Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 07:49 PM EDT

PDB ID	:	5BWK
Title	:	6.0 A Crystal structure of a Get3-Get4-Get5 intermediate complex from S.cerevisiae
Authors	:	Gristick, H.B.; Chartron, J.W.; Clemons, W.M.
Deposited on	:	2015-06-08
Resolution	:	6.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

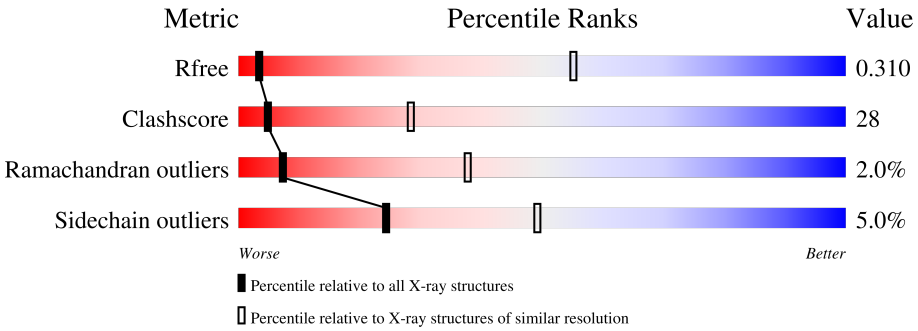
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1000 (8.00-3.88)
Clashscore	141614	1049 (8.00-3.90)
Ramachandran outliers	138981	1016 (8.00-3.86)
Sidechain outliers	138945	1017 (8.00-3.82)

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%

Mol	Chain	Length	Quality of chain
1	A	373	36% 40% 6% 18%
1	B	373	39% 38% 5% 18%
1	C	373	37% 39% 6% 18%
1	D	373	39% 38% 5% 18%
1	M	373	39% 36% 6% 18%
1	N	373	39% 36% 6% 18%
1	O	373	37% 40% 5% 18%

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Mol	Chain	Length	Quality of chain
1	P	373	40% 36% 5% 18%
2	E	319	61% 29% 9%
2	G	319	61% 29% 9%
2	I	319	62% 28% 9%
2	K	319	62% 28% 9%
2	Q	319	64% 26% 9%
2	S	319	60% 30% 9%
2	U	319	61% 29% 9%
2	W	319	62% 28% 9%
3	F	56	64% 32%
3	H	56	62% 34%
3	J	56	59% 38%
3	L	56	62% 34%
3	R	56	61% 36%
3	T	56	62% 32%
3	V	56	54% 43%
3	X	56	61% 36%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 41907 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 ATPase GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2402	1522	399	464	17			
1	B	304	Total	C	N	O	S	0	0	0
			2402	1522	399	464	17			
1	D	304	Total	C	N	O	S	0	0	0
			2402	1522	399	464	17			
1	M	304	Total	C	N	O	S	0	0	0
			2402	1522	399	464	17			
1	N	304	Total	C	N	O	S	0	0	0
			2402	1522	399	464	17			
1	O	304	Total	C	N	O	S	0	0	0
			2402	1522	399	464	17			
1	P	304	Total	C	N	O	S	0	0	0
			2402	1522	399	464	17			
1	C	304	Total	C	N	O	S	0	0	0
			2402	1522	399	464	17			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP B3LGZ3
A	-17	GLY	-	expression tag	UNP B3LGZ3
A	-16	GLY	-	expression tag	UNP B3LGZ3
A	-15	SER	-	expression tag	UNP B3LGZ3
A	-14	HIS	-	expression tag	UNP B3LGZ3
A	-13	HIS	-	expression tag	UNP B3LGZ3
A	-12	HIS	-	expression tag	UNP B3LGZ3
A	-11	HIS	-	expression tag	UNP B3LGZ3
A	-10	HIS	-	expression tag	UNP B3LGZ3
A	-9	HIS	-	expression tag	UNP B3LGZ3
A	-8	GLY	-	expression tag	UNP B3LGZ3
A	-7	GLU	-	expression tag	UNP B3LGZ3
A	-6	ASN	-	expression tag	UNP B3LGZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	expression tag	UNP B3LGZ3
A	-4	TYR	-	expression tag	UNP B3LGZ3
A	-3	PHE	-	expression tag	UNP B3LGZ3
A	-2	GLN	-	expression tag	UNP B3LGZ3
A	-1	SER	-	expression tag	UNP B3LGZ3
A	0	VAL	-	expression tag	UNP B3LGZ3
A	1	ASP	-	expression tag	UNP B3LGZ3
B	-18	MET	-	initiating methionine	UNP B3LGZ3
B	-17	GLY	-	expression tag	UNP B3LGZ3
B	-16	GLY	-	expression tag	UNP B3LGZ3
B	-15	SER	-	expression tag	UNP B3LGZ3
B	-14	HIS	-	expression tag	UNP B3LGZ3
B	-13	HIS	-	expression tag	UNP B3LGZ3
B	-12	HIS	-	expression tag	UNP B3LGZ3
B	-11	HIS	-	expression tag	UNP B3LGZ3
B	-10	HIS	-	expression tag	UNP B3LGZ3
B	-9	HIS	-	expression tag	UNP B3LGZ3
B	-8	GLY	-	expression tag	UNP B3LGZ3
B	-7	GLU	-	expression tag	UNP B3LGZ3
B	-6	ASN	-	expression tag	UNP B3LGZ3
B	-5	LEU	-	expression tag	UNP B3LGZ3
B	-4	TYR	-	expression tag	UNP B3LGZ3
B	-3	PHE	-	expression tag	UNP B3LGZ3
B	-2	GLN	-	expression tag	UNP B3LGZ3
B	-1	SER	-	expression tag	UNP B3LGZ3
B	0	VAL	-	expression tag	UNP B3LGZ3
B	1	ASP	-	expression tag	UNP B3LGZ3
D	-18	MET	-	initiating methionine	UNP B3LGZ3
D	-17	GLY	-	expression tag	UNP B3LGZ3
D	-16	GLY	-	expression tag	UNP B3LGZ3
D	-15	SER	-	expression tag	UNP B3LGZ3
D	-14	HIS	-	expression tag	UNP B3LGZ3
D	-13	HIS	-	expression tag	UNP B3LGZ3
D	-12	HIS	-	expression tag	UNP B3LGZ3
D	-11	HIS	-	expression tag	UNP B3LGZ3
D	-10	HIS	-	expression tag	UNP B3LGZ3
D	-9	HIS	-	expression tag	UNP B3LGZ3
D	-8	GLY	-	expression tag	UNP B3LGZ3
D	-7	GLU	-	expression tag	UNP B3LGZ3
D	-6	ASN	-	expression tag	UNP B3LGZ3
D	-5	LEU	-	expression tag	UNP B3LGZ3
D	-4	TYR	-	expression tag	UNP B3LGZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	PHE	-	expression tag	UNP B3LGZ3
D	-2	GLN	-	expression tag	UNP B3LGZ3
D	-1	SER	-	expression tag	UNP B3LGZ3
D	0	VAL	-	expression tag	UNP B3LGZ3
D	1	ASP	-	expression tag	UNP B3LGZ3
M	-18	MET	-	initiating methionine	UNP B3LGZ3
M	-17	GLY	-	expression tag	UNP B3LGZ3
M	-16	GLY	-	expression tag	UNP B3LGZ3
M	-15	SER	-	expression tag	UNP B3LGZ3
M	-14	HIS	-	expression tag	UNP B3LGZ3
M	-13	HIS	-	expression tag	UNP B3LGZ3
M	-12	HIS	-	expression tag	UNP B3LGZ3
M	-11	HIS	-	expression tag	UNP B3LGZ3
M	-10	HIS	-	expression tag	UNP B3LGZ3
M	-9	HIS	-	expression tag	UNP B3LGZ3
M	-8	GLY	-	expression tag	UNP B3LGZ3
M	-7	GLU	-	expression tag	UNP B3LGZ3
M	-6	ASN	-	expression tag	UNP B3LGZ3
M	-5	LEU	-	expression tag	UNP B3LGZ3
M	-4	TYR	-	expression tag	UNP B3LGZ3
M	-3	PHE	-	expression tag	UNP B3LGZ3
M	-2	GLN	-	expression tag	UNP B3LGZ3
M	-1	SER	-	expression tag	UNP B3LGZ3
M	0	VAL	-	expression tag	UNP B3LGZ3
M	1	ASP	-	expression tag	UNP B3LGZ3
N	-18	MET	-	initiating methionine	UNP B3LGZ3
N	-17	GLY	-	expression tag	UNP B3LGZ3
N	-16	GLY	-	expression tag	UNP B3LGZ3
N	-15	SER	-	expression tag	UNP B3LGZ3
N	-14	HIS	-	expression tag	UNP B3LGZ3
N	-13	HIS	-	expression tag	UNP B3LGZ3
N	-12	HIS	-	expression tag	UNP B3LGZ3
N	-11	HIS	-	expression tag	UNP B3LGZ3
N	-10	HIS	-	expression tag	UNP B3LGZ3
N	-9	HIS	-	expression tag	UNP B3LGZ3
N	-8	GLY	-	expression tag	UNP B3LGZ3
N	-7	GLU	-	expression tag	UNP B3LGZ3
N	-6	ASN	-	expression tag	UNP B3LGZ3
N	-5	LEU	-	expression tag	UNP B3LGZ3
N	-4	TYR	-	expression tag	UNP B3LGZ3
N	-3	PHE	-	expression tag	UNP B3LGZ3
N	-2	GLN	-	expression tag	UNP B3LGZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-1	SER	-	expression tag	UNP B3LGZ3
N	0	VAL	-	expression tag	UNP B3LGZ3
N	1	ASP	-	expression tag	UNP B3LGZ3
O	-18	MET	-	initiating methionine	UNP B3LGZ3
O	-17	GLY	-	expression tag	UNP B3LGZ3
O	-16	GLY	-	expression tag	UNP B3LGZ3
O	-15	SER	-	expression tag	UNP B3LGZ3
O	-14	HIS	-	expression tag	UNP B3LGZ3
O	-13	HIS	-	expression tag	UNP B3LGZ3
O	-12	HIS	-	expression tag	UNP B3LGZ3
O	-11	HIS	-	expression tag	UNP B3LGZ3
O	-10	HIS	-	expression tag	UNP B3LGZ3
O	-9	HIS	-	expression tag	UNP B3LGZ3
O	-8	GLY	-	expression tag	UNP B3LGZ3
O	-7	GLU	-	expression tag	UNP B3LGZ3
O	-6	ASN	-	expression tag	UNP B3LGZ3
O	-5	LEU	-	expression tag	UNP B3LGZ3
O	-4	TYR	-	expression tag	UNP B3LGZ3
O	-3	PHE	-	expression tag	UNP B3LGZ3
O	-2	GLN	-	expression tag	UNP B3LGZ3
O	-1	SER	-	expression tag	UNP B3LGZ3
O	0	VAL	-	expression tag	UNP B3LGZ3
O	1	ASP	-	expression tag	UNP B3LGZ3
P	-18	MET	-	initiating methionine	UNP B3LGZ3
P	-17	GLY	-	expression tag	UNP B3LGZ3
P	-16	GLY	-	expression tag	UNP B3LGZ3
P	-15	SER	-	expression tag	UNP B3LGZ3
P	-14	HIS	-	expression tag	UNP B3LGZ3
P	-13	HIS	-	expression tag	UNP B3LGZ3
P	-12	HIS	-	expression tag	UNP B3LGZ3
P	-11	HIS	-	expression tag	UNP B3LGZ3
P	-10	HIS	-	expression tag	UNP B3LGZ3
P	-9	HIS	-	expression tag	UNP B3LGZ3
P	-8	GLY	-	expression tag	UNP B3LGZ3
P	-7	GLU	-	expression tag	UNP B3LGZ3
P	-6	ASN	-	expression tag	UNP B3LGZ3
P	-5	LEU	-	expression tag	UNP B3LGZ3
P	-4	TYR	-	expression tag	UNP B3LGZ3
P	-3	PHE	-	expression tag	UNP B3LGZ3
P	-2	GLN	-	expression tag	UNP B3LGZ3
P	-1	SER	-	expression tag	UNP B3LGZ3
P	0	VAL	-	expression tag	UNP B3LGZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
P	1	ASP	-	expression tag	UNP B3LGZ3
C	-18	MET	-	initiating methionine	UNP B3LGZ3
C	-17	GLY	-	expression tag	UNP B3LGZ3
C	-16	GLY	-	expression tag	UNP B3LGZ3
C	-15	SER	-	expression tag	UNP B3LGZ3
C	-14	HIS	-	expression tag	UNP B3LGZ3
C	-13	HIS	-	expression tag	UNP B3LGZ3
C	-12	HIS	-	expression tag	UNP B3LGZ3
C	-11	HIS	-	expression tag	UNP B3LGZ3
C	-10	HIS	-	expression tag	UNP B3LGZ3
C	-9	HIS	-	expression tag	UNP B3LGZ3
C	-8	GLY	-	expression tag	UNP B3LGZ3
C	-7	GLU	-	expression tag	UNP B3LGZ3
C	-6	ASN	-	expression tag	UNP B3LGZ3
C	-5	LEU	-	expression tag	UNP B3LGZ3
C	-4	TYR	-	expression tag	UNP B3LGZ3
C	-3	PHE	-	expression tag	UNP B3LGZ3
C	-2	GLN	-	expression tag	UNP B3LGZ3
C	-1	SER	-	expression tag	UNP B3LGZ3
C	0	VAL	-	expression tag	UNP B3LGZ3
C	1	ASP	-	expression tag	UNP B3LGZ3

- Molecule 2 is a protein called Golgi to ER traffic protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	291	Total	C	N	O	S	0	0	0
			2406	1567	380	453	6			
2	G	291	Total	C	N	O	S	0	0	0
			2406	1567	380	453	6			
2	I	291	Total	C	N	O	S	0	0	0
			2406	1567	380	453	6			
2	K	291	Total	C	N	O	S	0	0	0
			2406	1567	380	453	6			
2	Q	291	Total	C	N	O	S	0	0	0
			2406	1567	380	453	6			
2	S	291	Total	C	N	O	S	0	0	0
			2406	1567	380	453	6			
2	U	291	Total	C	N	O	S	0	0	0
			2406	1567	380	453	6			
2	W	291	Total	C	N	O	S	0	0	0
			2406	1567	380	453	6			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	9	MET	-	initiating methionine	UNP Q12125
E	10	GLY	-	expression tag	UNP Q12125
E	258	ALA	LYS	conflict	UNP Q12125
E	260	ALA	LYS	conflict	UNP Q12125
E	312	GLY	-	expression tag	UNP Q12125
E	313	GLU	-	expression tag	UNP Q12125
E	314	ASN	-	expression tag	UNP Q12125
E	315	LEU	-	expression tag	UNP Q12125
E	316	TYR	-	expression tag	UNP Q12125
E	317	PHE	-	expression tag	UNP Q12125
E	318	GLN	-	expression tag	UNP Q12125
E	319	SER	-	expression tag	UNP Q12125
E	320	LEU	-	expression tag	UNP Q12125
E	321	GLU	-	expression tag	UNP Q12125
E	322	HIS	-	expression tag	UNP Q12125
E	323	HIS	-	expression tag	UNP Q12125
E	324	HIS	-	expression tag	UNP Q12125
E	325	HIS	-	expression tag	UNP Q12125
E	326	HIS	-	expression tag	UNP Q12125
E	327	HIS	-	expression tag	UNP Q12125
G	9	MET	-	initiating methionine	UNP Q12125
G	10	GLY	-	expression tag	UNP Q12125
G	258	ALA	LYS	conflict	UNP Q12125
G	260	ALA	LYS	conflict	UNP Q12125
G	312	GLY	-	expression tag	UNP Q12125
G	313	GLU	-	expression tag	UNP Q12125
G	314	ASN	-	expression tag	UNP Q12125
G	315	LEU	-	expression tag	UNP Q12125
G	316	TYR	-	expression tag	UNP Q12125
G	317	PHE	-	expression tag	UNP Q12125
G	318	GLN	-	expression tag	UNP Q12125
G	319	SER	-	expression tag	UNP Q12125
G	320	LEU	-	expression tag	UNP Q12125
G	321	GLU	-	expression tag	UNP Q12125
G	322	HIS	-	expression tag	UNP Q12125
G	323	HIS	-	expression tag	UNP Q12125
G	324	HIS	-	expression tag	UNP Q12125
G	325	HIS	-	expression tag	UNP Q12125
G	326	HIS	-	expression tag	UNP Q12125
G	327	HIS	-	expression tag	UNP Q12125
I	9	MET	-	initiating methionine	UNP Q12125
I	10	GLY	-	expression tag	UNP Q12125
I	258	ALA	LYS	conflict	UNP Q12125

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Chain	Residue	Modelled	Actual	Comment	Reference
I	260	ALA	LYS	conflict	UNP Q12125
I	312	GLY	-	expression tag	UNP Q12125
I	313	GLU	-	expression tag	UNP Q12125
I	314	ASN	-	expression tag	UNP Q12125
I	315	LEU	-	expression tag	UNP Q12125
I	316	TYR	-	expression tag	UNP Q12125
I	317	PHE	-	expression tag	UNP Q12125
I	318	GLN	-	expression tag	UNP Q12125
I	319	SER	-	expression tag	UNP Q12125
I	320	LEU	-	expression tag	UNP Q12125
I	321	GLU	-	expression tag	UNP Q12125
I	322	HIS	-	expression tag	UNP Q12125
I	323	HIS	-	expression tag	UNP Q12125
I	324	HIS	-	expression tag	UNP Q12125
I	325	HIS	-	expression tag	UNP Q12125
I	326	HIS	-	expression tag	UNP Q12125
I	327	HIS	-	expression tag	UNP Q12125
K	9	MET	-	initiating methionine	UNP Q12125
K	10	GLY	-	expression tag	UNP Q12125
K	258	ALA	LYS	conflict	UNP Q12125
K	260	ALA	LYS	conflict	UNP Q12125
K	312	GLY	-	expression tag	UNP Q12125
K	313	GLU	-	expression tag	UNP Q12125
K	314	ASN	-	expression tag	UNP Q12125
K	315	LEU	-	expression tag	UNP Q12125
K	316	TYR	-	expression tag	UNP Q12125
K	317	PHE	-	expression tag	UNP Q12125
K	318	GLN	-	expression tag	UNP Q12125
K	319	SER	-	expression tag	UNP Q12125
K	320	LEU	-	expression tag	UNP Q12125
K	321	GLU	-	expression tag	UNP Q12125
K	322	HIS	-	expression tag	UNP Q12125
K	323	HIS	-	expression tag	UNP Q12125
K	324	HIS	-	expression tag	UNP Q12125
K	325	HIS	-	expression tag	UNP Q12125
K	326	HIS	-	expression tag	UNP Q12125
K	327	HIS	-	expression tag	UNP Q12125
Q	9	MET	-	initiating methionine	UNP Q12125
Q	10	GLY	-	expression tag	UNP Q12125
Q	258	ALA	LYS	conflict	UNP Q12125
Q	260	ALA	LYS	conflict	UNP Q12125
Q	312	GLY	-	expression tag	UNP Q12125

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	313	GLU	-	expression tag	UNP Q12125
Q	314	ASN	-	expression tag	UNP Q12125
Q	315	LEU	-	expression tag	UNP Q12125
Q	316	TYR	-	expression tag	UNP Q12125
Q	317	PHE	-	expression tag	UNP Q12125
Q	318	GLN	-	expression tag	UNP Q12125
Q	319	SER	-	expression tag	UNP Q12125
Q	320	LEU	-	expression tag	UNP Q12125
Q	321	GLU	-	expression tag	UNP Q12125
Q	322	HIS	-	expression tag	UNP Q12125
Q	323	HIS	-	expression tag	UNP Q12125
Q	324	HIS	-	expression tag	UNP Q12125
Q	325	HIS	-	expression tag	UNP Q12125
Q	326	HIS	-	expression tag	UNP Q12125
Q	327	HIS	-	expression tag	UNP Q12125
S	9	MET	-	initiating methionine	UNP Q12125
S	10	GLY	-	expression tag	UNP Q12125
S	258	ALA	LYS	conflict	UNP Q12125
S	260	ALA	LYS	conflict	UNP Q12125
S	312	GLY	-	expression tag	UNP Q12125
S	313	GLU	-	expression tag	UNP Q12125
S	314	ASN	-	expression tag	UNP Q12125
S	315	LEU	-	expression tag	UNP Q12125
S	316	TYR	-	expression tag	UNP Q12125
S	317	PHE	-	expression tag	UNP Q12125
S	318	GLN	-	expression tag	UNP Q12125
S	319	SER	-	expression tag	UNP Q12125
S	320	LEU	-	expression tag	UNP Q12125
S	321	GLU	-	expression tag	UNP Q12125
S	322	HIS	-	expression tag	UNP Q12125
S	323	HIS	-	expression tag	UNP Q12125
S	324	HIS	-	expression tag	UNP Q12125
S	325	HIS	-	expression tag	UNP Q12125
S	326	HIS	-	expression tag	UNP Q12125
S	327	HIS	-	expression tag	UNP Q12125
U	9	MET	-	initiating methionine	UNP Q12125
U	10	GLY	-	expression tag	UNP Q12125
U	258	ALA	LYS	conflict	UNP Q12125
U	260	ALA	LYS	conflict	UNP Q12125
U	312	GLY	-	expression tag	UNP Q12125
U	313	GLU	-	expression tag	UNP Q12125
U	314	ASN	-	expression tag	UNP Q12125

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
U	315	LEU	-	expression tag	UNP Q12125
U	316	TYR	-	expression tag	UNP Q12125
U	317	PHE	-	expression tag	UNP Q12125
U	318	GLN	-	expression tag	UNP Q12125
U	319	SER	-	expression tag	UNP Q12125
U	320	LEU	-	expression tag	UNP Q12125
U	321	GLU	-	expression tag	UNP Q12125
U	322	HIS	-	expression tag	UNP Q12125
U	323	HIS	-	expression tag	UNP Q12125
U	324	HIS	-	expression tag	UNP Q12125
U	325	HIS	-	expression tag	UNP Q12125
U	326	HIS	-	expression tag	UNP Q12125
U	327	HIS	-	expression tag	UNP Q12125
W	9	MET	-	initiating methionine	UNP Q12125
W	10	GLY	-	expression tag	UNP Q12125
W	258	ALA	LYS	conflict	UNP Q12125
W	260	ALA	LYS	conflict	UNP Q12125
W	312	GLY	-	expression tag	UNP Q12125
W	313	GLU	-	expression tag	UNP Q12125
W	314	ASN	-	expression tag	UNP Q12125
W	315	LEU	-	expression tag	UNP Q12125
W	316	TYR	-	expression tag	UNP Q12125
W	317	PHE	-	expression tag	UNP Q12125
W	318	GLN	-	expression tag	UNP Q12125
W	319	SER	-	expression tag	UNP Q12125
W	320	LEU	-	expression tag	UNP Q12125
W	321	GLU	-	expression tag	UNP Q12125
W	322	HIS	-	expression tag	UNP Q12125
W	323	HIS	-	expression tag	UNP Q12125
W	324	HIS	-	expression tag	UNP Q12125
W	325	HIS	-	expression tag	UNP Q12125
W	326	HIS	-	expression tag	UNP Q12125
W	327	HIS	-	expression tag	UNP Q12125

- Molecule 3 is a protein called Ubiquitin-like protein MDY2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	54	Total	C	N	O	0	0	0
			429	280	70	79			
3	H	54	Total	C	N	O	0	0	0
			430	280	70	80			
3	J	54	Total	C	N	O	0	0	0
			430	280	70	80			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	L	54	Total 430	C 280	N 70	O 80	0	0	0
3	R	54	Total 430	C 280	N 70	O 80	0	0	0
3	T	54	Total 430	C 280	N 70	O 80	0	0	0
3	V	54	Total 430	C 280	N 70	O 80	0	0	0
3	X	54	Total 430	C 280	N 70	O 80	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

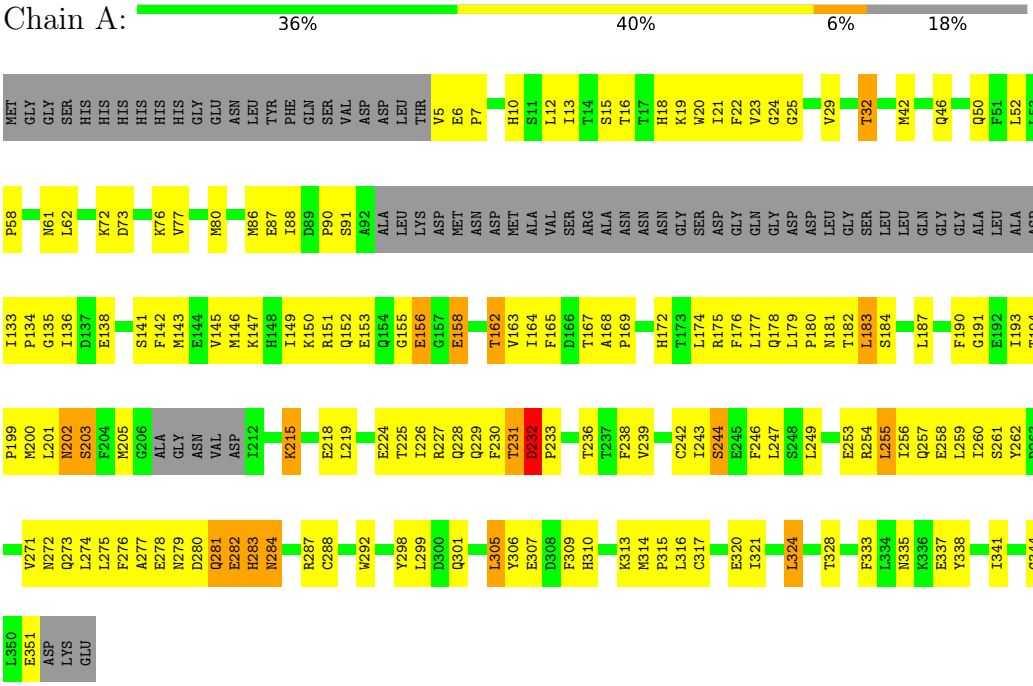
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Zn 1	0	0
4	D	1	Total 1	Zn 1	0	0
4	M	1	Total 1	Zn 1	0	0
4	O	1	Total 1	Zn 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

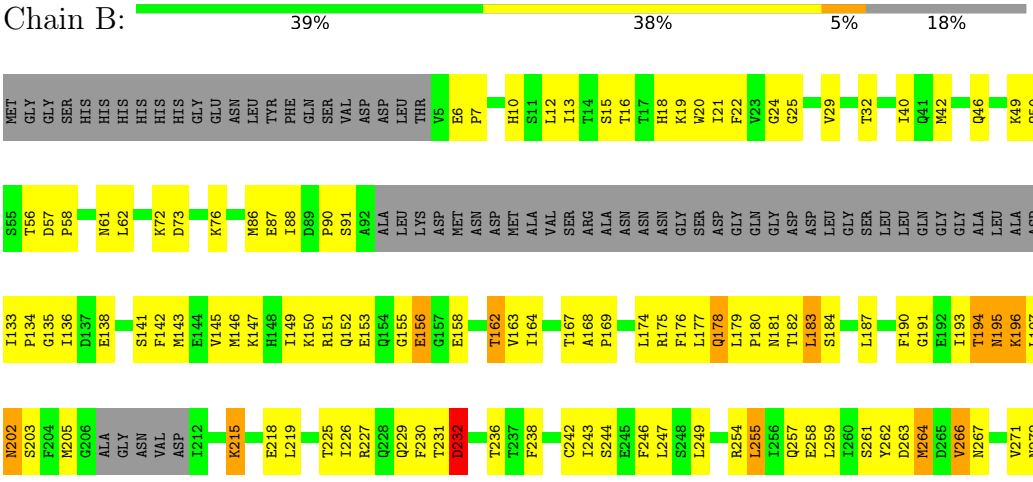
- Molecule 1: ATPase GET3

Chain A:



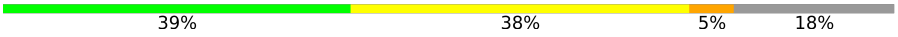
- Molecule 1: ATPase GET3

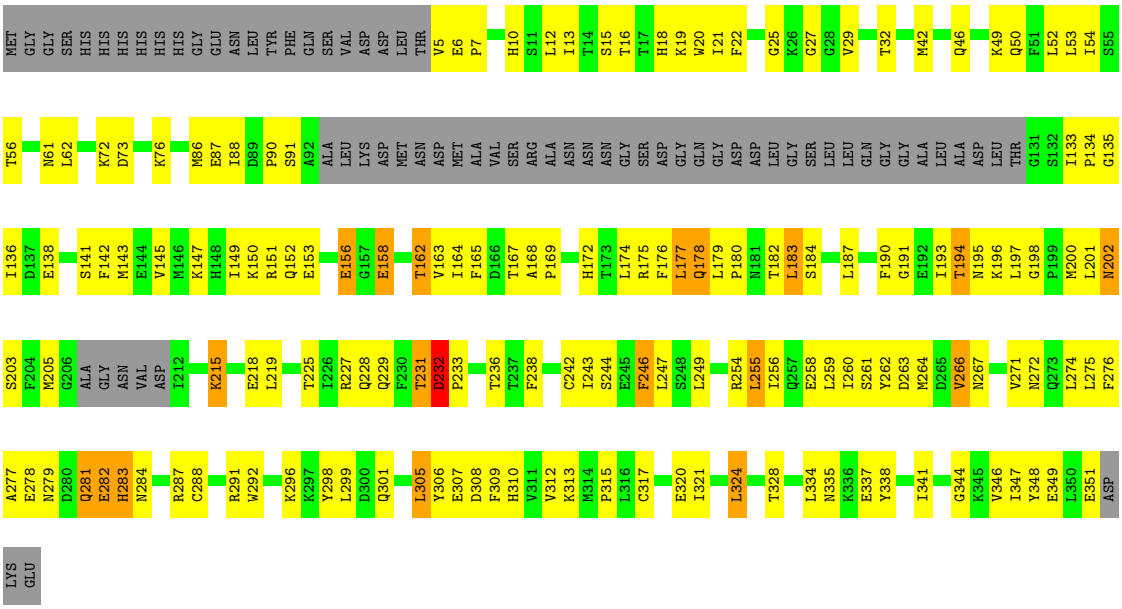
Chain B:



• Molecule 1: ATPase GET3

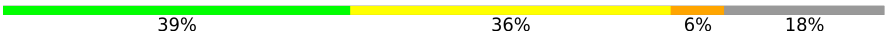
Chain D:

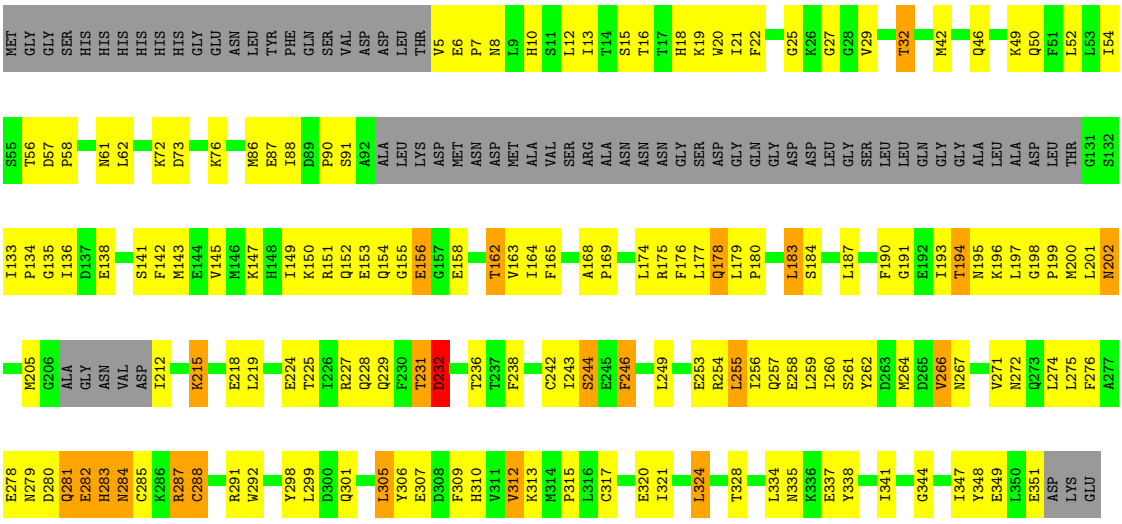




• Molecule 1: ATPase GET3

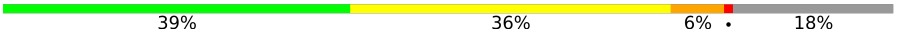
Chain M:

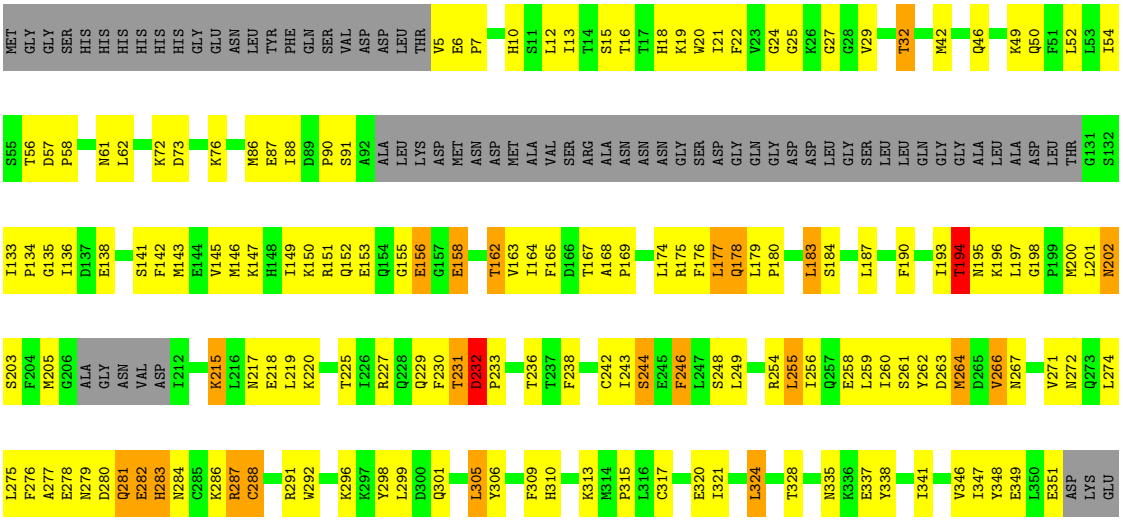




• Molecule 1: ATPase GET3

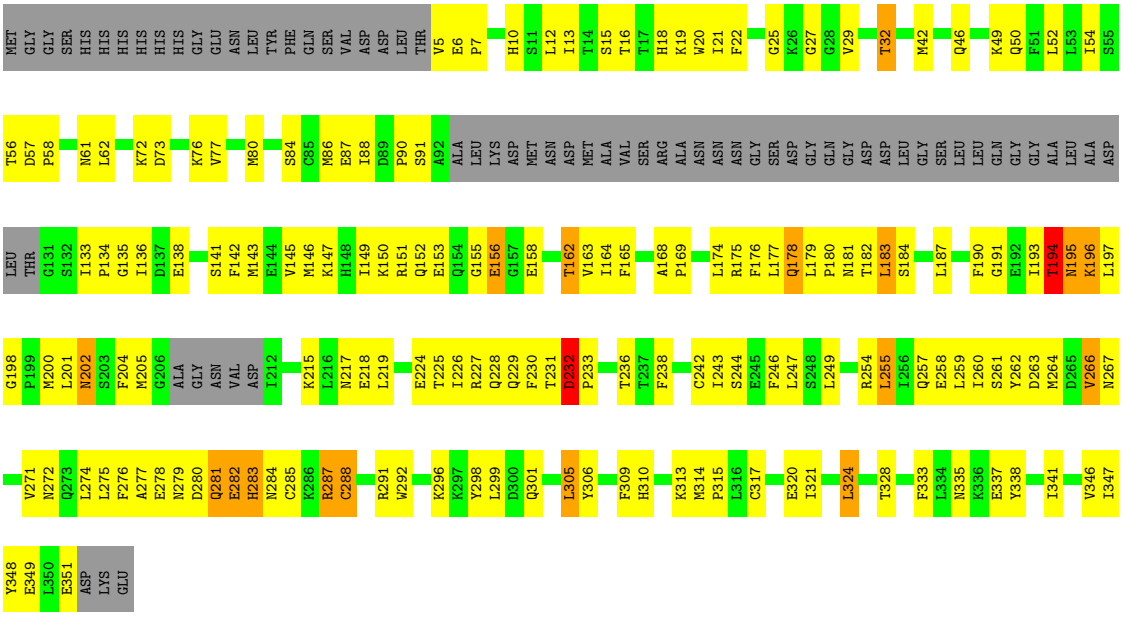
Chain N:





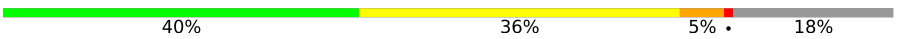
• Molecule 1: ATPase GET3

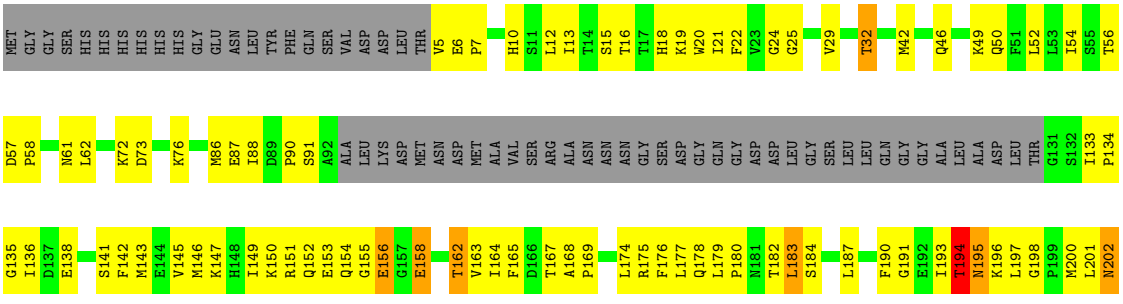
Chain O:

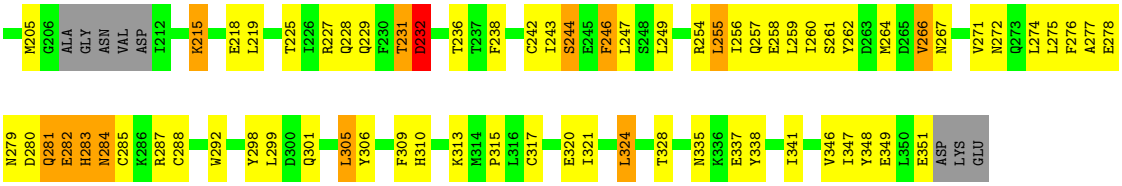


• Molecule 1: ATPase GET3

Chain P:

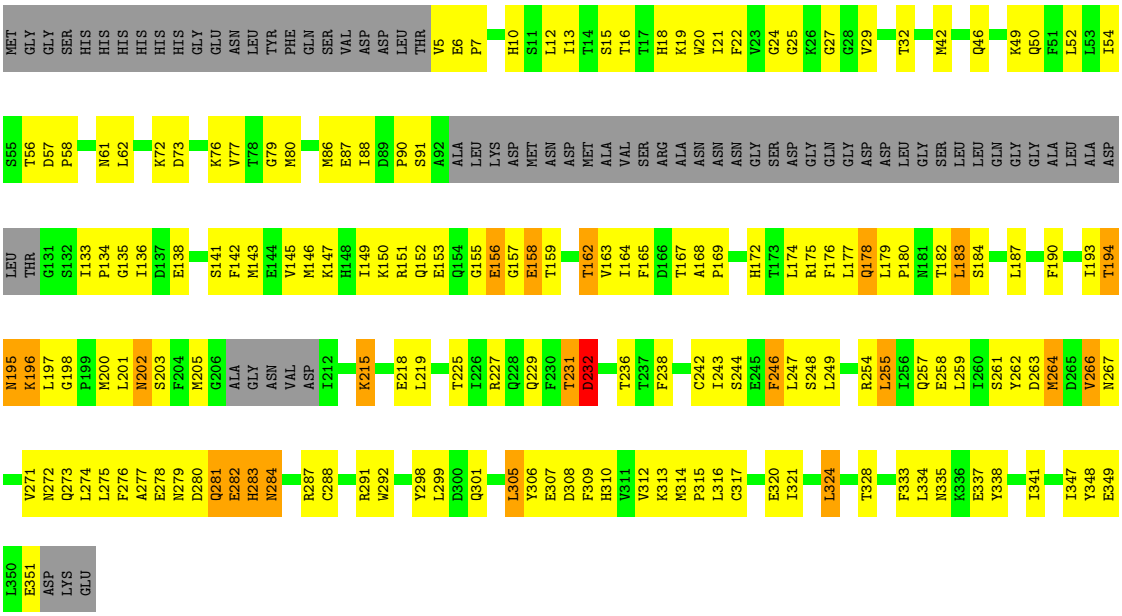






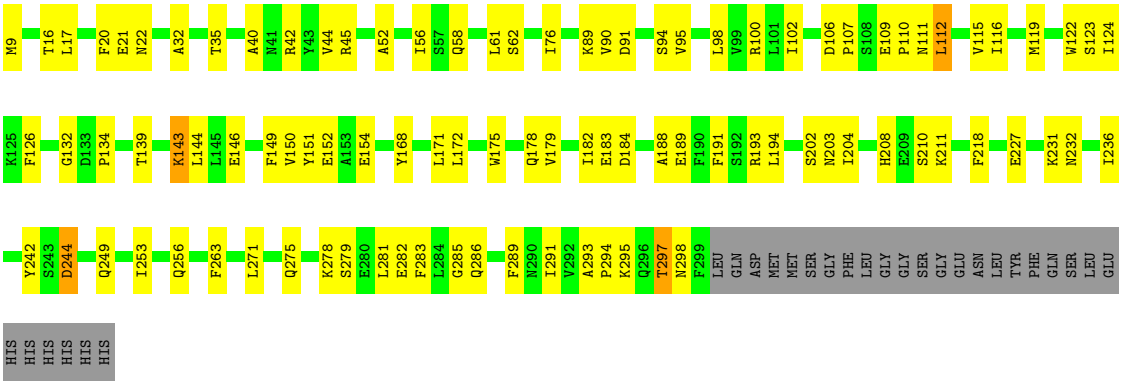
• Molecule 1: ATPase GET3

Chain C:



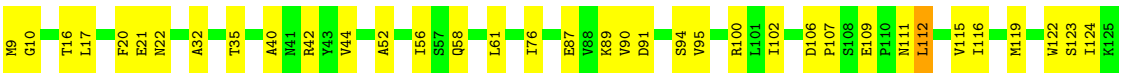
• Molecule 2: Golgi to ER traffic protein 4

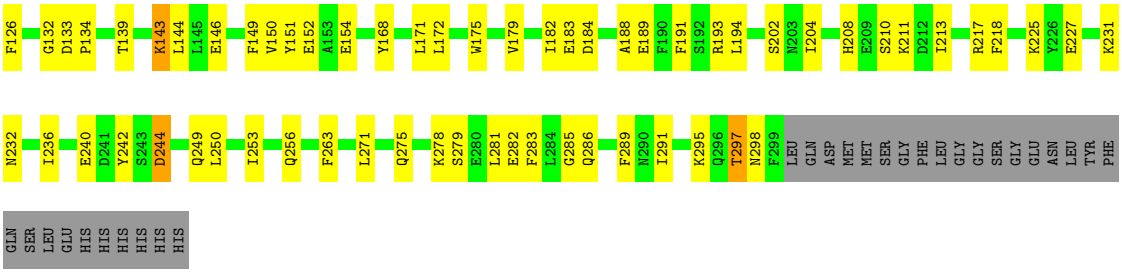
Chain E:



• Molecule 2: Golgi to ER traffic protein 4

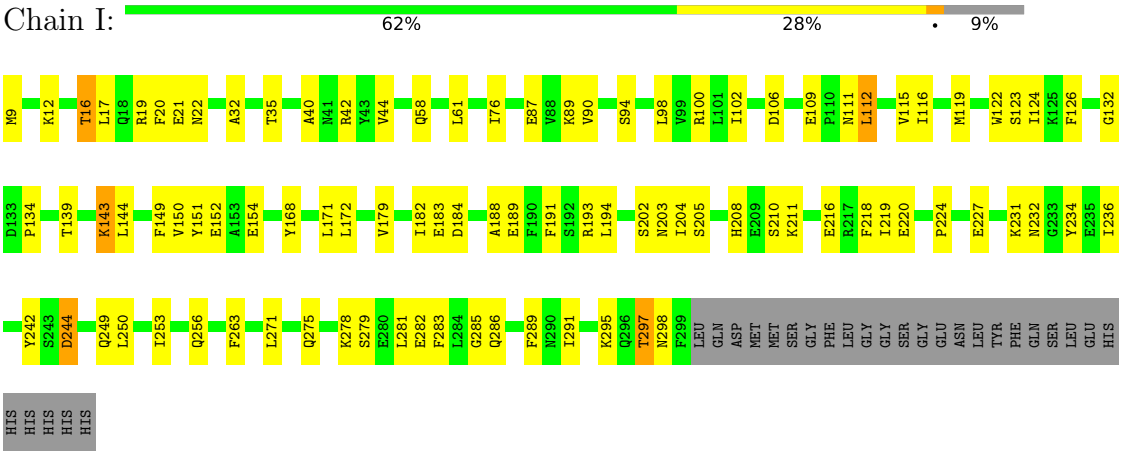
Chain G:





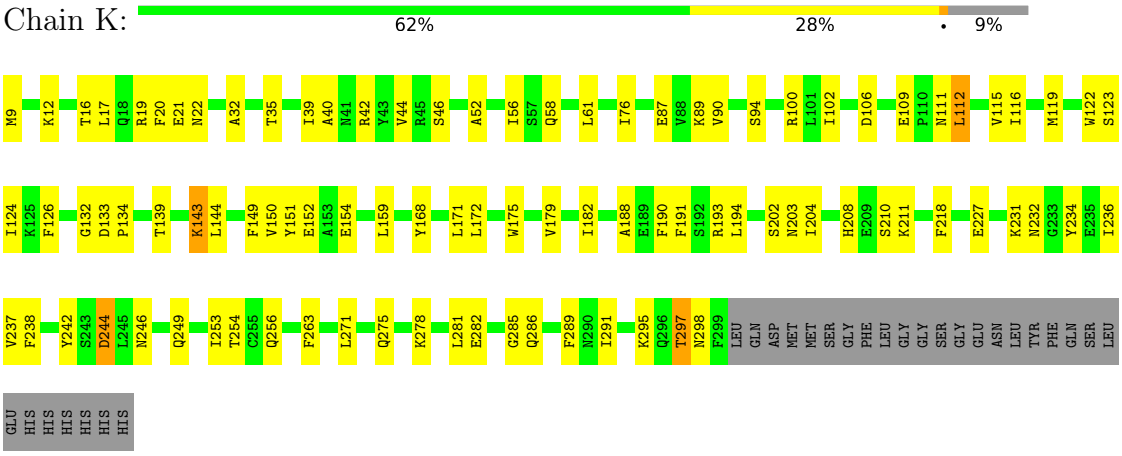
• Molecule 2: Golgi to ER traffic protein 4

Chain I:



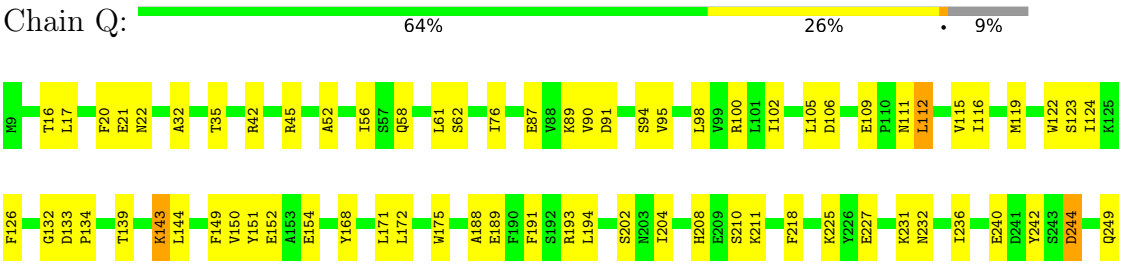
• Molecule 2: Golgi to ER traffic protein 4

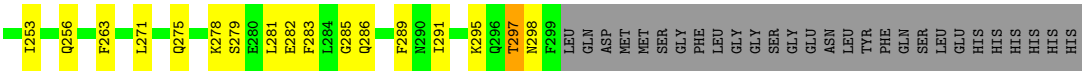
Chain K:



• Molecule 2: Golgi to ER traffic protein 4

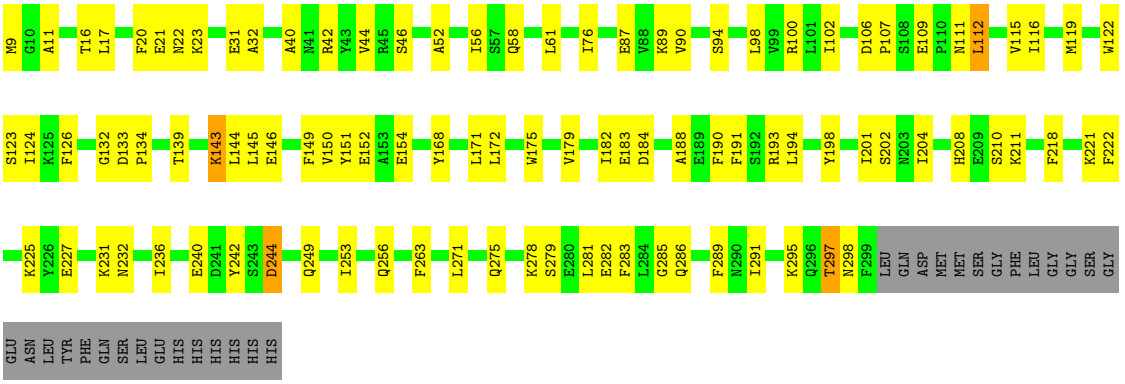
Chain Q:





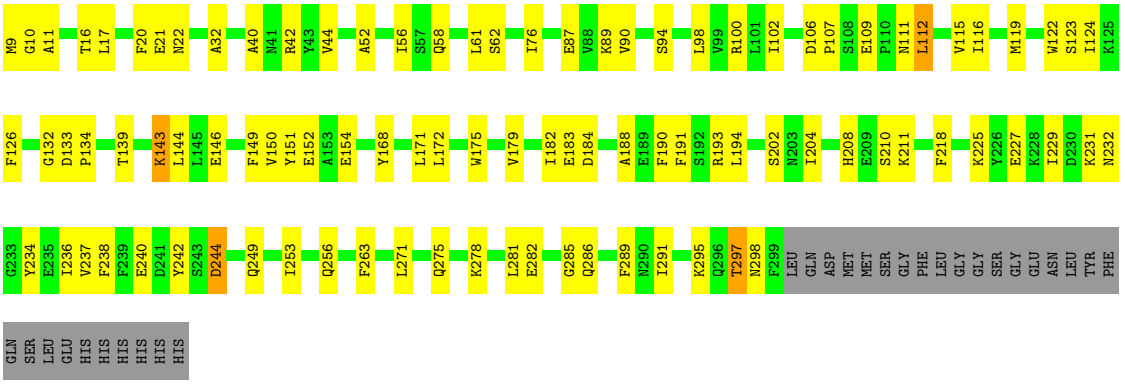
• Molecule 2: Golgi to ER traffic protein 4

Chain S:



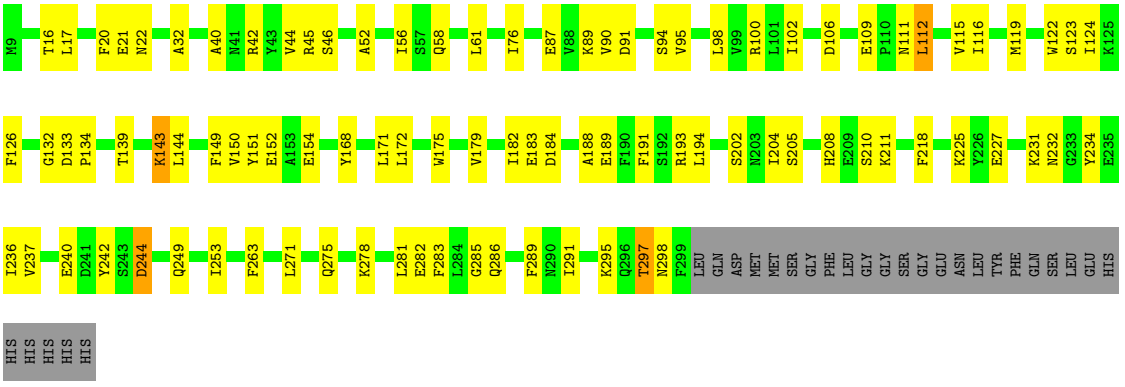
• Molecule 2: Golgi to ER traffic protein 4

Chain U:



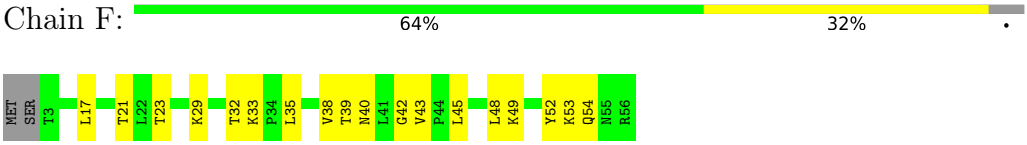
• Molecule 2: Golgi to ER traffic protein 4

Chain W:



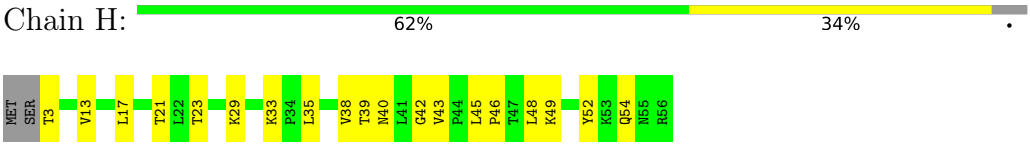
• Molecule 3: Ubiquitin-like protein MDY2

Chain F:



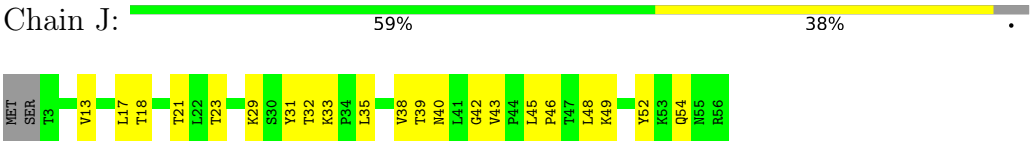
• Molecule 3: Ubiquitin-like protein MDY2

Chain H:



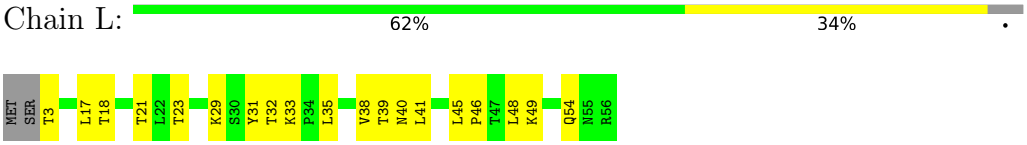
• Molecule 3: Ubiquitin-like protein MDY2

Chain J:



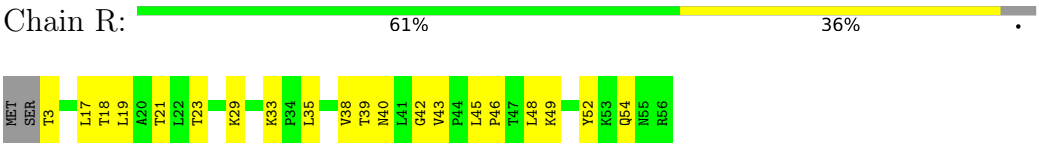
• Molecule 3: Ubiquitin-like protein MDY2

Chain L:



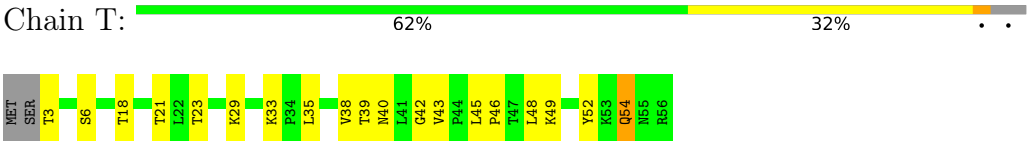
• Molecule 3: Ubiquitin-like protein MDY2

Chain R:



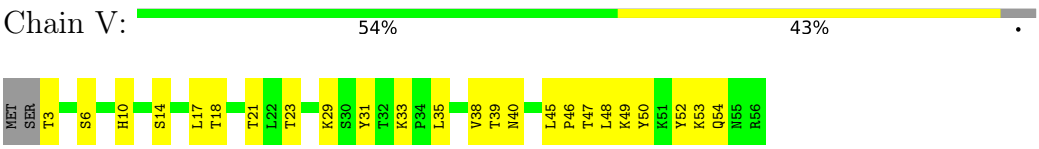
• Molecule 3: Ubiquitin-like protein MDY2

Chain T:



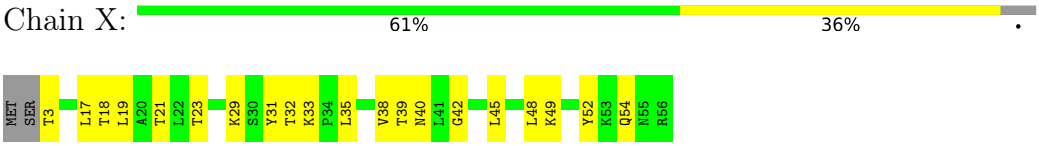
• Molecule 3: Ubiquitin-like protein MDY2

Chain V:



• Molecule 3: Ubiquitin-like protein MDY2

Chain X:


61%
36%
MET
SER
T3
L17
T18
L19
A20
T21
L22
T23
K29
S30
Y31
T32
K33
P34
L35
V38
T39
N40
L41
G42
L45
L48
K49
Y52
K53
Q54
N55
R56

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	152.43Å 127.33Å 210.26Å 90.00° 110.23° 90.00°	Depositor
Resolution (Å)	30.00 – 6.00 29.99 – 6.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-6.00) 96.5 (29.99-6.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 6.07Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.274 , 0.302 0.277 , 0.310	Depositor DCC
R_{free} test set	917 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	359.5	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 263.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	41907	wwPDB-VP
Average B, all atoms (Å^2)	361.0	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 20.29 % 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 8.9806e-03. 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: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/2444	0.47	0/3294
1	B	0.26	0/2444	0.47	0/3294
1	C	0.26	0/2444	0.47	0/3294
1	D	0.26	0/2444	0.47	0/3294
1	M	0.26	0/2444	0.47	0/3294
1	N	0.26	0/2444	0.47	0/3294
1	O	0.26	0/2444	0.47	0/3294
1	P	0.26	0/2444	0.47	0/3294
2	E	0.27	0/2465	0.41	0/3330
2	G	0.27	0/2465	0.41	0/3330
2	I	0.27	0/2465	0.41	0/3330
2	K	0.27	0/2465	0.41	0/3330
2	Q	0.27	0/2465	0.41	0/3330
2	S	0.27	0/2465	0.41	0/3330
2	U	0.27	0/2465	0.41	0/3330
2	W	0.27	0/2465	0.41	0/3330
3	F	0.26	0/440	0.44	0/597
3	H	0.26	0/441	0.44	0/597
3	J	0.26	0/441	0.45	0/597
3	L	0.26	0/441	0.44	0/597
3	R	0.26	0/441	0.44	0/597
3	T	0.26	0/441	0.44	0/597
3	V	0.26	0/441	0.44	0/597
3	X	0.26	0/441	0.44	0/597
All	All	0.27	0/42799	0.44	0/57768

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2402	0	2388	195	0
1	B	2402	0	2387	214	0
1	C	2402	0	2387	263	0
1	D	2402	0	2387	194	1
1	M	2402	0	2387	226	0
1	N	2402	0	2386	246	1
1	O	2402	0	2387	246	0
1	P	2402	0	2386	213	0
2	E	2406	0	2339	93	0
2	G	2406	0	2339	104	0
2	I	2406	0	2339	107	0
2	K	2406	0	2339	97	0
2	Q	2406	0	2339	87	0
2	S	2406	0	2339	94	0
2	U	2406	0	2339	103	0
2	W	2406	0	2339	92	0
3	F	429	0	452	30	0
3	H	430	0	452	25	0
3	J	430	0	452	33	0
3	L	430	0	452	27	0
3	R	430	0	452	25	0
3	T	430	0	452	25	0
3	V	430	0	452	37	0
3	X	430	0	452	28	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
All	All	41907	0	41423	2311	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (2311) 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:B:143:MET:CE	1:C:201:LEU:HB3	1.70	1.20
1:D:180:PRO:HG2	1:D:229:GLN:HE21	1.13	1.11
1:P:138:GLU:HG2	1:P:175:ARG:HB3	1.33	1.10
1:A:138:GLU:HG2	1:A:175:ARG:HB3	1.35	1.09
1:M:138:GLU:HG2	1:M:175:ARG:HB3	1.35	1.09
1:P:154:GLN:HG3	1:C:79:GLY:CA	1.82	1.08
1:D:174:LEU:HD22	1:D:177:LEU:HD11	1.38	1.06
1:C:138:GLU:HG2	1:C:175:ARG:HB3	1.37	1.06
1:D:138:GLU:HG2	1:D:175:ARG:HB3	1.39	1.04
1:P:174:LEU:O	1:P:177:LEU:HG	1.58	1.04
1:B:174:LEU:HD22	1:B:177:LEU:HD11	1.39	1.03
1:P:180:PRO:HG2	1:P:229:GLN:HE21	1.22	1.03
1:N:230:PHE:HA	2:S:9:MET:HE1	1.41	1.02
1:A:143:MET:SD	1:D:201:LEU:HD23	1.98	1.02
1:B:138:GLU:HG2	1:B:175:ARG:HB3	1.37	1.02
1:N:138:GLU:HG2	1:N:175:ARG:HB3	1.38	1.02
1:O:180:PRO:HG2	1:O:229:GLN:HE21	1.21	1.02
1:N:143:MET:HE2	1:O:197:LEU:HB2	1.41	1.02
1:O:138:GLU:HG2	1:O:175:ARG:HB3	1.36	1.02
1:B:180:PRO:HG2	1:B:229:GLN:HE21	1.22	1.01
1:M:199:PRO:HB3	1:C:156:GLU:HG2	1.43	1.01
1:A:180:PRO:HG2	1:A:229:GLN:HE21	1.25	1.00
1:M:180:PRO:HG2	1:M:229:GLN:HE21	1.24	1.00
1:N:180:PRO:HG2	1:N:229:GLN:HE21	1.26	1.00
1:N:174:LEU:HD22	1:N:177:LEU:HD11	1.44	1.00
1:N:143:MET:HE2	1:O:197:LEU:CB	1.93	0.99
1:O:174:LEU:HD22	1:O:177:LEU:HD11	1.45	0.99
1:A:174:LEU:HD22	1:A:177:LEU:HD11	1.43	0.98
2:I:42:ARG:HG3	1:C:257:GLN:OE1	1.64	0.97
1:M:212:ILE:HG21	1:C:155:GLY:CA	1.95	0.97
1:O:174:LEU:O	1:O:177:LEU:HG	1.64	0.97
1:P:154:GLN:CD	1:C:79:GLY:HA3	1.85	0.97
1:B:143:MET:HA	1:C:201:LEU:HD23	1.46	0.96
1:B:257:GLN:OE1	2:G:42:ARG:HG3	1.65	0.96
1:D:183:LEU:HD23	1:D:184:SER:H	1.30	0.96
1:C:180:PRO:HG2	1:C:229:GLN:HE21	1.31	0.96
1:A:201:LEU:HD23	1:D:143:MET:SD	2.05	0.95
1:N:197:LEU:HD13	1:O:147:LYS:NZ	1.82	0.95
1:N:183:LEU:HD23	1:N:184:SER:H	1.31	0.95
1:C:174:LEU:HD22	1:C:177:LEU:HD11	1.48	0.94
1:D:174:LEU:O	1:D:177:LEU:HG	1.65	0.94
1:A:174:LEU:O	1:A:177:LEU:HG	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:42:ARG:NH2	1:C:305:LEU:HD22	1.82	0.94
1:N:174:LEU:O	1:N:177:LEU:HG	1.68	0.93
1:P:183:LEU:HD23	1:P:184:SER:H	1.33	0.93
1:N:147:LYS:NZ	1:O:197:LEU:HD13	1.83	0.93
1:O:183:LEU:HD23	1:O:184:SER:H	1.32	0.93
1:B:143:MET:HA	1:C:201:LEU:CD2	1.98	0.93
1:B:143:MET:SD	1:C:201:LEU:HD23	2.09	0.92
1:B:143:MET:HE1	1:C:201:LEU:HB3	1.47	0.92
1:A:138:GLU:HB2	1:A:176:PHE:HB3	1.51	0.92
1:M:174:LEU:HD22	1:M:177:LEU:HD11	1.49	0.91
1:C:183:LEU:HD23	1:C:184:SER:N	1.85	0.91
1:M:138:GLU:HB2	1:M:176:PHE:HB3	1.50	0.91
1:B:183:LEU:HD23	1:B:184:SER:H	1.35	0.91
1:B:174:LEU:O	1:B:177:LEU:HG	1.70	0.91
1:M:174:LEU:O	1:M:177:LEU:HG	1.71	0.91
1:C:135:GLY:HA3	1:C:179:LEU:HD22	1.53	0.91
1:D:183:LEU:HD23	1:D:184:SER:N	1.87	0.90
1:C:138:GLU:HB2	1:C:176:PHE:HB3	1.53	0.90
1:P:154:GLN:CG	1:C:79:GLY:HA3	2.02	0.90
1:P:135:GLY:HA3	1:P:179:LEU:HD22	1.54	0.90
1:D:180:PRO:HG2	1:D:229:GLN:NE2	1.87	0.90
1:M:183:LEU:HD23	1:M:184:SER:H	1.37	0.89
1:O:183:LEU:HD23	1:O:184:SER:N	1.87	0.89
1:B:143:MET:HE3	1:C:201:LEU:HB3	1.52	0.89
1:P:183:LEU:HD23	1:P:184:SER:N	1.88	0.89
1:P:174:LEU:HD22	1:P:177:LEU:HD11	1.52	0.89
1:M:135:GLY:HA3	1:M:179:LEU:HD22	1.55	0.89
1:P:154:GLN:CG	1:C:79:GLY:CA	2.51	0.89
1:O:263:ASP:HB3	2:U:9:MET:SD	2.13	0.88
1:D:135:GLY:HA3	1:D:179:LEU:HD22	1.56	0.88
1:C:174:LEU:O	1:C:177:LEU:HG	1.74	0.88
1:C:183:LEU:HD23	1:C:184:SER:H	1.37	0.88
1:D:138:GLU:HB2	1:D:176:PHE:HB3	1.54	0.88
1:N:183:LEU:HD23	1:N:184:SER:N	1.88	0.88
1:A:135:GLY:HA3	1:A:179:LEU:HD22	1.55	0.87
1:O:138:GLU:HB2	1:O:176:PHE:HB3	1.56	0.87
1:P:138:GLU:HB2	1:P:176:PHE:HB3	1.55	0.87
1:A:183:LEU:HD23	1:A:184:SER:H	1.38	0.87
1:M:199:PRO:HD3	1:C:156:GLU:HB3	1.56	0.87
2:G:217:ARG:CZ	1:M:154:GLN:HE22	1.88	0.86
1:N:147:LYS:HZ2	1:O:197:LEU:HD13	1.34	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:135:GLY:HA3	1:O:179:LEU:HD22	1.57	0.86
1:B:138:GLU:HB2	1:B:176:PHE:HB3	1.56	0.86
1:B:183:LEU:HD23	1:B:184:SER:N	1.90	0.86
3:F:35:LEU:HD12	3:F:38:VAL:HG21	1.55	0.86
1:N:201:LEU:HD23	1:O:143:MET:SD	2.16	0.86
1:B:135:GLY:HA3	1:B:179:LEU:HD22	1.57	0.86
1:M:147:LYS:HZ1	1:P:197:LEU:HD13	1.41	0.86
1:M:183:LEU:HD23	1:M:184:SER:N	1.90	0.86
1:N:143:MET:HB3	1:O:197:LEU:HB2	1.55	0.85
1:P:317:CYS:SG	1:P:321:ILE:HD11	2.15	0.85
2:G:217:ARG:NH2	1:M:154:GLN:HE22	1.74	0.85
3:T:35:LEU:HD12	3:T:38:VAL:HG21	1.58	0.85
1:M:199:PRO:HD3	1:C:156:GLU:CG	2.07	0.85
1:N:143:MET:CB	1:O:197:LEU:HD12	2.07	0.85
1:P:154:GLN:HG3	1:C:79:GLY:HA2	1.56	0.84
3:X:35:LEU:HD12	3:X:38:VAL:HG21	1.58	0.84
1:A:183:LEU:HD23	1:A:184:SER:N	1.91	0.84
1:O:230:PHE:HA	2:U:9:MET:HE1	1.59	0.84
1:M:143:MET:SD	1:P:201:LEU:HD23	2.17	0.84
2:G:217:ARG:HG2	1:M:154:GLN:OE1	1.77	0.84
1:N:135:GLY:HA3	1:N:179:LEU:HD22	1.57	0.84
3:L:35:LEU:HD12	3:L:38:VAL:HG21	1.58	0.84
1:M:147:LYS:NZ	1:P:197:LEU:HD13	1.93	0.84
1:O:179:LEU:O	1:O:183:LEU:HD22	1.77	0.84
1:D:50:GLN:HE22	1:D:76:LYS:HE2	1.42	0.83
1:M:201:LEU:HD23	1:P:143:MET:SD	2.18	0.83
3:V:35:LEU:HD12	3:V:38:VAL:HG21	1.59	0.83
1:M:305:LEU:HD22	2:Q:42:ARG:NH2	1.93	0.83
3:J:35:LEU:HD12	3:J:38:VAL:HG21	1.60	0.83
1:N:138:GLU:HB2	1:N:176:PHE:HB3	1.60	0.83
1:O:218:GLU:HG3	1:O:219:LEU:N	1.91	0.83
1:D:305:LEU:HD22	2:K:42:ARG:HH21	1.44	0.83
1:N:190:PHE:CE2	1:O:183:LEU:HB2	2.14	0.83
1:M:199:PRO:HD3	1:C:156:GLU:CB	2.09	0.82
2:W:232:ASN:HB2	3:X:21:THR:HB	1.61	0.82
3:R:35:LEU:HD12	3:R:38:VAL:HG21	1.60	0.82
2:I:42:ARG:HH22	1:C:305:LEU:HD22	1.41	0.82
1:P:180:PRO:HG2	1:P:229:GLN:NE2	1.96	0.81
1:A:218:GLU:HG3	1:A:219:LEU:N	1.94	0.81
1:B:263:ASP:HB3	2:G:9:MET:SD	2.19	0.81
1:P:179:LEU:O	1:P:183:LEU:HD22	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:35:LEU:HD12	3:H:38:VAL:HG21	1.63	0.81
1:N:190:PHE:CZ	1:O:183:LEU:HG	2.16	0.81
1:D:218:GLU:HG3	1:D:219:LEU:N	1.96	0.81
1:M:50:GLN:HE22	1:M:76:LYS:HE2	1.46	0.81
1:N:183:LEU:HD11	1:O:194:THR:HG22	1.63	0.81
1:D:317:CYS:SG	1:D:321:ILE:HD11	2.22	0.80
1:M:199:PRO:CD	1:C:156:GLU:HB3	2.10	0.80
1:P:16:THR:HG22	1:P:46:GLN:NE2	1.96	0.80
1:B:179:LEU:O	1:B:183:LEU:HD22	1.80	0.80
1:B:50:GLN:HE22	1:B:76:LYS:HE2	1.47	0.80
1:B:201:LEU:HB3	1:C:143:MET:CE	2.12	0.80
1:C:218:GLU:HG3	1:C:219:LEU:N	1.95	0.80
2:E:202:SER:HB2	3:F:33:LYS:HB2	1.64	0.80
1:N:179:LEU:O	1:N:183:LEU:HD22	1.82	0.80
1:N:233:PRO:HB3	2:S:9:MET:N	1.97	0.80
1:M:199:PRO:CB	1:C:156:GLU:HG2	2.10	0.80
1:N:50:GLN:HE22	1:N:76:LYS:HE2	1.47	0.80
1:P:154:GLN:HG3	1:C:79:GLY:HA3	1.63	0.80
1:N:197:LEU:HD13	1:O:147:LYS:HZ1	1.44	0.79
1:C:13:ILE:HA	1:C:42:MET:HG2	1.64	0.79
1:A:50:GLN:HE22	1:A:76:LYS:HE2	1.47	0.79
1:O:180:PRO:HG2	1:O:229:GLN:NE2	1.97	0.79
1:P:29:VAL:HG21	1:P:242:CYS:HA	1.63	0.79
1:O:50:GLN:HE22	1:O:76:LYS:HE2	1.47	0.79
1:D:180:PRO:CG	1:D:229:GLN:HE21	1.93	0.79
1:B:218:GLU:HG3	1:B:219:LEU:N	1.97	0.79
1:M:187:LEU:HD11	1:P:190:PHE:CE1	2.17	0.79
1:N:180:PRO:HG2	1:N:229:GLN:NE2	1.98	0.79
1:P:218:GLU:HG3	1:P:219:LEU:N	1.98	0.79
1:D:202:ASN:HD22	1:D:202:ASN:N	1.79	0.78
1:M:179:LEU:O	1:M:183:LEU:HD22	1.83	0.78
1:A:16:THR:HG22	1:A:46:GLN:NE2	1.97	0.78
1:P:50:GLN:HE22	1:P:76:LYS:HE2	1.48	0.78
1:N:146:MET:HG3	1:O:201:LEU:HD22	1.65	0.78
1:N:230:PHE:HA	2:S:9:MET:CE	2.13	0.78
1:O:218:GLU:HG3	1:O:219:LEU:H	1.48	0.78
1:A:180:PRO:HG2	1:A:229:GLN:NE2	1.98	0.78
1:A:317:CYS:SG	1:A:321:ILE:HD11	2.23	0.78
1:B:180:PRO:HG2	1:B:229:GLN:NE2	1.98	0.78
1:M:180:PRO:HG2	1:M:229:GLN:NE2	1.99	0.78
2:I:279:SER:HB2	3:J:43:VAL:HG11	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:201:LEU:HD21	1:O:146:MET:HG3	1.66	0.78
1:M:218:GLU:HG3	1:M:219:LEU:N	1.98	0.78
1:N:146:MET:HG3	1:O:201:LEU:CD2	2.13	0.78
1:B:202:ASN:HD22	1:B:202:ASN:N	1.82	0.77
1:C:50:GLN:HE22	1:C:76:LYS:HE2	1.50	0.77
1:B:201:LEU:HD21	1:C:146:MET:HG3	1.66	0.77
1:N:183:LEU:HG	1:O:190:PHE:CZ	2.19	0.77
1:P:202:ASN:HD22	1:P:202:ASN:N	1.82	0.77
1:A:324:LEU:O	1:A:328:THR:HG23	1.83	0.77
1:N:194:THR:HG22	1:O:183:LEU:HD11	1.64	0.77
1:A:218:GLU:HG3	1:A:219:LEU:H	1.49	0.77
1:D:218:GLU:HG3	1:D:219:LEU:H	1.50	0.77
1:M:72:LYS:HE2	1:M:151:ARG:HH12	1.48	0.77
1:B:190:PHE:CZ	1:C:183:LEU:HG	2.19	0.77
1:B:143:MET:SD	1:C:196:LYS:HE2	2.25	0.76
1:N:317:CYS:SG	1:N:321:ILE:HD11	2.25	0.76
1:C:16:THR:HG22	1:C:46:GLN:NE2	2.00	0.76
1:M:13:ILE:HA	1:M:42:MET:HG2	1.67	0.76
1:A:202:ASN:HD22	1:A:202:ASN:N	1.83	0.76
1:N:143:MET:HB2	1:O:197:LEU:HD12	1.65	0.76
2:U:202:SER:HB2	3:V:33:LYS:HB2	1.66	0.76
1:D:13:ILE:HA	1:D:42:MET:HG2	1.68	0.76
2:U:106:ASP:HB3	2:U:109:GLU:HG2	1.66	0.76
1:N:20:TRP:HZ2	1:O:204:PHE:CE2	2.03	0.76
1:N:13:ILE:HA	1:N:42:MET:HG2	1.65	0.76
1:P:13:ILE:HA	1:P:42:MET:HG2	1.67	0.76
1:P:142:PHE:O	1:P:145:VAL:HG22	1.85	0.76
1:O:202:ASN:HD22	1:O:202:ASN:N	1.82	0.75
1:A:72:LYS:HE2	1:A:151:ARG:HH12	1.50	0.75
1:O:227:ARG:NH1	1:O:227:ARG:HB3	2.01	0.75
1:N:142:PHE:O	1:N:145:VAL:HG22	1.87	0.75
1:P:218:GLU:HG3	1:P:219:LEU:H	1.52	0.75
1:M:317:CYS:SG	1:M:321:ILE:HD11	2.26	0.75
2:U:175:TRP:CZ3	3:V:48:LEU:HD12	2.22	0.75
1:A:147:LYS:NZ	1:D:197:LEU:HD13	2.01	0.75
1:C:317:CYS:SG	1:C:321:ILE:HD11	2.26	0.75
1:A:305:LEU:HD22	2:E:42:ARG:NH2	2.01	0.74
1:M:212:ILE:HG21	1:C:155:GLY:HA3	1.68	0.74
1:D:16:THR:HG22	1:D:46:GLN:NE2	2.02	0.74
1:N:16:THR:HG22	1:N:46:GLN:NE2	2.02	0.74
1:D:29:VAL:HG21	1:D:242:CYS:HA	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LEU:HD23	1:C:143:MET:SD	2.26	0.74
1:N:218:GLU:HG3	1:N:219:LEU:N	2.01	0.74
1:O:324:LEU:O	1:O:328:THR:HG23	1.87	0.74
1:N:202:ASN:HD22	1:N:202:ASN:N	1.84	0.74
2:Q:275:GLN:NE2	2:Q:298:ASN:H	1.86	0.74
1:A:142:PHE:O	1:A:145:VAL:HG22	1.88	0.74
1:B:317:CYS:SG	1:B:321:ILE:HD11	2.28	0.74
1:M:29:VAL:HG21	1:M:242:CYS:HA	1.70	0.74
2:S:202:SER:HB2	3:T:33:LYS:HB2	1.70	0.74
1:C:324:LEU:O	1:C:328:THR:HG23	1.88	0.74
1:D:305:LEU:HD22	2:K:42:ARG:NH2	2.02	0.73
1:M:202:ASN:HD22	1:M:202:ASN:N	1.86	0.73
1:C:238:PHE:HB3	1:C:266:VAL:HG12	1.70	0.73
1:M:142:PHE:O	1:M:145:VAL:HG22	1.88	0.73
2:S:256:GLN:HE22	3:T:29:LYS:HG3	1.52	0.73
1:D:179:LEU:O	1:D:183:LEU:HD22	1.87	0.73
1:A:179:LEU:O	1:A:183:LEU:HD22	1.88	0.73
1:M:187:LEU:HG	1:P:190:PHE:CZ	2.23	0.73
2:K:106:ASP:HB3	2:K:109:GLU:HG2	1.69	0.73
1:O:16:THR:HG22	1:O:46:GLN:NE2	2.03	0.73
1:A:174:LEU:CD2	1:A:177:LEU:HD11	2.18	0.73
1:B:16:THR:HG22	1:B:46:GLN:NE2	2.04	0.73
1:N:187:LEU:HD22	1:O:187:LEU:HD22	1.70	0.73
1:M:143:MET:HE2	1:P:197:LEU:HB2	1.71	0.73
1:O:27:GLY:HA2	1:P:246:PHE:CD2	2.23	0.73
1:N:187:LEU:HD11	1:O:190:PHE:CE1	2.24	0.72
1:O:317:CYS:SG	1:O:321:ILE:HD11	2.29	0.72
1:D:72:LYS:HE2	1:D:151:ARG:HH12	1.51	0.72
1:C:142:PHE:O	1:C:145:VAL:HG22	1.88	0.72
1:A:13:ILE:HA	1:A:42:MET:HG2	1.71	0.72
1:B:301:GLN:O	1:B:305:LEU:HB2	1.89	0.72
1:B:324:LEU:O	1:B:328:THR:HG23	1.89	0.72
1:D:142:PHE:O	1:D:145:VAL:HG22	1.89	0.72
1:M:218:GLU:HG3	1:M:219:LEU:H	1.54	0.72
1:O:230:PHE:HA	2:U:9:MET:CE	2.19	0.72
1:P:324:LEU:O	1:P:328:THR:HG23	1.89	0.72
2:G:256:GLN:HE22	3:H:29:LYS:HG3	1.53	0.72
2:K:232:ASN:HB2	3:L:21:THR:HB	1.71	0.72
1:O:142:PHE:O	1:O:145:VAL:HG22	1.88	0.72
1:O:13:ILE:HA	1:O:42:MET:HG2	1.69	0.72
2:G:217:ARG:NE	1:M:154:GLN:HE22	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:72:LYS:HE2	1:N:151:ARG:HH12	1.53	0.72
2:S:106:ASP:HB3	2:S:109:GLU:HG2	1.72	0.72
3:T:39:THR:HG23	3:T:40:ASN:H	1.55	0.72
3:V:39:THR:HG23	3:V:40:ASN:H	1.54	0.72
3:X:39:THR:HG23	3:X:40:ASN:H	1.53	0.72
1:O:195:ASN:HD22	1:O:195:ASN:N	1.87	0.71
1:C:218:GLU:HG3	1:C:219:LEU:H	1.53	0.71
1:B:197:LEU:HD13	1:C:147:LYS:NZ	2.05	0.71
2:I:150:VAL:HG13	2:I:151:TYR:N	2.04	0.71
1:O:29:VAL:HG21	1:O:242:CYS:HA	1.71	0.71
2:Q:106:ASP:HB3	2:Q:109:GLU:HG2	1.70	0.71
1:C:72:LYS:HE2	1:C:151:ARG:HH12	1.54	0.71
2:I:76:ILE:HG21	2:I:115:VAL:HG13	1.73	0.71
2:E:76:ILE:HG21	2:E:115:VAL:HG13	1.72	0.71
3:L:39:THR:HG23	3:L:40:ASN:H	1.54	0.71
1:M:16:THR:HG22	1:M:46:GLN:NE2	2.04	0.71
2:S:144:LEU:HD13	2:S:152:GLU:HB3	1.71	0.71
1:A:29:VAL:HG21	1:A:242:CYS:HA	1.70	0.71
2:G:76:ILE:HG21	2:G:115:VAL:HG13	1.73	0.71
1:M:197:LEU:HD13	1:P:147:LYS:HZ1	1.56	0.71
1:D:174:LEU:CD2	1:D:177:LEU:HD11	2.19	0.71
1:D:324:LEU:O	1:D:328:THR:HG23	1.90	0.71
1:M:301:GLN:O	1:M:305:LEU:HB2	1.91	0.71
3:R:39:THR:HG23	3:R:40:ASN:H	1.56	0.71
1:O:72:LYS:HE2	1:O:151:ARG:HH12	1.56	0.70
1:N:324:LEU:O	1:N:328:THR:HG23	1.91	0.70
1:B:29:VAL:HG21	1:B:242:CYS:HA	1.73	0.70
2:K:76:ILE:HG21	2:K:115:VAL:HG13	1.72	0.70
1:N:227:ARG:HB3	1:N:227:ARG:NH1	2.05	0.70
2:S:76:ILE:HG21	2:S:115:VAL:HG13	1.74	0.70
2:U:134:PRO:HG3	3:V:35:LEU:HD23	1.72	0.70
1:M:324:LEU:O	1:M:328:THR:HG23	1.90	0.70
1:P:180:PRO:CG	1:P:229:GLN:HE21	2.01	0.70
1:B:13:ILE:HA	1:B:42:MET:HG2	1.71	0.70
2:E:275:GLN:NE2	2:E:298:ASN:H	1.90	0.70
1:P:195:ASN:HD22	1:P:195:ASN:N	1.90	0.70
1:B:142:PHE:O	1:B:145:VAL:HG22	1.92	0.70
1:N:29:VAL:HG21	1:N:242:CYS:HA	1.74	0.70
1:N:143:MET:HB3	1:O:197:LEU:HD12	1.73	0.70
1:C:242:CYS:O	1:C:271:VAL:HA	1.91	0.70
1:A:242:CYS:O	1:A:271:VAL:HA	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:134:PRO:HG3	3:H:35:LEU:HD23	1.73	0.69
2:W:106:ASP:HB3	2:W:109:GLU:HG2	1.72	0.69
1:C:180:PRO:HG2	1:C:229:GLN:NE2	2.05	0.69
1:B:180:PRO:CG	1:B:229:GLN:HE21	2.03	0.69
1:M:257:GLN:OE1	2:Q:42:ARG:HG3	1.92	0.69
2:W:144:LEU:HD13	2:W:152:GLU:HB3	1.75	0.69
2:I:144:LEU:HD13	2:I:152:GLU:HB3	1.73	0.69
1:A:180:PRO:CG	1:A:229:GLN:HE21	2.03	0.69
1:B:194:THR:HG22	1:C:183:LEU:HD11	1.75	0.69
2:I:283:PHE:CE1	3:J:42:GLY:HA2	2.27	0.69
1:C:301:GLN:O	1:C:305:LEU:HB2	1.92	0.69
3:J:39:THR:HG23	3:J:40:ASN:H	1.58	0.69
2:Q:76:ILE:HG21	2:Q:115:VAL:HG13	1.74	0.69
1:C:202:ASN:HD22	1:C:202:ASN:N	1.90	0.69
2:G:150:VAL:HB	3:H:52:TYR:CD2	2.28	0.69
1:B:218:GLU:HG3	1:B:219:LEU:H	1.55	0.69
1:B:238:PHE:HB3	1:B:266:VAL:HG12	1.75	0.69
3:F:39:THR:HG23	3:F:40:ASN:H	1.58	0.69
1:N:20:TRP:CZ2	1:O:204:PHE:CE2	2.81	0.69
1:N:218:GLU:HG3	1:N:219:LEU:H	1.55	0.69
1:P:133:ILE:HB	1:P:136:ILE:HD12	1.75	0.68
2:W:76:ILE:HG21	2:W:115:VAL:HG13	1.75	0.68
1:B:146:MET:HB2	1:C:201:LEU:HD22	1.75	0.68
2:G:106:ASP:HB3	2:G:109:GLU:HG2	1.73	0.68
3:H:39:THR:HG23	3:H:40:ASN:H	1.58	0.68
2:S:150:VAL:HG13	2:S:151:TYR:N	2.07	0.68
1:B:242:CYS:O	1:B:271:VAL:HA	1.93	0.68
1:M:242:CYS:O	1:M:271:VAL:HA	1.93	0.68
1:N:197:LEU:HD13	1:O:147:LYS:HZ3	1.58	0.68
1:P:138:GLU:CG	1:P:175:ARG:HB3	2.20	0.68
1:A:195:ASN:N	1:A:195:ASN:HD22	1.91	0.68
1:N:20:TRP:CZ2	1:O:204:PHE:HE2	2.12	0.68
1:B:201:LEU:HB3	1:C:143:MET:HE1	1.76	0.68
1:M:194:THR:HG22	1:P:183:LEU:HD11	1.76	0.68
1:O:174:LEU:CD2	1:O:177:LEU:HD11	2.22	0.68
1:O:301:GLN:O	1:O:305:LEU:HB2	1.92	0.68
2:U:144:LEU:HD13	2:U:152:GLU:HB3	1.76	0.68
1:A:238:PHE:HB3	1:A:266:VAL:HG12	1.75	0.68
2:E:106:ASP:HB3	2:E:109:GLU:HG2	1.73	0.68
2:E:279:SER:HB2	3:F:43:VAL:HG11	1.76	0.68
2:I:150:VAL:HB	3:J:52:TYR:CD2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:112:LEU:HD23	2:S:149:PHE:HE2	1.58	0.68
1:M:238:PHE:HB3	1:M:266:VAL:HG12	1.75	0.68
1:N:180:PRO:CG	1:N:229:GLN:HE21	2.05	0.68
1:O:27:GLY:HA2	1:P:246:PHE:CE2	2.28	0.68
1:P:72:LYS:HE2	1:P:151:ARG:HH12	1.57	0.68
1:P:238:PHE:HB3	1:P:266:VAL:HG12	1.76	0.68
2:I:150:VAL:HG13	2:I:151:TYR:H	1.58	0.67
1:N:29:VAL:HG22	1:N:243:ILE:HG23	1.76	0.67
2:U:17:LEU:HD13	2:U:58:GLN:HG2	1.76	0.67
1:O:242:CYS:O	1:O:271:VAL:HA	1.93	0.67
2:E:144:LEU:HD13	2:E:152:GLU:HB3	1.77	0.67
2:E:189:GLU:HB3	3:F:48:LEU:CD2	2.24	0.67
2:Q:275:GLN:HE22	2:Q:297:THR:HA	1.58	0.67
2:U:76:ILE:HG21	2:U:115:VAL:HG13	1.75	0.67
2:U:190:PHE:CE1	3:V:48:LEU:HD13	2.28	0.67
1:A:201:LEU:HB3	1:D:143:MET:HE1	1.77	0.67
1:N:238:PHE:HB3	1:N:266:VAL:HG12	1.75	0.67
2:S:150:VAL:HG13	2:S:151:TYR:H	1.60	0.67
1:A:22:PHE:HB2	1:A:238:PHE:HA	1.75	0.67
1:B:72:LYS:HE2	1:B:151:ARG:HH12	1.59	0.67
2:I:19:ARG:NH1	1:C:5:VAL:CG2	2.57	0.67
1:M:138:GLU:CG	1:M:175:ARG:HB3	2.20	0.67
1:M:201:LEU:O	1:M:205:MET:HG2	1.94	0.67
1:P:242:CYS:O	1:P:271:VAL:HA	1.95	0.67
2:Q:144:LEU:HD13	2:Q:152:GLU:HB3	1.77	0.67
1:A:138:GLU:CG	1:A:175:ARG:HB3	2.21	0.67
1:B:197:LEU:HB2	1:C:143:MET:HB3	1.75	0.67
1:D:29:VAL:HG22	1:D:243:ILE:HG23	1.76	0.67
2:K:144:LEU:HD13	2:K:152:GLU:HB3	1.76	0.67
1:N:301:GLN:O	1:N:305:LEU:HB2	1.95	0.67
2:U:278:LYS:HA	2:U:295:LYS:HE3	1.76	0.67
2:G:144:LEU:HD13	2:G:152:GLU:HB3	1.76	0.67
1:B:183:LEU:HB2	1:C:190:PHE:CE2	2.29	0.67
1:B:201:LEU:HD22	1:C:146:MET:HB2	1.76	0.67
2:G:112:LEU:HD11	2:G:143:LYS:HD2	1.76	0.67
1:C:179:LEU:O	1:C:183:LEU:HD22	1.95	0.67
1:D:301:GLN:O	1:D:305:LEU:HB2	1.93	0.67
1:N:260:ILE:HD13	2:S:42:ARG:HG2	1.75	0.67
1:M:212:ILE:HG21	1:C:155:GLY:HA2	1.77	0.66
1:P:301:GLN:O	1:P:305:LEU:HB2	1.94	0.66
1:B:201:LEU:CD2	1:C:146:MET:HG3	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:PHE:HB3	1:D:266:VAL:HG12	1.76	0.66
2:K:112:LEU:HD11	2:K:143:LYS:HD2	1.78	0.66
1:M:180:PRO:CG	1:M:229:GLN:HE21	2.04	0.66
1:O:238:PHE:HB3	1:O:266:VAL:HG12	1.76	0.66
2:Q:112:LEU:HD11	2:Q:143:LYS:HD2	1.76	0.66
1:A:305:LEU:HD22	2:E:42:ARG:HH21	1.60	0.66
2:E:150:VAL:HG13	2:E:151:TYR:N	2.10	0.66
2:I:106:ASP:HB3	2:I:109:GLU:HG2	1.76	0.66
1:N:227:ARG:HB3	1:N:227:ARG:HH11	1.60	0.66
1:P:202:ASN:HD22	1:P:202:ASN:H	1.41	0.66
2:U:150:VAL:HG13	2:U:151:TYR:N	2.09	0.66
2:U:271:LEU:HD22	2:U:298:ASN:ND2	2.11	0.66
1:C:29:VAL:HG22	1:C:243:ILE:HG23	1.77	0.66
1:A:197:LEU:HD13	1:D:147:LYS:HZ1	1.60	0.66
1:A:301:GLN:O	1:A:305:LEU:HB2	1.95	0.66
1:P:19:LYS:HA	1:P:162:THR:HA	1.78	0.66
1:A:19:LYS:HA	1:A:162:THR:HA	1.77	0.66
1:A:190:PHE:CE1	1:D:187:LEU:HD11	2.30	0.66
2:E:112:LEU:HD23	2:E:149:PHE:HE2	1.61	0.66
2:G:150:VAL:HG13	2:G:151:TYR:N	2.10	0.66
2:K:275:GLN:NE2	2:K:298:ASN:H	1.94	0.66
1:O:180:PRO:CG	1:O:229:GLN:HE21	2.01	0.66
2:W:150:VAL:HG13	2:W:151:TYR:N	2.09	0.66
2:E:256:GLN:HE22	3:F:29:LYS:HG3	1.60	0.66
2:I:19:ARG:NH1	1:C:5:VAL:HG23	2.10	0.66
2:Q:236:ILE:HD12	2:Q:249:GLN:HB3	1.77	0.66
2:S:175:TRP:CZ3	3:T:48:LEU:HD12	2.31	0.66
1:C:29:VAL:HG21	1:C:242:CYS:HA	1.76	0.66
1:A:174:LEU:HD13	1:A:177:LEU:HD11	1.78	0.66
1:N:202:ASN:HD22	1:N:202:ASN:H	1.44	0.66
2:Q:150:VAL:HG13	2:Q:151:TYR:N	2.10	0.66
1:D:227:ARG:HB3	1:D:227:ARG:NH1	2.10	0.66
2:E:275:GLN:HE22	2:E:297:THR:HA	1.59	0.66
2:G:17:LEU:HD13	2:G:58:GLN:HG2	1.77	0.66
1:B:29:VAL:HG22	1:B:243:ILE:HG23	1.78	0.66
2:E:112:LEU:HD11	2:E:143:LYS:HD2	1.77	0.66
2:K:236:ILE:HD12	2:K:249:GLN:HB3	1.78	0.66
1:O:178:GLN:HA	1:O:229:GLN:HE22	1.61	0.66
2:U:112:LEU:HD23	2:U:149:PHE:HE2	1.61	0.66
2:K:150:VAL:HG13	2:K:151:TYR:N	2.10	0.66
1:C:178:GLN:HA	1:C:229:GLN:HE22	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:16:THR:HG21	1:C:308:ASP:OD2	1.96	0.65
1:N:201:LEU:HD22	1:O:146:MET:HB2	1.76	0.65
1:A:147:LYS:HZ1	1:D:197:LEU:HD13	1.59	0.65
1:A:178:GLN:HA	1:A:229:GLN:HE22	1.60	0.65
1:D:19:LYS:HA	1:D:162:THR:HA	1.78	0.65
1:D:242:CYS:O	1:D:271:VAL:HA	1.96	0.65
2:G:278:LYS:HA	2:G:295:LYS:HE3	1.78	0.65
1:P:179:LEU:N	1:P:180:PRO:HD2	2.11	0.65
1:P:196:LYS:HG2	1:P:202:ASN:OD1	1.95	0.65
2:Q:232:ASN:HB2	3:R:21:THR:HB	1.78	0.65
2:I:208:HIS:NE2	3:J:29:LYS:HG2	2.11	0.65
1:M:197:LEU:HD13	1:P:147:LYS:NZ	2.10	0.65
1:O:179:LEU:N	1:O:180:PRO:HD2	2.10	0.65
2:U:240:GLU:HG2	3:V:6:SER:OG	1.97	0.65
2:G:202:SER:HB2	3:H:33:LYS:HB2	1.77	0.65
1:M:190:PHE:CZ	1:P:187:LEU:HG	2.31	0.65
1:O:201:LEU:O	1:O:205:MET:HG2	1.96	0.65
1:D:179:LEU:N	1:D:180:PRO:HD2	2.10	0.65
2:W:231:LYS:HE2	3:X:18:THR:OG1	1.97	0.65
1:A:179:LEU:N	1:A:180:PRO:HD2	2.10	0.65
1:M:29:VAL:HG22	1:M:243:ILE:HG23	1.79	0.65
2:W:150:VAL:HG13	2:W:151:TYR:H	1.61	0.65
1:B:22:PHE:HB2	1:B:238:PHE:HA	1.78	0.65
2:K:17:LEU:HD13	2:K:58:GLN:HG2	1.78	0.65
2:Q:278:LYS:HA	2:Q:295:LYS:HE3	1.79	0.65
1:C:179:LEU:N	1:C:180:PRO:HD2	2.12	0.65
1:A:187:LEU:HD11	1:D:190:PHE:CE1	2.31	0.65
1:M:305:LEU:HD22	2:Q:42:ARG:HH21	1.61	0.65
1:P:201:LEU:O	1:P:205:MET:HG2	1.97	0.65
1:C:22:PHE:HB2	1:C:238:PHE:HA	1.79	0.65
1:B:227:ARG:NH1	1:B:227:ARG:HB3	2.12	0.65
1:D:22:PHE:HB2	1:D:238:PHE:HA	1.77	0.65
2:S:278:LYS:HA	2:S:295:LYS:HE3	1.79	0.65
1:M:22:PHE:HB2	1:M:238:PHE:HA	1.78	0.64
2:U:112:LEU:HD11	2:U:143:LYS:HD2	1.79	0.64
1:B:306:TYR:HB3	1:B:309:PHE:HB2	1.79	0.64
1:N:174:LEU:CD2	1:N:177:LEU:HD11	2.25	0.64
2:I:19:ARG:HH12	1:C:5:VAL:CG2	2.09	0.64
1:M:287:ARG:HB2	1:N:288:CYS:SG	2.37	0.64
2:K:231:LYS:HE2	3:L:18:THR:OG1	1.97	0.64
1:N:19:LYS:HA	1:N:162:THR:HA	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:242:CYS:O	1:N:271:VAL:HA	1.98	0.64
1:B:195:ASN:HD22	1:B:195:ASN:N	1.93	0.64
2:K:175:TRP:CZ3	3:L:48:LEU:HD12	2.31	0.64
1:M:199:PRO:HD3	1:C:156:GLU:HG3	1.80	0.64
1:N:179:LEU:N	1:N:180:PRO:HD2	2.13	0.64
1:O:257:GLN:OE1	2:U:42:ARG:HG3	1.96	0.64
1:P:178:GLN:HA	1:P:229:GLN:HE22	1.62	0.64
2:I:203:ASN:OD1	3:J:32:THR:HG22	1.98	0.64
1:O:19:LYS:HA	1:O:162:THR:HA	1.78	0.64
1:P:22:PHE:HB2	1:P:238:PHE:HA	1.78	0.64
2:S:275:GLN:HE22	2:S:297:THR:HA	1.63	0.64
1:C:195:ASN:HD22	1:C:195:ASN:N	1.95	0.64
1:B:179:LEU:N	1:B:180:PRO:HD2	2.11	0.64
1:M:179:LEU:N	1:M:180:PRO:HD2	2.12	0.64
1:N:194:THR:CG2	1:O:183:LEU:HD11	2.27	0.64
1:A:187:LEU:HG	1:D:190:PHE:CZ	2.33	0.64
2:I:112:LEU:HD23	2:I:149:PHE:HE2	1.62	0.64
1:C:227:ARG:HB3	1:C:227:ARG:NH1	2.13	0.64
1:A:72:LYS:HE2	1:A:151:ARG:NH1	2.13	0.64
2:I:42:ARG:NH2	1:C:305:LEU:CD2	2.59	0.64
1:N:143:MET:HB3	1:O:197:LEU:CD1	2.28	0.64
1:O:133:ILE:HB	1:O:136:ILE:HD12	1.80	0.64
1:A:190:PHE:CZ	1:D:187:LEU:HG	2.32	0.64
2:G:275:GLN:NE2	2:G:298:ASN:H	1.96	0.64
2:K:134:PRO:HG3	3:L:35:LEU:HD23	1.79	0.64
1:N:306:TYR:HB3	1:N:309:PHE:HB2	1.79	0.64
1:O:20:TRP:HB2	1:O:236:THR:HG23	1.79	0.64
2:Q:17:LEU:HD13	2:Q:58:GLN:HG2	1.78	0.64
2:I:202:SER:HB2	3:J:33:LYS:HB2	1.80	0.63
2:W:236:ILE:HD12	2:W:249:GLN:HB3	1.79	0.63
1:D:306:TYR:HB3	1:D:309:PHE:HB2	1.79	0.63
1:P:174:LEU:CD2	1:P:177:LEU:HD11	2.26	0.63
1:C:19:LYS:HA	1:C:162:THR:HA	1.79	0.63
1:B:133:ILE:HB	1:B:136:ILE:HD12	1.79	0.63
1:N:201:LEU:HB3	1:O:143:MET:CE	2.29	0.63
1:N:274:LEU:CD1	1:N:313:LYS:HB3	2.29	0.63
1:P:16:THR:HG22	1:P:46:GLN:HE21	1.62	0.63
1:B:201:LEU:O	1:B:205:MET:HG2	1.98	0.63
1:D:133:ILE:HB	1:D:136:ILE:HD12	1.81	0.63
2:K:112:LEU:HD23	2:K:149:PHE:HE2	1.62	0.63
1:C:243:ILE:HA	1:C:271:VAL:HG13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:134:PRO:HG3	3:J:35:LEU:HD23	1.80	0.63
1:M:27:GLY:HA2	1:N:246:PHE:CE2	2.34	0.63
1:M:133:ILE:HB	1:M:136:ILE:HD12	1.81	0.63
2:U:236:ILE:HD12	2:U:249:GLN:HB3	1.81	0.63
2:W:275:GLN:HE22	2:W:297:THR:HA	1.62	0.63
1:C:180:PRO:CG	1:C:229:GLN:HE21	2.10	0.63
1:A:196:LYS:HG2	1:A:202:ASN:OD1	1.99	0.63
1:D:72:LYS:HE2	1:D:151:ARG:NH1	2.14	0.63
1:M:274:LEU:CD1	1:M:313:LYS:HB3	2.29	0.63
1:M:287:ARG:CB	1:N:288:CYS:SG	2.87	0.63
1:B:190:PHE:CE1	1:C:187:LEU:HD11	2.33	0.63
2:E:150:VAL:HG13	2:E:151:TYR:H	1.62	0.63
1:P:56:THR:HB	1:P:90:PRO:HG3	1.81	0.63
2:I:16:THR:CG2	1:C:308:ASP:HB2	2.27	0.63
1:M:212:ILE:HG22	1:C:156:GLU:OE1	1.99	0.63
1:N:143:MET:CB	1:O:197:LEU:HB2	2.26	0.63
1:O:29:VAL:HG22	1:O:243:ILE:HG23	1.81	0.63
1:P:257:GLN:OE1	2:W:42:ARG:HG3	1.98	0.63
2:W:271:LEU:HD22	2:W:298:ASN:ND2	2.13	0.63
1:D:50:GLN:NE2	1:D:76:LYS:HE2	2.13	0.63
2:E:17:LEU:HD13	2:E:58:GLN:HG2	1.79	0.63
1:A:257:GLN:OE1	2:E:42:ARG:HG3	1.99	0.62
1:A:306:TYR:HB3	1:A:309:PHE:HB2	1.81	0.62
2:I:42:ARG:HH22	1:C:305:LEU:CD2	2.12	0.62
1:M:306:TYR:HB3	1:M:309:PHE:HB2	1.81	0.62
1:N:243:ILE:HA	1:N:271:VAL:HG13	1.81	0.62
1:O:22:PHE:HB2	1:O:238:PHE:HA	1.80	0.62
2:Q:150:VAL:HG13	2:Q:151:TYR:H	1.62	0.62
2:U:256:GLN:HE22	3:V:29:LYS:HG3	1.64	0.62
2:E:278:LYS:HA	2:E:295:LYS:HE3	1.81	0.62
2:E:285:GLY:HA2	2:E:289:PHE:HD2	1.64	0.62
2:I:232:ASN:HB2	3:J:21:THR:CB	2.29	0.62
1:M:19:LYS:HA	1:M:162:THR:HA	1.80	0.62
1:P:174:LEU:HD13	1:P:177:LEU:HD11	1.80	0.62
1:D:267:ASN:HB2	2:K:12:LYS:HZ1	1.64	0.62
2:K:275:GLN:HE22	2:K:297:THR:HA	1.62	0.62
2:W:275:GLN:NE2	2:W:298:ASN:H	1.97	0.62
1:C:274:LEU:CD1	1:C:313:LYS:HB3	2.30	0.62
1:A:227:ARG:HB3	1:A:227:ARG:NH1	2.14	0.62
1:B:19:LYS:HA	1:B:162:THR:HA	1.81	0.62
1:B:56:THR:HB	1:B:90:PRO:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:116:ILE:HA	2:E:119:MET:HE2	1.81	0.62
2:W:112:LEU:HD11	2:W:143:LYS:HD2	1.82	0.62
1:A:202:ASN:HD22	1:A:202:ASN:H	1.45	0.62
1:D:201:LEU:O	1:D:205:MET:HG2	2.00	0.62
2:G:217:ARG:NH2	1:M:154:GLN:NE2	2.47	0.62
2:K:271:LEU:HD22	2:K:298:ASN:ND2	2.14	0.62
2:W:278:LYS:HA	2:W:295:LYS:HE3	1.81	0.62
2:G:275:GLN:HE22	2:G:297:THR:HA	1.64	0.62
1:A:29:VAL:HG22	1:A:243:ILE:HG23	1.82	0.62
1:M:246:PHE:CD2	1:N:27:GLY:HA2	2.35	0.62
1:C:133:ILE:HB	1:C:136:ILE:HD12	1.81	0.62
1:C:306:TYR:HB3	1:C:309:PHE:HB2	1.80	0.62
2:G:282:GLU:O	2:G:286:GLN:HG3	2.00	0.62
1:P:174:LEU:C	1:P:177:LEU:HG	2.20	0.62
1:P:227:ARG:NH1	1:P:227:ARG:HB3	2.14	0.62
1:B:183:LEU:HG	1:C:190:PHE:CZ	2.35	0.61
1:D:202:ASN:HD22	1:D:202:ASN:H	1.48	0.61
2:I:19:ARG:HH12	1:C:5:VAL:HG22	1.64	0.61
1:M:138:GLU:CB	1:M:176:PHE:HB3	2.27	0.61
1:N:22:PHE:HB2	1:N:238:PHE:HA	1.80	0.61
1:B:146:MET:HB2	1:C:201:LEU:CD2	2.31	0.61
2:G:112:LEU:HD23	2:G:149:PHE:HE2	1.65	0.61
1:N:72:LYS:HE2	1:N:151:ARG:NH1	2.14	0.61
1:N:143:MET:SD	1:O:196:LYS:HG3	2.39	0.61
1:P:274:LEU:CD1	1:P:313:LYS:HB3	2.30	0.61
1:C:202:ASN:HD22	1:C:202:ASN:H	1.46	0.61
2:E:271:LEU:HD22	2:E:298:ASN:ND2	2.15	0.61
2:K:191:PHE:HZ	2:K:211:LYS:HG3	1.66	0.61
1:N:238:PHE:HB3	1:N:266:VAL:CG1	2.30	0.61
1:P:20:TRP:HB2	1:P:236:THR:HG23	1.81	0.61
1:C:174:LEU:CD2	1:C:177:LEU:HD11	2.27	0.61
1:D:238:PHE:HB3	1:D:266:VAL:CG1	2.29	0.61
2:I:275:GLN:HE22	2:I:297:THR:HA	1.66	0.61
1:M:72:LYS:HE2	1:M:151:ARG:NH1	2.14	0.61
1:C:238:PHE:HB3	1:C:266:VAL:CG1	2.29	0.61
1:A:197:LEU:HD13	1:D:147:LYS:NZ	2.14	0.61
2:Q:112:LEU:HD23	2:Q:149:PHE:HE2	1.66	0.61
1:C:174:LEU:HD13	1:C:177:LEU:HD11	1.83	0.61
1:B:197:LEU:O	1:C:143:MET:CE	2.48	0.61
1:B:238:PHE:HB3	1:B:266:VAL:CG1	2.31	0.61
2:I:278:LYS:HA	2:I:295:LYS:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:288:CYS:SG	1:N:287:ARG:HB3	2.40	0.61
1:A:284:ASN:N	1:A:284:ASN:HD22	1.98	0.61
1:D:27:GLY:HA2	1:C:246:PHE:CD2	2.35	0.61
2:I:286:GLN:HG2	2:I:291:ILE:O	2.01	0.61
1:M:199:PRO:CG	1:C:156:GLU:HG2	2.30	0.61
2:W:112:LEU:HD23	2:W:149:PHE:HE2	1.65	0.61
1:A:143:MET:HE1	1:D:201:LEU:HB3	1.82	0.61
1:M:195:ASN:HD22	1:M:195:ASN:N	1.98	0.61
1:A:29:VAL:CG2	1:A:243:ILE:HG23	2.31	0.61
1:A:238:PHE:HB3	1:A:266:VAL:CG1	2.30	0.61
2:E:236:ILE:HD12	2:E:249:GLN:HB3	1.83	0.61
1:B:143:MET:HE3	1:C:201:LEU:CB	2.29	0.61
1:D:56:THR:HB	1:D:90:PRO:HG3	1.83	0.61
1:O:306:TYR:HB3	1:O:309:PHE:HB2	1.83	0.61
2:I:35:THR:HG22	1:C:307:GLU:OE2	2.01	0.60
2:I:232:ASN:HB2	3:J:21:THR:HB	1.82	0.60
2:S:17:LEU:HD13	2:S:58:GLN:HG2	1.83	0.60
2:S:134:PRO:HG3	3:T:35:LEU:HD23	1.82	0.60
2:U:150:VAL:HG13	2:U:151:TYR:H	1.64	0.60
2:U:271:LEU:HD22	2:U:298:ASN:HD21	1.66	0.60
1:A:281:GLN:O	1:A:282:GLU:HB2	2.00	0.60
1:D:274:LEU:CD1	1:D:313:LYS:HB3	2.31	0.60
1:O:281:GLN:O	1:O:282:GLU:HB2	2.00	0.60
1:P:16:THR:HA	1:P:46:GLN:HE22	1.67	0.60
1:D:20:TRP:HB2	1:D:236:THR:HG23	1.81	0.60
3:F:35:LEU:HA	3:F:38:VAL:HG23	1.84	0.60
1:M:20:TRP:HB2	1:M:236:THR:HG23	1.81	0.60
1:M:190:PHE:CE1	1:P:187:LEU:HD11	2.37	0.60
1:M:282:GLU:O	1:M:283:HIS:O	2.19	0.60
1:O:227:ARG:HB3	1:O:227:ARG:HH11	1.66	0.60
1:P:174:LEU:HB3	1:P:177:LEU:CD1	2.31	0.60
2:Q:271:LEU:HD22	2:Q:298:ASN:ND2	2.16	0.60
2:I:112:LEU:HD11	2:I:143:LYS:HD2	1.83	0.60
1:O:138:GLU:CG	1:O:175:ARG:HB3	2.22	0.60
1:A:247:LEU:HB3	1:B:247:LEU:HD13	1.83	0.60
1:D:138:GLU:CG	1:D:175:ARG:HB3	2.25	0.60
1:N:190:PHE:HE2	1:O:183:LEU:HB2	1.67	0.60
2:U:191:PHE:HZ	2:U:211:LYS:HG3	1.65	0.60
1:B:20:TRP:HB2	1:B:236:THR:HG23	1.82	0.60
1:B:178:GLN:HA	1:B:229:GLN:HE22	1.67	0.60
2:E:202:SER:HB2	3:F:33:LYS:CB	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:250:LEU:HD11	3:H:13:VAL:HG22	1.83	0.60
2:I:271:LEU:HD22	2:I:298:ASN:ND2	2.17	0.60
2:I:275:GLN:NE2	2:I:298:ASN:H	1.97	0.60
1:N:281:GLN:O	1:N:282:GLU:HB2	2.01	0.60
2:Q:285:GLY:HA2	2:Q:289:PHE:HD2	1.66	0.60
1:B:274:LEU:CD1	1:B:313:LYS:HB3	2.31	0.60
2:G:256:GLN:HE22	3:H:29:LYS:CG	2.14	0.60
1:N:143:MET:CE	1:O:197:LEU:HB2	2.26	0.60
1:P:306:TYR:HB3	1:P:309:PHE:HB2	1.82	0.60
1:C:281:GLN:O	1:C:282:GLU:HB2	2.02	0.60
1:B:305:LEU:HD22	2:G:42:ARG:NH2	2.16	0.60
1:D:281:GLN:O	1:D:282:GLU:HB2	2.02	0.60
1:O:56:THR:HB	1:O:90:PRO:HG3	1.84	0.60
1:P:281:GLN:O	1:P:282:GLU:HB2	2.01	0.60
2:W:191:PHE:HZ	2:W:211:LYS:HG3	1.67	0.60
2:K:190:PHE:CE1	3:L:48:LEU:HD13	2.36	0.60
1:N:56:THR:HB	1:N:90:PRO:HG3	1.82	0.60
2:E:286:GLN:HG2	2:E:291:ILE:O	2.01	0.59
2:G:271:LEU:HD22	2:G:298:ASN:ND2	2.17	0.59
1:P:284:ASN:HD22	1:P:284:ASN:N	1.99	0.59
2:S:275:GLN:NE2	2:S:298:ASN:H	2.00	0.59
3:X:39:THR:HG23	3:X:40:ASN:N	2.16	0.59
2:E:189:GLU:HB3	3:F:48:LEU:HD22	1.82	0.59
2:K:286:GLN:HG2	2:K:291:ILE:O	2.02	0.59
1:M:178:GLN:HA	1:M:229:GLN:HE22	1.65	0.59
2:W:17:LEU:HD13	2:W:58:GLN:HG2	1.84	0.59
1:C:284:ASN:HD22	1:C:284:ASN:N	2.00	0.59
1:D:198:GLY:CA	1:D:200:MET:H	2.15	0.59
1:D:267:ASN:O	1:D:310:HIS:HB2	2.02	0.59
1:O:202:ASN:HD22	1:O:202:ASN:H	1.50	0.59
1:O:238:PHE:HB3	1:O:266:VAL:CG1	2.32	0.59
1:P:347:ILE:C	1:P:349:GLU:H	2.05	0.59
1:M:56:THR:HB	1:M:90:PRO:HG3	1.83	0.59
1:A:201:LEU:O	1:A:205:MET:HG2	2.03	0.59
1:A:243:ILE:HA	1:A:271:VAL:HG13	1.84	0.59
1:A:274:LEU:CD1	1:A:313:LYS:HB3	2.32	0.59
1:B:174:LEU:CD2	1:B:177:LEU:HD11	2.22	0.59
1:B:281:GLN:O	1:B:282:GLU:HB2	2.02	0.59
2:K:204:ILE:HG12	3:L:31:TYR:HD2	1.66	0.59
1:O:274:LEU:CD1	1:O:313:LYS:HB3	2.32	0.59
1:B:183:LEU:HB2	1:C:190:PHE:HE2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:12:LYS:HD2	1:C:267:ASN:HB3	1.85	0.59
1:P:243:ILE:HA	1:P:271:VAL:HG13	1.84	0.59
2:S:150:VAL:HB	3:T:52:TYR:CD2	2.37	0.59
1:D:247:LEU:HD13	1:C:247:LEU:HB3	1.84	0.59
2:K:150:VAL:HG13	2:K:151:TYR:H	1.65	0.59
1:M:243:ILE:HA	1:M:271:VAL:HG13	1.84	0.59
2:S:208:HIS:NE2	3:T:29:LYS:HG2	2.18	0.59
2:G:94:SER:HB3	2:G:122:TRP:CH2	2.37	0.59
2:G:150:VAL:HG13	2:G:151:TYR:H	1.66	0.59
1:M:193:ILE:C	1:M:195:ASN:H	2.06	0.59
1:M:227:ARG:NH1	1:M:227:ARG:HB3	2.18	0.59
1:M:284:ASN:HD22	1:M:284:ASN:N	2.00	0.59
1:P:154:GLN:CG	1:C:79:GLY:HA2	2.24	0.59
1:M:281:GLN:O	1:M:282:GLU:HB2	2.02	0.59
3:T:35:LEU:HA	3:T:38:VAL:HG23	1.85	0.59
1:A:194:THR:HG22	1:D:183:LEU:HD11	1.84	0.59
1:M:199:PRO:CD	1:C:156:GLU:CG	2.78	0.59
1:N:198:GLY:CA	1:N:200:MET:H	2.16	0.59
1:O:196:LYS:HG2	1:O:202:ASN:OD1	2.03	0.59
1:C:72:LYS:HE2	1:C:151:ARG:NH1	2.16	0.59
1:B:243:ILE:HA	1:B:271:VAL:HG13	1.85	0.58
1:P:260:ILE:HD13	2:W:42:ARG:HG2	1.84	0.58
1:P:305:LEU:HD22	2:W:42:ARG:NH2	2.18	0.58
2:U:94:SER:HB3	2:U:122:TRP:CH2	2.37	0.58
1:C:56:THR:HB	1:C:90:PRO:HG3	1.85	0.58
1:A:72:LYS:CE	1:A:151:ARG:HH12	2.16	0.58
1:D:174:LEU:HD22	1:D:177:LEU:CD1	2.26	0.58
2:K:278:LYS:HA	2:K:295:LYS:HE3	1.85	0.58
3:L:35:LEU:HA	3:L:38:VAL:HG23	1.85	0.58
1:M:238:PHE:HB3	1:M:266:VAL:CG1	2.32	0.58
1:N:133:ILE:HB	1:N:136:ILE:HD12	1.85	0.58
1:N:267:ASN:O	1:N:310:HIS:HB2	2.02	0.58
2:Q:282:GLU:O	2:Q:286:GLN:HG3	2.03	0.58
2:U:275:GLN:HE22	2:U:297:THR:HA	1.68	0.58
1:A:56:THR:HB	1:A:90:PRO:HG3	1.84	0.58
1:B:284:ASN:HD22	1:B:284:ASN:N	2.00	0.58
1:D:29:VAL:CG2	1:D:243:ILE:HG23	2.33	0.58
2:I:232:ASN:HB2	3:J:21:THR:OG1	2.02	0.58
2:S:271:LEU:HD22	2:S:298:ASN:ND2	2.18	0.58
2:U:275:GLN:NE2	2:U:298:ASN:H	2.00	0.58
1:O:285:CYS:SG	1:P:285:CYS:SG	3.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:238:PHE:HB3	1:P:266:VAL:CG1	2.32	0.58
1:A:20:TRP:HB2	1:A:236:THR:HG23	1.84	0.58
1:B:29:VAL:CG2	1:B:243:ILE:HG23	2.34	0.58
2:K:285:GLY:HA2	2:K:289:PHE:HD2	1.68	0.58
1:M:347:ILE:C	1:M:349:GLU:H	2.06	0.58
1:A:258:GLU:HG2	1:A:262:TYR:CE2	2.38	0.58
1:D:196:LYS:HZ3	1:D:202:ASN:CG	2.07	0.58
1:D:243:ILE:HA	1:D:271:VAL:HG13	1.86	0.58
2:E:94:SER:HB3	2:E:122:TRP:CH2	2.38	0.58
2:I:16:THR:HG21	1:C:308:ASP:CB	2.34	0.58
1:N:183:LEU:HD11	1:O:194:THR:CG2	2.31	0.58
1:N:260:ILE:CD1	2:S:42:ARG:HD3	2.32	0.58
2:I:231:LYS:HE2	3:J:18:THR:OG1	2.04	0.58
1:O:198:GLY:CA	1:O:200:MET:H	2.17	0.58
1:D:54:ILE:HA	1:D:86:MET:O	2.03	0.58
1:N:12:LEU:O	1:N:12:LEU:HD22	2.04	0.58
1:O:194:THR:C	1:O:195:ASN:HD22	2.06	0.58
1:C:194:THR:C	1:C:195:ASN:HD22	2.07	0.58
1:B:143:MET:HE2	1:C:197:LEU:O	2.03	0.57
1:D:202:ASN:N	1:D:202:ASN:ND2	2.52	0.57
1:O:16:THR:HG22	1:O:46:GLN:HE21	1.69	0.57
2:S:112:LEU:HD11	2:S:143:LYS:HD2	1.85	0.57
1:C:32:THR:HG22	1:C:61:ASN:HD22	1.69	0.57
1:A:194:THR:C	1:A:195:ASN:HD22	2.08	0.57
1:M:205:MET:HG3	1:P:228:GLN:CD	2.24	0.57
1:N:54:ILE:HD11	1:N:88:ILE:HG12	1.86	0.57
1:C:201:LEU:O	1:C:205:MET:HG2	2.04	0.57
1:C:282:GLU:O	1:C:283:HIS:O	2.21	0.57
2:G:283:PHE:CE1	3:H:42:GLY:HA2	2.39	0.57
1:O:72:LYS:HE2	1:O:151:ARG:NH1	2.19	0.57
1:O:347:ILE:C	1:O:349:GLU:H	2.07	0.57
2:S:282:GLU:O	2:S:286:GLN:HG3	2.04	0.57
2:W:232:ASN:HB2	3:X:21:THR:CB	2.34	0.57
1:C:72:LYS:CE	1:C:151:ARG:HH12	2.18	0.57
1:A:174:LEU:HD22	1:A:177:LEU:CD1	2.29	0.57
1:A:347:ILE:C	1:A:349:GLU:H	2.06	0.57
1:N:20:TRP:HB2	1:N:236:THR:HG23	1.86	0.57
1:A:174:LEU:C	1:A:177:LEU:HG	2.25	0.57
1:B:198:GLY:CA	1:B:200:MET:H	2.17	0.57
2:G:217:ARG:HH21	1:M:154:GLN:HE22	1.50	0.57
1:N:217:ASN:ND2	1:O:217:ASN:OD1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ASN:HB3	1:A:341:ILE:HD13	1.87	0.57
1:B:282:GLU:O	1:B:283:HIS:O	2.22	0.57
1:O:282:GLU:O	1:O:283:HIS:O	2.21	0.57
1:P:72:LYS:HE2	1:P:151:ARG:NH1	2.20	0.57
1:A:174:LEU:HD13	1:A:177:LEU:CD1	2.35	0.57
2:G:278:LYS:HG3	2:G:295:LYS:HG2	1.87	0.57
2:I:16:THR:CG2	1:C:308:ASP:CB	2.81	0.57
2:I:236:ILE:HD12	2:I:249:GLN:HB3	1.86	0.57
2:S:94:SER:HB3	2:S:122:TRP:CH2	2.40	0.57
1:D:247:LEU:HB3	1:C:247:LEU:HD13	1.86	0.57
3:L:39:THR:HG23	3:L:40:ASN:N	2.18	0.57
1:N:147:LYS:HZ1	1:O:197:LEU:HD13	1.68	0.57
1:N:201:LEU:O	1:N:205:MET:HG2	2.04	0.57
1:N:233:PRO:HG3	2:S:11:ALA:H	1.68	0.57
2:U:282:GLU:O	2:U:286:GLN:HG3	2.04	0.57
1:D:72:LYS:CE	1:D:151:ARG:HH12	2.17	0.57
1:N:284:ASN:HD22	1:N:284:ASN:N	2.01	0.57
2:Q:94:SER:HB3	2:Q:122:TRP:CH2	2.39	0.57
2:W:94:SER:HB3	2:W:122:TRP:CH2	2.39	0.57
1:C:347:ILE:C	1:C:349:GLU:H	2.06	0.57
1:A:282:GLU:O	1:A:283:HIS:O	2.22	0.57
1:B:347:ILE:C	1:B:349:GLU:H	2.06	0.57
1:D:315:PRO:HB3	1:D:338:TYR:CE2	2.39	0.57
1:N:183:LEU:HB2	1:O:190:PHE:CE2	2.40	0.57
3:R:35:LEU:HA	3:R:38:VAL:HG23	1.87	0.57
2:S:236:ILE:HD12	2:S:249:GLN:HB3	1.87	0.57
3:X:35:LEU:HA	3:X:38:VAL:HG23	1.86	0.57
1:A:16:THR:HG22	1:A:46:GLN:HE21	1.69	0.56
1:A:247:LEU:HD13	1:B:247:LEU:HB3	1.87	0.56
1:B:227:ARG:HB3	1:B:227:ARG:HH11	1.69	0.56
2:I:17:LEU:HD13	2:I:58:GLN:HG2	1.87	0.56
2:K:94:SER:HB3	2:K:122:TRP:CH2	2.40	0.56
1:N:29:VAL:CG2	1:N:243:ILE:HG23	2.34	0.56
1:N:347:ILE:C	1:N:349:GLU:H	2.07	0.56
2:S:116:ILE:HA	2:S:119:MET:HE2	1.87	0.56
1:B:50:GLN:NE2	1:B:76:LYS:HE2	2.19	0.56
1:M:174:LEU:CD2	1:M:177:LEU:HD11	2.30	0.56
1:M:196:LYS:HG2	1:M:202:ASN:OD1	2.06	0.56
1:N:54:ILE:HA	1:N:86:MET:O	2.06	0.56
1:O:279:ASN:HB3	1:O:341:ILE:HD13	1.87	0.56
3:V:35:LEU:HA	3:V:38:VAL:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:285:GLY:HA2	2:G:289:PHE:HD2	1.69	0.56
1:N:196:LYS:HG2	1:N:202:ASN:OD1	2.05	0.56
1:N:260:ILE:HD11	2:S:42:ARG:HD3	1.86	0.56
1:O:174:LEU:HD13	1:O:177:LEU:HD11	1.85	0.56
1:P:256:ILE:O	1:P:260:ILE:HG13	2.05	0.56
2:Q:150:VAL:HB	3:R:52:TYR:CD2	2.39	0.56
1:C:138:GLU:CB	1:C:176:PHE:HB3	2.32	0.56
1:D:54:ILE:HD11	1:D:88:ILE:HG12	1.87	0.56
1:M:259:LEU:HD13	1:M:266:VAL:HG11	1.87	0.56
1:M:315:PRO:HB3	1:M:338:TYR:CE2	2.40	0.56
1:N:177:LEU:HD23	1:N:177:LEU:N	2.21	0.56
1:P:29:VAL:HG21	1:P:242:CYS:CA	2.34	0.56
2:S:285:GLY:HA2	2:S:289:PHE:HD2	1.68	0.56
1:B:202:ASN:HD22	1:B:202:ASN:H	1.53	0.56
2:G:250:LEU:HD21	3:H:13:VAL:HG13	1.87	0.56
1:N:178:GLN:HA	1:N:229:GLN:HE22	1.70	0.56
1:O:29:VAL:CG2	1:O:243:ILE:HG23	2.35	0.56
1:A:315:PRO:HB3	1:A:338:TYR:CE2	2.41	0.56
2:E:90:VAL:HG21	2:E:123:SER:HA	1.86	0.56
2:G:236:ILE:HD12	2:G:249:GLN:HB3	1.87	0.56
1:N:50:GLN:NE2	1:N:76:LYS:HE2	2.20	0.56
1:N:143:MET:HE2	1:O:197:LEU:HB3	1.85	0.56
1:N:146:MET:CG	1:O:201:LEU:HD22	2.35	0.56
2:S:191:PHE:HZ	2:S:211:LYS:HG3	1.70	0.56
1:B:197:LEU:HD13	1:C:147:LYS:HZ1	1.68	0.56
1:D:347:ILE:C	1:D:349:GLU:H	2.06	0.56
1:M:212:ILE:HD13	1:C:155:GLY:HA3	1.88	0.56
1:N:282:GLU:O	1:N:283:HIS:O	2.23	0.56
2:W:271:LEU:HD22	2:W:298:ASN:HD21	1.70	0.56
2:W:285:GLY:HA2	2:W:289:PHE:HD2	1.70	0.56
1:D:62:LEU:HB2	1:D:87:GLU:OE1	2.06	0.56
1:D:195:ASN:HD22	1:D:195:ASN:N	2.02	0.56
1:D:249:LEU:HD11	1:D:298:TYR:HB3	1.86	0.56
2:E:20:PHE:CE1	2:E:32:ALA:HB1	2.40	0.56
2:E:191:PHE:HZ	2:E:211:LYS:HG3	1.71	0.56
2:K:208:HIS:NE2	3:L:29:LYS:HG2	2.20	0.56
1:N:147:LYS:NZ	1:O:197:LEU:CD1	2.64	0.56
1:B:200:MET:HG2	1:C:150:LYS:HE2	1.88	0.56
1:B:201:LEU:HD13	1:C:146:MET:HB3	1.88	0.56
1:M:32:THR:HB	1:M:61:ASN:HD22	1.71	0.56
1:C:20:TRP:HB2	1:C:236:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:285:GLY:HA2	2:I:289:PHE:HD2	1.71	0.55
3:J:35:LEU:HA	3:J:38:VAL:HG23	1.87	0.55
1:O:254:ARG:HG3	1:O:255:LEU:N	2.21	0.55
1:P:282:GLU:O	1:P:283:HIS:O	2.24	0.55
1:C:254:ARG:HG3	1:C:255:LEU:N	2.22	0.55
1:A:307:GLU:CD	2:E:35:THR:HG22	2.27	0.55
1:N:16:THR:HA	1:N:46:GLN:HE22	1.72	0.55
1:N:315:PRO:HB3	1:N:338:TYR:CE2	2.41	0.55
1:O:178:GLN:NE2	1:O:261:SER:HB2	2.22	0.55
1:P:231:THR:O	1:P:231:THR:HG22	2.06	0.55
2:W:286:GLN:HG2	2:W:291:ILE:O	2.06	0.55
1:C:16:THR:HG22	1:C:46:GLN:HE21	1.68	0.55
1:C:32:THR:CG2	1:C:61:ASN:HD22	2.19	0.55
1:A:195:ASN:N	1:A:195:ASN:ND2	2.55	0.55
1:B:197:LEU:HB2	1:C:143:MET:CB	2.35	0.55
1:D:247:LEU:CB	1:C:247:LEU:HD13	2.37	0.55
1:D:305:LEU:O	2:K:42:ARG:NH2	2.36	0.55
1:D:308:ASP:OD2	2:K:39:ILE:HD13	2.06	0.55
2:G:279:SER:HB2	3:H:43:VAL:HG11	1.87	0.55
1:M:29:VAL:CG2	1:M:243:ILE:HG23	2.36	0.55
2:U:263:PHE:HB2	2:U:289:PHE:CE1	2.42	0.55
1:A:183:LEU:HD11	1:D:194:THR:HG22	1.88	0.55
1:A:243:ILE:HG22	1:A:272:ASN:O	2.05	0.55
1:A:267:ASN:O	1:A:310:HIS:HB2	2.05	0.55
1:B:193:ILE:C	1:B:195:ASN:H	2.10	0.55
1:D:282:GLU:O	1:D:283:HIS:O	2.25	0.55
2:K:232:ASN:HB2	3:L:21:THR:CB	2.35	0.55
1:A:259:LEU:HD13	1:A:266:VAL:HG11	1.89	0.55
2:I:234:TYR:HB2	3:J:21:THR:HG21	1.89	0.55
1:M:267:ASN:O	1:M:310:HIS:HB2	2.06	0.55
1:N:147:LYS:CE	1:O:197:LEU:HD22	2.36	0.55
1:P:32:THR:CB	1:P:61:ASN:HD22	2.20	0.55
1:P:315:PRO:HB3	1:P:338:TYR:CE2	2.42	0.55
2:Q:202:SER:HB2	3:R:33:LYS:HB2	1.87	0.55
1:C:29:VAL:CG2	1:C:243:ILE:HG23	2.37	0.55
1:A:143:MET:CE	1:D:201:LEU:HB3	2.35	0.55
1:A:174:LEU:HB3	1:A:177:LEU:CD1	2.37	0.55
1:D:305:LEU:CD2	2:K:42:ARG:NH2	2.69	0.55
1:N:138:GLU:CG	1:N:175:ARG:HB3	2.24	0.55
1:N:193:ILE:C	1:N:195:ASN:H	2.09	0.55
1:P:260:ILE:CG2	2:W:46:SER:OG	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:THR:HA	1:A:46:GLN:HE22	1.72	0.55
1:N:146:MET:HG3	1:O:201:LEU:HD21	1.88	0.55
1:N:187:LEU:HD22	1:O:187:LEU:CD2	2.36	0.55
1:N:187:LEU:HG	1:O:190:PHE:CZ	2.40	0.55
1:P:195:ASN:N	1:P:195:ASN:ND2	2.55	0.55
1:P:202:ASN:N	1:P:202:ASN:ND2	2.53	0.55
2:U:285:GLY:HA2	2:U:289:PHE:HD2	1.70	0.55
1:D:227:ARG:HB3	1:D:227:ARG:HH11	1.68	0.55
2:E:90:VAL:CG2	2:E:123:SER:HA	2.37	0.55
1:O:174:LEU:C	1:O:177:LEU:HG	2.25	0.55
1:O:259:LEU:HD13	1:O:266:VAL:HG11	1.89	0.55
1:P:138:GLU:CB	1:P:176:PHE:HB3	2.31	0.55
2:S:202:SER:HB2	3:T:33:LYS:CB	2.37	0.55
2:U:231:LYS:HE2	3:V:18:THR:OG1	2.07	0.55
2:W:90:VAL:HG21	2:W:123:SER:HA	1.89	0.55
1:B:267:ASN:O	1:B:310:HIS:HB2	2.06	0.55
3:F:39:THR:HG23	3:F:40:ASN:N	2.21	0.55
2:I:116:ILE:HA	2:I:119:MET:HE2	1.89	0.55
1:N:52:LEU:HD12	1:N:163:VAL:HG13	1.88	0.55
1:N:72:LYS:CE	1:N:151:ARG:HH12	2.18	0.55
2:Q:231:LYS:HE2	3:R:18:THR:OG1	2.07	0.55
2:S:256:GLN:HE22	3:T:29:LYS:CG	2.19	0.55
1:B:16:THR:HA	1:B:46:GLN:HE22	1.72	0.54
1:B:254:ARG:HG3	1:B:255:LEU:N	2.22	0.54
1:D:177:LEU:N	1:D:177:LEU:HD23	2.22	0.54
1:M:29:VAL:O	1:M:29:VAL:HG13	2.08	0.54
1:N:201:LEU:HB3	1:O:143:MET:SD	2.47	0.54
1:C:196:LYS:HG2	1:C:202:ASN:OD1	2.06	0.54
1:A:198:GLY:CA	1:A:200:MET:H	2.21	0.54
1:A:201:LEU:HB3	1:D:143:MET:CE	2.37	0.54
1:B:194:THR:C	1:B:195:ASN:HD22	2.10	0.54
1:D:178:GLN:HA	1:D:229:GLN:HE22	1.71	0.54
2:Q:286:GLN:HG2	2:Q:291:ILE:O	2.06	0.54
1:B:138:GLU:CG	1:B:175:ARG:HB3	2.23	0.54
1:D:279:ASN:HB3	1:D:341:ILE:HD13	1.89	0.54
1:P:198:GLY:CA	1:P:200:MET:H	2.21	0.54
2:U:208:HIS:NE2	3:V:29:LYS:HG2	2.23	0.54
2:U:286:GLN:HG2	2:U:291:ILE:O	2.06	0.54
2:W:202:SER:HB2	3:X:33:LYS:HB2	1.89	0.54
1:C:174:LEU:HD13	1:C:177:LEU:CD1	2.38	0.54
1:D:174:LEU:HD13	1:D:177:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:271:LEU:HD22	2:E:298:ASN:HD21	1.72	0.54
2:G:175:TRP:CZ3	3:H:48:LEU:HD12	2.42	0.54
2:I:94:SER:HB3	2:I:122:TRP:CH2	2.42	0.54
1:M:27:GLY:HA2	1:N:246:PHE:CD2	2.43	0.54
1:M:174:LEU:HD13	1:M:177:LEU:HD11	1.89	0.54
1:N:147:LYS:HZ1	1:O:197:LEU:HD22	1.73	0.54
1:N:201:LEU:CD2	1:O:146:MET:HG3	2.34	0.54
1:P:32:THR:HB	1:P:61:ASN:HD22	1.71	0.54
1:B:72:LYS:HE2	1:B:151:ARG:NH1	2.21	0.54
1:B:196:LYS:HZ3	1:B:202:ASN:CG	2.10	0.54
1:D:52:LEU:HD12	1:D:163:VAL:HG13	1.90	0.54
1:D:153:GLU:O	1:D:158:GLU:HA	2.07	0.54
2:K:271:LEU:HD22	2:K:298:ASN:HD21	1.71	0.54
2:U:281:LEU:HB2	2:U:295:LYS:HE2	1.90	0.54
1:C:54:ILE:HA	1:C:86:MET:O	2.07	0.54
1:C:259:LEU:HD13	1:C:266:VAL:HG11	1.88	0.54
1:B:196:LYS:HG3	1:C:143:MET:SD	2.46	0.54
1:D:16:THR:HG22	1:D:46:GLN:HE21	1.71	0.54
2:K:116:ILE:HA	2:K:119:MET:CE	2.38	0.54
1:O:243:ILE:HA	1:O:271:VAL:HG13	1.88	0.54
1:P:194:THR:C	1:P:195:ASN:HD22	2.11	0.54
2:W:204:ILE:HG12	3:X:31:TYR:HD2	1.71	0.54
1:B:174:LEU:HD22	1:B:177:LEU:CD1	2.27	0.54
1:D:305:LEU:CD2	2:K:42:ARG:HH21	2.18	0.54
2:E:208:HIS:NE2	3:F:29:LYS:HG2	2.22	0.54
2:G:61:LEU:HD22	2:G:100:ARG:NH2	2.23	0.54
2:K:20:PHE:CE1	2:K:32:ALA:HB1	2.43	0.54
2:K:90:VAL:HG21	2:K:123:SER:HA	1.88	0.54
1:N:195:ASN:HD22	1:N:195:ASN:N	2.05	0.54
1:N:202:ASN:N	1:N:202:ASN:ND2	2.56	0.54
2:Q:263:PHE:HB2	2:Q:289:PHE:CE1	2.42	0.54
3:V:39:THR:HG23	3:V:40:ASN:N	2.22	0.54
1:C:50:GLN:NE2	1:C:76:LYS:HE2	2.20	0.54
3:H:35:LEU:HA	3:H:38:VAL:HG23	1.90	0.54
2:K:234:TYR:HB2	3:L:21:THR:HG21	1.89	0.54
1:N:153:GLU:O	1:N:158:GLU:HA	2.08	0.54
1:O:16:THR:HA	1:O:46:GLN:HE22	1.73	0.54
1:A:193:ILE:C	1:A:195:ASN:H	2.11	0.54
1:M:174:LEU:HB3	1:M:177:LEU:HG	1.89	0.54
1:M:228:GLN:NE2	1:P:205:MET:SD	2.81	0.54
1:N:201:LEU:HD13	1:O:146:MET:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:138:GLU:HB3	1:O:176:PHE:HD1	1.73	0.54
1:C:279:ASN:HB3	1:C:341:ILE:HD13	1.89	0.54
1:D:193:ILE:C	1:D:195:ASN:H	2.11	0.54
2:K:202:SER:HB2	3:L:33:LYS:HB2	1.89	0.54
1:N:16:THR:HG22	1:N:46:GLN:HE21	1.73	0.54
1:O:284:ASN:HD22	1:O:284:ASN:N	2.05	0.54
1:P:227:ARG:HB3	1:P:227:ARG:HH11	1.71	0.54
2:Q:271:LEU:HD22	2:Q:298:ASN:HD21	1.73	0.54
2:S:112:LEU:HD23	2:S:149:PHE:CE2	2.41	0.54
2:W:90:VAL:CG2	2:W:123:SER:HA	2.38	0.54
1:D:138:GLU:CB	1:D:176:PHE:HB3	2.32	0.53
1:N:194:THR:CG2	1:O:183:LEU:CD1	2.86	0.53
1:N:259:LEU:HD13	1:N:266:VAL:HG11	1.89	0.53
2:Q:20:PHE:CE1	2:Q:32:ALA:HB1	2.43	0.53
2:Q:90:VAL:CG2	2:Q:123:SER:HA	2.38	0.53
2:W:61:LEU:HD22	2:W:100:ARG:NH2	2.23	0.53
1:C:138:GLU:CG	1:C:175:ARG:HB3	2.24	0.53
1:B:315:PRO:HB3	1:B:338:TYR:CE2	2.44	0.53
2:K:90:VAL:CG2	2:K:123:SER:HA	2.38	0.53
1:O:54:ILE:HA	1:O:86:MET:O	2.08	0.53
1:O:249:LEU:HD11	1:O:298:TYR:HB3	1.90	0.53
1:P:193:ILE:C	1:P:195:ASN:H	2.10	0.53
1:P:267:ASN:O	1:P:310:HIS:HB2	2.07	0.53
1:C:16:THR:HA	1:C:46:GLN:HE22	1.72	0.53
1:B:178:GLN:NE2	1:B:261:SER:HB2	2.22	0.53
1:B:259:LEU:HD13	1:B:266:VAL:HG11	1.90	0.53
1:D:284:ASN:HD22	1:D:284:ASN:N	2.04	0.53
1:M:199:PRO:HG3	1:C:156:GLU:CB	2.39	0.53
1:N:278:GLU:OE1	1:N:292:TRP:HZ3	1.92	0.53
1:D:233:PRO:HB3	2:K:9:MET:N	2.24	0.53
2:G:271:LEU:HD22	2:G:298:ASN:HD21	1.74	0.53
1:M:52:LEU:HD12	1:M:163:VAL:HG13	1.89	0.53
1:O:258:GLU:HG2	1:O:262:TYR:CE2	2.43	0.53
1:P:29:VAL:HG22	1:P:243:ILE:HG23	1.90	0.53
2:W:282:GLU:O	2:W:286:GLN:HG3	2.08	0.53
1:C:315:PRO:HB3	1:C:338:TYR:CE2	2.44	0.53
1:A:133:ILE:HB	1:A:136:ILE:HD12	1.91	0.53
2:K:116:ILE:HA	2:K:119:MET:HE2	1.90	0.53
1:O:263:ASP:O	2:U:9:MET:CE	2.57	0.53
1:D:174:LEU:C	1:D:177:LEU:HG	2.28	0.53
1:D:198:GLY:HA2	1:D:200:MET:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:202:ASN:N	1:O:202:ASN:ND2	2.54	0.53
1:P:52:LEU:HD12	1:P:163:VAL:HG13	1.90	0.53
1:D:16:THR:HA	1:D:46:GLN:HE22	1.74	0.53
2:E:263:PHE:HB2	2:E:289:PHE:CE1	2.44	0.53
2:G:20:PHE:CE1	2:G:32:ALA:HB1	2.44	0.53
2:I:19:ARG:NH1	1:C:5:VAL:N	2.57	0.53
2:I:90:VAL:CG2	2:I:123:SER:HA	2.39	0.53
1:O:233:PRO:CG	2:U:11:ALA:HB3	2.39	0.53
2:S:61:LEU:HD22	2:S:100:ARG:NH2	2.24	0.53
2:S:286:GLN:HG2	2:S:291:ILE:O	2.08	0.53
2:I:271:LEU:HD22	2:I:298:ASN:HD21	1.74	0.53
1:M:202:ASN:HD22	1:M:202:ASN:H	1.54	0.53
1:M:227:ARG:HB3	1:M:227:ARG:HH11	1.74	0.53
1:N:178:GLN:NE2	1:N:261:SER:HB2	2.24	0.53
1:O:193:ILE:C	1:O:195:ASN:H	2.11	0.53
1:P:174:LEU:HD13	1:P:177:LEU:CD1	2.39	0.53
2:Q:232:ASN:HB2	3:R:21:THR:CB	2.39	0.53
2:Q:278:LYS:HG3	2:Q:295:LYS:HG2	1.91	0.53
2:S:283:PHE:CE1	3:T:42:GLY:HA2	2.43	0.53
1:C:198:GLY:CA	1:C:200:MET:H	2.22	0.53
1:M:32:THR:CB	1:M:61:ASN:HD22	2.22	0.53
2:Q:90:VAL:HG21	2:Q:123:SER:HA	1.90	0.53
2:W:218:PHE:HZ	2:W:242:TYR:CZ	2.27	0.53
1:C:267:ASN:O	1:C:310:HIS:HB2	2.07	0.53
2:G:191:PHE:HZ	2:G:211:LYS:HG3	1.73	0.53
2:G:217:ARG:CG	1:M:154:GLN:OE1	2.53	0.53
1:O:134:PRO:O	1:O:179:LEU:HD22	2.09	0.53
1:P:54:ILE:HA	1:P:86:MET:O	2.07	0.53
2:Q:175:TRP:CZ3	3:R:48:LEU:HD12	2.44	0.53
2:U:90:VAL:CG2	2:U:123:SER:HA	2.39	0.53
2:U:191:PHE:CZ	2:U:211:LYS:HG3	2.44	0.53
1:C:227:ARG:HB3	1:C:227:ARG:HH11	1.74	0.53
1:A:54:ILE:HA	1:A:86:MET:O	2.10	0.52
1:A:254:ARG:HG3	1:A:255:LEU:N	2.24	0.52
1:B:54:ILE:HA	1:B:86:MET:O	2.10	0.52
2:I:116:ILE:HA	2:I:119:MET:CE	2.39	0.52
1:M:16:THR:HA	1:M:46:GLN:HE22	1.74	0.52
1:M:194:THR:C	1:M:195:ASN:HD22	2.13	0.52
1:N:201:LEU:HB3	1:O:143:MET:HE1	1.91	0.52
1:P:154:GLN:HG3	1:C:79:GLY:C	2.26	0.52
2:U:90:VAL:HG21	2:U:123:SER:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:GLN:NE2	1:C:261:SER:HB2	2.24	0.52
1:A:7:PRO:HG2	1:A:337:GLU:HG2	1.90	0.52
1:D:174:LEU:HB3	1:D:177:LEU:HG	1.90	0.52
2:E:112:LEU:HD23	2:E:149:PHE:CE2	2.43	0.52
1:M:54:ILE:HA	1:M:86:MET:O	2.10	0.52
1:N:143:MET:CG	1:O:197:LEU:HB2	2.40	0.52
1:O:179:LEU:HG	1:O:183:LEU:HD13	1.91	0.52
1:P:254:ARG:HG3	1:P:255:LEU:N	2.24	0.52
1:P:259:LEU:HD13	1:P:266:VAL:HG11	1.91	0.52
2:U:202:SER:HB2	3:V:33:LYS:CB	2.36	0.52
1:C:141:SER:O	1:C:145:VAL:HG13	2.09	0.52
1:A:54:ILE:HD11	1:A:88:ILE:HG12	1.92	0.52
1:A:202:ASN:N	1:A:202:ASN:ND2	2.55	0.52
1:N:147:LYS:HZ1	1:O:197:LEU:CD1	2.21	0.52
1:N:174:LEU:HB3	1:N:177:LEU:HG	1.92	0.52
1:N:249:LEU:HD11	1:N:298:TYR:HB3	1.91	0.52
1:O:315:PRO:HB3	1:O:338:TYR:CE2	2.45	0.52
1:P:201:LEU:HG	1:P:205:MET:CE	2.39	0.52
1:P:257:GLN:HE22	2:W:45:ARG:HB2	1.74	0.52
1:B:197:LEU:O	1:C:143:MET:HE2	2.08	0.52
1:M:199:PRO:CG	1:C:156:GLU:HB3	2.38	0.52
1:N:215:LYS:HA	1:N:218:GLU:HG2	1.90	0.52
1:N:279:ASN:HB3	1:N:341:ILE:HD13	1.91	0.52
2:Q:263:PHE:HB2	2:Q:289:PHE:CZ	2.45	0.52
2:W:20:PHE:CE1	2:W:32:ALA:HB1	2.44	0.52
1:D:259:LEU:HD13	1:D:266:VAL:HG11	1.90	0.52
1:M:258:GLU:HG2	1:M:262:TYR:CE2	2.43	0.52
2:S:116:ILE:HA	2:S:119:MET:CE	2.40	0.52
2:W:116:ILE:HA	2:W:119:MET:CE	2.40	0.52
1:B:195:ASN:N	1:B:195:ASN:ND2	2.58	0.52
1:D:21:ILE:HB	1:D:164:ILE:HD13	1.92	0.52
1:D:243:ILE:HG22	1:D:272:ASN:O	2.09	0.52
1:D:254:ARG:HG3	1:D:255:LEU:N	2.24	0.52
1:D:258:GLU:HG2	1:D:262:TYR:CE2	2.44	0.52
2:I:20:PHE:CE1	2:I:32:ALA:HB1	2.44	0.52
1:M:141:SER:O	1:M:145:VAL:HG13	2.09	0.52
1:M:254:ARG:HG3	1:M:255:LEU:N	2.25	0.52
3:R:49:LYS:N	3:R:49:LYS:HD2	2.24	0.52
2:S:263:PHE:HB2	2:S:289:PHE:CE1	2.45	0.52
1:B:54:ILE:HD11	1:B:88:ILE:HG12	1.92	0.52
1:B:196:LYS:O	1:B:197:LEU:C	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:258:GLU:HG2	1:N:262:TYR:CE2	2.45	0.52
1:N:263:ASP:HB3	2:S:9:MET:SD	2.50	0.52
1:O:6:GLU:O	1:O:310:HIS:HD2	1.92	0.52
3:R:39:THR:HG23	3:R:40:ASN:N	2.23	0.52
1:C:174:LEU:HB3	1:C:177:LEU:HG	1.92	0.52
1:A:184:SER:O	1:A:187:LEU:HB2	2.10	0.52
1:B:6:GLU:O	1:B:310:HIS:HD2	1.93	0.52
1:B:258:GLU:HG2	1:B:262:TYR:CE2	2.45	0.52
1:D:184:SER:O	1:D:187:LEU:HB2	2.10	0.52
1:D:196:LYS:NZ	1:D:202:ASN:CG	2.63	0.52
2:E:116:ILE:HA	2:E:119:MET:CE	2.39	0.52
2:G:286:GLN:HG2	2:G:291:ILE:O	2.09	0.52
2:I:263:PHE:HB2	2:I:289:PHE:CE1	2.45	0.52
2:K:263:PHE:HB2	2:K:289:PHE:CE1	2.45	0.52
1:N:147:LYS:HZ1	1:O:197:LEU:CD2	2.23	0.52
1:N:254:ARG:HG3	1:N:255:LEU:N	2.25	0.52
1:O:12:LEU:O	1:O:12:LEU:HD22	2.10	0.52
1:P:249:LEU:HD11	1:P:298:TYR:HB3	1.91	0.52
2:U:116:ILE:HA	2:U:119:MET:HE2	1.91	0.52
1:C:193:ILE:C	1:C:195:ASN:H	2.13	0.52
1:A:191:GLY:O	1:A:195:ASN:ND2	2.43	0.52
1:P:29:VAL:CG2	1:P:243:ILE:HG23	2.39	0.52
1:B:134:PRO:O	1:B:179:LEU:HD22	2.10	0.52
1:B:249:LEU:HD11	1:B:298:TYR:HB3	1.92	0.52
2:G:217:ARG:NE	1:M:154:GLN:NE2	2.57	0.52
2:Q:283:PHE:CE1	3:R:42:GLY:HA2	2.44	0.52
2:S:154:GLU:HG3	2:S:168:TYR:CE1	2.45	0.52
3:T:39:THR:HG23	3:T:40:ASN:N	2.22	0.52
2:U:112:LEU:HD23	2:U:149:PHE:CE2	2.44	0.52
2:W:116:ILE:HA	2:W:119:MET:HE2	1.91	0.52
2:W:150:VAL:HB	3:X:52:TYR:CD2	2.45	0.52
1:C:7:PRO:HG2	1:C:337:GLU:HG2	1.92	0.52
1:C:249:LEU:HD11	1:C:298:TYR:HB3	1.91	0.52
1:B:180:PRO:O	1:B:225:THR:HG21	2.10	0.51
1:M:187:LEU:HD21	1:P:190:PHE:CD1	2.45	0.51
3:T:35:LEU:HD12	3:T:38:VAL:CG2	2.36	0.51
1:A:227:ARG:HB3	1:A:227:ARG:HH11	1.74	0.51
1:B:174:LEU:HB3	1:B:177:LEU:HG	1.91	0.51
1:D:32:THR:HG22	1:D:61:ASN:HD22	1.75	0.51
1:N:217:ASN:CG	1:O:217:ASN:CG	2.69	0.51
2:Q:134:PRO:HG3	3:R:35:LEU:HD23	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:271:LEU:HD22	2:S:298:ASN:HD21	1.75	0.51
1:N:196:LYS:HG3	1:O:143:MET:SD	2.49	0.51
1:P:6:GLU:O	1:P:310:HIS:HD2	1.94	0.51
2:U:61:LEU:HD22	2:U:100:ARG:NH2	2.25	0.51
3:F:35:LEU:HD12	3:F:38:VAL:CG2	2.34	0.51
2:I:90:VAL:HG21	2:I:123:SER:HA	1.92	0.51
1:M:249:LEU:HD11	1:M:298:TYR:HB3	1.92	0.51
1:N:196:LYS:O	1:N:197:LEU:C	2.49	0.51
2:U:229:ILE:HD13	3:V:14:SER:HB2	1.93	0.51
3:V:49:LYS:HD2	3:V:49:LYS:N	2.26	0.51
1:C:153:GLU:O	1:C:158:GLU:HA	2.10	0.51
1:A:256:ILE:O	1:A:260:ILE:HG13	2.11	0.51
2:E:263:PHE:HB2	2:E:289:PHE:CZ	2.46	0.51
2:G:213:ILE:O	2:G:217:ARG:HG3	2.10	0.51
1:O:146:MET:HE2	1:O:149:ILE:HG13	1.92	0.51
2:S:90:VAL:CG2	2:S:123:SER:HA	2.41	0.51
1:A:15:SER:OG	1:A:18:HIS:HD2	1.94	0.51
1:D:29:VAL:HG21	1:D:242:CYS:CA	2.39	0.51
1:D:283:HIS:O	1:D:284:ASN:HB2	2.11	0.51
1:M:184:SER:O	1:M:187:LEU:HB2	2.11	0.51
1:C:32:THR:CB	1:C:61:ASN:HD22	2.24	0.51
1:D:7:PRO:HG2	1:D:337:GLU:HG2	1.93	0.51
2:E:134:PRO:HG3	3:F:35:LEU:HD23	1.92	0.51
1:M:145:VAL:O	1:M:149:ILE:HG12	2.10	0.51
1:N:29:VAL:HG13	1:N:29:VAL:O	2.11	0.51
1:O:174:LEU:HB3	1:O:177:LEU:CD1	2.41	0.51
1:B:143:MET:SD	1:C:196:LYS:CE	2.97	0.51
2:I:281:LEU:HB2	2:I:295:LYS:HE2	1.92	0.51
1:M:54:ILE:HD11	1:M:88:ILE:HG12	1.93	0.51
1:M:194:THR:HG22	1:P:183:LEU:CD1	2.39	0.51
1:O:50:GLN:NE2	1:O:76:LYS:HE2	2.19	0.51
1:O:191:GLY:O	1:O:195:ASN:ND2	2.43	0.51
1:O:267:ASN:O	1:O:310:HIS:HB2	2.09	0.51
3:T:49:LYS:HD2	3:T:49:LYS:N	2.25	0.51
1:A:249:LEU:HD11	1:A:298:TYR:HB3	1.93	0.51
1:B:138:GLU:CB	1:B:176:PHE:HB3	2.34	0.51
1:D:12:LEU:O	1:D:12:LEU:HD22	2.09	0.51
2:G:263:PHE:HB2	2:G:289:PHE:CE1	2.46	0.51
2:K:263:PHE:HB2	2:K:289:PHE:CZ	2.46	0.51
1:M:6:GLU:O	1:M:310:HIS:HD2	1.93	0.51
1:M:205:MET:SD	1:P:228:GLN:NE2	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:32:THR:CB	1:N:61:ASN:HD22	2.24	0.51
1:N:279:ASN:OD1	1:N:341:ILE:HD11	2.11	0.51
1:O:29:VAL:O	1:O:29:VAL:HG13	2.11	0.51
2:Q:61:LEU:HD22	2:Q:100:ARG:NH2	2.26	0.51
1:C:147:LYS:HA	1:C:150:LYS:HE3	1.93	0.51
1:A:32:THR:CB	1:A:61:ASN:HD22	2.24	0.51
1:B:143:MET:SD	1:C:201:LEU:HB3	2.47	0.51
2:K:112:LEU:HD23	2:K:149:PHE:CE2	2.45	0.51
1:N:143:MET:CE	1:O:197:LEU:O	2.59	0.51
1:N:174:LEU:HD13	1:N:177:LEU:HD11	1.93	0.51
1:O:174:LEU:HB3	1:O:177:LEU:HG	1.93	0.51
1:P:180:PRO:O	1:P:225:THR:HG21	2.10	0.51
2:Q:191:PHE:HZ	2:Q:211:LYS:HG3	1.76	0.51
1:M:243:ILE:HG22	1:M:272:ASN:O	2.11	0.50
1:M:288:CYS:SG	1:N:287:ARG:CB	2.99	0.50
1:O:32:THR:HG22	1:O:61:ASN:HD22	1.75	0.50
1:O:195:ASN:N	1:O:195:ASN:ND2	2.54	0.50
1:C:52:LEU:HD12	1:C:163:VAL:HG13	1.94	0.50
1:B:16:THR:HG22	1:B:46:GLN:HE21	1.76	0.50
2:G:218:PHE:HZ	2:G:242:TYR:CZ	2.29	0.50
1:P:134:PRO:O	1:P:179:LEU:HD22	2.10	0.50
2:W:191:PHE:CZ	2:W:211:LYS:HG3	2.45	0.50
2:W:204:ILE:CG1	3:X:31:TYR:HD2	2.24	0.50
1:B:196:LYS:NZ	1:B:202:ASN:CG	2.65	0.50
2:G:102:ILE:HG21	2:G:139:THR:HG22	1.94	0.50
2:G:217:ARG:HH21	1:M:154:GLN:NE2	2.07	0.50
2:I:124:ILE:HG12	2:I:132:GLY:N	2.27	0.50
1:O:138:GLU:CB	1:O:176:PHE:HB3	2.35	0.50
1:P:72:LYS:CE	1:P:151:ARG:HH12	2.24	0.50
2:Q:116:ILE:HA	2:Q:119:MET:CE	2.41	0.50
2:U:175:TRP:CZ2	3:V:48:LEU:HB2	2.45	0.50
3:X:35:LEU:HD12	3:X:38:VAL:CG2	2.36	0.50
1:B:201:LEU:HB3	1:C:143:MET:SD	2.52	0.50
1:D:29:VAL:HG13	1:D:29:VAL:O	2.11	0.50
2:G:90:VAL:HG21	2:G:123:SER:HA	1.92	0.50
2:G:116:ILE:HA	2:G:119:MET:CE	2.41	0.50
1:M:199:PRO:HG3	1:C:156:GLU:HB3	1.93	0.50
1:O:177:LEU:N	1:O:177:LEU:HD23	2.26	0.50
1:P:184:SER:O	1:P:187:LEU:HB2	2.11	0.50
2:U:218:PHE:HZ	2:U:242:TYR:CZ	2.29	0.50
1:A:138:GLU:CB	1:A:176:PHE:HB3	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:90:VAL:CG2	2:G:123:SER:HA	2.40	0.50
2:I:205:SER:HA	3:J:29:LYS:O	2.12	0.50
2:U:20:PHE:CE1	2:U:32:ALA:HB1	2.47	0.50
1:C:236:THR:HG22	1:C:264:MET:HE3	1.94	0.50
1:B:141:SER:O	1:B:145:VAL:HG13	2.12	0.50
1:D:267:ASN:HB3	2:K:12:LYS:HD2	1.93	0.50
1:O:145:VAL:O	1:O:149:ILE:HG12	2.11	0.50
1:P:279:ASN:HB3	1:P:341:ILE:HD13	1.92	0.50
2:W:263:PHE:HB2	2:W:289:PHE:CE1	2.47	0.50
1:A:12:LEU:O	1:A:12:LEU:HD22	2.12	0.50
1:A:178:GLN:NE2	1:A:261:SER:HB2	2.26	0.50
1:D:263:ASP:O	2:K:9:MET:SD	2.69	0.50
1:M:202:ASN:N	1:M:202:ASN:ND2	2.58	0.50
1:N:233:PRO:HG2	2:S:11:ALA:HB3	1.93	0.50
1:P:54:ILE:HD11	1:P:88:ILE:HG12	1.93	0.50
1:P:145:VAL:O	1:P:149:ILE:HG12	2.12	0.50
2:W:175:TRP:CZ3	3:X:48:LEU:HD12	2.47	0.50
1:A:178:GLN:CA	1:A:229:GLN:HE22	2.24	0.50
1:O:54:ILE:HD11	1:O:88:ILE:HG12	1.93	0.50
1:P:7:PRO:HG2	1:P:337:GLU:HG2	1.94	0.50
2:S:20:PHE:CE1	2:S:32:ALA:HB1	2.47	0.50
2:U:116:ILE:HA	2:U:119:MET:CE	2.41	0.50
2:W:204:ILE:HG22	2:W:208:HIS:HD2	1.77	0.50
1:A:52:LEU:HD12	1:A:163:VAL:HG13	1.93	0.50
1:B:147:LYS:HA	1:B:150:LYS:HE3	1.94	0.50
1:B:279:ASN:HB3	1:B:341:ILE:HD13	1.93	0.50
1:M:50:GLN:NE2	1:M:76:LYS:HE2	2.21	0.50
1:N:198:GLY:HA2	1:N:200:MET:H	1.76	0.50
1:O:62:LEU:HB2	1:O:87:GLU:OE1	2.12	0.50
2:S:102:ILE:HG21	2:S:139:THR:HG22	1.93	0.50
2:S:283:PHE:HE1	3:T:40:ASN:HD21	1.59	0.50
1:C:184:SER:O	1:C:187:LEU:HB2	2.11	0.50
1:A:32:THR:HB	1:A:61:ASN:HD22	1.77	0.49
1:B:202:ASN:N	1:B:202:ASN:ND2	2.55	0.49
1:D:246:PHE:CD2	1:C:27:GLY:HA2	2.47	0.49
2:E:278:LYS:HG3	2:E:295:LYS:HG2	1.94	0.49
3:H:35:LEU:HD12	3:H:38:VAL:CG2	2.40	0.49
1:N:6:GLU:O	1:N:310:HIS:HD2	1.94	0.49
1:P:258:GLU:HG2	1:P:262:TYR:CE2	2.46	0.49
2:S:90:VAL:HG21	2:S:123:SER:HA	1.93	0.49
2:U:263:PHE:HB2	2:U:289:PHE:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:49:LYS:N	3:X:49:LYS:HD2	2.27	0.49
1:C:6:GLU:O	1:C:310:HIS:HD2	1.95	0.49
1:C:258:GLU:HG2	1:C:262:TYR:CE2	2.46	0.49
1:D:278:GLU:OE1	1:D:292:TRP:HZ3	1.96	0.49
2:I:112:LEU:HD23	2:I:149:PHE:CE2	2.43	0.49
2:K:191:PHE:CZ	2:K:211:LYS:HG3	2.45	0.49
1:M:180:PRO:HA	1:M:183:LEU:HD21	1.94	0.49
1:O:52:LEU:HD12	1:O:163:VAL:HG13	1.94	0.49
1:P:275:LEU:HB2	1:P:292:TRP:CD1	2.47	0.49
2:Q:116:ILE:HA	2:Q:119:MET:HE2	1.95	0.49
1:A:147:LYS:HZ3	1:D:197:LEU:HD13	1.74	0.49
2:E:202:SER:CB	3:F:33:LYS:HB2	2.38	0.49
2:I:256:GLN:HE22	3:J:29:LYS:HG3	1.77	0.49
2:K:61:LEU:HD22	2:K:100:ARG:NH2	2.27	0.49
1:N:174:LEU:C	1:N:177:LEU:HG	2.31	0.49
1:O:72:LYS:CE	1:O:151:ARG:HH12	2.23	0.49
1:O:153:GLU:O	1:O:158:GLU:HA	2.12	0.49
2:U:229:ILE:HG21	3:V:14:SER:HA	1.93	0.49
2:W:208:HIS:NE2	3:X:29:LYS:HG2	2.27	0.49
1:B:155:GLY:O	1:B:156:GLU:HB2	2.11	0.49
1:B:196:LYS:HG2	1:B:202:ASN:OD1	2.13	0.49
1:D:6:GLU:O	1:D:310:HIS:HD2	1.96	0.49
1:N:32:THR:HG22	1:N:61:ASN:HD22	1.77	0.49
1:O:5:VAL:HG11	1:O:309:PHE:O	2.12	0.49
1:P:274:LEU:HD12	1:P:313:LYS:HB3	1.95	0.49
2:W:102:ILE:HG21	2:W:139:THR:HG22	1.93	0.49
1:C:243:ILE:HG22	1:C:272:ASN:O	2.13	0.49
1:A:180:PRO:O	1:A:225:THR:HG21	2.12	0.49
1:D:141:SER:O	1:D:145:VAL:HG13	2.12	0.49
2:I:208:HIS:CD2	3:J:29:LYS:HG2	2.47	0.49
2:I:231:LYS:HB3	3:J:18:THR:HA	1.94	0.49
1:N:260:ILE:HD13	2:S:42:ARG:CG	2.43	0.49
2:S:279:SER:HB2	3:T:43:VAL:HG11	1.94	0.49
2:U:179:VAL:HG13	3:V:50:TYR:CE1	2.47	0.49
1:C:135:GLY:HA3	1:C:179:LEU:CD2	2.36	0.49
1:B:12:LEU:O	1:B:12:LEU:HD22	2.12	0.49
2:K:102:ILE:HD11	2:K:119:MET:SD	2.53	0.49
1:N:143:MET:HB3	1:O:197:LEU:CB	2.35	0.49
1:A:29:VAL:HG21	1:A:242:CYS:CA	2.39	0.49
1:A:50:GLN:NE2	1:A:76:LYS:HE2	2.20	0.49
1:A:134:PRO:O	1:A:179:LEU:HD22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:GLU:OE1	2:K:35:THR:HG22	2.12	0.49
3:F:49:LYS:HD2	3:F:49:LYS:N	2.28	0.49
2:I:150:VAL:CG1	2:I:151:TYR:N	2.73	0.49
1:M:174:LEU:C	1:M:177:LEU:HG	2.32	0.49
1:N:32:THR:CG2	1:N:61:ASN:HD22	2.25	0.49
1:O:243:ILE:HG22	1:O:272:ASN:O	2.13	0.49
1:P:15:SER:OG	1:P:18:HIS:HD2	1.96	0.49
2:U:175:TRP:CE3	3:V:48:LEU:HD12	2.47	0.49
1:B:198:GLY:HA2	1:B:200:MET:H	1.78	0.49
1:D:260:ILE:HG21	2:K:46:SER:OG	2.13	0.49
1:M:16:THR:HG22	1:M:46:GLN:HE21	1.74	0.49
1:M:153:GLU:O	1:M:158:GLU:HA	2.12	0.49
1:N:32:THR:HB	1:N:61:ASN:HD22	1.76	0.49
1:N:62:LEU:HB2	1:N:87:GLU:OE1	2.13	0.49
2:S:191:PHE:CZ	2:S:211:LYS:HG3	2.48	0.49
2:U:124:ILE:HG12	2:U:132:GLY:N	2.27	0.49
2:W:278:LYS:HG3	2:W:295:LYS:HG2	1.94	0.49
1:C:178:GLN:CA	1:C:229:GLN:HE22	2.26	0.49
1:C:274:LEU:HD22	1:C:299:LEU:HD11	1.94	0.49
1:A:141:SER:O	1:A:145:VAL:HG13	2.12	0.49
1:B:177:LEU:N	1:B:177:LEU:HD23	2.28	0.49
1:B:243:ILE:HG22	1:B:272:ASN:O	2.12	0.49
1:D:5:VAL:HG11	1:D:309:PHE:O	2.13	0.49
3:H:49:LYS:N	3:H:49:LYS:HD2	2.28	0.49
2:I:150:VAL:CG1	2:I:151:TYR:H	2.23	0.49
3:L:35:LEU:HD12	3:L:38:VAL:CG2	2.36	0.49
1:M:196:LYS:O	1:M:197:LEU:C	2.51	0.49
1:M:198:GLY:CA	1:M:200:MET:H	2.26	0.49
1:N:134:PRO:O	1:N:179:LEU:HD22	2.13	0.49
1:O:32:THR:CB	1:O:61:ASN:HD22	2.26	0.49
1:O:141:SER:O	1:O:145:VAL:HG13	2.12	0.49
1:O:147:LYS:HA	1:O:150:LYS:HE3	1.95	0.49
1:O:283:HIS:O	1:O:284:ASN:HB2	2.13	0.49
2:W:263:PHE:HB2	2:W:289:PHE:CZ	2.48	0.49
1:C:62:LEU:HB2	1:C:87:GLU:OE1	2.13	0.49
1:A:187:LEU:HD21	1:D:190:PHE:CD1	2.48	0.49
2:E:283:PHE:HE1	3:F:40:ASN:HD21	1.60	0.49
2:G:236:ILE:HD11	2:G:253:ILE:HD12	1.95	0.49
2:I:191:PHE:HZ	2:I:211:LYS:HG3	1.76	0.49
2:I:204:ILE:HG22	2:I:208:HIS:HD2	1.77	0.49
3:J:35:LEU:HD12	3:J:38:VAL:CG2	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:49:LYS:N	3:L:49:LYS:HD2	2.28	0.49
1:M:180:PRO:O	1:M:225:THR:HG21	2.13	0.49
1:M:201:LEU:HG	1:M:205:MET:CE	2.43	0.49
1:N:7:PRO:HG2	1:N:337:GLU:HG2	1.94	0.49
1:O:32:THR:CG2	1:O:61:ASN:HD22	2.26	0.49
1:O:184:SER:O	1:O:187:LEU:HB2	2.13	0.49
1:P:178:GLN:CA	1:P:229:GLN:HE22	2.26	0.49
1:M:197:LEU:HB2	1:P:143:MET:HE2	1.95	0.48
1:M:275:LEU:HB2	1:M:292:TRP:CD1	2.48	0.48
1:B:10:HIS:HD2	1:B:335:ASN:ND2	2.12	0.48
1:D:153:GLU:HB3	1:D:158:GLU:O	2.13	0.48
3:J:49:LYS:N	3:J:49:LYS:HD2	2.28	0.48
2:K:154:GLU:HG3	2:K:168:TYR:CE1	2.48	0.48
1:M:12:LEU:O	1:M:12:LEU:HD22	2.13	0.48
1:M:29:VAL:HG21	1:M:242:CYS:CA	2.41	0.48
1:M:174:LEU:HD13	1:M:177:LEU:CD1	2.43	0.48
1:N:138:GLU:CB	1:N:176:PHE:HB3	2.36	0.48
1:N:274:LEU:HD12	1:N:313:LYS:HB3	1.95	0.48
1:O:174:LEU:HD13	1:O:177:LEU:CD1	2.44	0.48
1:P:62:LEU:HB2	1:P:87:GLU:OE1	2.13	0.48
1:P:243:ILE:HG22	1:P:272:ASN:O	2.12	0.48
1:A:174:LEU:CG	1:A:177:LEU:HD11	2.42	0.48
1:B:190:PHE:CE2	1:C:183:LEU:HB2	2.48	0.48
1:D:54:ILE:HD12	1:D:86:MET:HB3	1.95	0.48
2:K:134:PRO:CG	3:L:35:LEU:HD23	2.43	0.48
1:M:305:LEU:CD2	2:Q:42:ARG:NH2	2.71	0.48
1:N:145:VAL:O	1:N:149:ILE:HG12	2.13	0.48
2:Q:52:ALA:O	2:Q:56:ILE:HG13	2.13	0.48
2:S:150:VAL:CG1	2:S:151:TYR:H	2.26	0.48
2:U:227:GLU:OE2	3:V:10:HIS:NE2	2.46	0.48
1:C:281:GLN:O	1:C:282:GLU:CB	2.61	0.48
1:B:201:LEU:HD22	1:C:146:MET:CB	2.41	0.48
2:E:61:LEU:HD22	2:E:100:ARG:NH2	2.28	0.48
2:G:112:LEU:HD23	2:G:149:PHE:CE2	2.46	0.48
2:G:116:ILE:HA	2:G:119:MET:HE2	1.95	0.48
2:I:35:THR:HG22	1:C:307:GLU:CD	2.34	0.48
2:U:94:SER:HB3	2:U:122:TRP:CZ2	2.48	0.48
2:U:151:TYR:OH	3:V:47:THR:HG23	2.13	0.48
1:B:32:THR:HG22	1:B:61:ASN:HD22	1.77	0.48
1:D:145:VAL:O	1:D:149:ILE:HG12	2.14	0.48
3:H:39:THR:HG23	3:H:40:ASN:N	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:263:PHE:HB2	2:I:289:PHE:CZ	2.48	0.48
3:J:39:THR:HG23	3:J:40:ASN:N	2.26	0.48
2:K:218:PHE:HZ	2:K:242:TYR:CZ	2.32	0.48
1:M:177:LEU:N	1:M:177:LEU:HD23	2.29	0.48
1:N:243:ILE:HG22	1:N:272:ASN:O	2.13	0.48
1:P:32:THR:CG2	1:P:61:ASN:HD22	2.26	0.48
1:P:190:PHE:CD1	1:P:190:PHE:C	2.86	0.48
2:Q:112:LEU:HD23	2:Q:149:PHE:CE2	2.47	0.48
2:W:202:SER:HB2	3:X:33:LYS:CB	2.43	0.48
1:C:29:VAL:HG13	1:C:29:VAL:O	2.13	0.48
1:C:178:GLN:HA	1:C:229:GLN:NE2	2.26	0.48
1:A:247:LEU:CB	1:B:247:LEU:HD13	2.43	0.48
1:B:145:VAL:O	1:B:149:ILE:HG12	2.13	0.48
1:D:29:VAL:HG23	1:D:243:ILE:HG12	1.96	0.48
1:D:274:LEU:HD12	1:D:313:LYS:HB3	1.96	0.48
1:D:275:LEU:HB2	1:D:292:TRP:CD1	2.48	0.48
2:K:282:GLU:O	2:K:286:GLN:HG3	2.13	0.48
1:M:7:PRO:HG2	1:M:337:GLU:HG2	1.94	0.48
1:M:72:LYS:CE	1:M:151:ARG:HH12	2.20	0.48
1:C:145:VAL:O	1:C:149:ILE:HG12	2.14	0.48
1:C:276:PHE:HA	1:C:292:TRP:CZ2	2.49	0.48
1:B:72:LYS:CE	1:B:151:ARG:HH12	2.25	0.48
1:B:143:MET:HG3	1:C:196:LYS:HG3	1.95	0.48
1:P:260:ILE:HG22	2:W:46:SER:OG	2.13	0.48
1:A:174:LEU:CD1	1:A:177:LEU:HD11	2.42	0.48
1:A:275:LEU:HB2	1:A:292:TRP:CD1	2.49	0.48
2:G:115:VAL:HG12	2:G:119:MET:CE	2.43	0.48
1:N:231:THR:O	1:N:231:THR:HG22	2.14	0.48
1:O:180:PRO:O	1:O:225:THR:HG21	2.14	0.48
2:Q:102:ILE:HG21	2:Q:139:THR:HG22	1.94	0.48
1:C:153:GLU:HB3	1:C:158:GLU:O	2.13	0.48
1:A:274:LEU:HD12	1:A:313:LYS:HB3	1.96	0.48
1:B:143:MET:SD	1:C:201:LEU:CD2	2.94	0.48
2:G:204:ILE:HG22	2:G:208:HIS:HD2	1.79	0.48
2:K:194:LEU:HD22	2:K:210:SER:HB2	1.96	0.48
1:N:29:VAL:HG21	1:N:242:CYS:CA	2.44	0.48
1:N:180:PRO:HA	1:N:183:LEU:HD21	1.96	0.48
1:C:196:LYS:O	1:C:197:LEU:C	2.52	0.48
1:A:32:THR:HG22	1:A:61:ASN:HD22	1.79	0.48
1:A:145:VAL:O	1:A:149:ILE:HG12	2.13	0.48
1:B:52:LEU:HD12	1:B:163:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:LYS:O	1:D:197:LEU:C	2.51	0.48
2:G:52:ALA:O	2:G:56:ILE:HG13	2.14	0.48
2:I:61:LEU:HD22	2:I:100:ARG:NH2	2.29	0.48
1:M:134:PRO:O	1:M:179:LEU:HD22	2.13	0.48
1:M:276:PHE:HA	1:M:292:TRP:CZ2	2.49	0.48
1:N:153:GLU:HB3	1:N:158:GLU:O	2.14	0.48
1:C:134:PRO:O	1:C:179:LEU:HD22	2.14	0.48
1:A:196:LYS:NZ	1:A:202:ASN:CG	2.67	0.47
2:I:172:LEU:HD21	2:I:193:ARG:HD3	1.95	0.47
1:O:190:PHE:C	1:O:190:PHE:CD1	2.87	0.47
1:P:276:PHE:HA	1:P:292:TRP:CZ2	2.49	0.47
2:W:112:LEU:HD23	2:W:149:PHE:CE2	2.47	0.47
1:C:174:LEU:C	1:C:177:LEU:HG	2.33	0.47
1:D:134:PRO:O	1:D:179:LEU:HD22	2.13	0.47
1:D:174:LEU:HD13	1:D:177:LEU:CD1	2.44	0.47
1:D:196:LYS:HG2	1:D:202:ASN:OD1	2.13	0.47
2:I:283:PHE:HB2	3:J:43:VAL:HG23	1.96	0.47
2:K:52:ALA:O	2:K:56:ILE:HG13	2.15	0.47
1:N:184:SER:O	1:N:187:LEU:HB2	2.14	0.47
1:O:198:GLY:HA2	1:O:200:MET:H	1.79	0.47
3:R:35:LEU:HD12	3:R:38:VAL:CG2	2.38	0.47
2:U:102:ILE:HD11	2:U:119:MET:SD	2.54	0.47
1:C:202:ASN:N	1:C:202:ASN:ND2	2.60	0.47
1:B:138:GLU:HB3	1:B:176:PHE:HD1	1.78	0.47
2:I:42:ARG:HH21	1:C:305:LEU:HD22	1.76	0.47
2:I:102:ILE:HD11	2:I:119:MET:SD	2.55	0.47
2:I:218:PHE:HZ	2:I:242:TYR:CZ	2.32	0.47
1:M:259:LEU:CD1	1:M:266:VAL:HG11	2.45	0.47
1:N:147:LYS:NZ	1:O:197:LEU:HD22	2.29	0.47
1:C:174:LEU:HD22	1:C:177:LEU:CD1	2.34	0.47
1:A:6:GLU:O	1:A:310:HIS:HD2	1.96	0.47
1:D:195:ASN:N	1:D:195:ASN:ND2	2.62	0.47
2:I:204:ILE:HG12	3:J:31:TYR:HD2	1.80	0.47
1:P:50:GLN:NE2	1:P:76:LYS:HE2	2.21	0.47
1:P:141:SER:O	1:P:145:VAL:HG13	2.14	0.47
2:S:263:PHE:HB2	2:S:289:PHE:CZ	2.49	0.47
2:U:150:VAL:CG1	2:U:151:TYR:N	2.78	0.47
2:W:94:SER:HB3	2:W:122:TRP:CZ2	2.49	0.47
1:C:77:VAL:HG22	1:C:80:MET:HB2	1.95	0.47
1:B:29:VAL:O	1:B:29:VAL:HG13	2.13	0.47
1:B:283:HIS:O	1:B:284:ASN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:VAL:N	2:K:19:ARG:NH1	2.63	0.47
2:G:124:ILE:HG12	2:G:132:GLY:N	2.28	0.47
1:P:231:THR:O	1:P:232:ASP:O	2.32	0.47
2:S:150:VAL:CG1	2:S:151:TYR:N	2.75	0.47
2:S:204:ILE:HG22	2:S:208:HIS:HD2	1.79	0.47
1:C:215:LYS:HA	1:C:218:GLU:HG2	1.96	0.47
1:A:5:VAL:HG11	1:A:309:PHE:O	2.15	0.47
1:B:7:PRO:HG2	1:B:337:GLU:HG2	1.97	0.47
1:B:278:GLU:OE1	1:B:292:TRP:HZ3	1.97	0.47
1:D:138:GLU:HB3	1:D:176:PHE:HD1	1.79	0.47
2:K:204:ILE:CG1	3:L:31:TYR:HD2	2.28	0.47
1:M:29:VAL:HG23	1:M:243:ILE:HG12	1.96	0.47
1:O:178:GLN:CA	1:O:229:GLN:HE22	2.27	0.47
1:O:196:LYS:O	1:O:197:LEU:C	2.51	0.47
1:C:280:ASP:HB2	1:C:348:TYR:OH	2.14	0.47
1:A:147:LYS:HA	1:A:150:LYS:HE3	1.97	0.47
1:A:194:THR:HG22	1:D:183:LEU:CD1	2.45	0.47
1:B:10:HIS:HD2	1:B:335:ASN:HD21	1.63	0.47
1:B:15:SER:OG	1:B:18:HIS:HD2	1.97	0.47
1:B:32:THR:CB	1:B:61:ASN:HD22	2.27	0.47
1:B:180:PRO:HA	1:B:183:LEU:HD21	1.96	0.47
1:B:276:PHE:HA	1:B:292:TRP:CZ2	2.49	0.47
2:E:94:SER:HB3	2:E:122:TRP:CZ2	2.50	0.47
2:E:191:PHE:CZ	2:E:211:LYS:HG3	2.49	0.47
2:G:188:ALA:HB2	2:G:244:ASP:HB3	1.97	0.47
2:G:191:PHE:CZ	2:G:211:LYS:HG3	2.50	0.47
2:K:159:LEU:HD21	3:L:41:LEU:HD22	1.97	0.47
1:M:281:GLN:O	1:M:282:GLU:CB	2.63	0.47
1:N:190:PHE:CD1	1:N:190:PHE:C	2.87	0.47
1:N:217:ASN:OD1	1:O:217:ASN:ND2	2.47	0.47
1:P:154:GLN:HG3	1:C:79:GLY:O	2.15	0.47
2:Q:112:LEU:CD1	2:Q:143:LYS:HD2	2.44	0.47
2:Q:281:LEU:HB2	2:Q:295:LYS:HE2	1.95	0.47
1:C:15:SER:OG	1:C:18:HIS:HD2	1.97	0.47
1:C:146:MET:HE2	1:C:149:ILE:HG13	1.96	0.47
1:B:32:THR:CG2	1:B:61:ASN:HD22	2.28	0.47
1:D:32:THR:CG2	1:D:61:ASN:HD22	2.27	0.47
1:D:73:ASP:HA	1:D:152:GLN:CD	2.35	0.47
1:D:276:PHE:HA	1:D:292:TRP:CZ2	2.50	0.47
1:M:178:GLN:NE2	1:M:261:SER:HB2	2.30	0.47
1:M:305:LEU:HD22	2:Q:42:ARG:HH22	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:32:THR:HG22	1:P:61:ASN:HD22	1.80	0.47
1:P:153:GLU:O	1:P:158:GLU:HA	2.15	0.47
1:P:174:LEU:CG	1:P:177:LEU:HD11	2.45	0.47
1:P:196:LYS:O	1:P:197:LEU:C	2.52	0.47
2:Q:102:ILE:HD11	2:Q:119:MET:SD	2.55	0.47
2:U:17:LEU:CD1	2:U:58:GLN:HG2	2.44	0.47
2:U:102:ILE:HG21	2:U:139:THR:HG22	1.96	0.47
2:U:204:ILE:HG22	2:U:208:HIS:HD2	1.79	0.47
2:G:17:LEU:CD1	2:G:58:GLN:HG2	2.45	0.47
2:G:278:LYS:CG	2:G:295:LYS:HG2	2.44	0.47
1:M:54:ILE:HD11	1:M:88:ILE:CD1	2.45	0.47
1:M:195:ASN:N	1:M:195:ASN:ND2	2.63	0.47
1:O:178:GLN:HA	1:O:229:GLN:NE2	2.29	0.47
1:O:346:VAL:O	1:O:349:GLU:HB3	2.14	0.47
1:C:32:THR:HB	1:C:61:ASN:HD22	1.80	0.47
1:C:73:ASP:HA	1:C:152:GLN:CD	2.34	0.47
1:C:195:ASN:N	1:C:195:ASN:ND2	2.62	0.47
1:C:278:GLU:OE1	1:C:292:TRP:HZ3	1.98	0.47
1:A:32:THR:CG2	1:A:61:ASN:HD22	2.28	0.47
2:G:94:SER:HB3	2:G:122:TRP:CZ2	2.49	0.47
2:I:102:ILE:HG21	2:I:139:THR:HG22	1.97	0.47
2:U:87:GLU:HA	2:U:126:PHE:CZ	2.50	0.47
3:X:39:THR:HG23	3:X:40:ASN:OD1	2.15	0.47
2:G:189:GLU:HB3	3:H:48:LEU:CD2	2.45	0.46
2:K:102:ILE:HG21	2:K:139:THR:HG22	1.97	0.46
1:M:274:LEU:HD22	1:M:299:LEU:HD11	1.97	0.46
1:N:138:GLU:HB3	1:N:176:PHE:HD1	1.80	0.46
1:N:190:PHE:CE1	1:O:187:LEU:HD11	2.50	0.46
1:O:20:TRP:CB	1:O:236:THR:HG23	2.45	0.46
1:O:276:PHE:HA	1:O:292:TRP:CZ2	2.49	0.46
1:O:278:GLU:OE1	1:O:292:TRP:HZ3	1.97	0.46
1:P:279:ASN:OD1	1:P:341:ILE:HD11	2.14	0.46
2:S:218:PHE:HZ	2:S:242:TYR:CZ	2.33	0.46
2:U:202:SER:CB	3:V:33:LYS:HB2	2.42	0.46
1:B:73:ASP:HA	1:B:152:GLN:CD	2.35	0.46
1:D:73:ASP:HA	1:D:152:GLN:NE2	2.30	0.46
1:D:231:THR:O	1:D:231:THR:HG22	2.15	0.46
2:E:124:ILE:HG12	2:E:132:GLY:N	2.29	0.46
1:M:190:PHE:CD1	1:P:187:LEU:HD21	2.50	0.46
1:P:178:GLN:HA	1:P:229:GLN:NE2	2.28	0.46
3:V:35:LEU:HD12	3:V:38:VAL:CG2	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:205:SER:HB2	3:X:32:THR:HG23	1.97	0.46
1:B:174:LEU:HD13	1:B:177:LEU:HD11	1.97	0.46
2:G:111:ASN:O	2:G:112:LEU:C	2.54	0.46
1:M:153:GLU:HB3	1:M:158:GLU:O	2.15	0.46
1:M:190:PHE:CE2	1:P:183:LEU:HB2	2.50	0.46
1:M:193:ILE:C	1:M:195:ASN:N	2.69	0.46
1:A:259:LEU:CD1	1:A:266:VAL:HG11	2.46	0.46
1:A:281:GLN:O	1:A:282:GLU:CB	2.64	0.46
1:B:174:LEU:C	1:B:177:LEU:HG	2.32	0.46
2:G:263:PHE:HB2	2:G:289:PHE:CZ	2.51	0.46
2:I:12:LYS:HE3	1:C:267:ASN:HB2	1.98	0.46
2:K:40:ALA:O	2:K:44:VAL:HG23	2.14	0.46
1:N:21:ILE:HB	1:N:164:ILE:HD13	1.98	0.46
1:N:187:LEU:CD1	1:O:190:PHE:CE1	2.97	0.46
1:N:196:LYS:NZ	1:N:202:ASN:CG	2.69	0.46
1:N:281:GLN:O	1:N:282:GLU:CB	2.64	0.46
1:P:191:GLY:O	1:P:195:ASN:ND2	2.48	0.46
1:C:177:LEU:N	1:C:177:LEU:HD23	2.31	0.46
1:D:247:LEU:HD13	1:C:247:LEU:CB	2.46	0.46
1:M:155:GLY:O	1:M:156:GLU:HB2	2.16	0.46
2:W:87:GLU:HA	2:W:126:PHE:CZ	2.51	0.46
1:C:54:ILE:HD11	1:C:88:ILE:HG12	1.98	0.46
1:B:32:THR:HB	1:B:61:ASN:HD22	1.81	0.46
1:B:184:SER:O	1:B:187:LEU:HB2	2.14	0.46
2:K:94:SER:HB3	2:K:122:TRP:CZ2	2.50	0.46
1:M:138:GLU:HB3	1:M:176:PHE:HD1	1.79	0.46
1:M:285:CYS:SG	1:M:288:CYS:HB2	2.55	0.46
1:N:201:LEU:HG	1:N:205:MET:CE	2.46	0.46
1:P:174:LEU:HB3	1:P:177:LEU:HG	1.98	0.46
2:Q:256:GLN:HE22	3:R:29:LYS:HG3	1.81	0.46
2:U:232:ASN:HB2	3:V:21:THR:HB	1.96	0.46
1:D:281:GLN:O	1:D:282:GLU:CB	2.63	0.46
2:G:171:LEU:HD23	2:G:171:LEU:C	2.36	0.46
2:G:189:GLU:HB3	3:H:48:LEU:HD22	1.98	0.46
2:K:124:ILE:HG12	2:K:132:GLY:N	2.31	0.46
1:O:174:LEU:HD22	1:O:177:LEU:CD1	2.32	0.46
2:Q:218:PHE:HZ	2:Q:242:TYR:CZ	2.34	0.46
1:D:215:LYS:HA	1:D:218:GLU:HG2	1.97	0.46
2:G:154:GLU:HG3	2:G:168:TYR:CE1	2.51	0.46
2:K:115:VAL:HG12	2:K:119:MET:CE	2.46	0.46
1:N:10:HIS:HD2	1:N:335:ASN:HD21	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:138:GLU:HB3	1:P:176:PHE:HD1	1.81	0.46
1:P:179:LEU:HG	1:P:183:LEU:HD13	1.97	0.46
1:P:347:ILE:C	1:P:349:GLU:N	2.69	0.46
2:S:124:ILE:HG12	2:S:132:GLY:N	2.30	0.46
2:S:188:ALA:HB2	2:S:244:ASP:HB3	1.98	0.46
2:S:194:LEU:HD22	2:S:210:SER:HB2	1.96	0.46
1:B:230:PHE:HA	2:G:9:MET:HE1	1.97	0.46
1:B:347:ILE:C	1:B:349:GLU:N	2.69	0.46
2:E:112:LEU:CD1	2:E:143:LYS:HD2	2.46	0.46
2:E:189:GLU:HB3	3:F:48:LEU:HD21	1.98	0.46
2:E:232:ASN:HB2	3:F:21:THR:HB	1.98	0.46
1:O:32:THR:HB	1:O:61:ASN:HD22	1.80	0.46
1:O:180:PRO:HA	1:O:183:LEU:HD21	1.98	0.46
2:Q:94:SER:HB3	2:Q:122:TRP:CZ2	2.51	0.46
2:Q:124:ILE:HG12	2:Q:132:GLY:N	2.30	0.46
2:U:175:TRP:CH2	3:V:48:LEU:HD12	2.50	0.46
2:W:281:LEU:HB2	2:W:295:LYS:HE2	1.98	0.46
1:C:73:ASP:HA	1:C:152:GLN:NE2	2.31	0.46
1:B:143:MET:CE	1:C:197:LEU:O	2.63	0.46
1:B:263:ASP:O	2:G:9:MET:CE	2.64	0.46
1:D:15:SER:OG	1:D:18:HIS:HD2	1.99	0.46
2:G:227:GLU:O	2:G:227:GLU:HG3	2.16	0.46
1:N:5:VAL:HG11	1:N:309:PHE:O	2.16	0.46
1:N:236:THR:HG22	1:N:264:MET:HE3	1.97	0.46
1:P:260:ILE:CD1	2:W:42:ARG:HG2	2.47	0.46
2:W:124:ILE:HG12	2:W:132:GLY:N	2.31	0.46
2:W:171:LEU:HD23	2:W:171:LEU:C	2.36	0.46
3:X:19:LEU:HD12	3:X:19:LEU:O	2.14	0.46
1:C:10:HIS:HD2	1:C:335:ASN:ND2	2.14	0.46
1:C:259:LEU:CD1	1:C:266:VAL:HG11	2.46	0.46
1:A:138:GLU:HB3	1:A:176:PHE:HD1	1.80	0.45
1:A:233:PRO:HB3	2:E:9:MET:N	2.31	0.45
1:M:278:GLU:OE1	1:M:292:TRP:HZ3	1.99	0.45
1:O:16:THR:HB	1:O:49:LYS:CE	2.46	0.45
1:P:215:LYS:HA	1:P:218:GLU:HG2	1.98	0.45
1:P:278:GLU:OE1	1:P:292:TRP:HZ3	1.98	0.45
2:S:145:LEU:HG	3:T:54:GLN:HE22	1.80	0.45
2:U:278:LYS:HG3	2:U:295:LYS:HG2	1.98	0.45
1:A:283:HIS:O	1:A:284:ASN:HB2	2.17	0.45
1:D:180:PRO:O	1:D:225:THR:HG21	2.15	0.45
2:G:283:PHE:HE1	3:H:40:ASN:HD21	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:282:GLU:O	2:I:286:GLN:HG3	2.16	0.45
2:K:150:VAL:CG1	2:K:151:TYR:N	2.78	0.45
1:M:274:LEU:HD12	1:M:313:LYS:HB3	1.97	0.45
1:M:280:ASP:HB2	1:M:348:TYR:OH	2.16	0.45
1:N:20:TRP:HE3	1:N:165:PHE:HE2	1.64	0.45
1:N:197:LEU:O	1:O:143:MET:CE	2.64	0.45
1:N:283:HIS:O	1:N:284:ASN:HB2	2.16	0.45
1:O:15:SER:OG	1:O:18:HIS:HD2	1.99	0.45
1:O:21:ILE:HB	1:O:164:ILE:HD13	1.98	0.45
1:O:153:GLU:HB3	1:O:158:GLU:O	2.17	0.45
1:O:201:LEU:HG	1:O:205:MET:CE	2.47	0.45
2:Q:89:LYS:HA	2:Q:126:PHE:HB3	1.99	0.45
3:R:19:LEU:O	3:R:19:LEU:HD12	2.16	0.45
2:S:94:SER:HB3	2:S:122:TRP:CZ2	2.50	0.45
2:U:188:ALA:HB2	2:U:244:ASP:HB3	1.97	0.45
1:C:279:ASN:OD1	1:C:341:ILE:HD11	2.17	0.45
1:B:280:ASP:HB2	1:B:348:TYR:OH	2.16	0.45
2:G:116:ILE:HD13	2:G:144:LEU:HG	1.99	0.45
2:I:89:LYS:HA	2:I:126:PHE:HB3	1.97	0.45
2:K:89:LYS:HA	2:K:126:PHE:HB3	1.97	0.45
1:P:155:GLY:O	1:P:156:GLU:HB2	2.16	0.45
1:P:180:PRO:HA	1:P:183:LEU:HD21	1.98	0.45
2:W:91:ASP:O	2:W:95:VAL:HG23	2.17	0.45
1:C:12:LEU:O	1:C:12:LEU:HD22	2.17	0.45
1:B:281:GLN:O	1:B:282:GLU:CB	2.64	0.45
1:D:274:LEU:HD22	1:D:299:LEU:HD11	1.98	0.45
2:E:102:ILE:HD11	2:E:119:MET:SD	2.56	0.45
2:I:191:PHE:CZ	2:I:211:LYS:HG3	2.52	0.45
2:K:159:LEU:HD21	3:L:41:LEU:CD2	2.47	0.45
2:K:175:TRP:CH2	3:L:48:LEU:HD12	2.51	0.45
1:M:279:ASN:HB3	1:M:341:ILE:HD13	1.98	0.45
1:O:7:PRO:HG2	1:O:337:GLU:HG2	1.99	0.45
2:S:111:ASN:O	2:S:112:LEU:C	2.55	0.45
2:U:150:VAL:CG1	2:U:151:TYR:H	2.30	0.45
2:W:115:VAL:HG12	2:W:119:MET:CE	2.47	0.45
1:A:62:LEU:HB2	1:A:87:GLU:OE1	2.16	0.45
1:A:196:LYS:O	1:A:197:LEU:C	2.54	0.45
1:B:201:LEU:HG	1:B:205:MET:CE	2.47	0.45
2:E:111:ASN:O	2:E:112:LEU:C	2.55	0.45
2:G:179:VAL:HB	2:G:182:ILE:HD13	1.99	0.45
2:G:232:ASN:HB2	3:H:21:THR:OG1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:190:PHE:CD1	1:M:190:PHE:C	2.89	0.45
1:O:29:VAL:HG21	1:O:242:CYS:CA	2.42	0.45
2:Q:202:SER:HB2	3:R:33:LYS:CB	2.46	0.45
2:Q:204:ILE:HG22	2:Q:208:HIS:HD2	1.82	0.45
2:U:171:LEU:HD23	2:U:171:LEU:C	2.37	0.45
1:A:274:LEU:HD22	1:A:299:LEU:HD11	1.99	0.45
1:B:29:VAL:HG23	1:B:243:ILE:HG12	1.97	0.45
2:E:279:SER:CB	3:F:43:VAL:HG11	2.45	0.45
2:G:89:LYS:HA	2:G:126:PHE:HB3	1.98	0.45
2:I:87:GLU:HA	2:I:126:PHE:CZ	2.51	0.45
1:N:276:PHE:HA	1:N:292:TRP:CZ2	2.51	0.45
1:O:20:TRP:HE3	1:O:165:PHE:HE2	1.65	0.45
1:O:281:GLN:O	1:O:282:GLU:CB	2.64	0.45
1:P:257:GLN:NE2	2:W:45:ARG:CB	2.79	0.45
2:Q:279:SER:HB2	3:R:43:VAL:HG11	1.98	0.45
2:W:227:GLU:O	2:W:227:GLU:HG3	2.17	0.45
2:W:283:PHE:CE1	3:X:42:GLY:HA2	2.52	0.45
1:A:205:MET:O	1:D:228:GLN:HG2	2.15	0.45
2:E:89:LYS:HA	2:E:126:PHE:HB3	1.99	0.45
2:I:111:ASN:O	2:I:112:LEU:C	2.55	0.45
2:K:87:GLU:HA	2:K:126:PHE:CZ	2.52	0.45
1:N:15:SER:OG	1:N:18:HIS:HD2	1.99	0.45
1:N:196:LYS:HG3	1:O:143:MET:HG3	1.99	0.45
1:P:12:LEU:HD22	1:P:12:LEU:O	2.17	0.45
1:P:153:GLU:HB3	1:P:158:GLU:O	2.16	0.45
2:U:111:ASN:O	2:U:112:LEU:C	2.55	0.45
2:U:236:ILE:HD11	2:U:253:ILE:HD12	1.98	0.45
2:W:150:VAL:CG1	2:W:151:TYR:N	2.78	0.45
1:C:138:GLU:HB3	1:C:176:PHE:HD1	1.81	0.45
1:C:274:LEU:HD12	1:C:313:LYS:HB3	1.99	0.45
1:B:73:ASP:HA	1:B:152:GLN:NE2	2.32	0.45
2:E:218:PHE:HZ	2:E:242:TYR:CZ	2.35	0.45
2:K:171:LEU:HD23	2:K:171:LEU:C	2.38	0.45
1:N:286:LYS:H	1:N:286:LYS:HD3	1.81	0.45
1:O:54:ILE:HG13	1:O:86:MET:O	2.17	0.45
2:U:112:LEU:CD1	2:U:143:LYS:HD2	2.46	0.45
1:C:275:LEU:HD11	1:C:291:ARG:HD3	1.99	0.45
1:A:190:PHE:CD1	1:D:187:LEU:HD21	2.52	0.45
1:A:280:ASP:HB2	1:A:348:TYR:OH	2.17	0.45
1:B:16:THR:HB	1:B:49:LYS:CE	2.47	0.45
1:D:292:TRP:CZ3	1:D:296:LYS:HE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:150:VAL:CG1	2:E:151:TYR:N	2.78	0.45
2:E:256:GLN:HE22	3:F:29:LYS:CG	2.27	0.45
2:G:194:LEU:HD22	2:G:210:SER:HB2	1.99	0.45
2:K:17:LEU:CD1	2:K:58:GLN:HG2	2.46	0.45
1:M:187:LEU:CD1	1:P:190:PHE:CE1	2.94	0.45
1:M:256:ILE:O	1:M:260:ILE:HG13	2.17	0.45
1:N:10:HIS:HD2	1:N:335:ASN:ND2	2.14	0.45
1:O:279:ASN:OD1	1:O:341:ILE:HD11	2.17	0.45
1:P:73:ASP:HA	1:P:152:GLN:CD	2.38	0.45
1:P:198:GLY:HA2	1:P:200:MET:H	1.82	0.45
2:Q:154:GLU:HG3	2:Q:168:TYR:CE1	2.51	0.45
2:U:225:LYS:HB2	2:U:240:GLU:HB2	1.98	0.45
2:W:111:ASN:O	2:W:112:LEU:C	2.55	0.45
1:B:150:LYS:HE2	1:C:200:MET:HG2	1.99	0.45
2:E:171:LEU:HD23	2:E:171:LEU:C	2.37	0.45
2:E:172:LEU:HD21	2:E:193:ARG:HD3	1.98	0.45
2:E:204:ILE:HG22	2:E:208:HIS:HD2	1.81	0.45
2:I:188:ALA:HB2	2:I:244:ASP:HB3	1.99	0.45
1:M:15:SER:OG	1:M:18:HIS:HD2	2.00	0.45
1:N:29:VAL:HG23	1:N:243:ILE:HG12	1.98	0.45
1:P:20:TRP:HE3	1:P:165:PHE:HE2	1.65	0.45
1:P:257:GLN:NE2	2:W:45:ARG:HB2	2.31	0.45
2:W:89:LYS:HA	2:W:126:PHE:HB3	1.99	0.45
1:C:10:HIS:HD2	1:C:335:ASN:HD21	1.65	0.45
1:A:198:GLY:HA2	1:A:200:MET:H	1.81	0.44
1:A:276:PHE:HA	1:A:292:TRP:CZ2	2.52	0.44
1:B:168:ALA:HB1	1:B:169:PRO:HD2	1.99	0.44
1:B:274:LEU:HD12	1:B:313:LYS:HB3	1.98	0.44
1:D:20:TRP:HE3	1:D:165:PHE:HE2	1.65	0.44
1:D:247:LEU:HB3	1:C:247:LEU:HB3	1.98	0.44
2:K:172:LEU:HD21	2:K:193:ARG:HD3	1.99	0.44
1:M:199:PRO:CG	1:C:156:GLU:CG	2.96	0.44
1:N:141:SER:O	1:N:145:VAL:HG13	2.17	0.44
1:N:292:TRP:CZ3	1:N:296:LYS:HE2	2.52	0.44
1:P:29:VAL:HG23	1:P:243:ILE:HG12	1.99	0.44
2:U:40:ALA:O	2:U:44:VAL:HG23	2.17	0.44
2:U:168:TYR:CE2	2:U:194:LEU:HD23	2.52	0.44
2:U:194:LEU:HD22	2:U:210:SER:HB2	1.99	0.44
2:W:234:TYR:HB2	3:X:21:THR:HG21	1.99	0.44
1:A:172:HIS:HB3	1:A:258:GLU:OE2	2.17	0.44
1:A:215:LYS:HA	1:A:218:GLU:HG2	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:GLU:CD	2:G:35:THR:HG22	2.38	0.44
1:D:190:PHE:CD1	1:D:190:PHE:C	2.91	0.44
1:D:279:ASN:OD1	1:D:341:ILE:HD11	2.17	0.44
2:E:282:GLU:O	2:E:286:GLN:HG3	2.17	0.44
1:M:20:TRP:HE3	1:M:165:PHE:HE2	1.65	0.44
1:N:168:ALA:HB1	1:N:169:PRO:HD2	2.00	0.44
1:N:179:LEU:HG	1:N:183:LEU:HD13	2.00	0.44
1:N:274:LEU:HD22	1:N:299:LEU:HD11	1.98	0.44
1:O:196:LYS:NZ	1:O:202:ASN:CG	2.69	0.44
1:P:281:GLN:O	1:P:282:GLU:CB	2.65	0.44
2:S:89:LYS:HA	2:S:126:PHE:HB3	1.99	0.44
2:W:188:ALA:HB2	2:W:244:ASP:HB3	1.99	0.44
1:C:155:GLY:O	1:C:156:GLU:HB2	2.16	0.44
1:C:276:PHE:HA	1:C:292:TRP:CE2	2.52	0.44
1:C:347:ILE:C	1:C:349:GLU:N	2.70	0.44
1:B:143:MET:CG	1:C:196:LYS:HD2	2.47	0.44
2:E:179:VAL:HB	2:E:182:ILE:HD13	2.00	0.44
2:I:9:MET:HE1	1:C:263:ASP:O	2.17	0.44
2:I:94:SER:HB3	2:I:122:TRP:CZ2	2.52	0.44
2:I:202:SER:HB2	3:J:33:LYS:CB	2.46	0.44
2:K:111:ASN:O	2:K:112:LEU:C	2.55	0.44
1:M:347:ILE:C	1:M:349:GLU:N	2.70	0.44
1:N:20:TRP:HE3	1:N:165:PHE:CE2	2.35	0.44
1:O:29:VAL:HG23	1:O:243:ILE:HG12	1.99	0.44
2:S:52:ALA:O	2:S:56:ILE:HG13	2.17	0.44
2:U:154:GLU:HG3	2:U:168:TYR:CE1	2.52	0.44
2:W:168:TYR:CE2	2:W:194:LEU:HD23	2.52	0.44
1:A:155:GLY:O	1:A:156:GLU:HB2	2.18	0.44
1:B:153:GLU:O	1:B:158:GLU:HA	2.16	0.44
1:D:346:VAL:O	1:D:349:GLU:HB3	2.17	0.44
1:D:347:ILE:C	1:D:349:GLU:N	2.71	0.44
2:E:168:TYR:CE2	2:E:194:LEU:HD23	2.53	0.44
2:G:150:VAL:CG1	2:G:151:TYR:N	2.78	0.44
1:M:147:LYS:HZ1	1:P:197:LEU:CD1	2.22	0.44
1:N:233:PRO:CG	2:S:11:ALA:HB3	2.48	0.44
1:O:276:PHE:HA	1:O:292:TRP:CE2	2.53	0.44
1:P:281:GLN:HA	1:P:281:GLN:NE2	2.31	0.44
2:Q:111:ASN:O	2:Q:112:LEU:C	2.56	0.44
2:Q:231:LYS:HB2	3:R:17:LEU:HG	1.99	0.44
2:S:179:VAL:HB	2:S:182:ILE:HD13	2.00	0.44
2:U:89:LYS:HA	2:U:126:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:VAL:HG21	1:C:334:LEU:HD23	1.99	0.44
1:A:168:ALA:HB1	1:A:169:PRO:HD2	1.99	0.44
1:A:178:GLN:HA	1:A:229:GLN:NE2	2.30	0.44
1:A:230:PHE:HA	2:E:9:MET:HE1	2.00	0.44
1:B:230:PHE:CG	2:G:9:MET:HE3	2.52	0.44
1:B:259:LEU:CD1	1:B:266:VAL:HG11	2.47	0.44
1:D:276:PHE:HA	1:D:292:TRP:CE2	2.52	0.44
1:D:307:GLU:CD	2:K:35:THR:HG22	2.38	0.44
2:E:231:LYS:HB2	3:F:17:LEU:HG	1.99	0.44
2:G:112:LEU:CD1	2:G:143:LYS:HD2	2.47	0.44
2:G:208:HIS:NE2	3:H:29:LYS:HG2	2.32	0.44
2:K:236:ILE:HD11	2:K:253:ILE:HD12	2.00	0.44
1:M:178:GLN:CA	1:M:229:GLN:HE22	2.30	0.44
1:N:260:ILE:HG22	2:S:46:SER:OG	2.18	0.44
2:U:115:VAL:HG12	2:U:119:MET:CE	2.48	0.44
1:C:254:ARG:HG3	1:C:255:LEU:H	1.82	0.44
1:A:247:LEU:HD13	1:B:247:LEU:CB	2.46	0.44
1:D:180:PRO:HB2	1:D:225:THR:CG2	2.48	0.44
2:E:178:GLN:NE2	3:F:53:LYS:O	2.50	0.44
2:E:281:LEU:HB2	2:E:295:LYS:HE2	1.98	0.44
2:K:116:ILE:HD13	2:K:144:LEU:HG	1.99	0.44
1:N:180:PRO:O	1:N:225:THR:HG21	2.17	0.44
1:C:283:HIS:O	1:C:284:ASN:HB2	2.17	0.44
2:G:107:PRO:HB3	2:G:146:GLU:HB3	2.00	0.44
2:K:227:GLU:HG3	2:K:227:GLU:O	2.18	0.44
1:N:244:SER:OG	1:N:299:LEU:HG	2.18	0.44
1:N:259:LEU:CD1	1:N:266:VAL:HG11	2.47	0.44
1:O:247:LEU:CB	1:P:247:LEU:HD13	2.48	0.44
2:S:227:GLU:HG3	2:S:227:GLU:O	2.18	0.44
2:S:278:LYS:CG	2:S:295:LYS:HG2	2.48	0.44
1:A:77:VAL:HG22	1:A:80:MET:HB2	2.00	0.44
1:D:178:GLN:NE2	1:D:261:SER:HB2	2.32	0.44
2:K:112:LEU:CD1	2:K:143:LYS:HD2	2.46	0.44
1:M:5:VAL:HG11	1:M:309:PHE:O	2.18	0.44
1:M:215:LYS:HA	1:M:218:GLU:HG2	1.99	0.44
1:N:317:CYS:HG	1:N:321:ILE:HD11	1.83	0.44
1:O:247:LEU:HD13	1:P:247:LEU:HB3	2.00	0.44
1:A:20:TRP:HE3	1:A:165:PHE:HE2	1.66	0.44
1:D:147:LYS:HA	1:D:150:LYS:HE3	1.99	0.44
1:D:263:ASP:O	2:K:9:MET:HE1	2.17	0.44
2:E:52:ALA:O	2:E:56:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:39:THR:HG23	3:F:40:ASN:OD1	2.18	0.44
1:N:54:ILE:HD11	1:N:88:ILE:CD1	2.48	0.44
1:N:347:ILE:C	1:N:349:GLU:N	2.71	0.44
1:O:76:LYS:HD3	1:O:84:SER:OG	2.18	0.44
1:O:280:ASP:HB2	1:O:348:TYR:OH	2.18	0.44
1:P:16:THR:HB	1:P:49:LYS:CE	2.48	0.44
1:P:24:GLY:HA2	1:P:167:THR:OG1	2.17	0.44
1:P:147:LYS:HA	1:P:150:LYS:HE3	1.99	0.44
1:P:283:HIS:O	1:P:284:ASN:HB2	2.18	0.44
2:U:9:MET:CG	2:U:10:GLY:N	2.81	0.44
2:U:238:PHE:CE2	3:V:10:HIS:HB2	2.53	0.44
2:U:275:GLN:NE2	2:U:275:GLN:HA	2.33	0.44
1:D:32:THR:CB	1:D:61:ASN:HD22	2.31	0.43
1:D:172:HIS:HB3	1:D:258:GLU:OE2	2.17	0.43
2:E:116:ILE:HD13	2:E:144:LEU:HG	2.00	0.43
2:E:194:LEU:HD22	2:E:210:SER:HB2	1.99	0.43
2:I:250:LEU:HD11	3:J:13:VAL:HG22	1.99	0.43
1:N:231:THR:O	1:N:232:ASP:O	2.36	0.43
1:N:242:CYS:HB2	1:N:248:SER:OG	2.18	0.43
1:O:168:ALA:HB1	1:O:169:PRO:HD2	1.99	0.43
1:O:181:ASN:ND2	1:O:226:ILE:HG12	2.33	0.43
1:O:292:TRP:CZ3	1:O:296:LYS:HE2	2.53	0.43
1:P:193:ILE:C	1:P:195:ASN:N	2.72	0.43
2:Q:168:TYR:CE2	2:Q:194:LEU:HD23	2.53	0.43
2:Q:171:LEU:C	2:Q:171:LEU:HD23	2.38	0.43
2:Q:172:LEU:HD21	2:Q:193:ARG:HD3	1.99	0.43
2:S:171:LEU:HD23	2:S:171:LEU:C	2.38	0.43
2:S:236:ILE:HD11	2:S:253:ILE:HD12	2.00	0.43
2:U:227:GLU:HG3	2:U:227:GLU:O	2.18	0.43
3:V:39:THR:HG23	3:V:40:ASN:OD1	2.18	0.43
1:A:199:PRO:O	1:A:203:SER:HB2	2.18	0.43
2:E:40:ALA:O	2:E:44:VAL:HG23	2.17	0.43
2:G:87:GLU:HA	2:G:126:PHE:CZ	2.53	0.43
2:I:231:LYS:HB2	3:J:17:LEU:HG	2.00	0.43
1:M:135:GLY:HA3	1:M:179:LEU:CD2	2.39	0.43
1:M:253:GLU:OE1	2:Q:45:ARG:NH2	2.51	0.43
1:N:54:ILE:HD12	1:N:86:MET:HB3	2.00	0.43
1:N:194:THR:C	1:N:195:ASN:HD22	2.22	0.43
1:N:346:VAL:O	1:N:349:GLU:HB3	2.18	0.43
2:Q:189:GLU:HB3	3:R:48:LEU:CD2	2.48	0.43
2:Q:208:HIS:NE2	3:R:29:LYS:HG2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:204:ILE:HG22	2:K:208:HIS:HD2	1.84	0.43
1:M:168:ALA:HB1	1:M:169:PRO:HD2	2.00	0.43
1:N:20:TRP:CE3	1:N:165:PHE:HE2	2.36	0.43
1:N:276:PHE:HA	1:N:292:TRP:CE2	2.53	0.43
1:O:263:ASP:O	2:U:9:MET:HE2	2.19	0.43
1:P:135:GLY:HA3	1:P:179:LEU:CD2	2.37	0.43
1:A:10:HIS:HD2	1:A:335:ASN:ND2	2.16	0.43
1:B:276:PHE:HA	1:B:292:TRP:CE2	2.53	0.43
2:E:203:ASN:OD1	3:F:32:THR:HG22	2.17	0.43
2:E:236:ILE:HD11	2:E:253:ILE:HD12	1.99	0.43
2:G:133:ASP:HA	2:G:134:PRO:HD3	1.90	0.43
2:I:283:PHE:HE1	3:J:40:ASN:HD21	1.62	0.43
1:M:21:ILE:HB	1:M:164:ILE:HD13	2.01	0.43
1:N:16:THR:HB	1:N:49:LYS:CE	2.49	0.43
1:P:29:VAL:O	1:P:29:VAL:HG13	2.17	0.43
2:Q:87:GLU:HA	2:Q:126:PHE:CZ	2.53	0.43
2:W:189:GLU:HB3	3:X:48:LEU:CD2	2.49	0.43
1:B:191:GLY:O	1:B:195:ASN:ND2	2.51	0.43
1:B:346:VAL:O	1:B:349:GLU:HB3	2.18	0.43
1:D:16:THR:HB	1:D:49:LYS:CE	2.48	0.43
2:E:102:ILE:HG21	2:E:139:THR:HG22	1.99	0.43
2:K:168:TYR:CE2	2:K:194:LEU:HD23	2.54	0.43
2:K:278:LYS:HG3	2:K:295:LYS:HG2	2.00	0.43
1:M:253:GLU:OE1	2:Q:45:ARG:NH1	2.51	0.43
1:N:178:GLN:HA	1:N:229:GLN:NE2	2.34	0.43
1:O:135:GLY:HA3	1:O:179:LEU:CD2	2.40	0.43
1:O:196:LYS:HG3	1:O:202:ASN:HD21	1.84	0.43
1:O:274:LEU:HD12	1:O:313:LYS:HB3	1.99	0.43
2:S:275:GLN:NE2	2:S:275:GLN:HA	2.34	0.43
1:A:29:VAL:HG23	1:A:243:ILE:HG12	2.01	0.43
1:A:181:ASN:ND2	1:A:226:ILE:HG12	2.33	0.43
1:A:190:PHE:CD1	1:A:190:PHE:C	2.91	0.43
1:D:191:GLY:O	1:D:194:THR:OG1	2.35	0.43
1:D:259:LEU:CD1	1:D:266:VAL:HG11	2.48	0.43
2:I:171:LEU:C	2:I:171:LEU:HD23	2.39	0.43
2:K:179:VAL:HB	2:K:182:ILE:HD13	2.00	0.43
1:M:196:LYS:NZ	1:M:202:ASN:CG	2.72	0.43
1:O:16:THR:HB	1:O:49:LYS:HE2	2.00	0.43
1:O:198:GLY:CA	1:O:200:MET:N	2.82	0.43
3:V:45:LEU:HB3	3:V:46:PRO:HD2	2.01	0.43
2:W:52:ALA:O	2:W:56:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:HIS:HD2	1:D:335:ASN:ND2	2.17	0.43
1:D:193:ILE:C	1:D:195:ASN:N	2.72	0.43
1:D:275:LEU:HD11	1:D:291:ARG:HD3	1.99	0.43
2:G:40:ALA:O	2:G:44:VAL:HG23	2.18	0.43
2:K:231:LYS:HB2	3:L:17:LEU:HG	2.01	0.43
3:L:39:THR:HG23	3:L:40:ASN:OD1	2.18	0.43
1:M:32:THR:CG2	1:M:61:ASN:HD22	2.32	0.43
1:N:193:ILE:C	1:N:195:ASN:N	2.72	0.43
1:O:230:PHE:O	1:O:232:ASP:N	2.51	0.43
1:P:201:LEU:HG	1:P:205:MET:HE3	2.00	0.43
2:Q:116:ILE:HD13	2:Q:144:LEU:HG	2.01	0.43
2:W:202:SER:CB	3:X:33:LYS:HB2	2.49	0.43
1:C:24:GLY:HA2	1:C:167:THR:OG1	2.18	0.43
1:C:275:LEU:HB2	1:C:292:TRP:CD1	2.53	0.43
1:A:278:GLU:OE1	1:A:292:TRP:HZ3	2.02	0.43
1:D:27:GLY:HA2	1:C:246:PHE:CE2	2.53	0.43
2:E:232:ASN:HB2	3:F:21:THR:CB	2.48	0.43
2:G:9:MET:CG	2:G:10:GLY:N	2.82	0.43
1:M:193:ILE:O	1:M:195:ASN:N	2.52	0.43
1:N:275:LEU:HD11	1:N:291:ARG:HD3	2.00	0.43
1:O:174:LEU:CG	1:O:177:LEU:HD11	2.49	0.43
1:O:275:LEU:HD11	1:O:291:ARG:HD3	2.00	0.43
1:O:347:ILE:C	1:O:349:GLU:N	2.71	0.43
2:W:193:ARG:HA	3:X:45:LEU:HD13	2.01	0.43
1:C:180:PRO:O	1:C:225:THR:HG21	2.19	0.43
1:A:347:ILE:C	1:A:349:GLU:N	2.71	0.43
1:B:183:LEU:HG	1:C:190:PHE:HZ	1.80	0.43
1:B:193:ILE:C	1:B:195:ASN:N	2.72	0.43
1:B:292:TRP:CZ3	1:B:296:LYS:HE2	2.54	0.43
2:G:150:VAL:CG1	2:G:151:TYR:H	2.31	0.43
2:K:188:ALA:HB2	2:K:244:ASP:HB3	2.01	0.43
1:M:143:MET:HE2	1:P:197:LEU:CB	2.45	0.43
1:N:180:PRO:HA	1:N:183:LEU:CD2	2.49	0.43
1:O:155:GLY:O	1:O:156:GLU:HB2	2.17	0.43
1:P:179:LEU:N	1:P:180:PRO:CD	2.81	0.43
1:A:344:GLY:O	1:A:348:TYR:HD2	2.02	0.43
1:B:198:GLY:CA	1:B:200:MET:N	2.82	0.43
2:E:150:VAL:CG1	2:E:151:TYR:H	2.29	0.43
2:G:168:TYR:CE2	2:G:194:LEU:HD23	2.54	0.43
2:G:172:LEU:HD21	2:G:193:ARG:HD3	1.99	0.43
1:N:190:PHE:CZ	1:O:183:LEU:CG	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:254:ARG:HG3	1:O:255:LEU:H	1.83	0.43
1:O:260:ILE:HD13	2:U:42:ARG:HG2	2.01	0.43
1:P:276:PHE:HA	1:P:292:TRP:CE2	2.53	0.43
1:P:280:ASP:HB2	1:P:348:TYR:OH	2.19	0.43
2:S:281:LEU:HB2	2:S:295:LYS:HE2	2.00	0.43
2:U:204:ILE:HG12	3:V:31:TYR:HD2	1.83	0.43
1:C:29:VAL:HG23	1:C:243:ILE:HG12	2.00	0.43
1:A:29:VAL:O	1:A:29:VAL:HG13	2.19	0.42
1:B:236:THR:HG22	1:B:264:MET:HE3	2.00	0.42
2:E:179:VAL:HB	2:E:182:ILE:CD1	2.49	0.42
2:I:16:THR:HG21	1:C:308:ASP:CG	2.39	0.42
2:I:179:VAL:HB	2:I:182:ILE:HD13	2.01	0.42
1:M:276:PHE:HA	1:M:292:TRP:CE2	2.54	0.42
1:M:283:HIS:O	1:M:284:ASN:HB2	2.19	0.42
1:P:10:HIS:HD2	1:P:335:ASN:ND2	2.17	0.42
1:P:174:LEU:CD1	1:P:177:LEU:HD11	2.45	0.42
2:Q:188:ALA:HB2	2:Q:244:ASP:HB3	2.00	0.42
1:B:54:ILE:HD12	1:B:86:MET:HB3	2.00	0.42
1:B:200:MET:SD	1:C:150:LYS:HE2	2.59	0.42
1:B:215:LYS:HA	1:B:218:GLU:HG2	2.00	0.42
1:B:275:LEU:HB2	1:B:292:TRP:CD1	2.53	0.42
1:D:168:ALA:HB1	1:D:169:PRO:HD2	1.99	0.42
1:D:344:GLY:O	1:D:348:TYR:HD2	2.01	0.42
1:O:10:HIS:HD2	1:O:335:ASN:ND2	2.17	0.42
1:P:16:THR:CG2	1:P:46:GLN:NE2	2.75	0.42
2:Q:227:GLU:HG3	2:Q:227:GLU:O	2.18	0.42
2:S:116:ILE:HD13	2:S:144:LEU:HG	2.01	0.42
2:W:179:VAL:HB	2:W:182:ILE:HD13	2.01	0.42
1:C:168:ALA:HB1	1:C:169:PRO:HD2	1.99	0.42
1:C:198:GLY:HA2	1:C:200:MET:H	1.82	0.42
1:A:73:ASP:HA	1:A:152:GLN:CD	2.40	0.42
1:A:174:LEU:HB3	1:A:177:LEU:HG	2.01	0.42
1:A:244:SER:OG	1:A:299:LEU:HG	2.19	0.42
1:B:179:LEU:HG	1:B:183:LEU:HD13	2.01	0.42
1:D:52:LEU:HD22	1:D:53:LEU:N	2.34	0.42
1:D:247:LEU:C	1:C:247:LEU:HD13	2.40	0.42
2:K:281:LEU:HB2	2:K:295:LYS:HE2	2.01	0.42
1:N:190:PHE:CE2	1:O:183:LEU:CB	2.95	0.42
1:O:274:LEU:HD22	1:O:299:LEU:HD11	2.00	0.42
2:S:102:ILE:HD11	2:S:119:MET:SD	2.60	0.42
2:S:231:LYS:HE2	3:T:18:THR:OG1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:232:ASN:HB2	3:T:21:THR:HB	2.01	0.42
2:U:116:ILE:HD13	2:U:144:LEU:HG	2.00	0.42
2:W:102:ILE:HD11	2:W:119:MET:SD	2.59	0.42
1:C:180:PRO:HB2	1:C:225:THR:CG2	2.49	0.42
1:B:178:GLN:HE22	1:B:261:SER:HB2	1.83	0.42
1:B:274:LEU:HD22	1:B:299:LEU:HD11	2.00	0.42
1:D:194:THR:C	1:D:195:ASN:HD22	2.22	0.42
2:E:188:ALA:HB2	2:E:244:ASP:HB3	2.01	0.42
2:I:194:LEU:HD22	2:I:210:SER:HB2	2.01	0.42
2:I:275:GLN:NE2	2:I:275:GLN:HA	2.34	0.42
1:M:147:LYS:HZ2	1:P:197:LEU:HD13	1.78	0.42
1:N:24:GLY:HA2	1:N:167:THR:OG1	2.19	0.42
2:Q:105:LEU:CB	2:Q:143:LYS:HE2	2.50	0.42
2:S:23:LYS:HD3	2:S:31:GLU:HB3	2.01	0.42
3:V:52:TYR:O	3:V:53:LYS:HG3	2.20	0.42
2:W:98:LEU:O	2:W:102:ILE:HG13	2.19	0.42
1:A:138:GLU:H	1:A:138:GLU:CD	2.22	0.42
1:D:179:LEU:N	1:D:180:PRO:CD	2.81	0.42
2:E:91:ASP:O	2:E:95:VAL:HG23	2.19	0.42
2:I:216:GLU:O	2:I:220:GLU:HG3	2.20	0.42
2:I:283:PHE:CZ	3:J:42:GLY:HA2	2.54	0.42
1:M:179:LEU:N	1:M:180:PRO:CD	2.82	0.42
1:M:244:SER:OG	1:M:299:LEU:HG	2.18	0.42
1:M:279:ASN:OD1	1:M:341:ILE:HD11	2.19	0.42
1:P:154:GLN:OE1	1:C:79:GLY:HA3	2.19	0.42
1:C:172:HIS:HB3	1:C:258:GLU:OE2	2.19	0.42
1:A:201:LEU:HG	1:A:205:MET:CE	2.50	0.42
1:A:253:GLU:OE1	2:E:45:ARG:NH2	2.52	0.42
1:A:284:ASN:N	1:A:284:ASN:ND2	2.67	0.42
1:B:20:TRP:CB	1:B:236:THR:HG23	2.50	0.42
1:B:200:MET:CE	1:C:150:LYS:HE2	2.49	0.42
2:I:227:GLU:HG3	2:I:227:GLU:O	2.19	0.42
2:I:278:LYS:HG3	2:I:295:LYS:HG2	2.01	0.42
3:J:39:THR:HG23	3:J:40:ASN:OD1	2.20	0.42
2:K:193:ARG:HA	3:L:45:LEU:HD13	2.01	0.42
2:K:254:THR:HG22	2:K:289:PHE:HZ	1.85	0.42
1:N:198:GLY:CA	1:N:200:MET:N	2.81	0.42
1:O:22:PHE:CE1	1:O:174:LEU:HD21	2.54	0.42
1:O:227:ARG:HB3	1:O:227:ARG:CZ	2.50	0.42
1:O:281:GLN:HA	1:O:281:GLN:NE2	2.34	0.42
1:P:54:ILE:HD11	1:P:88:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:115:VAL:HG12	2:Q:119:MET:CE	2.49	0.42
2:S:133:ASP:HA	2:S:134:PRO:HD3	1.90	0.42
2:S:172:LEU:HD21	2:S:193:ARG:HD3	2.01	0.42
2:S:221:LYS:HD3	2:S:222:PHE:CE2	2.55	0.42
2:U:98:LEU:O	2:U:102:ILE:HG13	2.19	0.42
2:W:133:ASP:HA	2:W:134:PRO:HD3	1.90	0.42
1:C:174:LEU:HD22	1:C:177:LEU:HD21	2.02	0.42
1:C:242:CYS:HB2	1:C:248:SER:OG	2.20	0.42
1:A:23:VAL:HA	1:A:239:VAL:O	2.18	0.42
1:A:183:LEU:HG	1:D:190:PHE:CZ	2.54	0.42
2:G:225:LYS:HB2	2:G:240:GLU:HB2	2.00	0.42
2:I:9:MET:CE	1:C:263:ASP:O	2.68	0.42
2:I:116:ILE:HD13	2:I:144:LEU:HG	2.02	0.42
1:N:215:LYS:HB2	1:N:215:LYS:NZ	2.35	0.42
1:P:274:LEU:HD22	1:P:299:LEU:HD11	2.01	0.42
1:P:346:VAL:O	1:P:349:GLU:HB3	2.20	0.42
2:Q:150:VAL:CG1	2:Q:151:TYR:H	2.29	0.42
2:U:9:MET:HG2	2:U:10:GLY:H	1.85	0.42
2:U:172:LEU:HD21	2:U:193:ARG:HD3	2.02	0.42
2:U:179:VAL:HG22	3:V:50:TYR:CG	2.54	0.42
2:U:183:GLU:HG2	2:U:184:ASP:N	2.35	0.42
2:W:194:LEU:HD22	2:W:210:SER:HB2	2.00	0.42
1:B:24:GLY:HA2	1:B:167:THR:OG1	2.19	0.42
1:D:231:THR:O	1:D:232:ASP:O	2.38	0.42
1:D:312:VAL:HG21	1:D:334:LEU:HD23	2.02	0.42
2:E:227:GLU:HG3	2:E:227:GLU:O	2.18	0.42
2:G:179:VAL:HB	2:G:182:ILE:CD1	2.50	0.42
1:M:62:LEU:HB2	1:M:87:GLU:OE1	2.19	0.42
1:M:73:ASP:HA	1:M:152:GLN:CD	2.40	0.42
1:N:147:LYS:HA	1:N:150:LYS:HE3	2.01	0.42
1:P:178:GLN:NE2	1:P:261:SER:HB2	2.35	0.42
2:S:183:GLU:CG	2:S:184:ASP:N	2.82	0.42
2:U:256:GLN:HE22	3:V:29:LYS:CG	2.32	0.42
1:B:16:THR:HB	1:B:49:LYS:HE2	2.01	0.42
1:B:194:THR:CG2	1:C:183:LEU:HD11	2.47	0.42
2:G:231:LYS:HB2	3:H:17:LEU:HG	2.02	0.42
2:I:236:ILE:HD11	2:I:253:ILE:HD12	2.02	0.42
1:M:179:LEU:HG	1:M:183:LEU:HD13	2.02	0.42
1:M:180:PRO:HA	1:M:183:LEU:CD2	2.49	0.42
1:M:199:PRO:CD	1:C:156:GLU:CB	2.81	0.42
1:M:199:PRO:CG	1:C:156:GLU:CB	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:196:LYS:HE2	1:N:202:ASN:ND2	2.35	0.42
1:O:57:ASP:OD1	1:O:58:PRO:HD2	2.20	0.42
1:P:22:PHE:CE1	1:P:174:LEU:HD21	2.55	0.42
1:P:196:LYS:NZ	1:P:202:ASN:CG	2.73	0.42
2:U:133:ASP:HA	2:U:134:PRO:HD3	1.90	0.42
2:W:283:PHE:CZ	3:X:42:GLY:HA2	2.55	0.42
3:X:35:LEU:HD12	3:X:35:LEU:HA	1.92	0.42
1:C:231:THR:O	1:C:232:ASP:O	2.38	0.42
1:A:57:ASP:OD1	1:A:58:PRO:HD2	2.19	0.42
1:A:190:PHE:CZ	1:D:183:LEU:HG	2.55	0.42
1:D:263:ASP:O	2:K:9:MET:CE	2.67	0.42
2:E:232:ASN:HB2	3:F:21:THR:OG1	2.20	0.42
2:I:219:ILE:HA	2:I:224:PRO:HD2	2.02	0.42
2:K:133:ASP:HA	2:K:134:PRO:HD3	1.90	0.42
1:N:275:LEU:HB2	1:N:292:TRP:CD1	2.55	0.42
1:O:20:TRP:HE3	1:O:165:PHE:CE2	2.38	0.42
1:O:196:LYS:HG2	1:O:196:LYS:HZ3	1.67	0.42
2:U:234:TYR:HB2	3:V:21:THR:HG21	2.02	0.42
2:W:236:ILE:HD11	2:W:253:ILE:HD12	2.02	0.42
1:A:20:TRP:HE3	1:A:165:PHE:CE2	2.38	0.41
1:B:21:ILE:HB	1:B:164:ILE:HD13	2.02	0.41
1:B:146:MET:HE2	1:B:149:ILE:HG13	2.02	0.41
1:B:178:GLN:CA	1:B:229:GLN:HE22	2.32	0.41
1:D:198:GLY:CA	1:D:200:MET:N	2.81	0.41
1:O:259:LEU:CD1	1:O:266:VAL:HG11	2.49	0.41
1:O:275:LEU:HB2	1:O:292:TRP:CD1	2.55	0.41
3:R:35:LEU:HD12	3:R:35:LEU:HA	1.93	0.41
2:W:112:LEU:CD1	2:W:143:LYS:HD2	2.49	0.41
1:C:201:LEU:HG	1:C:205:MET:CE	2.51	0.41
1:B:56:THR:HB	1:B:90:PRO:CG	2.48	0.41
1:B:178:GLN:HA	1:B:229:GLN:NE2	2.32	0.41
1:B:180:PRO:HA	1:B:183:LEU:CD2	2.51	0.41
1:B:196:LYS:HG3	1:C:143:MET:HG3	2.01	0.41
1:D:198:GLY:C	1:D:200:MET:H	2.24	0.41
2:G:217:ARG:HE	1:M:154:GLN:NE2	2.17	0.41
2:I:183:GLU:CG	2:I:184:ASP:N	2.82	0.41
1:M:57:ASP:OD1	1:M:58:PRO:HD2	2.20	0.41
1:O:54:ILE:HD12	1:O:86:MET:HB3	2.02	0.41
1:O:193:ILE:C	1:O:195:ASN:N	2.73	0.41
1:O:233:PRO:HB3	2:U:9:MET:N	2.35	0.41
1:O:305:LEU:HD22	2:U:42:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:133:ASP:HA	2:Q:134:PRO:HD3	1.90	0.41
2:S:190:PHE:CE1	3:T:48:LEU:HD13	2.55	0.41
1:C:16:THR:HB	1:C:49:LYS:CE	2.50	0.41
1:A:281:GLN:HA	1:A:281:GLN:NE2	2.36	0.41
1:D:16:THR:HB	1:D:49:LYS:HE3	2.01	0.41
2:I:35:THR:CG2	1:C:307:GLU:CD	2.89	0.41
1:M:147:LYS:HA	1:M:150:LYS:HE3	2.02	0.41
1:M:191:GLY:O	1:M:194:THR:OG1	2.36	0.41
1:M:198:GLY:C	1:M:200:MET:H	2.23	0.41
1:M:312:VAL:HG21	1:M:334:LEU:HD23	2.00	0.41
1:N:198:GLY:C	1:N:200:MET:H	2.24	0.41
1:N:280:ASP:HB2	1:N:348:TYR:OH	2.20	0.41
1:O:77:VAL:HG22	1:O:80:MET:HB2	2.03	0.41
2:Q:61:LEU:HD22	2:Q:100:ARG:HH21	1.85	0.41
2:U:52:ALA:O	2:U:56:ILE:HG13	2.20	0.41
2:U:232:ASN:HB2	3:V:21:THR:CB	2.51	0.41
2:W:225:LYS:HB2	2:W:240:GLU:HB2	2.01	0.41
1:A:174:LEU:HD22	1:A:177:LEU:HD21	2.01	0.41
1:B:29:VAL:HG21	1:B:242:CYS:CA	2.44	0.41
2:E:183:GLU:CG	2:E:184:ASP:N	2.83	0.41
3:H:45:LEU:HB3	3:H:46:PRO:HD2	2.01	0.41
2:I:98:LEU:O	2:I:102:ILE:HG13	2.20	0.41
2:I:168:TYR:CE2	2:I:194:LEU:HD23	2.55	0.41
2:I:179:VAL:HB	2:I:182:ILE:CD1	2.50	0.41
1:M:187:LEU:CG	1:P:190:PHE:CZ	2.99	0.41
1:N:20:TRP:CB	1:N:236:THR:HG23	2.51	0.41
1:P:21:ILE:HB	1:P:164:ILE:HD13	2.02	0.41
1:P:73:ASP:HA	1:P:152:GLN:NE2	2.35	0.41
1:P:146:MET:HE2	1:P:149:ILE:HG13	2.03	0.41
1:P:198:GLY:C	1:P:200:MET:H	2.24	0.41
2:Q:150:VAL:CG1	2:Q:151:TYR:N	2.78	0.41
2:Q:191:PHE:CZ	2:Q:211:LYS:HG3	2.54	0.41
3:T:45:LEU:HB3	3:T:46:PRO:HD2	2.02	0.41
2:U:107:PRO:HB3	2:U:146:GLU:HB3	2.02	0.41
1:C:20:TRP:HE3	1:C:165:PHE:HE2	1.68	0.41
1:A:180:PRO:HB2	1:A:225:THR:CG2	2.50	0.41
1:A:236:THR:HG22	1:A:264:MET:HE3	2.02	0.41
1:B:57:ASP:OD1	1:B:58:PRO:HD2	2.20	0.41
1:B:62:LEU:HB2	1:B:87:GLU:OE1	2.21	0.41
1:B:146:MET:HG3	1:C:201:LEU:HD21	2.03	0.41
1:B:263:ASP:HB3	2:G:9:MET:CE	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:ILE:O	1:D:260:ILE:HG13	2.21	0.41
2:E:283:PHE:CE1	3:F:42:GLY:HA2	2.55	0.41
3:F:35:LEU:HD12	3:F:35:LEU:HA	1.91	0.41
1:M:20:TRP:HE3	1:M:165:PHE:CE2	2.39	0.41
1:M:231:THR:O	1:M:232:ASP:O	2.37	0.41
1:M:291:ARG:HD2	1:N:291:ARG:HD2	2.02	0.41
1:P:20:TRP:HE3	1:P:165:PHE:CE2	2.38	0.41
2:W:116:ILE:HD13	2:W:144:LEU:HG	2.02	0.41
2:W:172:LEU:HD21	2:W:193:ARG:HD3	2.02	0.41
1:C:273:GLN:C	1:C:316:LEU:HB2	2.40	0.41
1:A:16:THR:CG2	1:A:46:GLN:NE2	2.78	0.41
1:A:305:LEU:CD2	2:E:42:ARG:NH2	2.79	0.41
1:A:314:MET:CE	1:A:333:PHE:HB2	2.51	0.41
1:B:196:LYS:HG3	1:C:143:MET:CG	2.51	0.41
1:B:230:PHE:O	1:B:232:ASP:N	2.53	0.41
1:B:275:LEU:HD11	1:B:291:ARG:HD3	2.01	0.41
1:B:281:GLN:HA	1:B:281:GLN:NE2	2.36	0.41
2:E:175:TRP:CG	3:F:52:TYR:HD1	2.38	0.41
1:P:57:ASP:OD1	1:P:58:PRO:HD2	2.19	0.41
2:Q:17:LEU:CD1	2:Q:58:GLN:HG2	2.48	0.41
2:Q:91:ASP:O	2:Q:95:VAL:HG23	2.20	0.41
2:S:253:ILE:O	2:S:256:GLN:HB2	2.21	0.41
3:V:35:LEU:HD12	3:V:35:LEU:HA	1.92	0.41
2:W:154:GLU:HG3	2:W:168:TYR:CE1	2.55	0.41
2:W:275:GLN:NE2	2:W:275:GLN:HA	2.36	0.41
2:W:278:LYS:CG	2:W:295:LYS:HG2	2.51	0.41
1:C:29:VAL:HG21	1:C:242:CYS:CA	2.47	0.41
1:C:198:GLY:CA	1:C:200:MET:N	2.84	0.41
1:A:135:GLY:HA3	1:A:179:LEU:CD2	2.38	0.41
2:E:107:PRO:HB3	2:E:146:GLU:HB3	2.03	0.41
2:E:193:ARG:HA	3:F:45:LEU:HD13	2.02	0.41
2:G:9:MET:HG2	2:G:10:GLY:H	1.85	0.41
2:G:275:GLN:NE2	2:G:275:GLN:HA	2.35	0.41
2:K:202:SER:HB2	3:L:33:LYS:CB	2.50	0.41
1:M:178:GLN:HA	1:M:229:GLN:NE2	2.34	0.41
1:M:254:ARG:HG3	1:M:255:LEU:H	1.84	0.41
1:O:224:GLU:O	1:O:228:GLN:HG3	2.20	0.41
1:O:247:LEU:HB3	1:P:247:LEU:HB3	2.01	0.41
2:Q:105:LEU:HB2	2:Q:143:LYS:HE2	2.03	0.41
2:Q:193:ARG:HA	3:R:45:LEU:HD13	2.03	0.41
2:S:175:TRP:CH2	3:T:48:LEU:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:253:ILE:O	2:U:256:GLN:HB2	2.21	0.41
1:C:198:GLY:C	1:C:200:MET:H	2.24	0.41
1:A:21:ILE:HB	1:A:164:ILE:HD13	2.03	0.41
1:A:193:ILE:C	1:A:195:ASN:N	2.74	0.41
1:A:198:GLY:C	1:A:200:MET:H	2.24	0.41
1:B:286:LYS:H	1:B:286:LYS:HD3	1.84	0.41
1:D:20:TRP:HE3	1:D:165:PHE:CE2	2.39	0.41
2:K:238:PHE:HA	2:K:246:ASN:OD1	2.21	0.41
1:M:20:TRP:CB	1:M:236:THR:HG23	2.48	0.41
1:M:32:THR:HG22	1:M:61:ASN:HD22	1.86	0.41
1:N:20:TRP:CE3	1:N:165:PHE:CE2	3.09	0.41
1:N:196:LYS:HZ3	1:N:202:ASN:CG	2.24	0.41
1:O:288:CYS:SG	1:P:287:ARG:HB3	2.61	0.41
1:P:244:SER:OG	1:P:299:LEU:HG	2.21	0.41
1:C:281:GLN:NE2	1:C:281:GLN:HA	2.35	0.41
1:A:153:GLU:HB3	1:A:158:GLU:O	2.21	0.41
1:A:180:PRO:HB2	1:A:225:THR:HG23	2.03	0.41
1:A:198:GLY:CA	1:A:200:MET:N	2.83	0.41
1:A:272:ASN:O	1:A:273:GLN:HB2	2.21	0.41
1:B:22:PHE:CE1	1:B:174:LEU:HD21	2.55	0.41
1:B:40:ILE:HG21	1:B:328:THR:HG22	2.03	0.41
1:D:135:GLY:HA3	1:D:179:LEU:CD2	2.40	0.41
1:D:267:ASN:CB	2:K:12:LYS:HZ1	2.31	0.41
2:G:102:ILE:HD11	2:G:119:MET:SD	2.61	0.41
2:G:281:LEU:HB2	2:G:295:LYS:HE2	2.02	0.41
2:I:40:ALA:O	2:I:44:VAL:HG23	2.21	0.41
2:I:154:GLU:HG3	2:I:168:TYR:CE1	2.55	0.41
2:K:203:ASN:OD1	3:L:32:THR:HG22	2.20	0.41
1:M:205:MET:HG3	1:P:228:GLN:NE2	2.36	0.41
1:M:307:GLU:CD	2:Q:35:THR:HG22	2.41	0.41
1:N:230:PHE:CA	2:S:9:MET:CE	2.91	0.41
1:O:10:HIS:HD2	1:O:335:ASN:HD21	1.69	0.41
1:O:191:GLY:O	1:O:194:THR:OG1	2.31	0.41
1:P:20:TRP:CB	1:P:236:THR:HG23	2.48	0.41
1:P:56:THR:HB	1:P:90:PRO:CG	2.49	0.41
1:P:177:LEU:N	1:P:177:LEU:HD23	2.35	0.41
2:Q:225:LYS:HB2	2:Q:240:GLU:HB2	2.02	0.41
2:S:115:VAL:HG12	2:S:119:MET:CE	2.50	0.41
2:W:150:VAL:CG1	2:W:151:TYR:H	2.29	0.41
2:W:205:SER:HB3	3:X:32:THR:CG2	2.51	0.41
1:C:16:THR:CG2	1:C:46:GLN:NE2	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:LEU:N	1:C:180:PRO:CD	2.83	0.41
1:C:314:MET:CE	1:C:333:PHE:HB2	2.51	0.41
1:A:196:LYS:HZ3	1:A:202:ASN:CG	2.21	0.41
2:K:253:ILE:O	2:K:256:GLN:HB2	2.21	0.41
1:M:275:LEU:HD11	1:M:291:ARG:HD3	2.02	0.41
1:M:284:ASN:O	1:M:285:CYS:HB3	2.21	0.41
1:N:54:ILE:HG13	1:N:86:MET:O	2.21	0.41
1:N:73:ASP:HA	1:N:152:GLN:CD	2.41	0.41
1:N:174:LEU:HD13	1:N:177:LEU:CD1	2.51	0.41
1:N:197:LEU:HB2	1:O:143:MET:HE2	2.03	0.41
1:O:287:ARG:H	1:O:287:ARG:HG2	1.72	0.41
1:O:314:MET:CE	1:O:333:PHE:HB2	2.51	0.41
1:P:174:LEU:HB3	1:P:177:LEU:HD11	2.02	0.41
2:S:40:ALA:O	2:S:44:VAL:HG23	2.20	0.41
2:W:231:LYS:HB2	3:X:17:LEU:HG	2.02	0.41
1:C:57:ASP:OD1	1:C:58:PRO:HD2	2.21	0.41
1:A:10:HIS:HD2	1:A:335:ASN:HD21	1.69	0.40
1:A:153:GLU:O	1:A:158:GLU:HA	2.21	0.40
1:B:180:PRO:HB2	1:B:225:THR:CG2	2.51	0.40
2:E:109:GLU:HA	2:E:110:PRO:HD3	1.94	0.40
2:I:189:GLU:HB3	3:J:48:LEU:HD22	2.03	0.40
3:J:45:LEU:HB3	3:J:46:PRO:HD2	2.02	0.40
3:L:45:LEU:HB3	3:L:46:PRO:HD2	2.03	0.40
1:O:73:ASP:HA	1:O:152:GLN:CD	2.41	0.40
1:P:168:ALA:HB1	1:P:169:PRO:HD2	2.02	0.40
2:S:198:TYR:HD1	2:S:201:ILE:HD11	1.86	0.40
2:S:240:GLU:HG2	3:T:6:SER:OG	2.21	0.40
1:C:54:ILE:HD12	1:C:86:MET:HB3	2.03	0.40
1:A:24:GLY:HA2	1:A:167:THR:OG1	2.21	0.40
1:A:231:THR:O	1:A:232:ASP:O	2.39	0.40
1:A:273:GLN:C	1:A:316:LEU:HB2	2.42	0.40
1:B:179:LEU:N	1:B:180:PRO:CD	2.82	0.40
1:B:181:ASN:ND2	1:B:226:ILE:HG12	2.36	0.40
1:M:6:GLU:O	1:M:8:ASN:N	2.49	0.40
1:M:10:HIS:HD2	1:M:335:ASN:ND2	2.20	0.40
1:M:187:LEU:HD21	1:P:190:PHE:CG	2.56	0.40
1:N:155:GLY:O	1:N:156:GLU:HB2	2.22	0.40
1:P:5:VAL:HG11	1:P:309:PHE:O	2.22	0.40
1:P:10:HIS:HD2	1:P:335:ASN:HD21	1.70	0.40
1:P:180:PRO:HB2	1:P:225:THR:CG2	2.51	0.40
2:S:98:LEU:O	2:S:102:ILE:HG13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:183:GLU:HG2	2:W:184:ASP:N	2.37	0.40
1:C:180:PRO:HB2	1:C:225:THR:HG23	2.03	0.40
1:A:146:MET:HE2	1:A:149:ILE:HG13	2.03	0.40
1:D:260:ILE:CG2	2:K:46:SER:OG	2.70	0.40
2:E:98:LEU:O	2:E:102:ILE:HG13	2.22	0.40
2:E:293:ALA:HA	2:E:294:PRO:HD3	1.98	0.40
2:G:91:ASP:O	2:G:95:VAL:HG23	2.21	0.40
2:G:217:ARG:HE	1:M:154:GLN:HE22	1.63	0.40
1:N:178:GLN:CA	1:N:229:GLN:HE22	2.32	0.40
1:N:196:LYS:HG3	1:O:143:MET:CG	2.51	0.40
1:N:287:ARG:H	1:N:287:ARG:HG2	1.72	0.40
1:O:198:GLY:C	1:O:200:MET:H	2.24	0.40
2:Q:189:GLU:HB3	3:R:48:LEU:HD22	2.03	0.40
2:S:87:GLU:HA	2:S:126:PHE:CZ	2.56	0.40
2:S:225:LYS:HB2	2:S:240:GLU:HB2	2.02	0.40
2:U:179:VAL:HB	2:U:182:ILE:HD13	2.03	0.40
2:U:227:GLU:CD	3:V:10:HIS:CD2	2.95	0.40
2:U:231:LYS:HB2	3:V:17:LEU:HG	2.03	0.40
1:C:21:ILE:HB	1:C:164:ILE:HD13	2.03	0.40
1:C:157:GLY:O	1:C:159:THR:N	2.54	0.40
1:B:198:GLY:C	1:B:200:MET:H	2.24	0.40
1:B:226:ILE:O	1:B:226:ILE:HG22	2.20	0.40
2:E:115:VAL:HG12	2:E:119:MET:HE1	2.04	0.40
2:E:154:GLU:HG3	2:E:168:TYR:CE1	2.56	0.40
2:G:61:LEU:HD22	2:G:100:ARG:HH21	1.85	0.40
1:M:16:THR:HB	1:M:49:LYS:CE	2.50	0.40
1:M:224:GLU:O	1:M:228:GLN:HG3	2.21	0.40
1:N:57:ASP:OD1	1:N:58:PRO:HD2	2.21	0.40
1:N:256:ILE:O	1:N:260:ILE:HG13	2.21	0.40
1:P:198:GLY:CA	1:P:200:MET:N	2.83	0.40
1:P:259:LEU:CD1	1:P:266:VAL:HG11	2.51	0.40
2:Q:194:LEU:HD22	2:Q:210:SER:HB2	2.02	0.40
3:R:45:LEU:HB3	3:R:46:PRO:HD2	2.02	0.40
3:T:39:THR:HG23	3:T:40:ASN:OD1	2.21	0.40
1:C:20:TRP:HE3	1:C:165:PHE:CE2	2.40	0.40
1:A:54:ILE:HD11	1:A:88:ILE:CD1	2.52	0.40
1:A:224:GLU:O	1:A:228:GLN:HG3	2.21	0.40
2:E:115:VAL:HG12	2:E:119:MET:CE	2.51	0.40
2:G:183:GLU:CG	2:G:184:ASP:N	2.84	0.40
3:H:35:LEU:HD12	3:H:35:LEU:HA	1.92	0.40
3:H:39:THR:HG23	3:H:40:ASN:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:189:GLU:HB3	3:J:48:LEU:CD2	2.51	0.40
1:M:180:PRO:HB2	1:M:225:THR:CG2	2.51	0.40
1:M:231:THR:O	1:M:231:THR:HG22	2.21	0.40
1:M:344:GLY:O	1:M:348:TYR:HD2	2.04	0.40
1:N:230:PHE:O	1:N:232:ASP:N	2.55	0.40
1:O:179:LEU:N	1:O:180:PRO:CD	2.81	0.40
1:P:174:LEU:HB3	1:P:177:LEU:CG	2.52	0.40
1:P:174:LEU:CA	1:P:177:LEU:HG	2.52	0.40
2:Q:17:LEU:HD23	2:Q:17:LEU:HA	1.96	0.40
2:Q:98:LEU:O	2:Q:102:ILE:HG13	2.22	0.40
2:Q:253:ILE:O	2:Q:256:GLN:HB2	2.22	0.40
2:S:107:PRO:HB3	2:S:146:GLU:HB3	2.03	0.40
2:W:40:ALA:O	2:W:44:VAL:HG23	2.21	0.40
2:W:183:GLU:CG	2:W:184:ASP:N	2.85	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:GLU:OE1	1:N:220:LYS:NZ[1_655]	2.19	0.01

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	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	3	23
1	B	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	3	23
1	C	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	3	23
1	D	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	3	23
1	M	298/373 (80%)	257 (86%)	32 (11%)	9 (3%)	4	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	N	298/373 (80%)	257 (86%)	30 (10%)	11 (4%)	3 25
1	O	298/373 (80%)	260 (87%)	26 (9%)	12 (4%)	3 23
1	P	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	3 23
2	E	289/319 (91%)	269 (93%)	19 (7%)	1 (0%)	41 76
2	G	289/319 (91%)	270 (93%)	18 (6%)	1 (0%)	41 76
2	I	289/319 (91%)	269 (93%)	19 (7%)	1 (0%)	41 76
2	K	289/319 (91%)	269 (93%)	18 (6%)	2 (1%)	22 62
2	Q	289/319 (91%)	268 (93%)	20 (7%)	1 (0%)	41 76
2	S	289/319 (91%)	271 (94%)	17 (6%)	1 (0%)	41 76
2	U	289/319 (91%)	271 (94%)	16 (6%)	2 (1%)	22 62
2	W	289/319 (91%)	268 (93%)	19 (7%)	2 (1%)	22 62
3	F	52/56 (93%)	46 (88%)	6 (12%)	0	100 100
3	H	52/56 (93%)	46 (88%)	6 (12%)	0	100 100
3	J	52/56 (93%)	46 (88%)	6 (12%)	0	100 100
3	L	52/56 (93%)	46 (88%)	6 (12%)	0	100 100
3	R	52/56 (93%)	46 (88%)	6 (12%)	0	100 100
3	T	52/56 (93%)	46 (88%)	6 (12%)	0	100 100
3	V	52/56 (93%)	46 (88%)	6 (12%)	0	100 100
3	X	52/56 (93%)	46 (88%)	6 (12%)	0	100 100
All	All	5112/5984 (85%)	4582 (90%)	427 (8%)	103 (2%)	7 38

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	ASP
1	A	282	GLU
1	A	283	HIS
1	B	282	GLU
1	B	283	HIS
1	D	232	ASP
1	D	282	GLU
1	D	283	HIS
1	M	231	THR
1	M	232	ASP
1	M	282	GLU

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Mol	Chain	Res	Type
1	M	283	HIS
1	N	231	THR
1	N	232	ASP
1	N	282	GLU
1	N	283	HIS
1	O	231	THR
1	O	282	GLU
1	O	283	HIS
1	P	232	ASP
1	P	282	GLU
1	P	283	HIS
1	C	232	ASP
1	C	282	GLU
1	C	283	HIS
1	A	91	SER
1	A	231	THR
1	B	91	SER
1	B	231	THR
1	B	232	ASP
1	D	91	SER
1	D	231	THR
2	E	112	LEU
2	G	112	LEU
2	I	112	LEU
1	M	91	SER
1	N	91	SER
1	O	91	SER
1	O	232	ASP
1	P	91	SER
1	P	231	THR
2	S	112	LEU
2	W	112	LEU
1	C	91	SER
1	A	196	LYS
1	A	246	PHE
1	B	196	LYS
1	B	246	PHE
1	D	156	GLU
1	D	246	PHE
2	K	112	LEU
1	M	194	THR
1	N	156	GLU

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Mol	Chain	Res	Type
1	P	156	GLU
1	P	158	GLU
2	Q	112	LEU
2	U	112	LEU
1	C	156	GLU
1	C	158	GLU
1	C	231	THR
1	C	277	ALA
1	A	156	GLU
1	B	156	GLU
1	B	277	ALA
1	D	158	GLU
1	D	182	THR
1	D	277	ALA
1	M	156	GLU
1	M	246	PHE
1	N	158	GLU
1	N	277	ALA
1	O	156	GLU
1	O	182	THR
1	O	196	LYS
1	O	246	PHE
1	O	277	ALA
1	P	246	PHE
1	C	246	PHE
1	A	158	GLU
1	A	182	THR
1	B	194	THR
1	N	194	THR
1	N	246	PHE
1	P	182	THR
1	P	277	ALA
1	C	182	THR
1	C	196	LYS
1	A	277	ALA
1	B	182	THR
1	D	25	GLY
1	D	167	THR
1	N	25	GLY
1	O	25	GLY
1	O	194	THR
1	P	194	THR

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Mol	Chain	Res	Type
1	A	25	GLY
1	B	25	GLY
1	M	25	GLY
1	P	25	GLY
1	C	25	GLY
2	K	237	VAL
2	U	237	VAL
2	W	237	VAL

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	272/325 (84%)	252 (93%)	20 (7%)	13	38
1	B	272/325 (84%)	251 (92%)	21 (8%)	13	37
1	C	272/325 (84%)	251 (92%)	21 (8%)	13	37
1	D	272/325 (84%)	252 (93%)	20 (7%)	13	38
1	M	272/325 (84%)	252 (93%)	20 (7%)	13	38
1	N	272/325 (84%)	251 (92%)	21 (8%)	13	37
1	O	272/325 (84%)	252 (93%)	20 (7%)	13	38
1	P	272/325 (84%)	253 (93%)	19 (7%)	15	40
2	E	260/284 (92%)	253 (97%)	7 (3%)	44	66
2	G	260/284 (92%)	254 (98%)	6 (2%)	50	71
2	I	260/284 (92%)	254 (98%)	6 (2%)	50	71
2	K	260/284 (92%)	254 (98%)	6 (2%)	50	71
2	Q	260/284 (92%)	253 (97%)	7 (3%)	44	66
2	S	260/284 (92%)	254 (98%)	6 (2%)	50	71
2	U	260/284 (92%)	253 (97%)	7 (3%)	44	66
2	W	260/284 (92%)	254 (98%)	6 (2%)	50	71
3	F	50/52 (96%)	48 (96%)	2 (4%)	31	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	H	50/52 (96%)	47 (94%)	3 (6%)	19 44
3	J	50/52 (96%)	48 (96%)	2 (4%)	31 55
3	L	50/52 (96%)	47 (94%)	3 (6%)	19 44
3	R	50/52 (96%)	47 (94%)	3 (6%)	19 44
3	T	50/52 (96%)	47 (94%)	3 (6%)	19 44
3	V	50/52 (96%)	47 (94%)	3 (6%)	19 44
3	X	50/52 (96%)	47 (94%)	3 (6%)	19 44
All	All	4656/5288 (88%)	4421 (95%)	235 (5%)	24 49

All (235) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	162	THR
1	A	183	LEU
1	A	195	ASN
1	A	202	ASN
1	A	203	SER
1	A	215	LYS
1	A	232	ASP
1	A	244	SER
1	A	255	LEU
1	A	264	MET
1	A	266	VAL
1	A	281	GLN
1	A	284	ASN
1	A	287	ARG
1	A	288	CYS
1	A	305	LEU
1	A	320	GLU
1	A	324	LEU
1	A	351	GLU
1	B	162	THR
1	B	178	GLN
1	B	183	LEU
1	B	195	ASN
1	B	202	ASN
1	B	203	SER
1	B	215	LYS
1	B	232	ASP

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Mol	Chain	Res	Type
1	B	244	SER
1	B	255	LEU
1	B	264	MET
1	B	266	VAL
1	B	281	GLN
1	B	284	ASN
1	B	287	ARG
1	B	288	CYS
1	B	305	LEU
1	B	312	VAL
1	B	320	GLU
1	B	324	LEU
1	B	351	GLU
1	D	162	THR
1	D	177	LEU
1	D	178	GLN
1	D	183	LEU
1	D	194	THR
1	D	202	ASN
1	D	203	SER
1	D	215	LYS
1	D	232	ASP
1	D	244	SER
1	D	255	LEU
1	D	264	MET
1	D	266	VAL
1	D	281	GLN
1	D	287	ARG
1	D	288	CYS
1	D	305	LEU
1	D	320	GLU
1	D	324	LEU
1	D	351	GLU
2	E	16	THR
2	E	21	GLU
2	E	22	ASN
2	E	62	SER
2	E	143	LYS
2	E	244	ASP
2	E	297	THR
3	F	23	THR
3	F	54	GLN

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Mol	Chain	Res	Type
2	G	16	THR
2	G	21	GLU
2	G	22	ASN
2	G	143	LYS
2	G	244	ASP
2	G	297	THR
3	H	3	THR
3	H	23	THR
3	H	54	GLN
2	I	16	THR
2	I	21	GLU
2	I	22	ASN
2	I	143	LYS
2	I	244	ASP
2	I	297	THR
3	J	23	THR
3	J	54	GLN
2	K	16	THR
2	K	21	GLU
2	K	22	ASN
2	K	143	LYS
2	K	244	ASP
2	K	297	THR
3	L	3	THR
3	L	23	THR
3	L	54	GLN
1	M	32	THR
1	M	162	THR
1	M	178	GLN
1	M	183	LEU
1	M	202	ASN
1	M	215	LYS
1	M	232	ASP
1	M	244	SER
1	M	255	LEU
1	M	264	MET
1	M	266	VAL
1	M	281	GLN
1	M	284	ASN
1	M	287	ARG
1	M	288	CYS
1	M	305	LEU

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Mol	Chain	Res	Type
1	M	312	VAL
1	M	320	GLU
1	M	324	LEU
1	M	351	GLU
1	N	32	THR
1	N	162	THR
1	N	177	LEU
1	N	178	GLN
1	N	183	LEU
1	N	194	THR
1	N	202	ASN
1	N	203	SER
1	N	215	LYS
1	N	232	ASP
1	N	244	SER
1	N	255	LEU
1	N	264	MET
1	N	266	VAL
1	N	281	GLN
1	N	287	ARG
1	N	288	CYS
1	N	305	LEU
1	N	320	GLU
1	N	324	LEU
1	N	351	GLU
1	O	32	THR
1	O	162	THR
1	O	178	GLN
1	O	183	LEU
1	O	194	THR
1	O	195	ASN
1	O	202	ASN
1	O	215	LYS
1	O	232	ASP
1	O	244	SER
1	O	255	LEU
1	O	264	MET
1	O	266	VAL
1	O	281	GLN
1	O	287	ARG
1	O	288	CYS
1	O	305	LEU

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Mol	Chain	Res	Type
1	O	320	GLU
1	O	324	LEU
1	O	351	GLU
1	P	32	THR
1	P	162	THR
1	P	183	LEU
1	P	194	THR
1	P	195	ASN
1	P	202	ASN
1	P	215	LYS
1	P	232	ASP
1	P	244	SER
1	P	255	LEU
1	P	264	MET
1	P	266	VAL
1	P	281	GLN
1	P	284	ASN
1	P	288	CYS
1	P	305	LEU
1	P	320	GLU
1	P	324	LEU
1	P	351	GLU
2	Q	16	THR
2	Q	21	GLU
2	Q	22	ASN
2	Q	62	SER
2	Q	143	LYS
2	Q	244	ASP
2	Q	297	THR
3	R	3	THR
3	R	23	THR
3	R	54	GLN
2	S	16	THR
2	S	21	GLU
2	S	22	ASN
2	S	143	LYS
2	S	244	ASP
2	S	297	THR
3	T	3	THR
3	T	23	THR
3	T	54	GLN
2	U	16	THR

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Mol	Chain	Res	Type
2	U	21	GLU
2	U	22	ASN
2	U	62	SER
2	U	143	LYS
2	U	244	ASP
2	U	297	THR
3	V	3	THR
3	V	23	THR
3	V	54	GLN
2	W	16	THR
2	W	21	GLU
2	W	22	ASN
2	W	143	LYS
2	W	244	ASP
2	W	297	THR
3	X	3	THR
3	X	23	THR
3	X	54	GLN
1	C	162	THR
1	C	178	GLN
1	C	183	LEU
1	C	194	THR
1	C	195	ASN
1	C	202	ASN
1	C	203	SER
1	C	215	LYS
1	C	232	ASP
1	C	244	SER
1	C	255	LEU
1	C	264	MET
1	C	266	VAL
1	C	281	GLN
1	C	284	ASN
1	C	287	ARG
1	C	288	CYS
1	C	305	LEU
1	C	320	GLU
1	C	324	LEU
1	C	351	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (161) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	18	HIS
1	A	46	GLN
1	A	50	GLN
1	A	61	ASN
1	A	82	ASN
1	A	172	HIS
1	A	181	ASN
1	A	195	ASN
1	A	228	GLN
1	A	229	GLN
1	A	281	GLN
1	A	284	ASN
1	A	289	GLN
1	A	301	GLN
1	A	310	HIS
1	A	332	GLN
1	A	335	ASN
1	B	10	HIS
1	B	18	HIS
1	B	46	GLN
1	B	50	GLN
1	B	82	ASN
1	B	172	HIS
1	B	181	ASN
1	B	195	ASN
1	B	228	GLN
1	B	229	GLN
1	B	281	GLN
1	B	284	ASN
1	B	289	GLN
1	B	301	GLN
1	B	310	HIS
1	B	332	GLN
1	B	335	ASN
1	D	10	HIS
1	D	18	HIS
1	D	46	GLN
1	D	50	GLN
1	D	172	HIS
1	D	181	ASN
1	D	195	ASN
1	D	228	GLN

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Mol	Chain	Res	Type
1	D	229	GLN
1	D	281	GLN
1	D	284	ASN
1	D	289	GLN
1	D	301	GLN
1	D	310	HIS
1	D	332	GLN
1	D	335	ASN
2	E	275	GLN
2	E	298	ASN
2	G	256	GLN
2	G	275	GLN
2	G	298	ASN
3	H	54	GLN
2	I	275	GLN
2	I	298	ASN
2	K	275	GLN
2	K	298	ASN
1	M	10	HIS
1	M	18	HIS
1	M	46	GLN
1	M	50	GLN
1	M	61	ASN
1	M	82	ASN
1	M	154	GLN
1	M	172	HIS
1	M	181	ASN
1	M	195	ASN
1	M	228	GLN
1	M	229	GLN
1	M	281	GLN
1	M	284	ASN
1	M	289	GLN
1	M	301	GLN
1	M	310	HIS
1	M	332	GLN
1	M	335	ASN
1	N	10	HIS
1	N	18	HIS
1	N	46	GLN
1	N	50	GLN
1	N	61	ASN

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Mol	Chain	Res	Type
1	N	172	HIS
1	N	181	ASN
1	N	195	ASN
1	N	228	GLN
1	N	229	GLN
1	N	281	GLN
1	N	284	ASN
1	N	289	GLN
1	N	301	GLN
1	N	310	HIS
1	N	332	GLN
1	N	335	ASN
1	O	10	HIS
1	O	18	HIS
1	O	46	GLN
1	O	50	GLN
1	O	172	HIS
1	O	181	ASN
1	O	195	ASN
1	O	228	GLN
1	O	229	GLN
1	O	281	GLN
1	O	284	ASN
1	O	289	GLN
1	O	301	GLN
1	O	310	HIS
1	O	332	GLN
1	O	335	ASN
1	P	10	HIS
1	P	18	HIS
1	P	46	GLN
1	P	50	GLN
1	P	61	ASN
1	P	172	HIS
1	P	181	ASN
1	P	195	ASN
1	P	228	GLN
1	P	229	GLN
1	P	281	GLN
1	P	284	ASN
1	P	289	GLN
1	P	301	GLN

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Mol	Chain	Res	Type
1	P	310	HIS
1	P	332	GLN
1	P	335	ASN
2	Q	275	GLN
2	Q	298	ASN
3	R	54	GLN
2	S	256	GLN
2	S	275	GLN
2	S	298	ASN
3	T	54	GLN
2	U	275	GLN
2	U	298	ASN
3	V	54	GLN
2	W	275	GLN
2	W	298	ASN
3	X	54	GLN
1	C	10	HIS
1	C	18	HIS
1	C	46	GLN
1	C	50	GLN
1	C	61	ASN
1	C	82	ASN
1	C	172	HIS
1	C	181	ASN
1	C	195	ASN
1	C	228	GLN
1	C	229	GLN
1	C	281	GLN
1	C	284	ASN
1	C	289	GLN
1	C	301	GLN
1	C	310	HIS
1	C	332	GLN
1	C	335	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.