
3:C:47:TYR:HA	3:C:100:ILE:HD11	1.96	0.47
3:X:57:GLU:HB3	3:X:58:PRO:HD2	1.97	0.47
2:K:139:LEU:C	2:K:187:LEU:HD21	2.33	0.47
2:H:83:LEU:HD12	2:H:83:LEU:N	2.29	0.47
2:T:21:VAL:HA	2:T:58:TRP:O	2.15	0.47
1:D:23:MET:SD	2:E:133:HIS:CE1	3.08	0.47
1:D:23:MET:HG2	1:D:80:PHE:HD2	1.77	0.47
3:F:48:MET:HB2	3:F:100:ILE:CD1	2.45	0.47
1:Y:20:ASP:OD2	1:Y:89:ILE:CG1	2.62	0.47
2:K:104:LEU:HD12	2:K:188:GLN:O	2.15	0.47
3:C:65:LEU:C	3:C:65:LEU:HD23	2.35	0.47
2:K:10:CYS:HA	2:K:19:SER:O	2.13	0.47
1:M:88:ASN:HD21	2:N:42:ARG:HH12	1.62	0.47
2:K:171:THR:HG22	2:K:171:THR:O	2.15	0.47
2:W:22:TRP:CZ2	2:W:24:GLN:HB2	2.48	0.47
3:L:206:ASN:HA	3:L:210:GLY:O	2.14	0.47
1:V:81:ASP:CB	1:V:84:ASP:HB2	2.29	0.47
2:Z:13:ASN:HD21	2:Z:17:GLN:HB2	1.72	0.47
2:T:39:PRO:CG	2:T:42:ARG:HB2	2.45	0.47
1:P:31:TYR:OH	1:P:35:LYS:HB2	2.15	0.47
1:V:97:LYS:CG	1:V:98:GLY:H	2.24	0.47
2:K:13:ASN:CG	2:K:17:GLN:H	2.18	0.47
3:U:52:TRP:CD2	3:U:110:LEU:HD21	2.50	0.47
2:T:172:LEU:HD22	2:T:178:TYR:CE1	2.49	0.47
3:O:154:ASN:HD21	3:O:163:HIS:HE1	1.60	0.47
3:L:165:VAL:HG12	3:L:178:GLN:O	2.14	0.47
1:Y:94:LEU:CD2	1:Y:97:LYS:HE2	2.44	0.47
1:G:28:ILE:HD11	1:G:70:LEU:CD2	2.44	0.47
1:S:126:GLN:OE1	3:U:210:GLY:HA2	2.15	0.47
2:E:170:GLU:H	3:F:190:SER:HB3	1.80	0.47
3:C:180:VAL:HG11	3:C:185:LYS:O	2.15	0.47
3:I:165:VAL:HG21	3:I:186:PHE:CB	2.45	0.47
1:S:85:VAL:HG13	1:S:86:VAL:N	2.29	0.47
2:H:14:SER:O	2:H:132:SER:HB2	2.15	0.47
2:H:123:ASN:HD21	4:H:215:NAG:C2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:128:ASN:C	3:U:129:LEU:HD23	2.34	0.47
2:N:51:LEU:O	2:N:58:TRP:HA	2.14	0.47
2:K:44:TRP:CH2	2:K:64:LEU:HD13	2.50	0.47
1:M:16:HIS:HB3	2:N:134:TYR:CD2	2.50	0.47
1:P:44:PHE:CE2	1:P:114:ILE:HB	2.47	0.47
1:J:56:LEU:O	1:J:59:LEU:HB3	2.14	0.47
2:W:141:PHE:HB2	2:W:160:LEU:HD12	1.96	0.47
1:M:84:ASP:O	1:M:87:SER:HB2	2.14	0.47
1:A:112:ALA:HB1	1:A:116:GLU:HB2	1.96	0.47
2:K:204:ARG:HG2	2:K:205:THR:H	1.79	0.47
3:F:54:SER:O	3:F:55:SER:C	2.53	0.47
2:K:8:PHE:CE1	2:K:82:VAL:HG22	2.50	0.47
3:R:102:LEU:O	3:R:103:TYR:HB2	2.15	0.47
3:R:140:LEU:HD21	3:R:199:PHE:CD1	2.50	0.47
3:L:38:VAL:HG21	3:L:110:LEU:HG	1.97	0.47
3:L:49:ASN:ND2	4:L:233:NAG:C1	2.77	0.47
2:Q:147:SER:OG	2:Q:148:PRO:HD2	2.15	0.47
4:N:215:NAG:H4	4:O:233:NAG:C1	2.45	0.47
2:K:66:ALA:O	2:K:68:ASP:N	2.47	0.47
3:L:180:VAL:HG12	3:L:181:ASP:N	2.30	0.47
2:N:98:PHE:CE2	2:N:100:PRO:HA	2.50	0.47
2:Q:36:HIS:ND1	2:Q:47:THR:HG22	2.29	0.47
1:A:81:ASP:OD1	1:A:82:PRO:HD2	2.15	0.47
2:Z:125:SER:HA	2:Z:166:TRP:HA	1.95	0.47
1:G:46:MET:HB3	1:G:47:PRO:HD2	1.96	0.47
3:F:206:ASN:CG	3:F:207:PRO:CA	2.84	0.47
2:W:80:LEU:CD1	2:W:98:PHE:CB	2.93	0.47
4:O:234:NAG:O4	4:O:235:NAG:N2	2.47	0.47
2:Q:12:TYR:CD2	2:Q:100:PRO:HB3	2.50	0.47
2:K:35:VAL:HA	2:K:81:ARG:O	2.14	0.47
2:W:42:ARG:HH22	2:W:73:THR:HG23	1.79	0.47
1:V:20:ASP:OD2	2:W:134:TYR:HE2	1.98	0.47
2:N:146:LEU:HD22	2:N:152:TRP:CZ2	2.50	0.47
2:T:162:GLN:NE2	3:U:186:PHE:CE1	2.83	0.47
3:R:69:TYR:CE2	3:R:106:PHE:CD1	3.03	0.47
1:D:77:ASN:C	1:D:78:PHE:HD1	2.18	0.47
1:D:7:THR:CG2	1:D:10:THR:HB	2.44	0.47
3:F:126:LEU:O	3:F:129:LEU:HB2	2.15	0.47
3:I:40:CYS:O	3:I:41:PHE:CG	2.68	0.47
1:S:91:VAL:HG12	2:T:75:VAL:HG23	1.96	0.47
1:G:114:ILE:O	1:G:117:PHE:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:98:PHE:CE2	2:K:100:PRO:HG3	2.50	0.47
3:I:35:LEU:HD11	3:I:118:ARG:HG2	1.96	0.47
3:L:42:VAL:HG22	3:L:100:ILE:HD13	1.96	0.47
3:R:52:TRP:HE1	3:R:63:LEU:HD12	1.79	0.46
3:L:129:LEU:O	3:L:130:VAL:C	2.53	0.46
1:G:131:THR:CG2	1:G:131:THR:O	2.64	0.46
2:N:36:HIS:HB3	2:N:38:TRP:HE1	1.81	0.46
1:G:88:ASN:O	1:G:92:PHE:CD2	2.68	0.46
2:N:51:LEU:HB3	2:N:52:PRO:HD2	1.96	0.46
1:M:92:PHE:CE2	2:N:134:TYR:HE2	2.33	0.46
3:R:48:MET:CE	3:R:95:LEU:HD22	2.45	0.46
3:O:149:GLU:HG3	3:O:151:ASN:HD21	1.79	0.46
1:Y:114:ILE:O	1:Y:117:PHE:HB3	2.16	0.46
3:X:109:GLN:HG3	3:X:121:THR:HG22	1.97	0.46
3:O:192:ASP:OD1	3:O:194:GLN:HB2	2.15	0.46
3:U:139:THR:O	3:U:150:LEU:HD23	2.15	0.46
3:U:111:GLN:OE1	3:U:119:GLN:HB3	2.14	0.46
3:O:167:TYR:CE2	3:O:176:THR:HB	2.49	0.46
3:C:62:ASN:ND2	4:C:300:NAG:C8	2.78	0.46
3:F:86:SER:CB	3:F:91:SER:HB2	2.46	0.46
3:I:181:ASP:OD1	3:I:183:ARG:CD	2.61	0.46
2:W:121:ARG:HG2	2:W:170:GLU:OE2	2.15	0.46
3:U:131:ILE:HA	3:U:132:PRO:HD3	1.68	0.46
1:V:95:GLU:C	1:V:96:LEU:HD12	2.35	0.46
2:Z:70:GLN:HG2	2:Z:134:TYR:HE1	1.81	0.46
1:P:88:ASN:ND2	1:P:88:ASN:N	2.63	0.46
2:T:146:LEU:HD23	2:T:179:GLU:CB	2.45	0.46
2:B:146:LEU:HB2	2:B:152:TRP:CZ2	2.50	0.46
2:N:155:ALA:HA	2:N:156:PRO:HD3	1.69	0.46
2:Q:159:THR:HG22	2:Q:161:LYS:HG3	1.97	0.46
1:G:35:LYS:HE3	1:G:38:ARG:HB2	1.97	0.46
3:X:161:LEU:CD1	3:X:205:PHE:HD1	2.28	0.46
3:U:62:ASN:HD21	4:U:300:NAG:C2	2.28	0.46
2:K:106:LEU:HD23	2:K:184:VAL:HG13	1.97	0.46
3:X:62:ASN:CG	4:X:300:NAG:H83	2.35	0.46
3:U:64:THR:OG1	3:U:111:GLN:HB3	2.16	0.46
3:R:109:GLN:HA	3:R:120:ALA:O	2.16	0.46
2:Z:36:HIS:HB3	2:Z:38:TRP:HE1	1.81	0.46
2:B:117:VAL:O	2:B:206:LYS:HE2	2.16	0.46
2:W:114:VAL:HG22	2:W:124:ILE:HG12	1.98	0.46
2:K:144:ARG:NH1	2:K:152:TRP:HB3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:46:GLN:NE2	2:T:89:ARG:HA	2.30	0.46
2:H:64:LEU:HD23	2:H:64:LEU:N	2.30	0.46
2:W:159:THR:HG22	2:W:161:LYS:HG2	1.98	0.46
1:V:24:ILE:HG21	1:V:70:LEU:HD11	1.96	0.46
1:Y:57:GLN:NE2	1:Y:97:LYS:HZ2	2.13	0.46
3:X:62:ASN:HD21	4:X:300:NAG:C1	2.28	0.46
2:H:136:GLU:HB3	2:H:137:ARG:H	1.50	0.46
2:E:120:HIS:O	2:E:171:THR:N	2.49	0.46
2:H:38:TRP:CD1	2:H:81:ARG:NH2	2.84	0.46
2:H:15:ARG:HD2	2:H:68:ASP:O	2.16	0.46
3:O:84:LEU:HD11	3:O:94:GLN:HB2	1.98	0.46
1:V:88:ASN:ND2	2:W:73:THR:CG2	2.78	0.46
3:X:197:TYR:O	3:X:223:HIS:CA	2.60	0.46
2:K:161:LYS:NZ	3:L:185:LYS:HD3	2.27	0.46
1:S:117:PHE:HE1	1:S:121:TRP:CD1	2.33	0.46
3:F:140:LEU:CD2	3:F:150:LEU:HD13	2.45	0.46
1:V:19:LEU:HD21	2:W:136:GLU:HB2	1.98	0.46
1:M:20:ASP:OD1	1:M:23:MET:CE	2.64	0.46
1:A:59:LEU:HD13	1:A:121:TRP:CD1	2.51	0.46
2:Q:87:GLY:C	2:Q:89:ARG:H	2.19	0.46
2:H:112:LEU:HG	2:H:126:TRP:HB3	1.96	0.46
2:Q:107:MET:HG3	2:Q:108:ALA:N	2.30	0.46
3:X:42:VAL:HG22	3:X:48:MET:HB2	1.97	0.46
3:F:142:LYS:HG2	3:F:148:LEU:HB3	1.98	0.46
3:C:109:GLN:NE2	3:C:119:GLN:NE2	2.64	0.46
1:G:126:GLN:HE22	3:I:210:GLY:C	2.19	0.46
1:J:95:GLU:OE1	2:K:75:VAL:HB	2.16	0.46
2:Z:160:LEU:HD23	2:Z:160:LEU:HA	1.81	0.46
2:Q:119:THR:HA	2:Q:206:LYS:O	2.16	0.46
3:R:152:TRP:CE3	3:R:201:VAL:HG21	2.51	0.46
2:Z:183:ARG:HD3	2:Z:197:TRP:CE2	2.51	0.46
3:O:167:TYR:CD2	3:O:176:THR:HB	2.51	0.46
3:C:61:THR:OG1	3:C:114:ARG:NH2	2.33	0.46
3:X:149:GLU:HG2	3:X:151:ASN:HD21	1.81	0.46
2:Q:69:SER:OG	2:Q:71:LYS:HE2	2.16	0.46
2:N:174:PRO:HA	2:N:205:THR:HG21	1.98	0.46
3:X:128:ASN:O	3:X:212:ALA:HA	2.15	0.46
3:U:197:TYR:O	3:U:223:HIS:HA	2.15	0.46
2:H:105:ARG:HG2	2:H:105:ARG:HH21	1.80	0.46
1:S:53:LEU:HD22	1:S:96:LEU:HB3	1.98	0.46
2:E:122:CYS:O	2:E:168:CYS:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:121:ARG:NE	2:E:170:GLU:OE2	2.48	0.46
2:Z:80:LEU:HD13	2:Z:98:PHE:CB	2.46	0.46
1:G:67:GLU:OE2	1:G:83:ARG:HA	2.16	0.46
2:T:138:HIS:NE2	3:U:182:TYR:CE2	2.83	0.46
3:O:48:MET:HE3	3:O:95:LEU:HD12	1.98	0.46
1:V:62:GLU:C	1:V:65:PRO:HD2	2.35	0.46
1:Y:56:LEU:O	1:Y:59:LEU:N	2.49	0.46
1:P:7:THR:CG2	1:P:132:LEU:HD13	2.46	0.46
3:I:136:GLU:CB	3:I:137:ASN:HD22	2.29	0.46
1:J:7:THR:HG23	1:J:132:LEU:HD22	1.98	0.46
1:M:57:GLN:O	1:M:61:GLU:HG3	2.16	0.46
1:V:95:GLU:HG2	2:W:41:ARG:NH1	2.31	0.46
2:Z:173:THR:HA	2:Z:174:PRO:HD3	1.87	0.46
3:L:109:GLN:NE2	3:L:119:GLN:NE2	2.63	0.46
3:X:180:VAL:HG12	3:X:181:ASP:N	2.31	0.46
3:X:140:LEU:CG	3:X:222:ILE:HD11	2.45	0.46
1:P:62:GLU:OE2	1:P:65:PRO:HG3	2.15	0.46
2:T:124:ILE:HG21	2:T:201:LEU:HD23	1.97	0.46
3:R:68:TRP:CZ2	3:R:107:VAL:HG11	2.51	0.46
3:F:65:LEU:HD23	3:F:65:LEU:C	2.37	0.46
2:N:114:VAL:HG11	2:N:117:VAL:HG13	1.97	0.46
1:S:51:THR:HG22	1:S:51:THR:O	2.15	0.46
2:E:148:PRO:HG2	2:E:176:THR:HG23	1.97	0.46
1:M:121:TRP:O	1:M:124:PHE:HB3	2.16	0.46
1:D:60:GLU:OE2	1:D:94:LEU:HD21	2.17	0.45
1:A:35:LYS:HZ2	1:A:35:LYS:HB2	1.80	0.45
4:K:215:NAG:C4	4:K:216:NAG:C1	2.94	0.45
1:G:51:THR:OG1	1:G:52:GLU:N	2.48	0.45
2:H:46:GLN:NE2	2:H:47:THR:H	2.14	0.45
3:L:190:SER:O	3:L:191:VAL:HG13	2.16	0.45
2:Z:12:TYR:CZ	2:Z:14:SER:HA	2.50	0.45
3:X:157:LEU:HD11	3:X:161:LEU:HD13	1.96	0.45
3:U:148:LEU:HD12	3:U:148:LEU:C	2.37	0.45
2:T:50:LEU:HD23	2:T:60:CYS:HB2	1.98	0.45
2:B:39:PRO:HB2	2:B:42:ARG:HB2	1.98	0.45
3:O:61:THR:O	3:O:89:ILE:HG23	2.15	0.45
2:K:176:THR:HB	2:K:178:TYR:CE1	2.51	0.45
2:K:175:ASP:H	2:K:205:THR:HB	1.81	0.45
2:T:160:LEU:HD13	2:T:164:GLN:HB3	1.97	0.45
3:F:53:GLN:HG3	3:F:55:SER:OG	2.16	0.45
3:O:180:VAL:HG11	3:O:185:LYS:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:41:PHE:HB2	3:U:43:PHE:CE1	2.50	0.45
2:H:67:PRO:O	2:H:130:GLN:NE2	2.49	0.45
2:H:36:HIS:HE1	2:W:36:HIS:CE1	2.34	0.45
3:U:206:ASN:HD22	3:U:211:SER:HA	1.81	0.45
2:Z:73:THR:HG23	2:Z:75:VAL:HG22	1.97	0.45
2:W:132:SER:HG	2:W:134:TYR:HD1	1.64	0.45
1:P:36:LEU:O	1:P:39:MET:HB3	2.17	0.45
2:E:179:GLU:HG2	2:E:202:ALA:CB	2.44	0.45
2:T:201:LEU:HD12	2:T:202:ALA:N	2.31	0.45
1:A:13:GLN:NE2	2:B:75:VAL:HG12	2.32	0.45
2:W:112:LEU:HB3	2:W:201:LEU:HD22	1.99	0.45
2:T:14:SER:O	2:T:15:ARG:HG2	2.16	0.45
2:K:83:LEU:CD2	2:K:92:VAL:HG22	2.46	0.45
3:U:115:GLU:OE1	3:U:118:ARG:HD3	2.15	0.45
3:L:138:LEU:HD23	3:L:222:ILE:HG22	1.98	0.45
3:L:159:HIS:O	3:L:159:HIS:ND1	2.49	0.45
1:J:18:LEU:HD11	1:J:122:ILE:HG23	1.99	0.45
1:D:78:PHE:CD1	1:D:78:PHE:N	2.83	0.45
3:F:206:ASN:ND2	3:F:207:PRO:HB3	2.31	0.45
1:G:52:GLU:N	1:G:55:HIS:ND1	2.65	0.45
1:V:114:ILE:O	1:V:117:PHE:HB3	2.16	0.45
3:L:185:LYS:H	3:L:185:LYS:HG3	1.47	0.45
2:T:146:LEU:HD22	2:T:152:TRP:CE2	2.52	0.45
1:P:52:GLU:N	1:P:55:HIS:ND1	2.60	0.45
3:U:197:TYR:HB2	3:U:224:TRP:HB3	1.99	0.45
2:Z:141:PHE:CD2	2:Z:184:VAL:HG22	2.52	0.45
2:T:23:SER:CB	2:T:56:ALA:O	2.64	0.45
2:N:170:GLU:HB2	3:O:190:SER:HB3	1.98	0.45
1:S:57:GLN:HG3	1:S:61:GLU:OE2	2.16	0.45
2:W:153:GLU:H	2:W:153:GLU:CD	2.19	0.45
2:E:167:ILE:HD11	3:F:189:PRO:HB2	1.98	0.45
3:I:62:ASN:ND2	4:I:300:NAG:C1	2.68	0.45
2:H:118:GLU:OE1	2:H:121:ARG:HD3	2.16	0.45
2:W:183:ARG:HD2	2:W:194:TRP:HB3	1.98	0.45
2:N:17:GLN:NE2	2:N:63:ILE:HD11	2.32	0.45
3:O:48:MET:CE	3:O:95:LEU:HD12	2.46	0.45
2:N:172:LEU:HD22	2:N:178:TYR:CE1	2.52	0.45
1:D:92:PHE:CZ	2:E:73:THR:CG2	3.00	0.45
3:I:198:THR:OG1	3:I:223:HIS:CE1	2.69	0.45
2:Z:80:LEU:HD13	2:Z:98:PHE:HB3	1.98	0.45
2:W:76:ASP:HB2	2:W:100:PRO:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:16:ALA:O	2:K:64:LEU:HB2	2.17	0.45
1:P:87:SER:O	1:P:88:ASN:C	2.55	0.45
1:V:16:HIS:CG	2:W:134:TYR:HD2	2.34	0.45
1:A:66:LEU:HD12	1:A:66:LEU:O	2.16	0.45
2:N:158:LEU:HD23	3:O:147:GLN:NE2	2.30	0.45
3:I:100:ILE:O	3:I:100:ILE:HG22	2.16	0.45
3:I:87:GLU:O	3:I:89:ILE:HG13	2.15	0.45
3:C:106:PHE:O	3:C:124:LEU:N	2.48	0.45
3:F:126:LEU:HD22	3:F:129:LEU:HD12	1.98	0.45
3:F:62:ASN:ND2	4:F:300:NAG:C1	2.67	0.45
1:S:28:ILE:HD13	1:S:39:MET:CE	2.47	0.45
2:E:37:ALA:HB2	2:E:62:LEU:CD1	2.46	0.45
2:H:90:TRP:O	2:W:44:TRP:HA	2.16	0.45
3:R:62:ASN:ND2	4:R:300:NAG:H83	2.31	0.45
2:N:104:LEU:HD12	2:N:188:GLN:O	2.17	0.45
2:K:44:TRP:HH2	2:K:64:LEU:HD13	1.81	0.45
2:Z:162:GLN:HG2	2:Z:164:GLN:HB2	1.98	0.45
2:W:142:GLU:O	2:W:182:VAL:HG23	2.15	0.45
3:X:140:LEU:HD11	3:X:199:PHE:CD1	2.50	0.45
1:P:67:GLU:HG3	1:P:86:VAL:HG21	1.99	0.45
3:U:164:LEU:HA	3:U:179:SER:HA	1.99	0.45
2:T:112:LEU:CD1	2:T:112:LEU:H	2.29	0.45
1:Y:117:PHE:HE1	1:Y:121:TRP:HE1	1.63	0.45
3:R:152:TRP:CZ3	3:R:201:VAL:HG21	2.51	0.45
2:Z:109:PRO:HG3	2:Z:184:VAL:HG23	1.99	0.45
2:K:38:TRP:CZ3	2:K:45:GLN:CB	3.00	0.45
3:L:112:ASP:OD1	3:L:114:ARG:HG3	2.17	0.45
2:T:104:LEU:HB2	2:T:192:THR:OG1	2.16	0.45
2:Z:44:TRP:CH2	2:Z:72:LEU:HD21	2.50	0.45
3:L:148:LEU:O	3:L:188:LEU:N	2.50	0.45
2:B:65:GLY:HA3	2:B:71:LYS:HE3	1.98	0.45
3:L:57:GLU:HG2	3:L:58:PRO:CD	2.46	0.45
1:Y:51:THR:O	1:Y:52:GLU:HG3	2.17	0.45
2:W:10:CYS:C	2:W:11:PHE:CD1	2.90	0.45
2:H:185:LYS:HD3	2:H:194:TRP:CE2	2.51	0.45
3:F:35:LEU:CD2	3:F:118:ARG:CZ	2.95	0.45
3:O:134:ALA:HA	3:O:135:PRO:HD3	1.73	0.45
2:T:161:LYS:HD3	3:U:185:LYS:NZ	2.31	0.45
3:O:188:LEU:HD22	3:O:199:PHE:CE2	2.51	0.45
1:P:127:SER:HA	3:R:103:TYR:CE1	2.52	0.45
3:L:42:VAL:HG13	3:L:45:VAL:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:13:ASN:HB3	2:W:17:GLN:HB3	1.99	0.45
4:E:215:NAG:O4	4:F:233:NAG:H2	2.16	0.45
2:H:37:ALA:HB2	2:H:62:LEU:HD13	1.98	0.45
2:N:50:LEU:HD22	2:N:58:TRP:CB	2.41	0.45
3:I:61:THR:OG1	3:I:114:ARG:NH2	2.50	0.45
2:W:142:GLU:O	2:W:182:VAL:HA	2.16	0.45
2:E:186:PRO:HD2	2:E:192:THR:CG2	2.46	0.45
2:Z:36:HIS:HB3	2:Z:38:TRP:NE1	2.32	0.45
3:R:168:ARG:HG2	3:R:175:TRP:CE3	2.52	0.45
3:C:192:ASP:HB3	3:C:195:LYS:HD2	1.98	0.45
2:W:119:THR:HG22	2:W:206:LYS:C	2.37	0.45
1:D:31:TYR:HH	1:D:35:LYS:HE3	1.80	0.45
2:K:161:LYS:HZ3	3:L:185:LYS:NZ	2.15	0.45
2:W:70:GLN:CD	2:W:134:TYR:HE1	2.20	0.45
3:C:65:LEU:HD13	3:C:93:CYS:HB2	1.99	0.45
2:Q:142:GLU:HG3	2:Q:194:TRP:CH2	2.52	0.45
1:G:46:MET:HE3	1:G:46:MET:HB3	1.77	0.45
3:O:186:PHE:CD1	3:O:187:SER:N	2.85	0.45
3:X:171:TRP:H	3:X:171:TRP:HD1	1.64	0.45
1:J:125:CYS:O	1:J:129:ILE:CG2	2.58	0.44
2:W:117:VAL:HG12	2:W:118:GLU:N	2.31	0.44
2:T:38:TRP:HA	2:T:39:PRO:HD3	1.70	0.44
3:F:42:VAL:O	3:F:130:VAL:HA	2.17	0.44
1:V:127:SER:HA	3:X:103:TYR:CE1	2.51	0.44
2:E:124:ILE:O	2:E:124:ILE:HG22	2.17	0.44
2:T:82:VAL:CG1	2:T:94:ALA:H	2.31	0.44
1:M:69:VAL:HG11	1:M:114:ILE:HD12	1.99	0.44
3:O:46:GLU:O	3:O:47:TYR:HB3	2.17	0.44
2:E:155:ALA:HA	2:E:156:PRO:HD3	1.71	0.44
2:K:98:PHE:HE2	2:K:100:PRO:HG3	1.82	0.44
2:T:118:GLU:OE1	2:T:121:ARG:HD3	2.17	0.44
2:H:143:ALA:HB1	2:H:180:PHE:CE1	2.52	0.44
1:J:126:GLN:NE2	3:L:207:PRO:O	2.50	0.44
4:E:215:NAG:O4	4:F:233:NAG:C2	2.66	0.44
2:H:72:LEU:HD13	2:H:100:PRO:HG2	1.98	0.44
2:K:81:ARG:NE	2:K:95:ILE:HG22	2.30	0.44
2:T:167:ILE:HG21	2:T:180:PHE:CZ	2.52	0.44
3:I:168:ARG:HG2	3:I:175:TRP:CE3	2.52	0.44
3:F:45:VAL:O	3:F:45:VAL:CG1	2.64	0.44
3:I:159:HIS:CG	3:I:159:HIS:O	2.71	0.44
3:R:192:ASP:OD1	3:R:194:GLN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:42:PHE:CD2	1:J:69:VAL:HG22	2.51	0.44
1:A:124:PHE:O	1:A:127:SER:OG	2.33	0.44
1:Y:105:CYS:SG	1:Y:106:GLU:N	2.90	0.44
3:F:143:LEU:HD23	3:F:149:GLU:OE1	2.17	0.44
1:J:9:LYS:HB3	1:J:9:LYS:HE2	1.75	0.44
1:V:70:LEU:HB3	1:V:82:PRO:HB3	1.99	0.44
2:N:37:ALA:HB1	2:N:78:VAL:HG11	2.00	0.44
3:O:163:HIS:CE1	3:O:203:SER:OG	2.70	0.44
3:R:49:ASN:ND2	4:R:234:NAG:C1	2.80	0.44
2:Q:73:THR:O	2:Q:76:ASP:HB2	2.16	0.44
1:M:69:VAL:CG1	1:M:114:ILE:HD12	2.47	0.44
2:K:204:ARG:HG2	2:K:205:THR:N	2.31	0.44
3:I:188:LEU:HG	3:I:191:VAL:HG13	1.99	0.44
2:N:36:HIS:HB3	2:N:38:TRP:NE1	2.33	0.44
2:N:138:HIS:HB3	2:N:187:LEU:HD12	1.99	0.44
2:N:193:THR:HG22	2:N:194:TRP:N	2.33	0.44
3:C:102:LEU:HA	3:C:126:LEU:HB2	1.98	0.44
3:F:126:LEU:O	3:F:129:LEU:N	2.47	0.44
2:E:162:GLN:NE2	3:F:187:SER:HB2	2.32	0.44
3:L:62:ASN:HD21	4:L:300:NAG:H2	1.82	0.44
1:V:59:LEU:HB2	1:V:121:TRP:CZ2	2.53	0.44
3:U:167:TYR:HA	3:U:198:THR:O	2.17	0.44
3:R:44:ASN:ND2	3:R:133:TRP:CD1	2.86	0.44
3:F:144:SER:CB	3:F:147:GLN:HG3	2.47	0.44
2:H:158:LEU:HA	3:I:147:GLN:NE2	2.32	0.44
3:F:102:LEU:HD22	3:F:127:GLN:CA	2.45	0.44
3:F:102:LEU:HD23	3:F:126:LEU:CB	2.48	0.44
3:F:167:TYR:CE2	3:F:176:THR:CG2	3.01	0.44
1:J:53:LEU:CD1	1:J:96:LEU:HB3	2.32	0.44
2:B:37:ALA:HB2	2:B:62:LEU:HD13	1.98	0.44
1:Y:84:ASP:OD2	2:Z:71:LYS:NZ	2.47	0.44
3:X:131:ILE:HD11	3:X:214:HIS:HB2	2.00	0.44
1:P:86:VAL:O	1:P:87:SER:C	2.54	0.44
3:X:106:PHE:CE2	3:X:108:VAL:CG2	3.00	0.44
1:P:23:MET:HE3	1:P:23:MET:HB3	1.80	0.44
2:K:22:TRP:O	2:K:58:TRP:N	2.51	0.44
3:I:84:LEU:HD12	3:I:84:LEU:N	2.33	0.44
2:T:17:GLN:HG2	2:T:63:ILE:CD1	2.48	0.44
2:W:104:LEU:O	2:W:192:THR:HG23	2.18	0.44
3:C:205:PHE:CZ	3:C:209:CYS:HB2	2.53	0.44
1:D:82:PRO:HA	1:D:85:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:136:GLU:CG	2:E:137:ARG:H	2.31	0.44
3:F:158:ASN:O	3:F:159:HIS:ND1	2.50	0.44
3:I:207:PRO:HG2	3:O:117:ARG:HH21	90.92	0.44
1:J:36:LEU:HA	1:J:39:MET:HB3	1.99	0.44
2:T:73:THR:HA	2:T:101:PHE:CE1	2.51	0.44
2:T:138:HIS:NE2	3:U:182:TYR:HE2	2.15	0.44
2:Q:141:PHE:HA	2:Q:183:ARG:O	2.17	0.44
2:Q:136:GLU:HG3	2:Q:137:ARG:H	1.82	0.44
1:Y:67:GLU:HG2	1:Y:71:ASN:ND2	2.32	0.44
3:X:147:GLN:HG2	3:X:189:PRO:O	2.18	0.44
3:L:89:ILE:HG22	3:L:90:THR:H	1.83	0.44
3:R:102:LEU:HD22	3:R:127:GLN:HA	1.99	0.44
3:I:207:PRO:HG2	3:O:117:ARG:NH2	91.06	0.44
3:I:65:LEU:HD13	3:I:93:CYS:CB	2.48	0.44
1:V:68:GLU:O	1:V:71:ASN:N	2.51	0.44
2:B:44:TRP:CZ3	2:B:64:LEU:HD22	2.53	0.44
2:T:80:LEU:HD11	2:T:98:PHE:CG	2.53	0.44
3:L:57:GLU:HG3	3:L:58:PRO:HD2	1.97	0.44
2:T:84:CYS:SG	2:T:93:MET:HG3	2.58	0.44
2:N:83:LEU:CD2	2:N:92:VAL:HG22	2.48	0.44
1:Y:69:VAL:HA	1:Y:72:LEU:HG	2.00	0.44
3:I:140:LEU:HD13	3:I:224:TRP:CE3	2.53	0.44
3:F:102:LEU:O	3:F:104:GLN:N	2.50	0.44
3:F:44:ASN:HB3	3:F:46:GLU:HG3	1.98	0.44
3:F:48:MET:CE	3:F:95:LEU:HD12	2.48	0.44
2:E:162:GLN:HE22	3:F:187:SER:C	2.21	0.44
1:G:113:THR:HG23	1:G:116:GLU:CD	2.38	0.44
2:H:132:SER:OG	2:H:134:TYR:HD1	2.00	0.44
2:H:121:ARG:C	2:H:172:LEU:HD12	2.38	0.44
2:T:158:LEU:HD23	3:U:147:GLN:NE2	2.33	0.44
2:T:22:TRP:O	2:T:58:TRP:HE3	2.00	0.44
3:O:62:ASN:HD21	4:O:300:NAG:H2	1.83	0.44
3:U:62:ASN:ND2	4:U:300:NAG:C1	2.80	0.44
3:X:69:TYR:CE2	3:X:106:PHE:HD1	2.36	0.44
3:X:166:GLN:HB3	3:X:175:TRP:HE3	1.81	0.44
2:N:36:HIS:HB3	2:N:38:TRP:CD1	2.53	0.44
3:X:80:CYS:HB3	3:X:83:TYR:CE1	2.53	0.44
2:E:120:HIS:CE1	2:E:174:PRO:CG	3.00	0.44
1:D:24:ILE:HD11	1:D:85:VAL:HG22	2.00	0.44
1:A:18:LEU:CD1	1:A:122:ILE:HG23	2.47	0.44
1:G:126:GLN:NE2	3:I:210:GLY:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:88:ASN:ND2	2:T:42:ARG:HH22	2.16	0.44
1:J:31:TYR:CD2	1:J:36:LEU:HB2	2.52	0.44
3:U:146:SER:O	3:U:191:VAL:HG22	2.18	0.44
1:A:23:MET:SD	2:B:133:HIS:CE1	3.11	0.44
2:K:74:THR:HA	2:K:101:PHE:CD1	2.53	0.44
1:V:64:LYS:N	1:V:65:PRO:HD2	2.33	0.44
2:K:124:ILE:O	2:K:166:TRP:HA	2.17	0.44
2:Z:84:CYS:SG	2:Z:93:MET:HG3	2.58	0.44
2:Z:143:ALA:HA	2:Z:181:GLN:O	2.18	0.43
1:D:114:ILE:CG2	1:D:115:VAL:N	2.80	0.43
3:F:157:LEU:HD13	3:F:205:PHE:CD1	2.52	0.43
1:A:17:LEU:O	1:A:18:LEU:C	2.55	0.43
3:F:115:GLU:O	3:F:115:GLU:HG3	2.17	0.43
2:E:162:GLN:HE22	3:F:187:SER:HB2	1.83	0.43
2:B:20:CYS:O	2:B:59:ALA:HA	2.18	0.43
2:T:106:LEU:HA	2:T:106:LEU:HD23	1.78	0.43
2:K:138:HIS:C	2:K:187:LEU:CD1	2.86	0.43
2:Q:64:LEU:HD12	2:Q:72:LEU:HG	2.00	0.43
3:X:157:LEU:HD11	3:X:161:LEU:HD22	1.98	0.43
3:U:38:VAL:HG21	3:U:110:LEU:CD1	2.48	0.43
3:X:169:THR:HA	3:X:196:ARG:O	2.18	0.43
3:L:182:TYR:HE1	3:L:183:ARG:NH1	2.16	0.43
2:E:106:LEU:HD13	2:E:186:PRO:HG3	2.00	0.43
1:S:9:LYS:HB3	1:S:9:LYS:HE2	1.74	0.43
1:M:81:ASP:OD1	1:M:82:PRO:HD2	2.18	0.43
2:W:112:LEU:HD12	2:W:126:TRP:CB	2.48	0.43
2:T:15:ARG:HD2	2:T:68:ASP:OD1	2.17	0.43
2:H:104:LEU:O	2:H:192:THR:HG23	2.18	0.43
1:A:89:ILE:O	1:A:93:VAL:HG23	2.18	0.43
2:H:98:PHE:CE1	2:H:103:ASN:HB2	2.53	0.43
3:X:206:ASN:HA	3:X:210:GLY:O	2.18	0.43
1:J:57:GLN:O	1:J:61:GLU:HG3	2.18	0.43
2:Q:174:PRO:HA	2:Q:205:THR:CG2	2.46	0.43
2:Q:175:ASP:N	2:Q:205:THR:HB	2.33	0.43
3:I:47:TYR:C	3:I:47:TYR:CD1	2.92	0.43
3:O:154:ASN:ND2	3:O:163:HIS:HE1	2.14	0.43
3:O:138:LEU:HD12	3:O:138:LEU:N	2.31	0.43
2:Q:22:TRP:O	2:Q:58:TRP:HE3	2.01	0.43
4:F:234:NAG:H61	4:F:235:NAG:O7	2.18	0.43
2:T:129:SER:OG	2:T:130:GLN:N	2.51	0.43
2:N:39:PRO:HB2	2:N:42:ARG:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:116:PRO:HG2	2:Z:205:THR:O	2.17	0.43
2:W:150:HIS:HD2	2:W:154:GLU:OE1	2.00	0.43
2:W:166:TRP:C	2:W:166:TRP:CE3	2.91	0.43
2:E:13:ASN:HB2	2:E:17:GLN:HB3	2.00	0.43
1:D:66:LEU:HD11	1:D:70:LEU:HD11	1.99	0.43
3:F:159:HIS:CG	3:F:159:HIS:O	2.71	0.43
1:A:35:LYS:HD2	1:A:38:ARG:NH2	2.30	0.43
2:Z:138:HIS:HB3	2:Z:187:LEU:CD1	2.32	0.43
3:I:42:VAL:CG1	3:I:130:VAL:HG22	2.48	0.43
2:K:158:LEU:HA	3:L:147:GLN:NE2	2.33	0.43
2:H:115:VAL:HB	2:H:123:ASN:O	2.18	0.43
2:H:8:PHE:CE1	2:H:82:VAL:CG2	3.01	0.43
1:J:36:LEU:O	1:J:39:MET:HB3	2.17	0.43
2:W:142:GLU:HG3	2:W:194:TRP:CH2	2.54	0.43
2:K:161:LYS:HE2	3:L:185:LYS:HD3	2.00	0.43
1:P:88:ASN:O	1:P:89:ILE:C	2.57	0.43
2:N:63:ILE:HA	2:N:63:ILE:HD13	1.83	0.43
3:L:224:TRP:O	3:L:224:TRP:CD1	2.72	0.43
2:B:187:LEU:HD11	3:C:183:ARG:HD2	1.99	0.43
3:F:198:THR:OG1	3:F:223:HIS:CE1	2.71	0.43
2:H:38:TRP:HH2	2:W:83:LEU:HD21	1.82	0.43
3:O:163:HIS:CE1	3:O:203:SER:HG	2.37	0.43
2:W:50:LEU:CD2	2:W:60:CYS:HB2	2.49	0.43
2:N:146:LEU:HD11	2:N:151:THR:HA	1.99	0.43
3:O:173:HIS:HB3	1:V:45:TYR:CE2	2.53	0.43
1:S:64:LYS:N	1:S:65:PRO:CD	2.82	0.43
1:Y:31:TYR:HD2	1:Y:36:LEU:HB2	1.82	0.43
2:T:137:ARG:HE	2:T:137:ARG:HB2	1.61	0.43
2:N:183:ARG:HG3	2:N:194:TRP:CE3	2.54	0.43
3:U:47:TYR:HE1	3:U:49:ASN:HD21	1.64	0.43
1:D:122:ILE:O	1:D:125:CYS:HB2	2.19	0.43
1:D:82:PRO:O	1:D:85:VAL:HG12	2.17	0.43
3:I:106:PHE:CE2	3:I:108:VAL:CG1	3.01	0.43
1:S:36:LEU:O	1:S:40:LEU:HD12	2.19	0.43
1:S:56:LEU:HB3	1:S:93:VAL:HG13	2.00	0.43
2:T:80:LEU:HD12	2:T:98:PHE:HB2	2.00	0.43
2:T:159:THR:CG2	2:T:161:LYS:HE3	2.44	0.43
3:C:140:LEU:HD11	3:C:199:PHE:CE1	2.53	0.43
2:T:129:SER:O	2:T:130:GLN:C	2.56	0.43
2:H:107:MET:HE3	2:H:108:ALA:H	1.82	0.43
1:M:55:HIS:O	1:M:57:GLN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:104:LEU:O	2:T:192:THR:HG23	2.19	0.43
2:T:17:GLN:HG2	2:T:63:ILE:HD13	1.99	0.43
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.61	0.43
3:C:169:THR:C	3:C:171:TRP:N	2.72	0.43
1:D:13:GLN:HG2	2:E:75:VAL:HG12	1.99	0.43
1:D:52:GLU:H	1:D:55:HIS:CE1	2.37	0.43
3:I:132:PRO:HB3	3:I:161:LEU:HD21	2.01	0.43
2:B:119:THR:HG22	2:B:206:LYS:HB2	2.00	0.43
3:I:42:VAL:HG11	3:I:130:VAL:HG22	2.01	0.43
2:K:138:HIS:HA	2:K:187:LEU:CD1	2.48	0.43
2:H:98:PHE:CE2	2:H:100:PRO:HA	2.54	0.43
3:F:130:VAL:O	3:F:132:PRO:HD3	2.18	0.43
1:V:69:VAL:HA	1:V:72:LEU:CD2	2.44	0.43
3:O:164:LEU:HD12	3:O:165:VAL:N	2.34	0.43
2:N:70:GLN:NE2	2:N:134:TYR:CE1	2.86	0.43
1:D:62:GLU:HG3	1:D:117:PHE:CE1	2.47	0.43
3:L:183:ARG:HD2	3:L:183:ARG:HA	1.77	0.43
3:X:200:ARG:HG3	3:X:218:TRP:CZ3	2.53	0.43
3:R:40:CYS:C	3:R:41:PHE:CD1	2.92	0.43
3:I:188:LEU:HG	3:I:191:VAL:CG1	2.48	0.43
3:C:62:ASN:HD21	4:C:300:NAG:C2	2.32	0.43
1:S:16:HIS:CE1	2:T:134:TYR:HB3	2.54	0.43
2:E:143:ALA:O	2:E:158:LEU:HG	2.18	0.43
3:X:62:ASN:ND2	4:X:300:NAG:H83	2.34	0.43
2:Q:102:GLU:HA	2:Q:189:GLY:HA2	2.01	0.43
2:Q:177:GLN:HE21	2:Q:177:GLN:HB3	1.64	0.43
3:F:167:TYR:CZ	3:F:176:THR:HB	2.54	0.43
2:T:183:ARG:HD2	2:T:194:TRP:CB	2.44	0.43
2:W:114:VAL:HG11	2:W:117:VAL:CG2	2.48	0.43
1:J:88:ASN:O	1:J:89:ILE:C	2.55	0.43
3:L:165:VAL:O	3:L:177:GLU:HA	2.18	0.43
2:H:201:LEU:HD12	2:H:202:ALA:H	1.82	0.43
3:L:130:VAL:O	3:L:131:ILE:HD13	2.19	0.43
2:W:126:TRP:CZ2	2:W:164:GLN:O	2.72	0.43
2:W:179:GLU:HA	2:W:201:LEU:O	2.18	0.43
2:K:98:PHE:CZ	2:K:100:PRO:HA	2.54	0.43
1:J:113:THR:HG23	1:J:116:GLU:OE1	2.18	0.43
3:O:181:ASP:N	3:O:181:ASP:OD2	2.52	0.43
2:E:120:HIS:CE1	2:E:174:PRO:HG3	2.54	0.43
3:C:102:LEU:C	3:C:104:GLN:H	2.21	0.43
3:L:147:GLN:HG2	3:L:189:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:HIS:HB3	2:H:134:TYR:CD2	2.54	0.43
2:W:80:LEU:HD11	2:W:98:PHE:HB3	1.99	0.43
2:H:72:LEU:HD23	2:H:72:LEU:HA	1.67	0.43
2:Z:119:THR:HG22	2:Z:206:LYS:O	2.19	0.43
1:A:7:THR:CG2	1:A:132:LEU:HD13	2.48	0.43
1:V:125:CYS:C	1:V:127:SER:N	2.72	0.43
2:K:188:GLN:HG2	2:K:189:GLY:N	2.33	0.43
3:U:165:VAL:HG22	3:U:201:VAL:HG22	2.00	0.43
1:P:12:LEU:O	1:P:16:HIS:CD2	2.72	0.43
2:Q:73:THR:HG22	2:Q:75:VAL:H	1.83	0.43
2:N:11:PHE:HD1	2:N:105:ARG:HD3	1.83	0.43
2:Z:150:HIS:CD2	2:Z:154:GLU:OE1	2.72	0.43
2:B:138:HIS:CE1	3:C:182:TYR:CE2	3.07	0.43
3:F:128:ASN:ND2	3:F:211:SER:HB2	2.34	0.43
2:T:83:LEU:HB3	2:T:90:TRP:HE3	1.84	0.43
1:G:16:HIS:O	1:G:17:LEU:C	2.57	0.43
1:G:91:VAL:HG21	2:H:42:ARG:NH2	2.34	0.43
3:C:84:LEU:HD22	4:C:234:NAG:C6	2.40	0.43
1:P:126:GLN:OE1	3:R:210:GLY:HA2	2.19	0.43
1:M:23:MET:SD	2:N:133:HIS:CE1	3.11	0.43
3:I:140:LEU:CD1	3:I:224:TRP:HB2	2.49	0.43
1:M:46:MET:HB3	1:M:46:MET:HE3	1.85	0.43
3:U:138:LEU:HD12	3:U:138:LEU:N	2.34	0.43
1:A:81:ASP:HA	1:A:82:PRO:HD3	1.88	0.43
3:O:159:HIS:HA	3:O:182:TYR:HB2	2.01	0.43
2:W:155:ALA:HA	2:W:156:PRO:HD3	1.87	0.43
1:A:61:GLU:HB2	1:A:107:TYR:OH	2.19	0.42
2:Z:11:PHE:HA	2:Z:103:ASN:HB3	2.01	0.42
2:T:158:LEU:HD13	2:T:167:ILE:CD1	2.47	0.42
2:B:111:SER:HB2	2:B:127:GLU:HG3	2.00	0.42
2:K:16:ALA:HB1	2:K:65:GLY:N	2.33	0.42
2:T:119:THR:HG22	2:T:174:PRO:HB3	2.01	0.42
1:J:118:LEU:HD23	1:J:118:LEU:N	2.34	0.42
2:N:179:GLU:HA	2:N:201:LEU:O	2.18	0.42
1:Y:66:LEU:O	1:Y:70:LEU:HG	2.19	0.42
2:N:10:CYS:O	2:N:11:PHE:HD2	2.01	0.42
1:G:128:ILE:HD13	1:G:128:ILE:N	2.34	0.42
2:W:95:ILE:CG1	2:W:96:GLN:N	2.82	0.42
3:U:45:VAL:HG21	3:U:157:LEU:HD11	2.00	0.42
3:F:188:LEU:HA	3:F:189:PRO:HD2	1.86	0.42
1:D:63:LEU:HD23	1:D:66:LEU:HD23	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:83:LEU:HB3	2:T:90:TRP:CE3	2.54	0.42
3:I:131:ILE:HA	3:I:132:PRO:HD3	1.84	0.42
2:T:128:ILE:CG2	2:T:184:VAL:HG21	2.46	0.42
3:O:197:TYR:HB2	3:O:224:TRP:HB3	2.01	0.42
3:U:206:ASN:ND2	3:U:207:PRO:HA	2.34	0.42
1:S:91:VAL:HG12	2:T:75:VAL:CG2	2.49	0.42
3:X:131:ILE:HA	3:X:132:PRO:HD3	1.69	0.42
2:W:35:VAL:HA	2:W:81:ARG:O	2.19	0.42
1:P:62:GLU:OE2	1:P:62:GLU:HA	2.19	0.42
3:L:126:LEU:HA	3:L:129:LEU:HD12	2.01	0.42
1:M:82:PRO:O	1:M:85:VAL:HG12	2.19	0.42
3:I:48:MET:CB	3:I:100:ILE:HD11	2.49	0.42
3:I:188:LEU:HA	3:I:189:PRO:HD2	1.82	0.42
3:R:109:GLN:NE2	3:R:119:GLN:NE2	2.68	0.42
2:N:86:GLU:OE1	2:N:91:ARG:HD2	2.19	0.42
2:B:185:LYS:HB2	2:B:194:TRP:CE3	2.53	0.42
1:J:14:LEU:HA	1:J:14:LEU:HD12	1.89	0.42
1:J:37:THR:O	1:J:41:THR:HG23	2.20	0.42
1:D:60:GLU:O	1:D:63:LEU:HD12	2.19	0.42
3:F:68:TRP:HE3	3:F:77:VAL:HG13	1.84	0.42
3:X:164:LEU:HD12	3:X:165:VAL:N	2.33	0.42
2:N:115:VAL:HG11	4:N:215:NAG:O5	2.19	0.42
2:Q:72:LEU:CD1	2:Q:78:VAL:CG2	2.96	0.42
3:X:180:VAL:CG1	3:X:181:ASP:N	2.81	0.42
2:T:120:HIS:HA	2:T:172:LEU:O	2.19	0.42
3:C:204:ARG:HB2	3:C:215:TRP:CE3	2.54	0.42
3:L:167:TYR:N	3:L:176:THR:O	2.47	0.42
3:O:173:HIS:HB3	1:V:45:TYR:CZ	2.54	0.42
2:W:143:ALA:HB1	2:W:180:PHE:CZ	2.54	0.42
1:Y:28:ILE:O	1:Y:28:ILE:CG2	2.68	0.42
2:W:144:ARG:HD3	2:W:152:TRP:HE3	1.83	0.42
2:N:114:VAL:O	2:N:114:VAL:HG12	2.18	0.42
2:N:42:ARG:HD3	2:N:42:ARG:HA	1.88	0.42
2:N:82:VAL:O	2:N:93:MET:N	2.42	0.42
1:M:53:LEU:HD23	1:M:53:LEU:HA	1.79	0.42
1:Y:20:ASP:OD1	1:Y:85:VAL:CG2	2.66	0.42
1:G:92:PHE:CZ	2:H:134:TYR:CE2	3.07	0.42
1:Y:125:CYS:O	1:Y:126:GLN:C	2.57	0.42
2:E:128:ILE:H	2:E:128:ILE:HG13	1.59	0.42
1:G:54:LYS:HG3	1:G:103:PHE:CE2	2.53	0.42
3:I:138:LEU:HB2	3:I:222:ILE:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:151:ASN:ND2	3:L:185:LYS:HG2	2.34	0.42
2:Q:104:LEU:HD13	2:Q:135:PHE:CZ	2.54	0.42
1:P:123:THR:O	1:P:124:PHE:C	2.56	0.42
2:T:187:LEU:HD21	3:U:183:ARG:NH1	2.34	0.42
1:A:118:LEU:O	1:A:119:ASN:C	2.57	0.42
3:F:148:LEU:HD11	3:F:188:LEU:HD23	2.00	0.42
2:B:83:LEU:CD2	2:B:92:VAL:HA	2.50	0.42
3:R:42:VAL:CG1	3:R:45:VAL:HA	2.49	0.42
1:J:85:VAL:HG22	1:J:89:ILE:HD11	2.01	0.42
1:P:88:ASN:O	1:P:91:VAL:HB	2.20	0.42
3:O:207:PRO:C	3:O:208:LEU:HG	2.39	0.42
2:Z:141:PHE:HE1	2:Z:163:LYS:HA	1.85	0.42
1:M:14:LEU:CD1	1:M:128:ILE:HG21	2.49	0.42
3:U:63:LEU:HD23	3:U:112:ASP:HA	2.00	0.42
1:P:128:ILE:HG12	1:P:128:ILE:H	1.53	0.42
1:Y:62:GLU:HA	1:Y:62:GLU:OE2	2.19	0.42
3:L:206:ASN:CB	3:L:211:SER:HA	2.50	0.42
3:F:134:ALA:HA	3:F:135:PRO:HD3	1.81	0.42
2:E:162:GLN:NE2	3:F:186:PHE:CD1	2.88	0.42
2:H:73:THR:O	2:H:76:ASP:HB2	2.19	0.42
2:E:40:ASP:OD2	2:E:77:ILE:HB	2.19	0.42
1:V:66:LEU:HD12	1:V:114:ILE:HD11	1.97	0.42
3:U:149:GLU:OE1	3:U:185:LYS:HD2	2.20	0.42
1:M:20:ASP:OD1	1:M:85:VAL:CG2	2.68	0.42
3:R:40:CYS:O	3:R:129:LEU:HD22	2.19	0.42
3:X:61:THR:O	3:X:89:ILE:HG23	2.19	0.42
2:T:10:CYS:HA	2:T:19:SER:O	2.18	0.42
1:P:53:LEU:HA	1:P:53:LEU:HD23	1.86	0.42
3:I:128:ASN:O	3:I:212:ALA:CB	2.68	0.42
1:G:36:LEU:CD1	1:G:39:MET:HE3	2.50	0.42
1:G:88:ASN:O	1:G:92:PHE:HD2	2.03	0.42
3:U:205:PHE:O	3:U:206:ASN:HB2	2.20	0.42
2:W:42:ARG:NH2	2:W:73:THR:HG23	2.35	0.42
3:O:165:VAL:CG2	3:O:178:GLN:HB3	2.49	0.42
2:Q:121:ARG:HG2	2:Q:170:GLU:OE2	2.20	0.42
2:N:167:ILE:HD13	2:N:169:LEU:HD21	2.01	0.42
1:S:114:ILE:HG12	1:S:118:LEU:HD11	2.02	0.42
2:T:144:ARG:HD3	2:T:157:LEU:CD2	2.49	0.42
1:P:45:TYR:HB3	1:P:107:TYR:CD1	2.51	0.42
3:X:67:TYR:CD1	3:X:67:TYR:C	2.93	0.42
3:O:198:THR:HG21	1:V:104:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ALA:HB1	1:A:124:PHE:CD1	2.54	0.42
3:C:69:TYR:CE2	3:C:101:HIS:HB2	2.55	0.42
2:E:13:ASN:HB3	2:E:17:GLN:O	2.19	0.42
2:E:39:PRO:HA	2:E:78:VAL:HA	2.01	0.42
3:F:84:LEU:HD11	3:F:94:GLN:HB2	2.01	0.42
2:H:84:CYS:SG	2:H:93:MET:HG3	2.60	0.42
2:W:119:THR:HB	2:W:174:PRO:CG	2.35	0.42
3:L:188:LEU:HA	3:L:188:LEU:HD12	1.59	0.42
3:R:61:THR:CG2	3:R:62:ASN:N	2.83	0.42
2:W:141:PHE:HB2	2:W:160:LEU:HB2	2.02	0.42
2:Q:119:THR:O	2:Q:205:THR:HG21	2.20	0.42
3:L:126:LEU:C	3:L:128:ASN:N	2.72	0.42
3:U:139:THR:OG1	3:U:151:ASN:HB2	2.19	0.42
2:N:142:GLU:HG3	2:N:194:TRP:CZ2	2.54	0.42
2:N:35:VAL:HA	2:N:81:ARG:O	2.19	0.42
2:K:110:ILE:O	2:K:127:GLU:N	2.48	0.42
1:J:22:GLN:HG2	1:J:122:ILE:HD13	2.02	0.42
3:L:204:ARG:HB2	3:L:215:TRP:CE3	2.55	0.42
1:D:126:GLN:NE2	3:F:207:PRO:O	2.50	0.42
4:W:215:NAG:O4	4:X:233:NAG:C1	2.68	0.42
2:H:178:TYR:HB2	2:H:203:PHE:CZ	2.55	0.42
3:R:157:LEU:HD13	3:R:205:PHE:CE1	2.48	0.42
1:P:25:LEU:HD12	1:P:25:LEU:HA	1.77	0.42
1:P:25:LEU:HD21	1:P:119:ASN:ND2	2.35	0.42
1:A:56:LEU:O	1:A:59:LEU:HB3	2.19	0.42
2:K:183:ARG:O	2:K:194:TRP:CZ3	2.73	0.42
2:Q:158:LEU:HA	3:R:147:GLN:HE22	1.85	0.42
1:V:37:THR:O	1:V:41:THR:HG23	2.19	0.42
2:H:155:ALA:HA	2:H:156:PRO:HD3	1.81	0.42
3:C:208:LEU:HA	3:C:208:LEU:HD23	1.76	0.42
3:F:119:GLN:HE21	3:F:119:GLN:HB2	1.68	0.42
1:J:18:LEU:CD2	1:J:126:GLN:HG2	2.50	0.42
3:F:192:ASP:C	3:F:192:ASP:OD1	2.58	0.42
1:A:36:LEU:CD1	1:A:40:LEU:HG	2.50	0.42
2:Z:42:ARG:HB3	2:Z:44:TRP:CD1	2.55	0.42
1:S:24:ILE:HA	1:S:80:PHE:CE2	2.55	0.42
1:S:78:PHE:CD2	1:S:80:PHE:CE1	3.08	0.42
1:G:91:VAL:HG12	2:H:75:VAL:CG2	2.49	0.42
2:T:36:HIS:HB3	2:T:38:TRP:NE1	2.35	0.42
1:V:53:LEU:HD13	1:V:96:LEU:O	2.20	0.42
3:X:157:LEU:C	3:X:157:LEU:HD12	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:141:PHE:HB2	2:Q:160:LEU:HB2	2.00	0.42
2:K:117:VAL:O	2:K:206:LYS:HE2	2.20	0.42
3:L:126:LEU:C	3:L:128:ASN:H	2.22	0.42
2:N:117:VAL:HG12	2:N:122:CYS:SG	2.60	0.42
2:T:63:ILE:HD13	2:T:63:ILE:HA	1.87	0.42
1:P:14:LEU:HD23	1:P:14:LEU:HA	1.79	0.42
3:I:45:VAL:HG23	3:I:157:LEU:HD11	2.02	0.42
2:K:119:THR:O	2:K:174:PRO:HA	2.20	0.42
2:E:141:PHE:HD2	2:E:183:ARG:O	2.03	0.42
1:Y:131:THR:O	1:Y:131:THR:HG22	2.20	0.42
2:Q:171:THR:HG22	2:Q:171:THR:O	2.20	0.42
3:O:161:LEU:HD23	3:O:161:LEU:HA	1.84	0.42
2:E:167:ILE:HD11	3:F:189:PRO:CG	2.50	0.41
2:T:83:LEU:CB	2:T:90:TRP:CE3	3.03	0.41
1:V:14:LEU:HD21	1:V:53:LEU:HD21	2.02	0.41
1:V:69:VAL:HG11	1:V:114:ILE:CD1	2.50	0.41
3:X:161:LEU:HD11	3:X:205:PHE:HD1	1.85	0.41
2:N:37:ALA:HA	2:N:80:LEU:HD23	2.01	0.41
3:O:42:VAL:HG13	3:O:45:VAL:HA	2.02	0.41
2:Q:135:PHE:CE1	2:Q:186:PRO:HB3	2.55	0.41
3:X:69:TYR:CE1	3:X:101:HIS:ND1	2.86	0.41
1:Y:67:GLU:O	1:Y:71:ASN:CG	2.58	0.41
1:Y:18:LEU:HD11	1:Y:122:ILE:HG23	2.01	0.41
2:E:160:LEU:HD23	2:E:160:LEU:HA	1.74	0.41
1:M:31:TYR:OH	1:M:35:LYS:N	2.40	0.41
2:W:118:GLU:OE1	2:W:121:ARG:HD3	2.21	0.41
2:E:44:TRP:HB2	2:T:89:ARG:HD2	2.02	0.41
2:K:13:ASN:ND2	2:K:16:ALA:H	2.15	0.41
1:V:125:CYS:O	1:V:126:GLN:C	2.58	0.41
3:X:107:VAL:CG1	3:X:108:VAL:N	2.83	0.41
2:E:185:LYS:HA	2:E:186:PRO:HD3	1.71	0.41
2:T:118:GLU:OE1	2:T:121:ARG:HB2	2.20	0.41
3:L:61:THR:HG23	3:L:114:ARG:NH2	2.35	0.41
2:H:17:GLN:NE2	2:H:61:ASN:OD1	2.49	0.41
3:I:110:LEU:HD23	3:I:111:GLN:N	2.34	0.41
2:K:144:ARG:CD	2:K:152:TRP:CE3	3.02	0.41
2:T:73:THR:HG23	2:T:75:VAL:HG22	2.02	0.41
2:T:172:LEU:HA	2:T:172:LEU:HD23	1.88	0.41
1:S:127:SER:OG	3:U:103:TYR:HB3	2.19	0.41
1:Y:67:GLU:HG2	1:Y:71:ASN:HD21	1.85	0.41
2:K:178:TYR:HB2	2:K:203:PHE:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:133:THR:HG22	1:P:133:THR:O	2.20	0.41
3:C:154:ASN:HD21	3:C:163:HIS:CE1	2.35	0.41
1:M:36:LEU:HD12	1:M:40:LEU:HG	2.01	0.41
2:E:147:SER:HB2	2:E:148:PRO:HD2	2.01	0.41
1:D:6:SER:N	1:D:8:LYS:HG3	2.35	0.41
1:D:94:LEU:HD23	1:D:94:LEU:HA	1.78	0.41
3:F:158:ASN:O	3:F:159:HIS:HB3	2.20	0.41
2:B:37:ALA:HA	2:B:80:LEU:HD23	2.02	0.41
2:Z:13:ASN:C	2:Z:13:ASN:OD1	2.59	0.41
2:T:141:PHE:HA	2:T:183:ARG:O	2.20	0.41
1:S:24:ILE:HA	1:S:80:PHE:HE2	1.84	0.41
2:W:38:TRP:CZ3	2:W:45:GLN:CB	3.03	0.41
2:W:76:ASP:CB	2:W:100:PRO:HG2	2.50	0.41
1:V:69:VAL:HG11	1:V:114:ILE:HD12	2.03	0.41
2:K:161:LYS:HE2	3:L:185:LYS:CD	2.51	0.41
2:Q:155:ALA:HA	2:Q:156:PRO:HD3	1.81	0.41
2:Q:167:ILE:HG12	2:Q:168:CYS:H	1.83	0.41
1:P:28:ILE:O	1:P:28:ILE:CG2	2.68	0.41
3:X:149:GLU:HG2	3:X:151:ASN:ND2	2.35	0.41
2:Q:188:GLN:HG2	2:Q:189:GLY:N	2.36	0.41
3:I:157:LEU:HA	3:I:157:LEU:HD23	2.28	0.41
3:L:203:SER:C	3:L:215:TRP:CE3	2.94	0.41
2:Z:126:TRP:HH2	2:Z:167:ILE:HB	1.85	0.41
2:T:83:LEU:HD23	2:T:92:VAL:HA	2.02	0.41
3:I:152:TRP:CH2	3:I:184:HIS:O	2.72	0.41
1:G:40:LEU:HD21	1:G:115:VAL:HG23	2.02	0.41
3:X:52:TRP:CZ3	3:X:92:GLY:HA2	2.55	0.41
3:U:132:PRO:HB3	3:U:161:LEU:CD1	2.50	0.41
3:U:205:PHE:CZ	3:U:209:CYS:HB2	2.56	0.41
1:A:131:THR:O	1:A:132:LEU:HD23	2.20	0.41
3:X:167:TYR:CB	3:X:199:PHE:CE2	3.04	0.41
2:T:146:LEU:HD12	2:T:147:SER:N	2.36	0.41
1:M:83:ARG:HG3	1:M:84:ASP:N	2.34	0.41
2:K:184:VAL:HG13	2:K:184:VAL:O	2.19	0.41
1:A:91:VAL:HG12	2:B:75:VAL:CG2	2.50	0.41
2:N:81:ARG:CD	2:N:95:ILE:HG22	2.50	0.41
2:Z:50:LEU:HD23	2:Z:60:CYS:HB2	2.01	0.41
3:X:134:ALA:HB2	3:X:217:GLU:O	2.21	0.41
1:D:114:ILE:HG23	1:D:115:VAL:N	2.34	0.41
1:D:78:PHE:CD2	1:D:80:PHE:CE1	3.08	0.41
1:A:35:LYS:HZ1	1:A:73:ALA:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:68:ASP:OD1	2:H:130:GLN:HA	2.20	0.41
2:B:81:ARG:HG3	2:B:92:VAL:HG13	2.01	0.41
2:Z:18:ILE:HD11	2:Z:72:LEU:HD11	2.03	0.41
3:O:169:THR:HG23	3:O:197:TYR:CD2	2.55	0.41
3:O:140:LEU:CD1	3:O:224:TRP:HB2	2.51	0.41
1:G:63:LEU:HD23	1:G:63:LEU:HA	1.70	0.41
2:T:143:ALA:O	2:T:158:LEU:HB2	2.20	0.41
1:V:95:GLU:O	1:V:96:LEU:HD12	2.21	0.41
1:J:92:PHE:CZ	2:K:73:THR:HG23	2.56	0.41
1:J:20:ASP:OD2	1:J:85:VAL:HG23	2.20	0.41
1:J:86:VAL:O	1:J:87:SER:C	2.58	0.41
2:N:72:LEU:HD13	2:N:100:PRO:HG2	2.02	0.41
2:Q:104:LEU:HD13	2:Q:135:PHE:HZ	1.86	0.41
2:N:146:LEU:HD13	2:N:152:TRP:CD1	2.55	0.41
1:G:81:ASP:OD1	1:G:82:PRO:CD	2.68	0.41
2:Q:181:GLN:HG2	2:Q:198:SER:O	2.20	0.41
3:F:144:SER:HB3	3:F:147:GLN:HG3	2.02	0.41
3:F:66:HIS:ND1	3:F:79:LYS:HA	2.36	0.41
3:X:171:TRP:N	3:X:171:TRP:CD1	2.88	0.41
2:H:121:ARG:HG2	2:H:170:GLU:OE2	2.21	0.41
2:H:37:ALA:HB2	2:H:62:LEU:HD11	2.01	0.41
2:K:66:ALA:O	2:K:67:PRO:C	2.59	0.41
2:Z:73:THR:CG2	2:Z:75:VAL:HG22	2.51	0.41
2:Q:144:ARG:CD	2:Q:152:TRP:HE3	2.34	0.41
2:Q:135:PHE:O	2:Q:136:GLU:C	2.58	0.41
2:K:50:LEU:HD23	2:K:59:ALA:O	2.20	0.41
3:L:49:ASN:CG	4:L:233:NAG:C1	2.89	0.41
2:N:121:ARG:HD2	2:N:170:GLU:OE1	2.20	0.41
2:E:20:CYS:O	2:E:59:ALA:HA	2.20	0.41
3:F:167:TYR:CE2	3:F:176:THR:HG21	2.55	0.41
3:F:67:TYR:CE1	3:F:78:GLN:HB2	2.56	0.41
3:I:64:THR:OG1	3:I:111:GLN:HB3	2.21	0.41
2:H:40:ASP:OD2	2:H:77:ILE:HB	2.20	0.41
2:H:78:VAL:O	2:H:98:PHE:HB3	2.20	0.41
2:K:67:PRO:O	2:K:130:GLN:NE2	2.53	0.41
3:X:206:ASN:HD22	3:X:211:SER:HA	1.84	0.41
1:Y:94:LEU:HD23	1:Y:97:LYS:HE2	2.03	0.41
2:W:9:THR:HG22	2:W:11:PHE:HE1	1.85	0.41
2:N:20:CYS:HB2	2:N:60:CYS:CB	2.51	0.41
1:J:23:MET:HB3	1:J:23:MET:HE3	1.71	0.41
3:C:102:LEU:O	3:C:103:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:125:LYS:HB3	3:F:127:GLN:HE22	1.86	0.41
1:D:127:SER:HA	3:F:103:TYR:CD1	2.55	0.41
1:D:66:LEU:O	1:D:69:VAL:HB	2.20	0.41
2:W:83:LEU:CB	2:W:90:TRP:CE3	3.03	0.41
3:I:128:ASN:O	3:I:212:ALA:HA	2.20	0.41
2:B:82:VAL:O	2:B:83:LEU:HD23	2.21	0.41
2:Z:44:TRP:CH2	2:Z:64:LEU:HD13	2.56	0.41
1:G:20:ASP:OD1	2:H:133:HIS:NE2	2.52	0.41
2:K:146:LEU:HA	2:K:146:LEU:HD12	1.85	0.41
1:J:13:GLN:H	1:J:13:GLN:HG3	1.66	0.41
1:J:9:LYS:O	1:J:10:THR:C	2.58	0.41
3:O:163:HIS:ND1	3:O:203:SER:OG	2.49	0.41
2:Q:50:LEU:HA	2:Q:50:LEU:HD23	1.84	0.41
2:N:12:TYR:CZ	2:N:14:SER:HA	2.56	0.41
1:V:35:LYS:HD2	1:V:38:ARG:NH2	2.35	0.41
3:L:166:GLN:HB3	3:L:175:TRP:HB3	2.03	0.41
2:N:83:LEU:HD13	2:N:90:TRP:HB3	2.03	0.41
2:T:112:LEU:O	2:T:113:GLN:HG3	2.21	0.41
2:W:112:LEU:CD1	2:W:126:TRP:HB3	2.51	0.41
2:W:164:GLN:HA	3:X:178:GLN:HE22	1.85	0.41
2:W:9:THR:HG22	2:W:11:PHE:CE1	2.56	0.41
3:L:68:TRP:CD1	3:L:107:VAL:HB	2.56	0.41
3:L:68:TRP:CE3	3:L:77:VAL:HG13	2.53	0.41
2:Q:145:THR:O	2:Q:155:ALA:HB1	2.21	0.41
2:T:206:LYS:HA	2:T:207:PRO:HD3	1.88	0.41
2:K:20:CYS:O	2:K:59:ALA:HA	2.20	0.41
3:R:102:LEU:HD22	3:R:127:GLN:N	2.35	0.41
2:B:155:ALA:HA	2:B:156:PRO:HD3	1.80	0.41
2:K:93:MET:CE	2:K:93:MET:HA	2.50	0.41
1:M:8:LYS:O	1:M:11:GLN:HB3	2.20	0.41
1:J:81:ASP:HA	1:J:82:PRO:HD3	1.91	0.41
4:R:235:NAG:H2	4:R:235:NAG:H83	1.93	0.41
2:W:20:CYS:O	2:W:59:ALA:HA	2.20	0.41
1:G:45:TYR:CD1	1:G:111:THR:HG22	2.55	0.41
3:O:135:PRO:O	3:O:219:SER:HB3	2.20	0.41
1:P:88:ASN:H	1:P:88:ASN:ND2	2.19	0.41
1:M:118:LEU:O	1:M:119:ASN:C	2.59	0.41
4:X:300:NAG:H82	4:X:300:NAG:H2	1.94	0.41
3:X:61:THR:HG22	3:X:62:ASN:N	2.35	0.41
1:P:59:LEU:HD13	1:P:121:TRP:CD1	2.56	0.41
1:J:25:LEU:HD23	1:J:122:ILE:HD12	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:158:LEU:HD13	2:Z:167:ILE:HD11	2.04	0.40
3:C:142:LYS:HB2	3:C:142:LYS:HE3	1.75	0.40
3:I:204:ARG:HH11	3:O:117:ARG:HG3	95.70	0.40
2:T:106:LEU:HD11	2:T:186:PRO:HG3	2.03	0.40
1:G:92:PHE:HZ	2:H:134:TYR:CE2	2.38	0.40
2:H:83:LEU:HD21	2:W:38:TRP:HH2	1.85	0.40
2:Q:39:PRO:HD2	2:Q:44:TRP:O	2.22	0.40
2:Q:40:ASP:OD1	2:Q:41:ARG:HG3	2.21	0.40
1:M:44:PHE:CE2	1:M:114:ILE:HG13	2.56	0.40
1:Y:28:ILE:HD12	1:Y:114:ILE:HD13	2.03	0.40
3:X:87:GLU:O	3:X:89:ILE:HG13	2.21	0.40
3:L:135:PRO:HB2	3:L:219:SER:HB3	2.03	0.40
2:T:11:PHE:HB3	2:T:105:ARG:HB3	2.02	0.40
2:N:126:TRP:NE1	2:N:165:GLU:HA	2.36	0.40
3:C:157:LEU:HG	3:C:157:LEU:H	1.65	0.40
2:W:14:SER:O	2:W:15:ARG:HG2	2.21	0.40
3:F:133:TRP:HB2	3:F:155:ARG:HG3	2.02	0.40
2:Z:130:GLN:H	2:Z:130:GLN:HG3	1.52	0.40
2:K:132:SER:OG	2:K:134:TYR:HD1	2.04	0.40
3:F:63:LEU:HD13	3:F:110:LEU:HD21	2.03	0.40
2:K:81:ARG:HD2	2:K:95:ILE:HG22	1.99	0.40
2:N:51:LEU:CB	2:N:52:PRO:HD2	2.51	0.40
2:Z:162:GLN:N	2:Z:162:GLN:OE1	2.53	0.40
2:Q:160:LEU:HD23	2:Q:160:LEU:HA	1.89	0.40
2:Q:136:GLU:OE1	2:Q:136:GLU:HA	2.21	0.40
2:Z:54:SER:HB3	2:Z:57:SER:OG	2.21	0.40
2:Q:22:TRP:CE3	2:Q:82:VAL:HG11	2.56	0.40
1:S:65:PRO:O	1:S:66:LEU:C	2.60	0.40
3:L:68:TRP:NE1	3:L:107:VAL:HB	2.37	0.40
3:R:152:TRP:CE2	3:R:201:VAL:HG11	2.56	0.40
2:B:126:TRP:CE2	2:B:165:GLU:HA	2.56	0.40
3:R:67:TYR:HB2	3:R:106:PHE:CE1	2.56	0.40
2:T:104:LEU:HD13	2:T:135:PHE:CZ	2.56	0.40
1:J:81:ASP:OD1	1:J:82:PRO:HD2	2.21	0.40
1:A:14:LEU:O	1:A:15:GLU:C	2.59	0.40
2:E:167:ILE:HG13	3:F:189:PRO:HG3	2.03	0.40
2:Z:152:TRP:CZ3	2:Z:181:GLN:HB2	2.56	0.40
2:Z:143:ALA:HB1	2:Z:180:PHE:CE1	2.56	0.40
3:F:125:LYS:HB3	3:F:127:GLN:NE2	2.36	0.40
2:W:83:LEU:HB3	2:W:90:TRP:HE3	1.85	0.40
2:T:142:GLU:OE1	2:T:183:ARG:NE	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:11:PHE:O	2:Z:18:ILE:HA	2.22	0.40
3:L:191:VAL:CG1	3:L:197:TYR:CZ	3.03	0.40
3:O:65:LEU:HA	3:O:109:GLN:O	2.21	0.40
2:Q:36:HIS:HB3	2:Q:38:TRP:HE1	1.86	0.40
1:G:12:LEU:HD23	1:G:12:LEU:C	2.42	0.40
1:A:81:ASP:O	1:A:84:ASP:HB2	2.22	0.40
3:F:200:ARG:HD2	3:F:218:TRP:HB3	2.03	0.40
1:S:51:THR:O	1:S:52:GLU:HG3	2.20	0.40
1:Y:25:LEU:C	1:Y:27:GLY:H	2.25	0.40
1:M:48:LYS:HD3	1:M:108:ALA:HA	2.04	0.40
2:E:145:THR:OG1	2:E:169:LEU:HD21	2.22	0.40
3:F:102:LEU:C	3:F:104:GLN:N	2.75	0.40
2:W:91:ARG:HG2	2:W:93:MET:SD	2.62	0.40
3:R:52:TRP:NE1	3:R:63:LEU:HD12	2.37	0.40
1:G:64:LYS:N	1:G:65:PRO:HD2	2.37	0.40
2:T:36:HIS:HB3	2:T:38:TRP:HE1	1.86	0.40
2:E:48:CYS:SG	2:E:62:LEU:HD23	2.62	0.40
2:W:80:LEU:HD13	2:W:98:PHE:HB3	2.01	0.40
3:O:49:ASN:ND2	4:O:234:NAG:C1	2.85	0.40
2:Q:78:VAL:HG23	2:Q:100:PRO:HG3	2.04	0.40
3:X:167:TYR:HB3	3:X:199:PHE:CD2	2.56	0.40
2:B:104:LEU:HD13	2:B:135:PHE:CZ	2.56	0.40
2:T:170:GLU:OE2	2:T:170:GLU:HA	2.20	0.40
1:S:130:SER:C	1:S:132:LEU:H	2.24	0.40
3:U:35:LEU:HD22	3:U:63:LEU:HD13	2.04	0.40
2:N:16:ALA:O	2:N:64:LEU:HB2	2.22	0.40
2:T:20:CYS:O	2:T:59:ALA:HA	2.20	0.40
3:L:117:ARG:HA	3:L:117:ARG:HD3	1.86	0.40
3:X:148:LEU:C	3:X:148:LEU:HD12	2.42	0.40
2:E:13:ASN:HB3	2:E:17:GLN:H	1.86	0.40
3:I:134:ALA:HA	3:I:135:PRO:HD3	1.90	0.40
3:I:142:LYS:HD2	3:I:144:SER:O	2.22	0.40
3:F:138:LEU:C	3:F:222:ILE:HD13	2.42	0.40
2:E:37:ALA:HB2	2:E:62:LEU:HD13	2.03	0.40
2:H:32:SER:HB3	2:H:85:ARG:HB2	2.04	0.40
2:T:101:PHE:CZ	2:T:134:TYR:HD1	2.40	0.40
1:V:53:LEU:HA	1:V:53:LEU:HD23	1.86	0.40
1:V:68:GLU:HA	1:V:71:ASN:HB2	2.02	0.40
3:X:205:PHE:O	3:X:206:ASN:HB2	2.21	0.40
1:V:129:ILE:HA	1:V:132:LEU:HD12	2.04	0.40
1:M:16:HIS:HB3	2:N:134:TYR:HD2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:142:GLU:HA	2:E:158:LEU:O	2.22	0.40
3:X:154:ASN:ND2	3:X:163:HIS:CE1	2.84	0.40
3:O:111:GLN:HA	3:O:111:GLN:OE1	2.21	0.40
3:X:202:ARG:HD3	3:X:218:TRP:CZ2	2.57	0.40
1:A:59:LEU:HD13	1:A:121:TRP:CD2	2.57	0.40
3:L:107:VAL:HG22	3:L:123:MET:HG3	2.04	0.40
3:I:170:ASP:OD2	3:I:196:ARG:HB3	2.22	0.40
1:P:14:LEU:HD12	1:P:128:ILE:HB	2.03	0.40

All (4) 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)
3:I:173:HIS:NE2	1:b:45:TYR:OH[1_655]	1.67	0.53
2:Q:43:ARG:O	2:f:92:VAL:CG2[1_554]	1.98	0.22
3:I:173:HIS:CD2	1:b:45:TYR:OH[1_655]	2.02	0.18
2:E:204:ARG:O	1:P:45:TYR:OH[1_445]	2.16	0.04

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	115/136 (85%)	96 (84%)	18 (16%)	1 (1%)	21 68
1	D	115/136 (85%)	98 (85%)	17 (15%)	0	100 100
1	G	115/136 (85%)	102 (89%)	12 (10%)	1 (1%)	21 68
1	J	115/136 (85%)	108 (94%)	7 (6%)	0	100 100
1	M	115/136 (85%)	103 (90%)	10 (9%)	2 (2%)	11 56
1	P	115/136 (85%)	103 (90%)	10 (9%)	2 (2%)	11 56
1	S	115/136 (85%)	99 (86%)	16 (14%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	V	115/136 (85%)	100 (87%)	13 (11%)	2 (2%)	11 56
1	Y	114/136 (84%)	101 (89%)	12 (10%)	1 (1%)	21 68
1	b	113/136 (83%)	93 (82%)	19 (17%)	1 (1%)	21 68
1	e	115/136 (85%)	100 (87%)	13 (11%)	2 (2%)	11 56
1	h	115/136 (85%)	101 (88%)	14 (12%)	0	100 100
2	B	191/217 (88%)	180 (94%)	11 (6%)	0	100 100
2	E	192/217 (88%)	179 (93%)	13 (7%)	0	100 100
2	H	192/217 (88%)	175 (91%)	16 (8%)	1 (0%)	34 77
2	K	192/217 (88%)	176 (92%)	15 (8%)	1 (0%)	34 77
2	N	191/217 (88%)	179 (94%)	12 (6%)	0	100 100
2	Q	191/217 (88%)	179 (94%)	11 (6%)	1 (0%)	34 77
2	T	192/217 (88%)	176 (92%)	15 (8%)	1 (0%)	34 77
2	W	192/217 (88%)	172 (90%)	20 (10%)	0	100 100
2	Z	192/217 (88%)	175 (91%)	17 (9%)	0	100 100
2	c	192/217 (88%)	178 (93%)	14 (7%)	0	100 100
2	f	192/217 (88%)	181 (94%)	8 (4%)	3 (2%)	12 58
2	i	192/217 (88%)	180 (94%)	12 (6%)	0	100 100
3	C	184/202 (91%)	174 (95%)	10 (5%)	0	100 100
3	F	182/202 (90%)	169 (93%)	12 (7%)	1 (0%)	34 77
3	I	184/202 (91%)	165 (90%)	19 (10%)	0	100 100
3	L	189/202 (94%)	172 (91%)	13 (7%)	4 (2%)	9 53
3	O	189/202 (94%)	172 (91%)	17 (9%)	0	100 100
3	R	184/202 (91%)	169 (92%)	13 (7%)	2 (1%)	17 65
3	U	189/202 (94%)	179 (95%)	10 (5%)	0	100 100
3	X	189/202 (94%)	180 (95%)	8 (4%)	1 (0%)	34 77
3	a	189/202 (94%)	179 (95%)	10 (5%)	0	100 100
3	d	189/202 (94%)	173 (92%)	16 (8%)	0	100 100
3	g	189/202 (94%)	176 (93%)	13 (7%)	0	100 100
3	j	189/202 (94%)	174 (92%)	14 (7%)	1 (0%)	34 77
All	All	5924/6660 (89%)	5416 (91%)	480 (8%)	28 (0%)	34 77

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	71	ASN
3	L	127	GLN
2	Q	88	VAL
1	Y	66	LEU
3	L	187	SER
1	M	56	LEU
1	M	132	LEU
1	V	94	LEU
1	b	57	GLN
1	e	92	PHE
2	f	138	HIS
2	f	154	GLU
2	f	175	ASP
3	R	181	ASP
2	T	92	VAL
1	V	130	SER
3	X	155	ARG
1	A	74	HIS
1	G	131	THR
1	P	87	SER
3	j	45	VAL
2	K	67	PRO
3	L	206	ASN
1	e	82	PRO
1	P	89	ILE
3	F	193	GLY
2	H	53	VAL
3	R	113	PRO

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	115/128 (90%)	115 (100%)	0	100 100
1	D	115/128 (90%)	115 (100%)	0	100 100
1	G	115/128 (90%)	111 (96%)	4 (4%)	43 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	115/128 (90%)	109 (95%)	6 (5%)	29 69
1	M	115/128 (90%)	115 (100%)	0	100 100
1	P	115/128 (90%)	113 (98%)	2 (2%)	68 89
1	S	115/128 (90%)	114 (99%)	1 (1%)	84 93
1	V	115/128 (90%)	115 (100%)	0	100 100
1	Y	114/128 (89%)	113 (99%)	1 (1%)	84 93
1	b	113/128 (88%)	113 (100%)	0	100 100
1	e	115/128 (90%)	115 (100%)	0	100 100
1	h	115/128 (90%)	115 (100%)	0	100 100
2	B	179/194 (92%)	177 (99%)	2 (1%)	80 92
2	E	180/194 (93%)	178 (99%)	2 (1%)	80 92
2	H	180/194 (93%)	177 (98%)	3 (2%)	68 89
2	K	180/194 (93%)	178 (99%)	2 (1%)	80 92
2	N	179/194 (92%)	177 (99%)	2 (1%)	80 92
2	Q	179/194 (92%)	175 (98%)	4 (2%)	60 85
2	T	180/194 (93%)	178 (99%)	2 (1%)	80 92
2	W	180/194 (93%)	177 (98%)	3 (2%)	68 89
2	Z	180/194 (93%)	179 (99%)	1 (1%)	90 96
2	c	180/194 (93%)	180 (100%)	0	100 100
2	f	180/194 (93%)	179 (99%)	1 (1%)	90 96
2	i	180/194 (93%)	180 (100%)	0	100 100
3	C	182/194 (94%)	181 (100%)	1 (0%)	92 97
3	F	180/194 (93%)	178 (99%)	2 (1%)	80 92
3	I	182/194 (94%)	180 (99%)	2 (1%)	80 92
3	L	185/194 (95%)	181 (98%)	4 (2%)	60 85
3	O	185/194 (95%)	184 (100%)	1 (0%)	92 97
3	R	182/194 (94%)	182 (100%)	0	100 100
3	U	185/194 (95%)	184 (100%)	1 (0%)	92 97
3	X	185/194 (95%)	185 (100%)	0	100 100
3	a	185/194 (95%)	185 (100%)	0	100 100
3	d	185/194 (95%)	184 (100%)	1 (0%)	92 97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	g	185/194 (95%)	184 (100%)	1 (0%)	92 97
3	j	185/194 (95%)	184 (100%)	1 (0%)	92 97
All	All	5740/6192 (93%)	5690 (99%)	50 (1%)	84 93

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	15	ARG
2	B	81	ARG
3	C	143	LEU
2	E	15	ARG
2	E	96	GLN
3	F	119	GLN
3	F	159	HIS
1	G	20	ASP
1	G	53	LEU
1	G	104	MET
1	G	119	ASN
2	H	20	CYS
2	H	60	CYS
2	H	68	ASP
3	I	118	ARG
3	I	159	HIS
1	J	13	GLN
1	J	55	HIS
1	J	118	LEU
1	J	128	ILE
1	J	129	ILE
1	J	131	THR
2	K	46	GLN
2	K	154	GLU
3	L	59	GLN
3	L	146	SER
3	L	183	ARG
3	L	185	LYS
2	N	60	CYS
2	N	129	SER
3	O	149	GLU
1	P	119	ASN
1	P	128	ILE
2	Q	48	CYS

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Mol	Chain	Res	Type
2	Q	60	CYS
2	Q	68	ASP
2	Q	129	SER
1	S	20	ASP
2	T	61	ASN
2	T	68	ASP
3	U	150	LEU
2	W	60	CYS
2	W	138	HIS
2	W	144	ARG
1	Y	39	MET
2	Z	130	GLN
3	d	44	ASN
2	f	138	HIS
3	g	133	TRP
3	j	110	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
2	B	123	ASN
2	B	133	HIS
3	C	49	ASN
3	C	62	ASN
3	C	66	HIS
3	C	109	GLN
3	C	119	GLN
3	C	137	ASN
3	C	163	HIS
1	D	119	ASN
2	E	24	GLN
2	E	123	ASN
2	E	164	GLN
3	F	49	ASN
3	F	53	GLN
3	F	62	ASN
3	F	94	GLN
3	F	109	GLN
3	F	119	GLN
3	F	154	ASN
1	G	88	ASN

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Mol	Chain	Res	Type
1	G	126	GLN
2	H	13	ASN
2	H	123	ASN
2	H	130	GLN
2	H	164	GLN
3	I	49	ASN
3	I	62	ASN
3	I	137	ASN
3	I	223	HIS
1	J	88	ASN
1	J	126	GLN
2	K	24	GLN
2	K	123	ASN
3	L	49	ASN
3	L	62	ASN
3	L	109	GLN
3	L	119	GLN
3	L	151	ASN
3	L	154	ASN
1	M	11	GLN
1	M	88	ASN
2	N	17	GLN
2	N	24	GLN
2	N	123	ASN
2	N	133	HIS
2	N	164	GLN
2	N	181	GLN
3	O	49	ASN
3	O	62	ASN
3	O	137	ASN
3	O	141	HIS
3	O	151	ASN
3	O	154	ASN
3	O	178	GLN
3	O	184	HIS
1	P	88	ASN
2	Q	13	ASN
2	Q	36	HIS
2	Q	164	GLN
2	Q	177	GLN
3	R	49	ASN
3	R	62	ASN

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Mol	Chain	Res	Type
3	R	66	HIS
3	R	82	HIS
3	R	101	HIS
3	R	109	GLN
3	R	119	GLN
3	R	137	ASN
3	R	163	HIS
1	S	88	ASN
2	T	123	ASN
2	T	164	GLN
3	U	62	ASN
3	U	109	GLN
3	U	119	GLN
3	U	137	ASN
3	U	206	ASN
1	V	88	ASN
2	W	17	GLN
2	W	123	ASN
2	W	164	GLN
2	W	177	GLN
3	X	137	ASN
3	X	151	ASN
3	X	154	ASN
3	X	184	HIS
3	X	206	ASN
1	Y	13	GLN
1	Y	22	GLN
1	Y	88	ASN
2	Z	103	ASN
2	Z	123	ASN
2	Z	150	HIS
2	Z	164	GLN
3	a	62	ASN
3	a	66	HIS
3	a	101	HIS
3	a	109	GLN
3	a	119	GLN
3	a	147	GLN
3	a	151	ASN
3	a	154	ASN
3	a	206	ASN
1	b	13	GLN

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Mol	Chain	Res	Type
1	b	88	ASN
2	c	113	GLN
2	c	123	ASN
2	c	164	GLN
3	d	39	GLN
3	d	44	ASN
3	d	62	ASN
3	d	66	HIS
3	d	101	HIS
3	d	109	GLN
3	d	122	GLN
3	d	151	ASN
3	d	154	ASN
3	d	178	GLN
3	d	206	ASN
1	e	16	HIS
1	e	55	HIS
1	e	88	ASN
2	f	46	GLN
2	f	70	GLN
2	f	123	ASN
2	f	164	GLN
3	g	39	GLN
3	g	44	ASN
3	g	62	ASN
3	g	66	HIS
3	g	101	HIS
3	g	109	GLN
3	g	122	GLN
3	g	137	ASN
3	g	151	ASN
3	g	154	ASN
1	h	13	GLN
1	h	88	ASN
1	h	126	GLN
2	i	123	ASN
2	i	150	HIS
2	i	177	GLN
3	j	39	GLN
3	j	44	ASN
3	j	62	ASN
3	j	101	HIS

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Mol	Chain	Res	Type
3	j	109	GLN
3	j	122	GLN
3	j	147	GLN
3	j	154	ASN
3	j	163	HIS
3	j	178	GLN
3	j	184	HIS
3	j	206	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

54 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	215	-	14,14,15	0.51	0	15,19,21	1.11	0
4	NAG	C	233	-	14,14,15	0.59	0	15,19,21	0.82	0
4	NAG	C	234	-	14,14,15	0.51	0	15,19,21	1.42	2 (13%)
4	NAG	C	235	-	14,14,15	0.49	0	15,19,21	1.05	1 (6%)
4	NAG	C	300	-	14,14,15	0.55	0	15,19,21	1.32	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	400	-	14,14,15	0.52	0	15,19,21	0.65	0
4	NAG	E	215	-	14,14,15	0.73	1 (7%)	15,19,21	1.22	2 (13%)
4	NAG	F	233	-	14,14,15	0.52	0	15,19,21	1.53	2 (13%)
4	NAG	F	234	-	14,14,15	0.43	0	15,19,21	1.92	1 (6%)
4	NAG	F	235	-	14,14,15	0.48	0	15,19,21	0.76	0
4	NAG	F	300	-	14,14,15	0.53	0	15,19,21	1.08	1 (6%)
4	NAG	F	400	-	14,14,15	0.53	0	15,19,21	0.65	0
4	NAG	H	215	-	14,14,15	0.62	0	15,19,21	1.37	1 (6%)
4	NAG	I	233	-	14,14,15	0.67	0	15,19,21	0.98	1 (6%)
4	NAG	I	234	-	14,14,15	0.41	0	15,19,21	1.65	1 (6%)
4	NAG	I	235	-	14,14,15	0.52	0	15,19,21	0.68	0
4	NAG	I	300	-	14,14,15	0.52	0	15,19,21	1.26	2 (13%)
4	NAG	I	400	-	14,14,15	0.55	0	15,19,21	0.63	0
4	NAG	K	215	-	14,14,15	0.66	0	15,19,21	1.68	3 (20%)
4	NAG	K	216	-	14,14,15	0.49	0	15,19,21	1.68	3 (20%)
4	NAG	L	233	-	14,14,15	0.55	0	15,19,21	1.24	1 (6%)
4	NAG	L	234	-	14,14,15	0.51	0	15,19,21	0.98	1 (6%)
4	NAG	L	300	-	14,14,15	0.54	0	15,19,21	1.32	2 (13%)
4	NAG	L	400	-	14,14,15	0.56	0	15,19,21	0.70	0
4	NAG	N	215	-	14,14,15	0.70	0	15,19,21	1.52	2 (13%)
4	NAG	O	233	-	14,14,15	0.64	0	15,19,21	1.00	1 (6%)
4	NAG	O	234	-	14,14,15	0.44	0	15,19,21	1.14	2 (13%)
4	NAG	O	235	-	14,14,15	0.48	0	15,19,21	1.13	1 (6%)
4	NAG	O	300	-	14,14,15	0.53	0	15,19,21	1.64	2 (13%)
4	NAG	O	400	-	14,14,15	0.46	0	15,19,21	0.96	1 (6%)
4	NAG	Q	215	-	14,14,15	0.60	0	15,19,21	1.81	3 (20%)
4	NAG	R	233	-	14,14,15	0.60	0	15,19,21	1.17	1 (6%)
4	NAG	R	234	-	14,14,15	0.35	0	15,19,21	2.34	2 (13%)
4	NAG	R	235	-	14,14,15	0.53	0	15,19,21	0.75	0
4	NAG	R	300	-	14,14,15	0.60	0	15,19,21	1.09	1 (6%)
4	NAG	R	400	-	14,14,15	0.53	0	15,19,21	0.57	0
4	NAG	T	215	-	14,14,15	0.71	0	15,19,21	1.45	3 (20%)
4	NAG	U	233	-	14,14,15	0.56	0	15,19,21	2.15	5 (33%)
4	NAG	U	300	-	14,14,15	0.57	0	15,19,21	0.66	0
4	NAG	W	215	-	14,14,15	0.60	0	15,19,21	1.02	1 (6%)
4	NAG	X	233	-	14,14,15	0.55	0	15,19,21	1.97	4 (26%)
4	NAG	X	300	-	14,14,15	0.49	0	15,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	Z	215	-	14,14,15	0.58	0	15,19,21	0.98	1 (6%)
4	NAG	a	233	-	14,14,15	0.50	0	15,19,21	1.99	3 (20%)
4	NAG	a	300	-	14,14,15	0.46	0	15,19,21	0.77	0
4	NAG	c	215	-	14,14,15	0.69	0	15,19,21	1.58	3 (20%)
4	NAG	c	216	-	14,14,15	0.52	0	15,19,21	1.95	3 (20%)
4	NAG	d	300	-	14,14,15	0.47	0	15,19,21	0.70	0
4	NAG	f	215	-	14,14,15	0.69	0	15,19,21	1.19	2 (13%)
4	NAG	g	233	-	14,14,15	0.53	0	15,19,21	1.66	4 (26%)
4	NAG	g	300	-	14,14,15	0.46	0	15,19,21	0.94	0
4	NAG	i	215	-	14,14,15	0.66	0	15,19,21	1.46	2 (13%)
4	NAG	i	216	-	14,14,15	0.46	0	15,19,21	2.01	3 (20%)
4	NAG	j	300	-	14,14,15	0.52	0	15,19,21	0.68	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	215	-	-	0/6/23/26	0/1/1/1
4	NAG	C	233	-	-	0/6/23/26	0/1/1/1
4	NAG	C	234	-	-	0/6/23/26	0/1/1/1
4	NAG	C	235	-	-	0/6/23/26	0/1/1/1
4	NAG	C	300	-	-	0/6/23/26	0/1/1/1
4	NAG	C	400	-	-	0/6/23/26	0/1/1/1
4	NAG	E	215	-	-	0/6/23/26	0/1/1/1
4	NAG	F	233	-	-	0/6/23/26	0/1/1/1
4	NAG	F	234	-	-	0/6/23/26	0/1/1/1
4	NAG	F	235	-	-	0/6/23/26	0/1/1/1
4	NAG	F	300	-	-	0/6/23/26	0/1/1/1
4	NAG	F	400	-	-	0/6/23/26	0/1/1/1
4	NAG	H	215	-	-	0/6/23/26	0/1/1/1
4	NAG	I	233	-	-	0/6/23/26	0/1/1/1
4	NAG	I	234	-	-	0/6/23/26	0/1/1/1
4	NAG	I	235	-	-	0/6/23/26	0/1/1/1
4	NAG	I	300	-	-	2/6/23/26	0/1/1/1
4	NAG	I	400	-	-	0/6/23/26	0/1/1/1
4	NAG	K	215	-	-	0/6/23/26	0/1/1/1
4	NAG	K	216	-	-	0/6/23/26	0/1/1/1
4	NAG	L	233	-	-	0/6/23/26	0/1/1/1
4	NAG	L	234	-	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	L	300	-	-	0/6/23/26	0/1/1/1
4	NAG	L	400	-	-	1/6/23/26	0/1/1/1
4	NAG	N	215	-	-	0/6/23/26	0/1/1/1
4	NAG	O	233	-	-	0/6/23/26	0/1/1/1
4	NAG	O	234	-	-	0/6/23/26	0/1/1/1
4	NAG	O	235	-	-	0/6/23/26	0/1/1/1
4	NAG	O	300	-	-	0/6/23/26	0/1/1/1
4	NAG	O	400	-	-	0/6/23/26	0/1/1/1
4	NAG	Q	215	-	-	0/6/23/26	0/1/1/1
4	NAG	R	233	-	-	0/6/23/26	0/1/1/1
4	NAG	R	234	-	-	0/6/23/26	0/1/1/1
4	NAG	R	235	-	-	0/6/23/26	0/1/1/1
4	NAG	R	300	-	-	0/6/23/26	0/1/1/1
4	NAG	R	400	-	-	0/6/23/26	0/1/1/1
4	NAG	T	215	-	-	0/6/23/26	0/1/1/1
4	NAG	U	233	-	-	0/6/23/26	0/1/1/1
4	NAG	U	300	-	-	0/6/23/26	0/1/1/1
4	NAG	W	215	-	-	0/6/23/26	0/1/1/1
4	NAG	X	233	-	-	0/6/23/26	0/1/1/1
4	NAG	X	300	-	-	0/6/23/26	0/1/1/1
4	NAG	Z	215	-	-	0/6/23/26	0/1/1/1
4	NAG	a	233	-	-	0/6/23/26	0/1/1/1
4	NAG	a	300	-	-	0/6/23/26	0/1/1/1
4	NAG	c	215	-	-	0/6/23/26	0/1/1/1
4	NAG	c	216	-	-	0/6/23/26	0/1/1/1
4	NAG	d	300	-	-	0/6/23/26	0/1/1/1
4	NAG	f	215	-	-	0/6/23/26	0/1/1/1
4	NAG	g	233	-	-	0/6/23/26	0/1/1/1
4	NAG	g	300	-	-	0/6/23/26	0/1/1/1
4	NAG	i	215	-	-	0/6/23/26	0/1/1/1
4	NAG	i	216	-	-	0/6/23/26	0/1/1/1
4	NAG	j	300	-	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	215	NAG	O5-C1	-2.00	1.40	1.43

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	c	215	NAG	C2-N2-C7	-4.25	117.57	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	233	NAG	C2-N2-C7	-4.14	117.72	123.04
4	i	216	NAG	C4-C3-C2	-4.11	104.84	111.23
4	K	216	NAG	C4-C3-C2	-4.10	104.86	111.23
4	U	233	NAG	C4-C3-C2	-3.94	105.10	111.23
4	g	233	NAG	C2-N2-C7	-3.37	118.71	123.04
4	X	233	NAG	C4-C3-C2	-3.29	106.11	111.23
4	R	233	NAG	C2-N2-C7	-3.26	118.85	123.04
4	g	233	NAG	C4-C3-C2	-3.18	106.28	111.23
4	T	215	NAG	C1-O5-C5	-3.10	108.32	112.25
4	T	215	NAG	C2-N2-C7	-3.01	119.17	123.04
4	N	215	NAG	C2-N2-C7	-2.91	119.30	123.04
4	L	300	NAG	C2-N2-C7	-2.88	119.34	123.04
4	a	233	NAG	C4-C3-C2	-2.86	106.79	111.23
4	c	216	NAG	C4-C3-C2	-2.72	107.00	111.23
4	i	215	NAG	C1-O5-C5	-2.71	108.81	112.25
4	K	216	NAG	C2-N2-C7	-2.63	119.66	123.04
4	X	233	NAG	C2-N2-C7	-2.60	119.70	123.04
4	i	216	NAG	C2-N2-C7	-2.60	119.70	123.04
4	Q	215	NAG	C2-N2-C7	-2.51	119.81	123.04
4	f	215	NAG	O4-C4-C3	-2.47	104.78	110.34
4	C	234	NAG	C6-C5-C4	-2.40	107.09	113.02
4	C	235	NAG	C2-N2-C7	-2.40	119.96	123.04
4	K	215	NAG	C6-C5-C4	-2.23	107.51	113.02
4	C	300	NAG	O7-C7-C8	-2.21	118.00	122.06
4	W	215	NAG	O4-C4-C3	-2.20	105.38	110.34
4	U	233	NAG	C2-N2-C7	-2.15	120.28	123.04
4	K	215	NAG	C2-N2-C7	-2.13	120.30	123.04
4	R	234	NAG	C4-C3-C2	-2.11	107.95	111.23
4	c	215	NAG	O4-C4-C3	-2.11	105.60	110.34
4	O	400	NAG	C2-N2-C7	-2.09	120.36	123.04
4	C	300	NAG	C4-C3-C2	-2.07	108.00	111.23
4	E	215	NAG	C1-O5-C5	-2.01	109.69	112.25
4	I	300	NAG	C1-O5-C5	2.01	114.80	112.25
4	T	215	NAG	C3-C4-C5	2.01	113.70	110.20
4	O	234	NAG	C1-O5-C5	2.03	114.82	112.25
4	F	233	NAG	C3-C4-C5	2.19	114.02	110.20
4	U	233	NAG	C3-C2-N2	2.35	116.18	110.56
4	E	215	NAG	C3-C4-C5	2.39	114.36	110.20
4	g	233	NAG	C1-O5-C5	2.41	115.30	112.25
4	c	215	NAG	C3-C4-C5	2.41	114.40	110.20
4	L	300	NAG	C3-C4-C5	2.41	114.41	110.20
4	a	233	NAG	C3-C4-C5	2.42	114.42	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	216	NAG	C1-O5-C5	2.45	115.35	112.25
4	Z	215	NAG	C1-O5-C5	2.46	115.37	112.25
4	O	233	NAG	C3-C4-C5	2.54	114.62	110.20
4	O	234	NAG	O5-C5-C6	2.56	112.90	107.35
4	R	300	NAG	C3-C4-C5	2.65	114.82	110.20
4	f	215	NAG	C3-C4-C5	2.69	114.89	110.20
4	g	233	NAG	C3-C4-C5	2.74	114.97	110.20
4	C	300	NAG	C8-C7-N2	2.77	121.40	116.11
4	I	233	NAG	C3-C4-C5	2.77	115.03	110.20
4	F	300	NAG	C3-C4-C5	2.88	115.22	110.20
4	I	300	NAG	C3-C4-C5	2.92	115.29	110.20
4	U	233	NAG	C3-C4-C5	2.97	115.37	110.20
4	O	235	NAG	C1-O5-C5	3.05	116.12	112.25
4	L	234	NAG	C1-O5-C5	3.09	116.17	112.25
4	X	233	NAG	C3-C4-C5	3.11	115.62	110.20
4	Q	215	NAG	C1-O5-C5	3.13	116.22	112.25
4	c	216	NAG	C3-C4-C5	3.42	116.16	110.20
4	H	215	NAG	C3-C4-C5	3.47	116.24	110.20
4	L	233	NAG	C3-C4-C5	3.56	116.41	110.20
4	O	300	NAG	C3-C4-C5	3.59	116.46	110.20
4	i	215	NAG	C3-C4-C5	3.76	116.75	110.20
4	N	215	NAG	C3-C4-C5	3.97	117.11	110.20
4	O	300	NAG	C1-O5-C5	4.15	117.51	112.25
4	Q	215	NAG	C3-C4-C5	4.26	117.61	110.20
4	C	234	NAG	C1-O5-C5	4.34	117.75	112.25
4	K	215	NAG	C3-C4-C5	4.57	118.16	110.20
4	X	233	NAG	C1-O5-C5	4.61	118.10	112.25
4	c	216	NAG	C1-O5-C5	5.13	118.75	112.25
4	i	216	NAG	C1-O5-C5	5.13	118.76	112.25
4	I	234	NAG	C1-O5-C5	5.16	118.80	112.25
4	U	233	NAG	C1-O5-C5	5.33	119.02	112.25
4	a	233	NAG	C1-O5-C5	5.67	119.44	112.25
4	F	234	NAG	C1-O5-C5	6.61	120.64	112.25
4	R	234	NAG	C1-O5-C5	8.45	122.97	112.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	400	NAG	O7-C7-N2-C2
4	I	300	NAG	O7-C7-N2-C2
4	I	300	NAG	C8-C7-N2-C2

There are no ring outliers.

33 monomers are involved in 94 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	215	NAG	3	0
4	C	234	NAG	4	0
4	C	300	NAG	5	0
4	C	400	NAG	2	0
4	E	215	NAG	6	0
4	F	233	NAG	2	0
4	F	234	NAG	2	0
4	F	235	NAG	1	0
4	F	300	NAG	3	0
4	F	400	NAG	3	0
4	H	215	NAG	5	0
4	I	233	NAG	1	0
4	I	300	NAG	3	0
4	K	215	NAG	7	0
4	K	216	NAG	3	0
4	L	233	NAG	2	0
4	L	300	NAG	4	0
4	N	215	NAG	5	0
4	O	233	NAG	1	0
4	O	234	NAG	4	0
4	O	235	NAG	1	0
4	O	300	NAG	4	0
4	Q	215	NAG	4	0
4	R	234	NAG	1	0
4	R	235	NAG	1	0
4	R	300	NAG	4	0
4	T	215	NAG	5	0
4	U	233	NAG	2	0
4	U	300	NAG	5	0
4	W	215	NAG	5	0
4	X	233	NAG	2	0
4	X	300	NAG	4	0
4	Z	215	NAG	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	121/136 (88%)	-0.24	0 100 100	39, 76, 123, 170	0
1	D	121/136 (88%)	-0.10	0 100 100	34, 71, 130, 159	0
1	G	121/136 (88%)	-0.22	0 100 100	35, 75, 134, 184	0
1	J	121/136 (88%)	-0.13	0 100 100	30, 73, 117, 142	0
1	M	121/136 (88%)	-0.21	0 100 100	37, 75, 126, 167	0
1	P	121/136 (88%)	-0.20	0 100 100	30, 73, 128, 153	0
1	S	121/136 (88%)	-0.04	4 (3%) 50 34	46, 91, 137, 201	0
1	V	121/136 (88%)	0.16	9 (7%) 17 11	24, 88, 151, 419	0
1	Y	120/136 (88%)	0.00	3 (2%) 61 44	45, 100, 152, 199	0
1	b	119/136 (87%)	-0.00	3 (2%) 61 44	45, 96, 153, 177	0
1	e	121/136 (88%)	0.01	3 (2%) 61 44	22, 80, 131, 165	0
1	h	121/136 (88%)	0.01	3 (2%) 61 44	50, 93, 132, 185	0
2	B	195/217 (89%)	-0.13	1 (0%) 91 85	45, 76, 126, 155	0
2	E	196/217 (90%)	-0.09	0 100 100	30, 74, 118, 190	0
2	H	196/217 (90%)	-0.14	1 (0%) 91 85	41, 73, 122, 150	0
2	K	196/217 (90%)	-0.13	0 100 100	25, 72, 117, 135	0
2	N	195/217 (89%)	-0.17	2 (1%) 84 72	43, 74, 111, 141	0
2	Q	195/217 (89%)	-0.21	0 100 100	29, 69, 111, 146	0
2	T	196/217 (90%)	0.06	3 (1%) 76 62	36, 89, 140, 175	0
2	W	196/217 (90%)	0.03	5 (2%) 59 43	25, 88, 138, 210	0
2	Z	196/217 (90%)	-0.04	3 (1%) 76 62	45, 80, 125, 176	0
2	c	196/217 (90%)	0.02	6 (3%) 52 36	46, 82, 138, 208	0
2	f	196/217 (90%)	0.01	2 (1%) 84 72	23, 85, 133, 168	0
2	i	196/217 (90%)	0.02	3 (1%) 76 62	39, 94, 143, 168	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
3	C	188/202 (93%)	0.24	7 (3%) 45 30	42, 93, 157, 226	0
3	F	186/202 (92%)	0.29	10 (5%) 29 19	33, 86, 149, 214	0
3	I	188/202 (93%)	0.11	6 (3%) 51 35	56, 90, 158, 217	0
3	L	191/202 (94%)	0.19	3 (1%) 74 60	21, 82, 153, 218	0
3	O	191/202 (94%)	0.23	8 (4%) 40 26	38, 88, 156, 196	0
3	R	188/202 (93%)	0.21	10 (5%) 30 20	41, 86, 154, 231	0
3	U	191/202 (94%)	0.62	23 (12%) 6 5	83, 151, 224, 267	0
3	X	191/202 (94%)	0.96	39 (20%) 1 1	81, 156, 229, 291	0
3	a	191/202 (94%)	0.86	31 (16%) 3 2	80, 149, 221, 369	0
3	d	191/202 (94%)	0.75	26 (13%) 4 3	77, 149, 229, 281	0
3	g	191/202 (94%)	0.64	25 (13%) 5 4	82, 143, 195, 287	0
3	j	191/202 (94%)	0.71	27 (14%) 4 3	69, 140, 196, 284	0
All	All	6076/6660 (91%)	0.14	266 (4%) 38 25	21, 90, 178, 419	0

All (266) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	j	56	SER	12.8
3	a	113	PRO	8.8
3	d	58	PRO	8.2
3	U	54	SER	7.1
3	X	58	PRO	6.6
3	X	56	SER	6.5
3	a	156	PHE	6.5
3	U	55	SER	5.9
3	X	36	PRO	5.7
3	X	87	GLU	5.7
3	d	57	GLU	5.5
3	a	36	PRO	5.5
3	j	57	GLU	5.3
3	a	52	TRP	5.3
3	U	145	GLU	5.3
3	X	156	PHE	5.3
2	c	24	GLN	5.2
3	a	60	PRO	5.2
3	X	37	GLU	5.0
3	j	87	GLU	5.0
3	j	109	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
3	U	58	PRO	4.9
3	a	40	CYS	4.9
3	d	71	ASN	4.9
3	d	106	PHE	4.8
3	U	156	PHE	4.7
3	X	88	GLU	4.7
3	X	173	HIS	4.6
1	S	77	ASN	4.6
3	g	55	SER	4.6
3	X	53	GLN	4.5
3	a	108	VAL	4.4
3	X	68	TRP	4.4
3	g	59	GLN	4.3
3	X	55	SER	4.3
3	g	90	THR	4.2
3	C	55	SER	4.1
3	d	148	LEU	4.1
3	a	106	PHE	4.1
3	C	35	LEU	4.1
3	d	116	PRO	4.0
3	U	169	THR	4.0
3	g	109	GLN	4.0
3	d	192	ASP	4.0
3	X	86	SER	4.0
1	h	133	THR	4.0
3	C	173	HIS	3.9
3	X	63	LEU	3.9
1	b	77	ASN	3.9
3	U	63	LEU	3.9
1	V	39	MET	3.8
1	V	83	ARG	3.8
3	X	71	ASN	3.8
3	d	86	SER	3.8
3	j	55	SER	3.8
3	C	119	GLN	3.8
3	j	122	GLN	3.7
3	a	86	SER	3.7
1	V	42	PHE	3.6
3	X	46	GLU	3.5
3	C	110	LEU	3.5
2	f	24	GLN	3.5
3	d	34	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
3	a	63	LEU	3.5
3	d	107	VAL	3.5
3	R	75	ASP	3.5
3	X	54	SER	3.5
3	a	62	ASN	3.4
3	g	108	VAL	3.4
3	j	86	SER	3.4
3	g	60	PRO	3.3
3	a	107	VAL	3.3
3	j	154	ASN	3.3
3	X	122	GLN	3.3
3	j	85	PHE	3.3
3	X	201	VAL	3.3
3	g	200	ARG	3.3
3	j	62	ASN	3.3
3	d	85	PHE	3.3
3	g	64	THR	3.3
1	Y	77	ASN	3.2
3	g	34	PRO	3.2
3	d	156	PHE	3.2
3	a	50	CYS	3.2
3	F	159	HIS	3.2
3	a	45	VAL	3.2
3	j	45	VAL	3.2
3	X	45	VAL	3.1
3	X	113	PRO	3.1
3	j	66	HIS	3.1
3	a	69	TYR	3.1
3	O	63	LEU	3.1
3	X	85	PHE	3.1
3	O	37	GLU	3.1
3	d	55	SER	3.1
3	R	120	ALA	3.1
3	R	109	GLN	3.1
3	a	85	PHE	3.1
3	g	63	LEU	3.1
2	B	54	SER	3.1
3	j	96	GLN	3.1
3	g	51	THR	3.1
2	Z	204	ARG	3.0
3	d	108	VAL	3.0
2	W	55	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
3	a	112	ASP	3.0
3	X	221	PRO	3.0
1	V	91	VAL	3.0
3	j	145	GLU	3.0
3	g	112	ASP	3.0
1	h	39	MET	3.0
1	S	133	THR	3.0
3	F	191	VAL	2.9
3	R	57	GLU	2.9
3	U	45	VAL	2.9
1	V	133	THR	2.9
2	T	181	GLN	2.9
3	F	193	GLY	2.9
3	a	189	PRO	2.9
2	W	6	SER	2.9
3	j	70	LYS	2.9
3	U	90	THR	2.9
3	U	62	ASN	2.9
3	I	149	GLU	2.9
3	g	88	GLU	2.9
2	N	145	THR	2.9
3	U	116	PRO	2.9
1	V	132	LEU	2.8
3	j	61	THR	2.8
3	I	63	LEU	2.8
3	a	94	GLN	2.8
3	O	156	PHE	2.8
3	I	156	PHE	2.8
3	X	66	HIS	2.8
3	U	53	GLN	2.8
2	i	190	GLU	2.7
3	O	61	THR	2.7
3	a	98	LYS	2.7
3	F	55	SER	2.7
2	T	144	ARG	2.7
3	g	118	ARG	2.7
1	V	78	PHE	2.7
2	c	81	ARG	2.7
3	X	73	ASP	2.7
3	j	155	ARG	2.7
3	a	39	GLN	2.7
2	W	37	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
3	d	191	VAL	2.7
1	S	44	PHE	2.7
3	I	116	PRO	2.7
3	d	62	ASN	2.6
3	F	117	ARG	2.6
3	j	108	VAL	2.6
3	X	116	PRO	2.6
3	a	177	GLU	2.6
1	e	67	GLU	2.6
3	U	88	GLU	2.6
3	U	34	PRO	2.6
2	Z	178	TYR	2.6
3	j	69	TYR	2.6
3	R	173	HIS	2.6
1	e	77	ASN	2.6
3	F	61	THR	2.6
3	X	171	TRP	2.6
3	a	111	GLN	2.6
3	U	201	VAL	2.6
2	c	6	SER	2.6
3	X	107	VAL	2.6
1	e	133	THR	2.6
3	O	36	PRO	2.6
3	F	149	GLU	2.5
3	R	156	PHE	2.5
3	d	101	HIS	2.5
3	F	110	LEU	2.5
3	g	87	GLU	2.5
3	X	120	ALA	2.5
3	d	93	CYS	2.5
1	V	82	PRO	2.5
3	d	194	GLN	2.5
3	X	98	LYS	2.4
2	W	96	GLN	2.4
3	X	57	GLU	2.4
3	R	117	ARG	2.4
3	j	60	PRO	2.4
3	d	45	VAL	2.4
3	a	51	THR	2.4
2	N	56	ALA	2.4
3	R	65	LEU	2.4
3	R	76	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	a	34	PRO	2.4
3	a	53	GLN	2.4
3	g	113	PRO	2.4
3	U	200	ARG	2.4
3	j	107	VAL	2.4
3	F	156	PHE	2.4
3	X	38	VAL	2.4
3	X	99	GLU	2.4
3	X	69	TYR	2.4
2	c	113	GLN	2.3
3	O	109	GLN	2.3
1	b	7	THR	2.3
3	U	107	VAL	2.3
3	j	106	PHE	2.3
3	a	77	VAL	2.3
2	W	97	ASP	2.3
3	U	157	LEU	2.3
3	d	59	GLN	2.3
3	U	108	VAL	2.3
1	S	73	ALA	2.3
3	U	66	HIS	2.3
3	X	101	HIS	2.3
3	g	61	THR	2.3
3	d	90	THR	2.3
3	g	52	TRP	2.2
2	H	56	ALA	2.2
3	U	185	LYS	2.2
3	g	224	TRP	2.2
3	j	65	LEU	2.2
1	Y	131	THR	2.2
2	c	112	LEU	2.2
3	X	121	THR	2.2
3	O	62	ASN	2.2
3	g	98	LYS	2.2
3	C	117	ARG	2.2
3	L	115	GLU	2.2
3	a	217	GLU	2.2
3	I	71	ASN	2.2
3	d	222	ILE	2.2
2	i	24	GLN	2.2
3	a	79	LYS	2.2
2	f	76	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
3	L	35	LEU	2.2
3	a	188	LEU	2.2
3	d	51	THR	2.2
3	X	110	LEU	2.2
3	X	157	LEU	2.2
2	T	157	LEU	2.1
3	X	89	ILE	2.1
3	g	65	LEU	2.1
3	g	94	GLN	2.1
1	V	38	ARG	2.1
3	d	96	GLN	2.1
3	L	54	SER	2.1
3	R	159	HIS	2.1
1	Y	78	PHE	2.1
3	I	56	SER	2.1
3	U	133	TRP	2.1
3	g	96	GLN	2.1
1	b	44	PHE	2.1
3	j	54	SER	2.1
2	c	55	GLN	2.1
3	j	153	ASN	2.1
3	g	220	HIS	2.1
3	C	156	PHE	2.1
3	g	106	PHE	2.1
3	F	119	GLN	2.1
1	h	35	LYS	2.0
2	Z	7	GLN	2.0
3	O	59	GLN	2.0
3	U	178	GLN	2.0
3	X	123	MET	2.0
3	j	200	ARG	2.0
3	a	212	ALA	2.0
2	i	206	LYS	2.0
3	d	177	GLU	2.0
3	j	220	HIS	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	O	300	14/15	0.83	0.28	0.17	86,91,109,113	0
4	NAG	W	215	14/15	0.90	0.22	-0.00	62,71,83,86	0
4	NAG	E	215	14/15	0.86	0.29	-0.06	35,58,79,86	0
4	NAG	F	300	14/15	0.72	0.29	-0.07	69,80,84,88	0
4	NAG	L	300	14/15	0.90	0.26	-0.16	88,97,104,106	0
4	NAG	T	215	14/15	0.91	0.22	-0.22	38,53,67,68	0
4	NAG	Z	215	14/15	0.88	0.25	-0.24	68,76,81,85	0
4	NAG	Q	215	14/15	0.91	0.23	-0.25	38,48,65,67	0
4	NAG	R	300	14/15	0.86	0.23	-0.37	79,87,94,96	0
4	NAG	B	215	14/15	0.92	0.24	-0.43	33,46,76,79	0
4	NAG	I	300	14/15	0.85	0.23	-0.51	51,83,96,99	0
4	NAG	c	215	14/15	0.89	0.22	-0.51	58,66,80,84	0
4	NAG	H	215	14/15	0.92	0.22	-0.66	41,53,80,89	0
4	NAG	N	215	14/15	0.90	0.22	-0.75	47,54,79,80	0
4	NAG	f	215	14/15	0.94	0.19	-0.84	63,70,87,90	0
4	NAG	C	234	14/15	0.92	0.23	-0.98	89,105,113,116	0
4	NAG	g	300	14/15	0.61	0.28	-1.29	157,173,179,182	0
4	NAG	i	215	14/15	0.94	0.16	-1.36	52,67,74,82	0
4	NAG	a	300	14/15	0.71	0.27	-1.59	123,141,146,148	0
4	NAG	F	234	14/15	0.93	0.17	-1.60	81,109,119,125	0
4	NAG	C	300	14/15	0.87	0.22	-1.67	61,73,86,95	0
4	NAG	L	233	14/15	0.89	0.19	-2.27	66,89,100,106	0
4	NAG	O	234	14/15	0.94	0.14	-3.11	59,77,90,93	0
4	NAG	g	233	14/15	0.83	0.31	-	114,126,139,140	0
4	NAG	c	216	14/15	0.78	0.31	-	91,113,121,123	0
4	NAG	U	300	14/15	0.75	0.25	-	172,177,180,182	0
4	NAG	C	400	14/15	0.69	0.20	-	153,161,167,167	0
4	NAG	a	233	14/15	0.71	0.42	-	119,129,137,142	0
4	NAG	I	235	14/15	0.77	0.26	-	131,142,148,150	0
4	NAG	d	300	14/15	0.74	0.26	-	176,185,189,191	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	F	235	14/15	0.88	0.25	-	137,148,151,153	0
4	NAG	R	400	14/15	0.74	0.31	-	200,203,210,211	0
4	NAG	O	235	14/15	0.88	0.21	-	91,111,120,122	0
4	NAG	X	300	14/15	0.55	0.36	-	195,203,206,208	0
4	NAG	F	400	14/15	0.77	0.25	-	158,167,171,172	0
4	NAG	i	216	14/15	0.67	0.38	-	128,143,156,164	0
4	NAG	j	300	14/15	0.68	0.29	-	162,174,182,183	0
4	NAG	I	234	14/15	0.92	0.21	-	78,101,110,111	0
4	NAG	I	233	14/15	0.90	0.28	-	64,81,91,92	0
4	NAG	L	400	14/15	0.72	0.30	-	198,202,205,206	0
4	NAG	R	233	14/15	0.92	0.32	-	74,84,92,93	0
4	NAG	U	233	14/15	0.70	0.43	-	98,118,139,142	0
4	NAG	I	400	14/15	0.69	0.36	-	161,169,176,177	0
4	NAG	K	216	14/15	0.92	0.30	-	78,88,92,93	0
4	NAG	O	400	14/15	0.75	0.20	-	139,147,151,153	0
4	NAG	X	233	14/15	0.72	0.39	-	120,128,156,157	0
4	NAG	L	234	14/15	0.86	0.27	-	120,132,140,140	0
4	NAG	C	235	14/15	0.86	0.27	-	108,136,143,147	0
4	NAG	C	233	14/15	0.87	0.34	-	79,85,94,97	0
4	NAG	O	233	14/15	0.91	0.31	-	70,78,86,93	0
4	NAG	F	233	14/15	0.93	0.23	-	81,91,97,97	0
4	NAG	R	235	14/15	0.87	0.26	-	138,149,151,152	0
4	NAG	K	215	14/15	0.90	0.28	-	57,65,73,77	0
4	NAG	R	234	14/15	0.92	0.22	-	94,111,117,122	0

6.5 Other polymers (i)

There are no such residues in this entry.