Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:25 PM UTC

PDB ID	:	3QAZ / pdb_00003qaz
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

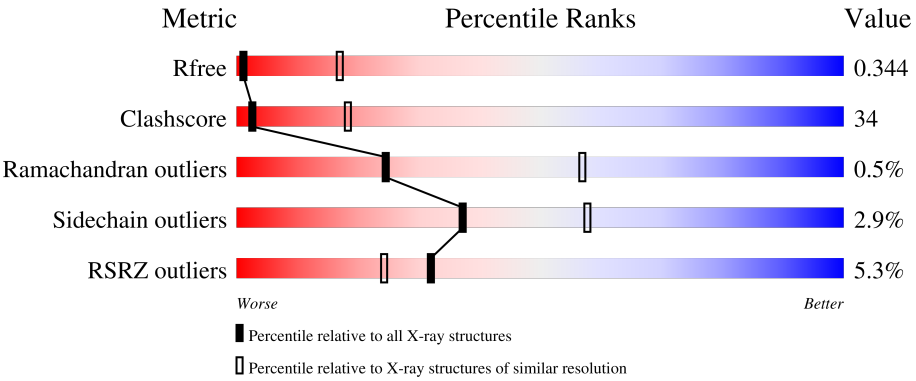
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (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}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 40% 45% 11%
1	D	136	3% 38% 48% 11%
1	G	136	3% 32% 54% 11%
1	J	136	4% 34% 51% 11%
1	M	136	5% 41% 46% 11%

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Mol	Chain	Length	Quality of chain
1	P	136	42% 43% 11%
1	S	136	3% 38% 47% 11%
1	V	136	12% 36% 49% 11%
1	Y	136	6% 33% 50% 5% 12%
1	b	136	31% 51% 6% 12%
1	e	136	8% 32% 51% 5% 11%
1	h	136	3% 40% 48% 11%
2	B	217	57% 32% 10%
2	E	217	45% 41% 5% 10%
2	H	217	45% 43% 10%
2	K	217	37% 52% 10%
2	N	217	42% 45% 10%
2	Q	217	3% 33% 55% 10%
2	T	217	33% 55% 10%
2	W	217	3% 38% 50% 10%
2	Z	217	3% 42% 45% 10%
2	c	217	5% 40% 48% 10%
2	f	217	31% 55% 10%
2	i	217	3% 37% 51% 10%
3	C	202	6% 62% 31% 7%
3	F	202	12% 38% 50% 8%
3	I	202	47% 43% 7%
3	L	202	6% 46% 44% 5%
3	O	202	8% 45% 44% 5%
3	R	202	50% 41% 7%

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Mol	Chain	Length	Quality of chain
3	U	202	7% 45% 47% • 5%
3	X	202	7% 46% 48% • 5%
3	a	202	13% 41% 52% • 5%
3	d	202	9% 49% 45% • 5%
3	g	202	7% 45% 47% • 5%
3	j	202	11% 48% 45% • 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 (i)

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:

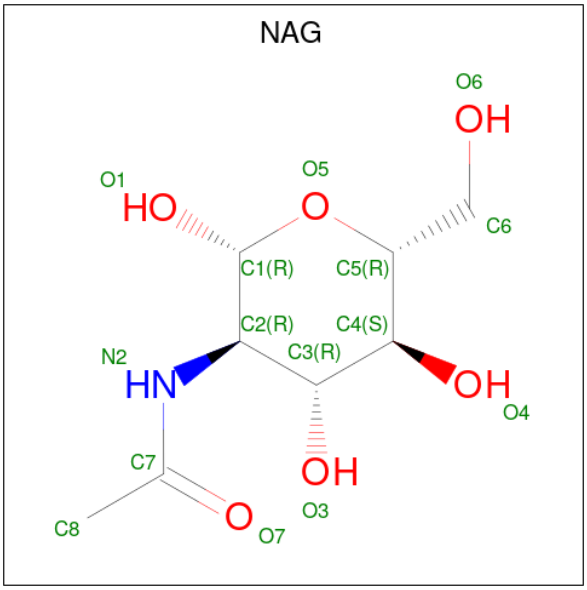
Chain	Residue	Modelled	Actual	Comment	Reference
C	31	ALA	-	expression tag	UNP P31785
C	32	ASP	-	expression tag	UNP P31785
C	33	PRO	-	expression tag	UNP P31785
C	53	GLN	ASN	engineered mutation	UNP P31785
F	31	ALA	-	expression tag	UNP P31785
F	32	ASP	-	expression tag	UNP P31785
F	33	PRO	-	expression tag	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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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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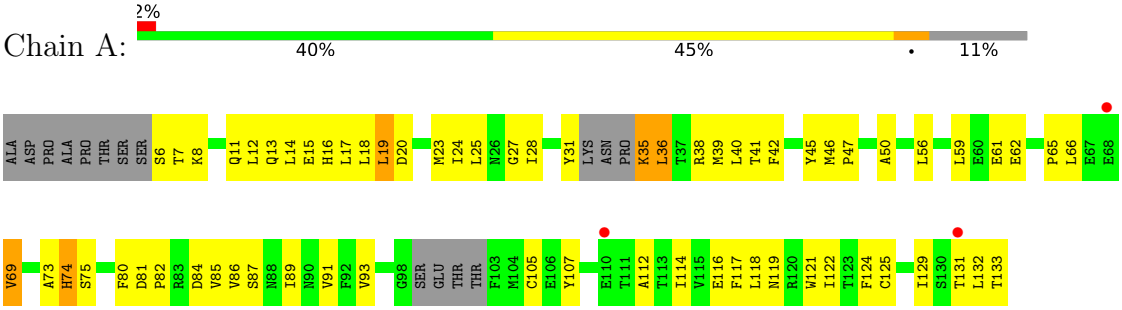
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	a	1	Total	C	N	O	0	0
			14	8	1	5		
4	a	1	Total	C	N	O	0	0
			14	8	1	5		
4	c	1	Total	C	N	O	0	0
			14	8	1	5		
4	c	1	Total	C	N	O	0	0
			14	8	1	5		
4	d	1	Total	C	N	O	0	0
			14	8	1	5		
4	f	1	Total	C	N	O	0	0
			14	8	1	5		
4	g	1	Total	C	N	O	0	0
			14	8	1	5		
4	g	1	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

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

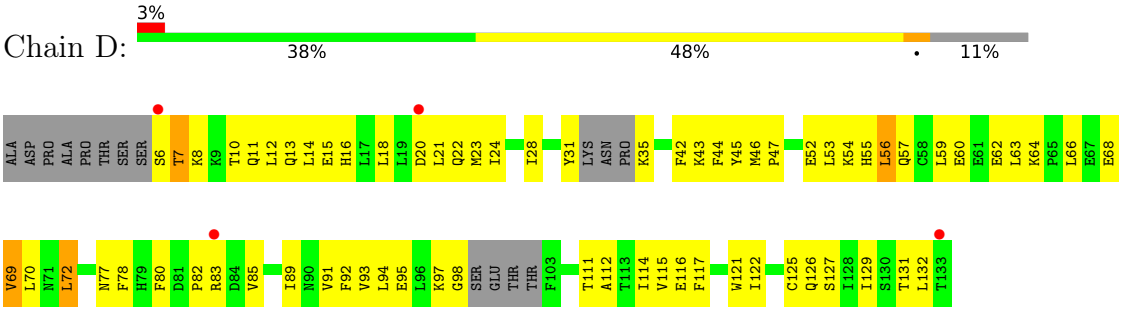
• Molecule 1: Interleukin-2

Chain A:



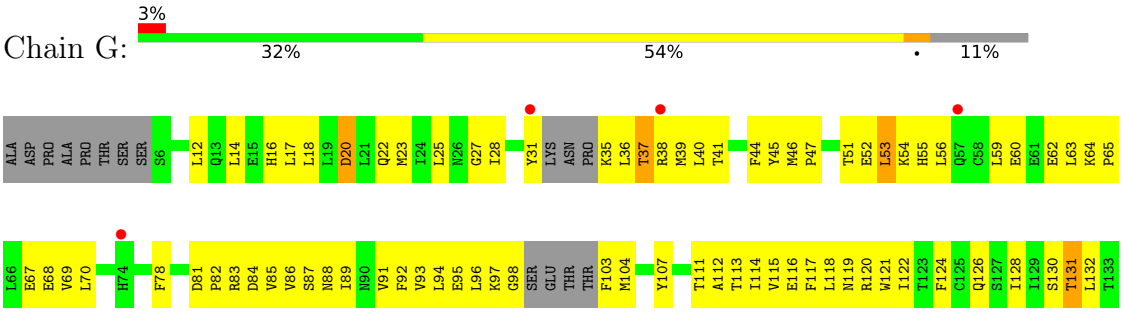
• Molecule 1: Interleukin-2

Chain D:



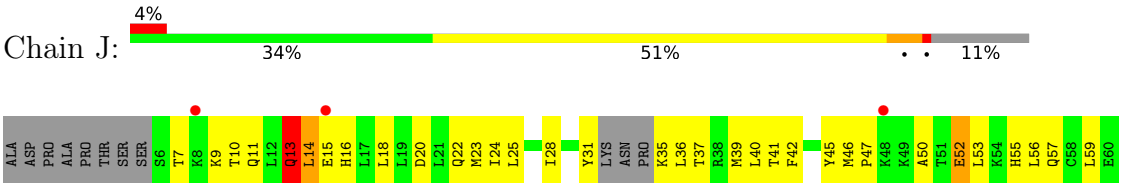
• Molecule 1: Interleukin-2

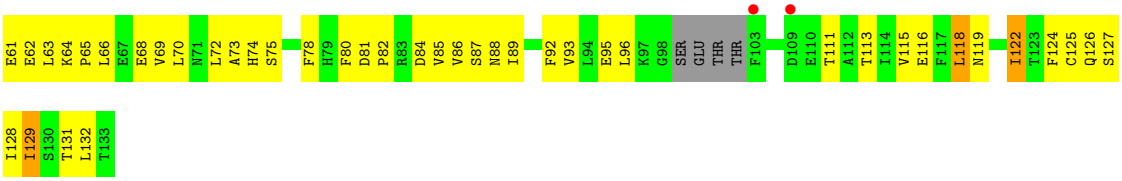
Chain G:



• Molecule 1: Interleukin-2

Chain J:

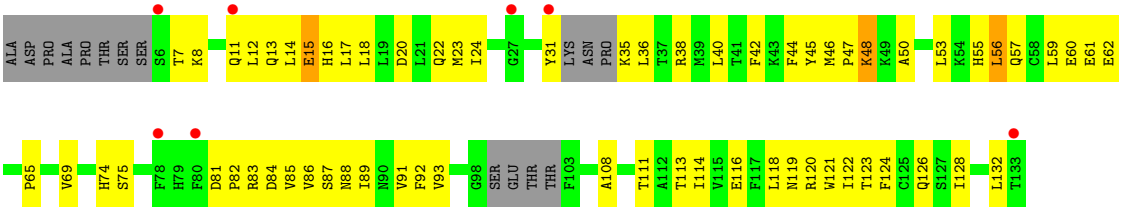




• Molecule 1: Interleukin-2

Chain M:

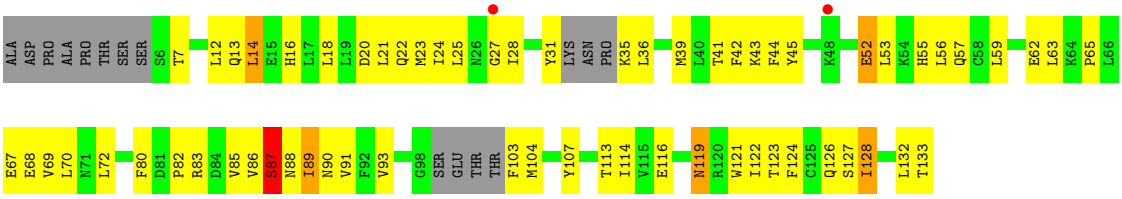




• Molecule 1: Interleukin-2

Chain P:

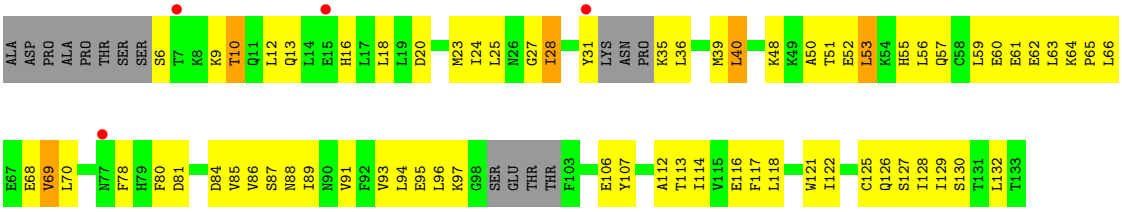




• Molecule 1: Interleukin-2

Chain S:

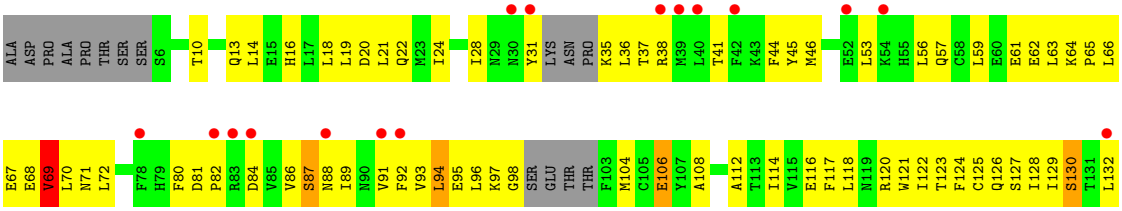




• Molecule 1: Interleukin-2

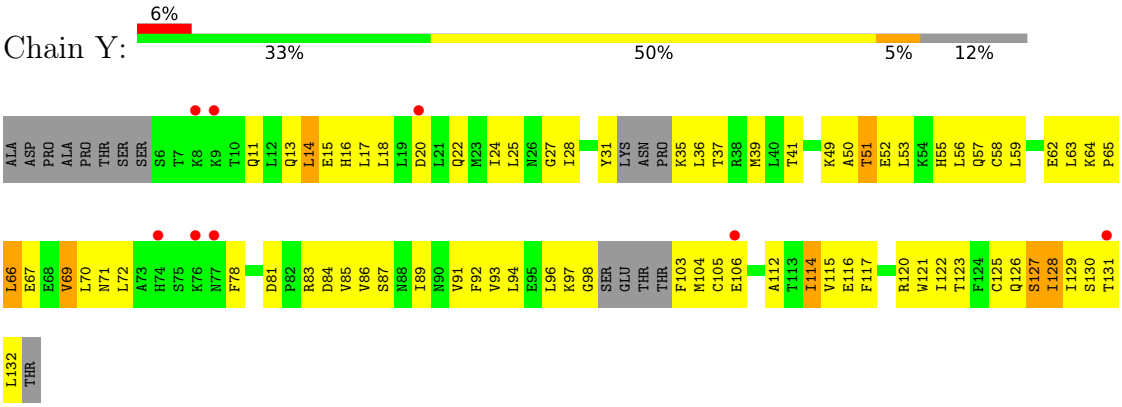
Chain V:



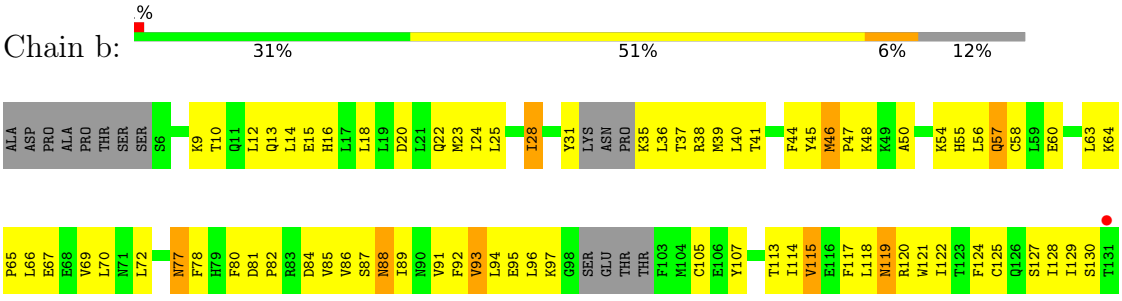




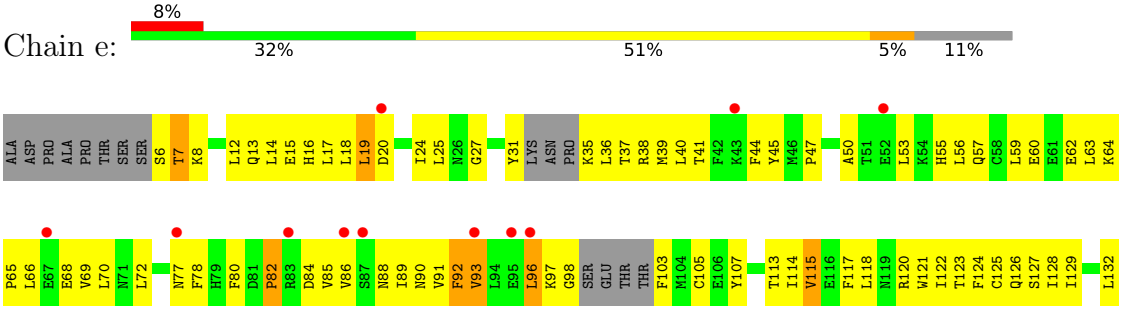
• Molecule 1: Interleukin-2



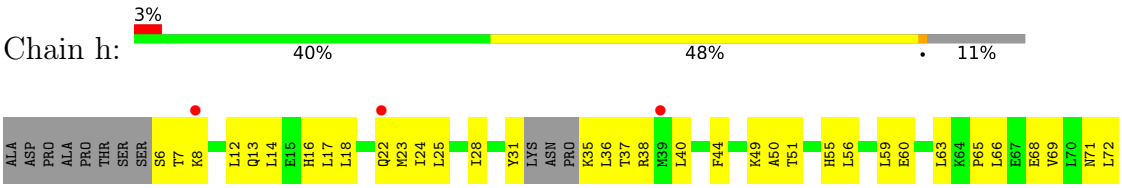
• Molecule 1: Interleukin-2

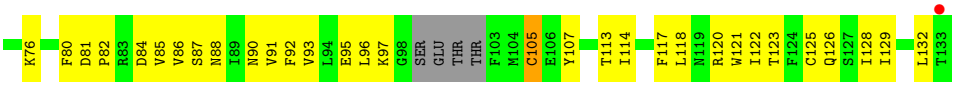


• Molecule 1: Interleukin-2



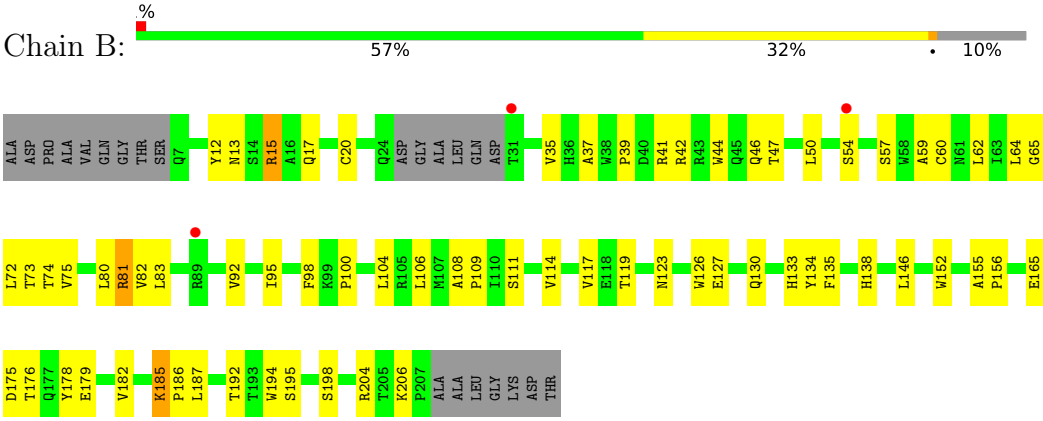
• Molecule 1: Interleukin-2





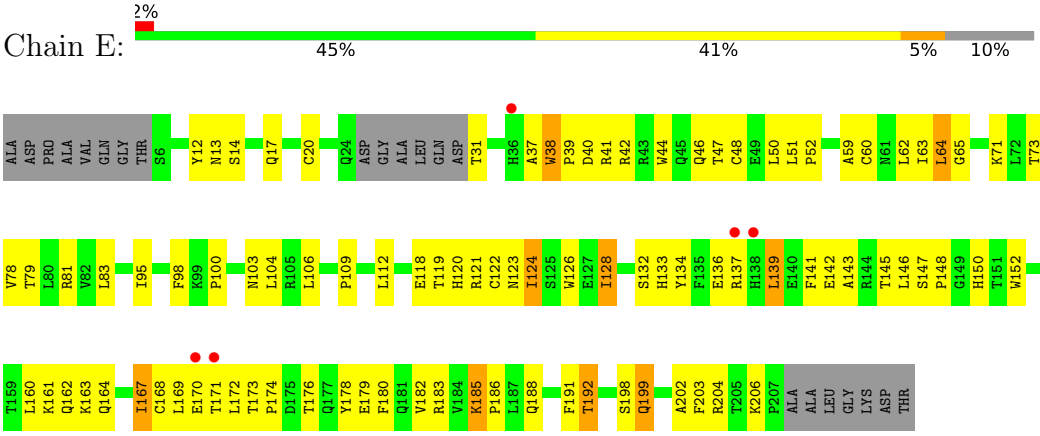
• Molecule 2: Interleukin-2 receptor subunit beta

Chain B:



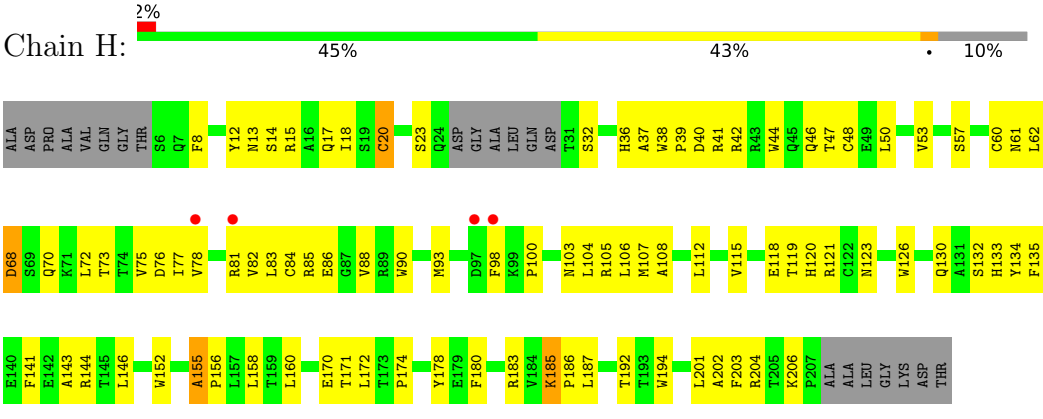
• Molecule 2: Interleukin-2 receptor subunit beta

Chain E:



• Molecule 2: Interleukin-2 receptor subunit beta

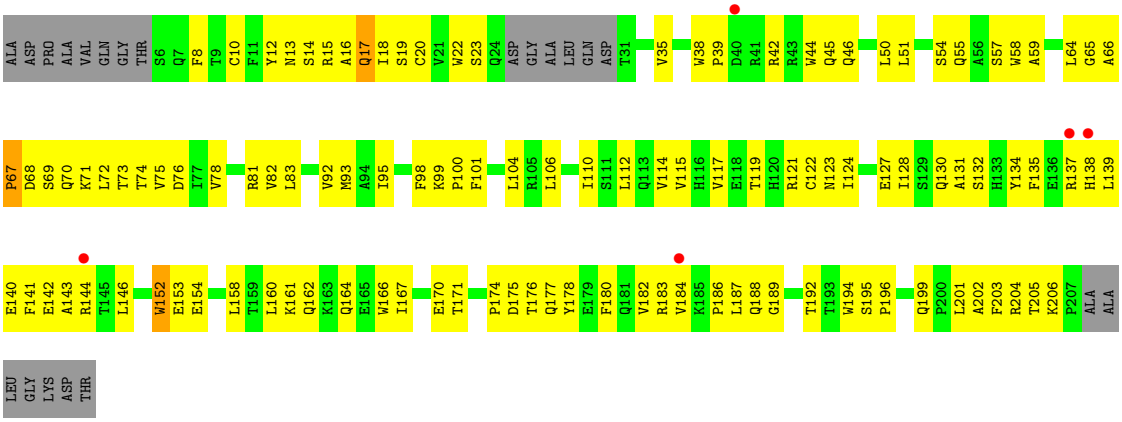
Chain H:



• Molecule 2: Interleukin-2 receptor subunit beta

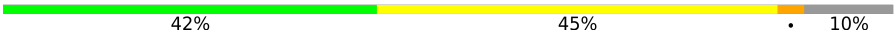
Chain K:

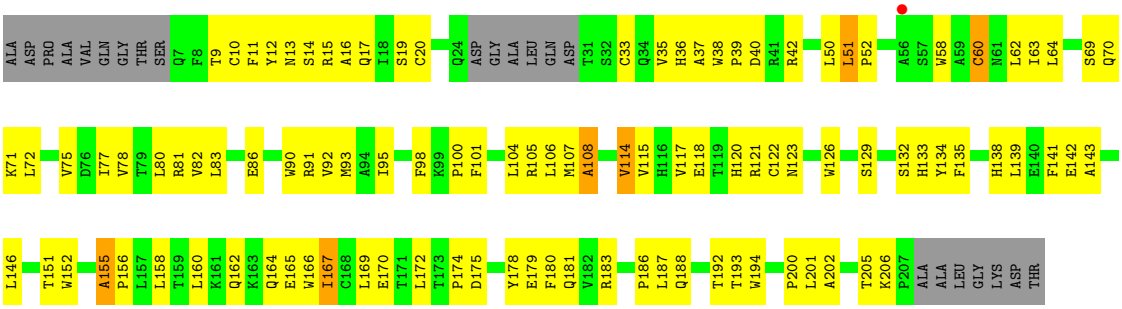




• Molecule 2: Interleukin-2 receptor subunit beta

Chain N:

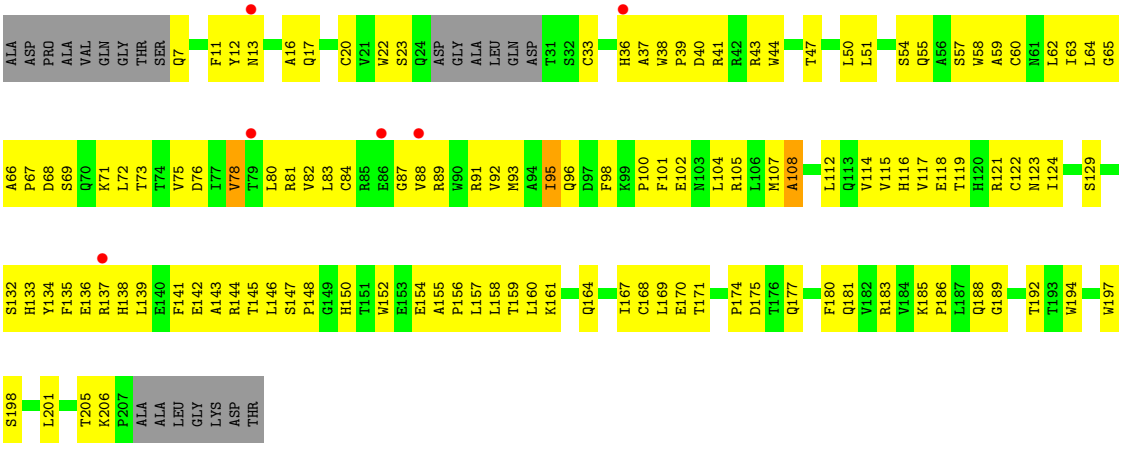




• Molecule 2: Interleukin-2 receptor subunit beta

Chain Q:

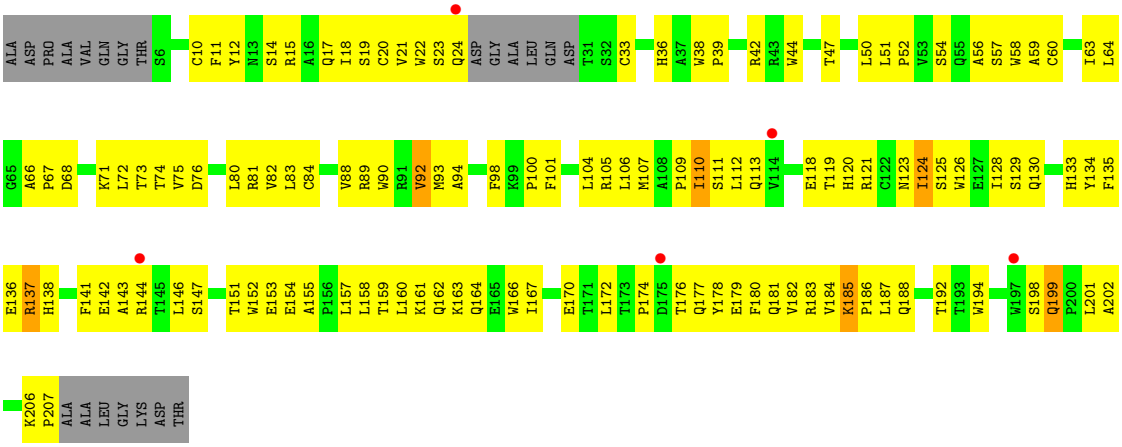




• Molecule 2: Interleukin-2 receptor subunit beta

Chain T:

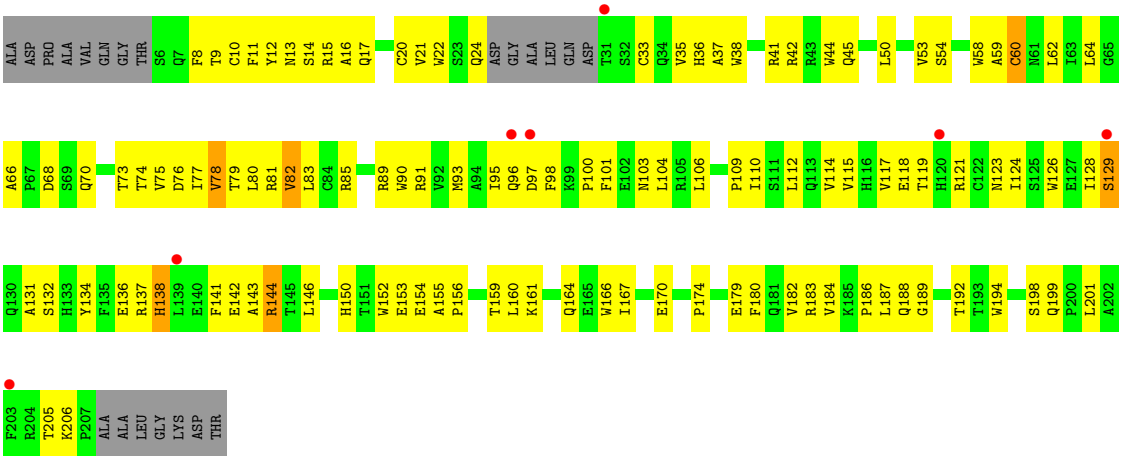




• Molecule 2: Interleukin-2 receptor subunit beta

Chain W:

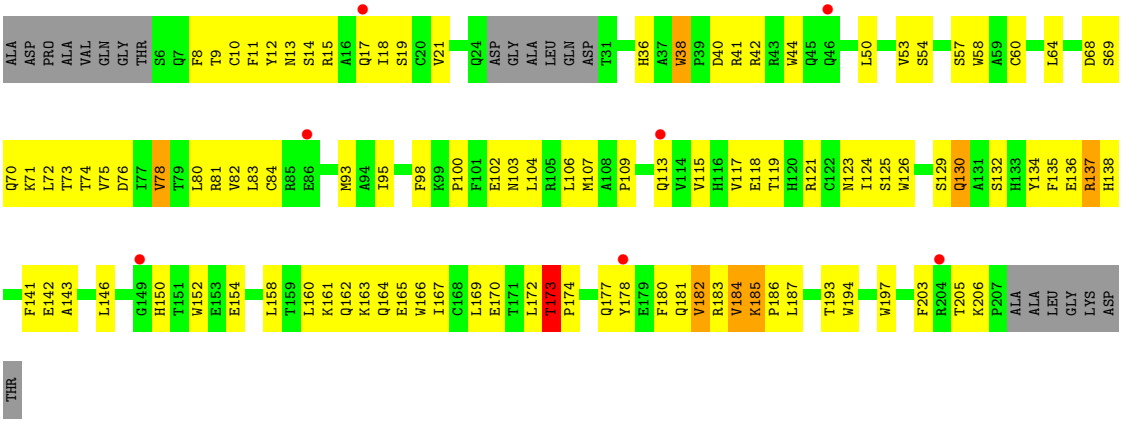




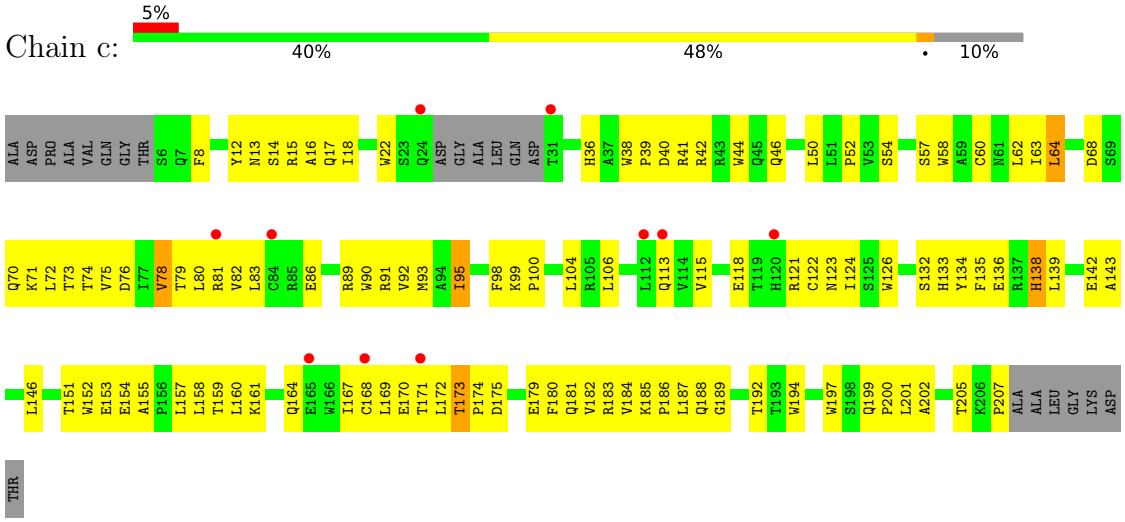
• Molecule 2: Interleukin-2 receptor subunit beta

Chain Z:

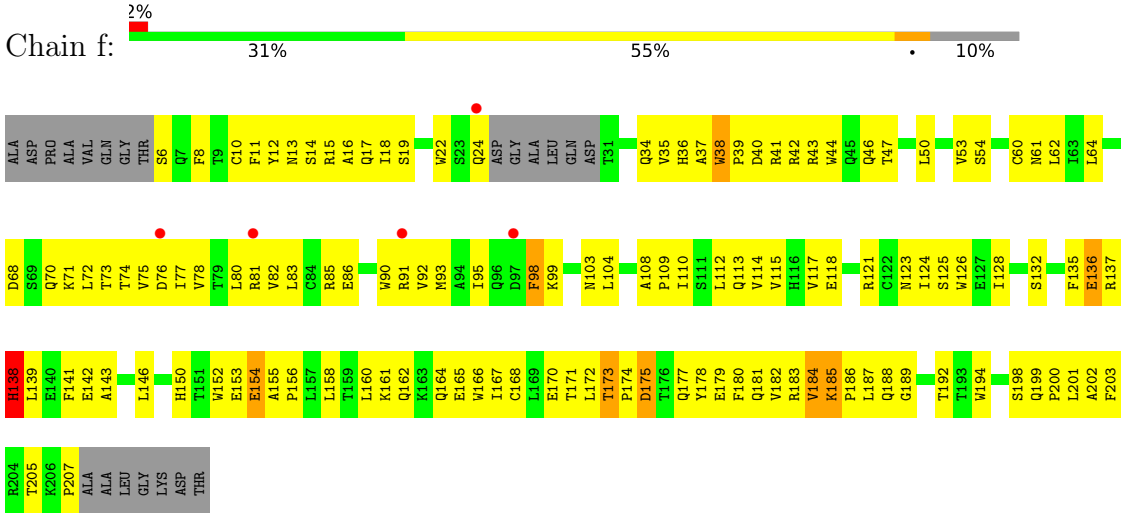




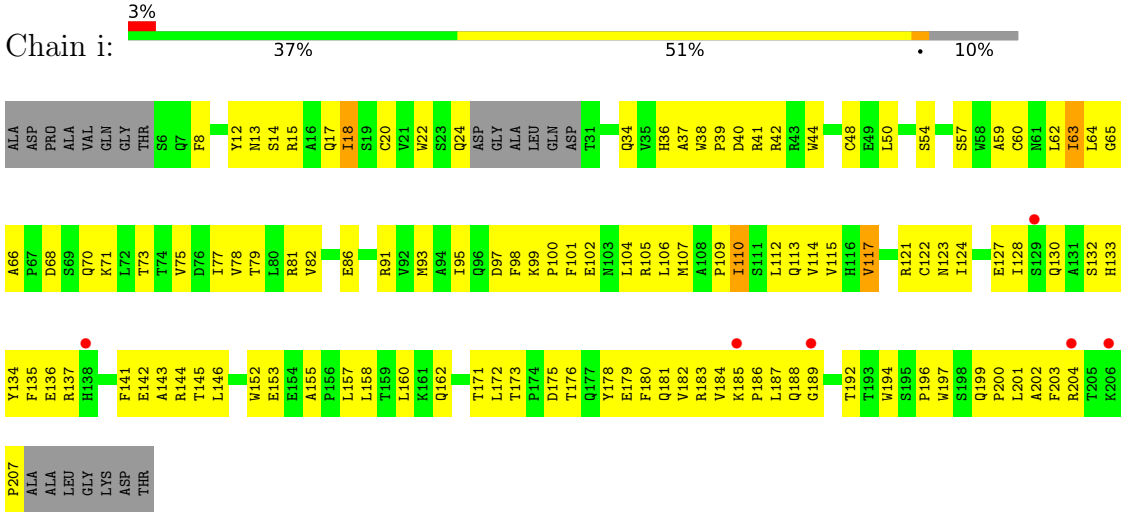
• Molecule 2: Interleukin-2 receptor subunit beta



• Molecule 2: Interleukin-2 receptor subunit beta

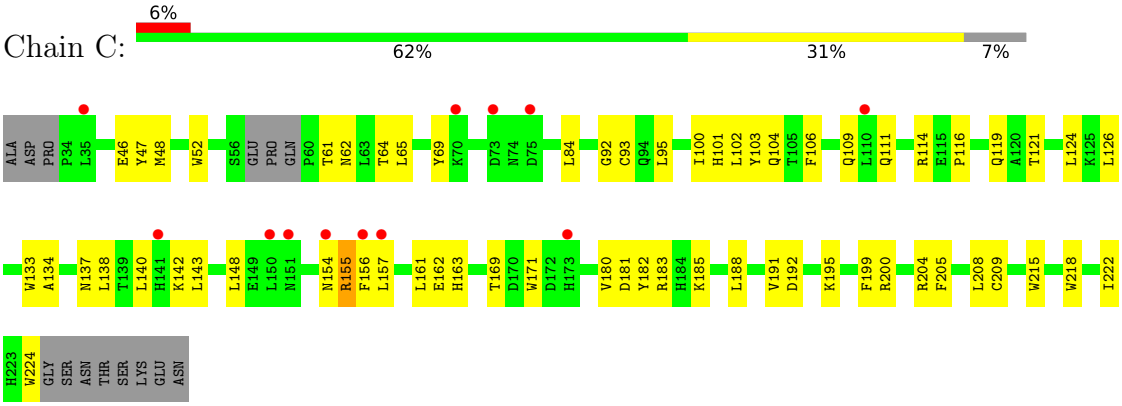


• Molecule 2: Interleukin-2 receptor subunit beta



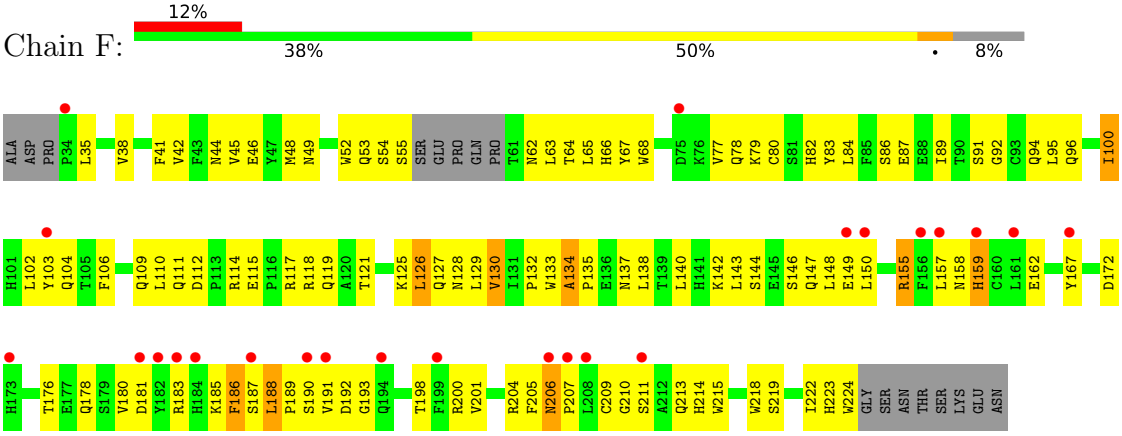
• Molecule 3: Cytokine receptor common subunit gamma

Chain C:



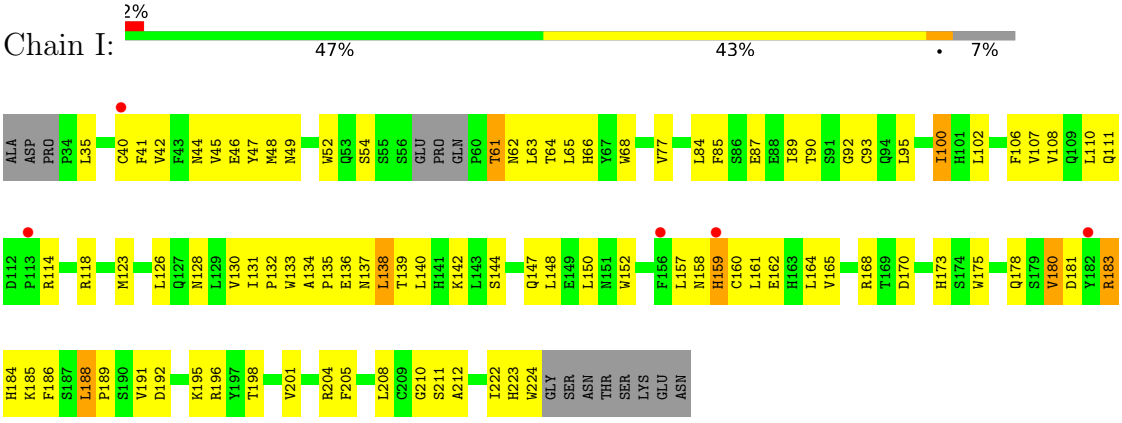
• Molecule 3: Cytokine receptor common subunit gamma

Chain F:



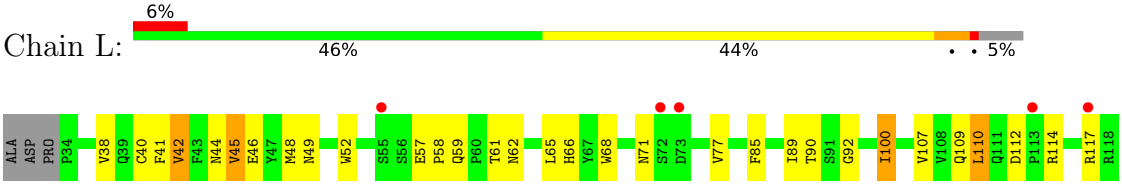
• Molecule 3: Cytokine receptor common subunit gamma

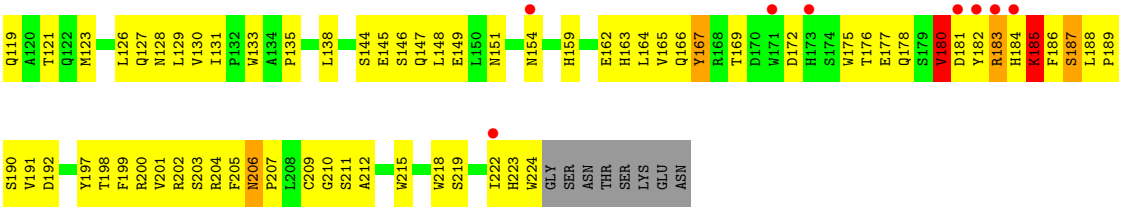
Chain I:



• Molecule 3: Cytokine receptor common subunit gamma

Chain L:

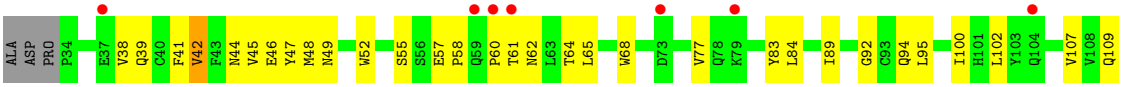


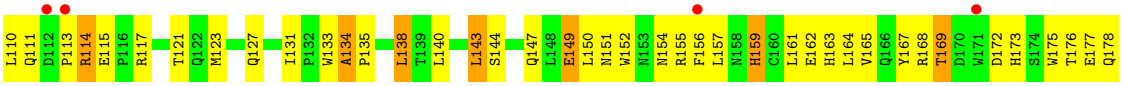


• Molecule 3: Cytokine receptor common subunit gamma

Chain O:





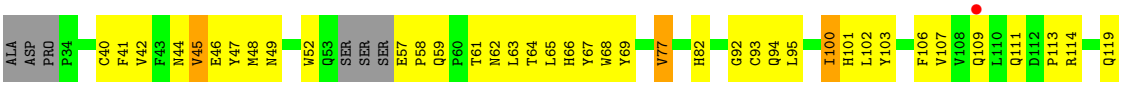


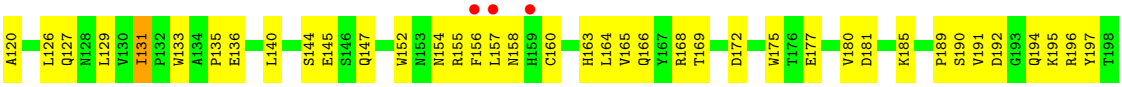


• Molecule 3: Cytokine receptor common subunit gamma

Chain R:





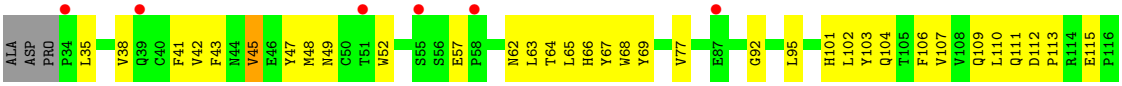


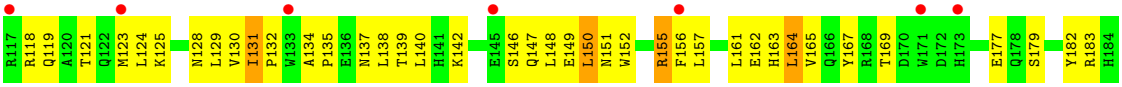


• Molecule 3: Cytokine receptor common subunit gamma

Chain U:



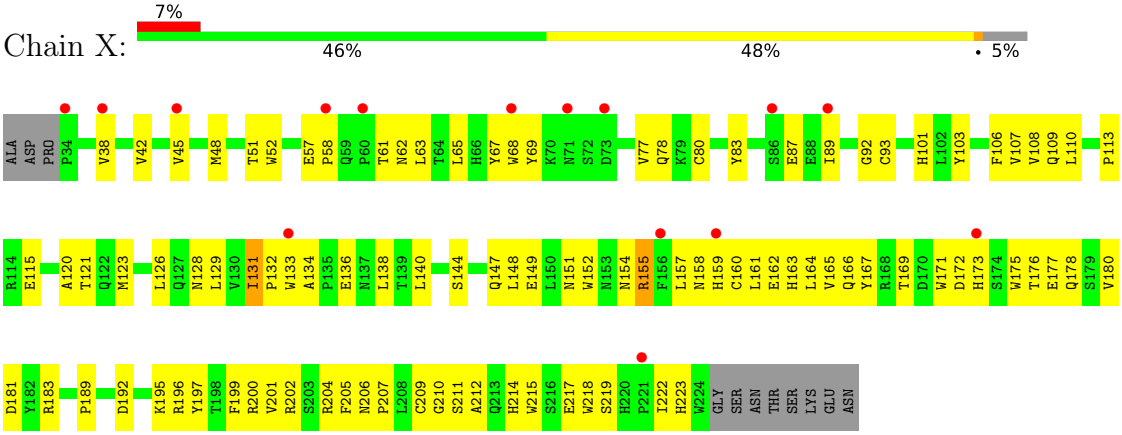






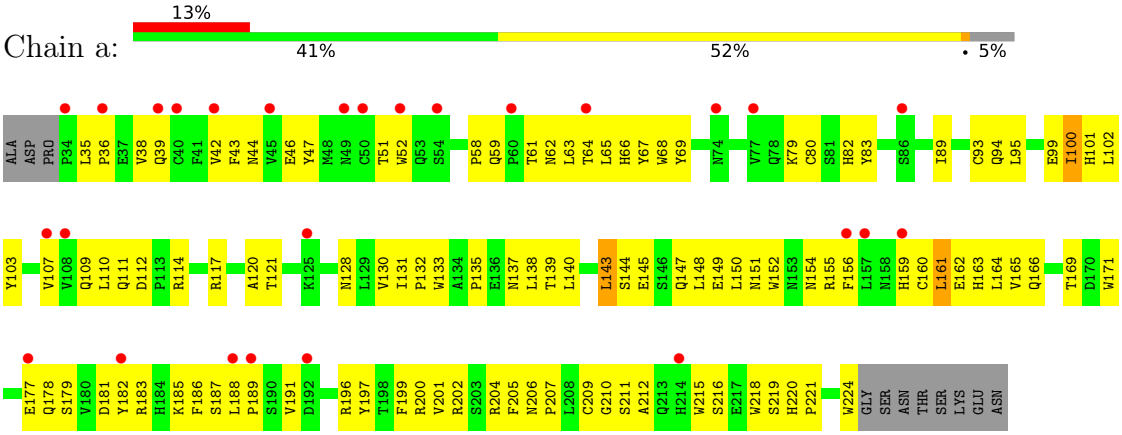
• Molecule 3: Cytokine receptor common subunit gamma

Chain X:



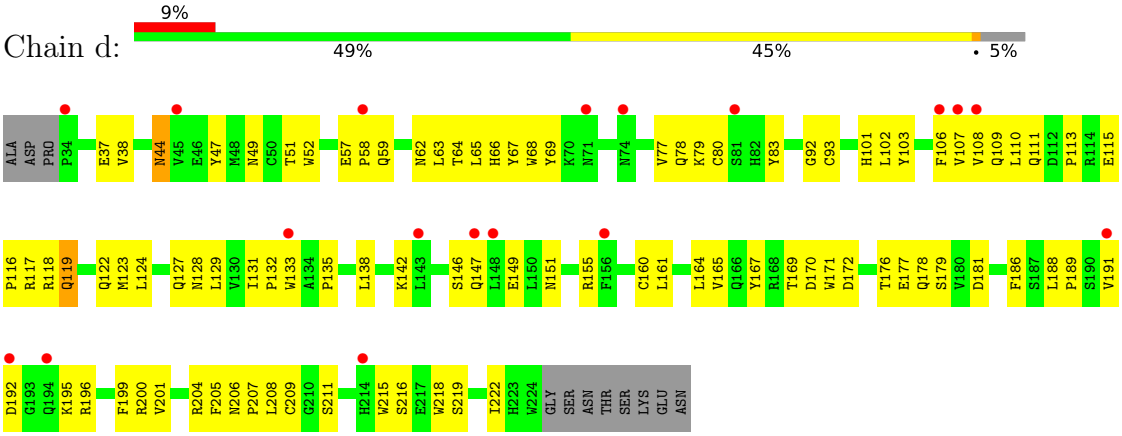
• Molecule 3: Cytokine receptor common subunit gamma

Chain a:



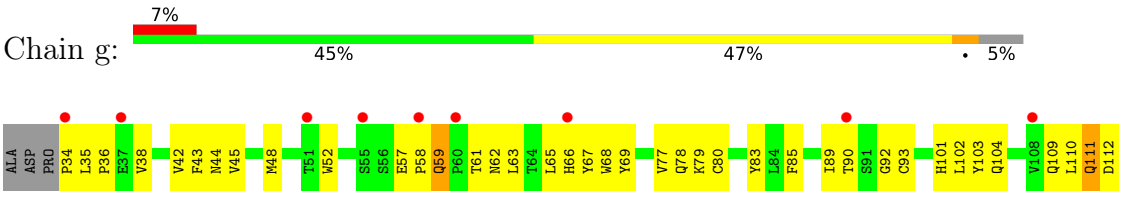
• Molecule 3: Cytokine receptor common subunit gamma

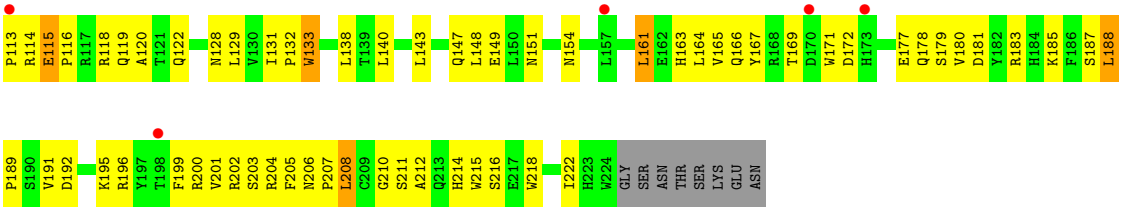
Chain d:



• Molecule 3: Cytokine receptor common subunit gamma

Chain g:

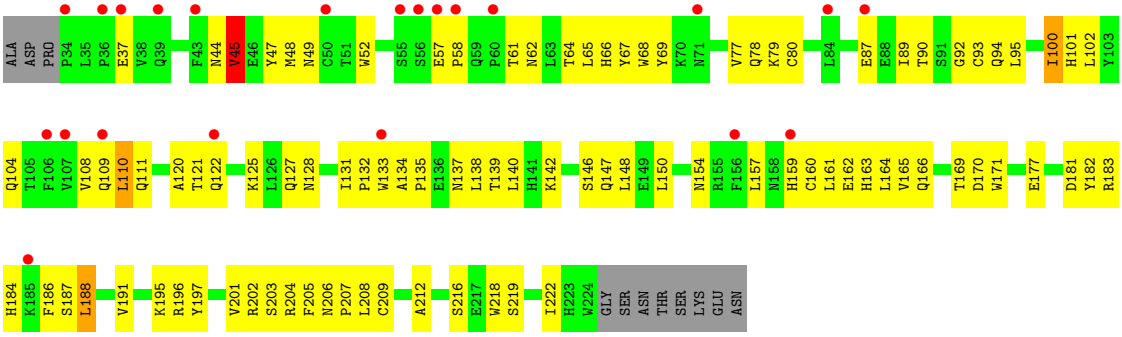




• Molecule 3: Cytokine receptor common subunit gamma

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) 94.5 (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 0.285 , 0.344	Depositor DCC
R_{free} test set	1881 reflections (1.67%)	wwPDB-VP
Wilson B-factor (Å^2)	82.1	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 92.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.036 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.88	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.39	0/1015	0.79	2/1367 (0.1%)
1	D	0.44	0/1015	0.84	2/1367 (0.1%)
1	G	0.43	0/1015	0.82	2/1367 (0.1%)
1	J	0.45	0/1015	0.91	3/1367 (0.2%)
1	M	0.37	0/1015	0.80	0/1367
1	P	0.42	0/1015	0.80	1/1367 (0.1%)
1	S	0.38	0/1015	0.79	1/1367 (0.1%)
1	V	0.48	0/1015	0.94	2/1367 (0.1%)
1	Y	0.41	0/1008	0.87	1/1357 (0.1%)
1	b	0.39	0/1000	0.83	1/1346 (0.1%)
1	e	0.52	0/1015	1.06	7/1367 (0.5%)
1	h	0.39	0/1015	0.83	2/1367 (0.1%)
2	B	0.44	0/1660	0.82	0/2264
2	E	0.46	0/1666	0.96	10/2272 (0.4%)
2	H	0.45	0/1666	0.86	3/2272 (0.1%)
2	K	0.48	0/1666	0.91	6/2272 (0.3%)
2	N	0.41	0/1660	0.91	6/2264 (0.3%)
2	Q	0.48	0/1660	0.89	3/2264 (0.1%)
2	T	0.42	0/1666	0.83	2/2272 (0.1%)
2	W	0.45	0/1666	0.87	4/2272 (0.2%)
2	Z	0.43	0/1666	0.85	4/2272 (0.2%)
2	c	0.44	0/1666	0.83	4/2272 (0.2%)
2	f	0.44	0/1666	0.93	8/2272 (0.4%)
2	i	0.42	0/1666	0.87	3/2272 (0.1%)
3	C	0.42	0/1658	0.84	5/2254 (0.2%)
3	F	0.41	0/1644	0.96	10/2235 (0.4%)
3	I	0.41	0/1658	0.87	3/2254 (0.1%)
3	L	0.49	0/1685	0.95	6/2294 (0.3%)
3	O	0.42	0/1685	0.92	8/2294 (0.3%)
3	R	0.38	0/1666	0.83	0/2267
3	U	0.33	0/1685	0.84	7/2294 (0.3%)
3	X	0.32	0/1685	0.81	2/2294 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
3	a	0.33	0/1685	0.78	1/2294 (0.0%)
3	d	0.32	0/1685	0.81	1/2294 (0.0%)
3	g	0.32	0/1685	0.80	4/2294 (0.2%)
3	j	0.36	0/1685	0.84	4/2294 (0.2%)
All	All	0.42	0/52238	0.87	128/70975 (0.2%)

There are no bond length outliers.

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	f	38	TRP	CA-C-N	10.81	130.57	119.76
2	f	38	TRP	C-N-CA	10.81	130.57	119.76
3	d	155	ARG	N-CA-C	10.03	121.80	111.07
3	O	114	ARG	N-CA-C	9.85	121.61	111.07
3	U	155	ARG	N-CA-C	9.78	121.53	111.07
2	W	129	SER	N-CA-C	9.69	121.44	111.07
3	j	188	LEU	CA-C-N	9.38	129.13	119.19
3	j	188	LEU	C-N-CA	9.38	129.13	119.19
1	V	69	VAL	N-CA-C	-8.85	101.59	110.62
1	Y	127	SER	N-CA-C	8.52	120.34	111.14
2	N	108	ALA	CA-C-N	8.37	128.44	119.90
2	N	108	ALA	C-N-CA	8.37	128.44	119.90
1	e	90	ASN	N-CA-C	8.00	120.00	111.28
3	F	188	LEU	CA-C-N	7.80	127.09	118.97
3	F	188	LEU	C-N-CA	7.80	127.09	118.97
2	E	155	ALA	CA-C-N	7.74	127.67	119.85
2	E	155	ALA	C-N-CA	7.74	127.67	119.85
3	L	185	LYS	N-CA-C	7.74	121.74	110.28
3	O	134	ALA	CA-C-N	7.72	127.65	119.85
3	O	134	ALA	C-N-CA	7.72	127.65	119.85
3	U	57	GLU	CA-C-N	7.58	126.85	118.97
3	U	57	GLU	C-N-CA	7.58	126.85	118.97
2	W	66	ALA	CA-C-N	-7.46	111.95	119.56
2	W	66	ALA	C-N-CA	-7.46	111.95	119.56
1	J	13	GLN	N-CA-C	7.43	119.17	111.14
2	Z	173	THR	CA-C-N	7.25	127.28	119.89
2	Z	173	THR	C-N-CA	7.25	127.28	119.89
2	N	155	ALA	CA-C-N	7.23	127.19	120.03
2	N	155	ALA	C-N-CA	7.23	127.19	120.03
1	e	7	THR	N-CA-C	-7.04	103.95	112.54
3	F	155	ARG	N-CA-C	7.03	118.59	111.07
2	N	51	LEU	CA-C-N	6.98	126.74	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	51	LEU	C-N-CA	6.98	126.74	119.76
2	E	199	GLN	N-CA-C	-6.82	101.18	109.57
3	L	184	HIS	N-CA-C	6.81	118.70	111.28
2	K	199	GLN	CA-C-N	6.74	127.14	119.93
2	K	199	GLN	C-N-CA	6.74	127.14	119.93
2	E	150	HIS	N-CA-C	6.74	120.36	110.59
2	c	99	LYS	CA-C-N	6.49	125.72	118.97
2	c	99	LYS	C-N-CA	6.49	125.72	118.97
1	e	86	VAL	CB-CA-C	-6.45	103.43	112.14
1	J	14	LEU	N-CA-C	-6.45	104.25	111.28
1	P	52	GLU	N-CA-C	6.41	118.91	109.24
3	g	115	GLU	CA-C-N	6.40	126.02	119.56
3	g	115	GLU	C-N-CA	6.40	126.02	119.56
1	A	19	LEU	N-CA-C	6.34	117.85	111.07
3	F	130	VAL	N-CA-C	6.30	116.75	106.72
3	L	167	TYR	N-CA-C	6.29	119.75	109.06
2	f	99	LYS	CA-C-N	6.25	127.65	119.84
2	f	99	LYS	C-N-CA	6.25	127.65	119.84
3	O	55	SER	N-CA-C	6.18	117.68	111.07
3	I	188	LEU	CA-C-N	6.09	127.45	119.84
3	I	188	LEU	C-N-CA	6.09	127.45	119.84
1	J	52	GLU	N-CA-C	6.07	118.18	109.14
3	I	100	ILE	N-CA-C	6.05	116.08	106.88
3	U	188	LEU	CA-C-N	6.00	125.39	118.85
3	U	188	LEU	C-N-CA	6.00	125.39	118.85
2	K	18	ILE	CB-CA-C	-5.99	103.74	111.53
3	F	134	ALA	CA-C-N	5.98	125.94	119.78
3	F	134	ALA	C-N-CA	5.98	125.94	119.78
3	L	100	ILE	N-CA-C	5.96	116.20	106.72
3	g	188	LEU	CA-C-N	5.95	125.56	119.56
3	g	188	LEU	C-N-CA	5.95	125.56	119.56
3	U	131	ILE	CA-C-N	5.91	126.38	119.99
3	U	131	ILE	C-N-CA	5.91	126.38	119.99
3	F	206	ASN	N-CA-C	5.89	113.52	108.22
2	i	66	ALA	N-CA-C	-5.81	102.27	109.64
1	A	36	LEU	N-CA-C	-5.81	105.69	112.89
2	Q	108	ALA	CA-C-N	5.72	125.66	119.76
2	Q	108	ALA	C-N-CA	5.72	125.66	119.76
2	E	185	LYS	CA-C-N	5.70	127.69	120.51
2	E	185	LYS	C-N-CA	5.70	127.69	120.51
3	O	188	LEU	CA-C-N	5.68	125.53	119.28
3	O	188	LEU	C-N-CA	5.68	125.53	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	h	105	CYS	N-CA-C	5.68	117.78	108.52
2	i	99	LYS	CA-C-N	5.66	125.77	119.32
2	i	99	LYS	C-N-CA	5.66	125.77	119.32
3	F	172	ASP	N-CA-C	5.65	118.03	110.35
1	V	87	SER	N-CA-C	-5.64	105.04	111.07
1	D	7	THR	N-CA-C	-5.62	106.19	113.16
2	c	173	THR	CA-C-N	5.62	125.57	119.78
2	c	173	THR	C-N-CA	5.62	125.57	119.78
1	h	7	THR	N-CA-C	-5.62	105.04	112.34
2	Z	38	TRP	CA-C-N	5.62	126.40	120.11
2	Z	38	TRP	C-N-CA	5.62	126.40	120.11
1	b	77	ASN	N-CA-C	5.60	117.08	110.97
2	Q	124	ILE	N-CA-C	5.60	115.92	107.75
1	e	77	ASN	N-CA-C	5.58	119.35	112.54
1	e	96	LEU	N-CA-C	5.45	117.22	111.28
3	j	134	ALA	CA-C-N	5.44	125.44	119.90
3	j	134	ALA	C-N-CA	5.44	125.44	119.90
1	G	37	THR	N-CA-C	-5.41	105.08	110.97
2	K	99	LYS	CA-C-N	5.38	125.45	119.32
2	K	99	LYS	C-N-CA	5.38	125.45	119.32
3	O	131	ILE	CA-C-N	5.36	125.26	119.85
3	O	131	ILE	C-N-CA	5.36	125.26	119.85
2	f	173	THR	CA-C-N	5.35	125.29	119.78
2	f	173	THR	C-N-CA	5.35	125.29	119.78
3	C	155	ARG	N-CA-C	5.34	117.11	111.28
1	e	115	VAL	N-CA-C	5.34	115.55	110.42
3	C	134	ALA	CA-C-N	5.33	125.34	119.90
3	C	134	ALA	C-N-CA	5.33	125.34	119.90
2	E	38	TRP	CA-C-N	5.33	125.09	119.76
2	E	38	TRP	C-N-CA	5.33	125.09	119.76
2	K	152	TRP	N-CA-C	5.32	117.49	111.11
1	e	93	VAL	N-CA-C	5.29	116.02	110.62
2	f	98	PHE	N-CA-C	5.29	117.24	108.20
3	L	180	VAL	N-CA-C	5.22	117.21	109.17
3	F	100	ILE	N-CA-C	5.20	115.26	107.51
3	X	115	GLU	CA-C-N	5.19	124.85	119.56
3	X	115	GLU	C-N-CA	5.19	124.85	119.56
2	f	136	GLU	CB-CA-C	-5.18	110.18	117.23
3	L	200	ARG	N-CA-C	5.17	116.39	108.52
3	a	100	ILE	N-CA-C	5.17	113.81	106.53
1	S	53	LEU	N-CA-C	5.16	117.57	111.33
2	T	199	GLN	CA-C-N	-5.14	114.61	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	199	GLN	C-N-CA	-5.14	114.61	119.76
2	E	173	THR	CA-C-N	5.12	126.23	119.84
2	E	173	THR	C-N-CA	5.12	126.23	119.84
1	G	86	VAL	N-CA-C	-5.11	105.52	110.42
3	C	188	LEU	CA-C-N	5.10	125.17	119.87
3	C	188	LEU	C-N-CA	5.10	125.17	119.87
2	W	82	VAL	CB-CA-C	-5.07	104.15	111.34
1	D	72	LEU	N-CA-C	-5.05	106.28	112.90
3	F	186	PHE	N-CA-C	5.03	117.26	108.76
2	H	155	ALA	CA-C-N	5.03	125.01	120.03
2	H	155	ALA	C-N-CA	5.03	125.01	120.03
2	H	136	GLU	CB-CA-C	-5.03	110.39	117.23

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	65	0
1	D	998	0	1015	105	0
1	G	998	0	1015	75	0
1	J	998	0	1015	82	0
1	M	998	0	1015	64	0
1	P	998	0	1015	66	1
1	S	998	0	1015	76	0
1	V	998	0	1015	96	0
1	Y	991	0	1008	81	0
1	b	983	0	997	95	2
1	e	998	0	1015	89	0
1	h	998	0	1015	71	0
2	B	1612	0	1565	62	0
2	E	1618	0	1570	127	1
2	H	1618	0	1570	107	0
2	K	1618	0	1570	148	0
2	N	1612	0	1565	117	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Q	1612	0	1565	117	1
2	T	1618	0	1570	160	0
2	W	1618	0	1570	159	0
2	Z	1618	0	1570	123	0
2	c	1618	0	1570	129	0
2	f	1618	0	1570	134	1
2	i	1618	0	1570	134	0
3	C	1605	0	1512	51	0
3	F	1592	0	1499	156	0
3	I	1605	0	1512	89	2
3	L	1630	0	1533	109	0
3	O	1630	0	1533	109	0
3	R	1612	0	1517	81	0
3	U	1630	0	1533	107	0
3	X	1630	0	1533	103	0
3	a	1630	0	1533	128	0
3	d	1630	0	1533	95	0
3	g	1630	0	1533	112	0
3	j	1630	0	1533	103	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	8	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	4	0
4	c	28	0	26	1	0
4	d	14	0	13	3	0
4	f	14	0	13	3	0
4	g	28	0	26	7	0
4	i	28	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	j	14	0	13	4	0
All	All	51562	0	49986	3461	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 34.

All (3461) 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
1:e:50:ALA:HB3	1:e:120:ARG:NH2	1.63	1.12
3:F:206:ASN:OD1	3:F:210:GLY:O	1.70	1.10
2:Z:158:LEU:HA	3:a:147:GLN:HE22	1.17	1.10
2:W:110:ILE:HG12	2:W:129:SER:HB2	1.36	1.07
1:e:50:ALA:HB3	1:e:120:ARG:HH22	1.18	1.06
2:f:82:VAL:HG13	2:f:93:MET:HB2	1.33	1.05
1:h:56:LEU:HB3	1:h:93:VAL:HG13	1.38	1.03
3:g:138:LEU:HB3	3:g:222:ILE:HD13	1.41	1.03
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:O:114:ARG:O	2:i:204:ARG:N	1.93	1.00
3:a:38:VAL:HG22	3:a:52:TRP:HB3	1.41	0.99
1:D:42:PHE:HE1	1:D:72:LEU:HD11	1.24	0.99
2:i:109:PRO:HG3	2:i:184:VAL:HG23	1.44	0.99
2:f:123:ASN:HD21	4:f:215:NAG:C1	1.75	0.99
2:K:138:HIS:C	2:K:187:LEU:HG	1.89	0.97
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
3:d:107:VAL:HG22	3:d:123:MET:HG2	1.47	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
1:b:87:SER:HB3	2:c:42:ARG:HH12	1.30	0.95
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:123:ASN:HD21	4:i:215:NAG:C1	1.79	0.94
2:Z:13:ASN:ND2	2:Z:17:GLN:HB2	1.82	0.94
1:J:16:HIS:CE1	2:K:134:TYR:HB3	2.02	0.94
3:L:52:TRP:CZ3	3:L:92:GLY:HA2	2.03	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
3:O:169:THR:H	3:O:172:ASP:HB2	1.31	0.92
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
1:b:66:LEU:HD12	1:b:117:PHE:HE2	1.34	0.90
2:i:65:GLY:HA3	2:i:71:LYS:HE3	1.54	0.90
3:F:62:ASN:HD21	4:F:300:NAG:C1	1.85	0.89
3:j:164:LEU:HD11	3:j:177:GLU:HB2	1.52	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
3:g:35:LEU:HD13	3:g:110:LEU:HD12	1.55	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
2:K:146:LEU:HB2	2:K:152:TRP:CH2	2.09	0.88
3:L:169:THR:H	3:L:172:ASP:HB2	1.39	0.88
3:a:52:TRP:HZ3	3:a:65:LEU:HD12	1.39	0.88
2:c:183:ARG:HD2	2:c:194:TRP:HB3	1.55	0.87
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
1:b:13:GLN:HE21	2:c:75:VAL:HG12	1.39	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
2:i:44:TRP:CZ3	2:i:64:LEU:HD22	2.10	0.86
1:J:15:GLU:HG2	1:J:129:ILE:CD1	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:f:126:TRP:HZ3	2:f:167:ILE:HG22	1.43	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
2:i:128:ILE:HG22	2:i:184:VAL:HG21	1.61	0.83
1:M:56:LEU:HB3	1:M:93:VAL:HG13	1.60	0.83
2:E:162:GLN:CD	3:F:187:SER:H	1.85	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
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
1:h:56:LEU:HD11	1:h:96:LEU:HD23	1.59	0.82
1:A:20:ASP:HB2	1:A:23:MET:HE2	1.59	0.82
1:e:44:PHE:HE1	1:e:65:PRO:HB2	1.44	0.82
3:d:66:HIS:HE1	3:d:79:LYS:HG2	1.42	0.82
2:E:162:GLN:HE22	3:F:187:SER:CA	1.92	0.82
2:i:101:PHE:HA	2:i:104:LEU:HD21	1.60	0.82
2:Q:12:TYR:OH	2:Q:72:LEU:HB2	1.79	0.82
2:i:12:TYR:CE2	2:i:14:SER:HA	2.14	0.82
2:H:18:ILE:HB	2:H:62:LEU:HB2	1.60	0.82
3:L:204:ARG:HD3	3:L:212:ALA:O	1.80	0.82
1:P:31:TYR:HH	1:P:35:LYS:N	1.78	0.82
3:g:35:LEU:HB3	3:g:110:LEU:HD11	1.61	0.81
1:J:31:TYR:OH	1:J:35:LYS:HB3	1.80	0.81
2:c:13:ASN:HD21	2:c:16:ALA:H	1.25	0.81
3:g:164:LEU:HD11	3:g:177:GLU:HB2	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:j:164:LEU:HD21	3:j:177:GLU:OE1	1.79	0.81
2:K:81:ARG:CD	2:K:95:ILE:HG22	2.11	0.81
2:N:175:ASP:H	2:N:205:THR:HB	1.44	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
3:O:114:ARG:HB3	2:i:202:ALA:O	1.80	0.80
3:g:140:LEU:HD11	3:g:222:ILE:HD12	1.63	0.80
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
1:D:20:ASP:OD1	1:D:23:MET:HE2	1.80	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:a:164:LEU:HD11	3:a:177:GLU:HB2	1.61	0.80
2:f:13:ASN:ND2	2:f:17:GLN:HB2	1.96	0.80
3:X:158:ASN:O	3:X:159:HIS:HB2	1.80	0.80
1:b:31:TYR:HH	1:b:35:LYS:N	1.78	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:b:87:SER:HB3	2:c:42:ARG:NH1	1.97	0.79
1:h:36:LEU:HD12	1:h:36:LEU:O	1.82	0.79
1:V:120:ARG:O	1:V:123:THR:HB	1.82	0.79
3:j:205:PHE:CZ	3:j:209:CYS:HB2	2.17	0.79
3:d:149:GLU:HG2	3:d:151:ASN:HD21	1.46	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:h:66:LEU:HD12	1:h:117:PHE:HE2	1.48	0.79
3:j:47:TYR:HE1	3:j:49:ASN:HD21	1.29	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
3:d:80:CYS:HB3	3:d:83:TYR:CE1	2.18	0.79
3:R:156:PHE:HD2	3:R:157:LEU:HG	1.48	0.78
2:Z:12:TYR:CE2	2:Z:14:SER:HA	2.18	0.78
3:d:37:GLU:HG3	3:d:122:GLN:HE22	1.47	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:Z:158:LEU:HA	3:a:147:GLN:NE2	1.95	0.78
2:c:73:THR:HG22	2:c:76:ASP:OD1	1.84	0.78
1:e:24:ILE:HD11	1:e:89:ILE:HD11	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:185:LYS:HB2	2:f:194:TRP:CE3	2.18	0.78
3:g:42:VAL:HG22	3:g:48:MET:HB2	1.64	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
3:g:69:TYR:CZ	3:g:101:HIS:HB2	2.19	0.77
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
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:a:139:THR:O	3:a:150:LEU:HD12	1.82	0.77
2:c:175:ASP:OD1	2:c:207:PRO:HG3	1.83	0.77
2:i:109:PRO:HG3	2:i:184:VAL:CG2	2.14	0.77
2:i:114:VAL:HG11	2:i:117:VAL:HG22	1.66	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:U:148:LEU:HD21	3:U:191:VAL:HG11	1.66	0.77
3:X:165:VAL:HG22	3:X:201:VAL:HG22	1.63	0.77
2:K:167:ILE:HG21	2:K:180:PHE:CZ	2.20	0.77
2:c:54:SER:HB3	2:c:57:SER:HB2	1.64	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:K:14:SER:HG	2:K:135:PHE:HE2	1.33	0.76
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:i:13:ASN:ND2	2:i:17:GLN:HG2	2.00	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
2:f:40:ASP:HB3	2:f:77:ILE:HB	1.65	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
3:a:161:LEU:HD22	3:a:204:ARG:O	1.86	0.76
2:f:73:THR:HG22	2:f:76:ASP:OD1	1.84	0.76
2:H:50:LEU:HD23	2:H:60:CYS:HB2	1.68	0.76
3:g:65:LEU:HD13	3:g:93:CYS:HB2	1.67	0.76
3:R:163:HIS:ND1	3:R:203:SER:HB3	2.00	0.76
3:g:192:ASP:OD2	3:g:195:LYS:HG3	1.85	0.76
1:V:124:PHE:O	1:V:128:ILE:HG12	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:g:38:VAL:HG22	3:g:52:TRP:HB3	1.67	0.75
2:Z:73:THR:HG22	2:Z:76:ASP:OD1	1.85	0.75
1:e:120:ARG:O	1:e:123:THR:HB	1.85	0.75
1:h:50:ALA:HA	1:h:55:HIS:ND1	2.01	0.75
3:F:183:ARG:HD3	3:F:185:LYS:HE2	1.67	0.75
3:g:138:LEU:HB3	3:g:222:ILE:CD1	2.15	0.75
3:F:62:ASN:CG	4:F:300:NAG:H83	2.11	0.75
2:f:71:LYS:O	2:f:72:LEU:HD23	1.86	0.75
1:h:69:VAL:O	1:h:72:LEU:HG	1.85	0.75
2:B:13:ASN:ND2	2:B:17:GLN:HB3	2.00	0.75
1:J:66:LEU:O	1:J:70:LEU:HD12	1.86	0.75
1:M:16:HIS:HD1	2:N:134:TYR:HB3	1.51	0.75
2:Z:82:VAL:O	2:Z:83:LEU:HD23	1.87	0.75
3:F:204:ARG:HH21	3:F:213:GLN:HA	1.50	0.75
2:E:164:GLN:HE21	3:F:178:GLN:HG2	1.52	0.75
2:W:115:VAL:HB	2:W:123:ASN:HD22	1.52	0.75
2:W:161:LYS:O	3:X:183:ARG:NH2	2.19	0.74
2:Z:143:ALA:HB3	2:Z:158:LEU:HB2	1.69	0.74
2:i:37:ALA:HB2	2:i:62:LEU:HD13	1.67	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:c:89:ARG:HG2	2:c:89:ARG:HH11	1.49	0.74
2:K:137:ARG:O	3:L:181:ASP:HB3	1.87	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
1:b:56:LEU:CD1	1:b:96:LEU:HD23	2.17	0.74
1:P:23:MET:HE1	2:Q:133:HIS:CE1	2.23	0.74
1:b:66:LEU:HD12	1:b:117:PHE:CE2	2.21	0.74
3:F:117:ARG:HH21	2:c:207:PRO:CG	2.00	0.74
2:Z:164:GLN:NE2	3:a:178:GLN:HG2	2.02	0.74
1:V:69:VAL:O	1:V:72:LEU:HB2	1.87	0.74
1:h:81:ASP:HB3	1:h:84:ASP:HB2	1.69	0.74
3:X:197:TYR:O	3:X:223:HIS:HA	1.88	0.74
1:D:16:HIS:HB3	2:E:134:TYR:CD2	2.22	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
3:U:52:TRP:HZ3	3:U:65:LEU:HD12	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:a:80:CYS:HB3	3:a:83:TYR:CE1	2.22	0.73
1:e:44:PHE:CE1	1:e:65:PRO:HB2	2.22	0.73
2:i:44:TRP:HZ3	2:i:64:LEU:HD22	1.53	0.73
1:A:74:HIS:CG	1:A:75:SER:H	2.05	0.73
3:F:68:TRP:HH2	3:F:109:GLN:NE2	1.85	0.73
1:J:88:ASN:ND2	2:K:42:ARG:HH22	1.85	0.73
2:K:143:ALA:HB1	2:K:180:PHE:CE1	2.23	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
3:d:52:TRP:HZ3	3:d:65:LEU:HD12	1.52	0.73
2:i:50:LEU:HD23	2:i:60:CYS:HB2	1.70	0.73
1:D:18:LEU:HD11	1:D:122:ILE:HG23	1.71	0.73
2:E:119:THR:HB	2:E:174:PRO:HG3	1.69	0.73
2:W:82:VAL:HB	2:W:93:MET:HB2	1.71	0.73
3:j:57:GLU:HB3	3:j:58:PRO:HD2	1.71	0.73
2:K:121:ARG:HG2	2:K:170:GLU:OE1	1.88	0.73
2:N:69:SER:HB2	2:N:71:LYS:HE2	1.68	0.73
2:N:123:ASN:ND2	4:N:215:NAG:C1	2.51	0.73
2:T:172:LEU:HD22	2:T:178:TYR:CZ	2.23	0.73
1:b:28:ILE:O	1:b:36:LEU:HD11	1.86	0.73
3:d:138:LEU:HB3	3:d:222:ILE:HD13	1.70	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
3:d:204:ARG:HH21	3:d:215:TRP:NE1	1.85	0.73
2:W:13:ASN:HD21	2:W:16:ALA:H	1.34	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
2:T:109:PRO:HG3	2:T:184:VAL:CG2	2.18	0.73
3:U:192:ASP:OD2	3:U:195:LYS:HE3	1.88	0.73
2:f:114:VAL:HG11	2:f:117:VAL:HG22	1.71	0.73
3:g:52:TRP:HZ3	3:g:65:LEU:HD12	1.54	0.73
3:C:84:LEU:CD2	4:C:234:NAG:H62	2.19	0.73
1:D:95:GLU:CD	2:E:41:ARG:HH12	1.97	0.73
1:e:125:CYS:O	1:e:129:ILE:HG13	1.88	0.73
3:g:62:ASN:HD21	4:g:300:NAG:C1	2.02	0.73
2:Q:115:VAL:CG1	4:Q:215:NAG:H62	2.18	0.72
3:U:204:ARG:HH21	3:U:215:TRP:NE1	1.86	0.72
1:e:39:MET:HG3	1:e:72:LEU:HD12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:161:LYS:HZ3	3:L:185:LYS:HD3	1.54	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
3:a:169:THR:HG22	3:a:197:TYR:CE2	2.23	0.72
2:f:12:TYR:CE2	2:f:14:SER:HA	2.25	0.72
3:g:183:ARG:HH11	3:g:183:ARG:HG3	1.54	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:F:52:TRP:NE1	3:F:63:LEU:HD12	2.05	0.72
3:F:117:ARG:HH21	2:c:207:PRO:HG2	1.53	0.72
2:i:112:LEU:HB3	2:i:201:LEU:HD22	1.71	0.72
3:j:68:TRP:HB3	3:j:77:VAL:HA	1.72	0.72
2:B:114:VAL:CG1	2:B:117:VAL:HG23	2.20	0.72
2:K:104:LEU:O	2:K:192:THR:HG23	1.89	0.72
1:V:95:GLU:HG3	2:W:41:ARG:HH12	1.55	0.72
2:Z:164:GLN:HE21	3:a:178:GLN:HG2	1.55	0.72
2:E:128:ILE:HD12	2:E:128:ILE:O	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
3:a:147:GLN:HG2	3:a:189:PRO:O	1.90	0.72
1:b:13:GLN:NE2	2:c:75:VAL:HG12	2.05	0.72
1:b:56:LEU:HD11	1:b:96:LEU:HD23	1.72	0.72
3:I:138:LEU:H	3:I:138:LEU:HD12	1.54	0.71
2:Q:174:PRO:HA	2:Q:205:THR:HG21	1.72	0.71
3:a:38:VAL:HG13	3:a:51:THR:O	1.90	0.71
3:F:52:TRP:HE1	3:F:63:LEU:HD12	1.55	0.71
1:M:35:LYS:HD2	1:M:38:ARG:HH21	1.54	0.71
3:O:62:ASN:ND2	4:O:300:NAG:H83	2.05	0.71
3:g:132:PRO:HB3	3:g:161:LEU:HD21	1.72	0.71
1:G:31:TYR:HH	1:G:35:LYS:N	1.87	0.71
3:U:147:GLN:HG2	3:U:189:PRO:O	1.90	0.71
2:B:123:ASN:HD21	4:B:215:NAG:C1	2.02	0.71
1:D:11:GLN:HB2	1:D:132:LEU:HD22	1.70	0.71
3:R:154:ASN:HD21	3:R:163:HIS:CE1	2.09	0.71
2:f:13:ASN:O	2:f:14:SER:HB3	1.89	0.71
1:h:31:TYR:HH	1:h:35:LYS:N	1.88	0.71
1:h:125:CYS:O	1:h:129:ILE:HG13	1.91	0.71
3:R:48:MET:HB2	3:R:100:ILE:HD11	1.72	0.71
2:i:124:ILE:HD11	2:i:203:PHE:CD2	2.26	0.71
2:T:183:ARG:HD2	2:T:194:TRP:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:a:62:ASN:HD21	4:a:300:NAG:C1	2.04	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
2:T:138:HIS:CE1	3:U:182:TYR:CD2	2.79	0.70
2:W:189:GLY:HA3	2:W:192:THR:OG1	1.91	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:d:132:PRO:O	3:d:216:SER:HB2	1.90	0.70
2:f:139:LEU:HD23	2:f:186:PRO:HA	1.71	0.70
3:F:206:ASN:CG	3:F:207:PRO:HA	2.16	0.70
1:G:44:PHE:HE2	1:G:114:ILE:HB	1.56	0.70
3:O:42:VAL:HG22	3:O:100:ILE:HD13	1.73	0.70
2:W:110:ILE:HG12	2:W:129:SER:CB	2.19	0.70
1:D:7:THR:HG22	1:D:132:LEU:HD11	1.72	0.70
2:E:112:LEU:HG	2:E:126:TRP:HB3	1.74	0.70
3:I:168:ARG:HG2	3:I:175:TRP:CZ3	2.26	0.70
2:i:82:VAL:HG12	2:i:93:MET:HB2	1.72	0.70
3:U:188:LEU:HD11	3:U:199:PHE:HE1	1.55	0.70
1:b:37:THR:HA	1:b:40:LEU:HB2	1.73	0.70
2:c:167:ILE:HG21	2:c:180:PHE:CZ	2.27	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
1:e:24:ILE:CD1	1:e:89:ILE:HD11	2.21	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:33:CYS:HB3	2:Q:50:LEU:HD12	1.74	0.70
2:Q:160:LEU:HD13	2:Q:164:GLN:HB3	1.72	0.70
2:c:124:ILE:HD13	2:c:201:LEU:HD23	1.74	0.70
3:d:147:GLN:HG2	3:d:189:PRO:O	1.92	0.70
1:Y:128:ILE:O	1:Y:132:LEU:HG	1.91	0.69
3:j:52:TRP:CD2	3:j:110:LEU:HD11	2.27	0.69
2:T:98:PHE:CE2	2:T:100:PRO:HA	2.27	0.69
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:f:37:ALA:HB2	2:f:62:LEU:HD13	1.74	0.69
3:U:62:ASN:ND2	4:U:300:NAG:H83	2.07	0.69
2:W:12:TYR:CE2	2:W:14:SER:HA	2.27	0.69
3:X:68:TRP:HB3	3:X:77:VAL:HA	1.74	0.69
3:L:57:GLU:CG	3:L:58:PRO:HD2	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:e:66:LEU:HD23	1:e:66:LEU:O	1.91	0.69
3:g:204:ARG:HG2	3:g:205:PHE:N	2.07	0.69
2:N:12:TYR:CE2	2:N:14:SER:HA	2.28	0.69
3:j:148:LEU:HD11	3:j:188:LEU:HD12	1.75	0.69
3:a:149:GLU:OE1	3:a:185:LYS:HD2	1.93	0.69
2:c:121:ARG:HG2	2:c:170:GLU:OE2	1.93	0.69
1:D:122:ILE:O	1:D:126:GLN:HG3	1.93	0.69
3:O:107:VAL:HG22	3:O:123:MET:HG2	1.73	0.69
2:Q:91:ARG:HD3	2:Q:93:MET:HE1	1.73	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
2:W:13:ASN:O	2:W:14:SER:OG	2.09	0.69
2:f:114:VAL:HG11	2:f:117:VAL:CG2	2.22	0.69
1:h:23:MET:HE1	2:i:133:HIS:CE1	2.28	0.69
1:M:122:ILE:O	1:M:126:GLN:HG3	1.93	0.69
3:R:57:GLU:HB3	3:R:58:PRO:HD2	1.75	0.69
2:T:159:THR:HG21	2:T:161:LYS:HE3	1.75	0.69
1:S:125:CYS:O	1:S:129:ILE:HG13	1.93	0.69
2:W:35:VAL:HG23	2:W:50:LEU:HD11	1.73	0.69
2:Z:104:LEU:HD22	2:Z:135:PHE:HZ	1.58	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:a:52:TRP:CZ3	3:a:65:LEU:HD12	2.26	0.68
3:g:52:TRP:CZ3	3:g:65:LEU:HD12	2.27	0.68
3:F:188:LEU:HD21	3:F:191:VAL:HG12	1.74	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:Q:17:GLN:CG	2:Q:63:ILE:HD13	2.23	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
2:c:123:ASN:HD21	4:c:215:NAG:C1	2.07	0.68
1:A:16:HIS:CE1	2:B:134:TYR:HB3	2.29	0.68
3:L:188:LEU:HD12	3:L:189:PRO:HD2	1.76	0.68
3:X:154:ASN:HD21	3:X:163:HIS:CE1	2.10	0.68
3:a:152:TRP:HE1	3:a:163:HIS:CD2	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:45:VAL:O	3:F:45:VAL:HG12	1.93	0.68
1:M:87:SER:O	1:M:91:VAL:HG23	1.94	0.68
1:S:127:SER:HA	3:U:103:TYR:CD1	2.29	0.68
2:f:112:LEU:HG	2:f:126:TRP:HB3	1.76	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
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
2:i:54:SER:HB3	2:i:57:SER:HB2	1.75	0.67
3:O:57:GLU:HG2	3:O:58:PRO:CD	2.23	0.67
1:V:31:TYR:HH	1:V:35:LYS:N	1.92	0.67
1:J:45:TYR:HE1	1:J:111:THR:HG22	1.58	0.67
2:i:15:ARG:HD3	2:i:68:ASP:O	1.93	0.67
2:i:183:ARG:HD2	2:i:194:TRP:HB3	1.75	0.67
2:N:17:GLN:HG2	2:N:63:ILE:HD13	1.76	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
3:g:207:PRO:HG2	3:g:208:LEU:HD23	1.76	0.67
1:G:112:ALA:HB1	1:G:116:GLU:HB2	1.77	0.67
1:P:52:GLU:O	1:P:55:HIS:HB2	1.95	0.67
2:Q:98:PHE:CE2	2:Q:100:PRO:HA	2.29	0.67
2:Q:117:VAL:HG12	2:Q:122:CYS:SG	2.35	0.67
1:V:95:GLU:CG	2:W:41:ARG:HH12	2.08	0.67
2:W:119:THR:HG22	2:W:206:LYS:O	1.93	0.67
3:d:66:HIS:CE1	3:d:79:LYS:HG2	2.28	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
2:f:73:THR:CG2	2:f:75:VAL:HG22	2.25	0.67
3:R:206:ASN:OD1	3:R:207:PRO:HA	1.95	0.67
3:a:169:THR:HG22	3:a:197:TYR:HE2	1.60	0.67
2:f:172:LEU:HD22	2:f:178:TYR:CE1	2.28	0.67
2:i:110:ILE:HD12	2:i:127:GLU:HB2	1.77	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
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
3:a:42:VAL:HB	3:a:130:VAL:HG22	1.77	0.67
3:g:38:VAL:HG23	3:g:110:LEU:HD23	1.77	0.67
3:g:44:ASN:HD22	3:g:133:TRP:H	1.40	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:j:109:GLN:HE21	3:j:121:THR:HG22	1.60	0.67
3:F:48:MET:CB	3:F:100:ILE:HD11	2.25	0.66
3:a:200:ARG:HG3	3:a:218:TRP:CZ3	2.30	0.66
2:i:18:ILE:HD12	2:i:64:LEU:HD11	1.76	0.66
3:X:154:ASN:HD21	3:X:163:HIS:HE1	1.41	0.66
3:d:62:ASN:ND2	4:d:300:NAG:H83	2.11	0.66
1:e:15:GLU:O	1:e:18:LEU:HB3	1.95	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:e:14:LEU:HD21	1:e:125:CYS:HA	1.78	0.66
1:h:23:MET:SD	1:h:80:PHE:HB3	2.35	0.66
2:B:68:ASP:OD1	2:B:130:GLN:HG2	1.95	0.66
1:D:10:THR:O	1:D:14:LEU:HD12	1.94	0.66
2:f:36:HIS:HB3	2:f:38:TRP:HE1	1.61	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:g:52:TRP:CZ3	3:g:92:GLY:HA2	2.31	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
1:e:127:SER:HA	3:g:103:TYR:CE1	2.30	0.66
2:i:42:ARG:HB3	2:i:44:TRP:NE1	2.10	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
2:B:108:ALA:HB1	2:B:198:SER:HA	1.78	0.66
1:J:45:TYR:CE1	1:J:111:THR:HG22	2.30	0.66
1:M:16:HIS:CE1	2:N:134:TYR:HB3	2.31	0.66
3:U:188:LEU:HD11	3:U:199:PHE:CE1	2.31	0.66
1:D:16:HIS:ND1	2:E:134:TYR:HD2	1.93	0.65
1:J:63:LEU:HD23	1:J:66:LEU:HD23	1.78	0.65
2:W:15:ARG:HD3	2:W:68:ASP:O	1.97	0.65
2:W:21:VAL:HA	2:W:58:TRP:O	1.95	0.65
3:F:140:LEU:HD23	3:F:150:LEU:HD13	1.78	0.65
3:L:166:GLN:HG2	3:L:177:GLU:HB3	1.77	0.65
2:Z:15:ARG:HD2	2:Z:130:GLN:CB	2.26	0.65
3:a:62:ASN:ND2	4:a:300:NAG:H83	2.12	0.65
2:E:198:SER:O	2:E:199:GLN:C	2.38	0.65
3:I:135:PRO:HG2	3:I:201:VAL:HG12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:71:LYS:O	2:K:72:LEU:HD23	1.95	0.65
3:a:46:GLU:HG3	3:a:47:TYR:HD2	1.61	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
2:K:13:ASN:HD21	2:K:16:ALA:H	1.45	0.65
2:K:128:ILE:HD12	2:K:131:ALA:HB3	1.78	0.65
1:M:18:LEU:O	1:M:22:GLN:HG3	1.97	0.65
2:W:98:PHE:O	2:W:100:PRO:HD3	1.96	0.65
1:Y:20:ASP:OD1	1:Y:85:VAL:HG23	1.97	0.65
3:g:140:LEU:CD1	3:g:222:ILE:HD12	2.27	0.65
2:Z:69:SER:OG	2:Z:71:LYS:HE2	1.96	0.65
1:e:56:LEU:HD22	1:e:93:VAL:HG22	1.77	0.65
1:h:16:HIS:HB3	1:h:92:PHE:CE2	2.32	0.65
3:C:140:LEU:HD22	3:C:148:LEU:HD23	1.78	0.65
3:O:46:GLU:CD	3:O:133:TRP:HE1	2.05	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:g:80:CYS:HB3	3:g:83:TYR:CE1	2.32	0.65
3:g:132:PRO:HD2	3:g:216:SER:HB3	1.78	0.65
2:K:138:HIS:HA	2:K:187:LEU:HD12	1.77	0.65
2:Q:36:HIS:HD2	2:Q:83:LEU:HG	1.61	0.65
2:Q:114:VAL:HG11	2:Q:117:VAL:HG13	1.79	0.65
2:T:123:ASN:ND2	4:T:215:NAG:C1	2.53	0.65
3:X:107:VAL:HG22	3:X:123:MET:HG2	1.77	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
3:R:169:THR:H	3:R:172:ASP:HB2	1.62	0.65
1:V:59:LEU:HB2	1:V:121:TRP:CE2	2.32	0.65
1:b:127:SER:HA	3:d:103:TYR:CE1	2.32	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
1:G:12:LEU:O	1:G:12:LEU:HD23	1.96	0.64
3:I:52:TRP:HZ3	3:I:65:LEU:HD12	1.62	0.64
1:P:20:ASP:O	1:P:24:ILE:HD12	1.95	0.64
2:Z:129:SER:O	2:Z:130:GLN:C	2.37	0.64
3:a:66:HIS:HE1	3:a:79:LYS:HG2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:LEU:HD23	1:D:132:LEU:O	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:164:LEU:HD11	3:L:177:GLU:HB2	1.79	0.64
3:L:191:VAL:HB	3:L:197:TYR:CE1	2.32	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
3:F:87:GLU:O	3:F:89:ILE:HG13	1.97	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:K:146:LEU:HD13	2:K:152:TRP:CE3	2.33	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
1:S:70:LEU:HD22	1:S:78:PHE:CE2	2.32	0.64
1:b:24:ILE:HD11	1:b:85:VAL:HG21	1.78	0.64
3:F:204:ARG:NH2	3:F:213:GLN:HA	2.11	0.64
2:N:158:LEU:HA	3:O:147:GLN:NE2	2.12	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
1:Y:97:LYS:HG3	1:Y:98:GLY:H	1.63	0.64
2:f:126:TRP:CZ3	2:f:167:ILE:HG22	2.30	0.64
3:j:166:GLN:HG2	3:j:177:GLU:HB3	1.79	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
2:Z:161:LYS:HD3	3:a:185:LYS:HE3	1.79	0.64
3:j:157:LEU:HD23	3:j:205:PHE:HE1	1.63	0.64
1:D:16:HIS:HB3	2:E:134:TYR:CE2	2.33	0.64
2:T:185:LYS:HB2	2:T:194:TRP:CE3	2.32	0.64
2:W:188:GLN:HG2	2:W:189:GLY:N	2.12	0.64
1:J:86:VAL:HA	1:J:89:ILE:HD12	1.80	0.64
2:H:82:VAL:C	2:H:83:LEU:HD12	2.22	0.63
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
2:K:114:VAL:CG1	2:K:117:VAL:HG13	2.27	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:i:104:LEU:O	2:i:192:THR:HG23	1.99	0.63
2:E:38:TRP:CE3	2:T:81:ARG:NH1	2.67	0.63
1:G:56:LEU:HD13	1:G:124:PHE:CE2	2.34	0.63
3:I:165:VAL:HG11	3:I:186:PHE:CD2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:158:LEU:HA	3:O:147:GLN:HE22	1.64	0.63
1:P:25:LEU:HD22	1:P:122:ILE:HD12	1.80	0.63
2:Q:118:GLU:OE1	2:Q:121:ARG:HD3	1.98	0.63
3:a:61:THR:O	3:a:89:ILE:HG23	1.97	0.63
1:b:28:ILE:O	1:b:28:ILE:HG22	1.98	0.63
3:d:62:ASN:HD21	4:d:300:NAG:C1	2.12	0.63
3:d:165:VAL:HG22	3:d:201:VAL:HG22	1.81	0.63
3:g:62:ASN:HD21	4:g:300:NAG:C2	2.11	0.63
1:A:114:ILE:O	1:A:117:PHE:HB3	1.99	0.63
3:F:46:GLU:CD	3:F:133:TRP:HE1	2.06	0.63
2:Q:72:LEU:CD1	2:Q:78:VAL:HG21	2.28	0.63
3:U:42:VAL:HG22	3:U:48:MET:HB2	1.79	0.63
1:Y:97:LYS:HG3	1:Y:98:GLY:N	2.13	0.63
2:Z:126:TRP:NE1	2:Z:165:GLU:HA	2.12	0.63
2:Z:169:LEU:HB3	2:Z:172:LEU:HD21	1.80	0.63
2:c:12:TYR:CE2	2:c:14:SER:HA	2.33	0.63
2:c:139:LEU:HD23	2:c:186:PRO:HA	1.79	0.63
3:j:138:LEU:HB2	3:j:222:ILE:HG21	1.79	0.63
1:D:91:VAL:HG13	2:E:41:ARG:HD2	1.80	0.63
3:F:62:ASN:HB3	2:c:113:GLN:HE22	1.63	0.63
1:S:127:SER:HA	3:U:103:TYR:CE1	2.34	0.63
2:Z:121:ARG:HG2	2:Z:170:GLU:OE2	1.98	0.63
2:c:14:SER:HB3	2:c:104:LEU:HD22	1.79	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
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:b:39:MET:HG3	1:b:69:VAL:HG13	1.80	0.63
2:i:158:LEU:HA	3:j:147:GLN:NE2	2.14	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
2:N:146:LEU:HD22	2:N:152:TRP:CE2	2.34	0.63
1:V:24:ILE:O	1:V:28:ILE:HG13	1.99	0.63
3:d:123:MET:O	3:d:124:LEU:HD23	1.98	0.63
3:j:138:LEU:HB3	3:j:222:ILE:HD13	1.81	0.63
3:j:171:TRP:CD1	3:j:171:TRP:H	2.16	0.63
1:A:125:CYS:O	1:A:129:ILE:HG13	1.98	0.63
1:G:89:ILE:O	1:G:93:VAL:HG23	1.98	0.63
2:K:44:TRP:CZ3	2:K:64:LEU:HD22	2.34	0.63
2:N:162:GLN:OE1	2:N:162:GLN:N	2.32	0.63
2:f:175:ASP:OD1	2:f:207:PRO:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:158:LEU:HA	3:j:147:GLN:HE22	1.64	0.63
2:N:181:GLN:HE21	2:N:200:PRO:HD3	1.64	0.62
1:P:44:PHE:HE2	1:P:114:ILE:HB	1.64	0.62
2:f:141:PHE:CE2	2:f:184:VAL:HG22	2.34	0.62
2:K:106:LEU:HD22	2:K:186:PRO:HD3	1.81	0.62
3:R:206:ASN:HA	3:R:210:GLY:O	1.99	0.62
2:T:74:THR:HA	2:T:101:PHE:HB2	1.81	0.62
3:U:169:THR:HG22	3:U:197:TYR:CE2	2.33	0.62
2:c:86:GLU:O	2:c:86:GLU:HG2	1.99	0.62
3:j:109:GLN:HG3	3:j:120:ALA:O	1.99	0.62
1:A:18:LEU:HD11	1:A:122:ILE:HG23	1.82	0.62
1:D:56:LEU:HG	1:D:93:VAL:HG13	1.80	0.62
3:F:140:LEU:CD1	3:F:224:TRP:HB2	2.29	0.62
3:F:180:VAL:HG12	3:F:181:ASP:O	1.98	0.62
2:N:17:GLN:HA	2:N:62:LEU:O	1.99	0.62
1:b:87:SER:CB	2:c:42:ARG:HH12	2.08	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
2:W:188:GLN:HG2	2:W:189:GLY:H	1.64	0.62
1:e:17:LEU:CD1	1:e:89:ILE:HG23	2.29	0.62
3:g:67:TYR:CE1	3:g:78:GLN:HB2	2.35	0.62
3:j:157:LEU:HD23	3:j:205:PHE:CE1	2.34	0.62
3:R:59:GLN:OE1	3:R:114:ARG:NH2	2.33	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
2:f:143:ALA:HB1	2:f:180:PHE:CZ	2.34	0.62
3:j:165:VAL:HG22	3:j:201:VAL:CG2	2.28	0.62
3:C:64:THR:OG1	3:C:111:GLN:HB3	2.00	0.62
2:E:73:THR:O	2:E:76:ASP:HB2	1.99	0.62
3:I:52:TRP:CD1	3:I:54:SER:HG	2.18	0.62
2:N:40:ASP:OD2	2:N:77:ILE:HB	1.99	0.62
2:W:85:ARG:HD3	2:W:90:TRP:CE2	2.34	0.62
1:Y:127:SER:HA	3:a:103:TYR:CE1	2.34	0.62
1:e:85:VAL:O	1:e:89:ILE:HG13	2.00	0.62
1:A:35:LYS:HD2	1:A:38:ARG:HH21	1.64	0.62
2:B:106:LEU:HD11	2:B:186:PRO:HG3	1.82	0.62
2:T:73:THR:HG22	2:T:76:ASP:OD1	2.00	0.62
2:W:82:VAL:O	2:W:83:LEU:HD23	1.99	0.62
1:b:88:ASN:HD22	1:b:88:ASN:N	1.98	0.62
1:h:56:LEU:CD1	1:h:96:LEU:HD23	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:c:98:PHE:CE2	2:c:100:PRO:HA	2.34	0.62
2:B:81:ARG:NH1	2:B:95:ILE:HD12	2.14	0.62
3:F:48:MET:HB3	3:F:100:ILE:HD11	1.82	0.62
2:K:141:PHE:CE2	2:K:184:VAL:HB	2.34	0.62
2:K:161:LYS:NZ	3:L:149:GLU:OE2	2.33	0.62
3:O:138:LEU:HD12	3:O:138:LEU:H	1.65	0.62
2:W:36:HIS:ND1	2:W:38:TRP:NE1	2.46	0.62
3:a:66:HIS:CE1	3:a:79:LYS:HG2	2.35	0.62
1:e:13:GLN:NE2	2:f:75:VAL:HG12	2.14	0.62
3:g:66:HIS:CE1	3:g:79:LYS:HG2	2.34	0.62
3:g:149:GLU:HG2	3:g:151:ASN:HD21	1.65	0.62
2:H:13:ASN:HB2	2:H:17:GLN:HB3	1.82	0.61
3:I:162:GLU:OE2	3:I:204:ARG:HD2	1.99	0.61
2:T:146:LEU:HB3	2:T:179:GLU:HB2	1.81	0.61
1:h:91:VAL:HG13	2:i:41:ARG:HD2	1.82	0.61
2:i:115:VAL:HB	2:i:123:ASN:HD22	1.64	0.61
3:I:128:ASN:C	3:I:212:ALA:HB2	2.25	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
3:d:132:PRO:HD2	3:d:216:SER:HB3	1.82	0.61
2:B:104:LEU:O	2:B:192:THR:HG23	1.99	0.61
1:D:11:GLN:O	1:D:11:GLN:HG2	2.00	0.61
1:P:22:GLN:HG2	1:P:122:ILE:HD13	1.81	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: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
1:G:60:GLU:OE2	1:G:94:LEU:HD21	2.01	0.61
3:L:148:LEU:HD11	3:L:188:LEU:HD23	1.82	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
2:i:132:SER:OG	2:i:134:TYR:HD1	1.83	0.61
1:P:36:LEU:HD12	1:P:39:MET:HB3	1.81	0.61
1:P:85:VAL:O	1:P:89:ILE:HG13	2.00	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
3:X:65:LEU:HD13	3:X:93:CYS:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:39:PRO:HB2	2:f:42:ARG:HB2	1.83	0.61
2:f:166:TRP:HZ3	2:f:168:CYS:HB2	1.64	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
3:a:160:CYS:C	3:a:161:LEU:HD23	2.26	0.61
2:c:122:CYS:HB2	2:c:172:LEU:HD11	1.82	0.61
3:g:171:TRP:CE2	3:g:195:LYS:HG2	2.34	0.61
2:B:204:ARG:HD3	1:D:43:LYS:O	2.00	0.61
2:E:186:PRO:HD2	2:E:192:THR:HG21	1.83	0.61
2:K:140:GLU:HG3	2:K:187:LEU:HD21	1.83	0.61
4:T:215:NAG:H61	4:U:233:NAG:H82	1.81	0.61
1:e:38:ARG:HA	1:e:41:THR:HG23	1.83	0.61
1:e:84:ASP:C	1:e:88:ASN:HD22	2.08	0.61
1:h:120:ARG:O	1:h:123:THR:HB	2.00	0.61
1:S:40:LEU:HD23	1:S:113:THR:HB	1.81	0.61
3:d:65:LEU:HD13	3:d:93:CYS:HB2	1.83	0.61
3:d:167:TYR:CE1	3:d:188:LEU:HD11	2.36	0.61
3:I:47:TYR:HE1	3:I:49:ASN:ND2	1.99	0.61
2:K:144:ARG:HH11	2:K:152:TRP:HB3	1.66	0.61
2:T:44:TRP:CH2	2:T:64:LEU:HD13	2.36	0.61
2:W:115:VAL:CB	2:W:123:ASN:HD22	2.13	0.61
1:e:66:LEU:HD12	1:e:117:PHE:HE2	1.65	0.61
2:i:123:ASN:ND2	4:i:215:NAG:C1	2.58	0.61
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:Z:13:ASN:HD22	2:Z:17:GLN:HB2	1.64	0.60
2:c:36:HIS:HB3	2:c:38:TRP:HE1	1.66	0.60
3:C:137:ASN:ND2	4:C:400:NAG:C1	2.64	0.60
1:M:42:PHE:CD2	1:M:69:VAL:HG22	2.36	0.60
1:P:18:LEU:HD11	1:P:122:ILE:HG23	1.82	0.60
1:P:62:GLU:O	1:P:65:PRO:HG2	2.01	0.60
2:W:137:ARG:NH2	3:X:162:GLU:OE1	2.34	0.60
1:Y:91:VAL:HG13	2:Z:41:ARG:HD3	1.83	0.60
2:i:172:LEU:HD22	2:i:178:TYR:CE1	2.36	0.60
2:W:14:SER:HB3	2:W:104:LEU:HD22	1.83	0.60
1:b:95:GLU:HG2	1:b:95:GLU:O	2.01	0.60
2:f:181:GLN:HG2	2:f:198:SER:O	2.00	0.60
3:j:44:ASN:HD22	3:j:133:TRP:H	1.46	0.60
2:E:109:PRO:HG2	2:E:182:VAL:HG13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:48:MET:HE3	3:I:95:LEU:HD12	1.82	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
3:a:137:ASN:O	3:a:139:THR:HG23	2.01	0.60
2:c:93:MET:O	2:c:93:MET:HE3	2.01	0.60
1:e:56:LEU:HB3	1:e:93:VAL:HG13	1.84	0.60
1:D:16:HIS:ND1	2:E:134:TYR:CD2	2.69	0.60
3:L:41:PHE:O	3:L:48:MET:HG3	2.01	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:a:62:ASN:HD21	4:a:300:NAG:C2	2.14	0.60
3:g:38:VAL:H	3:g:122:GLN:HE22	1.48	0.60
1:h:13:GLN:NE2	2:i:75:VAL:HG12	2.17	0.60
3:j:135:PRO:HG2	3:j:201:VAL:O	2.02	0.60
3:j:137:ASN:O	3:j:139:THR:HG23	2.02	0.60
3:C:200:ARG:HG3	3:C:218:TRP:CE3	2.37	0.60
2:E:152:TRP:O	2:E:155:ALA:HB3	2.01	0.60
1:P:24:ILE:HG23	1:P:70:LEU:HD21	1.83	0.60
3:U:148:LEU:HD11	3:U:188:LEU:HD12	1.83	0.60
1:Y:14:LEU:HD11	1:Y:53:LEU:HD21	1.82	0.60
2:Z:117:VAL:O	2:Z:118:GLU:HG3	2.02	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
1:M:12:LEU:O	1:M:16:HIS:HD2	1.85	0.60
3:U:142:LYS:HA	3:U:148:LEU:HA	1.83	0.60
2:W:78:VAL:O	2:W:80:LEU:CD1	2.50	0.60
2:Z:164:GLN:HE21	3:a:178:GLN:CG	2.14	0.60
1:b:24:ILE:HA	1:b:80:PHE:CE2	2.37	0.60
2:i:141:PHE:CE2	2:i:184:VAL:HG22	2.36	0.60
3:j:169:THR:CG2	3:j:195:LYS:HB3	2.32	0.60
2:E:123:ASN:HD21	4:E:215:NAG:C2	2.14	0.60
2:E:164:GLN:NE2	3:F:178:GLN:HG2	2.16	0.60
3:L:44:ASN:HB3	3:L:46:GLU:HG3	1.83	0.60
1:S:10:THR:HA	1:S:13:GLN:HE21	1.66	0.60
2:W:80:LEU:HD13	2:W:98:PHE:HB2	1.84	0.60
1:Y:67:GLU:O	1:Y:71:ASN:ND2	2.35	0.60
2:Z:54:SER:H	2:Z:57:SER:HB2	1.65	0.60
2:c:50:LEU:HD23	2:c:60:CYS:HB2	1.83	0.60
1:h:40:LEU:HD23	1:h:113:THR:HB	1.84	0.60
3:I:181:ASP:CG	3:I:183:ARG:HH11	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:83:LEU:CD2	2:N:92:VAL:HA	2.32	0.60
1:b:10:THR:HG22	1:b:14:LEU:HD12	1.83	0.60
3:g:63:LEU:HD13	3:g:110:LEU:HD13	1.84	0.60
1:h:44:PHE:CZ	1:h:69:VAL:HG21	2.37	0.60
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: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
1:J:56:LEU:HB3	1:J:93:VAL:HG13	1.83	0.59
3:O:44:ASN:HB3	3:O:46:GLU:HG3	1.83	0.59
3:U:62:ASN:HD21	4:U:300:NAG:C1	2.14	0.59
2:W:98:PHE:HE2	2:W:100:PRO:HA	1.62	0.59
3:a:143:LEU:HD12	3:a:147:GLN:HB3	1.84	0.59
2:E:164:GLN:HE21	3:F:178:GLN:CG	2.16	0.59
2:Z:117:VAL:HG23	2:Z:206:LYS:HE2	1.83	0.59
1:b:81:ASP:HB3	1:b:84:ASP:HB2	1.84	0.59
2:i:115:VAL:HB	2:i:123:ASN:ND2	2.17	0.59
2:i:171:THR:HG22	2:i:171:THR:O	2.02	0.59
1:D:24:ILE:HG23	1:D:70:LEU:HD21	1.85	0.59
2:Q:71:LYS:O	2:Q:72:LEU:HD23	2.03	0.59
2:Q:101:PHE:CD2	2:Q:104:LEU:HD11	2.38	0.59
1:S:85:VAL:O	1:S:89:ILE:HG13	2.02	0.59
3:U:52:TRP:CZ3	3:U:65:LEU:HD12	2.37	0.59
2:i:142:GLU:HG3	2:i:194:TRP:CH2	2.37	0.59
3:F:117:ARG:NH2	2:c:207:PRO:HG2	2.17	0.59
1:S:117:PHE:CE1	1:S:121:TRP:CD1	2.91	0.59
3:U:65:LEU:HD23	3:U:66:HIS:N	2.17	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
1:G:62:GLU:O	1:G:65:PRO:HG2	2.03	0.59
1:P:20:ASP:OD2	2:Q:134:TYR:OH	2.18	0.59
2:W:118:GLU:O	2:W:205:THR:HB	2.02	0.59
3:X:202:ARG:HG3	3:X:215:TRP:CE3	2.37	0.59
2:c:164:GLN:HE21	3:d:178:GLN:HG2	1.67	0.59
3:g:164:LEU:HD12	3:g:165:VAL:N	2.17	0.59
1:A:31:TYR:HH	1:A:35:LYS:N	2.00	0.59
3:C:138:LEU:HB3	3:C:222:ILE:HD13	1.83	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
2:K:138:HIS:CB	2:K:187:LEU:HD12	2.31	0.59
3:R:145:GLU:OE1	3:R:145:GLU:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:180:VAL:HG11	3:R:185:LYS:O	2.02	0.59
2:T:109:PRO:CG	2:T:184:VAL:HG23	2.28	0.59
2:T:128:ILE:HG22	2:T:184:VAL:HG21	1.84	0.59
1:b:50:ALA:HA	1:b:55:HIS:ND1	2.17	0.59
2:c:86:GLU:OE2	2:c:91:ARG:HB2	2.01	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
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:V:118:LEU:O	1:V:122:ILE:HG13	2.02	0.59
2:W:109:PRO:HG3	2:W:184:VAL:CG2	2.32	0.59
2:W:132:SER:OG	2:W:134:TYR:HD1	1.86	0.59
1:A:85:VAL:HG13	1:A:86:VAL:H	1.65	0.59
2:B:123:ASN:HD21	4:B:215:NAG:C2	2.15	0.59
2:K:93:MET:HA	2:K:93:MET:HE3	1.85	0.59
2:N:106:LEU:HD11	2:N:186:PRO:HG3	1.83	0.59
1:V:86:VAL:HG12	1:V:89:ILE:HD12	1.85	0.59
1:b:88:ASN:ND2	2:c:42:ARG:HH22	2.00	0.59
2:f:37:ALA:HA	2:f:80:LEU:HD23	1.84	0.59
2:K:73:THR:O	2:K:76:ASP:HB2	2.03	0.59
3:O:150:LEU:HD22	3:O:152:TRP:CE3	2.38	0.59
2:W:80:LEU:HD13	2:W:98:PHE:CB	2.33	0.59
2:Z:14:SER:O	2:Z:132:SER:HB2	2.03	0.59
1:b:125:CYS:O	1:b:129:ILE:HG13	2.02	0.59
2:K:14:SER:OG	2:K:135:PHE:HE2	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:Q:132:SER:HG	2:Q:134:TYR:HD1	1.49	0.59
2:Q:138:HIS:O	2:Q:139:LEU:HG	2.03	0.59
2:T:39:PRO:HG2	2:T:42:ARG:HB2	1.85	0.59
1:V:56:LEU:O	1:V:57:GLN:C	2.45	0.59
1:V:68:GLU:C	1:V:71:ASN:H	2.11	0.59
3:d:63:LEU:HB3	3:d:110:LEU:HD11	1.85	0.59
3:j:171:TRP:H	3:j:171:TRP:HD1	1.50	0.59
1:A:74:HIS:CG	1:A:75:SER:N	2.71	0.58
2:N:160:LEU:HD13	2:N:164:GLN:HB3	1.85	0.58
2:W:128:ILE:HG13	2:W:128:ILE:O	2.02	0.58
1:e:37:THR:HA	1:e:40:LEU:HD12	1.85	0.58
3:C:169:THR:C	3:C:171:TRP:H	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:141:PHE:CD2	2:T:184:VAL:HG22	2.38	0.58
1:V:45:TYR:CD2	1:V:62:GLU:HG3	2.38	0.58
2:W:83:LEU:HB3	2:W:90:TRP:CE3	2.38	0.58
2:f:40:ASP:OD1	2:f:41:ARG:N	2.36	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:L:62:ASN:HD21	4:L:300:NAG:C2	2.16	0.58
2:Q:123:ASN:HD21	4:Q:215:NAG:C1	2.16	0.58
2:W:138:HIS:HB3	2:W:187:LEU:CD1	2.32	0.58
3:d:149:GLU:HG2	3:d:151:ASN:ND2	2.15	0.58
3:j:165:VAL:HG22	3:j:201:VAL:HG22	1.83	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
3:L:126:LEU:O	3:L:128:ASN:N	2.36	0.58
2:W:167:ILE:HG21	2:W:180:PHE:CZ	2.38	0.58
1:Y:13:GLN:NE2	2:Z:75:VAL:HG12	2.18	0.58
1:Y:37:THR:O	1:Y:41:THR:HG23	2.02	0.58
1:b:69:VAL:HA	1:b:72:LEU:HD12	1.86	0.58
2:c:8:PHE:HB2	2:c:22:TRP:HD1	1.67	0.58
3:g:38:VAL:CG2	3:g:110:LEU:HD23	2.33	0.58
3:I:106:PHE:CE2	3:I:108:VAL:HG13	2.38	0.58
3:O:147:GLN:HG2	3:O:189:PRO:O	2.02	0.58
2:Q:37:ALA:HA	2:Q:80:LEU:HD23	1.85	0.58
2:W:118:GLU:OE1	2:W:121:ARG:HB2	2.03	0.58
2:Z:82:VAL:C	2:Z:83:LEU:HD23	2.27	0.58
1:e:7:THR:HG23	1:e:132:LEU:HD22	1.83	0.58
1:D:24:ILE:HD11	1:D:85:VAL:CG2	2.34	0.58
1:G:95:GLU:HG3	1:G:95:GLU:O	2.03	0.58
3:O:48:MET:HE3	3:O:95:LEU:HD12	1.85	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
3:a:171:TRP:H	3:a:171:TRP:CD1	2.21	0.58
2:c:143:ALA:HB1	2:c:180:PHE:CZ	2.39	0.58
2:f:109:PRO:HG3	2:f:184:VAL:CG2	2.34	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
2:T:98:PHE:O	2:T:100:PRO:HD3	2.03	0.58
3:U:52:TRP:CE3	3:U:110:LEU:HD21	2.38	0.58
2:c:13:ASN:ND2	2:c:16:ALA:H	1.98	0.58
2:c:122:CYS:HB2	2:c:172:LEU:CD1	2.34	0.58
2:B:172:LEU:HD22	2:B:178:TYR:CZ	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:68:TRP:CE3	3:R:77:VAL:HG13	2.39	0.58
3:j:87:GLU:O	3:j:89:ILE:HG13	2.04	0.58
1:A:36:LEU:HD13	1:A:39:MET:HE3	1.86	0.58
2:B:106:LEU:O	2:B:195:SER:HB2	2.04	0.58
2:E:64:LEU:N	2:E:64:LEU:HD23	2.18	0.58
3:F:41:PHE:O	3:F:48:MET:HG3	2.04	0.58
3:F:148:LEU:HG	3:F:191:VAL:HG11	1.86	0.58
2:H:12:TYR:CD1	2:H:13:ASN:N	2.72	0.58
2:H:146:LEU:HD22	2:H:152:TRP:CZ2	2.39	0.58
2:H:146:LEU:HD13	2:H:152:TRP:CD2	2.38	0.58
2:N:167:ILE:HG21	2:N:180:PHE:CZ	2.39	0.58
3:X:166:GLN:HB3	3:X:175:TRP:CE3	2.39	0.58
1:b:56:LEU:HD22	1:b:93:VAL:HG22	1.85	0.58
1:b:64:LYS:N	1:b:65:PRO:HD2	2.18	0.58
1:h:117:PHE:CE1	1:h:121:TRP:CD1	2.92	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
1:M:15:GLU:OE2	3:O:208:LEU:HD22	2.03	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
3:d:63:LEU:HD13	3:d:110:LEU:HD21	1.86	0.58
3:g:205:PHE:O	3:g:212:ALA:HB3	2.04	0.58
1:h:65:PRO:O	1:h:69:VAL:HG23	2.03	0.58
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
3:O:115:GLU:HA	2:i:204:ARG:HB3	1.86	0.57
3:O:206:ASN:HA	3:O:210:GLY:O	2.03	0.57
2:W:136:GLU:OE2	3:X:207:PRO:HG3	2.04	0.57
2:f:36:HIS:CE1	2:f:47:THR:HG22	2.39	0.57
2:f:136:GLU:OE2	3:g:207:PRO:HG3	2.03	0.57
2:f:171:THR:O	2:f:171:THR:HG22	2.04	0.57
2:i:183:ARG:NE	2:i:197:TRP:CZ2	2.72	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
3:F:106:PHE:CD2	3:F:126:LEU:HD21	2.39	0.57
2:K:124:ILE:HD11	2:K:203:PHE:CE2	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
3:a:80:CYS:HB3	3:a:83:TYR:HE1	1.68	0.57
2:f:115:VAL:HB	2:f:123:ASN:HD22	1.69	0.57
2:f:162:GLN:HE22	3:g:187:SER:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:95:GLU:HG3	1:h:95:GLU:O	2.02	0.57
1:h:117:PHE:CE1	1:h:121:TRP:HD1	2.22	0.57
2:i:104:LEU:HD13	2:i:135:PHE:CZ	2.39	0.57
2:E:103:ASN:OD1	2:E:191:PHE:HB2	2.04	0.57
4:K:215:NAG:H4	4:K:216:NAG:C1	2.33	0.57
3:L:206:ASN:HB2	3:L:207:PRO:HA	1.86	0.57
3:R:41:PHE:HD2	3:R:131:ILE:HD11	1.69	0.57
1:S:64:LYS:N	1:S:65:PRO:HD2	2.19	0.57
2:c:89:ARG:HG2	2:c:89:ARG:NH1	2.16	0.57
3:j:186:PHE:CG	3:j:187:SER:N	2.72	0.57
2:W:123:ASN:ND2	4:W:215:NAG:C1	2.64	0.57
3:a:44:ASN:ND2	3:a:156:PHE:CD2	2.73	0.57
1:e:12:LEU:C	1:e:12:LEU:HD23	2.30	0.57
2:i:37:ALA:HB2	2:i:62:LEU:CD1	2.34	0.57
2:H:46:GLN:OE1	2:W:89:ARG:HA	2.04	0.57
3:X:128:ASN:C	3:X:129:LEU:HD23	2.29	0.57
2:Z:106:LEU:HD11	2:Z:186:PRO:CG	2.32	0.57
3:a:52:TRP:CD2	3:a:110:LEU:HD21	2.40	0.57
2:f:85:ARG:HG3	2:f:90:TRP:CZ3	2.38	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:S:95:GLU:HG3	1:S:95:GLU:O	2.02	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:a:69:TYR:CE1	3:a:101:HIS:HD2	2.23	0.57
1:e:126:GLN:HG2	3:g:208:LEU:O	2.04	0.57
1:M:13:GLN:HG2	2:N:75:VAL:CG1	2.35	0.57
2:N:205:THR:HG22	2:N:206:LYS:N	2.19	0.57
3:O:102:LEU:HD22	3:O:127:GLN:HA	1.86	0.57
3:O:117:ARG:HG3	2:i:204:ARG:NH1	2.19	0.57
2:c:8:PHE:CE1	2:c:82:VAL:CG2	2.87	0.57
2:i:44:TRP:CH2	2:i:64:LEU:HD22	2.38	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:K:106:LEU:O	2:K:195:SER:HB2	2.05	0.57
2:W:36:HIS:HB3	2:W:38:TRP:NE1	2.20	0.57
2:c:13:ASN:CG	2:c:17:GLN:H	2.13	0.57
3:d:57:GLU:HB3	3:d:58:PRO:HD2	1.85	0.57
2:i:8:PHE:HD1	2:i:22:TRP:HB2	1.69	0.57
2:i:109:PRO:CG	2:i:184:VAL:HG23	2.27	0.57
2:K:13:ASN:O	2:K:14:SER:CB	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:165:VAL:HG13	3:a:201:VAL:HG22	1.87	0.57
1:A:24:ILE:O	1:A:28:ILE:HG13	2.04	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
2:H:50:LEU:CD2	2:H:60:CYS:HB2	2.35	0.57
1:J:62:GLU:HA	1:J:62:GLU:OE2	2.04	0.57
1:J:78:PHE:CD2	1:J:80:PHE:CZ	2.92	0.57
2:K:69:SER:HB2	2:K:71:LYS:HE2	1.86	0.57
2:K:112:LEU:O	2:K:201:LEU:HD22	2.04	0.57
3:O:52:TRP:CH2	3:O:92:GLY:HA2	2.40	0.57
1:S:87:SER:O	1:S:91:VAL:HG23	2.05	0.57
1:Y:24:ILE:HD11	1:Y:89:ILE:HD11	1.87	0.57
3:g:109:GLN:HA	3:g:120:ALA:O	2.05	0.57
2:i:199:GLN:HB3	2:i:200:PRO:HD2	1.87	0.57
1:D:18:LEU:O	1:D:22:GLN:HG3	2.04	0.56
2:E:14:SER:O	2:E:132:SER:HB2	2.05	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
2:c:14:SER:O	2:c:132:SER:HB2	2.04	0.56
1:e:60:GLU:O	1:e:63:LEU:HB2	2.05	0.56
1:h:16:HIS:HB3	1:h:92:PHE:CZ	2.39	0.56
3:j:47:TYR:HB2	3:j:95:LEU:O	2.05	0.56
2:H:106:LEU:HD11	2:H:186:PRO:HG3	1.87	0.56
2:K:81:ARG:HD3	2:K:95:ILE:HG22	1.86	0.56
2:K:138:HIS:C	2:K:187:LEU:CG	2.74	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
1:Y:28:ILE:HG12	1:Y:78:PHE:CZ	2.41	0.56
2:f:35:VAL:O	2:f:36:HIS:HD2	1.87	0.56
1:A:17:LEU:CD1	1:A:89:ILE:HG23	2.36	0.56
1:A:87:SER:O	1:A:91:VAL:HG23	2.05	0.56
3:F:102:LEU:C	3:F:104:GLN:H	2.12	0.56
2:H:144:ARG:HH11	2:H:152:TRP:HB3	1.71	0.56
1:J:16:HIS:ND1	2:K:134:TYR:HB3	2.20	0.56
2:K:175:ASP:N	2:K:205:THR:HB	2.20	0.56
2:Q:13:ASN:ND2	2:Q:17:GLN:HB3	2.19	0.56
3:R:65:LEU:HD23	3:R:66:HIS:N	2.20	0.56
4:W:215:NAG:H83	3:X:176:THR:HG21	1.87	0.56
1:Y:117:PHE:CE1	1:Y:121:TRP:CD1	2.94	0.56
1:e:82:PRO:O	1:e:85:VAL:HG12	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:15:ARG:HD3	2:f:68:ASP:O	2.06	0.56
2:i:113:GLN:O	2:i:124:ILE:HG23	2.05	0.56
3:F:188:LEU:CD2	3:F:191:VAL:HG12	2.35	0.56
2:H:172:LEU:HD22	2:H:178:TYR:CE1	2.40	0.56
1:J:126:GLN:HA	1:J:129:ILE:CG2	2.36	0.56
1:M:35:LYS:HD2	1:M:38:ARG:NH2	2.21	0.56
2:Q:37:ALA:HB2	2:Q:62:LEU:HD13	1.88	0.56
2:W:77:ILE:HA	2:W:100:PRO:HD3	1.87	0.56
2:W:164:GLN:NE2	3:X:178:GLN:HG2	2.20	0.56
3:X:157:LEU:HD13	3:X:160:CYS:HB2	1.87	0.56
1:Y:28:ILE:HG12	1:Y:78:PHE:HZ	1.69	0.56
1:e:53:LEU:HD21	1:e:128:ILE:HG21	1.87	0.56
3:j:150:LEU:HB3	3:j:186:PHE:HB3	1.87	0.56
3:I:158:ASN:O	3:I:159:HIS:HB3	2.04	0.56
1:J:84:ASP:O	1:J:87:SER:HB2	2.05	0.56
3:O:52:TRP:HZ3	3:O:65:LEU:HD12	1.68	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:V:117:PHE:CE1	1:V:121:TRP:HD1	2.23	0.56
3:a:109:GLN:HA	3:a:120:ALA:O	2.05	0.56
2:i:121:ARG:C	2:i:172:LEU:HD12	2.31	0.56
3:C:48:MET:CE	3:C:95:LEU:HD12	2.36	0.56
1:D:16:HIS:HB3	2:E:134:TYR:HD2	1.67	0.56
2:H:37:ALA:HB2	2:H:62:LEU:CD1	2.35	0.56
1:M:85:VAL:O	1:M:89:ILE:HG13	2.05	0.56
1:S:28:ILE:O	1:S:36:LEU:HD11	2.06	0.56
2:T:143:ALA:HB3	2:T:158:LEU:HB2	1.87	0.56
2:c:142:GLU:O	2:c:182:VAL:HA	2.05	0.56
1:e:59:LEU:O	1:e:63:LEU:HG	2.05	0.56
2:i:144:ARG:HD2	2:i:181:GLN:OE1	2.04	0.56
3:j:169:THR:HG21	3:j:195:LYS:HB3	1.87	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
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:b:15:GLU:O	1:b:18:LEU:HB3	2.06	0.56
2:E:162:GLN:OE1	2:E:162:GLN:N	2.38	0.56
3:F:205:PHE:CZ	3:F:209:CYS:HB2	2.40	0.56
2:K:195:SER:HB2	2:K:196:PRO:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:g:65:LEU:O	3:g:80:CYS:HB2	2.06	0.56
3:C:140:LEU:HD13	3:C:224:TRP:HB2	1.88	0.56
3:F:167:TYR:CD1	3:F:167:TYR:C	2.84	0.56
2:N:164:GLN:HG2	2:N:166:TRP:O	2.06	0.56
1:S:24:ILE:HD11	1:S:89:ILE:HD11	1.88	0.56
1:S:31:TYR:HB3	1:S:36:LEU:HD13	1.88	0.56
2:W:11:PHE:HA	2:W:103:ASN:HB3	1.88	0.56
2:W:164:GLN:HE21	3:X:178:GLN:HG2	1.71	0.56
2:f:146:LEU:HD22	2:f:152:TRP:CE2	2.41	0.56
2:i:42:ARG:HB3	2:i:44:TRP:CD1	2.41	0.56
2:i:143:ALA:HB1	2:i:181:GLN:O	2.05	0.56
3:j:169:THR:HA	3:j:196:ARG:O	2.05	0.56
3:j:202:ARG:HD3	3:j:218:TRP:CE2	2.40	0.56
3:L:68:TRP:HE3	3:L:77:VAL:HG13	1.71	0.56
3:R:44:ASN:HB3	3:R:46:GLU:HG3	1.87	0.56
2:Z:74:THR:HG23	2:Z:75:VAL:HG13	1.88	0.56
1:b:37:THR:HA	1:b:40:LEU:HD12	1.87	0.56
1:G:53:LEU:HD22	1:G:96:LEU:HD22	1.88	0.55
2:N:146:LEU:HD13	2:N:152:TRP:CG	2.40	0.55
3:O:62:ASN:HD21	4:O:300:NAG:C2	2.19	0.55
1:V:68:GLU:O	1:V:72:LEU:CD2	2.52	0.55
3:X:165:VAL:HG22	3:X:201:VAL:CG2	2.36	0.55
1:b:24:ILE:HD11	1:b:85:VAL:CG2	2.36	0.55
2:c:70:GLN:HG2	2:c:134:TYR:HE1	1.70	0.55
1:S:69:VAL:HG11	1:S:114:ILE:HD12	1.89	0.55
1:S:117:PHE:CE1	1:S:121:TRP:HD1	2.24	0.55
2:T:106:LEU:HD12	2:T:184:VAL:HG12	1.87	0.55
2:T:112:LEU:N	2:T:112:LEU:HD12	2.20	0.55
3:U:109:GLN:HE21	3:U:121:THR:HG22	1.71	0.55
3:X:133:TRP:HB3	3:X:155:ARG:HG3	1.88	0.55
1:Y:22:GLN:HG2	1:Y:122:ILE:HD13	1.86	0.55
2:Z:160:LEU:HD13	2:Z:164:GLN:HB3	1.89	0.55
3:d:135:PRO:HG2	3:d:201:VAL:O	2.05	0.55
2:i:98:PHE:CE2	2:i:100:PRO:HA	2.41	0.55
3:j:132:PRO:O	3:j:216:SER:HB2	2.06	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
2:E:50:LEU:HD23	2:E:60:CYS:HB2	1.87	0.55
2:H:20:CYS:HB2	2:H:60:CYS:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:215:NAG:O4	4:I:233:NAG:C1	2.55	0.55
3:I:62:ASN:HD21	4:I:300:NAG:C2	2.18	0.55
3:I:128:ASN:OD1	3:I:211:SER:HB2	2.06	0.55
2:K:114:VAL:HG13	2:K:117:VAL:HG13	1.86	0.55
2:K:143:ALA:HB1	2:K:180:PHE:CZ	2.42	0.55
2:K:183:ARG:HG3	2:K:194:TRP:CE3	2.40	0.55
1:S:28:ILE:O	1:S:28:ILE:HG22	2.06	0.55
2:T:170:GLU:H	3:U:190:SER:HB3	1.70	0.55
1:Y:31:TYR:OH	1:Y:35:LYS:HE3	2.07	0.55
1:b:16:HIS:CE1	2:c:134:TYR:HB3	2.41	0.55
1:b:24:ILE:HA	1:b:80:PHE:HE2	1.71	0.55
1:e:66:LEU:HD11	1:e:118:LEU:HD21	1.89	0.55
1:e:91:VAL:HG12	2:f:75:VAL:CG2	2.36	0.55
3:g:62:ASN:O	3:g:113:PRO:HD3	2.05	0.55
2:i:142:GLU:O	2:i:182:VAL:HG23	2.06	0.55
2:i:185:LYS:HB2	2:i:194:TRP:HA	1.88	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:Q:183:ARG:HG2	2:Q:197:TRP:CZ3	2.41	0.55
3:U:140:LEU:HD12	3:U:222:ILE:HD11	1.88	0.55
2:W:44:TRP:CH2	2:W:64:LEU:HD13	2.41	0.55
3:d:171:TRP:H	3:d:171:TRP:CD1	2.24	0.55
2:i:17:GLN:HB3	2:i:63:ILE:HD13	1.87	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
3:C:148:LEU:HD13	3:C:191:VAL:HG21	1.89	0.55
3:R:65:LEU:HD23	3:R:65:LEU:C	2.31	0.55
3:R:135:PRO:HG2	3:R:201:VAL:HG12	1.89	0.55
3:R:204:ARG:HD2	3:R:212:ALA:O	2.06	0.55
1:V:112:ALA:HB1	1:V:116:GLU:HB2	1.87	0.55
3:X:161:LEU:HD12	3:X:205:PHE:HA	1.88	0.55
2:Z:118:GLU:OE1	2:Z:121:ARG:HB2	2.07	0.55
1:b:117:PHE:CE1	1:b:121:TRP:CD1	2.95	0.55
1:e:127:SER:HA	3:g:103:TYR:CD1	2.41	0.55
2:f:13:ASN:O	2:f:14:SER:CB	2.55	0.55
1:A:35:LYS:HB2	1:A:35:LYS:NZ	2.22	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:G:45:TYR:HB3	1:G:107:TYR:HD1	1.72	0.55
3:O:64:THR:HG22	3:O:83:TYR:OH	2.06	0.55
1:S:56:LEU:HD22	1:S:93:VAL:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:39:PRO:CB	2:T:42:ARG:HB2	2.37	0.55
2:T:144:ARG:HD3	2:T:157:LEU:HD23	1.89	0.55
2:W:50:LEU:HD23	2:W:60:CYS:HB2	1.89	0.55
1:A:69:VAL:HG11	1:A:114:ILE:HD12	1.88	0.55
3:C:162:GLU:OE2	3:C:204:ARG:HD2	2.07	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
1:P:16:HIS:ND1	2:Q:134:TYR:CD2	2.75	0.55
2:Q:84:CYS:HB2	2:Q:93:MET:HE3	1.89	0.55
1:b:23:MET:HE1	2:c:133:HIS:CE1	2.41	0.55
2:f:121:ARG:HG2	2:f:170:GLU:OE2	2.07	0.55
2:f:185:LYS:HB2	2:f:194:TRP:CZ3	2.40	0.55
2:i:18:ILE:O	2:i:18:ILE:HG22	2.05	0.55
2:E:104:LEU:HB2	2:E:192:THR:OG1	2.06	0.55
2:E:178:TYR:HB2	2:E:203:PHE:CZ	2.41	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
4:K:215:NAG:O4	4:K:216:NAG:C7	2.54	0.55
2:Q:143:ALA:HB1	2:Q:180:PHE:CE1	2.41	0.55
2:T:141:PHE:HE1	2:T:163:LYS:HA	1.70	0.55
1:Y:112:ALA:HB1	1:Y:116:GLU:HB2	1.88	0.55
3:a:35:LEU:HD21	3:a:63:LEU:HD22	1.88	0.55
1:b:16:HIS:HB3	2:c:134:TYR:CD2	2.41	0.55
2:c:44:TRP:CH2	2:c:64:LEU:HD13	2.41	0.55
3:d:169:THR:O	3:d:172:ASP:HB2	2.07	0.55
2:f:44:TRP:CH2	2:f:64:LEU:HD22	2.41	0.55
2:f:187:LEU:HD11	3:g:183:ARG:NH1	2.22	0.55
3:g:68:TRP:HB3	3:g:77:VAL:HA	1.88	0.55
3:g:165:VAL:HG22	3:g:201:VAL:HG22	1.89	0.55
1:h:85:VAL:HG13	1:h:86:VAL:N	2.21	0.55
2:E:104:LEU:HD12	2:E:188:GLN:O	2.07	0.55
3:O:68:TRP:HE3	3:O:77:VAL:HG13	1.71	0.55
3:O:150:LEU:HD23	3:O:151:ASN:N	2.22	0.55
3:O:157:LEU:HD13	3:O:205:PHE:CD1	2.42	0.55
2:T:113:GLN:O	2:T:124:ILE:HG23	2.07	0.55
3:U:68:TRP:HB3	3:U:77:VAL:HA	1.88	0.55
1:V:45:TYR:HD2	1:V:62:GLU:HG3	1.71	0.55
2:W:36:HIS:HB3	2:W:38:TRP:CD1	2.41	0.55
4:W:215:NAG:H61	4:X:233:NAG:H82	1.89	0.55
1:b:60:GLU:OE1	1:b:94:LEU:HD21	2.07	0.55
2:c:50:LEU:HD22	2:c:58:TRP:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:64:THR:OG1	3:d:111:GLN:HB3	2.06	0.55
2:f:73:THR:HG23	2:f:75:VAL:H	1.72	0.55
3:j:48:MET:HB2	3:j:100:ILE:HD11	1.89	0.55
3:C:46:GLU:CD	3:C:133:TRP:HE1	2.15	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
2:W:146:LEU:HD22	2:W:152:TRP:CE2	2.41	0.55
3:X:152:TRP:HE1	3:X:163:HIS:CE1	2.25	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
3:O:62:ASN:HD21	4:O:300:NAG:C1	2.20	0.54
2:T:88:VAL:HG23	2:T:89:ARG:H	1.72	0.54
2:W:118:GLU:C	2:W:206:LYS:HB2	2.33	0.54
3:X:106:PHE:HE2	3:X:108:VAL:CG2	2.20	0.54
2:f:85:ARG:HG3	2:f:90:TRP:CH2	2.42	0.54
3:g:149:GLU:HG2	3:g:151:ASN:ND2	2.21	0.54
3:j:62:ASN:HD21	4:j:300:NAG:C2	2.19	0.54
3:F:207:PRO:HA	3:F:210:GLY:O	2.08	0.54
3:L:130:VAL:HB	3:L:205:PHE:CD2	2.42	0.54
1:S:9:LYS:O	1:S:13:GLN:HG3	2.08	0.54
2:f:14:SER:OG	2:f:132:SER:HB2	2.07	0.54
2:i:136:GLU:OE2	3:j:207:PRO:HG3	2.07	0.54
1:A:7:THR:HG23	1:A:132:LEU:HD13	1.89	0.54
1:D:11:GLN:CG	1:D:129:ILE:HG23	2.36	0.54
3:F:67:TYR:C	3:F:67:TYR:CD1	2.86	0.54
3:F:68:TRP:CH2	3:F:109:GLN:NE2	2.73	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
2:T:88:VAL:HG23	2:T:89:ARG:N	2.23	0.54
3:U:186:PHE:CE2	3:U:187:SER:O	2.61	0.54
2:f:183:ARG:HD2	2:f:194:TRP:HB3	1.89	0.54
1:h:14:LEU:HD21	1:h:128:ILE:HB	1.88	0.54
3:j:47:TYR:CE1	3:j:49:ASN:ND2	2.72	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
1:h:6:SER:C	1:h:8:LYS:N	2.62	0.54
2:B:126:TRP:NE1	2:B:165:GLU:HA	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:LEU:HD13	1:G:124:PHE:HE2	1.72	0.54
1:J:126:GLN:CD	3:L:210:GLY:HA2	2.32	0.54
1:P:45:TYR:HB3	1:P:107:TYR:HD1	1.72	0.54
1:P:88:ASN:HD22	1:P:88:ASN:N	2.05	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
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
3:a:204:ARG:HH21	3:a:215:TRP:NE1	2.06	0.54
1:A:61:GLU:OE2	1:A:105:CYS:HB3	2.08	0.54
2:K:137:ARG:NH2	3:L:162:GLU:OE1	2.40	0.54
3:L:145:GLU:OE1	3:L:145:GLU:HA	2.06	0.54
3:O:39:GLN:HB2	3:O:41:PHE:HE1	1.72	0.54
3:R:144:SER:HB3	3:R:147:GLN:HB2	1.89	0.54
2:T:66:ALA:O	2:T:67:PRO:C	2.50	0.54
1:V:35:LYS:HD2	1:V:38:ARG:HH21	1.73	0.54
1:V:46:MET:HB2	1:V:108:ALA:HB3	1.90	0.54
2:W:13:ASN:CG	2:W:17:GLN:H	2.15	0.54
3:X:132:PRO:CB	3:X:161:LEU:HD21	2.36	0.54
3:a:191:VAL:HB	3:a:197:TYR:CE1	2.43	0.54
1:e:45:TYR:HD2	1:e:62:GLU:HG3	1.71	0.54
2:i:14:SER:O	2:i:132:SER:HB2	2.08	0.54
1:D:11:GLN:O	1:D:15:GLU:HB2	2.07	0.54
2:N:141:PHE:HB2	2:N:160:LEU:HB2	1.89	0.54
3:O:157:LEU:HD13	3:O:205:PHE:CE1	2.42	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:Z:162:GLN:HE22	3:a:187:SER:HB3	1.72	0.54
3:d:188:LEU:HD22	3:d:199:PHE:HZ	1.73	0.54
1:h:82:PRO:O	1:h:85:VAL:HG12	2.08	0.54
1:D:69:VAL:CG1	1:D:114:ILE:HD12	2.35	0.54
3:I:110:LEU:HD23	3:I:110:LEU:C	2.33	0.54
1:M:24:ILE:HG22	1:M:118:LEU:HD11	1.88	0.54
2:N:132:SER:OG	2:N:134:TYR:HD1	1.90	0.54
2:T:142:GLU:O	2:T:182:VAL:HG23	2.07	0.54
2:Z:146:LEU:HD22	2:Z:152:TRP:CE2	2.43	0.54
2:c:122:CYS:HB3	2:c:169:LEU:HB2	1.90	0.54
3:g:143:LEU:HD11	3:g:147:GLN:OE1	2.08	0.54
3:g:167:TYR:HB3	3:g:199:PHE:CD1	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:73:THR:HA	2:T:101:PHE:HE1	1.73	0.54
3:U:204:ARG:HH21	3:U:215:TRP:HE1	1.56	0.54
3:X:62:ASN:O	3:X:113:PRO:HD3	2.08	0.54
2:Z:143:ALA:O	2:Z:158:LEU:HG	2.08	0.54
2:c:153:GLU:C	2:c:155:ALA:H	2.15	0.54
1:h:66:LEU:HD12	1:h:117:PHE:CE2	2.36	0.54
2:i:86:GLU:OE2	2:i:91:ARG:HB2	2.08	0.54
2:E:31:THR:O	2:E:31:THR:HG22	2.08	0.54
3:I:164:LEU:HD12	3:I:178:GLN:O	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:J:122:ILE:O	1:J:126:GLN:HG3	2.07	0.54
3:L:166:GLN:HA	3:L:176:THR:O	2.07	0.54
1:M:82:PRO:O	1:M:86:VAL:HG23	2.07	0.54
2:Q:54:SER:OG	2:Q:55:GLN:N	2.41	0.54
2:Q:66:ALA:HB1	2:Q:67:PRO:HD2	1.89	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
1:Y:91:VAL:HG13	2:Z:41:ARG:CD	2.37	0.54
1:b:16:HIS:HB3	1:b:92:PHE:CZ	2.42	0.54
3:g:66:HIS:HE1	3:g:79:LYS:HG2	1.73	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
2:Z:102:GLU:C	2:Z:103:ASN:HD22	2.16	0.53
3:a:150:LEU:C	3:a:151:ASN:HD22	2.16	0.53
2:c:39:PRO:HG2	2:c:42:ARG:HB2	1.90	0.53
3:d:65:LEU:HD13	3:d:93:CYS:CB	2.38	0.53
1:e:12:LEU:CD2	2:f:74:THR:HG21	2.38	0.53
2:f:158:LEU:HD23	3:g:147:GLN:NE2	2.23	0.53
3:F:204:ARG:HB2	3:F:215:TRP:CE3	2.43	0.53
3:R:136:GLU:CD	3:R:155:ARG:HD3	2.33	0.53
2:W:50:LEU:HD22	2:W:58:TRP:HB3	1.90	0.53
2:c:167:ILE:HG12	2:c:168:CYS:N	2.23	0.53
2:i:160:LEU:HD22	2:i:162:GLN:NE2	2.23	0.53
3:C:62:ASN:ND2	4:C:300:NAG:H83	2.23	0.53
1:D:131:THR:O	1:D:131:THR:CG2	2.57	0.53
2:H:15:ARG:NH1	2:H:70:GLN:HB2	2.22	0.53
2:H:146:LEU:HD22	2:H:152:TRP:CE2	2.44	0.53
3:O:84:LEU:HD21	4:O:234:NAG:C6	2.36	0.53
2:Q:150:HIS:HB3	2:Q:154:GLU:OE1	2.08	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
1:Y:31:TYR:HB3	1:Y:36:LEU:HD13	1.89	0.53
2:c:160:LEU:HD13	2:c:164:GLN:HB3	1.89	0.53
3:F:94:GLN:HE21	3:F:96:GLN:NE2	2.07	0.53
1:M:16:HIS:HD1	2:N:134:TYR:CB	2.19	0.53
2:Q:11:PHE:HD1	2:Q:105:ARG:HD3	1.73	0.53
2:W:73:THR:OG1	2:W:75:VAL:HG22	2.08	0.53
3:X:144:SER:HB3	3:X:147:GLN:HG3	1.91	0.53
1:Y:28:ILE:O	1:Y:28:ILE:HG22	2.08	0.53
3:a:67:TYR:CE2	3:a:95:LEU:HD21	2.44	0.53
2:f:44:TRP:CZ2	2:f:72:LEU:HD21	2.43	0.53
2:i:22:TRP:CZ2	2:i:24:GLN:HB2	2.43	0.53
3:F:183:ARG:HD3	3:F:185:LYS:CE	2.37	0.53
2:H:160:LEU:HD21	3:I:189:PRO:HG3	1.90	0.53
2:N:146:LEU:HD22	2:N:152:TRP:NE1	2.23	0.53
2:N:146:LEU:HD13	2:N:152:TRP:CD2	2.43	0.53
1:S:112:ALA:HB1	1:S:116:GLU:CB	2.38	0.53
3:U:62:ASN:HD21	4:U:300:NAG:H83	1.72	0.53
1:Y:120:ARG:O	1:Y:123:THR:HB	2.09	0.53
2:f:73:THR:HG23	2:f:75:VAL:HG22	1.89	0.53
1:h:37:THR:HA	1:h:40:LEU:HD12	1.89	0.53
2:i:124:ILE:HD11	2:i:203:PHE:HD2	1.71	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
3:I:140:LEU:HD22	3:I:148:LEU:HD13	1.90	0.53
3:L:148:LEU:HD12	3:L:188:LEU:HB3	1.90	0.53
3:R:64:THR:OG1	3:R:111:GLN:HB3	2.09	0.53
2:T:44:TRP:HH2	2:T:72:LEU:HD21	1.74	0.53
2:T:198:SER:O	2:T:199:GLN:C	2.52	0.53
3:a:138:LEU:H	3:a:138:LEU:HD12	1.72	0.53
3:a:165:VAL:HG22	3:a:201:VAL:HG22	1.91	0.53
2:c:199:GLN:OE1	2:c:200:PRO:HD2	2.08	0.53
1:e:64:LYS:N	1:e:65:PRO:HD2	2.24	0.53
3:C:154:ASN:HD21	3:C:163:HIS:HE1	1.54	0.53
3:I:158:ASN:O	3:I:159:HIS:CB	2.55	0.53
3:L:192:ASP:N	3:L:197:TYR:OH	2.33	0.53
3:O:144:SER:HB3	3:O:147:GLN:HB2	1.90	0.53
2:Q:87:GLY:O	2:Q:89:ARG:N	2.42	0.53
3:U:164:LEU:HD12	3:U:165:VAL:N	2.24	0.53
3:a:171:TRP:H	3:a:171:TRP:HD1	1.56	0.53
2:f:82:VAL:HG13	2:f:93:MET:CB	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:j:65:LEU:HD22	3:j:80:CYS:SG	2.49	0.53
3:F:110:LEU:HD23	3:F:110:LEU:C	2.33	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
3:X:65:LEU:HD13	3:X:93:CYS:CB	2.37	0.53
1:h:25:LEU:HD22	1:h:122:ILE:CD1	2.39	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
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
1:Y:28:ILE:O	1:Y:36:LEU:HD11	2.08	0.53
2:Z:42:ARG:HB3	2:Z:44:TRP:NE1	2.24	0.53
2:Z:166:TRP:C	2:Z:166:TRP:CE3	2.87	0.53
2:c:146:LEU:HD22	2:c:152:TRP:CE2	2.43	0.53
2:i:36:HIS:HB3	2:i:38:TRP:HE1	1.72	0.53
3:F:128:ASN:CG	3:F:211:SER:HB2	2.33	0.53
1:G:18:LEU:HD11	1:G:122:ILE:HG23	1.91	0.53
2:H:185:LYS:HB2	2:H:194:TRP:CE3	2.44	0.53
1:J:10:THR:HA	1:J:13:GLN:OE1	2.08	0.53
3:L:202:ARG:HD2	3:L:215:TRP:HB3	1.91	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
1:V:28:ILE:O	1:V:28:ILE:HG22	2.09	0.53
2:Z:44:TRP:HH2	2:Z:72:LEU:HD21	1.74	0.53
3:a:154:ASN:HD21	3:a:163:HIS:CE1	2.27	0.53
1:b:81:ASP:OD1	1:b:82:PRO:HD2	2.09	0.53
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:R:62:ASN:ND2	4:R:300:NAG:C1	2.69	0.52
2:W:85:ARG:HD3	2:W:90:TRP:CZ2	2.44	0.52
3:X:109:GLN:HA	3:X:120:ALA:O	2.10	0.52
1:b:92:PHE:CE1	2:c:73:THR:OG1	2.62	0.52
2:f:113:GLN:O	2:f:124:ILE:HG23	2.09	0.52
2:i:128:ILE:CG2	2:i:184:VAL:HG21	2.36	0.52
2:i:187:LEU:HD21	3:j:183:ARG:NH1	2.25	0.52
4:C:234:NAG:O7	4:C:234:NAG:H3	2.08	0.52
2:E:139:LEU:HB2	2:E:163:LYS:HB2	1.91	0.52
2:H:135:PHE:CE1	2:H:186:PRO:HB3	2.44	0.52
2:N:71:LYS:O	2:N:72:LEU:HD23	2.08	0.52
1:Y:126:GLN:OE1	3:a:210:GLY:HA2	2.09	0.52
2:Z:21:VAL:HA	2:Z:58:TRP:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:41:ARG:O	2:Z:42:ARG:HD3	2.09	0.52
2:Z:141:PHE:HA	2:Z:183:ARG:O	2.08	0.52
2:c:18:ILE:HB	2:c:62:LEU:HB2	1.91	0.52
2:c:143:ALA:HA	2:c:197:TRP:HZ3	1.73	0.52
1:A:85:VAL:HG13	1:A:86:VAL:N	2.23	0.52
1:A:85:VAL:O	1:A:89:ILE:HG13	2.10	0.52
1:D:24:ILE:HD11	1:D:85:VAL:HG21	1.91	0.52
2:E:124:ILE:HG21	2:E:180:PHE:CD2	2.45	0.52
2:K:51:LEU:C	2:K:58:TRP:HD1	2.16	0.52
1:P:63:LEU:HD13	1:P:90:ASN:HB2	1.91	0.52
3:U:204:ARG:HB2	3:U:215:TRP:CE3	2.44	0.52
3:X:68:TRP:HE3	3:X:77:VAL:HG13	1.73	0.52
3:X:204:ARG:HG2	3:X:205:PHE:N	2.25	0.52
1:Y:28:ILE:HD11	1:Y:70:LEU:CD2	2.39	0.52
1:Y:69:VAL:HG11	1:Y:114:ILE:HD12	1.91	0.52
3:a:164:LEU:HD12	3:a:165:VAL:N	2.23	0.52
2:i:188:GLN:HG2	2:i:189:GLY:H	1.73	0.52
3:j:140:LEU:HD21	3:j:150:LEU:HD13	1.91	0.52
1:A:31:TYR:HD2	1:A:36:LEU:HB2	1.74	0.52
2:E:172:LEU:HD22	2:E:178:TYR:CE1	2.45	0.52
1:J:88:ASN:HD21	2:K:42:ARG:HH22	1.52	0.52
2:N:17:GLN:HE21	2:N:63:ILE:HD11	1.74	0.52
2:N:162:GLN:HG3	3:O:178:GLN:HE21	1.74	0.52
3:R:67:TYR:HB2	3:R:106:PHE:CZ	2.44	0.52
3:X:192:ASP:OD2	3:X:195:LYS:HG3	2.10	0.52
1:Y:117:PHE:HE1	1:Y:121:TRP:NE1	2.06	0.52
2:Z:8:PHE:CE1	2:Z:82:VAL:HG22	2.44	0.52
2:Z:160:LEU:CD1	2:Z:164:GLN:HB3	2.39	0.52
3:d:128:ASN:C	3:d:129:LEU:HD23	2.34	0.52
2:f:118:GLU:O	2:f:205:THR:HG22	2.09	0.52
2:B:50:LEU:CD2	2:B:60:CYS:HB2	2.38	0.52
2:E:162:GLN:HE22	3:F:187:SER:CB	2.22	0.52
2:K:101:PHE:HA	2:K:104:LEU:HD21	1.91	0.52
2:K:142:GLU:HA	2:K:158:LEU:O	2.10	0.52
2:K:162:GLN:OE1	2:K:162:GLN:N	2.43	0.52
2:N:143:ALA:HB1	2:N:180:PHE:HE1	1.73	0.52
1:S:28:ILE:HG12	1:S:78:PHE:HZ	1.73	0.52
2:Z:15:ARG:HD3	2:Z:68:ASP:O	2.09	0.52
2:Z:107:MET:HB2	2:Z:129:SER:HB3	1.91	0.52
1:e:44:PHE:CZ	1:e:69:VAL:HG21	2.45	0.52
2:f:83:LEU:HA	2:f:91:ARG:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:56:LEU:HD13	1:h:93:VAL:HA	1.92	0.52
2:E:42:ARG:NH2	2:E:76:ASP:OD1	2.38	0.52
2:K:54:SER:OG	2:K:55:GLN:N	2.43	0.52
2:K:139:LEU:C	2:K:187:LEU:HD21	2.33	0.52
1:P:82:PRO:O	1:P:86:VAL:HG23	2.10	0.52
2:Q:144:ARG:NH1	2:Q:152:TRP:HB3	2.23	0.52
2:T:52:PRO:HA	2:T:57:SER:O	2.10	0.52
2:T:166:TRP:NE1	4:T:215:NAG:H3	2.25	0.52
3:U:123:MET:O	3:U:124:LEU:HD23	2.09	0.52
1:b:124:PHE:CE2	1:b:128:ILE:HG13	2.45	0.52
2:c:83:LEU:HB3	2:c:90:TRP:HB3	1.92	0.52
2:c:171:THR:O	2:c:171:THR:HG22	2.10	0.52
2:f:164:GLN:NE2	3:g:178:GLN:HG2	2.24	0.52
3:C:65:LEU:HD23	3:C:65:LEU:C	2.35	0.52
3:C:133:TRP:HB2	3:C:155:ARG:HG3	1.91	0.52
3:F:49:ASN:ND2	4:F:234:NAG:C1	2.73	0.52
1:G:84:ASP:O	1:G:87:SER:HB2	2.10	0.52
1:J:46:MET:HB3	1:J:47:PRO:HD2	1.89	0.52
2:K:142:GLU:O	2:K:182:VAL:HA	2.10	0.52
3:L:198:THR:HG23	3:L:223:HIS:CE1	2.44	0.52
3:O:162:GLU:OE2	3:O:204:ARG:HD2	2.09	0.52
2:Q:16:ALA:HB1	2:Q:65:GLY:N	2.25	0.52
3:R:69:TYR:CE1	3:R:101:HIS:HD2	2.27	0.52
1:S:65:PRO:O	1:S:68:GLU:N	2.42	0.52
2:T:22:TRP:CZ2	2:T:24:GLN:HB2	2.44	0.52
2:W:74:THR:HA	2:W:101:PHE:CD1	2.44	0.52
1:Y:64:LYS:N	1:Y:65:PRO:HD2	2.24	0.52
1:e:31:TYR:CE2	1:e:35:LYS:N	2.77	0.52
2:f:35:VAL:O	2:f:36:HIS:CD2	2.62	0.52
4:f:215:NAG:O4	4:g:233:NAG:C1	2.58	0.52
2:i:86:GLU:O	2:i:86:GLU:HG2	2.10	0.52
1:D:77:ASN:C	1:D:78:PHE:HD1	2.18	0.52
2:K:13:ASN:CG	2:K:17:GLN:H	2.18	0.52
2:Q:98:PHE:CZ	2:Q:100:PRO:HA	2.44	0.52
2:T:137:ARG:NH2	3:U:162:GLU:OE1	2.38	0.52
3:U:68:TRP:CE3	3:U:77:VAL:HG13	2.41	0.52
1:Y:17:LEU:HD23	1:Y:125:CYS:SG	2.49	0.52
1:Y:63:LEU:O	1:Y:66:LEU:HB3	2.09	0.52
2:Z:124:ILE:HD11	2:Z:203:PHE:CE2	2.44	0.52
2:c:122:CYS:CB	2:c:172:LEU:HD11	2.40	0.52
3:F:54:SER:O	3:F:55:SER:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:74:HIS:CG	1:J:75:SER:N	2.78	0.52
2:Q:101:PHE:HD2	2:Q:104:LEU:HD11	1.72	0.52
1:S:40:LEU:O	1:S:113:THR:HG22	2.10	0.52
1:S:94:LEU:HD23	1:S:97:LYS:HE2	1.92	0.52
3:U:128:ASN:C	3:U:129:LEU:HD23	2.34	0.52
1:Y:15:GLU:O	1:Y:18:LEU:HB3	2.09	0.52
1:b:67:GLU:HB2	1:b:86:VAL:HG21	1.92	0.52
1:h:23:MET:HE1	2:i:133:HIS:NE2	2.25	0.52
1:D:7:THR:CG2	1:D:132:LEU:HD11	2.40	0.52
1:P:21:LEU:HA	1:P:24:ILE:HD13	1.92	0.52
2:T:54:SER:H	2:T:57:SER:HB2	1.74	0.52
2:T:112:LEU:HD12	2:T:112:LEU:H	1.75	0.52
2:Z:12:TYR:O	2:Z:104:LEU:HA	2.10	0.52
2:Z:161:LYS:HD3	3:a:185:LYS:CE	2.40	0.52
2:c:185:LYS:HG2	2:c:186:PRO:O	2.10	0.52
1:e:56:LEU:HD12	1:e:97:LYS:HB3	1.92	0.52
2:f:37:ALA:HB2	2:f:62:LEU:CD1	2.40	0.52
1:h:56:LEU:HB3	1:h:93:VAL:CG1	2.27	0.52
3:j:138:LEU:HD21	3:j:219:SER:OG	2.09	0.52
2:B:39:PRO:HD2	2:B:44:TRP:O	2.10	0.51
1:D:131:THR:O	1:D:131:THR:HG22	2.09	0.51
2:H:72:LEU:HD13	2:H:100:PRO:CG	2.40	0.51
1:M:113:THR:HG23	1:M:116:GLU:OE1	2.10	0.51
3:O:60:PRO:HB3	3:O:89:ILE:HD11	1.91	0.51
1:P:42:PHE:CE1	1:P:72:LEU:HD11	2.44	0.51
2:Q:118:GLU:O	2:Q:205:THR:HG23	2.10	0.51
3:R:61:THR:HG22	3:R:62:ASN:N	2.25	0.51
1:S:84:ASP:O	1:S:87:SER:HB2	2.10	0.51
1:V:19:LEU:CD2	2:W:136:GLU:HB2	2.39	0.51
1:Y:57:GLN:CD	1:Y:97:LYS:HZ2	2.18	0.51
3:a:46:GLU:O	3:a:47:TYR:HB3	2.10	0.51
2:f:40:ASP:OD1	2:f:41:ARG:HB2	2.10	0.51
2:f:78:VAL:O	2:f:98:PHE:HB3	2.10	0.51
1:A:11:GLN:NE2	1:A:133:THR:OG1	2.39	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
4:C:300:NAG:H82	2:Z:113:GLN:OE1	2.10	0.51
2:E:51:LEU:HB3	2:E:52:PRO:HD2	1.91	0.51
3:F:206:ASN:CG	3:F:207:PRO:CA	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:150:LEU:O	3:I:185:LYS:HA	2.10	0.51
2:K:13:ASN:O	2:K:14:SER:HB3	2.09	0.51
1:S:50:ALA:HA	1:S:55:HIS:ND1	2.25	0.51
4:T:215:NAG:H61	4:U:233:NAG:C8	2.41	0.51
3:X:171:TRP:CD1	3:X:171:TRP:H	2.28	0.51
2:Z:177:GLN:O	2:Z:178:TYR:CD2	2.64	0.51
1:e:56:LEU:HB3	1:e:93:VAL:CG1	2.40	0.51
3:g:36:PRO:O	3:g:110:LEU:HD21	2.10	0.51
2:i:104:LEU:HD13	2:i:135:PHE:HZ	1.73	0.51
1:D:66:LEU:CD1	1:D:70:LEU:HD11	2.39	0.51
2:E:44:TRP:CH2	2:E:64:LEU:HD13	2.46	0.51
2:E:119:THR:HG22	2:E:206:LYS:O	2.10	0.51
1:G:81:ASP:OD1	1:G:82:PRO:HD2	2.10	0.51
1:J:24:ILE:HG23	1:J:70:LEU:HD21	1.92	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
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
3:U:68:TRP:CE3	3:U:77:VAL:HG22	2.45	0.51
3:X:62:ASN:CG	4:X:300:NAG:H83	2.35	0.51
3:a:132:PRO:HB3	3:a:161:LEU:HD11	1.92	0.51
3:a:133:TRP:CD1	3:a:155:ARG:HG3	2.45	0.51
3:d:169:THR:HG22	3:d:170:ASP:N	2.26	0.51
3:g:57:GLU:HB3	3:g:58:PRO:HD2	1.92	0.51
2:i:144:ARG:HD3	2:i:152:TRP:CE3	2.44	0.51
1:D:43:LYS:HB3	1:D:111:THR:OG1	2.11	0.51
1:D:97:LYS:HG3	1:D:98:GLY:H	1.76	0.51
3:L:129:LEU:O	3:L:130:VAL:C	2.53	0.51
1:M:122:ILE:O	1:M:126:GLN:CG	2.58	0.51
3:O:205:PHE:CZ	3:O:209:CYS:HB2	2.45	0.51
2:W:13:ASN:ND2	2:W:16:ALA:H	2.05	0.51
3:X:67:TYR:CE1	3:X:78:GLN:HB2	2.46	0.51
2:Z:71:LYS:O	2:Z:72:LEU:HD23	2.09	0.51
2:c:138:HIS:HB3	2:c:187:LEU:CD1	2.41	0.51
2:c:142:GLU:HA	2:c:158:LEU:O	2.10	0.51
1:A:62:GLU:HA	1:A:62:GLU:OE2	2.10	0.51
2:B:109:PRO:HG2	2:B:182:VAL:HG13	1.92	0.51
3:F:206:ASN:OD1	3:F:210:GLY:C	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:62:GLU:O	1:J:65:PRO:HG2	2.10	0.51
2:T:12:TYR:CE2	2:T:14:SER:HA	2.45	0.51
3:U:42:VAL:O	3:U:130:VAL:HA	2.10	0.51
3:U:140:LEU:HD11	3:U:199:PHE:CD2	2.46	0.51
3:d:167:TYR:CE2	3:d:176:THR:HB	2.45	0.51
1:e:39:MET:CG	1:e:72:LEU:HD12	2.39	0.51
1:e:92:PHE:CZ	2:f:73:THR:OG1	2.63	0.51
2:f:158:LEU:HA	3:g:147:GLN:HE22	1.75	0.51
2:f:160:LEU:HD13	2:f:164:GLN:HB3	1.93	0.51
3:g:85:PHE:CE2	3:g:90:THR:HG22	2.46	0.51
3:U:204:ARG:HG2	3:U:205:PHE:N	2.26	0.51
1:V:95:GLU:C	1:V:96:LEU:HD12	2.35	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
3:g:44:ASN:ND2	3:g:133:TRP:HB2	2.25	0.51
1:h:95:GLU:O	1:h:95:GLU:CG	2.59	0.51
2:E:13:ASN:O	2:E:13:ASN:OD1	2.29	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:Q:115:VAL:HG11	4:Q:215:NAG:C6	2.28	0.51
1:Y:127:SER:OG	3:a:103:TYR:HB3	2.10	0.51
3:a:42:VAL:O	3:a:130:VAL:HA	2.10	0.51
1:b:69:VAL:O	1:b:72:LEU:HB2	2.10	0.51
2:c:82:VAL:C	2:c:83:LEU:HD23	2.35	0.51
3:g:102:LEU:C	3:g:104:GLN:H	2.19	0.51
3:g:171:TRP:CD1	3:g:171:TRP:H	2.28	0.51
1:h:114:ILE:O	1:h:118:LEU:HG	2.10	0.51
3:j:160:CYS:HB3	3:j:205:PHE:CE1	2.46	0.51
1:D:12:LEU:O	1:D:12:LEU:HD23	2.10	0.51
2:E:12:TYR:CD2	2:E:100:PRO:HB3	2.46	0.51
1:G:59:LEU:HD13	1:G:121:TRP:CG	2.46	0.51
2:H:46:GLN:HG3	2:H:62:LEU:HD22	1.92	0.51
1:P:67:GLU:OE2	1:P:83:ARG:HA	2.11	0.51
3:R:136:GLU:OE2	3:R:155:ARG:HD3	2.11	0.51
1:S:28:ILE:HG12	1:S:78:PHE:CZ	2.46	0.51
1:V:24:ILE:HG23	1:V:80:PHE:CZ	2.45	0.51
3:X:154:ASN:ND2	3:X:163:HIS:HE1	2.08	0.51
3:a:164:LEU:HD12	3:a:165:VAL:H	1.76	0.51
3:a:191:VAL:HB	3:a:197:TYR:OH	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:73:THR:OG1	2:c:74:THR:N	2.44	0.51
3:d:44:ASN:ND2	3:d:133:TRP:H	2.08	0.51
3:j:125:LYS:HB3	3:j:127:GLN:NE2	2.26	0.51
2:H:139:LEU:HD23	2:H:186:PRO:HA	1.93	0.51
3:L:182:TYR:CD1	3:L:183:ARG:HD3	2.46	0.51
2:N:10:CYS:HA	2:N:19:SER:O	2.11	0.51
2:T:112:LEU:HG	2:T:126:TRP:HB3	1.93	0.51
3:X:38:VAL:HG13	3:X:51:THR:O	2.10	0.51
3:g:63:LEU:HD23	3:g:112:ASP:HA	1.93	0.51
3:F:140:LEU:HD13	3:F:224:TRP:HB2	1.92	0.51
3:F:162:GLU:OE2	3:F:204:ARG:HD3	2.10	0.51
1:G:126:GLN:HE22	3:I:210:GLY:C	2.19	0.51
2:H:12:TYR:HD1	2:H:13:ASN:H	1.59	0.51
3:L:188:LEU:CD2	3:L:199:PHE:CZ	2.94	0.51
1:M:46:MET:HB3	1:M:47:PRO:HD2	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
1:V:97:LYS:HG3	1:V:98:GLY:N	2.20	0.51
3:d:65:LEU:O	3:d:80:CYS:HB2	2.11	0.51
3:d:169:THR:HA	3:d:196:ARG:O	2.11	0.51
1:e:14:LEU:HD12	1:e:96:LEU:HD21	1.93	0.51
1:e:20:ASP:OD1	1:e:85:VAL:HG23	2.11	0.51
2:f:81:ARG:HG2	2:f:95:ILE:HD13	1.91	0.51
3:g:128:ASN:OD1	3:g:211:SER:HB2	2.10	0.51
2:B:73:THR:CG2	2:B:74:THR:N	2.74	0.50
1:G:103:PHE:CD1	1:G:104:MET:N	2.79	0.50
2:H:39:PRO:HG3	2:H:44:TRP:CZ3	2.46	0.50
1:J:74:HIS:CD2	1:J:75:SER:H	2.29	0.50
2:K:74:THR:N	2:K:101:PHE:CD1	2.78	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:Q:87:GLY:C	2:Q:89:ARG:H	2.19	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
2:W:146:LEU:HB3	2:W:179:GLU:HB2	1.92	0.50
3:a:204:ARG:HB2	3:a:215:TRP:CE3	2.46	0.50
2:f:128:ILE:HG12	2:f:165:GLU:OE1	2.10	0.50
3:g:62:ASN:HD21	4:g:300:NAG:H2	1.76	0.50
3:j:89:ILE:HG22	3:j:90:THR:N	2.26	0.50
2:B:146:LEU:HB2	2:B:152:TRP:CH2	2.46	0.50
1:D:46:MET:HB3	1:D:47:PRO:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:48:MET:HB2	3:F:100:ILE:HD11	1.93	0.50
2:H:141:PHE:HA	2:H:183:ARG:O	2.11	0.50
2:K:78:VAL:O	2:K:98:PHE:HB3	2.11	0.50
2:K:162:GLN:NE2	2:K:164:GLN:OE1	2.44	0.50
3:L:89:ILE:HG22	3:L:90:THR:N	2.26	0.50
3:O:175:TRP:HE1	1:V:106:GLU:HG3	1.76	0.50
2:T:167:ILE:HG21	2:T:180:PHE:CE1	2.46	0.50
3:U:204:ARG:HG3	3:U:214:HIS:O	2.12	0.50
1:V:62:GLU:C	1:V:65:PRO:HD2	2.35	0.50
2:W:106:LEU:HD12	2:W:106:LEU:N	2.27	0.50
3:a:132:PRO:HD2	3:a:216:SER:HB3	1.92	0.50
3:g:68:TRP:HE3	3:g:77:VAL:HG13	1.76	0.50
3:g:166:GLN:HG2	3:g:177:GLU:HB3	1.94	0.50
2:i:8:PHE:HB2	2:i:22:TRP:HD1	1.75	0.50
1:A:23:MET:SD	1:A:80:PHE:HB3	2.50	0.50
1:D:112:ALA:HB1	1:D:116:GLU:HB2	1.92	0.50
3:F:65:LEU:C	3:F:65:LEU:HD23	2.37	0.50
1:G:18:LEU:CD2	3:I:208:LEU:HA	2.41	0.50
3:L:129:LEU:O	3:L:131:ILE:HG12	2.12	0.50
1:M:45:TYR:CE1	1:M:111:THR:HG22	2.46	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
2:T:159:THR:HG22	2:T:161:LYS:HG3	1.92	0.50
1:V:127:SER:O	1:V:130:SER:HB3	2.12	0.50
2:W:106:LEU:HD13	2:W:186:PRO:HD3	1.93	0.50
2:W:141:PHE:HA	2:W:183:ARG:O	2.11	0.50
1:Y:69:VAL:O	1:Y:72:LEU:HG	2.11	0.50
1:Y:103:PHE:CG	1:Y:104:MET:N	2.79	0.50
3:a:95:LEU:HD22	3:a:99:GLU:OE1	2.12	0.50
3:a:200:ARG:HG3	3:a:218:TRP:CE3	2.46	0.50
1:b:60:GLU:HB2	1:b:93:VAL:HG11	1.94	0.50
2:c:104:LEU:HD13	2:c:135:PHE:CZ	2.46	0.50
2:f:124:ILE:HD11	2:f:203:PHE:CD2	2.47	0.50
2:i:203:PHE:CD1	2:i:203:PHE:C	2.89	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:K:39:PRO:HA	2:K:78:VAL:HA	1.94	0.50
3:O:150:LEU:HD22	3:O:152:TRP:HE3	1.76	0.50
3:R:191:VAL:HG23	3:R:197:TYR:CE1	2.46	0.50
3:U:148:LEU:HD12	3:U:148:LEU:C	2.37	0.50
1:V:91:VAL:HG12	2:W:75:VAL:CG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:36:HIS:CG	2:W:38:TRP:HE1	2.30	0.50
1:Y:11:GLN:O	1:Y:15:GLU:HG3	2.11	0.50
3:a:62:ASN:HD21	4:a:300:NAG:H2	1.75	0.50
2:f:11:PHE:O	2:f:18:ILE:HA	2.12	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
3:L:85:PHE:HA	3:L:89:ILE:O	2.11	0.50
1:M:20:ASP:OD1	1:M:23:MET:HE2	2.11	0.50
3:O:188:LEU:HD22	3:O:199:PHE:HE2	1.77	0.50
2:W:141:PHE:CD2	2:W:184:VAL:HG22	2.47	0.50
2:Z:8:PHE:CE1	2:Z:82:VAL:CG2	2.95	0.50
3:a:128:ASN:O	3:a:212:ALA:HA	2.12	0.50
1:b:78:PHE:CD1	1:b:80:PHE:CZ	3.00	0.50
1:b:82:PRO:O	1:b:85:VAL:HG12	2.12	0.50
2:c:78:VAL:O	2:c:80:LEU:HG	2.12	0.50
1:e:56:LEU:HD22	1:e:93:VAL:CG2	2.41	0.50
2:f:167:ILE:HG21	2:f:180:PHE:CZ	2.47	0.50
1:h:17:LEU:HA	1:h:92:PHE:HD2	1.76	0.50
2:i:102:GLU:HA	2:i:189:GLY:HA2	1.93	0.50
3:j:165:VAL:O	3:j:177:GLU:HA	2.12	0.50
1:D:23:MET:HE3	1:D:80:PHE:HB3	1.93	0.50
2:E:143:ALA:HB3	2:E:158:LEU:HD12	1.94	0.50
1:P:132:LEU:O	1:P:133:THR:CB	2.60	0.50
2:T:44:TRP:HH2	2:T:64:LEU:HD13	1.75	0.50
2:T:107:MET:HB2	2:T:129:SER:HB3	1.93	0.50
2:T:162:GLN:HE21	2:T:164:GLN:NE2	2.09	0.50
1:V:93:VAL:HG23	1:V:94:LEU:H	1.77	0.50
2:W:153:GLU:H	2:W:153:GLU:CD	2.19	0.50
1:Y:127:SER:HA	3:a:103:TYR:CD1	2.46	0.50
3:a:140:LEU:HD23	3:a:149:GLU:O	2.12	0.50
1:b:80:PHE:CD1	1:b:80:PHE:C	2.90	0.50
3:d:52:TRP:CZ3	3:d:65:LEU:HD12	2.40	0.50
1:h:91:VAL:HG12	2:i:75:VAL:CG2	2.42	0.50
2:i:63:ILE:O	2:i:63:ILE:HG22	2.10	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
1:G:53:LEU:CD2	1:G:96:LEU:HD22	2.42	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:O:198:THR:HG21	1:V:104:MET:HE2	1.93	0.50
1:S:48:LYS:HD3	1:S:107:TYR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:148:LEU:CD2	3:U:191:VAL:HG11	2.37	0.50
3:X:204:ARG:HH21	3:X:215:TRP:NE1	2.10	0.50
2:Z:115:VAL:HG11	4:Z:215:NAG:O5	2.11	0.50
3:d:160:CYS:HB3	3:d:205:PHE:CE1	2.47	0.50
1:A:36:LEU:HA	1:A:39:MET:HB3	1.93	0.50
1:D:24:ILE:O	1:D:28:ILE:HG13	2.12	0.50
1:D:68:GLU:HA	1:D:68:GLU:OE2	2.12	0.50
2:E:39:PRO:HB2	2:E:42:ARG:HB2	1.94	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
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
1:P:87:SER:O	1:P:88:ASN:C	2.55	0.50
3:R:62:ASN:HD21	4:R:300:NAG:C2	2.25	0.50
3:U:138:LEU:H	3:U:138:LEU:HD12	1.77	0.50
2:f:73:THR:HG21	2:f:75:VAL:HG22	1.92	0.50
1:h:86:VAL:O	1:h:90:ASN:N	2.40	0.50
3:F:167:TYR:OH	3:F:176:THR:HG21	2.11	0.50
1:G:14:LEU:HD13	1:G:128:ILE:HB	1.93	0.50
2:K:128:ILE:HD12	2:K:131:ALA:CB	2.41	0.50
1:V:57:GLN:HG3	1:V:61:GLU:OE2	2.11	0.50
1:e:6:SER:N	1:e:8:LYS:HG3	2.26	0.50
3:g:208:LEU:HD23	3:g:208:LEU:N	2.27	0.50
2:i:36:HIS:HB3	2:i:38:TRP:NE1	2.27	0.50
3:j:62:ASN:ND2	4:j:300:NAG:H83	2.27	0.50
1:D:89:ILE:O	1:D:92:PHE:HB2	2.12	0.49
1:D:91:VAL:HG12	2:E:75:VAL:CG2	2.42	0.49
3:F:138:LEU:HD21	3:F:219:SER:OG	2.12	0.49
3:F:158:ASN:O	3:F:159:HIS:CB	2.60	0.49
1:G:131:THR:HG22	1:G:131:THR:O	2.11	0.49
1:J:88:ASN:ND2	2:K:42:ARG:NH2	2.57	0.49
3:L:109:GLN:HE21	3:L:121:THR:CG2	2.25	0.49
1:M:36:LEU:HD12	1:M:36:LEU:O	2.12	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:W:10:CYS:C	2:W:11:PHE:CD1	2.90	0.49
2:W:37:ALA:HB2	2:W:62:LEU:HD22	1.94	0.49
2:Z:81:ARG:HE	2:Z:95:ILE:HD12	1.77	0.49
2:c:8:PHE:HB2	2:c:22:TRP:CD1	2.47	0.49
2:E:44:TRP:HH2	2:E:64:LEU:HD13	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:143:ALA:HB1	2:E:180:PHE:CE1	2.47	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
1:P:113:THR:OG1	1:P:116:GLU:HG3	2.12	0.49
3:U:38:VAL:HG21	3:U:110:LEU:HD13	1.93	0.49
3:U:69:TYR:CE1	3:U:101:HIS:ND1	2.80	0.49
2:Z:10:CYS:HA	2:Z:19:SER:O	2.11	0.49
2:Z:126:TRP:HZ3	2:Z:167:ILE:HG22	1.77	0.49
1:e:17:LEU:HD11	1:e:89:ILE:HG23	1.94	0.49
2:B:173:THR:HB	2:B:176:THR:OG1	2.12	0.49
1:D:16:HIS:CB	2:E:134:TYR:HD2	2.26	0.49
2:E:161:LYS:N	3:F:187:SER:OG	2.34	0.49
2:E:171:THR:O	2:E:171:THR:HG22	2.13	0.49
1:G:113:THR:HG23	1:G:116:GLU:CD	2.38	0.49
1:J:65:PRO:HA	1:J:68:GLU:HB2	1.93	0.49
1:V:46:MET:SD	1:V:112:ALA:HB3	2.52	0.49
1:V:91:VAL:HG12	2:W:75:VAL:HG21	1.94	0.49
2:Z:109:PRO:HG3	2:Z:184:VAL:CG2	2.42	0.49
3:d:171:TRP:H	3:d:171:TRP:HD1	1.60	0.49
1:e:13:GLN:HG2	2:f:75:VAL:HG12	1.93	0.49
1:e:105:CYS:SG	1:e:107:TYR:CE1	3.06	0.49
1:h:18:LEU:CD1	1:h:122:ILE:HG23	2.42	0.49
1:D:60:GLU:CA	1:D:63:LEU:HD12	2.36	0.49
2:E:167:ILE:HD11	3:F:189:PRO:CB	2.43	0.49
3:F:103:TYR:OH	3:F:209:CYS:HB3	2.13	0.49
3:F:144:SER:OG	3:F:147:GLN:HG3	2.13	0.49
3:F:204:ARG:HB2	3:F:215:TRP:CD2	2.47	0.49
2:H:23:SER:HB3	2:H:57:SER:OG	2.12	0.49
2:Q:158:LEU:HD23	3:R:147:GLN:NE2	2.27	0.49
2:Q:205:THR:HG22	2:Q:206:LYS:N	2.26	0.49
1:S:23:MET:HE3	1:S:80:PHE:HB3	1.95	0.49
1:S:28:ILE:O	1:S:28:ILE:CG2	2.61	0.49
2:T:23:SER:HB2	2:T:56:ALA:O	2.12	0.49
2:T:83:LEU:HB3	2:T:90:TRP:HB3	1.93	0.49
2:T:176:THR:HG22	2:T:177:GLN:O	2.12	0.49
3:U:134:ALA:HB2	3:U:217:GLU:O	2.12	0.49
1:V:87:SER:O	1:V:91:VAL:HG23	2.12	0.49
2:W:70:GLN:CD	2:W:134:TYR:HE1	2.20	0.49
2:W:119:THR:HG22	2:W:206:LYS:C	2.37	0.49
2:W:143:ALA:HB1	2:W:180:PHE:CE1	2.47	0.49
3:X:157:LEU:CD1	3:X:161:LEU:HD13	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:40:ASP:OD2	2:Z:41:ARG:NH1	2.45	0.49
3:a:143:LEU:HD21	3:a:149:GLU:HB2	1.95	0.49
3:a:162:GLU:OE2	3:a:204:ARG:HD2	2.11	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
1:G:28:ILE:HD11	1:G:70:LEU:HD21	1.94	0.49
1:J:47:PRO:CG	1:J:50:ALA:HB2	2.43	0.49
2:K:8:PHE:CE1	2:K:82:VAL:CG2	2.95	0.49
1:M:50:ALA:HB3	1:M:120:ARG:NH2	2.27	0.49
3:U:67:TYR:HE2	3:U:95:LEU:HD21	1.75	0.49
2:W:78:VAL:CG2	2:W:100:PRO:HG3	2.42	0.49
2:c:71:LYS:O	2:c:72:LEU:HD23	2.12	0.49
3:g:35:LEU:HD13	3:g:110:LEU:CD1	2.37	0.49
1:G:114:ILE:O	1:G:118:LEU:HD12	2.11	0.49
2:H:138:HIS:HB2	2:H:187:LEU:HG	1.95	0.49
2:K:162:GLN:HG3	3:L:178:GLN:HE21	1.76	0.49
2:K:201:LEU:HD12	2:K:202:ALA:H	1.77	0.49
3:L:44:ASN:ND2	3:L:133:TRP:CD1	2.80	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:R:82:HIS:HD2	3:R:94:GLN:HB3	1.77	0.49
3:a:64:THR:OG1	3:a:111:GLN:HB3	2.13	0.49
3:a:165:VAL:HG11	3:a:186:PHE:CD2	2.48	0.49
3:d:161:LEU:HA	3:d:204:ARG:O	2.12	0.49
1:e:56:LEU:HD11	1:e:96:LEU:HD23	1.94	0.49
2:f:112:LEU:HB3	2:f:201:LEU:HD22	1.95	0.49
2:i:143:ALA:HB1	2:i:180:PHE:CZ	2.47	0.49
2:i:144:ARG:CD	2:i:152:TRP:CE3	2.95	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
2:E:118:GLU:OE1	2:E:121:ARG:HD3	2.10	0.49
3:F:65:LEU:HD23	3:F:66:HIS:N	2.28	0.49
1:G:64:LYS:O	1:G:68:GLU:HG2	2.12	0.49
2:H:171:THR:O	2:H:171:THR:HG22	2.12	0.49
3:I:204:ARG:HG2	3:I:205:PHE:N	2.27	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
3:X:157:LEU:HD12	3:X:157:LEU:O	2.12	0.49
1:Y:18:LEU:CD1	1:Y:122:ILE:HG23	2.43	0.49
2:c:118:GLU:O	2:c:205:THR:HG22	2.13	0.49
3:g:62:ASN:CG	4:g:300:NAG:H83	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:183:ARG:HG3	3:g:183:ARG:NH1	2.24	0.49
3:j:68:TRP:CE3	3:j:77:VAL:HG22	2.48	0.49
3:j:132:PRO:HG3	3:j:161:LEU:HD22	1.94	0.49
1:A:31:TYR:CD2	1:A:36:LEU:HB2	2.48	0.49
1:A:81:ASP:HB3	1:A:84:ASP:HB2	1.95	0.49
2:B:72:LEU:HD13	2:B:100:PRO:HG2	1.95	0.49
2:H:40:ASP:OD1	2:H:41:ARG:N	2.46	0.49
1:P:41:THR:O	1:P:43:LYS:HG3	2.12	0.49
3:R:192:ASP:OD1	3:R:195:LYS:HG3	2.12	0.49
2:T:181:GLN:HG2	2:T:198:SER:O	2.13	0.49
3:U:106:PHE:O	3:U:124:LEU:N	2.46	0.49
2:W:79:THR:HA	2:W:97:ASP:HA	1.93	0.49
3:a:143:LEU:CD2	3:a:149:GLU:HB2	2.42	0.49
1:h:36:LEU:HD12	1:h:36:LEU:C	2.38	0.49
2:B:81:ARG:HH11	2:B:95:ILE:HD12	1.76	0.49
2:H:121:ARG:C	2:H:172:LEU:HD12	2.38	0.49
3:I:85:PHE:CE2	3:I:90:THR:HG22	2.48	0.49
2:K:101:PHE:HD2	2:K:188:GLN:OE1	1.96	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
3:a:65:LEU:HD13	3:a:93:CYS:HB3	1.93	0.49
3:a:148:LEU:C	3:a:148:LEU:HD12	2.38	0.49
1:b:85:VAL:O	1:b:89:ILE:HG13	2.13	0.49
1:e:53:LEU:HA	1:e:124:PHE:HZ	1.78	0.49
1:h:117:PHE:HE1	1:h:121:TRP:CD1	2.30	0.49
1:A:59:LEU:HD13	1:A:121:TRP:CG	2.47	0.49
1:G:62:GLU:OE2	1:G:62:GLU:HA	2.12	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:K:201:LEU:HD12	2:K:202:ALA:N	2.27	0.49
2:Q:145:THR:OG1	2:Q:169:LEU:HD13	2.12	0.49
1:S:81:ASP:CB	1:S:84:ASP:HB2	2.40	0.49
2:c:36:HIS:HB3	2:c:38:TRP:NE1	2.28	0.49
3:g:43:PHE:HB3	3:g:133:TRP:CZ3	2.47	0.49
1:D:59:LEU:HD13	1:D:121:TRP:CG	2.47	0.48
2:E:47:THR:CG2	2:E:48:CYS:N	2.76	0.48
2:E:162:GLN:HE22	3:F:187:SER:C	2.21	0.48
1:G:78:PHE:N	1:G:78:PHE:CD1	2.80	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:Z:78:VAL:O	2:Z:98:PHE:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:205:PHE:CZ	3:a:209:CYS:HB2	2.48	0.48
2:c:126:TRP:HZ3	2:c:167:ILE:HG22	1.78	0.48
3:g:165:VAL:HG22	3:g:201:VAL:CG2	2.43	0.48
1:h:35:LYS:O	1:h:38:ARG:HB3	2.13	0.48
3:j:138:LEU:HD23	3:j:222:ILE:HG12	1.95	0.48
2:E:98:PHE:O	2:E:100:PRO:HD3	2.12	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
1:S:128:ILE:O	1:S:132:LEU:HD23	2.14	0.48
3:U:45:VAL:CG2	3:U:157:LEU:HD11	2.43	0.48
1:V:24:ILE:CG2	1:V:70:LEU:HD11	2.43	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
3:a:82:HIS:ND1	3:a:94:GLN:HB3	2.28	0.48
1:e:12:LEU:HA	1:e:15:GLU:HG3	1.95	0.48
2:f:13:ASN:HD21	2:f:16:ALA:H	1.60	0.48
2:f:109:PRO:HG3	2:f:184:VAL:HG23	1.95	0.48
3:g:154:ASN:HD21	3:g:163:HIS:HE1	1.60	0.48
2:i:175:ASP:O	2:i:175:ASP:OD2	2.31	0.48
1:A:17:LEU:O	1:A:18:LEU:C	2.55	0.48
2:B:98:PHE:CE2	2:B:100:PRO:HA	2.48	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:L:154:ASN:HD21	3:L:163:HIS:CE1	2.31	0.48
3:O:143:LEU:CD2	3:O:149:GLU:HB3	2.43	0.48
1:P:86:VAL:O	1:P:87:SER:C	2.54	0.48
2:Q:114:VAL:CG1	2:Q:117:VAL:HG13	2.42	0.48
1:S:6:SER:HA	1:S:9:LYS:HE2	1.95	0.48
2:T:44:TRP:CH2	2:T:72:LEU:HD21	2.48	0.48
3:U:167:TYR:HB3	3:U:199:PHE:CD1	2.48	0.48
2:i:40:ASP:OD2	2:i:77:ILE:HB	2.12	0.48
1:A:45:TYR:OH	2:H:204:ARG:O	2.24	0.48
3:C:61:THR:HG1	3:C:114:ARG:HH22	1.54	0.48
2:E:103:ASN:OD1	2:E:191:PHE:CB	2.60	0.48
2:H:83:LEU:HD21	2:W:38:TRP:CH2	2.49	0.48
3:I:48:MET:HB2	3:I:100:ILE:HD11	1.95	0.48
2:K:23:SER:HB3	2:K:57:SER:OG	2.14	0.48
2:K:138:HIS:C	2:K:187:LEU:CD1	2.86	0.48
2:K:183:ARG:HD2	2:K:194:TRP:HB3	1.96	0.48
2:N:15:ARG:NH1	2:N:70:GLN:OE1	2.42	0.48
2:Q:167:ILE:HG12	2:Q:168:CYS:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:74:THR:N	2:T:101:PHE:CD1	2.81	0.48
2:T:118:GLU:HA	2:T:206:LYS:HD2	1.94	0.48
1:V:92:PHE:O	1:V:96:LEU:HD13	2.13	0.48
3:X:201:VAL:O	3:X:219:SER:HB3	2.14	0.48
1:e:124:PHE:O	1:e:127:SER:HB2	2.13	0.48
1:h:6:SER:C	1:h:8:LYS:H	2.21	0.48
3:j:61:THR:O	3:j:89:ILE:HG23	2.14	0.48
2:E:146:LEU:HD22	2:E:152:TRP:CE2	2.48	0.48
3:I:47:TYR:C	3:I:47:TYR:CD1	2.92	0.48
3:L:169:THR:N	3:L:172:ASP:HB2	2.19	0.48
2:W:166:TRP:CE3	2:W:166:TRP:C	2.91	0.48
1:Y:49:LYS:HB3	1:Y:49:LYS:HE2	1.68	0.48
3:a:43:PHE:O	3:a:44:ASN:C	2.56	0.48
1:b:54:LYS:HA	1:b:97:LYS:HB2	1.94	0.48
2:c:151:THR:OG1	2:c:154:GLU:HG3	2.14	0.48
2:c:153:GLU:C	2:c:155:ALA:N	2.72	0.48
2:f:125:SER:HA	2:f:166:TRP:HA	1.95	0.48
3:j:52:TRP:CH2	3:j:110:LEU:HD21	2.47	0.48
3:j:67:TYR:CE1	3:j:78:GLN:HB2	2.48	0.48
2:B:146:LEU:HB3	2:B:179:GLU:HB2	1.95	0.48
1:J:126:GLN:HA	1:J:129:ILE:HG22	1.95	0.48
2:N:114:VAL:CG1	2:N:117:VAL:HG13	2.44	0.48
3:O:155:ARG:HG3	3:O:156:PHE:CD2	2.49	0.48
1:P:88:ASN:O	1:P:89:ILE:C	2.57	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:W:115:VAL:HG21	2:W:123:ASN:ND2	2.28	0.48
1:Y:87:SER:O	1:Y:91:VAL:HG23	2.14	0.48
3:d:38:VAL:HG13	3:d:51:THR:O	2.13	0.48
3:d:47:TYR:HE1	3:d:49:ASN:HD21	1.62	0.48
3:d:169:THR:CG2	3:d:195:LYS:HB3	2.42	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
3:O:110:LEU:HD23	3:O:110:LEU:HA	1.58	0.48
1:P:80:PHE:CD1	1:P:80:PHE:O	2.67	0.48
1:P:103:PHE:CG	1:P:104:MET:N	2.81	0.48
2:T:33:CYS:O	2:T:50:LEU:HB2	2.14	0.48
3:U:52:TRP:CH2	3:U:92:GLY:HA2	2.48	0.48
3:X:160:CYS:HB3	3:X:205:PHE:CE1	2.48	0.48
2:Z:9:THR:HG22	2:Z:11:PHE:HE1	1.77	0.48
2:Z:146:LEU:HD22	2:Z:152:TRP:NE1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:44:ASN:HD21	3:a:156:PHE:HD2	1.61	0.48
3:g:128:ASN:C	3:g:129:LEU:HD23	2.38	0.48
2:i:144:ARG:NH1	2:i:197:TRP:CE2	2.82	0.48
3:j:166:GLN:NE2	3:j:218:TRP:CH2	2.82	0.48
2:B:46:GLN:HG3	2:B:47:THR:N	2.28	0.48
1:D:52:GLU:OE1	1:D:54:LYS:HE2	2.14	0.48
1:J:24:ILE:HD11	1:J:85:VAL:HG21	1.94	0.48
2:N:181:GLN:NE2	2:N:200:PRO:HD3	2.26	0.48
3:O:198:THR:HG21	1:V:104:MET:CE	2.44	0.48
2:Q:83:LEU:HD22	2:Q:92:VAL:HG22	1.96	0.48
1:S:18:LEU:HD11	1:S:122:ILE:HG23	1.95	0.48
2:T:129:SER:O	2:T:130:GLN:C	2.56	0.48
2:W:136:GLU:HG2	2:W:137:ARG:N	2.29	0.48
3:a:38:VAL:HG12	3:a:39:GLN:N	2.29	0.48
2:c:118:GLU:OE1	2:c:121:ARG:HB2	2.14	0.48
3:d:206:ASN:ND2	3:d:211:SER:HA	2.29	0.48
1:G:45:TYR:HE1	1:G:111:THR:CG2	2.26	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
2:K:176:THR:HG22	2:K:177:GLN:N	2.29	0.48
1:M:16:HIS:ND1	2:N:134:TYR:CD2	2.77	0.48
1:b:28:ILE:HD11	1:b:70:LEU:HD22	1.96	0.48
1:b:63:LEU:HG	1:b:86:VAL:HG13	1.95	0.48
2:c:188:GLN:HG2	2:c:189:GLY:N	2.29	0.48
3:d:169:THR:HG21	3:d:195:LYS:HB3	1.95	0.48
3:g:181:ASP:OD1	3:g:183:ARG:NH1	2.47	0.48
3:j:138:LEU:HD11	3:j:219:SER:HB2	1.95	0.48
2:K:12:TYR:CD1	2:K:13:ASN:N	2.82	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
3:O:102:LEU:HD22	3:O:127:GLN:CA	2.44	0.48
3:O:164:LEU:HD11	3:O:177:GLU:HB2	1.96	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:R:166:GLN:HG2	3:R:177:GLU:HB3	1.95	0.48
1:S:27:GLY:O	1:S:78:PHE:HE1	1.97	0.48
1:V:20:ASP:OD2	2:W:134:TYR:CE2	2.67	0.48
1:Y:18:LEU:HD11	1:Y:22:GLN:NE2	2.28	0.48
1:b:46:MET:HE1	1:b:120:ARG:HD3	1.96	0.48
3:d:206:ASN:HD22	3:d:211:SER:HA	1.78	0.48
3:j:162:GLU:OE2	3:j:206:ASN:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:11:GLN:HB2	1:J:132:LEU:HD13	1.95	0.47
1:P:28:ILE:O	1:P:28:ILE:HG22	2.14	0.47
3:R:69:TYR:CE1	3:R:101:HIS:CD2	3.02	0.47
1:S:60:GLU:O	1:S:63:LEU:HB2	2.14	0.47
3:U:137:ASN:O	3:U:139:THR:HG23	2.14	0.47
2:f:46:GLN:HE21	2:f:47:THR:N	2.12	0.47
2:f:95:ILE:HG23	2:f:95:ILE:O	2.13	0.47
3:j:169:THR:HG22	3:j:170:ASP:N	2.28	0.47
3:C:102:LEU:C	3:C:104:GLN:H	2.21	0.47
3:F:146:SER:O	3:F:191:VAL:HG22	2.14	0.47
1:J:24:ILE:CG2	1:J:118:LEU:HD11	2.44	0.47
2:K:83:LEU:HD21	2:K:92:VAL:HG22	1.96	0.47
3:L:135:PRO:HG2	3:L:201:VAL:HG12	1.95	0.47
3:O:113:PRO:HB2	2:i:114:VAL:HB	1.96	0.47
3:R:65:LEU:HD13	3:R:93:CYS:HB3	1.96	0.47
3:R:169:THR:HA	3:R:196:ARG:O	2.14	0.47
1:V:95:GLU:CG	2:W:41:ARG:NH1	2.77	0.47
1:V:125:CYS:C	1:V:127:SER:N	2.72	0.47
3:X:68:TRP:CE3	3:X:77:VAL:HG13	2.48	0.47
1:Y:56:LEU:HD23	1:Y:121:TRP:HZ3	1.79	0.47
3:a:143:LEU:HD12	3:a:147:GLN:CB	2.43	0.47
3:a:205:PHE:CE2	3:a:210:GLY:HA3	2.49	0.47
2:c:136:GLU:OE2	3:d:207:PRO:HG3	2.14	0.47
2:c:153:GLU:N	2:c:153:GLU:OE2	2.47	0.47
3:g:38:VAL:H	3:g:122:GLN:NE2	2.11	0.47
3:j:142:LYS:HB2	3:j:142:LYS:HE3	1.54	0.47
3:C:47:TYR:HA	3:C:100:ILE:HD11	1.96	0.47
1:G:16:HIS:O	1:G:17:LEU:C	2.57	0.47
1:J:88:ASN:O	1:J:89:ILE:C	2.55	0.47
3:O:168:ARG:HB2	3:O:172:ASP:HB3	1.95	0.47
3:O:207:PRO:C	3:O:208:LEU:HG	2.39	0.47
2:T:98:PHE:HE2	2:T:100:PRO:HA	1.77	0.47
3:X:57:GLU:HB3	3:X:58:PRO:HD2	1.97	0.47
1:b:56:LEU:HD13	1:b:93:VAL:HG22	1.96	0.47
1:e:14:LEU:HD22	1:e:129:ILE:HG12	1.96	0.47
2:f:142:GLU:O	2:f:182:VAL:HA	2.14	0.47
2:i:86:GLU:OE2	2:i:91:ARG:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:LEU:HD12	2:H:83:LEU:N	2.29	0.47
3:R:40:CYS:C	3:R:41:PHE:CD1	2.92	0.47
2:T:21:VAL:HA	2:T:58:TRP:O	2.15	0.47
2:c:46:GLN:NE2	2:c:63:ILE:O	2.44	0.47
2:c:106:LEU:HD11	2:c:186:PRO:HG3	1.96	0.47
3:d:167:TYR:HB2	3:d:199:PHE:CE2	2.49	0.47
3:g:138:LEU:HA	3:g:151:ASN:O	2.13	0.47
3:j:62:ASN:HD21	4:j:300:NAG:H2	1.79	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
2:K:10:CYS:HA	2:K:19:SER:O	2.13	0.47
2:K:104:LEU:HD12	2:K:188:GLN:O	2.15	0.47
2:K:171:THR:O	2:K:171:THR:HG22	2.15	0.47
1:M:88:ASN:HD21	2:N:42:ARG:HH12	1.62	0.47
2:W:22:TRP:CZ2	2:W:24:GLN:HB2	2.48	0.47
1:Y:20:ASP:OD2	1:Y:89:ILE:CG1	2.62	0.47
3:a:164:LEU:O	3:a:201:VAL:HG13	2.15	0.47
2:i:8:PHE:CE1	2:i:82:VAL:CG2	2.97	0.47
2:i:65:GLY:CA	2:i:71:LYS:HE3	2.33	0.47
1:G:28:ILE:HD11	1:G:70:LEU:CD2	2.44	0.47
2:K:161:LYS:NZ	3:L:185:LYS:HD3	2.27	0.47
3:L:165:VAL:HG12	3:L:178:GLN:O	2.14	0.47
3:L:206:ASN:HA	3:L:210:GLY:O	2.14	0.47
3:O:154:ASN:HD21	3:O:163:HIS:HE1	1.60	0.47
1:P:31:TYR:OH	1:P:35:LYS:HB2	2.15	0.47
1:S:126:GLN:OE1	3:U:210:GLY:HA2	2.15	0.47
2:T:39:PRO:CG	2:T:42:ARG:HB2	2.45	0.47
2:T:172:LEU:HD22	2:T:178:TYR:CE1	2.49	0.47
3:U:52:TRP:CD2	3:U:110:LEU:HD21	2.50	0.47
1:V:81:ASP:CB	1:V:84:ASP:HB2	2.29	0.47
1:V:97:LYS:CG	1:V:98:GLY:H	2.24	0.47
1:Y:94:LEU:CD2	1:Y:97:LYS:HE2	2.44	0.47
2:Z:13:ASN:HD21	2:Z:17:GLN:HB2	1.72	0.47
2:c:83:LEU:HB2	2:c:90:TRP:CE3	2.49	0.47
2:f:14:SER:OG	2:f:132:SER:CB	2.62	0.47
2:i:107:MET:HG3	2:i:130:GLN:OE1	2.14	0.47
3:j:138:LEU:CB	3:j:222:ILE:HG21	2.44	0.47
1:A:112:ALA:HB1	1:A:116:GLU:HB2	1.96	0.47
1:A:118:LEU:O	1:A:119:ASN:C	2.57	0.47
3:C:180:VAL:HG11	3:C:185:LYS:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:170:GLU:H	3:F:190:SER:HB3	1.80	0.47
3:F:192:ASP:C	3:F:192:ASP:OD1	2.58	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
3:I:165:VAL:HG21	3:I:186:PHE:CB	2.45	0.47
1:J:56:LEU:O	1:J:59:LEU:HB3	2.14	0.47
2:K:8:PHE:CE1	2:K:82:VAL:HG22	2.50	0.47
2:K:44:TRP:CH2	2:K:64:LEU:HD13	2.50	0.47
2:K:204:ARG:HG2	2:K:205:THR:H	1.79	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
1:M:16:HIS:HB3	2:N:134:TYR:CD2	2.50	0.47
1:M:84:ASP:O	1:M:87:SER:HB2	2.14	0.47
2:N:51:LEU:O	2:N:58:TRP:HA	2.14	0.47
1:P:44:PHE:CE2	1:P:114:ILE:HB	2.47	0.47
1:P:123:THR:O	1:P:124:PHE:C	2.56	0.47
2:Q:147:SER:OG	2:Q:148:PRO:HD2	2.15	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
1:S:85:VAL:HG13	1:S:86:VAL:N	2.29	0.47
2:W:141:PHE:HB2	2:W:160:LEU:HD12	1.96	0.47
1:Y:125:CYS:O	1:Y:126:GLN:C	2.57	0.47
2:Z:161:LYS:HD3	3:a:185:LYS:NZ	2.30	0.47
1:b:88:ASN:HD22	2:c:42:ARG:HH22	1.61	0.47
1:b:105:CYS:SG	1:b:107:TYR:CE1	3.08	0.47
2:c:106:LEU:CD1	2:c:186:PRO:HD3	2.44	0.47
2:f:82:VAL:CG1	2:f:93:MET:HB2	2.22	0.47
3:g:148:LEU:C	3:g:148:LEU:HD12	2.40	0.47
2:i:81:ARG:CD	2:i:95:ILE:HG12	2.45	0.47
3:j:67:TYR:CD1	3:j:67:TYR:C	2.92	0.47
1:A:81:ASP:OD1	1:A:82:PRO:HD2	2.15	0.47
1:G:46:MET:HB3	1:G:47:PRO:HD2	1.96	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
4:N:215:NAG:H4	4:O:233:NAG:C1	2.45	0.47
2:Q:36:HIS:ND1	2:Q:47:THR:HG22	2.29	0.47
2:Z:125:SER:HA	2:Z:166:TRP:HA	1.95	0.47
3:a:160:CYS:O	3:a:161:LEU:HD23	2.15	0.47
3:a:204:ARG:HB2	3:a:215:TRP:CZ3	2.49	0.47
1:b:69:VAL:HG12	1:b:70:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:128:ASN:O	3:g:129:LEU:HD23	2.14	0.47
2:K:35:VAL:HA	2:K:81:ARG:O	2.14	0.47
3:L:126:LEU:C	3:L:128:ASN:H	2.22	0.47
2:N:146:LEU:HD22	2:N:152:TRP:CZ2	2.50	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
3:R:69:TYR:CE2	3:R:106:PHE:CD1	3.03	0.47
2:T:162:GLN:NE2	3:U:186:PHE:CE1	2.83	0.47
1:V:20:ASP:OD2	2:W:134:TYR:HE2	1.98	0.47
2:W:42:ARG:HH22	2:W:73:THR:HG23	1.79	0.47
2:W:80:LEU:CD1	2:W:98:PHE:CB	2.93	0.47
3:X:67:TYR:CD1	3:X:67:TYR:C	2.93	0.47
2:Z:164:GLN:HG3	3:a:178:GLN:NE2	2.29	0.47
2:c:159:THR:HG22	2:c:161:LYS:CG	2.45	0.47
2:f:39:PRO:CB	2:f:42:ARG:HB2	2.45	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
1:G:114:ILE:O	1:G:117:PHE:HB3	2.15	0.47
2:H:107:MET:HE3	2:H:108:ALA:H	1.80	0.47
3:I:35:LEU:HD11	3:I:118:ARG:HG2	1.96	0.47
3:I:40:CYS:O	3:I:41:PHE:CG	2.68	0.47
2:K:98:PHE:CE2	2:K:100:PRO:HG3	2.50	0.47
3:L:42:VAL:HG22	3:L:100:ILE:HD13	1.96	0.47
1:S:91:VAL:HG12	2:T:75:VAL:HG23	1.96	0.47
1:b:56:LEU:O	1:b:58:CYS:N	2.47	0.47
1:b:86:VAL:O	1:b:87:SER:C	2.58	0.47
2:c:146:LEU:HD23	2:c:179:GLU:HB2	1.97	0.47
3:d:44:ASN:HD22	3:d:132:PRO:HA	1.80	0.47
3:d:192:ASP:OD2	3:d:195:LYS:HG3	2.14	0.47
1:e:25:LEU:C	1:e:27:GLY:H	2.23	0.47
2:f:40:ASP:OD1	2:f:41:ARG:CB	2.63	0.47
1:h:50:ALA:HB3	1:h:120:ARG:NH2	2.30	0.47
2:i:8:PHE:CE1	2:i:82:VAL:HG23	2.49	0.47
2:i:144:ARG:HD3	2:i:152:TRP:HE3	1.78	0.47
1:G:131:THR:O	1:G:131:THR:CG2	2.64	0.46
3:L:126:LEU:C	3:L:128:ASN:N	2.72	0.46
2:N:36:HIS:HB3	2:N:38:TRP:HE1	1.81	0.46
3:R:52:TRP:HE1	3:R:63:LEU:HD12	1.79	0.46
1:b:57:GLN:HA	1:b:97:LYS:HE2	1.96	0.46
2:c:12:TYR:HB2	2:c:18:ILE:HG12	1.98	0.46
2:c:164:GLN:NE2	3:d:178:GLN:HG2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:13:GLN:CD	2:f:75:VAL:HG12	2.40	0.46
2:f:146:LEU:HD23	2:f:179:GLU:HB2	1.97	0.46
1:G:88:ASN:O	1:G:92:PHE:CD2	2.68	0.46
1:M:92:PHE:CE2	2:N:134:TYR:HE2	2.33	0.46
2:N:51:LEU:HB3	2:N:52:PRO:HD2	1.96	0.46
3:O:149:GLU:HG3	3:O:151:ASN:HD21	1.79	0.46
3:O:167:TYR:CE2	3:O:176:THR:HB	2.49	0.46
3:O:192:ASP:OD1	3:O:194:GLN:HB2	2.15	0.46
3:R:48:MET:CE	3:R:95:LEU:HD22	2.45	0.46
3:U:111:GLN:OE1	3:U:119:GLN:HB3	2.14	0.46
3:U:139:THR:O	3:U:150:LEU:HD23	2.15	0.46
3:X:109:GLN:HG3	3:X:121:THR:HG22	1.97	0.46
1:Y:114:ILE:O	1:Y:117:PHE:HB3	2.16	0.46
3:d:188:LEU:HG	3:d:191:VAL:HG12	1.97	0.46
3:d:200:ARG:CZ	3:d:218:TRP:CE2	2.98	0.46
2:f:137:ARG:HB2	3:g:181:ASP:HB3	1.98	0.46
3:j:154:ASN:HD22	3:j:184:HIS:CD2	2.33	0.46
3:j:222:ILE:O	3:j:222:ILE:HG13	2.13	0.46
2:B:146:LEU:HB2	2:B:152:TRP:CZ2	2.50	0.46
2:B:204:ARG:O	1:D:45:TYR:OH	2.32	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:N:155:ALA:HA	2:N:156:PRO:HD3	1.69	0.46
1:P:88:ASN:N	1:P:88:ASN:ND2	2.63	0.46
2:Q:159:THR:HG22	2:Q:161:LYS:HG3	1.97	0.46
2:T:146:LEU:HD23	2:T:179:GLU:CB	2.45	0.46
3:U:131:ILE:HA	3:U:132:PRO:HD3	1.68	0.46
2:W:121:ARG:HG2	2:W:170:GLU:OE2	2.15	0.46
3:X:157:LEU:HD12	3:X:157:LEU:C	2.40	0.46
1:Y:67:GLU:O	1:Y:71:ASN:CG	2.58	0.46
2:Z:70:GLN:HG2	2:Z:134:TYR:HE1	1.81	0.46
2:c:83:LEU:CD2	2:c:92:VAL:HG22	2.45	0.46
2:f:153:GLU:C	2:f:155:ALA:N	2.72	0.46
1:h:24:ILE:O	1:h:28:ILE:HG13	2.14	0.46
1:G:35:LYS:HE3	1:G:38:ARG:HB2	1.97	0.46
2:K:106:LEU:HD23	2:K:184:VAL:HG13	1.97	0.46
3:R:109:GLN:HA	3:R:120:ALA:O	2.16	0.46
3:U:62:ASN:HD21	4:U:300:NAG:C2	2.28	0.46
3:U:64:THR:OG1	3:U:111:GLN:HB3	2.16	0.46
1:V:125:CYS:O	1:V:126:GLN:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:161:LEU:CD1	3:X:205:PHE:HD1	2.28	0.46
2:Z:36:HIS:HB3	2:Z:38:TRP:HE1	1.81	0.46
2:c:82:VAL:O	2:c:83:LEU:HD23	2.15	0.46
2:c:179:GLU:HG2	2:c:201:LEU:O	2.16	0.46
1:e:57:GLN:HG3	1:e:57:GLN:O	2.15	0.46
1:e:97:LYS:O	1:e:98:GLY:C	2.59	0.46
2:f:46:GLN:HE21	2:f:47:THR:H	1.63	0.46
2:f:118:GLU:OE1	2:f:121:ARG:HD3	2.14	0.46
2:B:117:VAL:O	2:B:206:LYS:HE2	2.16	0.46
2:E:46:GLN:NE2	2:T:89:ARG:HA	2.30	0.46
2:H:64:LEU:N	2:H:64:LEU:HD23	2.30	0.46
2:H:136:GLU:HB3	2:H:137:ARG:H	1.50	0.46
2:K:144:ARG:NH1	2:K:152:TRP:HB3	2.30	0.46
1:V:24:ILE:HG21	1:V:70:LEU:HD11	1.96	0.46
2:W:114:VAL:HG22	2:W:124:ILE:HG12	1.98	0.46
2:W:159:THR:HG22	2:W:161:LYS:HG2	1.98	0.46
3:X:62:ASN:HD21	4:X:300:NAG:C1	2.28	0.46
2:c:15:ARG:HD2	2:c:68:ASP:O	2.15	0.46
2:c:39:PRO:HB2	2:c:42:ARG:HB2	1.96	0.46
3:d:37:GLU:HG3	3:d:122:GLN:NE2	2.22	0.46
1:e:16:HIS:O	1:e:17:LEU:C	2.57	0.46
1:e:16:HIS:HB3	1:e:92:PHE:CZ	2.51	0.46
1:A:59:LEU:HD13	1:A:121:TRP:CD1	2.51	0.46
2:E:120:HIS:O	2:E:171:THR:N	2.49	0.46
3:F:140:LEU:CD2	3:F:150:LEU:HD13	2.45	0.46
2:H:15:ARG:HD2	2:H:68:ASP:O	2.16	0.46
2:H:38:TRP:CD1	2:H:81:ARG:NH2	2.84	0.46
2:H:112:LEU:HG	2:H:126:TRP:HB3	1.96	0.46
1:M:20:ASP:OD1	1:M:23:MET:CE	2.64	0.46
3:O:84:LEU:HD11	3:O:94:GLN:HB2	1.98	0.46
2:Q:107:MET:HG3	2:Q:108:ALA:N	2.30	0.46
1:S:117:PHE:HE1	1:S:121:TRP:CD1	2.33	0.46
1:V:19:LEU:HD21	2:W:136:GLU:HB2	1.98	0.46
1:V:88:ASN:ND2	2:W:73:THR:CG2	2.78	0.46
3:X:42:VAL:HG22	3:X:48:MET:HB2	1.97	0.46
3:X:197:TYR:O	3:X:223:HIS:CA	2.60	0.46
2:Z:13:ASN:C	2:Z:13:ASN:OD1	2.59	0.46
3:a:169:THR:HG22	3:a:197:TYR:CD2	2.50	0.46
1:b:88:ASN:N	1:b:88:ASN:ND2	2.62	0.46
1:e:14:LEU:O	1:e:14:LEU:HD23	2.15	0.46
3:C:61:THR:OG1	3:C:114:ARG:NH2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:109:GLN:NE2	3:C:119:GLN:NE2	2.64	0.46
3:F:142:LYS:HG2	3:F:148:LEU:HB3	1.98	0.46
1:J:95:GLU:OE1	2:K:75:VAL:HB	2.16	0.46
3:L:203:SER:C	3:L:215:TRP:CE3	2.94	0.46
3:O:167:TYR:CD2	3:O:176:THR:HB	2.51	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
3:X:149:GLU:HG2	3:X:151:ASN:HD21	1.81	0.46
2:Z:160:LEU:HA	2:Z:160:LEU:HD23	1.81	0.46
2:Z:183:ARG:HD3	2:Z:197:TRP:CE2	2.51	0.46
3:a:191:VAL:HB	3:a:197:TYR:HE1	1.80	0.46
1:b:12:LEU:C	1:b:12:LEU:HD23	2.40	0.46
3:d:115:GLU:OE1	3:d:118:ARG:HD3	2.16	0.46
1:e:114:ILE:O	1:e:117:PHE:HB3	2.16	0.46
2:f:199:GLN:OE1	2:f:200:PRO:HD2	2.15	0.46
3:g:115:GLU:HA	3:g:116:PRO:HD3	1.71	0.46
2:i:143:ALA:HA	2:i:197:TRP:HZ3	1.81	0.46
2:i:153:GLU:C	2:i:155:ALA:N	2.73	0.46
3:j:66:HIS:CE1	3:j:79:LYS:HG2	2.51	0.46
1:A:36:LEU:HA	1:A:39:MET:HE2	1.98	0.46
2:H:105:ARG:HG2	2:H:105:ARG:HH21	1.80	0.46
1:J:86:VAL:O	1:J:87:SER:C	2.58	0.46
2:K:139:LEU:N	2:K:187:LEU:HG	2.28	0.46
2:N:174:PRO:HA	2:N:205:THR:HG21	1.98	0.46
2:Q:69:SER:OG	2:Q:71:LYS:HE2	2.16	0.46
1:S:53:LEU:HD22	1:S:96:LEU:HB3	1.98	0.46
3:U:197:TYR:O	3:U:223:HIS:HA	2.15	0.46
3:X:128:ASN:O	3:X:212:ALA:HA	2.15	0.46
2:Z:136:GLU:OE2	3:a:207:PRO:HG3	2.16	0.46
2:c:8:PHE:HD1	2:c:22:TRP:HB2	1.80	0.46
3:d:205:PHE:CZ	3:d:209:CYS:HB2	2.50	0.46
1:e:62:GLU:C	1:e:65:PRO:HD2	2.39	0.46
3:g:171:TRP:NE1	3:g:195:LYS:HG2	2.31	0.46
2:i:105:ARG:HH21	2:i:196:PRO:HD3	1.80	0.46
2:E:121:ARG:NE	2:E:170:GLU:OE2	2.48	0.46
2:E:122:CYS:O	2:E:168:CYS:HA	2.16	0.46
1:G:67:GLU:OE2	1:G:83:ARG:HA	2.16	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
2:K:66:ALA:O	2:K:67:PRO:C	2.59	0.46
1:M:57:GLN:O	1:M:61:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:163:HIS:ND1	3:O:203:SER:OG	2.49	0.46
1:P:7:THR:CG2	1:P:132:LEU:HD13	2.46	0.46
2:Q:135:PHE:O	2:Q:136:GLU:C	2.58	0.46
2:T:138:HIS:NE2	3:U:182:TYR:CE2	2.83	0.46
1:Y:56:LEU:O	1:Y:59:LEU:N	2.49	0.46
2:Z:80:LEU:HD13	2:Z:98:PHE:CB	2.46	0.46
2:f:35:VAL:HA	2:f:81:ARG:O	2.16	0.46
2:f:150:HIS:HB3	2:f:154:GLU:HB2	1.97	0.46
2:f:164:GLN:HE21	3:g:178:GLN:HG2	1.81	0.46
3:g:62:ASN:ND2	4:g:300:NAG:C1	2.75	0.46
3:g:171:TRP:H	3:g:171:TRP:HD1	1.63	0.46
3:j:69:TYR:CZ	3:j:101:HIS:HB2	2.51	0.46
2:E:148:PRO:HG2	2:E:176:THR:HG23	1.97	0.46
3:L:109:GLN:NE2	3:L:119:GLN:NE2	2.63	0.46
1:M:121:TRP:O	1:M:124:PHE:HB3	2.16	0.46
2:N:114:VAL:HG11	2:N:117:VAL:HG13	1.97	0.46
1:P:62:GLU:OE2	1:P:65:PRO:HG3	2.15	0.46
3:R:68:TRP:CZ2	3:R:107:VAL:HG11	2.51	0.46
1:S:51:THR:HG22	1:S:51:THR:O	2.15	0.46
2:T:124:ILE:HG21	2:T:201:LEU:HD23	1.97	0.46
1:V:95:GLU:HG2	2:W:41:ARG:NH1	2.31	0.46
3:X:140:LEU:CG	3:X:222:ILE:HD11	2.45	0.46
3:X:180:VAL:HG12	3:X:181:ASP:N	2.31	0.46
2:Z:173:THR:HA	2:Z:174:PRO:HD3	1.87	0.46
3:d:204:ARG:HB2	3:d:215:TRP:CE3	2.50	0.46
3:g:128:ASN:CG	3:g:211:SER:HB2	2.40	0.46
3:j:102:LEU:C	3:j:104:GLN:H	2.24	0.46
1:A:35:LYS:HB2	1:A:35:LYS:HZ2	1.80	0.45
2:B:39:PRO:HB2	2:B:42:ARG:HB2	1.98	0.45
1:D:60:GLU:OE2	1:D:94:LEU:HD21	2.17	0.45
3:F:53:GLN:HG3	3:F:55:SER:OG	2.16	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
2:K:175:ASP:H	2:K:205:THR:HB	1.81	0.45
2:K:176:THR:HB	2:K:178:TYR:CE1	2.51	0.45
4:K:215:NAG:C4	4:K:216:NAG:C1	2.94	0.45
3:L:49:ASN:CG	4:L:233:NAG:C1	2.89	0.45
3:L:190:SER:O	3:L:191:VAL:HG13	2.16	0.45
3:O:61:THR:O	3:O:89:ILE:HG23	2.15	0.45
3:O:180:VAL:HG11	3:O:185:LYS:O	2.15	0.45
2:T:50:LEU:HD23	2:T:60:CYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:160:LEU:HD13	2:T:164:GLN:HB3	1.97	0.45
3:U:41:PHE:HB2	3:U:43:PHE:CE1	2.50	0.45
3:X:157:LEU:HD11	3:X:161:LEU:HD13	1.96	0.45
1:Y:57:GLN:NE2	1:Y:97:LYS:HZ2	2.13	0.45
2:Z:12:TYR:CZ	2:Z:14:SER:HA	2.50	0.45
3:d:63:LEU:CB	3:d:110:LEU:HD11	2.46	0.45
3:d:106:PHE:CE2	3:d:108:VAL:HG13	2.51	0.45
3:j:52:TRP:CZ3	3:j:92:GLY:HA2	2.51	0.45
1:A:13:GLN:NE2	2:B:75:VAL:HG12	2.32	0.45
2:E:179:GLU:HG2	2:E:202:ALA:CB	2.44	0.45
2:H:36:HIS:HE1	2:W:36:HIS:CE1	2.34	0.45
2:H:67:PRO:O	2:H:130:GLN:NE2	2.49	0.45
1:J:9:LYS:O	1:J:10:THR:C	2.58	0.45
2:K:83:LEU:CD2	2:K:92:VAL:HG22	2.46	0.45
3:L:138:LEU:HD23	3:L:222:ILE:HG22	1.98	0.45
3:L:159:HIS:ND1	3:L:159:HIS:O	2.49	0.45
1:P:36:LEU:O	1:P:39:MET:HB3	2.17	0.45
2:T:14:SER:O	2:T:15:ARG:HG2	2.16	0.45
2:T:201:LEU:HD12	2:T:202:ALA:N	2.31	0.45
3:U:115:GLU:OE1	3:U:118:ARG:HD3	2.15	0.45
3:U:206:ASN:HD22	3:U:211:SER:HA	1.81	0.45
2:W:112:LEU:HB3	2:W:201:LEU:HD22	1.99	0.45
2:Z:73:THR:HG23	2:Z:75:VAL:HG22	1.97	0.45
3:a:200:ARG:NE	3:a:218:TRP:CE2	2.84	0.45
1:b:117:PHE:CE1	1:b:121:TRP:HD1	2.34	0.45
2:c:81:ARG:HG2	2:c:95:ILE:HD13	1.98	0.45
2:c:121:ARG:C	2:c:172:LEU:HD12	2.42	0.45
1:h:60:GLU:O	1:h:63:LEU:HB2	2.16	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:J:18:LEU:HD11	1:J:122:ILE:HG23	1.99	0.45
3:L:185:LYS:H	3:L:185:LYS:HG3	1.47	0.45
1:M:118:LEU:O	1:M:119:ASN:C	2.59	0.45
2:N:170:GLU:HB2	3:O:190:SER:HB3	1.98	0.45
1:P:52:GLU:N	1:P:55:HIS:ND1	2.60	0.45
1:S:57:GLN:HG3	1:S:61:GLU:OE2	2.16	0.45
2:T:23:SER:CB	2:T:56:ALA:O	2.64	0.45
2:T:146:LEU:HD22	2:T:152:TRP:CE2	2.52	0.45
3:U:197:TYR:HB2	3:U:224:TRP:HB3	1.99	0.45
1:V:114:ILE:O	1:V:117:PHE:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:141:PHE:CD2	2:Z:184:VAL:HG22	2.52	0.45
1:e:121:TRP:O	1:e:122:ILE:C	2.60	0.45
2:f:98:PHE:HE1	2:f:103:ASN:HD22	1.60	0.45
2:f:188:GLN:HG2	2:f:189:GLY:H	1.81	0.45
3:g:169:THR:O	3:g:172:ASP:HB2	2.16	0.45
2:E:167:ILE:HD11	3:F:189:PRO:HB2	1.98	0.45
2:H:118:GLU:OE1	2:H:121:ARG:HD3	2.16	0.45
3:I:62:ASN:ND2	4:I:300:NAG:C1	2.68	0.45
2:N:17:GLN:NE2	2:N:63:ILE:HD11	2.32	0.45
2:N:172:LEU:HD22	2:N:178:TYR:CE1	2.52	0.45
2:W:183:ARG:HD2	2:W:194:TRP:HB3	1.98	0.45
1:b:18:LEU:CD2	3:d:208:LEU:HA	2.46	0.45
2:c:73:THR:HG23	2:c:75:VAL:H	1.80	0.45
3:d:131:ILE:HA	3:d:132:PRO:HD3	1.71	0.45
1:A:14:LEU:O	1:A:15:GLU:C	2.59	0.45
1:A:66:LEU:HD12	1:A:66:LEU:O	2.16	0.45
1:D:92:PHE:CZ	2:E:73:THR:CG2	3.00	0.45
3:I:87:GLU:O	3:I:89:ILE:HG13	2.15	0.45
3:I:100:ILE:O	3:I:100:ILE:HG22	2.16	0.45
3:I:198:THR:OG1	3:I:223:HIS:CE1	2.69	0.45
2:K:16:ALA:O	2:K:64:LEU:HB2	2.17	0.45
2:N:158:LEU:HD23	3:O:147:GLN:NE2	2.30	0.45
1:S:65:PRO:O	1:S:66:LEU:C	2.60	0.45
1:V:16:HIS:CG	2:W:134:TYR:HD2	2.34	0.45
2:W:76:ASP:HB2	2:W:100:PRO:HG2	1.98	0.45
2:Z:80:LEU:HD13	2:Z:98:PHE:HB3	1.98	0.45
3:a:165:VAL:HG22	3:a:201:VAL:CG2	2.46	0.45
2:c:159:THR:HG22	2:c:161:LYS:HG2	1.98	0.45
2:c:184:VAL:HG22	2:c:185:LYS:N	2.31	0.45
1:e:93:VAL:O	1:e:97:LYS:HG2	2.16	0.45
2:f:162:GLN:HE21	2:f:164:GLN:NE2	2.15	0.45
3:g:188:LEU:HG	3:g:191:VAL:HG12	1.99	0.45
3:g:200:ARG:CZ	3:g:218:TRP:CE2	3.00	0.45
2:i:34:GLN:HG2	2:i:48:CYS:O	2.16	0.45
3:j:131:ILE:HA	3:j:132:PRO:HD3	1.71	0.45
3:j:169:THR:HG22	3:j:171:TRP:H	1.81	0.45
3:j:171:TRP:CD1	3:j:171:TRP:N	2.84	0.45
3:C:106:PHE:O	3:C:124:LEU:N	2.48	0.45
2:E:37:ALA:HB2	2:E:62:LEU:CD1	2.46	0.45
3:F:62:ASN:ND2	4:F:300:NAG:C1	2.67	0.45
3:F:126:LEU:HD22	3:F:129:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:LEU:HD23	1:G:12:LEU:C	2.42	0.45
2:H:90:TRP:O	2:W:44:TRP:HA	2.16	0.45
2:K:38:TRP:CZ3	2:K:45:GLN:CB	3.00	0.45
2:K:44:TRP:HH2	2:K:64:LEU:HD13	1.81	0.45
3:L:112:ASP:OD1	3:L:114:ARG:HG3	2.17	0.45
2:N:104:LEU:HD12	2:N:188:GLN:O	2.17	0.45
1:P:67:GLU:HG3	1:P:86:VAL:HG21	1.99	0.45
3:R:62:ASN:ND2	4:R:300:NAG:H83	2.31	0.45
3:R:152:TRP:CZ3	3:R:201:VAL:HG21	2.51	0.45
1:S:28:ILE:HD13	1:S:39:MET:CE	2.47	0.45
2:T:104:LEU:HB2	2:T:192:THR:OG1	2.16	0.45
2:T:112:LEU:H	2:T:112:LEU:CD1	2.29	0.45
3:U:164:LEU:HA	3:U:179:SER:HA	1.99	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:Y:25:LEU:C	1:Y:27:GLY:H	2.25	0.45
1:Y:117:PHE:HE1	1:Y:121:TRP:HE1	1.63	0.45
2:Z:109:PRO:HG3	2:Z:184:VAL:HG23	1.99	0.45
2:Z:162:GLN:HG2	2:Z:164:GLN:HB2	1.98	0.45
2:f:50:LEU:HA	2:f:60:CYS:HB2	1.98	0.45
3:g:205:PHE:O	3:g:206:ASN:HB2	2.15	0.45
3:j:65:LEU:HD22	3:j:80:CYS:HB2	1.98	0.45
3:j:163:HIS:CD2	3:j:203:SER:OG	2.70	0.45
2:B:65:GLY:HA3	2:B:71:LYS:HE3	1.98	0.45
2:H:185:LYS:HD3	2:H:194:TRP:CE2	2.51	0.45
3:L:57:GLU:HG2	3:L:58:PRO:CD	2.46	0.45
3:L:148:LEU:O	3:L:188:LEU:N	2.50	0.45
1:Y:51:THR:O	1:Y:52:GLU:HG3	2.17	0.45
2:Z:44:TRP:CH2	2:Z:72:LEU:HD21	2.50	0.45
3:a:112:ASP:OD1	3:a:114:ARG:HG3	2.16	0.45
1:b:95:GLU:O	1:b:95:GLU:CG	2.64	0.45
2:f:153:GLU:O	2:f:155:ALA:N	2.49	0.45
3:j:171:TRP:CE2	3:j:195:LYS:HG2	2.52	0.45
3:F:35:LEU:CD2	3:F:118:ARG:CZ	2.95	0.45
3:F:102:LEU:C	3:F:104:GLN:N	2.75	0.45
3:F:138:LEU:C	3:F:222:ILE:HD13	2.42	0.45
3:L:42:VAL:HG13	3:L:45:VAL:HA	1.97	0.45
3:O:134:ALA:HA	3:O:135:PRO:HD3	1.73	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
2:T:161:LYS:HD3	3:U:185:LYS:NZ	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:148:LEU:C	3:X:148:LEU:HD12	2.42	0.45
3:d:38:VAL:HG22	3:d:52:TRP:HB3	1.98	0.45
1:e:65:PRO:O	1:e:69:VAL:HG23	2.17	0.45
3:g:59:GLN:HB3	3:g:114:ARG:NH2	2.32	0.45
1:h:95:GLU:HB2	2:i:41:ARG:HH12	1.81	0.45
3:j:52:TRP:CZ3	3:j:110:LEU:HD21	2.52	0.45
2:E:186:PRO:HD2	2:E:192:THR:CG2	2.46	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
3:I:61:THR:OG1	3:I:114:ARG:NH2	2.50	0.45
1:M:59:LEU:O	1:M:60:GLU:C	2.60	0.45
2:N:50:LEU:HD22	2:N:58:TRP:CB	2.41	0.45
2:N:107:MET:HE3	2:N:108:ALA:H	1.82	0.45
3:R:168:ARG:HG2	3:R:175:TRP:CE3	2.52	0.45
1:S:130:SER:C	1:S:132:LEU:H	2.24	0.45
2:W:13:ASN:HB3	2:W:17:GLN:HB3	1.99	0.45
2:W:142:GLU:O	2:W:182:VAL:HA	2.16	0.45
2:Z:36:HIS:HB3	2:Z:38:TRP:NE1	2.32	0.45
2:c:124:ILE:HD13	2:c:201:LEU:CD2	2.44	0.45
1:e:78:PHE:CD1	1:e:80:PHE:CZ	3.05	0.45
2:f:173:THR:HA	2:f:174:PRO:HD3	1.78	0.45
1:h:118:LEU:O	1:h:122:ILE:HG13	2.17	0.45
3:C:65:LEU:HD13	3:C:93:CYS:HB2	1.99	0.45
3:C:192:ASP:HB3	3:C:195:LYS:HD2	1.98	0.45
3:F:62:ASN:CB	2:c:113:GLN:HE22	2.27	0.45
3:O:48:MET:CE	3:O:95:LEU:HD12	2.46	0.45
3:O:186:PHE:CD1	3:O:187:SER:N	2.85	0.45
2:Q:142:GLU:HG3	2:Q:194:TRP:CH2	2.52	0.45
3:R:46:GLU:CD	3:R:133:TRP:HE1	2.25	0.45
2:W:70:GLN:CD	2:W:134:TYR:CE1	2.94	0.45
3:X:171:TRP:H	3:X:171:TRP:HD1	1.64	0.45
3:a:152:TRP:NE1	3:a:163:HIS:CD2	2.82	0.45
3:d:142:LYS:HG3	3:d:142:LYS:O	2.15	0.45
2:E:155:ALA:HA	2:E:156:PRO:HD3	1.71	0.44
3:F:42:VAL:O	3:F:130:VAL:HA	2.17	0.44
2:H:143:ALA:HB1	2:H:180:PHE:CE1	2.52	0.44
1:J:125:CYS:O	1:J:129:ILE:CG2	2.58	0.44
2:K:98:PHE:HE2	2:K:100:PRO:HG3	1.82	0.44
1:M:69:VAL:HG11	1:M:114:ILE:HD12	1.99	0.44
2:T:38:TRP:HA	2:T:39:PRO:HD3	1.70	0.44
2:T:82:VAL:CG1	2:T:94:ALA:H	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:118:GLU:OE1	2:T:121:ARG:HD3	2.17	0.44
1:V:127:SER:HA	3:X:103:TYR:CE1	2.51	0.44
2:W:117:VAL:HG12	2:W:118:GLU:N	2.31	0.44
1:Y:86:VAL:O	1:Y:87:SER:C	2.60	0.44
3:a:202:ARG:HG2	3:a:218:TRP:CH2	2.52	0.44
1:e:55:HIS:C	1:e:57:GLN:N	2.74	0.44
1:e:68:GLU:OE2	1:e:68:GLU:HA	2.17	0.44
1:h:93:VAL:O	1:h:97:LYS:HG2	2.17	0.44
2:i:146:LEU:HD22	2:i:152:TRP:CE2	2.52	0.44
4:E:215:NAG:O4	4:F:233:NAG:C2	2.66	0.44
3:F:45:VAL:O	3:F:45:VAL:CG1	2.64	0.44
1:G:46:MET:HE3	1:G:120:ARG:HG2	1.98	0.44
2:H:72:LEU:HD13	2:H:100:PRO:HG2	1.98	0.44
3:I:160:CYS:C	3:I:161:LEU:HD12	2.42	0.44
3:I:168:ARG:HG2	3:I:175:TRP:CE3	2.52	0.44
1:J:42:PHE:CD2	1:J:69:VAL:HG22	2.51	0.44
1:J:126:GLN:NE2	3:L:207:PRO:O	2.50	0.44
2:K:81:ARG:NE	2:K:95:ILE:HG22	2.30	0.44
3:R:192:ASP:OD1	3:R:194:GLN:HB2	2.17	0.44
2:T:167:ILE:HG21	2:T:180:PHE:CZ	2.52	0.44
1:Y:105:CYS:SG	1:Y:106:GLU:N	2.90	0.44
3:a:42:VAL:HB	3:a:130:VAL:HA	1.99	0.44
1:b:40:LEU:HD23	1:b:113:THR:HB	1.99	0.44
2:c:158:LEU:HD13	2:c:167:ILE:CD1	2.47	0.44
1:e:19:LEU:HD21	2:f:136:GLU:HB2	1.99	0.44
1:e:114:ILE:HG23	1:e:115:VAL:N	2.32	0.44
3:g:164:LEU:HD12	3:g:164:LEU:C	2.41	0.44
3:j:49:ASN:OD1	3:j:94:GLN:HB2	2.18	0.44
3:F:143:LEU:HD23	3:F:149:GLU:OE1	2.17	0.44
3:I:188:LEU:HG	3:I:191:VAL:HG13	1.99	0.44
1:J:9:LYS:HB3	1:J:9:LYS:HE2	1.75	0.44
1:J:126:GLN:HB3	3:L:209:CYS:C	2.43	0.44
2:K:204:ARG:HG2	2:K:205:THR:N	2.31	0.44
1:M:69:VAL:CG1	1:M:114:ILE:HD12	2.47	0.44
2:N:36:HIS:HB3	2:N:38:TRP:NE1	2.33	0.44
2:N:37:ALA:HB1	2:N:78:VAL:HG11	2.00	0.44
2:N:138:HIS:HB3	2:N:187:LEU:HD12	1.99	0.44
3:O:163:HIS:CE1	3:O:203:SER:OG	2.70	0.44
2:Q:73:THR:O	2:Q:76:ASP:HB2	2.16	0.44
3:R:49:ASN:ND2	4:R:234:NAG:C1	2.80	0.44
1:S:25:LEU:C	1:S:27:GLY:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:70:LEU:HB3	1:V:82:PRO:HB3	1.99	0.44
1:b:56:LEU:C	1:b:58:CYS:N	2.76	0.44
3:g:34:PRO:N	3:g:118:ARG:HH11	2.15	0.44
3:C:102:LEU:HA	3:C:126:LEU:HB2	1.98	0.44
2:E:162:GLN:NE2	3:F:187:SER:HB2	2.32	0.44
3:F:126:LEU:O	3:F:129:LEU:N	2.47	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:L:62:ASN:HD21	4:L:300:NAG:H2	1.82	0.44
3:R:44:ASN:ND2	3:R:133:TRP:CD1	2.86	0.44
3:U:167:TYR:HA	3:U:198:THR:O	2.17	0.44
1:V:59:LEU:HB2	1:V:121:TRP:CZ2	2.53	0.44
3:X:181:ASP:C	3:X:181:ASP:OD2	2.60	0.44
3:a:165:VAL:O	3:a:177:GLU:HA	2.18	0.44
3:a:166:GLN:HB2	3:a:200:ARG:HG2	1.98	0.44
1:b:46:MET:O	1:b:107:TYR:HB3	2.16	0.44
2:B:37:ALA:HB2	2:B:62:LEU:HD13	1.98	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
3:I:84:LEU:HD12	3:I:84:LEU:N	2.33	0.44
1:J:53:LEU:CD1	1:J:96:LEU:HB3	2.32	0.44
2:K:22:TRP:O	2:K:58:TRP:N	2.51	0.44
1:M:123:THR:O	1:M:124:PHE:C	2.57	0.44
3:O:46:GLU:O	3:O:47:TYR:HB3	2.17	0.44
2:T:17:GLN:HG2	2:T:63:ILE:CD1	2.48	0.44
3:X:106:PHE:CE2	3:X:108:VAL:CG2	3.00	0.44
3:X:131:ILE:HD11	3:X:214:HIS:HB2	2.00	0.44
1:Y:84:ASP:OD2	2:Z:71:LYS:NZ	2.47	0.44
2:Z:117:VAL:C	2:Z:118:GLU:HG3	2.42	0.44
3:a:161:LEU:CD2	3:a:205:PHE:HA	2.46	0.44
1:b:18:LEU:HD23	3:d:208:LEU:HD22	2.00	0.44
3:d:164:LEU:HD12	3:d:165:VAL:H	1.83	0.44
1:h:14:LEU:CD2	1:h:128:ILE:HB	2.48	0.44
2:i:188:GLN:HG2	2:i:189:GLY:N	2.31	0.44
3:j:169:THR:OG1	3:j:197:TYR:CE2	2.71	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
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
1:J:36:LEU:HA	1:J:39:MET:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:89:ILE:HG22	3:L:90:THR:H	1.83	0.44
1:M:126:GLN:CD	3:O:210:GLY:HA2	2.43	0.44
3:O:117:ARG:HH21	2:i:207:PRO:HG2	1.83	0.44
2:Q:136:GLU:HG3	2:Q:137:ARG:H	1.82	0.44
2:Q:141:PHE:HA	2:Q:183:ARG:O	2.17	0.44
3:R:102:LEU:HD22	3:R:127:GLN:HA	1.99	0.44
1:S:80:PHE:CD1	1:S:80:PHE:C	2.96	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
1:V:123:THR:O	1:V:124:PHE:C	2.61	0.44
2:W:104:LEU:O	2:W:192:THR:HG23	2.18	0.44
3:X:147:GLN:HG2	3:X:189:PRO:O	2.18	0.44
1:Y:67:GLU:HG2	1:Y:71:ASN:ND2	2.32	0.44
2:Z:98:PHE:C	2:Z:98:PHE:CD2	2.95	0.44
1:b:115:VAL:O	1:b:119:ASN:HB2	2.18	0.44
2:c:98:PHE:C	2:c:98:PHE:CD2	2.96	0.44
3:d:68:TRP:HB3	3:d:77:VAL:HA	1.99	0.44
1:e:65:PRO:O	1:e:68:GLU:N	2.47	0.44
2:f:158:LEU:HD13	2:f:167:ILE:HD11	1.98	0.44
1:h:28:ILE:HG22	1:h:28:ILE:O	2.18	0.44
2:B:44:TRP:CZ3	2:B:64:LEU:HD22	2.53	0.44
3:I:65:LEU:HD13	3:I:93:CYS:CB	2.48	0.44
3:I:140:LEU:HD13	3:I:224:TRP:CE3	2.53	0.44
3:L:57:GLU:HG3	3:L:58:PRO:HD2	1.97	0.44
2:N:83:LEU:CD2	2:N:92:VAL:HG22	2.48	0.44
3:O:117:ARG:NH2	2:i:207:PRO:HG2	2.33	0.44
2:T:80:LEU:HD11	2:T:98:PHE:CG	2.53	0.44
2:T:84:CYS:SG	2:T:93:MET:HG3	2.58	0.44
1:V:68:GLU:O	1:V:71:ASN:N	2.51	0.44
1:Y:69:VAL:HA	1:Y:72:LEU:HG	2.00	0.44
1:b:56:LEU:O	1:b:57:GLN:C	2.60	0.44
2:c:185:LYS:HD2	2:c:192:THR:HG22	2.00	0.44
3:d:167:TYR:CD2	3:d:176:THR:HB	2.52	0.44
1:e:47:PRO:HA	1:e:107:TYR:HA	2.00	0.44
2:f:8:PHE:HD1	2:f:22:TRP:HB2	1.83	0.44
3:g:38:VAL:N	3:g:122:GLN:HE22	2.14	0.44
3:j:64:THR:OG1	3:j:111:GLN:HB3	2.17	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
3:F:102:LEU:O	3:F:104:GLN:N	2.50	0.44
2:H:132:SER:OG	2:H:134:TYR:HD1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:36:HIS:HB3	2:N:38:TRP:CD1	2.53	0.44
3:O:62:ASN:HD21	4:O:300:NAG:H2	1.83	0.44
1:S:28:ILE:HD13	1:S:39:MET:HE2	1.99	0.44
2:T:22:TRP:O	2:T:58:TRP:HE3	2.00	0.44
2:T:158:LEU:HD23	3:U:147:GLN:NE2	2.33	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:80:CYS:HB3	3:X:83:TYR:CE1	2.53	0.44
3:X:166:GLN:HB3	3:X:175:TRP:HE3	1.81	0.44
1:Y:130:SER:HB3	3:a:103:TYR:HE1	1.83	0.44
3:a:109:GLN:HE21	3:a:121:THR:HG22	1.81	0.44
3:a:188:LEU:HD11	3:a:199:PHE:HE1	1.83	0.44
2:c:83:LEU:CB	2:c:90:TRP:CE3	3.01	0.44
3:d:171:TRP:CD1	3:d:171:TRP:N	2.86	0.44
3:d:205:PHE:O	3:d:206:ASN:HB2	2.18	0.44
1:e:44:PHE:HE1	1:e:65:PRO:CB	2.21	0.44
1:e:92:PHE:CE1	2:f:73:THR:OG1	2.66	0.44
2:f:70:GLN:NE2	2:f:72:LEU:O	2.50	0.44
1:h:16:HIS:CE1	2:i:134:TYR:HB3	2.53	0.44
2:i:12:TYR:HE2	2:i:101:PHE:CE1	2.35	0.44
2:i:110:ILE:CD1	2:i:127:GLU:HB2	2.47	0.44
2:i:153:GLU:N	2:i:153:GLU:CD	2.76	0.44
3:j:44:ASN:C	3:j:45:VAL:HG23	2.41	0.44
3:j:62:ASN:HD21	4:j:300:NAG:C1	2.30	0.44
1:A:18:LEU:CD1	1:A:122:ILE:HG23	2.47	0.44
1:A:23:MET:SD	2:B:133:HIS:CE1	3.11	0.44
1:D:24:ILE:HD11	1:D:85:VAL:HG22	2.00	0.44
2:E:120:HIS:CE1	2:E:174:PRO:CG	3.00	0.44
1:G:126:GLN:NE2	3:I:210:GLY:O	2.51	0.44
1:J:31:TYR:CD2	1:J:36:LEU:HB2	2.52	0.44
2:K:74:THR:HA	2:K:101:PHE:CD1	2.53	0.44
2:K:124:ILE:O	2:K:166:TRP:HA	2.17	0.44
3:R:206:ASN:CG	3:R:207:PRO:HA	2.42	0.44
1:S:88:ASN:ND2	2:T:42:ARG:HH22	2.16	0.44
3:U:146:SER:O	3:U:191:VAL:HG22	2.18	0.44
1:V:64:LYS:N	1:V:65:PRO:HD2	2.33	0.44
1:Y:28:ILE:HD13	1:Y:39:MET:HE3	2.00	0.44
2:Z:84:CYS:SG	2:Z:93:MET:HG3	2.58	0.44
3:a:144:SER:HB3	3:a:147:GLN:HB2	2.00	0.44
3:a:181:ASP:OD2	3:a:183:ARG:HG3	2.17	0.44
3:a:204:ARG:HH21	3:a:215:TRP:HE1	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:118:LEU:O	1:b:122:ILE:HG13	2.18	0.44
1:e:113:THR:O	1:e:114:ILE:C	2.61	0.44
1:h:22:GLN:O	1:h:25:LEU:HB3	2.18	0.44
1:h:76:LYS:HD2	1:h:76:LYS:O	2.18	0.44
2:i:68:ASP:OD1	2:i:130:GLN:HG2	2.18	0.44
2:i:101:PHE:HA	2:i:104:LEU:CD2	2.40	0.44
2:B:20:CYS:O	2:B:59:ALA:HA	2.18	0.43
1:D:114:ILE:CG2	1:D:115:VAL:N	2.80	0.43
2:E:106:LEU:HD13	2:E:186:PRO:HG3	2.00	0.43
2:E:162:GLN:HE22	3:F:187:SER:HB2	1.83	0.43
3:F:115:GLU:HG3	3:F:115:GLU:O	2.17	0.43
3:F:157:LEU:HD13	3:F:205:PHE:CD1	2.52	0.43
2:H:104:LEU:O	2:H:192:THR:HG23	2.18	0.43
3:L:182:TYR:HE1	3:L:183:ARG:NH1	2.16	0.43
1:M:81:ASP:OD1	1:M:82:PRO:HD2	2.18	0.43
3:O:114:ARG:HB3	2:i:203:PHE:HA	2.00	0.43
2:Q:64:LEU:HD12	2:Q:72:LEU:HG	2.00	0.43
1:S:9:LYS:HE2	1:S:9:LYS:HB3	1.74	0.43
2:T:15:ARG:HD2	2:T:68:ASP:OD1	2.17	0.43
2:T:106:LEU:HA	2:T:106:LEU:HD23	1.78	0.43
3:U:38:VAL:HG21	3:U:110:LEU:CD1	2.48	0.43
2:W:112:LEU:HD12	2:W:126:TRP:CB	2.48	0.43
2:W:153:GLU:CD	2:W:153:GLU:N	2.76	0.43
3:X:157:LEU:HD11	3:X:161:LEU:HD22	1.98	0.43
3:X:169:THR:HA	3:X:196:ARG:O	2.18	0.43
2:Z:143:ALA:HA	2:Z:181:GLN:O	2.18	0.43
2:f:104:LEU:HD13	2:f:135:PHE:CE1	2.53	0.43
2:i:203:PHE:CD1	2:i:203:PHE:O	2.71	0.43
3:j:138:LEU:CD2	3:j:222:ILE:HG12	2.48	0.43
1:A:89:ILE:O	1:A:93:VAL:HG23	2.18	0.43
3:C:116:PRO:HG2	2:Z:205:THR:O	2.17	0.43
1:D:10:THR:C	1:D:14:LEU:HD12	2.42	0.43
4:F:234:NAG:H61	4:F:235:NAG:O7	2.18	0.43
2:H:98:PHE:CE1	2:H:103:ASN:HB2	2.53	0.43
1:J:57:GLN:O	1:J:61:GLU:HG3	2.18	0.43
2:N:39:PRO:HB2	2:N:42:ARG:HB2	2.00	0.43
3:O:138:LEU:HD12	3:O:138:LEU:N	2.31	0.43
3:O:154:ASN:ND2	3:O:163:HIS:HE1	2.14	0.43
2:Q:22:TRP:O	2:Q:58:TRP:HE3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:158:ASN:C	3:R:160:CYS:H	2.26	0.43
2:T:129:SER:OG	2:T:130:GLN:N	2.51	0.43
2:W:150:HIS:HD2	2:W:154:GLU:OE1	2.00	0.43
3:X:206:ASN:HA	3:X:210:GLY:O	2.18	0.43
3:a:135:PRO:HG2	3:a:201:VAL:O	2.19	0.43
2:f:35:VAL:HG13	2:f:81:ARG:O	2.18	0.43
2:f:60:CYS:SG	2:f:61:ASN:N	2.90	0.43
3:g:169:THR:HA	3:g:196:ARG:O	2.18	0.43
1:h:25:LEU:HD22	1:h:122:ILE:HD12	1.99	0.43
2:i:106:LEU:HD13	2:i:186:PRO:HD3	1.99	0.43
1:A:35:LYS:HD2	1:A:38:ARG:NH2	2.30	0.43
1:D:66:LEU:HD11	1:D:70:LEU:HD11	1.99	0.43
2:E:13:ASN:HB2	2:E:17:GLN:HB3	2.00	0.43
3:F:114:ARG:HB3	2:c:202:ALA:O	2.18	0.43
3:F:159:HIS:O	3:F:159:HIS:CG	2.71	0.43
2:H:8:PHE:CE1	2:H:82:VAL:CG2	3.01	0.43
2:H:115:VAL:HB	2:H:123:ASN:O	2.18	0.43
3:I:42:VAL:CG1	3:I:130:VAL:HG22	2.48	0.43
1:J:36:LEU:O	1:J:39:MET:HB3	2.17	0.43
2:K:158:LEU:HA	3:L:147:GLN:NE2	2.33	0.43
2:K:161:LYS:HE2	3:L:185:LYS:HD3	2.00	0.43
3:L:224:TRP:O	3:L:224:TRP:CD1	2.72	0.43
2:N:63:ILE:HD13	2:N:63:ILE:HA	1.83	0.43
3:U:65:LEU:HD23	3:U:65:LEU:C	2.43	0.43
2:W:142:GLU:HG3	2:W:194:TRP:CH2	2.54	0.43
1:Y:51:THR:C	1:Y:52:GLU:HG3	2.43	0.43
2:Z:138:HIS:HB3	2:Z:187:LEU:CD1	2.32	0.43
1:b:44:PHE:CZ	1:b:69:VAL:HG21	2.53	0.43
2:c:39:PRO:CB	2:c:42:ARG:HB2	2.48	0.43
3:d:77:VAL:HG12	3:d:78:GLN:N	2.33	0.43
2:f:155:ALA:HA	2:f:156:PRO:HD3	1.90	0.43
1:A:41:THR:O	1:A:42:PHE:C	2.60	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
2:N:146:LEU:HD11	2:N:151:THR:HA	1.99	0.43
2:N:183:ARG:HG3	2:N:194:TRP:CE3	2.54	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
2:T:137:ARG:HE	2:T:137:ARG:HB2	1.61	0.43
3:U:47:TYR:HE1	3:U:49:ASN:HD21	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:50:LEU:CD2	2:W:60:CYS:HB2	2.49	0.43
1:Y:31:TYR:HD2	1:Y:36:LEU:HB2	1.82	0.43
3:d:62:ASN:O	3:d:113:PRO:HD3	2.18	0.43
1:e:36:LEU:O	1:e:39:MET:N	2.50	0.43
2:f:6:SER:N	2:f:24:GLN:OE1	2.51	0.43
1:h:86:VAL:O	1:h:87:SER:C	2.59	0.43
2:i:160:LEU:HD22	2:i:162:GLN:HE22	1.83	0.43
3:j:202:ARG:HD3	3:j:218:TRP:CZ2	2.53	0.43
1:A:19:LEU:HA	1:A:19:LEU:HD23	1.61	0.43
3:C:140:LEU:HD11	3:C:199:PHE:CE1	2.53	0.43
1:D:82:PRO:O	1:D:83:ARG:C	2.61	0.43
1:D:82:PRO:O	1:D:85:VAL:HG12	2.17	0.43
1:D:122:ILE:O	1:D:125:CYS:HB2	2.19	0.43
3:I:106:PHE:CE2	3:I:108:VAL:CG1	3.01	0.43
1:M:55:HIS:O	1:M:57:GLN:N	2.51	0.43
2:N:193:THR:HG22	2:N:194:TRP:N	2.33	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:17:GLN:HG2	2:T:63:ILE:HD13	1.99	0.43
2:T:80:LEU:HD12	2:T:98:PHE:HB2	2.00	0.43
2:T:104:LEU:O	2:T:192:THR:HG23	2.19	0.43
2:T:159:THR:CG2	2:T:161:LYS:HE3	2.44	0.43
1:b:127:SER:O	1:b:130:SER:HB3	2.18	0.43
3:d:117:ARG:HD3	3:d:117:ARG:HA	1.71	0.43
2:f:104:LEU:HB2	2:f:192:THR:OG1	2.18	0.43
3:g:179:SER:O	3:g:180:VAL:HG23	2.18	0.43
2:B:119:THR:HG22	2:B:206:LYS:HB2	2.00	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
1:D:62:GLU:HG3	1:D:117:PHE:CE1	2.47	0.43
3:F:130:VAL:O	3:F:132:PRO:HD3	2.18	0.43
2:H:98:PHE:CE2	2:H:100:PRO:HA	2.54	0.43
3:I:42:VAL:HG11	3:I:130:VAL:HG22	2.01	0.43
3:I:132:PRO:HB3	3:I:161:LEU:HD21	2.01	0.43
3:I:188:LEU:HG	3:I:191:VAL:CG1	2.48	0.43
2:K:68:ASP:O	2:K:69:SER:C	2.61	0.43
2:K:138:HIS:HA	2:K:187:LEU:CD1	2.48	0.43
3:L:183:ARG:HD2	3:L:183:ARG:HA	1.77	0.43
2:N:70:GLN:NE2	2:N:134:TYR:CE1	2.86	0.43
3:O:156:PHE:O	3:O:157:LEU:C	2.60	0.43
3:O:164:LEU:HD12	3:O:165:VAL:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:153:GLU:H	2:T:153:GLU:CD	2.25	0.43
1:V:66:LEU:O	1:V:67:GLU:C	2.62	0.43
1:V:69:VAL:HA	1:V:72:LEU:CD2	2.44	0.43
3:X:200:ARG:HG3	3:X:218:TRP:CZ3	2.53	0.43
3:d:149:GLU:HA	3:d:186:PHE:O	2.19	0.43
2:f:158:LEU:HD22	3:g:189:PRO:HB2	2.00	0.43
1:h:66:LEU:HD23	1:h:66:LEU:C	2.44	0.43
3:C:62:ASN:HD21	4:C:300:NAG:C2	2.32	0.43
2:E:143:ALA:O	2:E:158:LEU:HG	2.18	0.43
1:G:22:GLN:O	1:G:23:MET:C	2.59	0.43
1:M:55:HIS:C	1:M:57:GLN:N	2.76	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
1:S:16:HIS:CE1	2:T:134:TYR:HB3	2.54	0.43
2:T:112:LEU:C	2:T:201:LEU:HD22	2.44	0.43
3:X:62:ASN:ND2	4:X:300:NAG:H83	2.34	0.43
2:Z:137:ARG:NH1	3:a:179:SER:OG	2.50	0.43
3:a:131:ILE:HA	3:a:132:PRO:HD3	1.72	0.43
3:g:38:VAL:HG23	3:g:110:LEU:CD2	2.47	0.43
2:i:146:LEU:HB3	2:i:179:GLU:HB2	2.00	0.43
3:j:146:SER:O	3:j:191:VAL:HG22	2.19	0.43
3:F:167:TYR:CZ	3:F:176:THR:HB	2.54	0.43
2:H:201:LEU:HD12	2:H:202:ALA:H	1.82	0.43
3:I:136:GLU:C	3:I:137:ASN:HD22	2.26	0.43
1:J:113:THR:HG23	1:J:116:GLU:OE1	2.18	0.43
2:K:98:PHE:CZ	2:K:100:PRO:HA	2.54	0.43
3:L:130:VAL:O	3:L:131:ILE:HD13	2.19	0.43
3:L:165:VAL:O	3:L:177:GLU:HA	2.18	0.43
3:O:181:ASP:OD2	3:O:181:ASP:N	2.52	0.43
1:S:130:SER:C	1:S:132:LEU:N	2.74	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
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
1:b:31:TYR:HD1	1:b:77:ASN:OD1	2.01	0.43
3:d:188:LEU:HD12	3:d:188:LEU:HA	1.87	0.43
3:d:204:ARG:HG2	3:d:205:PHE:N	2.34	0.43
2:f:10:CYS:HA	2:f:19:SER:O	2.19	0.43
3:g:103:TYR:N	3:g:103:TYR:CD2	2.84	0.43
2:i:142:GLU:O	2:i:182:VAL:HA	2.18	0.43
2:i:160:LEU:HA	3:j:187:SER:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:THR:CG2	1:A:132:LEU:HD13	2.48	0.43
2:E:120:HIS:CE1	2:E:174:PRO:HG3	2.54	0.43
1:G:16:HIS:HB3	2:H:134:TYR:CD2	2.54	0.43
1:G:60:GLU:CD	1:G:94:LEU:HD21	2.43	0.43
2:H:72:LEU:HA	2:H:72:LEU:HD23	1.67	0.43
2:K:188:GLN:HG2	2:K:189:GLY:N	2.33	0.43
3:L:147:GLN:HG2	3:L:189:PRO:HA	2.01	0.43
2:N:11:PHE:HD1	2:N:105:ARG:HD3	1.83	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
3:U:165:VAL:HG22	3:U:201:VAL:HG22	2.00	0.43
1:V:130:SER:C	1:V:132:LEU:H	2.27	0.43
2:W:80:LEU:HD11	2:W:98:PHE:HB3	1.99	0.43
1:Y:130:SER:HB2	3:a:103:TYR:OH	2.19	0.43
2:Z:119:THR:HG22	2:Z:206:LYS:O	2.19	0.43
2:Z:150:HIS:CD2	2:Z:154:GLU:OE1	2.72	0.43
3:a:102:LEU:O	3:a:103:TYR:HB2	2.18	0.43
3:a:117:ARG:HD3	3:a:117:ARG:HA	1.70	0.43
3:d:131:ILE:HD13	3:d:215:TRP:O	2.18	0.43
1:e:55:HIS:HD2	1:e:103:PHE:CZ	2.36	0.43
3:g:169:THR:CG2	3:g:195:LYS:HB3	2.49	0.43
1:h:68:GLU:O	1:h:69:VAL:C	2.61	0.43
2:i:36:HIS:HB3	2:i:38:TRP:CD1	2.53	0.43
2:i:121:ARG:HD2	3:j:195:LYS:NZ	2.34	0.43
1:A:81:ASP:HA	1:A:82:PRO:HD3	1.88	0.43
2:B:138:HIS:CE1	3:C:182:TYR:CE2	3.07	0.43
3:C:84:LEU:HD22	4:C:234:NAG:C6	2.40	0.43
3:F:128:ASN:ND2	3:F:211:SER:HB2	2.34	0.43
1:G:91:VAL:HG21	2:H:42:ARG:NH2	2.34	0.43
3:I:140:LEU:CD1	3:I:224:TRP:HB2	2.49	0.43
1:M:23:MET:SD	2:N:133:HIS:CE1	3.11	0.43
3:O:159:HIS:HA	3:O:182:TYR:HB2	2.01	0.43
1:P:126:GLN:OE1	3:R:210:GLY:HA2	2.19	0.43
2:T:83:LEU:HB3	2:T:90:TRP:HE3	1.84	0.43
3:U:138:LEU:HD12	3:U:138:LEU:N	2.34	0.43
2:W:155:ALA:HA	2:W:156:PRO:HD3	1.87	0.43
3:d:67:TYR:CD1	3:d:67:TYR:C	2.97	0.43
3:g:62:ASN:ND2	4:g:300:NAG:H83	2.34	0.43
3:g:63:LEU:HA	3:g:111:GLN:O	2.19	0.43
1:h:88:ASN:ND2	2:i:42:ARG:HH22	2.17	0.43
2:i:38:TRP:HA	2:i:39:PRO:HD3	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:C	1:A:27:GLY:H	2.28	0.42
1:A:61:GLU:HB2	1:A:107:TYR:OH	2.19	0.42
2:B:111:SER:HB2	2:B:127:GLU:HG3	2.00	0.42
1:G:25:LEU:C	1:G:27:GLY:H	2.25	0.42
1:G:128:ILE:HD13	1:G:128:ILE:N	2.34	0.42
1:J:23:MET:HE3	1:J:23:MET:HB3	1.75	0.42
1:J:118:LEU:N	1:J:118:LEU:HD23	2.34	0.42
2:K:16:ALA:HB1	2:K:65:GLY:N	2.33	0.42
2:N:10:CYS:O	2:N:11:PHE:HD2	2.01	0.42
2:N:179:GLU:HA	2:N:201:LEU:O	2.18	0.42
2:T:119:THR:HG22	2:T:174:PRO:HB3	2.01	0.42
2:T:158:LEU:HD13	2:T:167:ILE:CD1	2.47	0.42
3:U:45:VAL:HG21	3:U:157:LEU:HD11	2.00	0.42
3:U:67:TYR:CD1	3:U:67:TYR:C	2.97	0.42
2:W:95:ILE:CG1	2:W:96:GLN:N	2.82	0.42
1:Y:66:LEU:O	1:Y:70:LEU:HG	2.19	0.42
2:Z:11:PHE:HA	2:Z:103:ASN:HB3	2.01	0.42
1:b:23:MET:SD	1:b:80:PHE:HB3	2.58	0.42
1:b:114:ILE:HG12	1:b:118:LEU:HG	2.01	0.42
2:c:52:PRO:HA	2:c:58:TRP:HA	2.00	0.42
1:e:45:TYR:CE2	1:e:62:GLU:OE1	2.71	0.42
3:g:205:PHE:CD2	3:g:210:GLY:HA3	2.54	0.42
1:h:12:LEU:HD23	1:h:12:LEU:C	2.44	0.42
3:j:100:ILE:O	3:j:100:ILE:HG22	2.18	0.42
2:B:185:LYS:HB2	2:B:194:TRP:CE3	2.53	0.42
1:D:63:LEU:HD23	1:D:66:LEU:HD23	1.99	0.42
3:F:188:LEU:HA	3:F:189:PRO:HD2	1.86	0.42
3:I:48:MET:CB	3:I:100:ILE:HD11	2.49	0.42
3:I:131:ILE:HA	3:I:132:PRO:HD3	1.84	0.42
3:I:188:LEU:HA	3:I:189:PRO:HD2	1.82	0.42
3:L:126:LEU:HA	3:L:129:LEU:HD12	2.01	0.42
1:M:13:GLN:CD	2:N:75:VAL:HG12	2.43	0.42
1:M:82:PRO:O	1:M:85:VAL:HG12	2.19	0.42
2:N:86:GLU:OE1	2:N:91:ARG:HD2	2.19	0.42
3:O:197:TYR:HB2	3:O:224:TRP:HB3	2.01	0.42
1:P:62:GLU:OE2	1:P:62:GLU:HA	2.19	0.42
2:Q:87:GLY:C	2:Q:89:ARG:N	2.75	0.42
3:R:109:GLN:NE2	3:R:119:GLN:NE2	2.68	0.42
1:S:62:GLU:C	1:S:65:PRO:HD2	2.44	0.42
1:S:91:VAL:HG12	2:T:75:VAL:CG2	2.49	0.42
2:T:83:LEU:HB3	2:T:90:TRP:CE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:128:ILE:CG2	2:T:184:VAL:HG21	2.46	0.42
3:U:206:ASN:ND2	3:U:207:PRO:HA	2.34	0.42
2:W:35:VAL:HA	2:W:81:ARG:O	2.19	0.42
3:X:131:ILE:HA	3:X:132:PRO:HD3	1.69	0.42
1:Y:56:LEU:C	1:Y:58:CYS:N	2.75	0.42
1:b:85:VAL:HG13	1:b:86:VAL:N	2.33	0.42
1:e:56:LEU:HB2	1:e:97:LYS:HD3	2.00	0.42
3:g:80:CYS:HB3	3:g:83:TYR:CZ	2.53	0.42
2:i:143:ALA:HB2	2:i:182:VAL:HG23	2.01	0.42
1:A:6:SER:C	1:A:8:LYS:N	2.74	0.42
3:C:204:ARG:HB2	3:C:215:TRP:CE3	2.54	0.42
1:D:23:MET:HE3	1:D:80:PHE:CB	2.50	0.42
1:D:60:GLU:O	1:D:63:LEU:HD12	2.19	0.42
2:E:63:ILE:C	2:E:64:LEU:HD23	2.44	0.42
2:E:124:ILE:O	2:E:124:ILE:HG22	2.17	0.42
3:F:68:TRP:HE3	3:F:77:VAL:HG13	1.84	0.42
1:G:130:SER:C	1:G:132:LEU:H	2.27	0.42
1:J:14:LEU:HD12	1:J:14:LEU:HA	1.89	0.42
1:J:37:THR:O	1:J:41:THR:HG23	2.20	0.42
3:L:167:TYR:N	3:L:176:THR:O	2.47	0.42
1:M:53:LEU:HD23	1:M:53:LEU:HA	1.79	0.42
2:N:13:ASN:OD1	2:N:13:ASN:C	2.61	0.42
2:N:42:ARG:HA	2:N:42:ARG:HD3	1.88	0.42
2:N:82:VAL:O	2:N:93:MET:N	2.42	0.42
2:N:114:VAL:O	2:N:114:VAL:HG12	2.18	0.42
2:N:115:VAL:HG11	4:N:215:NAG:O5	2.19	0.42
3:O:173:HIS:HB3	1:V:45:TYR:CZ	2.54	0.42
2:Q:72:LEU:CD1	2:Q:78:VAL:CG2	2.96	0.42
2:T:120:HIS:HA	2:T:172:LEU:O	2.19	0.42
1:V:63:LEU:C	1:V:65:PRO:HD2	2.44	0.42
2:W:143:ALA:HB1	2:W:180:PHE:CZ	2.54	0.42
2:W:144:ARG:HD3	2:W:152:TRP:HE3	1.83	0.42
3:X:164:LEU:HD12	3:X:165:VAL:N	2.33	0.42
3:X:180:VAL:CG1	3:X:181:ASP:N	2.81	0.42
1:Y:28:ILE:O	1:Y:28:ILE:CG2	2.68	0.42
3:a:58:PRO:HG2	3:a:59:GLN:H	1.85	0.42
3:a:138:LEU:HD21	3:a:219:SER:OG	2.19	0.42
2:c:115:VAL:HB	2:c:123:ASN:HD22	1.83	0.42
2:c:142:GLU:CD	2:c:157:LEU:HD11	2.44	0.42
1:e:118:LEU:O	1:e:122:ILE:HG13	2.18	0.42
3:g:202:ARG:HG3	3:g:215:TRP:CE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:69:VAL:C	1:h:71:ASN:H	2.27	0.42
1:D:95:GLU:CD	2:E:41:ARG:NH1	2.73	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
1:G:92:PHE:CZ	2:H:134:TYR:CE2	3.07	0.42
3:I:138:LEU:HB2	3:I:222:ILE:CG2	2.49	0.42
3:I:181:ASP:CG	3:I:183:ARG:CD	2.93	0.42
3:L:151:ASN:ND2	3:L:185:LYS:HG2	2.34	0.42
1:P:55:HIS:C	1:P:57:GLN:N	2.77	0.42
2:Q:104:LEU:HD13	2:Q:135:PHE:CZ	2.54	0.42
2:T:187:LEU:HD21	3:U:183:ARG:NH1	2.34	0.42
1:Y:20:ASP:OD1	1:Y:85:VAL:CG2	2.66	0.42
1:b:16:HIS:CB	1:b:92:PHE:CZ	3.02	0.42
1:b:64:LYS:N	1:b:65:PRO:CD	2.82	0.42
2:c:139:LEU:HD23	2:c:186:PRO:CA	2.48	0.42
3:d:102:LEU:HD22	3:d:127:GLN:HA	2.01	0.42
1:e:7:THR:CG2	1:e:132:LEU:HD22	2.49	0.42
3:g:110:LEU:HD12	3:g:110:LEU:C	2.44	0.42
1:h:69:VAL:C	1:h:71:ASN:N	2.77	0.42
2:i:70:GLN:HG2	2:i:134:TYR:HE1	1.84	0.42
2:B:83:LEU:CD2	2:B:92:VAL:HA	2.50	0.42
3:F:148:LEU:HD11	3:F:188:LEU:HD23	2.00	0.42
1:J:85:VAL:HG22	1:J:89:ILE:HD11	2.01	0.42
1:M:14:LEU:CD1	1:M:128:ILE:HG21	2.49	0.42
1:P:88:ASN:O	1:P:91:VAL:HB	2.20	0.42
1:P:128:ILE:H	1:P:128:ILE:HG12	1.53	0.42
2:Q:112:LEU:C	2:Q:201:LEU:HD22	2.44	0.42
3:R:42:VAL:CG1	3:R:45:VAL:HA	2.49	0.42
3:U:63:LEU:HD23	3:U:112:ASP:HA	2.00	0.42
1:Y:62:GLU:HA	1:Y:62:GLU:OE2	2.19	0.42
2:Z:141:PHE:HE1	2:Z:163:LYS:HA	1.85	0.42
3:d:204:ARG:HH21	3:d:215:TRP:HE1	1.62	0.42
2:f:117:VAL:HG12	2:f:118:GLU:N	2.34	0.42
2:E:40:ASP:OD2	2:E:77:ILE:HB	2.19	0.42
2:E:162:GLN:NE2	3:F:186:PHE:CD1	2.88	0.42
3:F:134:ALA:HA	3:F:135:PRO:HD3	1.81	0.42
2:H:13:ASN:HD21	2:H:130:GLN:CD	2.27	0.42
2:H:73:THR:O	2:H:76:ASP:HB2	2.19	0.42
3:L:109:GLN:CD	3:L:119:GLN:NE2	2.78	0.42
3:L:206:ASN:CB	3:L:211:SER:HA	2.50	0.42
1:M:20:ASP:OD1	1:M:85:VAL:CG2	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:53:LEU:HD23	1:P:53:LEU:HA	1.86	0.42
3:R:40:CYS:O	3:R:129:LEU:HD22	2.19	0.42
2:T:10:CYS:HA	2:T:19:SER:O	2.18	0.42
3:U:149:GLU:OE1	3:U:185:LYS:HD2	2.20	0.42
1:V:66:LEU:HD12	1:V:114:ILE:HD11	1.97	0.42
3:X:61:THR:O	3:X:89:ILE:HG23	2.19	0.42
3:a:169:THR:HA	3:a:196:ARG:O	2.19	0.42
1:b:16:HIS:HB3	2:c:134:TYR:HD2	1.83	0.42
2:c:113:GLN:O	2:c:124:ILE:HG23	2.20	0.42
3:d:109:GLN:NE2	3:d:119:GLN:OE1	2.52	0.42
2:f:77:ILE:HG22	2:f:78:VAL:N	2.35	0.42
1:h:126:GLN:HG2	3:j:208:LEU:O	2.19	0.42
2:i:183:ARG:CZ	2:i:197:TRP:CZ2	3.02	0.42
3:j:148:LEU:C	3:j:148:LEU:HD12	2.44	0.42
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
1:G:88:ASN:O	1:G:92:PHE:HD2	2.03	0.42
3:I:128:ASN:O	3:I:212:ALA:CB	2.68	0.42
2:N:167:ILE:HD13	2:N:169:LEU:HD21	2.01	0.42
3:O:165:VAL:CG2	3:O:178:GLN:HB3	2.49	0.42
1:P:25:LEU:C	1:P:27:GLY:H	2.28	0.42
1:P:45:TYR:HB3	1:P:107:TYR:CD1	2.51	0.42
2:Q:121:ARG:HG2	2:Q:170:GLU:OE2	2.20	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
2:W:42:ARG:NH2	2:W:73:THR:HG23	2.35	0.42
3:a:220:HIS:HA	3:a:221:PRO:HD2	1.92	0.42
1:b:22:GLN:O	1:b:25:LEU:HB3	2.19	0.42
2:c:160:LEU:HD23	2:c:160:LEU:HA	1.79	0.42
1:e:25:LEU:C	1:e:27:GLY:N	2.76	0.42
2:i:122:CYS:HB2	2:i:172:LEU:CD1	2.49	0.42
3:j:166:GLN:HG2	3:j:177:GLU:CB	2.47	0.42
3:j:204:ARG:HG2	3:j:205:PHE:N	2.34	0.42
1:D:14:LEU:O	1:D:15:GLU:C	2.62	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:K:110:ILE:O	2:K:127:GLU:N	2.48	0.42
3:L:188:LEU:HD12	3:L:188:LEU:HA	1.59	0.42
2:N:35:VAL:HA	2:N:81:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:142:GLU:HG3	2:N:194:TRP:CZ2	2.54	0.42
2:Q:119:THR:O	2:Q:205:THR:HG21	2.20	0.42
3:R:61:THR:CG2	3:R:62:ASN:N	2.83	0.42
2:T:154:GLU:O	2:T:155:ALA:C	2.63	0.42
3:U:139:THR:OG1	3:U:151:ASN:HB2	2.19	0.42
3:U:205:PHE:O	3:U:206:ASN:HB2	2.20	0.42
2:W:119:THR:HB	2:W:174:PRO:CG	2.35	0.42
2:W:141:PHE:HB2	2:W:160:LEU:HB2	2.02	0.42
1:b:46:MET:SD	1:b:120:ARG:HG2	2.60	0.42
1:b:92:PHE:O	1:b:96:LEU:HB2	2.19	0.42
3:d:165:VAL:O	3:d:177:GLU:HA	2.20	0.42
3:d:181:ASP:C	3:d:181:ASP:OD2	2.61	0.42
2:f:161:LYS:HD2	3:g:185:LYS:HZ1	1.84	0.42
1:h:85:VAL:CG1	1:h:86:VAL:N	2.83	0.42
3:j:68:TRP:CD2	3:j:77:VAL:HG22	2.55	0.42
1:A:56:LEU:O	1:A:59:LEU:HB3	2.19	0.42
3:C:208:LEU:HD23	3:C:208:LEU:HA	1.76	0.42
1:D:126:GLN:NE2	3:F:207:PRO:O	2.50	0.42
3:F:119:GLN:HE21	3:F:119:GLN:HB2	1.68	0.42
2:H:155:ALA:HA	2:H:156:PRO:HD3	1.81	0.42
2:H:178:TYR:HB2	2:H:203:PHE:CZ	2.55	0.42
1:J:22:GLN:HG2	1:J:122:ILE:HD13	2.02	0.42
2:K:183:ARG:O	2:K:194:TRP:CZ3	2.73	0.42
3:L:204:ARG:HB2	3:L:215:TRP:CE3	2.55	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
2:Q:158:LEU:HA	3:R:147:GLN:HE22	1.85	0.42
3:R:157:LEU:HD13	3:R:205:PHE:CE1	2.48	0.42
1:V:21:LEU:O	1:V:22:GLN:C	2.63	0.42
1:V:37:THR:O	1:V:41:THR:HG23	2.19	0.42
4:W:215:NAG:O4	4:X:233:NAG:C1	2.68	0.42
1:b:16:HIS:CB	2:c:134:TYR:HD2	2.32	0.42
3:d:69:TYR:CE1	3:d:101:HIS:HD2	2.38	0.42
2:i:143:ALA:CB	2:i:181:GLN:O	2.67	0.42
2:i:175:ASP:O	2:i:175:ASP:CG	2.63	0.42
1:A:36:LEU:CD1	1:A:40:LEU:HG	2.50	0.42
2:E:141:PHE:HD2	2:E:183:ARG:O	2.03	0.42
1:G:91:VAL:HG12	2:H:75:VAL:CG2	2.49	0.42
3:I:45:VAL:HG23	3:I:157:LEU:HD11	2.02	0.42
3:I:128:ASN:C	3:I:212:ALA:CB	2.92	0.42
1:J:18:LEU:CD2	1:J:126:GLN:HG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:117:VAL:O	2:K:206:LYS:HE2	2.20	0.42
2:K:119:THR:O	2:K:174:PRO:HA	2.20	0.42
2:N:117:VAL:HG12	2:N:122:CYS:SG	2.60	0.42
3:O:161:LEU:HD23	3:O:161:LEU:HA	1.84	0.42
1:P:14:LEU:HD23	1:P:14:LEU:HA	1.79	0.42
1:P:126:GLN:CD	3:R:210:GLY:HA2	2.45	0.42
2:Q:141:PHE:HB2	2:Q:160:LEU:HB2	2.00	0.42
2:Q:171:THR:O	2:Q:171:THR:HG22	2.20	0.42
1:S:24:ILE:HA	1:S:80:PHE:CE2	2.55	0.42
1:S:63:LEU:C	1:S:65:PRO:HD2	2.45	0.42
1:S:78:PHE:CD2	1:S:80:PHE:CE1	3.08	0.42
2:T:36:HIS:HB3	2:T:38:TRP:NE1	2.35	0.42
2:T:63:ILE:HD13	2:T:63:ILE:HA	1.87	0.42
1:V:53:LEU:HD13	1:V:96:LEU:O	2.20	0.42
2:W:13:ASN:C	2:W:14:SER:HG	2.18	0.42
2:W:117:VAL:C	2:W:118:GLU:HG3	2.45	0.42
1:Y:131:THR:O	1:Y:131:THR:HG22	2.20	0.42
2:Z:42:ARG:HB3	2:Z:44:TRP:CD1	2.55	0.42
3:a:112:ASP:OD2	3:a:114:ARG:NH1	2.53	0.42
3:a:143:LEU:CD1	3:a:147:GLN:HB3	2.48	0.42
2:f:36:HIS:HB3	2:f:38:TRP:NE1	2.32	0.42
3:g:203:SER:O	3:g:215:TRP:HE3	2.03	0.42
2:i:98:PHE:O	2:i:100:PRO:HD3	2.20	0.42
2:i:185:LYS:HA	2:i:186:PRO:HD3	1.83	0.42
2:E:41:ARG:C	2:E:42:ARG:HD3	2.45	0.41
2:E:160:LEU:HD23	2:E:160:LEU:HA	1.74	0.41
2:E:167:ILE:HD11	3:F:189:PRO:CG	2.50	0.41
1:G:97:LYS:O	1:G:98:GLY:C	2.63	0.41
3:I:181:ASP:CG	3:I:183:ARG:HD3	2.45	0.41
1:M:17:LEU:O	1:M:18:LEU:C	2.63	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
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:69:TYR:CE1	3:X:101:HIS:ND1	2.86	0.41
3:X:161:LEU:HD11	3:X:205:PHE:HD1	1.85	0.41
1:Y:18:LEU:HD11	1:Y:122:ILE:HG23	2.01	0.41
3:a:42:VAL:CB	3:a:130:VAL:HG22	2.47	0.41
3:a:68:TRP:CZ2	3:a:107:VAL:HG11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:23:MET:HE2	2:c:133:HIS:CD2	2.55	0.41
2:i:73:THR:HG22	2:i:134:TYR:OH	2.19	0.41
2:E:44:TRP:HB2	2:T:89:ARG:HD2	2.02	0.41
2:E:185:LYS:HA	2:E:186:PRO:HD3	1.71	0.41
2:K:13:ASN:ND2	2:K:16:ALA:H	2.15	0.41
3:L:61:THR:HG23	3:L:114:ARG:NH2	2.35	0.41
1:M:31:TYR:OH	1:M:35:LYS:N	2.40	0.41
2:T:118:GLU:OE1	2:T:121:ARG:HB2	2.20	0.41
2:W:118:GLU:OE1	2:W:121:ARG:HD3	2.21	0.41
3:X:107:VAL:CG1	3:X:108:VAL:N	2.83	0.41
3:a:165:VAL:HG11	3:a:186:PHE:CE2	2.55	0.41
1:b:38:ARG:HA	1:b:41:THR:HG23	2.02	0.41
1:b:66:LEU:HD11	1:b:118:LEU:HD21	2.02	0.41
1:b:92:PHE:HE2	2:c:134:TYR:HE2	1.67	0.41
2:f:8:PHE:CD1	2:f:22:TRP:HB2	2.55	0.41
2:f:115:VAL:HG11	4:f:215:NAG:H62	2.02	0.41
3:g:52:TRP:HZ3	3:g:65:LEU:CD1	2.28	0.41
3:j:37:GLU:HA	3:j:122:GLN:HE22	1.85	0.41
3:j:108:VAL:HG12	3:j:122:GLN:O	2.20	0.41
3:j:181:ASP:OD2	3:j:183:ARG:HB2	2.19	0.41
3:j:205:PHE:O	3:j:212:ALA:HB3	2.20	0.41
3:C:154:ASN:HD21	3:C:163:HIS:CE1	2.35	0.41
1:D:6:SER:N	1:D:8:LYS:HG3	2.35	0.41
2:E:147:SER:HB2	2:E:148:PRO:HD2	2.01	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:K:178:TYR:HB2	2:K:203:PHE:CE1	2.54	0.41
3:L:186:PHE:C	3:L:187:SER:O	2.63	0.41
1:M:36:LEU:HD12	1:M:40:LEU:HG	2.01	0.41
1:P:133:THR:O	1:P:133:THR:HG22	2.20	0.41
1:S:127:SER:OG	3:U:103:TYR:HB3	2.19	0.41
2:T:73:THR:HG23	2:T:75:VAL:HG22	2.02	0.41
2:T:172:LEU:HD23	2:T:172:LEU:HA	1.88	0.41
1:Y:67:GLU:HG2	1:Y:71:ASN:HD21	1.85	0.41
2:c:83:LEU:CD2	2:c:92:VAL:HA	2.50	0.41
3:d:63:LEU:HA	3:d:111:GLN:O	2.20	0.41
3:g:204:ARG:NH2	3:g:215:TRP:NE1	2.68	0.41
2:i:176:THR:HB	2:i:178:TYR:CE1	2.56	0.41
3:j:159:HIS:ND1	3:j:182:TYR:HB2	2.35	0.41
2:B:37:ALA:HA	2:B:80:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:LEU:HD23	1:D:94:LEU:HA	1.78	0.41
1:G:130:SER:C	1:G:132:LEU:N	2.78	0.41
2:K:161:LYS:HE2	3:L:185:LYS:CD	2.51	0.41
1:P:28:ILE:O	1:P:28:ILE:CG2	2.68	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
2:Q:188:GLN:HG2	2:Q:189:GLY:N	2.36	0.41
1:S:24:ILE:HA	1:S:80:PHE:HE2	1.84	0.41
2:T:141:PHE:HA	2:T:183:ARG:O	2.20	0.41
1:V:69:VAL:HG11	1:V:114:ILE:HD12	2.03	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
2:W:198:SER:O	2:W:199:GLN:C	2.62	0.41
3:X:149:GLU:HG2	3:X:151:ASN:ND2	2.35	0.41
2:c:183:ARG:HG3	2:c:197:TRP:CD2	2.55	0.41
1:e:65:PRO:O	1:e:69:VAL:N	2.52	0.41
2:f:53:VAL:HG12	2:f:54:SER:N	2.34	0.41
1:h:129:ILE:HA	1:h:132:LEU:HD12	2.02	0.41
2:i:157:LEU:HD23	2:i:157:LEU:HA	1.86	0.41
1:A:91:VAL:HG12	2:B:75:VAL:CG2	2.50	0.41
1:A:131:THR:O	1:A:132:LEU:HD23	2.20	0.41
1:G:40:LEU:HD21	1:G:115:VAL:HG23	2.02	0.41
3:I:152:TRP:CH2	3:I:184:HIS:O	2.72	0.41
2:K:184:VAL:HG13	2:K:184:VAL:O	2.19	0.41
1:M:83:ARG:HG3	1:M:84:ASP:N	2.34	0.41
2:N:81:ARG:CD	2:N:95:ILE:HG22	2.50	0.41
2:T:83:LEU:HD23	2:T:92:VAL:HA	2.02	0.41
2:T:146:LEU:HD12	2:T:147:SER:N	2.36	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
3:X:52:TRP:CZ3	3:X:92:GLY:HA2	2.55	0.41
3:X:134:ALA:HB2	3:X:217:GLU:O	2.21	0.41
3:X:167:TYR:CB	3:X:199:PHE:CE2	3.04	0.41
2:Z:50:LEU:HD23	2:Z:60:CYS:HB2	2.01	0.41
2:Z:126:TRP:HH2	2:Z:167:ILE:HB	1.85	0.41
2:c:91:ARG:HG2	2:c:93:MET:SD	2.61	0.41
1:A:35:LYS:HZ1	1:A:73:ALA:HA	1.85	0.41
2:B:81:ARG:HG3	2:B:92:VAL:HG13	2.01	0.41
1:D:78:PHE:CD2	1:D:80:PHE:CE1	3.08	0.41
1:D:114:ILE:HG23	1:D:115:VAL:N	2.34	0.41
3:F:66:HIS:ND1	3:F:79:LYS:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:144:SER:HB3	3:F:147:GLN:HG3	2.02	0.41
3:F:158:ASN:O	3:F:159:HIS:HB3	2.20	0.41
1:G:63:LEU:HD23	1:G:63:LEU:HA	1.70	0.41
1:G:81:ASP:OD1	1:G:82:PRO:CD	2.68	0.41
2:H:68:ASP:OD1	2:H:130:GLN:HA	2.20	0.41
1:J:20:ASP:OD2	1:J:85:VAL:HG23	2.20	0.41
1:J:92:PHE:CZ	2:K:73:THR:HG23	2.56	0.41
2:N:72:LEU:HD13	2:N:100:PRO:HG2	2.02	0.41
2:N:146:LEU:HD13	2:N:152:TRP:CD1	2.55	0.41
3:O:140:LEU:CD1	3:O:224:TRP:HB2	2.51	0.41
3:O:169:THR:HG23	3:O:197:TYR:CD2	2.55	0.41
2:Q:104:LEU:HD13	2:Q:135:PHE:HZ	1.86	0.41
2:Q:181:GLN:HG2	2:Q:198:SER:O	2.20	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
3:X:171:TRP:CD1	3:X:171:TRP:N	2.88	0.41
2:Z:18:ILE:HD11	2:Z:72:LEU:HD11	2.03	0.41
3:a:159:HIS:HA	3:a:182:TYR:HB2	2.02	0.41
1:b:31:TYR:O	1:b:31:TYR:CG	2.74	0.41
1:e:114:ILE:HG12	1:e:118:LEU:HG	2.01	0.41
2:f:46:GLN:NE2	2:f:47:THR:H	2.18	0.41
2:f:46:GLN:CG	2:f:62:LEU:HD22	2.51	0.41
2:i:179:GLU:HA	2:i:201:LEU:O	2.20	0.41
3:j:47:TYR:HE1	3:j:49:ASN:ND2	2.07	0.41
3:C:169:THR:C	3:C:171:TRP:N	2.72	0.41
3:F:186:PHE:CD2	3:F:186:PHE:C	2.97	0.41
2:H:37:ALA:HB2	2:H:62:LEU:HD11	2.01	0.41
2:H:48:CYS:C	2:H:60:CYS:SG	3.04	0.41
2:H:121:ARG:HG2	2:H:170:GLU:OE2	2.21	0.41
1:J:10:THR:O	1:J:11:GLN:C	2.64	0.41
2:K:50:LEU:HD23	2:K:59:ALA:O	2.20	0.41
3:L:203:SER:C	3:L:215:TRP:HE3	2.28	0.41
1:M:7:THR:O	1:M:8:LYS:C	2.62	0.41
2:N:121:ARG:HD2	2:N:170:GLU:OE1	2.20	0.41
2:Q:144:ARG:CD	2:Q:152:TRP:HE3	2.34	0.41
3:U:102:LEU:C	3:U:104:GLN:H	2.29	0.41
2:Z:73:THR:CG2	2:Z:75:VAL:HG22	2.51	0.41
3:d:115:GLU:HA	3:d:116:PRO:HD3	1.92	0.41
1:e:37:THR:HA	1:e:40:LEU:HB2	2.02	0.41
3:g:35:LEU:HD12	3:g:119:GLN:C	2.46	0.41
3:g:61:THR:O	3:g:89:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:ASP:O	1:D:21:LEU:C	2.64	0.41
2:E:20:CYS:O	2:E:59:ALA:HA	2.20	0.41
3:F:67:TYR:CE1	3:F:78:GLN:HB2	2.56	0.41
3:F:167:TYR:CE2	3:F:176:THR:HG21	2.55	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
3:I:64:THR:OG1	3:I:111:GLN:HB3	2.21	0.41
2:K:67:PRO:O	2:K:130:GLN:NE2	2.53	0.41
2:N:20:CYS:HB2	2:N:60:CYS:CB	2.51	0.41
2:N:133:HIS:C	2:N:135:PHE:N	2.77	0.41
3:R:48:MET:HE1	3:R:95:LEU:HD22	2.02	0.41
2:W:9:THR:HG22	2:W:11:PHE:HE1	1.85	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:c:44:TRP:CH2	2:c:72:LEU:HD21	2.56	0.41
3:d:178:GLN:HE21	3:d:179:SER:N	2.18	0.41
2:f:108:ALA:O	2:f:110:ILE:HG23	2.20	0.41
1:h:44:PHE:CZ	1:h:66:LEU:HA	2.55	0.41
2:B:13:ASN:OD1	2:B:13:ASN:C	2.64	0.41
2:B:82:VAL:O	2:B:83:LEU:HD23	2.21	0.41
2:B:155:ALA:HA	2:B:156:PRO:HD3	1.80	0.41
3:C:102:LEU:O	3:C:103:TYR:HB2	2.20	0.41
1:D:66:LEU:O	1:D:69:VAL:HB	2.20	0.41
1:D:127:SER:HA	3:F:103:TYR:CD1	2.55	0.41
3:F:125:LYS:HB3	3:F:127:GLN:HE22	1.86	0.41
1:G:20:ASP:OD1	2:H:133:HIS:NE2	2.52	0.41
2:H:63:ILE:C	2:H:64:LEU:HD23	2.45	0.41
3:I:65:LEU:HD23	3:I:65:LEU:C	2.46	0.41
3:I:128:ASN:O	3:I:212:ALA:HA	2.20	0.41
3:I:133:TRP:O	3:I:134:ALA:C	2.64	0.41
1:J:13:GLN:HG3	1:J:13:GLN:H	1.66	0.41
1:J:81:ASP:HA	1:J:82:PRO:HD3	1.91	0.41
2:K:20:CYS:O	2:K:59:ALA:HA	2.20	0.41
2:K:146:LEU:HD12	2:K:146:LEU:HA	1.85	0.41
3:L:68:TRP:CE3	3:L:77:VAL:HG13	2.53	0.41
3:L:68:TRP:CD1	3:L:107:VAL:HB	2.56	0.41
3:L:166:GLN:HB3	3:L:175:TRP:HB3	2.03	0.41
1:M:8:LYS:O	1:M:11:GLN:HB3	2.20	0.41
2:N:12:TYR:CZ	2:N:14:SER:HA	2.56	0.41
2:N:83:LEU:HD13	2:N:90:TRP:HB3	2.03	0.41
3:O:179:SER:C	3:O:180:VAL:CG2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:186:PHE:CD1	3:O:186:PHE:C	2.98	0.41
2:Q:50:LEU:HD23	2:Q:50:LEU:HA	1.84	0.41
2:Q:145:THR:O	2:Q:155:ALA:HB1	2.21	0.41
3:R:102:LEU:HD22	3:R:127:GLN:N	2.35	0.41
4:R:235:NAG:H83	4:R:235:NAG:H2	1.93	0.41
2:T:112:LEU:O	2:T:113:GLN:HG3	2.21	0.41
2:T:206:LYS:HA	2:T:207:PRO:HD3	1.88	0.41
1:V:35:LYS:HD2	1:V:38:ARG:NH2	2.35	0.41
2:W:9:THR:HG22	2:W:11:PHE:CE1	2.56	0.41
2:W:20:CYS:O	2:W:59:ALA:HA	2.20	0.41
2:W:83:LEU:CB	2:W:90:TRP:CE3	3.03	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:Z:44:TRP:CH2	2:Z:64:LEU:HD13	2.56	0.41
3:a:204:ARG:HD3	3:a:212:ALA:O	2.21	0.41
1:b:20:ASP:OD2	2:c:134:TYR:OH	2.26	0.41
2:c:40:ASP:OD1	2:c:41:ARG:N	2.54	0.41
2:c:64:LEU:HD23	2:c:64:LEU:N	2.36	0.41
2:c:173:THR:HA	2:c:174:PRO:HD3	1.82	0.41
3:d:149:GLU:CG	3:d:151:ASN:HD21	2.24	0.41
4:d:300:NAG:H82	4:d:300:NAG:H2	1.93	0.41
1:e:12:LEU:HD23	1:e:12:LEU:O	2.21	0.41
1:e:45:TYR:CD2	1:e:62:GLU:OE1	2.74	0.41
2:f:86:GLU:O	2:f:86:GLU:HG2	2.21	0.41
2:f:138:HIS:HB3	2:f:187:LEU:HD12	2.03	0.41
2:f:179:GLU:HG2	2:f:202:ALA:HA	2.03	0.41
2:i:153:GLU:C	2:i:155:ALA:H	2.28	0.41
1:D:63:LEU:O	1:D:64:LYS:C	2.63	0.41
3:F:62:ASN:CB	2:c:113:GLN:NE2	2.84	0.41
1:G:45:TYR:CD1	1:G:111:THR:HG22	2.55	0.41
1:J:20:ASP:CG	1:J:85:VAL:HG23	2.46	0.41
3:O:135:PRO:O	3:O:219:SER:HB3	2.20	0.41
1:P:59:LEU:HD13	1:P:121:TRP:CD1	2.56	0.41
1:P:88:ASN:ND2	1:P:88:ASN:H	2.19	0.41
4:X:300:NAG:H82	4:X:300:NAG:H2	1.94	0.41
2:Z:162:GLN:NE2	3:a:187:SER:HB3	2.35	0.41
2:c:181:GLN:HB3	2:c:197:TRP:CE3	2.56	0.41
1:e:12:LEU:HD11	2:f:188:GLN:NE2	2.36	0.41
1:e:66:LEU:O	1:e:70:LEU:HG	2.21	0.41
2:f:13:ASN:ND2	2:f:16:ALA:H	2.19	0.41
2:f:138:HIS:ND1	2:f:138:HIS:N	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:175:ASP:N	2:f:205:THR:HB	2.36	0.41
3:j:65:LEU:HD13	3:j:93:CYS:CB	2.51	0.41
3:j:128:ASN:O	3:j:212:ALA:HA	2.21	0.41
3:j:140:LEU:HD23	3:j:150:LEU:HA	2.03	0.41
1:A:12:LEU:HD23	1:A:12:LEU:C	2.46	0.40
3:C:142:LYS:HB2	3:C:142:LYS:HE3	1.75	0.40
3:C:157:LEU:H	3:C:157:LEU:HG	1.65	0.40
2:E:132:SER:C	2:E:134:TYR:N	2.79	0.40
1:G:92:PHE:HZ	2:H:134:TYR:CE2	2.38	0.40
2:H:13:ASN:C	2:H:15:ARG:H	2.28	0.40
2:H:83:LEU:HD21	2:W:38:TRP:HH2	1.85	0.40
1:J:25:LEU:HD23	1:J:122:ILE:HD12	2.01	0.40
3:L:135:PRO:HB2	3:L:219:SER:HB3	2.03	0.40
1:M:44:PHE:CE2	1:M:114:ILE:HG13	2.56	0.40
2:N:33:CYS:C	2:N:50:LEU:HB2	2.45	0.40
2:N:126:TRP:NE1	2:N:165:GLU:HA	2.36	0.40
3:O:117:ARG:HG3	2:i:204:ARG:HH11	1.86	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:S:23:MET:HE1	2:T:133:HIS:CE1	2.56	0.40
2:T:11:PHE:HB3	2:T:105:ARG:HB3	2.02	0.40
2:T:106:LEU:HD11	2:T:186:PRO:HG3	2.03	0.40
3:X:87:GLU:O	3:X:89:ILE:HG13	2.21	0.40
1:Y:28:ILE:HD12	1:Y:114:ILE:HD13	2.03	0.40
2:Z:158:LEU:HD13	2:Z:167:ILE:HD11	2.04	0.40
3:a:69:TYR:CE1	3:a:101:HIS:CD2	3.06	0.40
3:a:197:TYR:HB2	3:a:224:TRP:HB3	2.02	0.40
3:a:206:ASN:HD22	3:a:211:SER:HA	1.85	0.40
2:c:143:ALA:HA	2:c:181:GLN:O	2.20	0.40
3:d:167:TYR:HB2	3:d:199:PHE:CD2	2.56	0.40
2:f:34:GLN:N	2:f:50:LEU:HD12	2.36	0.40
1:h:105:CYS:SG	1:h:107:TYR:CE1	3.14	0.40
3:j:132:PRO:HG3	3:j:161:LEU:CD2	2.51	0.40
3:j:206:ASN:CG	3:j:207:PRO:HA	2.46	0.40
2:B:126:TRP:CE2	2:B:165:GLU:HA	2.56	0.40
3:F:48:MET:HE3	3:F:95:LEU:HD12	2.04	0.40
3:F:63:LEU:HD13	3:F:110:LEU:HD21	2.03	0.40
3:F:133:TRP:HB2	3:F:155:ARG:HG3	2.02	0.40
2:H:120:HIS:C	2:H:172:LEU:HB2	2.45	0.40
1:J:81:ASP:OD1	1:J:82:PRO:HD2	2.21	0.40
2:K:81:ARG:HD2	2:K:95:ILE:HG22	1.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:132:SER:OG	2:K:134:TYR:HD1	2.04	0.40
3:L:68:TRP:NE1	3:L:107:VAL:HB	2.37	0.40
2:N:51:LEU:CB	2:N:52:PRO:HD2	2.51	0.40
2:Q:13:ASN:HD22	2:Q:17:GLN:C	2.28	0.40
2:Q:22:TRP:CE3	2:Q:82:VAL:HG11	2.56	0.40
2:Q:136:GLU:OE1	2:Q:136:GLU:HA	2.21	0.40
2:Q:160:LEU:HD23	2:Q:160:LEU:HA	1.89	0.40
3:R:67:TYR:HB2	3:R:106:PHE:CE1	2.56	0.40
3:R:152:TRP:CE2	3:R:201:VAL:HG11	2.56	0.40
2:T:104:LEU:HD13	2:T:135:PHE:CZ	2.56	0.40
2:W:14:SER:O	2:W:15:ARG:HG2	2.21	0.40
2:Z:54:SER:HB3	2:Z:57:SER:OG	2.21	0.40
2:Z:130:GLN:H	2:Z:130:GLN:HG3	1.52	0.40
2:Z:162:GLN:OE1	2:Z:162:GLN:N	2.53	0.40
3:d:146:SER:O	3:d:191:VAL:HG22	2.21	0.40
3:g:102:LEU:C	3:g:104:GLN:N	2.79	0.40
1:h:51:THR:O	1:h:51:THR:HG22	2.22	0.40
1:A:81:ASP:O	1:A:84:ASP:HB2	2.22	0.40
3:C:154:ASN:CG	3:C:161:LEU:HD12	2.46	0.40
2:E:145:THR:OG1	2:E:169:LEU:HD21	2.22	0.40
2:E:167:ILE:HG13	3:F:189:PRO:HG3	2.03	0.40
3:F:68:TRP:CD1	3:F:68:TRP:C	3.00	0.40
3:F:125:LYS:HB3	3:F:127:GLN:NE2	2.36	0.40
3:F:200:ARG:HD2	3:F:218:TRP:HB3	2.03	0.40
3:I:159:HIS:O	3:I:159:HIS:CG	2.71	0.40
2:K:152:TRP:O	2:K:153:GLU:C	2.65	0.40
4:K:215:NAG:O3	4:K:216:NAG:O5	2.33	0.40
3:L:191:VAL:CG1	3:L:197:TYR:CZ	3.03	0.40
1:M:48:LYS:HD3	1:M:108:ALA:HA	2.04	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:S:51:THR:O	1:S:52:GLU:HG3	2.20	0.40
2:T:142:GLU:OE1	2:T:183:ARG:NE	2.55	0.40
2:W:83:LEU:HB3	2:W:90:TRP:HE3	1.85	0.40
2:Z:11:PHE:O	2:Z:18:ILE:HA	2.22	0.40
2:Z:143:ALA:HB1	2:Z:180:PHE:CE1	2.56	0.40
2:Z:152:TRP:CZ3	2:Z:181:GLN:HB2	2.56	0.40
3:a:36:PRO:HB2	3:a:52:TRP:HB2	2.02	0.40
1:b:18:LEU:HD21	3:d:208:LEU:HA	2.02	0.40
1:b:28:ILE:O	1:b:28:ILE:CG2	2.68	0.40
1:b:47:PRO:O	1:b:48:LYS:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:94:LEU:HD23	1:b:94:LEU:HA	1.54	0.40
2:c:175:ASP:N	2:c:205:THR:HB	2.36	0.40
3:d:106:PHE:O	3:d:124:LEU:N	2.51	0.40
2:f:40:ASP:CG	2:f:41:ARG:HG2	2.46	0.40
2:f:44:TRP:CH2	2:f:72:LEU:HD21	2.57	0.40
1:h:17:LEU:HA	1:h:92:PHE:CD2	2.55	0.40
2:i:18:ILE:HG21	2:i:62:LEU:HD12	2.02	0.40
2:i:20:CYS:O	2:i:59:ALA:HA	2.21	0.40
2:B:104:LEU:HD13	2:B:135:PHE:CZ	2.56	0.40
2:E:48:CYS:SG	2:E:62:LEU:HD23	2.62	0.40
1:G:64:LYS:N	1:G:65:PRO:HD2	2.37	0.40
3:L:117:ARG:HA	3:L:117:ARG:HD3	1.86	0.40
2:N:16:ALA:O	2:N:64:LEU:HB2	2.22	0.40
3:O:49:ASN:ND2	4:O:234:NAG:C1	2.85	0.40
1:P:124:PHE:C	1:P:124:PHE:CD2	3.00	0.40
2:Q:78:VAL:HG23	2:Q:100:PRO:HG3	2.04	0.40
3:R:52:TRP:NE1	3:R:63:LEU:HD12	2.37	0.40
2:T:20:CYS:O	2:T:59:ALA:HA	2.20	0.40
2:T:36:HIS:HB3	2:T:38:TRP:HE1	1.86	0.40
2:T:170:GLU:OE2	2:T:170:GLU:HA	2.20	0.40
3:U:35:LEU:HD22	3:U:63:LEU:HD13	2.04	0.40
2:W:80:LEU:HD13	2:W:98:PHE:HB3	2.01	0.40
2:W:91:ARG:HG2	2:W:93:MET:SD	2.62	0.40
3:X:167:TYR:HB3	3:X:199:PHE:CD2	2.56	0.40
1:Y:25:LEU:C	1:Y:27:GLY:N	2.79	0.40
3:a:100:ILE:O	3:a:100:ILE:HG22	2.21	0.40
2:c:83:LEU:CB	2:c:90:TRP:HE3	2.34	0.40
3:d:44:ASN:HD22	3:d:133:TRP:H	1.70	0.40
3:d:52:TRP:CZ3	3:d:92:GLY:HA2	2.56	0.40
3:d:135:PRO:HB2	3:d:219:SER:HB3	2.02	0.40
3:g:131:ILE:HD11	3:g:214:HIS:HB2	2.04	0.40
3:g:140:LEU:HA	3:g:149:GLU:O	2.20	0.40
1:h:69:VAL:O	1:h:71:ASN:N	2.54	0.40
2:i:79:THR:HG23	2:i:97:ASP:OD1	2.21	0.40
3:j:52:TRP:CE2	3:j:110:LEU:HD11	2.55	0.40
3:j:65:LEU:CD2	3:j:80:CYS:HB2	2.51	0.40
3:j:132:PRO:HB3	3:j:161:LEU:HD11	2.02	0.40
1:A:59:LEU:HD13	1:A:121:TRP:CD2	2.57	0.40
2:E:13:ASN:HB3	2:E:17:GLN:H	1.86	0.40
2:E:37:ALA:HB2	2:E:62:LEU:HD13	2.03	0.40
2:E:142:GLU:HA	2:E:158:LEU:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:205:PHE:CE2	3:F:209:CYS:C	2.99	0.40
2:H:32:SER:HB3	2:H:85:ARG:HB2	2.04	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:I:170:ASP:OD2	3:I:196:ARG:HB3	2.22	0.40
3:L:107:VAL:HG22	3:L:123:MET:HG3	2.04	0.40
1:M:16:HIS:HB3	2:N:134:TYR:HD2	1.85	0.40
3:O:111:GLN:OE1	3:O:111:GLN:HA	2.21	0.40
1:P:14:LEU:HD12	1:P:128:ILE:HB	2.03	0.40
2:T:101:PHE:CZ	2:T:134:TYR:HD1	2.40	0.40
1:V:53:LEU:HD23	1:V:53:LEU:HA	1.86	0.40
1:V:68:GLU:HA	1:V:71:ASN:HB2	2.02	0.40
1:V:129:ILE:HA	1:V:132:LEU:HD12	2.04	0.40
3:X:154:ASN:ND2	3:X:163:HIS:CE1	2.84	0.40
3:X:202:ARG:HD3	3:X:218:TRP:CZ2	2.57	0.40
3:X:205:PHE:O	3:X:206:ASN:HB2	2.21	0.40
3:a:145:GLU:OE1	3:a:145:GLU:HA	2.22	0.40
1:b:9:LYS:HB3	1:b:9:LYS:HE2	1.67	0.40
1:b:28:ILE:HG23	1:b:39:MET:HE3	2.03	0.40
2:c:79:THR:HG23	2:c:95:ILE:HD11	2.03	0.40
3:d:111:GLN:OE1	3:d:119:GLN:HB3	2.22	0.40
2:f:35:VAL:HG12	2:f:36:HIS:N	2.37	0.40
2:f:43:ARG:HA	2:f:43:ARG:HD2	1.97	0.40
2:f:177:GLN:O	2:f:178:TYR:CD2	2.74	0.40
1:h:59:LEU:HD13	1:h:121:TRP:CD1	2.56	0.40
2:i:63:ILE:HD13	2:i:63:ILE:HA	1.97	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%)	14 45
1	D	115/136 (85%)	98 (85%)	17 (15%)	0	100 100
1	G	115/136 (85%)	102 (89%)	12 (10%)	1 (1%)	14 45
1	J	115/136 (85%)	108 (94%)	7 (6%)	0	100 100
1	M	115/136 (85%)	103 (90%)	10 (9%)	2 (2%)	7 34
1	P	115/136 (85%)	103 (90%)	10 (9%)	2 (2%)	7 34
1	S	115/136 (85%)	99 (86%)	16 (14%)	0	100 100
1	V	115/136 (85%)	100 (87%)	13 (11%)	2 (2%)	7 34
1	Y	114/136 (84%)	101 (89%)	12 (10%)	1 (1%)	14 45
1	b	113/136 (83%)	93 (82%)	19 (17%)	1 (1%)	14 45
1	e	115/136 (85%)	100 (87%)	13 (11%)	2 (2%)	7 34
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%)	24 57
2	K	192/217 (88%)	176 (92%)	15 (8%)	1 (0%)	24 57
2	N	191/217 (88%)	179 (94%)	12 (6%)	0	100 100
2	Q	191/217 (88%)	179 (94%)	11 (6%)	1 (0%)	24 57
2	T	192/217 (88%)	176 (92%)	15 (8%)	1 (0%)	24 57
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%)	7 35
2	i	192/217 (88%)	180 (94%)	12 (6%)	0	100 100
3	C	184/202 (91%)	174 (95%)	10 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	F	182/202 (90%)	169 (93%)	12 (7%)	1 (0%)	24 57
3	I	184/202 (91%)	165 (90%)	19 (10%)	0	100 100
3	L	189/202 (94%)	172 (91%)	13 (7%)	4 (2%)	5 31
3	O	189/202 (94%)	172 (91%)	17 (9%)	0	100 100
3	R	184/202 (91%)	169 (92%)	13 (7%)	2 (1%)	11 41
3	U	189/202 (94%)	179 (95%)	10 (5%)	0	100 100
3	X	189/202 (94%)	180 (95%)	8 (4%)	1 (0%)	24 57
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%)	24 57
All	All	5924/6660 (89%)	5416 (91%)	480 (8%)	28 (0%)	24 57

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

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Mol	Chain	Res	Type
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%)	113 (98%)	2 (2%)	53	67
1	D	115/128 (90%)	113 (98%)	2 (2%)	53	67
1	G	115/128 (90%)	112 (97%)	3 (3%)	40	60
1	J	115/128 (90%)	108 (94%)	7 (6%)	17	43
1	M	115/128 (90%)	113 (98%)	2 (2%)	53	67
1	P	115/128 (90%)	110 (96%)	5 (4%)	26	50
1	S	115/128 (90%)	110 (96%)	5 (4%)	26	50
1	V	115/128 (90%)	113 (98%)	2 (2%)	53	67
1	Y	114/128 (89%)	108 (95%)	6 (5%)	20	45
1	b	113/128 (88%)	106 (94%)	7 (6%)	16	42
1	e	115/128 (90%)	114 (99%)	1 (1%)	70	74
1	h	115/128 (90%)	114 (99%)	1 (1%)	70	74
2	B	179/194 (92%)	176 (98%)	3 (2%)	53	67
2	E	180/194 (93%)	172 (96%)	8 (4%)	25	49
2	H	180/194 (93%)	175 (97%)	5 (3%)	38	58
2	K	180/194 (93%)	177 (98%)	3 (2%)	53	67
2	N	179/194 (92%)	174 (97%)	5 (3%)	38	58
2	Q	179/194 (92%)	172 (96%)	7 (4%)	28	52
2	T	180/194 (93%)	174 (97%)	6 (3%)	33	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	W	180/194 (93%)	176 (98%)	4 (2%)	45	63
2	Z	180/194 (93%)	173 (96%)	7 (4%)	28	52
2	c	180/194 (93%)	176 (98%)	4 (2%)	45	63
2	f	180/194 (93%)	177 (98%)	3 (2%)	53	67
2	i	180/194 (93%)	172 (96%)	8 (4%)	25	49
3	C	182/194 (94%)	181 (100%)	1 (0%)	81	81
3	F	180/194 (93%)	176 (98%)	4 (2%)	45	63
3	I	182/194 (94%)	176 (97%)	6 (3%)	33	56
3	L	185/194 (95%)	177 (96%)	8 (4%)	26	50
3	O	185/194 (95%)	175 (95%)	10 (5%)	20	45
3	R	182/194 (94%)	176 (97%)	6 (3%)	33	56
3	U	185/194 (95%)	181 (98%)	4 (2%)	45	63
3	X	185/194 (95%)	180 (97%)	5 (3%)	39	59
3	a	185/194 (95%)	183 (99%)	2 (1%)	65	73
3	d	185/194 (95%)	182 (98%)	3 (2%)	55	68
3	g	185/194 (95%)	179 (97%)	6 (3%)	34	56
3	j	185/194 (95%)	182 (98%)	3 (2%)	55	68
All	All	5740/6192 (93%)	5576 (97%)	164 (3%)	37	58

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	69	VAL
2	B	15	ARG
2	B	81	ARG
2	B	185	LYS
3	C	143	LEU
1	D	56	LEU
1	D	69	VAL
2	E	64	LEU
2	E	75	VAL
2	E	79	THR
2	E	124	ILE
2	E	128	ILE
2	E	139	LEU

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Mol	Chain	Res	Type
2	E	167	ILE
2	E	192	THR
3	F	38	VAL
3	F	126	LEU
3	F	159	HIS
3	F	201	VAL
1	G	20	ASP
1	G	53	LEU
1	G	119	ASN
2	H	20	CYS
2	H	68	ASP
2	H	86	GLU
2	H	88	VAL
2	H	185	LYS
3	I	61	THR
3	I	77	VAL
3	I	138	LEU
3	I	159	HIS
3	I	180	VAL
3	I	183	ARG
1	J	13	GLN
1	J	28	ILE
1	J	118	LEU
1	J	122	ILE
1	J	128	ILE
1	J	129	ILE
1	J	131	THR
2	K	17	GLN
2	K	46	GLN
2	K	154	GLU
3	L	42	VAL
3	L	45	VAL
3	L	59	GLN
3	L	110	LEU
3	L	146	SER
3	L	180	VAL
3	L	183	ARG
3	L	185	LYS
1	M	15	GLU
1	M	48	LYS
2	N	9	THR
2	N	60	CYS

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Mol	Chain	Res	Type
2	N	114	VAL
2	N	129	SER
2	N	167	ILE
3	O	38	VAL
3	O	42	VAL
3	O	138	LEU
3	O	143	LEU
3	O	149	GLU
3	O	159	HIS
3	O	169	THR
3	O	180	VAL
3	O	183	ARG
3	O	206	ASN
1	P	13	GLN
1	P	14	LEU
1	P	87	SER
1	P	119	ASN
1	P	128	ILE
2	Q	60	CYS
2	Q	68	ASP
2	Q	78	VAL
2	Q	95	ILE
2	Q	116	HIS
2	Q	129	SER
2	Q	185	LYS
3	R	45	VAL
3	R	77	VAL
3	R	100	ILE
3	R	126	LEU
3	R	131	ILE
3	R	165	VAL
1	S	10	THR
1	S	20	ASP
1	S	28	ILE
1	S	40	LEU
1	S	69	VAL
2	T	18	ILE
2	T	110	ILE
2	T	124	ILE
2	T	137	ARG
2	T	151	THR
2	T	185	LYS

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Mol	Chain	Res	Type
3	U	45	VAL
3	U	150	LEU
3	U	164	LEU
3	U	222	ILE
1	V	69	VAL
1	V	106	GLU
2	W	60	CYS
2	W	78	VAL
2	W	138	HIS
2	W	144	ARG
3	X	45	VAL
3	X	126	LEU
3	X	131	ILE
3	X	136	GLU
3	X	173	HIS
1	Y	14	LEU
1	Y	51	THR
1	Y	69	VAL
1	Y	114	ILE
1	Y	115	VAL
1	Y	128	ILE
2	Z	78	VAL
2	Z	130	GLN
2	Z	137	ARG
2	Z	173	THR
2	Z	182	VAL
2	Z	184	VAL
2	Z	185	LYS
3	a	143	LEU
3	a	161	LEU
1	b	28	ILE
1	b	46	MET
1	b	88	ASN
1	b	91	VAL
1	b	93	VAL
1	b	115	VAL
1	b	119	ASN
2	c	64	LEU
2	c	78	VAL
2	c	95	ILE
2	c	138	HIS
3	d	44	ASN

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Mol	Chain	Res	Type
3	d	59	GLN
3	d	119	GLN
1	e	19	LEU
2	f	138	HIS
2	f	184	VAL
2	f	185	LYS
3	g	45	VAL
3	g	59	GLN
3	g	111	GLN
3	g	133	TRP
3	g	161	LEU
3	g	208	LEU
1	h	49	LYS
2	i	18	ILE
2	i	63	ILE
2	i	78	VAL
2	i	110	ILE
2	i	117	VAL
2	i	137	ARG
2	i	145	THR
2	i	173	THR
3	j	45	VAL
3	j	100	ILE
3	j	110	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (194) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	90	ASN
2	B	123	ASN
2	B	133	HIS
3	C	44	ASN
3	C	49	ASN
3	C	62	ASN
3	C	74	ASN
3	C	82	HIS
3	C	109	GLN
3	C	119	GLN
3	C	137	ASN
3	C	163	HIS
1	D	22	GLN

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Mol	Chain	Res	Type
1	D	88	ASN
1	D	90	ASN
1	D	119	ASN
2	E	24	GLN
2	E	123	ASN
2	E	164	GLN
2	E	181	GLN
3	F	49	ASN
3	F	53	GLN
3	F	62	ASN
3	F	94	GLN
3	F	119	GLN
3	F	154	ASN
1	G	88	ASN
1	G	90	ASN
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	74	ASN
3	I	137	ASN
3	I	223	HIS
1	J	22	GLN
1	J	88	ASN
1	J	126	GLN
2	K	17	GLN
2	K	123	ASN
3	L	49	ASN
3	L	53	GLN
3	L	62	ASN
3	L	104	GLN
3	L	109	GLN
3	L	111	GLN
3	L	119	GLN
3	L	154	ASN
1	M	11	GLN
1	M	74	HIS
1	M	88	ASN
2	N	17	GLN

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Mol	Chain	Res	Type
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	109	GLN
3	O	137	ASN
3	O	151	ASN
3	O	154	ASN
3	O	184	HIS
1	P	74	HIS
1	P	88	ASN
2	Q	13	ASN
2	Q	36	HIS
2	Q	164	GLN
2	Q	188	GLN
3	R	49	ASN
3	R	62	ASN
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	147	GLN
3	R	163	HIS
1	S	11	GLN
1	S	16	HIS
1	S	88	ASN
1	S	90	ASN
2	T	123	ASN
2	T	164	GLN
3	U	49	ASN
3	U	62	ASN
3	U	109	GLN
3	U	119	GLN
3	U	206	ASN
1	V	74	HIS
1	V	88	ASN
1	V	126	GLN

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Mol	Chain	Res	Type
2	W	17	GLN
2	W	123	ASN
2	W	164	GLN
2	W	177	GLN
3	X	59	GLN
3	X	71	ASN
3	X	94	GLN
3	X	137	ASN
3	X	151	ASN
3	X	153	ASN
3	X	154	ASN
3	X	184	HIS
3	X	194	GLN
3	X	206	ASN
1	Y	11	GLN
1	Y	13	GLN
1	Y	22	GLN
1	Y	88	ASN
2	Z	24	GLN
2	Z	96	GLN
2	Z	103	ASN
2	Z	123	ASN
2	Z	150	HIS
2	Z	164	GLN
3	a	53	GLN
3	a	62	ASN
3	a	66	HIS
3	a	101	HIS
3	a	109	GLN
3	a	119	GLN
3	a	128	ASN
3	a	147	GLN
3	a	151	ASN
3	a	154	ASN
3	a	184	HIS
3	a	206	ASN
1	b	13	GLN
1	b	88	ASN
2	c	113	GLN
2	c	123	ASN
2	c	164	GLN
3	d	39	GLN

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Mol	Chain	Res	Type
3	d	44	ASN
3	d	49	ASN
3	d	62	ASN
3	d	66	HIS
3	d	101	HIS
3	d	109	GLN
3	d	122	GLN
3	d	141	HIS
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	74	HIS
1	e	119	ASN
2	f	46	GLN
2	f	70	GLN
2	f	123	ASN
2	f	133	HIS
2	f	164	GLN
3	g	39	GLN
3	g	44	ASN
3	g	49	ASN
3	g	59	GLN
3	g	62	ASN
3	g	66	HIS
3	g	82	HIS
3	g	101	HIS
3	g	122	GLN
3	g	137	ASN
3	g	151	ASN
3	g	153	ASN
3	g	154	ASN
3	g	184	HIS
3	g	206	ASN
3	g	223	HIS
1	h	13	GLN
1	h	57	GLN
1	h	88	ASN
1	h	90	ASN
2	i	116	HIS

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Mol	Chain	Res	Type
2	i	123	ASN
2	i	177	GLN
3	j	39	GLN
3	j	44	ASN
3	j	62	ASN
3	j	101	HIS
3	j	109	GLN
3	j	122	GLN
3	j	147	GLN
3	j	153	ASN
3	j	154	ASN
3	j	206	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	C	400	-	14,14,15	0.53	0	17,19,21	0.77	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	i	215	-	14,14,15	0.66	0	17,19,21	1.56	3 (17%)
4	NAG	O	400	-	14,14,15	0.48	0	17,19,21	0.86	0
4	NAG	F	300	-	14,14,15	0.54	0	17,19,21	1.17	2 (11%)
4	NAG	U	300	-	14,14,15	0.58	0	17,19,21	0.75	0
4	NAG	K	215	-	14,14,15	0.66	0	17,19,21	1.85	4 (23%)
4	NAG	L	234	-	14,14,15	0.52	0	17,19,21	0.92	1 (5%)
4	NAG	I	400	-	14,14,15	0.56	0	17,19,21	0.60	0
4	NAG	R	233	-	14,14,15	0.60	0	17,19,21	1.33	2 (11%)
4	NAG	F	233	-	14,14,15	0.52	0	17,19,21	1.87	3 (17%)
4	NAG	U	233	-	14,14,15	0.56	0	17,19,21	2.13	5 (29%)
4	NAG	a	300	-	14,14,15	0.47	0	17,19,21	0.87	1 (5%)
4	NAG	I	235	-	14,14,15	0.53	0	17,19,21	0.63	0
4	NAG	X	300	-	14,14,15	0.50	0	17,19,21	0.58	0
4	NAG	Q	215	-	14,14,15	0.60	0	17,19,21	1.91	5 (29%)
4	NAG	H	215	-	14,14,15	0.62	0	17,19,21	1.38	2 (11%)
4	NAG	C	234	-	14,14,15	0.52	0	17,19,21	1.50	3 (17%)
4	NAG	O	233	-	14,14,15	0.64	0	17,19,21	1.41	2 (11%)
4	NAG	a	233	-	14,14,15	0.50	0	17,19,21	1.93	4 (23%)
4	NAG	j	300	-	14,14,15	0.53	0	17,19,21	0.74	0
4	NAG	I	234	-	14,14,15	0.41	0	17,19,21	1.55	1 (5%)
4	NAG	B	215	-	14,14,15	0.52	0	17,19,21	1.13	1 (5%)
4	NAG	X	233	-	14,14,15	0.55	0	17,19,21	2.06	6 (35%)
4	NAG	F	400	-	14,14,15	0.56	0	17,19,21	0.78	0
4	NAG	R	300	-	14,14,15	0.61	0	17,19,21	1.38	2 (11%)
4	NAG	d	300	-	14,14,15	0.48	0	17,19,21	0.67	0
4	NAG	F	235	-	14,14,15	0.49	0	17,19,21	0.69	0
4	NAG	L	300	-	14,14,15	0.55	0	17,19,21	1.55	3 (17%)
4	NAG	L	233	-	14,14,15	0.56	0	17,19,21	1.23	1 (5%)
4	NAG	F	234	-	14,14,15	0.44	0	17,19,21	1.93	2 (11%)
4	NAG	C	300	-	14,14,15	0.56	0	17,19,21	1.40	4 (23%)
4	NAG	I	233	-	14,14,15	0.67	0	17,19,21	1.46	2 (11%)
4	NAG	f	215	-	14,14,15	0.70	0	17,19,21	1.39	3 (17%)
4	NAG	O	300	-	14,14,15	0.53	0	17,19,21	1.73	4 (23%)
4	NAG	i	216	-	14,14,15	0.46	0	17,19,21	2.07	6 (35%)
4	NAG	c	216	-	14,14,15	0.52	0	17,19,21	1.96	4 (23%)
4	NAG	C	233	-	14,14,15	0.59	0	17,19,21	1.36	1 (5%)
4	NAG	g	300	-	14,14,15	0.47	0	17,19,21	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	235	-	14,14,15	0.50	0	17,19,21	0.97	1 (5%)
4	NAG	T	215	-	14,14,15	0.72	0	17,19,21	1.46	2 (11%)
4	NAG	L	400	-	14,14,15	0.59	0	17,19,21	0.92	0
4	NAG	W	215	-	14,14,15	0.61	0	17,19,21	0.98	1 (5%)
4	NAG	R	235	-	14,14,15	0.54	0	17,19,21	0.72	0
4	NAG	g	233	-	14,14,15	0.54	0	17,19,21	1.94	7 (41%)
4	NAG	I	300	-	14,14,15	0.53	0	17,19,21	1.43	2 (11%)
4	NAG	K	216	-	14,14,15	0.49	0	17,19,21	1.84	5 (29%)
4	NAG	R	234	-	14,14,15	0.36	0	17,19,21	2.38	4 (23%)
4	NAG	R	400	-	14,14,15	0.54	0	17,19,21	0.67	0
4	NAG	c	215	-	14,14,15	0.70	0	17,19,21	1.65	4 (23%)
4	NAG	O	235	-	14,14,15	0.50	0	17,19,21	1.00	1 (5%)
4	NAG	Z	215	-	14,14,15	0.60	0	17,19,21	1.57	2 (11%)
4	NAG	O	234	-	14,14,15	0.45	0	17,19,21	1.06	1 (5%)
4	NAG	E	215	-	14,14,15	0.73	0	17,19,21	1.51	2 (11%)
4	NAG	N	215	-	14,14,15	0.70	0	17,19,21	1.65	3 (17%)

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	C	400	-	-	2/6/23/26	0/1/1/1
4	NAG	i	215	-	-	3/6/23/26	0/1/1/1
4	NAG	O	400	-	-	2/6/23/26	0/1/1/1
4	NAG	F	300	-	-	3/6/23/26	0/1/1/1
4	NAG	U	300	-	-	4/6/23/26	0/1/1/1
4	NAG	K	215	-	-	4/6/23/26	0/1/1/1
4	NAG	L	234	-	-	4/6/23/26	0/1/1/1
4	NAG	I	400	-	-	2/6/23/26	0/1/1/1
4	NAG	R	233	-	-	0/6/23/26	0/1/1/1
4	NAG	F	233	-	-	2/6/23/26	0/1/1/1
4	NAG	U	233	-	-	2/6/23/26	0/1/1/1
4	NAG	a	300	-	-	2/6/23/26	0/1/1/1
4	NAG	I	235	-	-	2/6/23/26	0/1/1/1
4	NAG	X	300	-	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	Q	215	-	-	1/6/23/26	0/1/1/1
4	NAG	H	215	-	-	4/6/23/26	0/1/1/1
4	NAG	C	234	-	-	4/6/23/26	0/1/1/1
4	NAG	O	233	-	-	0/6/23/26	0/1/1/1
4	NAG	a	233	-	-	0/6/23/26	0/1/1/1
4	NAG	j	300	-	-	2/6/23/26	0/1/1/1
4	NAG	I	234	-	-	4/6/23/26	0/1/1/1
4	NAG	B	215	-	-	2/6/23/26	0/1/1/1
4	NAG	X	233	-	-	2/6/23/26	0/1/1/1
4	NAG	F	400	-	-	2/6/23/26	0/1/1/1
4	NAG	R	300	-	-	4/6/23/26	0/1/1/1
4	NAG	d	300	-	-	4/6/23/26	0/1/1/1
4	NAG	F	235	-	-	2/6/23/26	0/1/1/1
4	NAG	L	300	-	-	4/6/23/26	0/1/1/1
4	NAG	L	233	-	-	3/6/23/26	0/1/1/1
4	NAG	F	234	-	-	3/6/23/26	0/1/1/1
4	NAG	C	300	-	-	4/6/23/26	0/1/1/1
4	NAG	I	233	-	-	2/6/23/26	0/1/1/1
4	NAG	f	215	-	-	2/6/23/26	0/1/1/1
4	NAG	O	300	-	-	3/6/23/26	0/1/1/1
4	NAG	i	216	-	-	2/6/23/26	0/1/1/1
4	NAG	c	216	-	-	1/6/23/26	0/1/1/1
4	NAG	C	233	-	-	2/6/23/26	0/1/1/1
4	NAG	g	300	-	-	2/6/23/26	0/1/1/1
4	NAG	C	235	-	-	4/6/23/26	0/1/1/1
4	NAG	T	215	-	-	3/6/23/26	0/1/1/1
4	NAG	L	400	-	-	2/6/23/26	0/1/1/1
4	NAG	W	215	-	-	0/6/23/26	0/1/1/1
4	NAG	R	235	-	-	2/6/23/26	0/1/1/1
4	NAG	g	233	-	-	4/6/23/26	0/1/1/1
4	NAG	I	300	-	-	4/6/23/26	0/1/1/1
4	NAG	K	216	-	-	1/6/23/26	0/1/1/1
4	NAG	R	234	-	-	3/6/23/26	0/1/1/1
4	NAG	R	400	-	-	2/6/23/26	0/1/1/1
4	NAG	c	215	-	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	O	235	-	-	2/6/23/26	0/1/1/1
4	NAG	Z	215	-	-	5/6/23/26	0/1/1/1
4	NAG	O	234	-	-	3/6/23/26	0/1/1/1
4	NAG	E	215	-	-	2/6/23/26	0/1/1/1
4	NAG	N	215	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	234	NAG	C1-O5-C5	8.05	122.97	112.19
4	F	234	NAG	C1-O5-C5	6.31	120.64	112.19
4	a	233	NAG	C1-O5-C5	5.41	119.44	112.19
4	U	233	NAG	C1-O5-C5	5.10	119.02	112.19
4	Z	215	NAG	O5-C1-C2	5.02	119.06	111.29
4	I	234	NAG	C1-O5-C5	4.93	118.80	112.19
4	i	216	NAG	C1-O5-C5	4.91	118.76	112.19
4	c	216	NAG	C1-O5-C5	4.90	118.75	112.19
4	I	233	NAG	O5-C1-C2	-4.80	103.86	111.29
4	F	233	NAG	O5-C1-C2	-4.74	103.96	111.29
4	C	233	NAG	O5-C1-C2	-4.54	104.27	111.29
4	X	233	NAG	C1-O5-C5	4.41	118.10	112.19
4	O	233	NAG	O5-C1-C2	-4.39	104.50	111.29
4	K	215	NAG	C3-C4-C5	4.37	118.16	110.23
4	E	215	NAG	O5-C1-C2	-4.28	104.66	111.29
4	i	216	NAG	C4-C3-C2	-4.21	104.84	111.02
4	K	216	NAG	C4-C3-C2	-4.20	104.86	111.02
4	C	234	NAG	C1-O5-C5	4.16	117.75	112.19
4	R	234	NAG	O5-C1-C2	4.10	117.63	111.29
4	Q	215	NAG	C3-C4-C5	4.07	117.61	110.23
4	U	233	NAG	C4-C3-C2	-4.04	105.10	111.02
4	O	300	NAG	C1-O5-C5	3.98	117.51	112.19
4	c	215	NAG	C2-N2-C7	-3.97	117.57	122.90
4	K	215	NAG	O5-C1-C2	-3.97	105.14	111.29
4	R	300	NAG	O5-C1-C2	-3.91	105.24	111.29
4	F	233	NAG	C2-N2-C7	-3.86	117.72	122.90
4	N	215	NAG	C3-C4-C5	3.79	117.11	110.23
4	N	215	NAG	O5-C1-C2	-3.74	105.50	111.29
4	g	233	NAG	O5-C1-C2	-3.72	105.54	111.29
4	i	215	NAG	C3-C4-C5	3.59	116.75	110.23
4	L	300	NAG	O5-C1-C2	-3.55	105.80	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	f	215	NAG	O5-C1-C2	-3.53	105.82	111.29
4	R	233	NAG	O5-C1-C2	-3.46	105.94	111.29
4	O	300	NAG	C3-C4-C5	3.43	116.46	110.23
4	L	233	NAG	C3-C4-C5	3.41	116.41	110.23
4	X	233	NAG	C4-C3-C2	-3.35	106.11	111.02
4	H	215	NAG	C3-C4-C5	3.32	116.24	110.23
4	F	234	NAG	O5-C1-C2	3.30	116.40	111.29
4	Q	215	NAG	O5-C1-C2	-3.29	106.20	111.29
4	c	216	NAG	C3-C4-C5	3.27	116.16	110.23
4	X	233	NAG	O5-C5-C4	3.24	118.71	110.83
4	c	216	NAG	O5-C5-C4	3.24	118.70	110.83
4	g	233	NAG	C4-C3-C2	-3.23	106.28	111.02
4	C	300	NAG	C8-C7-N2	3.18	121.40	116.12
4	g	233	NAG	C2-N2-C7	-3.13	118.71	122.90
4	c	215	NAG	O5-C1-C2	-3.12	106.46	111.29
4	U	233	NAG	O5-C5-C4	3.05	118.24	110.83
4	K	216	NAG	O5-C1-C2	-3.03	106.60	111.29
4	R	233	NAG	C2-N2-C7	-3.02	118.85	122.90
4	Q	215	NAG	C1-O5-C5	3.01	116.22	112.19
4	L	234	NAG	C1-O5-C5	2.98	116.17	112.19
4	X	233	NAG	C3-C4-C5	2.97	115.62	110.23
4	O	235	NAG	C1-O5-C5	2.93	116.12	112.19
4	i	215	NAG	O5-C1-C2	-2.93	106.75	111.29
4	a	233	NAG	C4-C3-C2	-2.89	106.79	111.02
4	T	215	NAG	C1-O5-C5	-2.88	108.32	112.19
4	C	300	NAG	O5-C1-C2	-2.84	106.90	111.29
4	U	233	NAG	C3-C4-C5	2.83	115.37	110.23
4	a	233	NAG	O5-C5-C4	2.82	117.69	110.83
4	X	233	NAG	O5-C1-C2	-2.82	106.93	111.29
4	I	300	NAG	O5-C1-C2	-2.80	106.96	111.29
4	I	300	NAG	C3-C4-C5	2.79	115.29	110.23
4	T	215	NAG	C2-N2-C7	-2.78	119.17	122.90
4	F	300	NAG	C3-C4-C5	2.75	115.22	110.23
4	C	234	NAG	O5-C1-C2	2.74	115.54	111.29
4	c	216	NAG	C4-C3-C2	-2.74	107.00	111.02
4	Q	215	NAG	O5-C5-C4	2.72	117.45	110.83
4	O	234	NAG	O5-C5-C6	2.69	112.90	107.66
4	O	300	NAG	O5-C1-C2	-2.68	107.14	111.29
4	N	215	NAG	C2-N2-C7	-2.68	119.30	122.90
4	L	300	NAG	C2-N2-C7	-2.65	119.34	122.90
4	I	233	NAG	C3-C4-C5	2.65	115.03	110.23
4	O	300	NAG	O5-C5-C4	2.62	117.21	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	g	233	NAG	C3-C4-C5	2.62	114.97	110.23
4	g	233	NAG	O5-C5-C4	2.60	117.15	110.83
4	f	215	NAG	C3-C4-C5	2.57	114.89	110.23
4	R	300	NAG	C3-C4-C5	2.53	114.82	110.23
4	i	215	NAG	C1-O5-C5	-2.52	108.81	112.19
4	U	233	NAG	O5-C1-C2	-2.45	107.50	111.29
4	O	233	NAG	C3-C4-C5	2.42	114.62	110.23
4	K	216	NAG	C2-N2-C7	-2.42	119.66	122.90
4	g	233	NAG	C1-C2-N2	2.42	114.24	110.43
4	C	234	NAG	C6-C5-C4	-2.41	107.09	113.02
4	i	216	NAG	O5-C1-C2	-2.40	107.57	111.29
4	X	233	NAG	C2-N2-C7	-2.39	119.70	122.90
4	i	216	NAG	C2-N2-C7	-2.38	119.70	122.90
4	i	216	NAG	O5-C5-C4	2.38	116.61	110.83
4	Z	215	NAG	C1-O5-C5	2.38	115.37	112.19
4	f	215	NAG	O4-C4-C3	-2.38	104.78	110.38
4	K	216	NAG	C1-O5-C5	2.36	115.35	112.19
4	H	215	NAG	O5-C1-C2	-2.35	107.65	111.29
4	i	216	NAG	C1-C2-N2	2.33	114.11	110.43
4	g	233	NAG	C1-O5-C5	2.33	115.30	112.19
4	a	233	NAG	C3-C4-C5	2.31	114.42	110.23
4	K	216	NAG	O5-C5-C4	2.31	116.44	110.83
4	Q	215	NAG	C2-N2-C7	-2.31	119.81	122.90
4	L	300	NAG	C3-C4-C5	2.30	114.41	110.23
4	c	215	NAG	C3-C4-C5	2.30	114.40	110.23
4	E	215	NAG	C3-C4-C5	2.27	114.36	110.23
4	C	300	NAG	O7-C7-C8	-2.27	118.00	122.05
4	C	400	NAG	O5-C1-C2	-2.25	107.81	111.29
4	K	215	NAG	C6-C5-C4	-2.24	107.51	113.02
4	F	300	NAG	O5-C1-C2	-2.21	107.86	111.29
4	C	235	NAG	C2-N2-C7	-2.20	119.96	122.90
4	K	215	NAG	O5-C5-C4	2.14	116.04	110.83
4	W	215	NAG	O4-C4-C3	-2.12	105.38	110.38
4	R	234	NAG	C4-C3-C2	-2.09	107.95	111.02
4	R	234	NAG	O5-C5-C4	2.09	115.91	110.83
4	B	215	NAG	O5-C1-C2	-2.09	108.06	111.29
4	F	233	NAG	C3-C4-C5	2.09	114.02	110.23
4	C	300	NAG	C4-C3-C2	-2.06	108.00	111.02
4	c	215	NAG	O4-C4-C3	-2.03	105.60	110.38
4	a	300	NAG	O5-C1-C2	-2.03	108.16	111.29

There are no chirality outliers.

All (135) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	234	NAG	C3-C2-N2-C7
4	C	300	NAG	C8-C7-N2-C2
4	C	300	NAG	O7-C7-N2-C2
4	C	400	NAG	C8-C7-N2-C2
4	C	400	NAG	O7-C7-N2-C2
4	F	234	NAG	C3-C2-N2-C7
4	F	234	NAG	C8-C7-N2-C2
4	F	234	NAG	O7-C7-N2-C2
4	F	300	NAG	C8-C7-N2-C2
4	F	300	NAG	O7-C7-N2-C2
4	F	400	NAG	C8-C7-N2-C2
4	F	400	NAG	O7-C7-N2-C2
4	I	234	NAG	C3-C2-N2-C7
4	I	234	NAG	C8-C7-N2-C2
4	I	234	NAG	O7-C7-N2-C2
4	I	300	NAG	C8-C7-N2-C2
4	I	300	NAG	O7-C7-N2-C2
4	I	400	NAG	C8-C7-N2-C2
4	I	400	NAG	O7-C7-N2-C2
4	K	215	NAG	O7-C7-N2-C2
4	L	233	NAG	C8-C7-N2-C2
4	L	233	NAG	O7-C7-N2-C2
4	L	300	NAG	C8-C7-N2-C2
4	L	300	NAG	O7-C7-N2-C2
4	L	400	NAG	C8-C7-N2-C2
4	L	400	NAG	O7-C7-N2-C2
4	O	234	NAG	C3-C2-N2-C7
4	O	234	NAG	C8-C7-N2-C2
4	O	234	NAG	O7-C7-N2-C2
4	O	235	NAG	C8-C7-N2-C2
4	O	235	NAG	O7-C7-N2-C2
4	O	400	NAG	C8-C7-N2-C2
4	O	400	NAG	O7-C7-N2-C2
4	R	234	NAG	C3-C2-N2-C7
4	R	234	NAG	C8-C7-N2-C2
4	R	234	NAG	O7-C7-N2-C2
4	R	300	NAG	C8-C7-N2-C2
4	R	300	NAG	O7-C7-N2-C2
4	R	400	NAG	C8-C7-N2-C2
4	R	400	NAG	O7-C7-N2-C2
4	X	300	NAG	C8-C7-N2-C2
4	X	300	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	d	300	NAG	C8-C7-N2-C2
4	d	300	NAG	O7-C7-N2-C2
4	g	300	NAG	C8-C7-N2-C2
4	g	300	NAG	O7-C7-N2-C2
4	j	300	NAG	C8-C7-N2-C2
4	j	300	NAG	O7-C7-N2-C2
4	K	215	NAG	C8-C7-N2-C2
4	i	216	NAG	C8-C7-N2-C2
4	i	216	NAG	O7-C7-N2-C2
4	L	300	NAG	O5-C5-C6-O6
4	g	233	NAG	O5-C5-C6-O6
4	f	215	NAG	C4-C5-C6-O6
4	L	300	NAG	C4-C5-C6-O6
4	g	233	NAG	C4-C5-C6-O6
4	E	215	NAG	C8-C7-N2-C2
4	E	215	NAG	O7-C7-N2-C2
4	I	235	NAG	C8-C7-N2-C2
4	i	215	NAG	C8-C7-N2-C2
4	i	215	NAG	O7-C7-N2-C2
4	f	215	NAG	O5-C5-C6-O6
4	C	235	NAG	C4-C5-C6-O6
4	C	235	NAG	C8-C7-N2-C2
4	I	235	NAG	O7-C7-N2-C2
4	I	233	NAG	C4-C5-C6-O6
4	C	235	NAG	O5-C5-C6-O6
4	C	235	NAG	O7-C7-N2-C2
4	F	235	NAG	C8-C7-N2-C2
4	F	235	NAG	O7-C7-N2-C2
4	L	234	NAG	C8-C7-N2-C2
4	L	234	NAG	O7-C7-N2-C2
4	O	300	NAG	C8-C7-N2-C2
4	O	300	NAG	O7-C7-N2-C2
4	R	235	NAG	C8-C7-N2-C2
4	R	235	NAG	O7-C7-N2-C2
4	U	300	NAG	C8-C7-N2-C2
4	U	300	NAG	O7-C7-N2-C2
4	Z	215	NAG	C8-C7-N2-C2
4	a	300	NAG	C8-C7-N2-C2
4	a	300	NAG	O7-C7-N2-C2
4	I	233	NAG	O5-C5-C6-O6
4	I	300	NAG	O5-C5-C6-O6
4	L	234	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	R	300	NAG	O5-C5-C6-O6
4	L	234	NAG	C4-C5-C6-O6
4	F	233	NAG	C8-C7-N2-C2
4	T	215	NAG	C8-C7-N2-C2
4	C	300	NAG	C4-C5-C6-O6
4	B	215	NAG	C4-C5-C6-O6
4	C	300	NAG	O5-C5-C6-O6
4	X	300	NAG	C4-C5-C6-O6
4	Z	215	NAG	O7-C7-N2-C2
4	X	300	NAG	O5-C5-C6-O6
4	C	233	NAG	C8-C7-N2-C2
4	T	215	NAG	O7-C7-N2-C2
4	F	300	NAG	O5-C5-C6-O6
4	U	300	NAG	C4-C5-C6-O6
4	U	300	NAG	O5-C5-C6-O6
4	U	233	NAG	C8-C7-N2-C2
4	g	233	NAG	C8-C7-N2-C2
4	d	300	NAG	C4-C5-C6-O6
4	C	234	NAG	C8-C7-N2-C2
4	F	233	NAG	O7-C7-N2-C2
4	B	215	NAG	O5-C5-C6-O6
4	d	300	NAG	O5-C5-C6-O6
4	K	215	NAG	O5-C5-C6-O6
4	L	233	NAG	C3-C2-N2-C7
4	c	215	NAG	O5-C5-C6-O6
4	C	233	NAG	O7-C7-N2-C2
4	U	233	NAG	O7-C7-N2-C2
4	I	234	NAG	C4-C5-C6-O6
4	K	215	NAG	C4-C5-C6-O6
4	g	233	NAG	O7-C7-N2-C2
4	C	234	NAG	O7-C7-N2-C2
4	H	215	NAG	C8-C7-N2-C2
4	X	233	NAG	C8-C7-N2-C2
4	c	215	NAG	C8-C7-N2-C2
4	H	215	NAG	O7-C7-N2-C2
4	Z	215	NAG	C4-C5-C6-O6
4	O	300	NAG	O5-C5-C6-O6
4	X	233	NAG	O7-C7-N2-C2
4	c	216	NAG	C4-C5-C6-O6
4	T	215	NAG	C4-C5-C6-O6
4	C	234	NAG	C1-C2-N2-C7
4	Z	215	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	c	215	NAG	O7-C7-N2-C2
4	K	216	NAG	C8-C7-N2-C2
4	Q	215	NAG	C8-C7-N2-C2
4	I	300	NAG	C4-C5-C6-O6
4	H	215	NAG	O5-C5-C6-O6
4	R	300	NAG	C4-C5-C6-O6
4	Z	215	NAG	O5-C5-C6-O6
4	H	215	NAG	C4-C5-C6-O6
4	i	215	NAG	O5-C5-C6-O6

There are no ring outliers.

41 monomers are involved in 118 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	400	NAG	2	0
4	i	215	NAG	2	0
4	F	300	NAG	3	0
4	U	300	NAG	5	0
4	K	215	NAG	8	0
4	F	233	NAG	2	0
4	U	233	NAG	2	0
4	a	300	NAG	4	0
4	X	300	NAG	4	0
4	Q	215	NAG	4	0
4	H	215	NAG	5	0
4	C	234	NAG	4	0
4	O	233	NAG	1	0
4	j	300	NAG	4	0
4	B	215	NAG	3	0
4	X	233	NAG	2	0
4	F	400	NAG	3	0
4	R	300	NAG	4	0
4	d	300	NAG	3	0
4	F	235	NAG	1	0
4	L	300	NAG	4	0
4	L	233	NAG	2	0
4	F	234	NAG	2	0
4	C	300	NAG	5	0
4	I	233	NAG	1	0
4	f	215	NAG	3	0
4	O	300	NAG	4	0
4	g	300	NAG	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	T	215	NAG	5	0
4	W	215	NAG	5	0
4	R	235	NAG	1	0
4	g	233	NAG	1	0
4	I	300	NAG	3	0
4	K	216	NAG	4	0
4	R	234	NAG	1	0
4	c	215	NAG	1	0
4	O	235	NAG	1	0
4	Z	215	NAG	3	0
4	O	234	NAG	4	0
4	E	215	NAG	6	0
4	N	215	NAG	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	121/136 (88%)	0.09	3 (2%) 58 40	39, 76, 123, 170	0
1	D	121/136 (88%)	0.31	4 (3%) 49 34	34, 71, 130, 159	0
1	G	121/136 (88%)	0.18	4 (3%) 49 34	35, 75, 134, 184	0
1	J	121/136 (88%)	0.21	5 (4%) 41 30	30, 73, 117, 142	0
1	M	121/136 (88%)	0.21	7 (5%) 29 23	37, 75, 126, 167	0
1	P	121/136 (88%)	0.06	2 (1%) 69 47	30, 73, 128, 153	0
1	S	121/136 (88%)	0.19	4 (3%) 49 34	46, 91, 137, 201	0
1	V	121/136 (88%)	0.81	16 (13%) 7 10	24, 88, 151, 419	0
1	Y	120/136 (88%)	0.41	8 (6%) 24 20	45, 100, 152, 199	0
1	b	119/136 (87%)	0.28	1 (0%) 82 62	45, 96, 153, 177	0
1	e	121/136 (88%)	0.70	11 (9%) 15 16	22, 80, 131, 165	0
1	h	121/136 (88%)	0.46	4 (3%) 49 34	50, 93, 132, 185	0
2	B	195/217 (89%)	0.17	3 (1%) 72 50	45, 76, 126, 155	0
2	E	196/217 (90%)	0.30	5 (2%) 57 39	30, 74, 118, 190	0
2	H	196/217 (90%)	0.14	5 (2%) 57 39	41, 73, 122, 150	0
2	K	196/217 (90%)	0.35	5 (2%) 57 39	25, 72, 117, 135	0
2	N	195/217 (89%)	0.11	1 (0%) 87 71	43, 74, 111, 141	0
2	Q	195/217 (89%)	0.15	6 (3%) 51 35	29, 69, 111, 146	0
2	T	196/217 (90%)	0.41	5 (2%) 57 39	36, 89, 140, 175	0
2	W	196/217 (90%)	0.30	7 (3%) 46 32	25, 88, 138, 210	0
2	Z	196/217 (90%)	0.26	7 (3%) 46 32	45, 80, 125, 176	0
2	c	196/217 (90%)	0.40	10 (5%) 33 25	46, 82, 138, 208	0
2	f	196/217 (90%)	0.28	5 (2%) 57 39	23, 85, 133, 168	0
2	i	196/217 (90%)	0.40	6 (3%) 51 35	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%)	0.54	12 (6%) 25 21	42, 93, 157, 226	0
3	F	186/202 (92%)	0.68	24 (12%) 7 11	33, 86, 149, 214	0
3	I	188/202 (93%)	0.33	5 (2%) 56 38	56, 90, 158, 217	0
3	L	191/202 (94%)	0.57	13 (6%) 23 20	21, 82, 153, 218	0
3	O	191/202 (94%)	0.43	16 (8%) 17 17	38, 88, 156, 196	0
3	R	188/202 (93%)	0.27	4 (2%) 63 44	41, 86, 154, 231	0
3	U	191/202 (94%)	0.77	15 (7%) 18 17	83, 151, 224, 267	0
3	X	191/202 (94%)	0.81	15 (7%) 18 17	81, 156, 229, 291	0
3	a	191/202 (94%)	1.01	27 (14%) 6 9	80, 149, 221, 369	0
3	d	191/202 (94%)	0.77	18 (9%) 14 16	77, 149, 229, 281	0
3	g	191/202 (94%)	0.74	14 (7%) 21 19	82, 143, 195, 287	0
3	j	191/202 (94%)	0.77	22 (11%) 9 12	69, 140, 196, 284	0
All	All	6076/6660 (91%)	0.42	319 (5%) 32 24	21, 90, 178, 419	0

All (319) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	159	HIS	7.5
3	F	156	PHE	6.4
1	V	83	ARG	5.3
3	a	156	PHE	5.0
3	d	71	ASN	5.0
3	L	181	ASP	4.8
1	V	91	VAL	4.8
3	d	58	PRO	4.6
1	e	52	GLU	4.6
3	F	208	LEU	4.5
2	c	112	LEU	4.5
3	L	184	HIS	4.5
2	E	171	THR	4.4
1	h	133	THR	4.3
3	L	182	TYR	4.3
1	A	131	THR	4.3
1	Y	77	ASN	4.3
3	a	40	CYS	4.2
3	F	182	TYR	4.1
3	F	191	VAL	4.1
1	V	92	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
3	d	148	LEU	4.0
3	a	45	VAL	4.0
3	a	36	PRO	3.9
2	W	139	LEU	3.9
1	V	38	ARG	3.9
2	f	97	ASP	3.9
2	c	24	GLN	3.9
3	R	159	HIS	3.8
3	d	194	GLN	3.8
2	Z	204	ARG	3.7
1	P	48	LYS	3.7
3	U	58	PRO	3.7
3	a	50	CYS	3.7
2	f	76	ASP	3.7
3	d	191	VAL	3.7
2	c	113	GLN	3.7
3	O	184	HIS	3.6
3	R	109	GLN	3.6
1	M	27	GLY	3.6
1	Y	106	GLU	3.6
1	V	42	PHE	3.6
3	F	183	ARG	3.6
2	W	97	ASP	3.6
3	L	171	TRP	3.5
1	S	77	ASN	3.5
3	j	43	PHE	3.5
3	O	213	GLN	3.5
3	I	159	HIS	3.5
1	V	39	MET	3.4
3	d	45	VAL	3.4
3	L	55	SER	3.3
1	V	52	GLU	3.3
2	i	189	GLY	3.3
3	g	34	PRO	3.3
2	E	138	HIS	3.3
3	R	157	LEU	3.3
3	d	156	PHE	3.2
3	d	108	VAL	3.2
2	K	40	ASP	3.2
3	g	108	VAL	3.2
3	X	221	PRO	3.2
2	Q	13	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
3	g	55	SER	3.2
1	V	82	PRO	3.2
2	B	89	ARG	3.2
3	a	39	GLN	3.2
3	a	182	TYR	3.2
1	V	132	LEU	3.2
3	U	39	GLN	3.1
3	j	109	GLN	3.1
1	e	93	VAL	3.1
3	X	58	PRO	3.1
3	O	171	TRP	3.1
3	R	156	PHE	3.1
2	H	78	VAL	3.1
2	c	81	ARG	3.1
1	D	6	SER	3.0
3	X	38	VAL	3.0
3	F	75	ASP	3.0
3	F	181	ASP	3.0
3	g	113	PRO	3.0
3	C	173	HIS	3.0
3	X	173	HIS	3.0
3	j	159	HIS	3.0
1	S	31	TYR	3.0
2	i	138	HIS	3.0
1	e	67	GLU	3.0
3	j	122	GLN	3.0
3	C	157	LEU	2.9
2	K	144	ARG	2.9
3	F	206	ASN	2.9
2	Z	17	GLN	2.9
3	O	61	THR	2.9
3	U	156	PHE	2.9
2	W	120	HIS	2.9
3	X	156	PHE	2.9
3	j	71	ASN	2.9
3	F	187	SER	2.8
3	j	56	SER	2.8
2	E	137	ARG	2.8
1	Y	74	HIS	2.8
3	L	72	SER	2.8
3	U	145	GLU	2.8
3	j	87	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	S	7	THR	2.8
3	F	199	PHE	2.8
3	C	110	LEU	2.8
2	T	24	GLN	2.8
3	O	59	GLN	2.8
1	M	78	PHE	2.8
2	Q	137	ARG	2.8
3	U	55	SER	2.8
3	a	60	PRO	2.8
3	F	167	TYR	2.8
1	P	27	GLY	2.8
1	e	77	ASN	2.8
3	X	71	ASN	2.8
3	F	173	HIS	2.7
3	d	192	ASP	2.7
3	a	108	VAL	2.7
2	H	98	PHE	2.7
2	W	203	PHE	2.7
1	e	87	SER	2.7
2	Z	178	TYR	2.7
3	F	184	HIS	2.7
3	j	36	PRO	2.7
1	M	31	TYR	2.7
3	g	51	THR	2.7
3	d	81	SER	2.7
2	W	31	THR	2.7
1	J	48	LYS	2.7
1	e	83	ARG	2.6
3	j	60	PRO	2.6
2	K	137	ARG	2.6
3	U	117	ARG	2.6
3	X	89	ILE	2.6
1	G	31	TYR	2.6
3	F	190	SER	2.6
1	V	54	LYS	2.6
3	I	113	PRO	2.6
3	C	151	ASN	2.6
1	D	83	ARG	2.6
3	a	189	PRO	2.6
3	O	73	ASP	2.6
3	a	54	SER	2.6
3	j	39	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
3	g	170	ASP	2.6
1	h	22	GLN	2.6
2	Q	79	THR	2.5
3	F	149	GLU	2.5
2	H	97	ASP	2.5
3	X	73	ASP	2.5
3	L	222	ILE	2.5
3	g	173	HIS	2.5
1	Y	76	LYS	2.5
1	G	38	ARG	2.5
3	O	113	PRO	2.5
1	Y	8	LYS	2.5
1	J	103	PHE	2.5
1	D	133	THR	2.5
2	Q	36	HIS	2.5
1	e	95	GLU	2.5
2	T	197	TRP	2.5
2	Z	86	GLU	2.5
2	c	165	GLU	2.5
3	U	133	TRP	2.5
3	j	185	LYS	2.5
3	j	34	PRO	2.5
1	V	40	LEU	2.5
3	F	161	LEU	2.5
3	I	182	TYR	2.5
3	X	159	HIS	2.5
1	J	15	GLU	2.5
3	a	177	GLU	2.5
3	U	171	TRP	2.5
1	J	8	LYS	2.5
2	c	84	CYS	2.5
3	O	112	ASP	2.5
2	B	31	THR	2.5
3	g	90	THR	2.5
3	a	42	VAL	2.5
3	U	173	HIS	2.4
1	Y	20	ASP	2.4
2	K	138	HIS	2.4
3	a	52	TRP	2.4
1	V	88	ASN	2.4
2	f	81	ARG	2.4
2	i	204	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	133	THR	2.4
2	i	206	LYS	2.4
3	I	40	CYS	2.4
1	G	74	HIS	2.4
2	E	36	HIS	2.4
3	F	34	PRO	2.4
2	Z	149	GLY	2.4
1	M	6	SER	2.4
1	A	68	GLU	2.4
2	c	120	HIS	2.4
3	g	58	PRO	2.4
3	X	86	SER	2.4
2	c	168	CYS	2.4
2	f	24	GLN	2.4
3	j	50	CYS	2.4
1	V	30	ASN	2.4
3	d	34	PRO	2.4
3	C	35	LEU	2.4
2	B	54	SER	2.3
3	a	86	SER	2.3
3	U	123	MET	2.3
1	J	109	ASP	2.3
1	M	80	PHE	2.3
3	L	173	HIS	2.3
3	C	154	ASN	2.3
1	D	20	ASP	2.3
3	L	113	PRO	2.3
3	d	214	HIS	2.3
3	C	156	PHE	2.3
3	F	150	LEU	2.3
3	C	75	ASP	2.3
3	O	37	GLU	2.3
3	L	183	ARG	2.3
3	F	157	LEU	2.3
1	h	8	LYS	2.3
3	a	159	HIS	2.3
3	d	133	TRP	2.3
3	I	156	PHE	2.3
3	d	106	PHE	2.3
3	F	103	TYR	2.3
1	e	43	LYS	2.3
3	O	60	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	c	171	THR	2.2
3	d	147	GLN	2.2
3	d	107	VAL	2.2
3	L	73	ASP	2.2
3	d	143	LEU	2.2
3	L	154	ASN	2.2
3	X	133	TRP	2.2
3	j	133	TRP	2.2
1	Y	9	LYS	2.2
1	e	86	VAL	2.2
3	j	37	GLU	2.2
2	T	175	ASP	2.2
3	O	156	PHE	2.2
3	d	74	ASN	2.2
2	H	138	HIS	2.2
3	C	141	HIS	2.2
2	N	56	ALA	2.2
2	T	144	ARG	2.2
1	S	15	GLU	2.2
3	F	207	PRO	2.2
3	a	34	PRO	2.2
2	c	31	THR	2.2
1	V	84	ASP	2.2
3	O	79	LYS	2.2
3	a	125	LYS	2.2
2	W	96	GLN	2.2
2	Z	113	GLN	2.2
3	C	150	LEU	2.2
3	O	182	TYR	2.2
3	X	45	VAL	2.2
1	V	78	PHE	2.2
3	j	156	PHE	2.2
3	F	194	GLN	2.2
3	a	188	LEU	2.2
2	f	91	ARG	2.2
3	j	107	VAL	2.2
3	X	34	PRO	2.2
3	g	37	GLU	2.2
1	e	96	LEU	2.2
3	a	192	ASP	2.1
3	U	87	GLU	2.1
3	g	198	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	h	39	MET	2.1
2	W	129	SER	2.1
2	i	129	SER	2.1
1	V	31	TYR	2.1
3	g	60	PRO	2.1
3	g	157	LEU	2.1
3	L	117	ARG	2.1
3	a	74	ASN	2.1
1	e	20	ASP	2.1
1	A	110	GLU	2.1
3	a	64	THR	2.1
3	F	211	SER	2.1
2	K	184	VAL	2.1
3	U	192	ASP	2.1
3	a	157	LEU	2.1
3	U	51	THR	2.1
1	M	11	GLN	2.1
3	a	107	VAL	2.1
3	j	84	LEU	2.1
3	g	66	HIS	2.1
3	C	73	ASP	2.1
3	U	34	PRO	2.1
3	j	58	PRO	2.1
1	Y	131	THR	2.1
2	E	170	GLU	2.1
2	Z	46	GLN	2.1
3	O	104	GLN	2.1
3	j	106	PHE	2.1
2	T	114	VAL	2.1
3	X	60	PRO	2.0
2	H	81	ARG	2.0
3	U	185	LYS	2.0
3	j	57	GLU	2.0
1	G	57	GLN	2.0
3	a	77	VAL	2.0
3	a	49	ASN	2.0
3	O	197	TYR	2.0
2	i	185	LYS	2.0
3	C	70	LYS	2.0
2	Q	86	GLU	2.0
2	Q	88	VAL	2.0
1	b	131	THR	2.0

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Mol	Chain	Res	Type	RSRZ
3	a	214	HIS	2.0
3	X	68	TRP	2.0
3	O	181	ASP	2.0
3	j	55	SER	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 oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	O	400	14/15	0.31	0.21	139,147,151,153	0
4	NAG	a	300	14/15	0.36	0.14	123,141,146,148	0
4	NAG	d	300	14/15	0.36	0.20	176,185,189,191	0
4	NAG	X	300	14/15	0.40	0.14	195,203,206,208	0
4	NAG	g	300	14/15	0.40	0.19	157,173,179,182	0
4	NAG	a	233	14/15	0.41	0.19	119,129,137,142	0
4	NAG	L	400	14/15	0.41	0.20	198,202,205,206	0
4	NAG	I	235	14/15	0.43	0.18	131,142,148,150	0
4	NAG	F	400	14/15	0.47	0.22	158,167,171,172	0
4	NAG	j	300	14/15	0.50	0.17	162,174,182,183	0
4	NAG	F	235	14/15	0.53	0.14	137,148,151,153	0
4	NAG	I	400	14/15	0.53	0.19	161,169,176,177	0
4	NAG	R	235	14/15	0.54	0.12	138,149,151,152	0
4	NAG	R	400	14/15	0.54	0.20	200,203,210,211	0
4	NAG	C	300	14/15	0.62	0.19	61,73,86,95	0
4	NAG	i	216	14/15	0.67	0.17	128,143,156,164	0
4	NAG	O	235	14/15	0.68	0.13	91,111,120,122	0
4	NAG	C	235	14/15	0.69	0.14	108,136,143,147	0
4	NAG	F	300	14/15	0.70	0.14	69,80,84,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	L	234	14/15	0.70	0.13	120,132,140,140	0
4	NAG	X	233	14/15	0.71	0.14	120,128,156,157	0
4	NAG	U	233	14/15	0.73	0.19	98,118,139,142	0
4	NAG	U	300	14/15	0.74	0.14	172,177,180,182	0
4	NAG	L	300	14/15	0.75	0.14	88,97,104,106	0
4	NAG	C	400	14/15	0.76	0.14	153,161,167,167	0
4	NAG	O	300	14/15	0.77	0.17	86,91,109,113	0
4	NAG	I	300	14/15	0.80	0.12	51,83,96,99	0
4	NAG	O	233	14/15	0.81	0.14	70,78,86,93	0
4	NAG	c	216	14/15	0.81	0.13	91,113,121,123	0
4	NAG	K	216	14/15	0.82	0.16	78,88,92,93	0
4	NAG	R	300	14/15	0.82	0.12	79,87,94,96	0
4	NAG	F	234	14/15	0.85	0.13	81,109,119,125	0
4	NAG	g	233	14/15	0.86	0.11	114,126,139,140	0
4	NAG	C	233	14/15	0.86	0.12	79,85,94,97	0
4	NAG	C	234	14/15	0.87	0.11	89,105,113,116	0
4	NAG	I	233	14/15	0.87	0.12	64,81,91,92	0
4	NAG	R	234	14/15	0.88	0.10	94,111,117,122	0
4	NAG	F	233	14/15	0.88	0.12	81,91,97,97	0
4	NAG	W	215	14/15	0.89	0.11	62,71,83,86	0
4	NAG	O	234	14/15	0.89	0.09	59,77,90,93	0
4	NAG	L	233	14/15	0.89	0.09	66,89,100,106	0
4	NAG	Z	215	14/15	0.89	0.12	68,76,81,85	0
4	NAG	I	234	14/15	0.90	0.10	78,101,110,111	0
4	NAG	R	233	14/15	0.91	0.12	74,84,92,93	0
4	NAG	c	215	14/15	0.91	0.10	58,66,80,84	0
4	NAG	T	215	14/15	0.91	0.12	38,53,67,68	0
4	NAG	K	215	14/15	0.91	0.12	57,65,73,77	0
4	NAG	i	215	14/15	0.93	0.09	52,67,74,82	0
4	NAG	E	215	14/15	0.93	0.10	35,58,79,86	0
4	NAG	f	215	14/15	0.93	0.09	63,70,87,90	0
4	NAG	B	215	14/15	0.94	0.10	33,46,76,79	0
4	NAG	N	215	14/15	0.94	0.08	47,54,79,80	0
4	NAG	Q	215	14/15	0.95	0.10	38,48,65,67	0
4	NAG	H	215	14/15	0.95	0.09	41,53,80,89	0

6.5 Other polymers (i)

There are no such residues in this entry.