Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:05 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

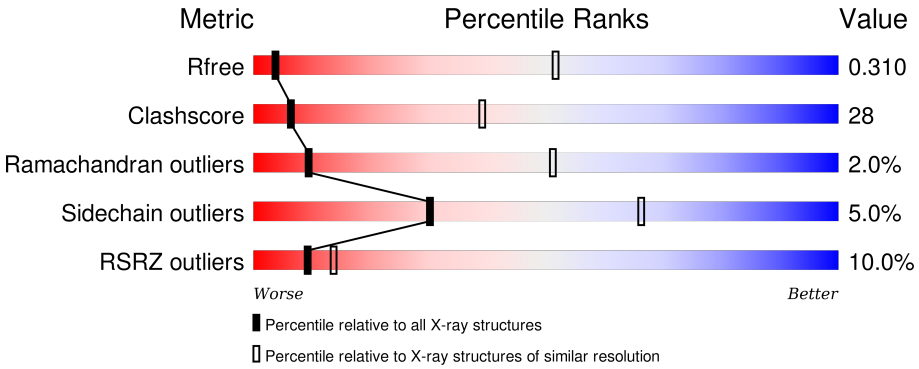
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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}	91344	1002 (8.30-3.66)
Clashscore	102246	1050 (8.30-3.70)
Ramachandran outliers	100387	1023 (8.30-3.66)
Sidechain outliers	100360	1012 (8.30-3.64)
RSRZ outliers	91569	1001 (8.30-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	373	9% 36% 40% 6% 18%
1	B	373	11% 39% 38% 5% 18%
1	C	373	11% 37% 39% 6% 18%
1	D	373	10% 39% 38% 5% 18%
1	M	373	8% 39% 36% 6% 18%

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Mol	Chain	Length	Quality of chain
1	N	373	8% 39% 36% 6% 18%
1	O	373	9% 37% 40% 5% 18%
1	P	373	7% 40% 36% 5% 18%
2	E	319	8% 61% 29% 9%
2	G	319	6% 61% 29% 9%
2	I	319	5% 62% 28% 9%
2	K	319	9% 62% 28% 9%
2	Q	319	8% 64% 26% 9%
2	S	319	8% 60% 30% 9%
2	U	319	6% 61% 29% 9%
2	W	319	8% 62% 28% 9%
3	F	56	16% 64% 32%
3	H	56	9% 63% 34%
3	J	56	9% 59% 38%
3	L	56	21% 63% 34%
3	R	56	13% 61% 36%
3	T	56	13% 63% 32%
3	V	56	14% 54% 43%
3	X	56	14% 61% 36%

2 Entry composition

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

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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			

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

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

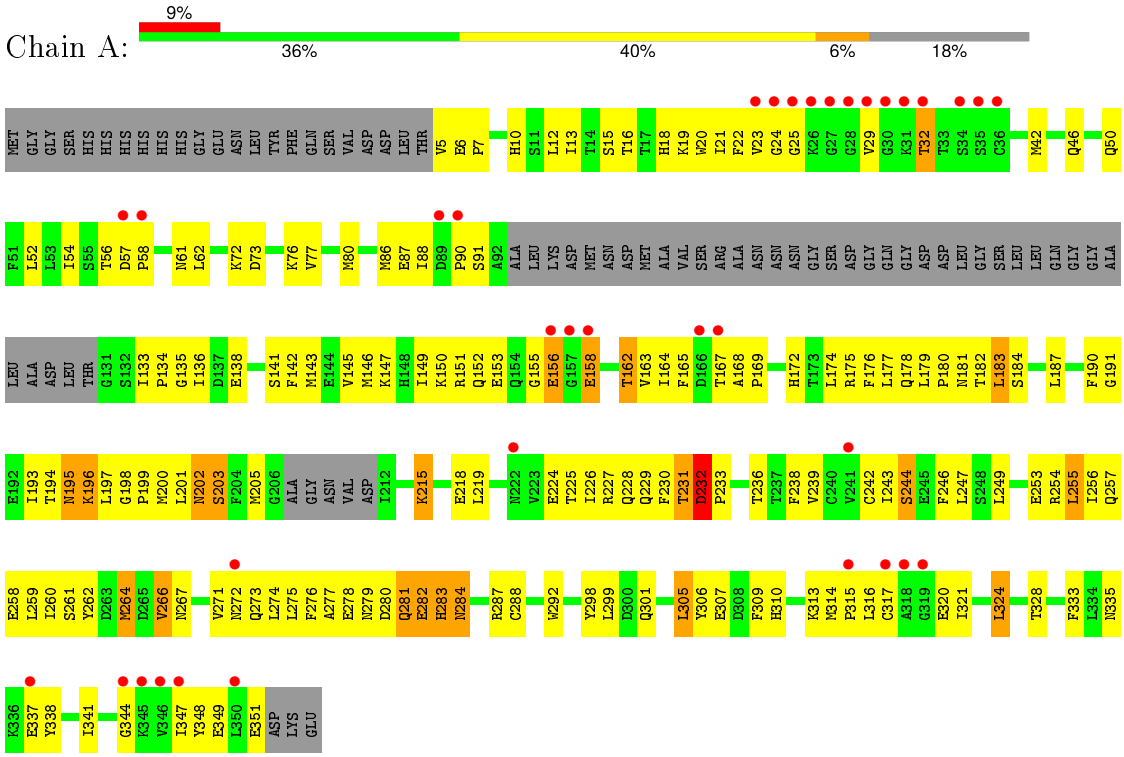
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	M	1	Total	Zn	0	0
			1	1		

3 Residue-property plots (i)

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

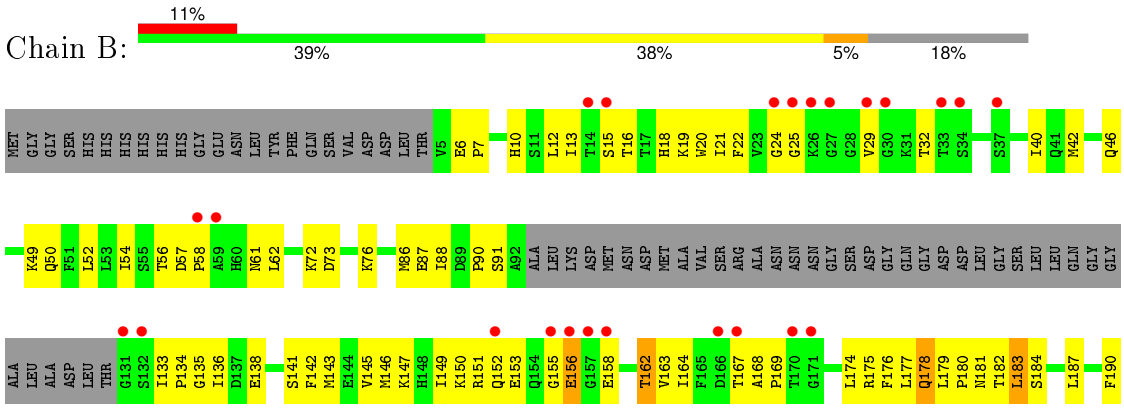
- Molecule 1: ATPase GET3

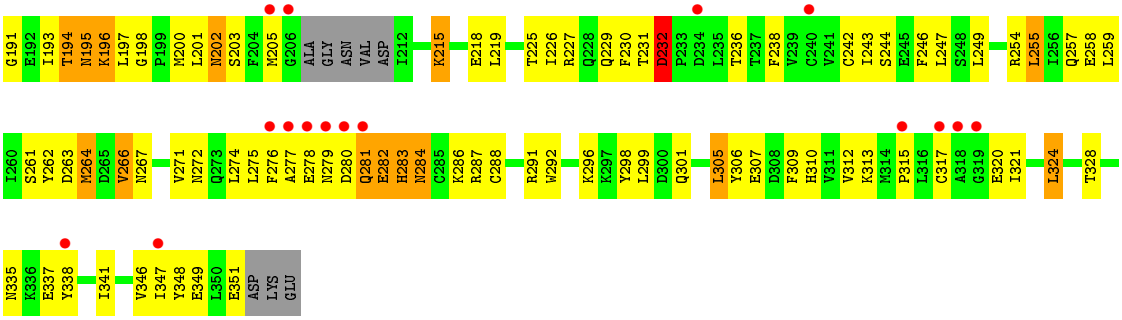
Chain A:



- Molecule 1: ATPase GET3

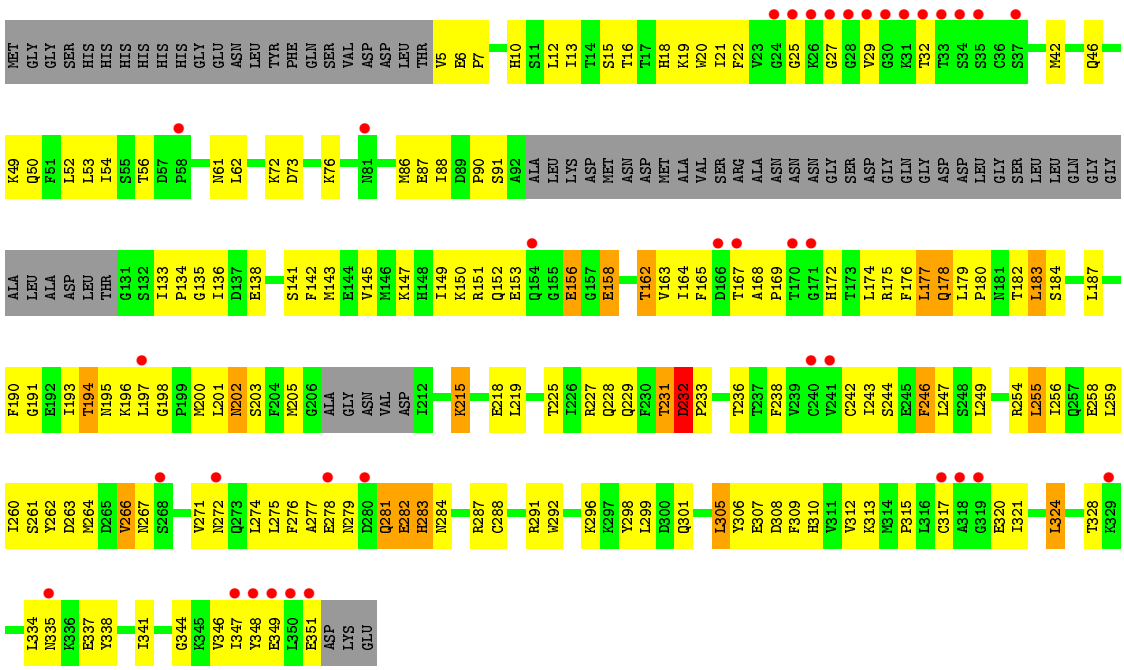
Chain B:





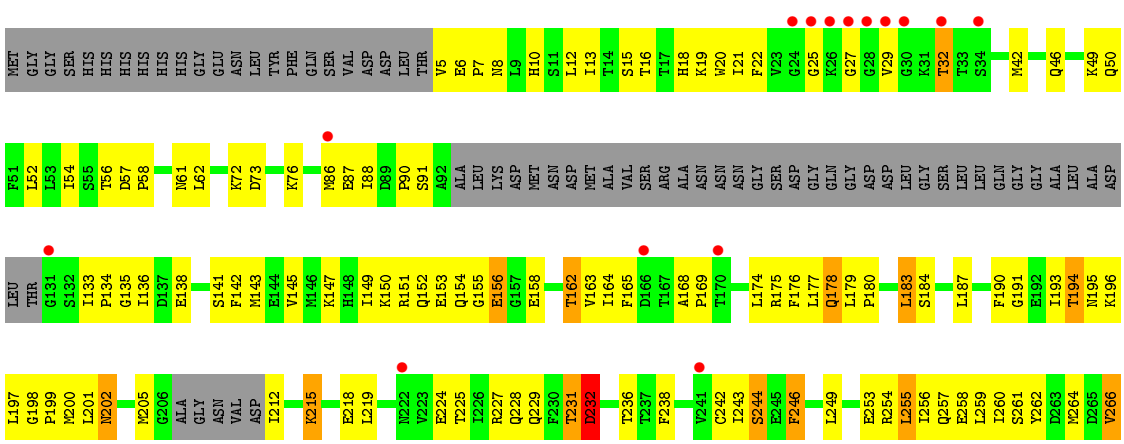
- Molecule 1: ATPase GET3

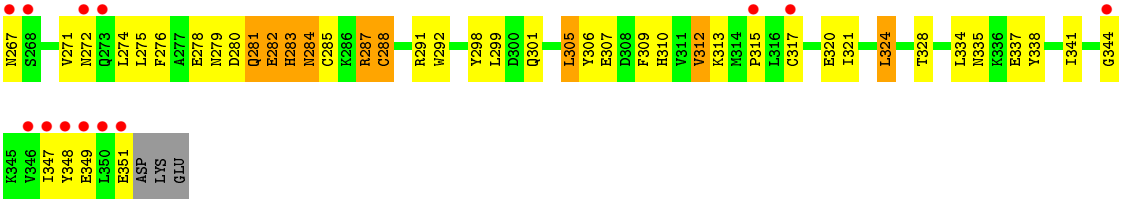
Chain D:



- Molecule 1: ATPase GET3

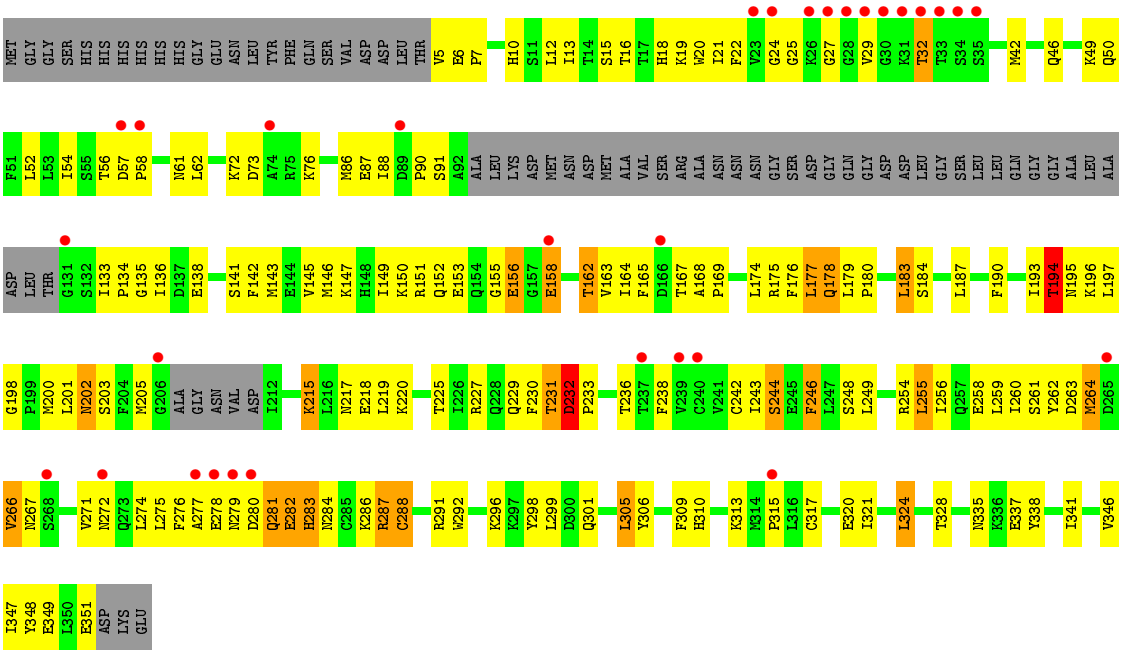
Chain M:





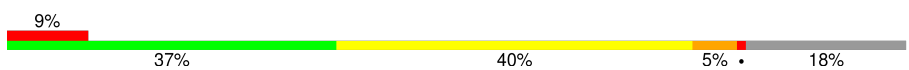
- Molecule 1: ATPase GET3

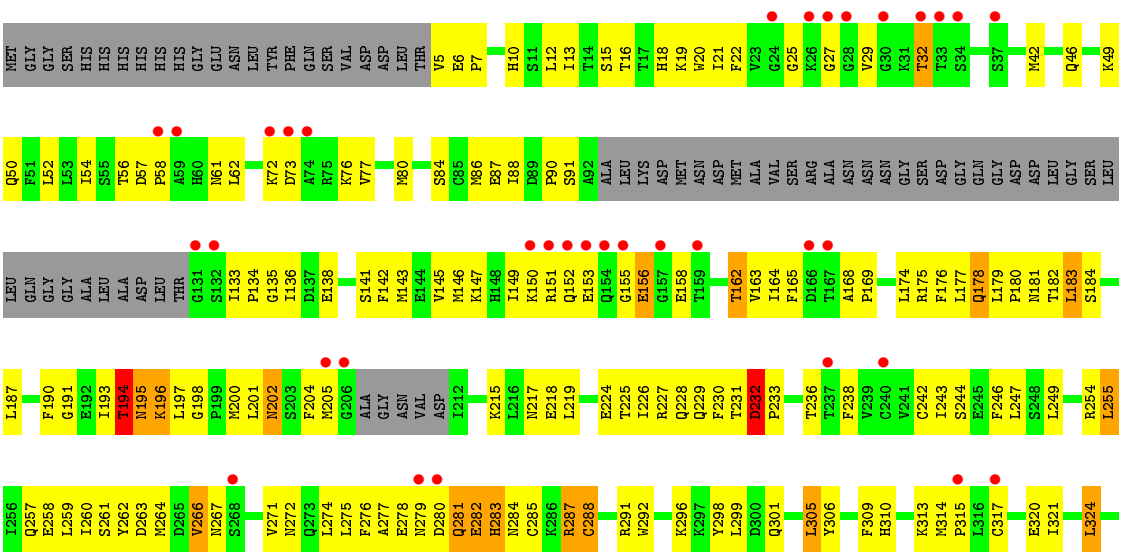
Chain N:



- Molecule 1: ATPase GET3

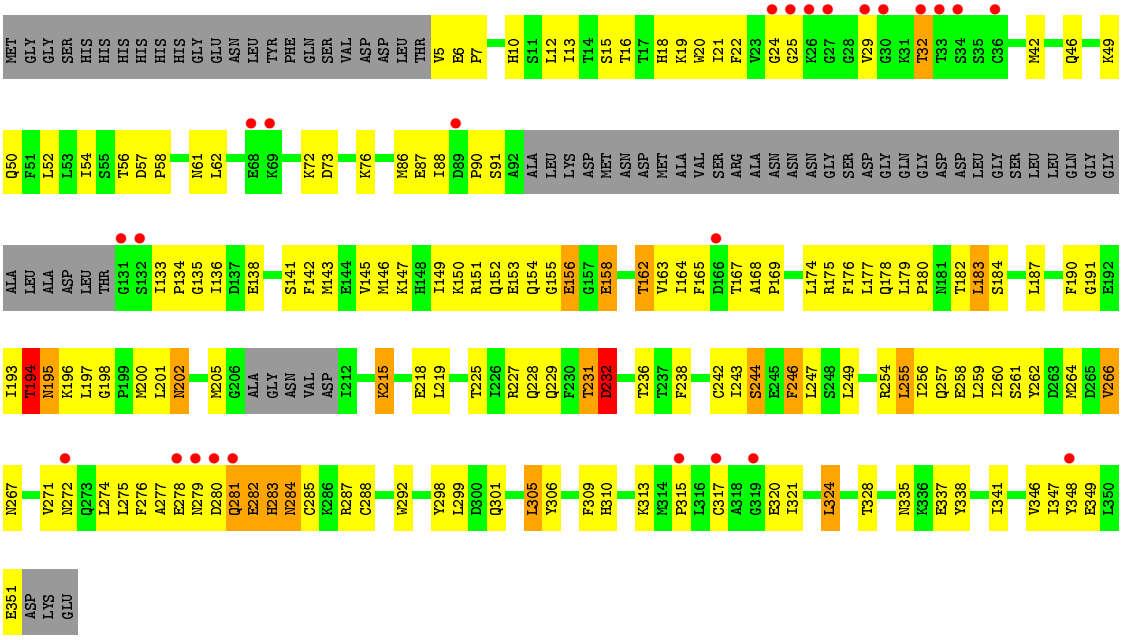
Chain O:





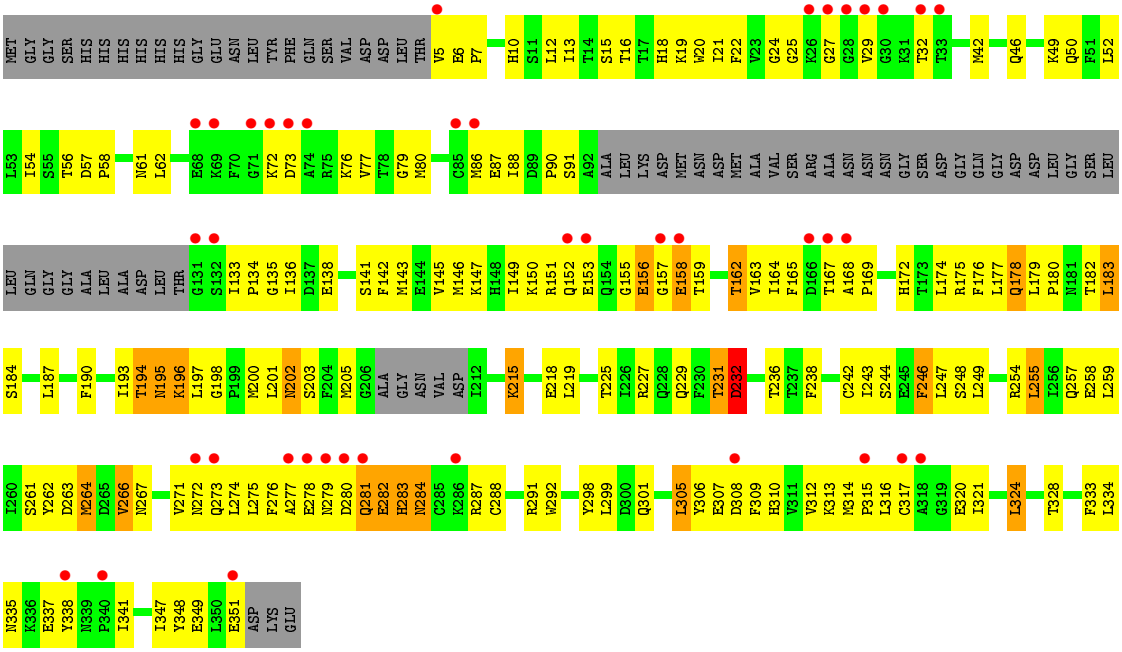
• Molecule 1: ATPase GET3

Chain P:



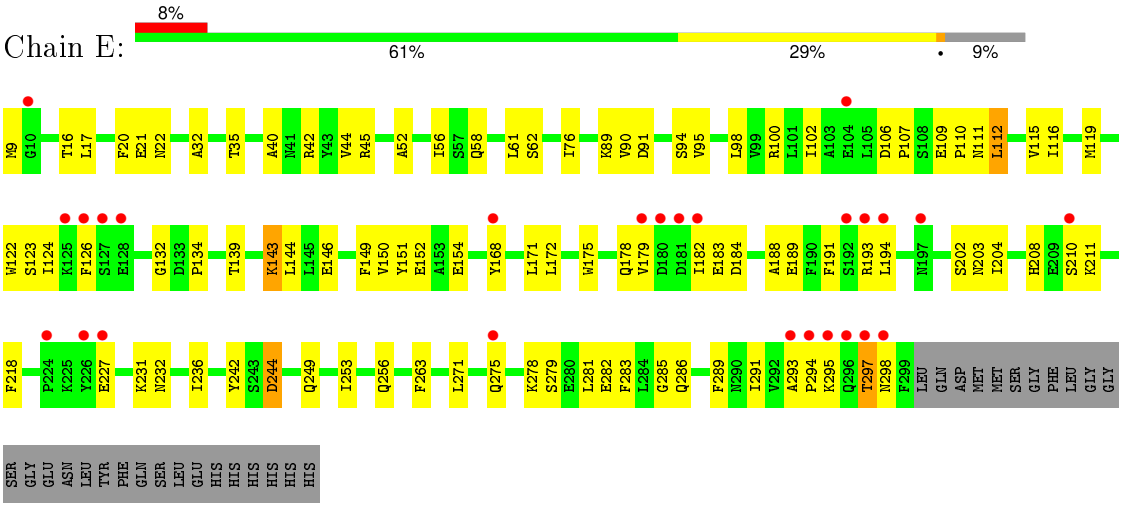
• Molecule 1: ATPase GET3

Chain C:



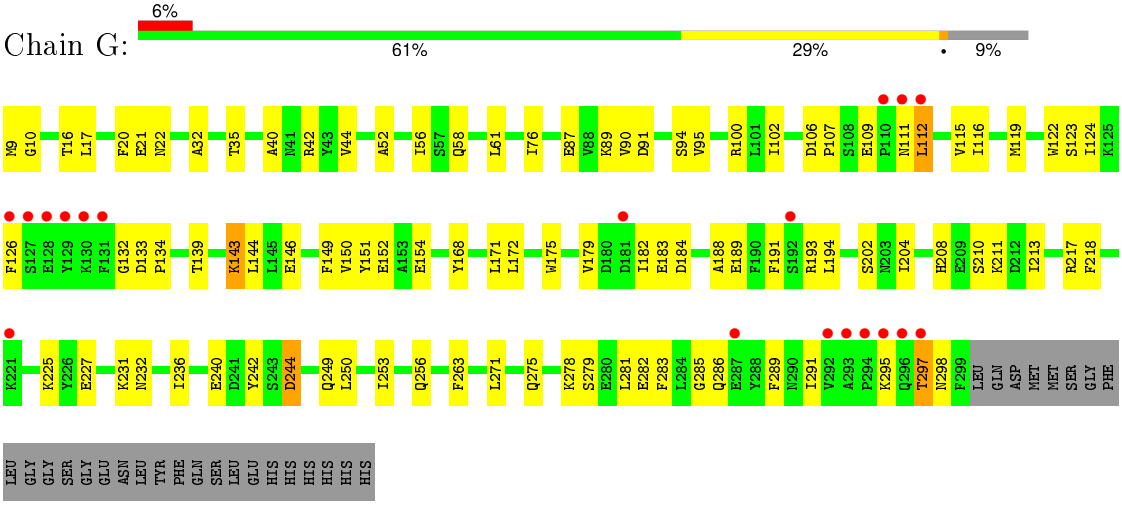
• Molecule 2: Golgi to ER traffic protein 4

Chain E:



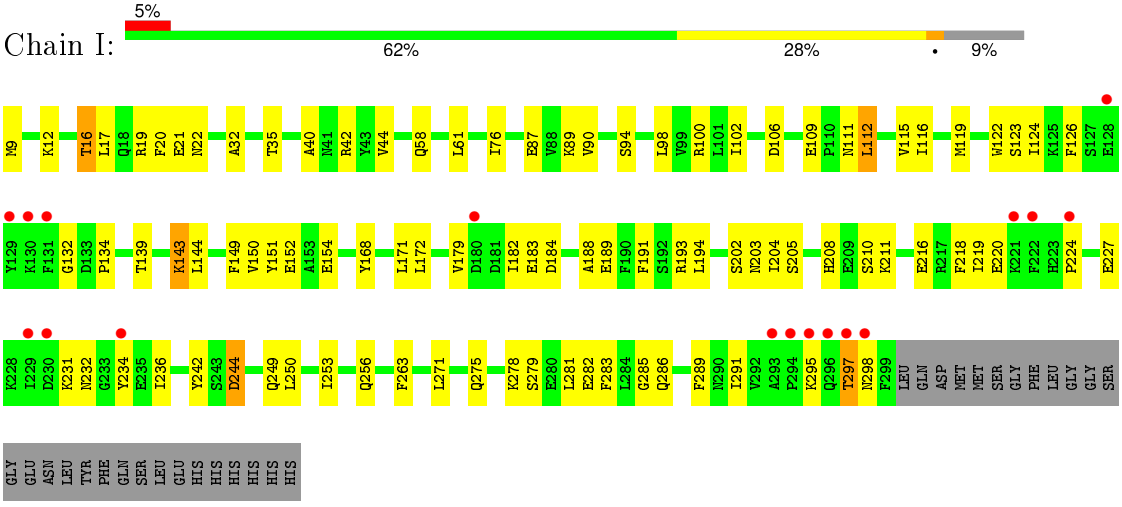
- Molecule 2: Golgi to ER traffic protein 4

Chain G:

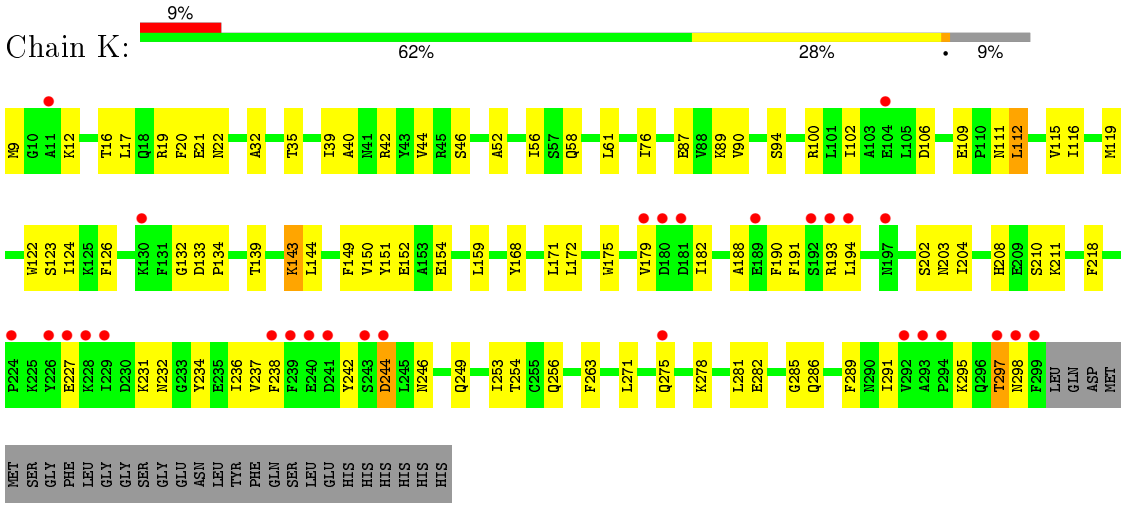


- Molecule 2: Golgi to ER traffic protein 4

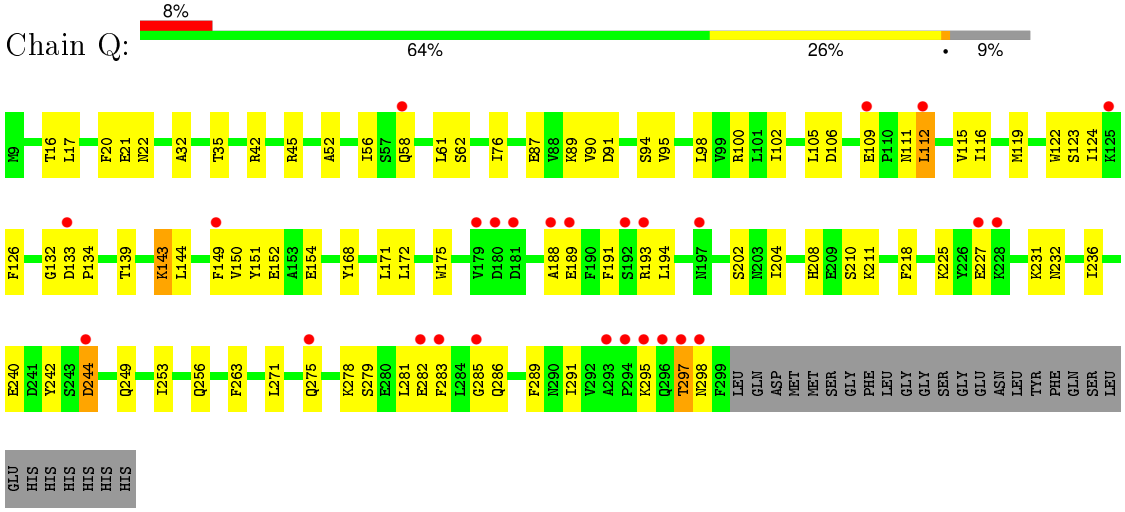
Chain I:



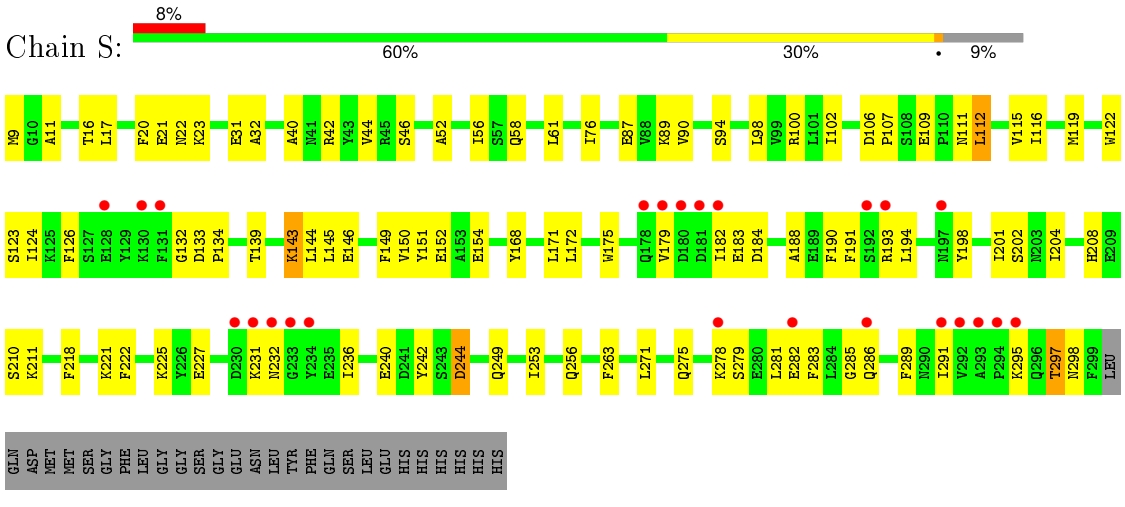
- Molecule 2: Golgi to ER traffic protein 4



• Molecule 2: Golgi to ER traffic protein 4

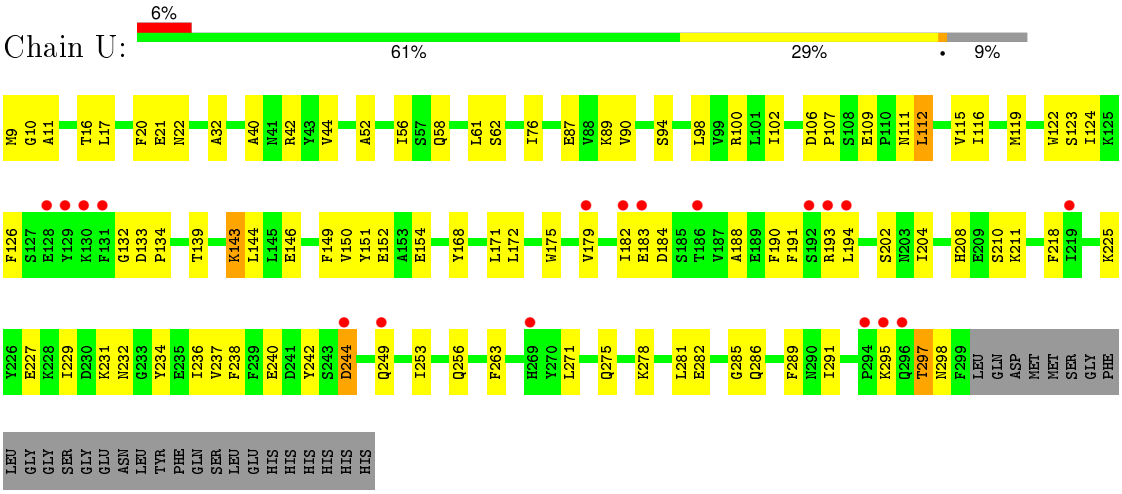


• Molecule 2: Golgi to ER traffic protein 4



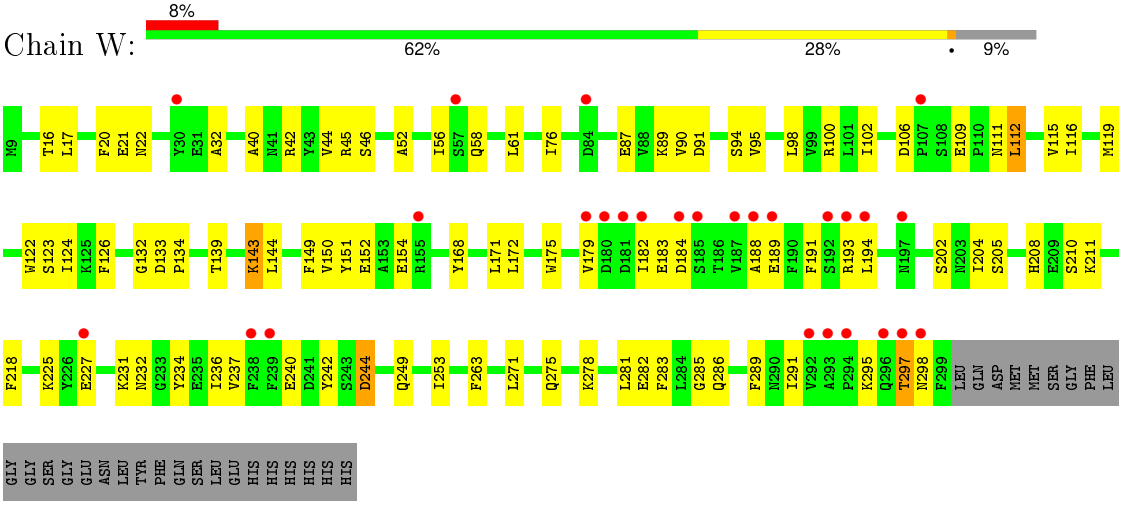
• Molecule 2: Golgi to ER traffic protein 4

Chain U:



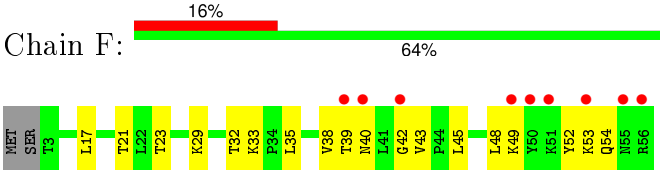
- Molecule 2: Golgi to ER traffic protein 4

Chain W:



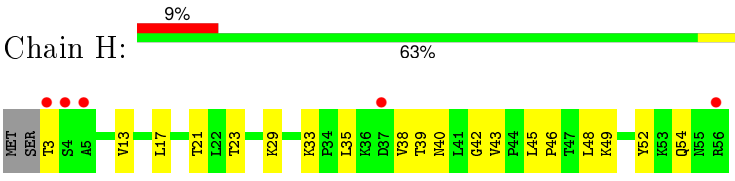
- Molecule 3: Ubiquitin-like protein MDY2

Chain F:



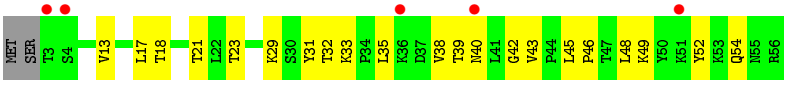
- Molecule 3: Ubiquitin-like protein MDY2

Chain H:



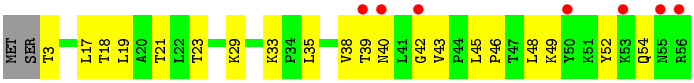
- Molecule 3: Ubiquitin-like protein MDY2

Chain J:

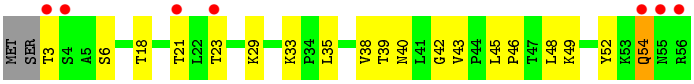


• Molecule 3: Ubiquitin-like protein MDY2

• Molecule 3: Ubiquitin-like protein MDY2



• Molecule 3: Ubiquitin-like protein MDY2



• Molecule 3: Ubiquitin-like protein MDY2

• Molecule 3: Ubiquitin-like protein MDY2

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	No test flags present.	DCC
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 , 262.4	EDS
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 18379 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.26	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:C:138:GLU:HG2	1:C:175:ARG:HB3	1.37	1.06
1:D:174:LEU:HD22	1:D:177:LEU:HD11	1.38	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:N:180:PRO:HG2	1:N:229:GLN:HE21	1.26	1.00
1:M:180:PRO:HG2	1:M:229:GLN:HE21	1.24	1.00
1:A:180:PRO:HG2	1:A:229:GLN:HE21	1.25	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:P:154:GLN:CD	1:C:79:GLY:HA3	1.85	0.97
1:O:174:LEU:O	1:O:177:LEU:HG	1.64	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:P:183:LEU:HD23	1:P:184:SER:H	1.33	0.93
1:N:174:LEU:O	1:N:177:LEU:HG	1.68	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:O:183:LEU:HD23	1:O:184:SER:N	1.87	0.89
1:M:183:LEU:HD23	1:M:184:SER:H	1.37	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:P:154:GLN:CG	1:C:79:GLY:CA	2.51	0.89
1:M:135:GLY:HA3	1:M:179:LEU:HD22	1.55	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:183:LEU:HD23	1:C:184:SER:H	1.37	0.88
1:C:174:LEU:O	1:C:177:LEU:HG	1.74	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:P:138:GLU:HB2	1:P:176:PHE:HB3	1.55	0.87
1:O:138:GLU:HB2	1:O:176:PHE:HB3	1.56	0.87
1:A:135:GLY:HA3	1:A:179:LEU:HD22	1.55	0.87
1:M:199:PRO:HD3	1:C:156:GLU:HB3	1.56	0.87
1:A:183:LEU:HD23	1:A:184:SER:H	1.38	0.87
2:G:217:ARG:CZ	1:M:154:GLN:HE22	1.88	0.86
1:O:135:GLY:HA3	1:O:179:LEU:HD22	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:147:LYS:HZ2	1:O:197:LEU:HD13	1.34	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
1:N:135:GLY:HA3	1:N:179:LEU:HD22	1.57	0.84
2:G:217:ARG:HG2	1:M:154:GLN:OE1	1.77	0.84
1:M:147:LYS:NZ	1:P:197:LEU:HD13	1.93	0.84
3:L:35:LEU:HD12	3:L:38:VAL:HG21	1.58	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
3:V:35:LEU:HD12	3:V:38:VAL:HG21	1.59	0.83
1:M:201:LEU:HD23	1:P:143:MET:SD	2.18	0.83
1:M:305:LEU:HD22	2:Q:42:ARG:NH2	1.93	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
3:J:35:LEU:HD12	3:J:38:VAL:HG21	1.60	0.83
1:N:190:PHE:CE2	1:O:183:LEU:HB2	2.14	0.83
1:D:305:LEU:HD22	2:K:42:ARG:HH21	1.44	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)
1:N:190:PHE:CZ	1:O:183:LEU:HG	2.16	0.81
3:H:35:LEU:HD12	3:H:38:VAL:HG21	1.63	0.81
1:N:183:LEU:HD11	1:O:194:THR:HG22	1.63	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:M:199:PRO:CD	1:C:156:GLU:HB3	2.10	0.80
1:D:317:CYS:SG	1:D:321:ILE:HD11	2.22	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:C:218:GLU:HG3	1:C:219:LEU:N	1.95	0.80
1:B:201:LEU:HB3	1:C:143:MET:CE	2.12	0.80
1:N:233:PRO:HB3	2:S:9:MET:N	1.97	0.80
1:N:179:LEU:O	1:N:183:LEU:HD22	1.82	0.80
2:E:202:SER:HB2	3:F:33:LYS:HB2	1.64	0.80
1:M:199:PRO:CB	1:C:156:GLU:HG2	2.10	0.80
1:P:154:GLN:HG3	1:C:79:GLY:HA3	1.63	0.80
1:N:50:GLN:HE22	1:N:76:LYS:HE2	1.47	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: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:A:50:GLN:HE22	1:A:76:LYS:HE2	1.47	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:N:180:PRO:HG2	1:N:229:GLN:NE2	1.98	0.79
1:M:187:LEU:HD11	1:P:190:PHE:CE1	2.17	0.79
1:B:218:GLU:HG3	1:B:219:LEU:N	1.97	0.79
1:P:218:GLU:HG3	1:P:219:LEU:N	1.98	0.79
1:M:179:LEU:O	1:M:183:LEU:HD22	1.83	0.78
1:D:202:ASN:HD22	1:D:202:ASN:N	1.79	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: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:N:146:MET:HG3	1:O:201:LEU:HD22	1.65	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
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
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:N:146:MET:HG3	1:O:201:LEU:CD2	2.13	0.78
1:M:218:GLU:HG3	1:M:219:LEU:N	1.98	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:N:183:LEU:HG	1:O:190:PHE:CZ	2.19	0.77
1:B:201:LEU:HD21	1:C:146:MET:HG3	1.66	0.77
1:P:202:ASN:HD22	1:P:202:ASN:N	1.82	0.77
1:N:194:THR:HG22	1:O:183:LEU:HD11	1.64	0.77
1:A:324:LEU:O	1:A:328:THR:HG23	1.83	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: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:A:202:ASN:N	1:A:202:ASN:HD22	1.83	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:142:PHE:O	1:P:145:VAL:HG22	1.85	0.76
1:P:13:ILE:HA	1:P:42:MET:HG2	1.67	0.76
1:O:202:ASN:N	1:O:202:ASN:HD22	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:P:218:GLU:HG3	1:P:219:LEU:H	1.52	0.75
1:N:142:PHE:O	1:N:145:VAL:HG22	1.87	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:M:212:ILE:HG21	1:C:155:GLY:HA3	1.68	0.74
1:A:305:LEU:HD22	2:E:42:ARG:NH2	2.01	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:N	1:N:202:ASN:HD22	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:M:29:VAL:HG21	1:M:242:CYS:HA	1.70	0.74
1:B:317:CYS:SG	1:B:321:ILE:HD11	2.28	0.74
1:C:324:LEU:O	1:C:328:THR:HG23	1.88	0.74
2:S:202:SER:HB2	3:T:33:LYS:HB2	1.70	0.74
1:M:202:ASN:HD22	1:M:202:ASN:N	1.86	0.73
1:D:305:LEU:HD22	2:K:42:ARG:NH2	2.02	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:M:187:LEU:HG	1:P:190:PHE:CZ	2.23	0.73
1:A:179:LEU:O	1:A:183:LEU:HD22	1.88	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:N:187:LEU:HD22	1:O:187:LEU:HD22	1.70	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: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:C:142:PHE:O	1:C:145:VAL:HG22	1.88	0.72
1:D:72:LYS:HE2	1:D:151:ARG:HH12	1.51	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:O:230:PHE:HA	2:U:9:MET:CE	2.19	0.72
1:M:218:GLU:HG3	1:M:219:LEU:H	1.54	0.72
1:P:324:LEU:O	1:P:328:THR:HG23	1.89	0.72
1:D:142:PHE:O	1:D:145:VAL:HG22	1.89	0.72
1:B:324:LEU:O	1:B: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)
3:V:39:THR:HG23	3:V:40:ASN:H	1.54	0.72
1:N:72:LYS:HE2	1:N:151:ARG:HH12	1.53	0.72
3:X:39:THR:HG23	3:X:40:ASN:H	1.53	0.72
3:T:39:THR:HG23	3:T:40:ASN:H	1.55	0.72
2:S:106:ASP:HB3	2:S:109:GLU:HG2	1.72	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:Q:106:ASP:HB3	2:Q:109:GLU:HG2	1.70	0.71
2:I:150:VAL:HG13	2:I:151:TYR:N	2.04	0.71
1:C:72:LYS:HE2	1:C:151:ARG:HH12	1.54	0.71
1:O:29:VAL:HG21	1:O:242:CYS:HA	1.71	0.71
2:I:76:ILE:HG21	2:I:115:VAL:HG13	1.73	0.71
3:L:39:THR:HG23	3:L:40:ASN:H	1.54	0.71
2:E:76:ILE:HG21	2:E:115:VAL:HG13	1.72	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:M:197:LEU:HD13	1:P:147:LYS:HZ1	1.56	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:D:174:LEU:CD2	1:D:177:LEU:HD11	2.19	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:D:324:LEU:O	1:D:328:THR:HG23	1.90	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
2:S:76:ILE:HG21	2:S:115:VAL:HG13	1.74	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:NH1	1:N:227:ARG:HB3	2.05	0.70
2:U:134:PRO:HG3	3:V:35:LEU:HD23	1.72	0.70
1:P:180:PRO:CG	1:P:229:GLN:HE21	2.01	0.70
1:M:324:LEU:O	1:M:328:THR:HG23	1.90	0.70
2:E:275:GLN:NE2	2:E:298:ASN:H	1.90	0.70
1:B:13:ILE:HA	1:B:42:MET:HG2	1.71	0.70
1:P:195:ASN:N	1:P:195:ASN:HD22	1.90	0.70
1:B:142:PHE:O	1:B:145:VAL:HG22	1.92	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:N:29:VAL:HG21	1:N:242:CYS:HA	1.74	0.70
1:C:180:PRO:HG2	1:C:229:GLN:NE2	2.05	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
1:A:242:CYS:O	1:A:271:VAL:HA	1.92	0.69
2:W:106:ASP:HB3	2:W:109:GLU:HG2	1.72	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
1:C:301:GLN:O	1:C:305:LEU:HB2	1.92	0.69
2:I:283:PHE:CE1	3:J:42:GLY:HA2	2.27	0.69
1:C:202:ASN:N	1:C:202:ASN:HD22	1.90	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
2:G:150:VAL:HB	3:H:52:TYR:CD2	2.28	0.69
1:B:238:PHE:HB3	1:B:266:VAL:HG12	1.75	0.69
1:B:218:GLU:HG3	1:B:219:LEU:H	1.55	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
3:F:39:THR:HG23	3:F:40:ASN:H	1.58	0.69
2:W:76:ILE:HG21	2:W:115:VAL:HG13	1.75	0.68
1:P:133:ILE:HB	1:P:136:ILE:HD12	1.75	0.68
1:B:146:MET:HB2	1:C:201:LEU:HD22	1.75	0.68
2:S:150:VAL:HG13	2:S:151:TYR:N	2.07	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
1:M:242:CYS:O	1:M:271:VAL:HA	1.93	0.68
1:B:242:CYS:O	1:B: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:HD22	1:A:195:ASN:N	1.91	0.68
1:N:20:TRP:CZ2	1:O:204:PHE:HE2	2.12	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:B:201:LEU:HB3	1:C:143:MET:HE1	1.76	0.68
2:U:144:LEU:HD13	2:U:152:GLU:HB3	1.76	0.68
1:O:301:GLN:O	1:O:305:LEU:HB2	1.92	0.68
2:I:150:VAL:HB	3:J:52:TYR:CD2	2.29	0.68
2:E:106:ASP:HB3	2:E:109:GLU:HG2	1.73	0.68
1:A:238:PHE:HB3	1:A:266:VAL:HG12	1.75	0.68
2:E:279:SER:HB2	3:F:43:VAL:HG11	1.76	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:P:238:PHE:HB3	1:P:266:VAL:HG12	1.76	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:M:238:PHE:HB3	1:M:266:VAL:HG12	1.75	0.68
1:P:72:LYS:HE2	1:P:151:ARG:HH12	1.57	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:U:190:PHE:CE1	3:V:48:LEU:HD13	2.28	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
1:A:201:LEU:HB3	1:D:143:MET:HE1	1.77	0.67
2:S:150:VAL:HG13	2:S:151:TYR:H	1.60	0.67
1:N:238:PHE:HB3	1:N:266:VAL:HG12	1.75	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: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: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
2:U:278:LYS:HA	2:U:295:LYS:HE3	1.76	0.67
1:N:301:GLN:O	1:N:305:LEU:HB2	1.95	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:C:179:LEU:O	1:C:183:LEU:HD22	1.95	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: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:M:180:PRO:CG	1:M:229:GLN:HE21	2.04	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:238:PHE:HB3	1:O:266:VAL:HG12	1.76	0.66
1:B:201:LEU:CD2	1:C:146:MET:HG3	2.24	0.66
1:D:238:PHE:HB3	1:D:266:VAL:HG12	1.76	0.66
2:Q:112:LEU:HD11	2:Q:143:LYS:HD2	1.76	0.66
2:K:112:LEU:HD11	2:K:143:LYS:HD2	1.78	0.66
1:P:202:ASN:H	1:P:202:ASN:HD22	1.41	0.66
1:A:305:LEU:HD22	2:E:42:ARG:HH21	1.60	0.66
1:N:227:ARG:HH11	1:N:227:ARG:HB3	1.60	0.66
1:C:29:VAL:HG22	1:C:243:ILE:HG23	1.77	0.66
2:U:271:LEU:HD22	2:U:298:ASN:ND2	2.11	0.66
2:U:150:VAL:HG13	2:U:151:TYR:N	2.09	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: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:190:PHE:CE1	1:D:187:LEU:HD11	2.30	0.66
1:O:180:PRO:CG	1:O:229:GLN:HE21	2.01	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:A:19:LYS:HA	1:A:162:THR:HA	1.77	0.66
2:E:112:LEU:HD23	2:E:149:PHE:HE2	1.61	0.66
2:W:150:VAL:HG13	2:W:151:TYR:N	2.09	0.66
1:C:29:VAL:HG21	1:C:242:CYS:HA	1.76	0.66
2:I:19:ARG:NH1	1:C:5:VAL:HG23	2.10	0.66
2:E:256:GLN:HE22	3:F:29:LYS:HG3	1.60	0.66
2:S:175:TRP:CZ3	3:T:48:LEU:HD12	2.31	0.66
2:Q:236:ILE:HD12	2:Q:249:GLN:HB3	1.77	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
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:D:227:ARG:HB3	1:D:227:ARG:NH1	2.10	0.66
1:O:178:GLN:HA	1:O:229:GLN:HE22	1.61	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:U:112:LEU:HD23	2:U:149:PHE:HE2	1.61	0.66
2:K:236:ILE:HD12	2:K:249:GLN:HB3	1.78	0.66
1:C:178:GLN:HA	1:C:229:GLN:HE22	1.59	0.66
2:K:150:VAL:HG13	2:K:151:TYR:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:201:LEU:HD22	1:O:146:MET:HB2	1.76	0.65
2:I:16:THR:HG21	1:C:308:ASP:OD2	1.96	0.65
1:P:179:LEU:N	1:P:180:PRO:HD2	2.11	0.65
1:A:178:GLN:HA	1:A:229:GLN:HE22	1.60	0.65
1:A:147:LYS:HZ1	1:D:197:LEU:HD13	1.59	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:D:19:LYS:HA	1:D:162:THR:HA	1.78	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
1:O:179:LEU:N	1:O:180:PRO:HD2	2.10	0.65
1:M:197:LEU:HD13	1:P:147:LYS:NZ	2.10	0.65
2:I:208:HIS:NE2	3:J:29:LYS:HG2	2.11	0.65
2:U:240:GLU:HG2	3:V:6:SER:OG	1.97	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
2:G:202:SER:HB2	3:H:33:LYS:HB2	1.77	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
1:C:179:LEU:N	1:C:180:PRO:HD2	2.12	0.65
2:Q:278:LYS:HA	2:Q:295:LYS:HE3	1.79	0.65
2:K:17:LEU:HD13	2:K:58:GLN:HG2	1.78	0.65
1:A:187:LEU:HD11	1:D:190:PHE:CE1	2.31	0.65
1:P:201:LEU:O	1:P:205:MET:HG2	1.97	0.65
1:M:305:LEU:HD22	2:Q:42:ARG:HH21	1.61	0.65
1:C:22:PHE:HB2	1:C:238:PHE:HA	1.79	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:B:227:ARG:HB3	1:B:227:ARG:NH1	2.12	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:N:174:LEU:CD2	1:N:177:LEU:HD11	2.25	0.64
1:B:306:TYR:HB3	1:B:309:PHE:HB2	1.79	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
1:N:242:CYS:O	1:N:271:VAL:HA	1.98	0.64
2:K:231:LYS:HE2	3:L:18:THR:OG1	1.97	0.64

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:PRO:CG	1:C:229:GLN:HE21	2.10	0.63
2:I:134:PRO:HG3	3:J:35:LEU:HD23	1.80	0.63
2:W:275:GLN:HE22	2:W:297:THR:HA	1.62	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
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:287:ARG:CB	1:N:288:CYS:SG	2.87	0.63
1:M:274:LEU:CD1	1:M:313:LYS:HB3	2.29	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
1:N:143:MET:CB	1:O:197:LEU:HB2	2.26	0.63
1:M:212:ILE:HG22	1:C:156:GLU:OE1	1.99	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:I:16:THR:CG2	1:C:308:ASP:HB2	2.27	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:O:22:PHE:HB2	1:O:238:PHE:HA	1.80	0.62
2:I:42:ARG:HH22	1:C:305:LEU:CD2	2.12	0.62
1:A:257:GLN:OE1	2:E:42:ARG:HG3	1.99	0.62
1:N:243:ILE:HA	1:N:271:VAL:HG13	1.81	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
1:A:306:TYR:HB3	1:A:309:PHE:HB2	1.81	0.62
1:M:306:TYR:HB3	1:M:309:PHE:HB2	1.81	0.62
1:P:174:LEU:HD13	1:P:177:LEU:HD11	1.80	0.62
2:E:285:GLY:HA2	2:E:289:PHE:HD2	1.64	0.62
1:M:19:LYS:HA	1:M:162:THR:HA	1.80	0.62
2:E:278:LYS:HA	2:E:295:LYS:HE3	1.81	0.62
2:I:232:ASN:HB2	3:J:21:THR:CB	2.29	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:D:267:ASN:HB2	2:K:12:LYS:HZ1	1.64	0.62
1:B:56:THR:HB	1:B:90:PRO:HG3	1.80	0.62
1:B:19:LYS:HA	1:B:162:THR:HA	1.81	0.62
1:A:227:ARG:NH1	1:A:227:ARG:HB3	2.14	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: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
1:A:202:ASN:H	1:A:202:ASN:HD22	1.45	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
1:P:174:LEU:C	1:P:177:LEU:HG	2.20	0.62
2:G:282:GLU:O	2:G:286:GLN:HG3	2.00	0.62
1:P:227:ARG:HB3	1:P:227:ARG:NH1	2.14	0.62
1:M:138:GLU:CB	1:M:176:PHE:HB3	2.27	0.61
1:B:183:LEU:HG	1:C:190:PHE:CZ	2.35	0.61
1:D:202:ASN:H	1:D:202:ASN:HD22	1.48	0.61
1:N:22:PHE:HB2	1:N:238:PHE:HA	1.80	0.61
2:I:19:ARG:HH12	1:C:5:VAL:HG22	1.64	0.61
1:B:146:MET:HB2	1:C:201:LEU:CD2	2.31	0.61
1:C:202:ASN:HD22	1:C:202:ASN:H	1.46	0.61
1:N:143:MET:SD	1:O:196:LYS:HG3	2.39	0.61
1:N:72:LYS:HE2	1:N:151:ARG:NH1	2.14	0.61
2:G:112:LEU:HD23	2:G:149:PHE:HE2	1.65	0.61
1:P:274:LEU:CD1	1:P:313:LYS:HB3	2.30	0.61
1:C:174:LEU:CD2	1:C:177:LEU:HD11	2.27	0.61
2:E:271:LEU:HD22	2:E:298:ASN:ND2	2.15	0.61
1:N:238:PHE:HB3	1:N:266:VAL:CG1	2.30	0.61
2:K:191:PHE:HZ	2:K:211:LYS:HG3	1.66	0.61
1:P:20:TRP:HB2	1:P:236:THR:HG23	1.81	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: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:C:174:LEU:HD13	1:C:177:LEU:HD11	1.83	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:B:238:PHE:HB3	1:B:266:VAL:CG1	2.31	0.61
1:B:197:LEU:O	1:C:143:MET:CE	2.48	0.61
1:M:288:CYS:SG	1:N:287:ARG:HB3	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:278:LYS:HA	2:I:295:LYS:HE3	1.82	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
2:I:286:GLN:HG2	2:I:291:ILE:O	2.01	0.61
1:D:27:GLY:HA2	1:C:246:PHE:CD2	2.35	0.61
1:A:284:ASN:HD22	1:A:284:ASN:N	1.98	0.61
1:M:195:ASN:HD22	1:M:195:ASN:N	1.98	0.61
1:A:143:MET:HE1	1:D:201:LEU:HB3	1.82	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:O:306:TYR:HB3	1:O:309:PHE:HB2	1.83	0.61
1:D:56:THR:HB	1:D:90:PRO:HG3	1.83	0.61
2:S:134:PRO:HG3	3:T:35:LEU:HD23	1.82	0.60
2:U:271:LEU:HD22	2:U:298:ASN:HD21	1.66	0.60
2:U:150:VAL:HG13	2:U:151:TYR:H	1.64	0.60
2:I:232:ASN:HB2	3:J:21:THR:HB	1.82	0.60
2:I:35:THR:HG22	1:C:307:GLU:OE2	2.01	0.60
2:S:17:LEU:HD13	2:S:58:GLN:HG2	1.83	0.60
1:P:16:THR:HA	1:P:46:GLN:HE22	1.67	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:174:LEU:HB3	1:P:177:LEU:CD1	2.31	0.60
1:M:190:PHE:CE1	1:P:187:LEU:HD11	2.37	0.60
3:F:35:LEU:HA	3:F:38:VAL:HG23	1.84	0.60
1:O:227:ARG:HH11	1:O:227:ARG:HB3	1.66	0.60
2:Q:271:LEU:HD22	2:Q:298:ASN:ND2	2.16	0.60
1:M:282:GLU:O	1:M:283:HIS:O	2.19	0.60
1:M:20:TRP:HB2	1:M:236:THR:HG23	1.81	0.60
1:D:20:TRP:HB2	1:D:236:THR:HG23	1.81	0.60
1:O:138:GLU:CG	1:O:175:ARG:HB3	2.22	0.60
2:I:112:LEU:HD11	2:I:143:LYS:HD2	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
1:A:247:LEU:HB3	1:B:247:LEU:HD13	1.83	0.60
2:U:191:PHE:HZ	2:U:211:LYS:HG3	1.65	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
2:G:250:LEU:HD11	3:H:13:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:TRP:HB2	1:B:236:THR:HG23	1.82	0.60
2:I:275:GLN:NE2	2:I:298:ASN:H	1.97	0.60
2:I:271:LEU:HD22	2:I:298:ASN:ND2	2.17	0.60
2:Q:285:GLY:HA2	2:Q:289:PHE:HD2	1.66	0.60
1:N:281:GLN:O	1:N:282:GLU:HB2	2.01	0.60
1:N:143:MET:CE	1:O:197:LEU:HB2	2.26	0.60
2:G:256:GLN:HE22	3:H:29:LYS:CG	2.14	0.60
1:C:281:GLN:O	1:C:282:GLU:HB2	2.02	0.60
1:P:306:TYR:HB3	1:P:309:PHE:HB2	1.82	0.60
1:B:274:LEU:CD1	1:B:313:LYS:HB3	2.31	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
2:W:191:PHE:HZ	2:W:211:LYS:HG3	1.67	0.60
1:P:281:GLN:O	1:P:282:GLU:HB2	2.01	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
3:X:39:THR:HG23	3:X:40:ASN:N	2.16	0.59
2:S:275:GLN:NE2	2:S:298:ASN:H	2.00	0.59
2:G:271:LEU:HD22	2:G:298:ASN:ND2	2.17	0.59
1:P:284:ASN:N	1:P:284:ASN:HD22	1.99	0.59
2:E:286:GLN:HG2	2:E:291:ILE:O	2.01	0.59
1:M:178:GLN:HA	1:M:229:GLN:HE22	1.65	0.59
2:E:189:GLU:HB3	3:F:48:LEU:HD22	1.82	0.59
1:C:284:ASN:HD22	1:C:284:ASN:N	2.00	0.59
2:W:17:LEU:HD13	2:W:58:GLN:HG2	1.84	0.59
2:K:286:GLN:HG2	2:K:291:ILE:O	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:D:267:ASN:O	1:D:310:HIS:HB2	2.02	0.59
1:D:198:GLY:CA	1:D:200:MET:H	2.15	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:B:174:LEU:CD2	1:B:177:LEU:HD11	2.22	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
2:K:204:ILE:HG12	3:L:31:TYR:HD2	1.66	0.59
1:B:281:GLN:O	1:B:282:GLU:HB2	2.02	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)
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
2:I:12:LYS:HD2	1:C:267:ASN:HB3	1.85	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:K:150:VAL:HG13	2:K:151:TYR:H	1.65	0.59
1:D:247:LEU:HD13	1:C:247:LEU:HB3	1.84	0.59
1:P:154:GLN:CG	1:C:79:GLY:HA2	2.24	0.59
1:M:193:ILE:C	1:M:195:ASN:H	2.06	0.59
2:G:150:VAL:HG13	2:G:151:TYR:H	1.66	0.59
1:M:284:ASN:N	1:M:284:ASN:HD22	2.00	0.59
2:G:94:SER:HB3	2:G:122:TRP:CH2	2.37	0.59
1:M:227:ARG:NH1	1:M:227:ARG:HB3	2.18	0.59
3:T:35:LEU:HA	3:T:38:VAL:HG23	1.85	0.59
1:M:281:GLN:O	1:M:282:GLU:HB2	2.02	0.59
1:A:194:THR:HG22	1:D:183:LEU:HD11	1.84	0.59
1:O:196:LYS:HG2	1:O:202:ASN:OD1	2.03	0.59
1:M:199:PRO:CD	1:C:156:GLU:CG	2.78	0.59
1:C:72:LYS:HE2	1:C:151:ARG:NH1	2.16	0.59
1:N:198:GLY:CA	1:N:200:MET:H	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:D:174:LEU:HD22	1:D:177:LEU:CD1	2.26	0.58
3:L:35:LEU:HA	3:L:38:VAL:HG23	1.85	0.58
1:A:72:LYS:CE	1:A:151:ARG:HH12	2.16	0.58
1:M:238:PHE:HB3	1:M:266:VAL:CG1	2.32	0.58
1:N:267:ASN:O	1:N:310:HIS:HB2	2.02	0.58
1:N:133:ILE:HB	1:N:136:ILE:HD12	1.85	0.58
2:K:278:LYS:HA	2:K:295:LYS:HE3	1.85	0.58
2:U:275:GLN:HE22	2:U:297:THR:HA	1.68	0.58
2:Q:282:GLU:O	2:Q:286:GLN:HG3	2.03	0.58
1:D:29:VAL:CG2	1:D:243:ILE:HG23	2.33	0.58
2:U:275:GLN:NE2	2:U:298:ASN:H	2.00	0.58
2:S:271:LEU:HD22	2:S:298:ASN:ND2	2.18	0.58
2:I:232:ASN:HB2	3:J:21:THR:OG1	2.02	0.58
1:B:284:ASN:N	1:B:284:ASN:HD22	2.00	0.58
1:A:56:THR:HB	1:A:90:PRO:HG3	1.84	0.58
1:P:238:PHE:HB3	1:P:266:VAL:CG1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:285:CYS:SG	1:P:285:CYS:SG	3.00	0.58
1:B:29:VAL:CG2	1:B:243:ILE:HG23	2.34	0.58
1:A:20:TRP:HB2	1:A:236:THR:HG23	1.84	0.58
1:M:347:ILE:C	1:M:349:GLU:H	2.06	0.58
2:K:285:GLY:HA2	2:K:289:PHE:HD2	1.68	0.58
1:N:183:LEU:HD11	1:O:194:THR:CG2	2.31	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
1:N:260:ILE:CD1	2:S:42:ARG:HD3	2.32	0.58
2:I:16:THR:HG21	1:C:308:ASP:CB	2.34	0.58
1:A:258:GLU:HG2	1:A:262:TYR:CE2	2.38	0.58
2:E:94:SER:HB3	2:E:122:TRP:CH2	2.38	0.58
1:O:198:GLY:CA	1:O:200:MET:H	2.17	0.58
2:I:231:LYS:HE2	3:J:18:THR:OG1	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: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:B:143:MET:HE2	1:C:197:LEU:O	2.03	0.57
1:D:202:ASN:ND2	1:D:202:ASN:N	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:C:201:LEU:O	1:C:205:MET:HG2	2.04	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:C:282:GLU:O	1:C:283:HIS:O	2.21	0.57
1:N:54:ILE:HD11	1:N:88:ILE:HG12	1.86	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:O:72:LYS:HE2	1:O:151:ARG:NH1	2.19	0.57
2:G:283:PHE:CE1	3:H:42:GLY:HA2	2.39	0.57
2:S:282:GLU:O	2:S:286:GLN:HG3	2.04	0.57
1:O:347:ILE:C	1:O:349:GLU:H	2.07	0.57
1:A:174:LEU:HD22	1:A:177:LEU:CD1	2.29	0.57
1:N:20:TRP:HB2	1:N:236:THR:HG23	1.86	0.57
1:A:347:ILE:C	1:A:349:GLU:H	2.06	0.57
1:A:174:LEU:C	1:A:177:LEU:HG	2.25	0.57
2:G:217:ARG:HH21	1:M:154:GLN:HE22	1.50	0.57
1:B:198:GLY:CA	1:B:200:MET:H	2.17	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:P:72:LYS:HE2	1:P:151:ARG:NH1	2.20	0.57
1:O:282:GLU:O	1:O:283:HIS:O	2.21	0.57
1:B:282:GLU:O	1:B:283:HIS:O	2.22	0.57
1:A:279:ASN:HB3	1:A:341:ILE:HD13	1.87	0.57
1:A:174:LEU:HD13	1:A:177:LEU:CD1	2.35	0.57
2:I:16:THR:CG2	1:C:308:ASP:CB	2.81	0.57
2:G:278:LYS:HG3	2:G:295:LYS:HG2	1.87	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:N:233:PRO:HG3	2:S:11:ALA:H	1.68	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
3:L:39:THR:HG23	3:L:40:ASN:N	2.18	0.57
1:D:247:LEU:HB3	1:C:247:LEU:HD13	1.86	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:W:94:SER:HB3	2:W:122:TRP:CH2	2.39	0.57
2:Q:94:SER:HB3	2:Q:122:TRP:CH2	2.39	0.57
1:C:347:ILE:C	1:C:349:GLU:H	2.06	0.57
1:N:183:LEU:HB2	1:O:190:PHE:CE2	2.40	0.57
3:X:35:LEU:HA	3:X:38:VAL:HG23	1.86	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
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:A:16:THR:HG22	1:A:46:GLN:HE21	1.69	0.56
2:S:116:ILE:HA	2:S:119:MET:HE2	1.87	0.56
1:N:29:VAL:CG2	1:N:243:ILE:HG23	2.34	0.56
1:B:227:ARG:HB3	1:B:227:ARG:HH11	1.69	0.56
1:A:247:LEU:HD13	1:B:247:LEU:HB3	1.87	0.56
1:N:347:ILE:C	1:N:349:GLU:H	2.07	0.56
2:K:94:SER:HB3	2:K:122:TRP:CH2	2.40	0.56
2:I:17:LEU:HD13	2:I:58:GLN:HG2	1.87	0.56
1:M:174:LEU:CD2	1:M:177:LEU:HD11	2.30	0.56
3:V:35:LEU:HA	3:V:38:VAL:HG23	1.87	0.56
1:M:196:LYS:HG2	1:M:202:ASN:OD1	2.06	0.56
1:B:50:GLN:NE2	1:B:76:LYS:HE2	2.19	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:35:LEU:HA	3:J:38:VAL:HG23	1.87	0.55
2:I:285:GLY:HA2	2:I:289:PHE:HD2	1.71	0.55
1:P:282:GLU:O	1:P:283:HIS:O	2.24	0.55
1:O:254:ARG:HG3	1:O:255:LEU:N	2.21	0.55
1:C:254:ARG:HG3	1:C:255:LEU:N	2.22	0.55
1:O:178:GLN:NE2	1:O:261:SER:HB2	2.22	0.55
1:C:16:THR:HG22	1:C:46:GLN:HE21	1.68	0.55
1:N:16:THR:HA	1:N:46:GLN:HE22	1.72	0.55
1:C:32:THR:CG2	1:C:61:ASN:HD22	2.19	0.55
1:N:315:PRO:HB3	1:N:338:TYR:CE2	2.41	0.55
2:W:286:GLN:HG2	2:W:291:ILE:O	2.06	0.55
1:A:307:GLU:CD	2:E:35:THR:HG22	2.27	0.55
1:P:231:THR:HG22	1:P:231:THR:O	2.06	0.55
1:A:195:ASN:N	1:A:195:ASN:ND2	2.55	0.55
1:D:305:LEU:O	2:K:42:ARG:NH2	2.36	0.55
1:B:197:LEU:HB2	1:C:143:MET:CB	2.35	0.55
1:M:29:VAL:CG2	1:M:243:ILE:HG23	2.36	0.55
1:D:247:LEU:CB	1:C:247:LEU:HD13	2.37	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
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:B:193:ILE:C	1:B:195:ASN:H	2.10	0.55
2:K:232:ASN:HB2	3:L:21:THR:CB	2.35	0.55
1:A:243:ILE:HG22	1:A:272:ASN:O	2.05	0.55
1:D:282:GLU:O	1:D:283:HIS:O	2.25	0.55
1:A:267:ASN:O	1:A:310:HIS:HB2	2.05	0.55
1:N:147:LYS:CE	1:O:197:LEU:HD22	2.36	0.55
1:C:29:VAL:CG2	1:C:243:ILE:HG23	2.37	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:P:32:THR:CB	1:P:61:ASN:HD22	2.20	0.55
2:Q:202:SER:HB2	3:R:33:LYS:HB2	1.87	0.55
1:M:267:ASN:O	1:M:310:HIS:HB2	2.06	0.55
1:P:315:PRO:HB3	1:P:338:TYR:CE2	2.42	0.55
1:A:143:MET:CE	1:D:201:LEU:HB3	2.35	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: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: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: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:202:ASN:ND2	1:P:202:ASN:N	2.53	0.55
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:P:195:ASN:N	1:P:195:ASN:ND2	2.55	0.55
2:U:285:GLY:HA2	2:U:289:PHE:HD2	1.70	0.55
1:P:138:GLU:CB	1:P:176:PHE:HB3	2.31	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
2:S:202:SER:HB2	3:T:33:LYS:CB	2.37	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
2:W:90:VAL:HG21	2:W:123:SER:HA	1.89	0.55
2:U:231:LYS:HE2	3:V:18:THR:OG1	2.07	0.55
2:S:256:GLN:HE22	3:T:29:LYS:CG	2.19	0.55
1:N:72:LYS:CE	1:N:151:ARG:HH12	2.18	0.55
2:I:116:ILE:HA	2:I:119:MET:HE2	1.89	0.55
3:F:39:THR:HG23	3:F:40:ASN:N	2.21	0.55
2:Q:231:LYS:HE2	3:R:18:THR:OG1	2.07	0.55
1:B:267:ASN:O	1:B:310:HIS:HB2	2.06	0.55
1:N:52:LEU:HD12	1:N:163:VAL:HG13	1.88	0.55
1:C:196:LYS:HG2	1:C:202:ASN:OD1	2.06	0.54
1:D:177:LEU:HD23	1:D:177:LEU:N	2.22	0.54
1:N:201:LEU:HB3	1:O:143:MET:SD	2.47	0.54
1:M:29:VAL:O	1:M:29:VAL:HG13	2.08	0.54
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:178:GLN:HA	1:D:229:GLN:HE22	1.71	0.54
1:B:194:THR:C	1:B:195:ASN:HD22	2.10	0.54
1:A:201:LEU:HB3	1:D:143:MET:CE	2.37	0.54
2:Q:286:GLN:HG2	2:Q:291:ILE:O	2.06	0.54
1:A:198:GLY:CA	1:A:200:MET:H	2.21	0.54
1:B:138:GLU:CG	1:B:175:ARG:HB3	2.23	0.54
1:C:174:LEU:HD13	1:C:177:LEU:CD1	2.38	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: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
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)
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:M:174:LEU:HD13	1:M:177:LEU:HD11	1.89	0.54
2:E:271:LEU:HD22	2:E:298:ASN:HD21	1.72	0.54
1:M:27:GLY:HA2	1:N:246:PHE:CD2	2.43	0.54
1:P:32:THR:HB	1:P:61:ASN:HD22	1.71	0.54
2:I:94:SER:HB3	2:I:122:TRP:CH2	2.42	0.54
2:G:175:TRP:CZ3	3:H:48:LEU:HD12	2.42	0.54
1:B:196:LYS:HZ3	1:B:202:ASN:CG	2.10	0.54
1:C:259:LEU:HD13	1:C:266:VAL:HG11	1.88	0.54
1:B:72:LYS:HE2	1:B:151:ARG:NH1	2.21	0.54
2:U:281:LEU:HB2	2:U:295:LYS:HE2	1.90	0.54
2:K:271:LEU:HD22	2:K:298:ASN:HD21	1.71	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
1:C:54:ILE:HA	1:C:86:MET:O	2.07	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
1:O:243:ILE:HA	1:O:271:VAL:HG13	1.88	0.54
2:K:116:ILE:HA	2:K:119:MET:CE	2.38	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: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
1:D:305:LEU:CD2	2:K:42:ARG:HH21	2.18	0.54
1:C:50:GLN:NE2	1:C:76:LYS:HE2	2.20	0.54
3:V:39:THR:HG23	3:V:40:ASN:N	2.22	0.54
2:E:208:HIS:NE2	3:F:29:LYS:HG2	2.22	0.54
2:Q:263:PHE:HB2	2:Q:289:PHE:CE1	2.42	0.54
2:K:90:VAL:HG21	2:K:123:SER:HA	1.88	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
3:H:35:LEU:HA	3:H:38:VAL:HG23	1.90	0.54
1:O:16:THR:HA	1:O:46:GLN:HE22	1.73	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:A:193:ILE:C	1:A:195:ASN:H	2.11	0.54
1:O:138:GLU:HB3	1:O:176:PHE:HD1	1.73	0.54
1:N:201:LEU:HD13	1:O:146:MET:HB3	1.90	0.54
1:M:174:LEU:HB3	1:M:177:LEU:HG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:228:GLN:NE2	1:P:205:MET:SD	2.81	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
1:N:16:THR:HG22	1:N:46:GLN:HE21	1.73	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
1:P:227:ARG:HB3	1:P:227:ARG:HH11	1.71	0.54
1:O:284:ASN:N	1:O:284:ASN:HD22	2.05	0.54
2:W:90:VAL:CG2	2:W:123:SER:HA	2.38	0.54
2:K:202:SER:HB2	3:L:33:LYS:HB2	1.89	0.54
1:C:138:GLU:CG	1:C:175:ARG:HB3	2.24	0.53
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:W:61:LEU:HD22	2:W:100:ARG:NH2	2.23	0.53
2:Q:90:VAL:CG2	2:Q:123:SER:HA	2.38	0.53
2:Q:20:PHE:CE1	2:Q:32:ALA:HB1	2.43	0.53
1:C:16:THR:HA	1:C:46:GLN:HE22	1.72	0.53
1:P:193:ILE:C	1:P:195:ASN:H	2.10	0.53
2:K:90:VAL:CG2	2:K:123:SER:HA	2.38	0.53
1:B:315:PRO:HB3	1:B:338:TYR:CE2	2.44	0.53
1:P:267:ASN:O	1:P:310:HIS:HB2	2.07	0.53
1:O:249:LEU:HD11	1:O:298:TYR:HB3	1.90	0.53
1:O:54:ILE:HA	1:O:86:MET:O	2.08	0.53
1:B:259:LEU:HD13	1:B:266:VAL:HG11	1.90	0.53
1:B:178:GLN:NE2	1:B:261:SER:HB2	2.22	0.53
1:M:199:PRO:HG3	1:C:156:GLU:CB	2.39	0.53
1:D:284:ASN:HD22	1:D:284:ASN:N	2.04	0.53
1:N:278:GLU:OE1	1:N:292:TRP:HZ3	1.92	0.53
1:P:29:VAL:HG22	1:P:243:ILE:HG23	1.90	0.53
2:G:271:LEU:HD22	2:G:298:ASN:HD21	1.74	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: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:D:233:PRO:HB3	2:K:9:MET:N	2.24	0.53
1:O:263:ASP:O	2:U:9:MET:CE	2.57	0.53
2:K:116:ILE:HA	2:K:119:MET:HE2	1.90	0.53
1:A:133:ILE:HB	1:A:136:ILE:HD12	1.91	0.53
1:D:174:LEU:C	1:D:177:LEU:HG	2.28	0.53
1:O:202:ASN:N	1:O:202:ASN:ND2	2.54	0.53

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ILE:HA	1:A:86:MET:O	2.10	0.52
1:D:174:LEU:HB3	1:D:177:LEU:HG	1.90	0.52
1:P:259:LEU:HD13	1:P:266:VAL:HG11	1.91	0.52
1:O:179:LEU:HG	1:O:183:LEU:HD13	1.91	0.52
1:N:143:MET:CG	1:O:197:LEU:HB2	2.40	0.52
1:C:141:SER:O	1:C:145:VAL:HG13	2.09	0.52
2:U:202:SER:HB2	3:V:33:LYS:CB	2.36	0.52
2:E:112:LEU:HD23	2:E:149:PHE:CE2	2.43	0.52
1:A:7:PRO:HG2	1:A:337:GLU:HG2	1.90	0.52
1:M:54:ILE:HA	1:M:86:MET:O	2.10	0.52
1:P:254:ARG:HG3	1:P:255:LEU:N	2.24	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:P:201:LEU:HG	1:P:205:MET:CE	2.39	0.52
1:A:202:ASN:ND2	1:A:202:ASN:N	2.55	0.52
1:P:257:GLN:HE22	2:W:45:ARG:HB2	1.74	0.52
1:A:54:ILE:HD11	1:A:88:ILE:HG12	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:M:199:PRO:CG	1:C:156:GLU:HB3	2.38	0.52
1:B:197:LEU:O	1:C:143:MET:HE2	2.08	0.52
1:N:215:LYS:HA	1:N:218:GLU:HG2	1.90	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:N:279:ASN:HB3	1:N:341:ILE:HD13	1.91	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: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
1:B:195:ASN:N	1:B:195:ASN:ND2	2.58	0.52
1:D:243:ILE:HG22	1:D:272:ASN:O	2.09	0.52
1:M:141:SER:O	1:M:145:VAL:HG13	2.09	0.52
2:S:263:PHE:HB2	2:S:289:PHE:CE1	2.45	0.52
1:M:254:ARG:HG3	1:M:255:LEU:N	2.25	0.52
1:D:254:ARG:HG3	1:D:255:LEU:N	2.24	0.52
1:D:21:ILE:HB	1:D:164:ILE:HD13	1.92	0.52
2:I:20:PHE:CE1	2:I:32:ALA:HB1	2.44	0.52
3:R:49:LYS:N	3:R:49:LYS:HD2	2.24	0.52
1:D:258:GLU:HG2	1:D:262:TYR:CE2	2.44	0.52
1:N:263:ASP:HB3	2:S:9:MET:SD	2.50	0.52
1:C:174:LEU:HB3	1:C:177:LEU:HG	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:LYS:O	1:B:197:LEU:C	2.48	0.52
3:R:39:THR:HG23	3:R:40:ASN:N	2.23	0.52
1:B:54:ILE:HD11	1:B:88:ILE:HG12	1.92	0.52
1:O:6:GLU:O	1:O:310:HIS:HD2	1.92	0.52
1:N:258:GLU:HG2	1:N:262:TYR:CE2	2.45	0.52
1:D:184:SER:O	1:D:187:LEU:HB2	2.10	0.52
1:N:147:LYS:HZ1	1:O:197:LEU:CD2	2.23	0.52
1:A:184:SER:O	1:A: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: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
2:G:286:GLN:HG2	2:G:291:ILE:O	2.09	0.52
2:K:263:PHE:HB2	2:K:289:PHE:CE1	2.45	0.52
2:I:263:PHE:HB2	2:I:289:PHE:CE1	2.45	0.52
1:B:6:GLU:O	1:B:310:HIS:HD2	1.93	0.52
1:P:249:LEU:HD11	1:P:298:TYR:HB3	1.91	0.52
1:N:254:ARG:HG3	1:N:255:LEU:N	2.25	0.52
1:B:258:GLU:HG2	1:B:262:TYR:CE2	2.45	0.52
1:O:12:LEU:O	1:O:12:LEU:HD22	2.10	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
2:G:217:ARG:NE	1:M:154:GLN:NE2	2.57	0.52
3:T:39:THR:HG23	3:T:40:ASN:N	2.22	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
2:U:112:LEU:HD23	2:U:149:PHE:CE2	2.44	0.52
2:S:154:GLU:HG3	2:S:168:TYR:CE1	2.45	0.52
2:Q:283:PHE:CE1	3:R:42:GLY:HA2	2.44	0.52
1:B:249:LEU:HD11	1:B:298:TYR:HB3	1.92	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:B:174:LEU:HB3	1:B:177:LEU:HG	1.91	0.51
2:Q:134:PRO:HG3	3:R:35:LEU:HD23	1.90	0.51
2:S:271:LEU:HD22	2:S:298:ASN:HD21	1.75	0.51
1:A:227:ARG:HH11	1:A:227:ARG:HB3	1.74	0.51
1:N:217:ASN:CG	1:O:217:ASN:CG	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:THR:HG22	1:D:61:ASN:HD22	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
1:N:196:LYS:O	1:N:197:LEU:C	2.49	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:C:153:GLU:O	1:C:158:GLU:HA	2.10	0.51
1:M:249:LEU:HD11	1:M:298:TYR:HB3	1.92	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:O:146:MET:HE2	1:O:149:ILE:HG13	1.92	0.51
2:G:213:ILE:O	2:G:217:ARG:HG3	2.10	0.51
2:E:263:PHE:HB2	2:E:289:PHE:CZ	2.46	0.51
1:A:256:ILE:O	1:A:260:ILE:HG13	2.11	0.51
2:S:90:VAL:CG2	2:S:123:SER:HA	2.41	0.51
1:M:184:SER:O	1:M:187:LEU:HB2	2.11	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:C:32:THR:CB	1:C:61:ASN:HD22	2.24	0.51
1:A:15:SER:OG	1:A:18:HIS:HD2	1.94	0.51
1:O:174:LEU:HB3	1:O:177:LEU:CD1	2.41	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:D:7:PRO:HG2	1:D:337:GLU:HG2	1.93	0.51
1:B:143:MET:SD	1:C:196:LYS:CE	2.97	0.51
1:M:194:THR:HG22	1:P:183:LEU:CD1	2.39	0.51
1:O:191:GLY:O	1:O:195:ASN:ND2	2.43	0.51
1:O:50:GLN:NE2	1:O:76:LYS:HE2	2.19	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: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:B:138:GLU:CB	1:B:176:PHE:HB3	2.34	0.51
1:M:205:MET:SD	1:P:228:GLN:NE2	2.84	0.51
1:C:147:LYS:HA	1:C:150:LYS:HE3	1.93	0.51
1:O:29:VAL:O	1:O:29:VAL:HG13	2.11	0.51
2:K:263:PHE:HB2	2:K:289:PHE:CZ	2.46	0.51
2:G:263:PHE:HB2	2:G:289:PHE:CE1	2.46	0.51
1:M:6:GLU:O	1:M:310:HIS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:279:ASN:OD1	1:N:341:ILE:HD11	2.11	0.51
1:N:32:THR:CB	1:N:61:ASN:HD22	2.24	0.51
1:A:249:LEU:HD11	1:A:298:TYR:HB3	1.93	0.51
2:Q:61:LEU:HD22	2:Q:100:ARG:NH2	2.26	0.51
1:D:12:LEU:O	1:D:12:LEU:HD22	2.09	0.51
1:B:143:MET:SD	1:C:201:LEU:HB3	2.47	0.51
1:P:180:PRO:O	1:P:225:THR:HG21	2.10	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
2:K:112:LEU:HD23	2:K:149:PHE:CE2	2.45	0.51
2:Q:191:PHE:HZ	2:Q:211:LYS:HG3	1.76	0.51
1:A:32:THR:CB	1:A:61:ASN:HD22	2.24	0.51
1:O:195:ASN:ND2	1:O:195:ASN:N	2.54	0.50
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:C:52:LEU:HD12	1:C:163:VAL:HG13	1.94	0.50
1:P:134:PRO:O	1:P:179:LEU:HD22	2.10	0.50
1:B:16:THR:HG22	1:B:46:GLN:HE21	1.76	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
2:G:218:PHE:HZ	2:G:242:TYR:CZ	2.29	0.50
1:O:138:GLU:CB	1:O:176:PHE:HB3	2.35	0.50
2:G:217:ARG:HH21	1:M:154:GLN:NE2	2.07	0.50
3:X:35:LEU:HD12	3:X:38:VAL:CG2	2.36	0.50
1:B:196:LYS:NZ	1:B:202:ASN:CG	2.65	0.50
2:U:175:TRP:CZ2	3:V:48:LEU:HB2	2.45	0.50
2:G:102:ILE:HG21	2:G:139:THR:HG22	1.94	0.50
2:Q:116:ILE:HA	2:Q:119:MET:CE	2.41	0.50
1:P:72:LYS:CE	1:P:151:ARG:HH12	2.24	0.50
2:I:124:ILE:HG12	2:I:132:GLY:N	2.27	0.50
1:P:184:SER:O	1:P:187:LEU:HB2	2.11	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:B:201:LEU:HB3	1:C:143:MET:SD	2.52	0.50
1:D:29:VAL:O	1:D:29:VAL:HG13	2.11	0.50
2:G:116:ILE:HA	2:G:119:MET:CE	2.41	0.50
2:G:90:VAL:HG21	2:G:123:SER:HA	1.92	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:I:205:SER:HA	3:J:29:LYS:O	2.12	0.50
1:C:236:THR:HG22	1:C:264:MET:HE3	1.94	0.50
2:G:90:VAL:CG2	2:G:123:SER:HA	2.40	0.50
2:U:20:PHE:CE1	2:U:32:ALA:HB1	2.47	0.50
1:B:141:SER:O	1:B:145:VAL:HG13	2.12	0.50
1:O:145:VAL:O	1:O:149:ILE:HG12	2.11	0.50
1:D:267:ASN:HB3	2:K:12:LYS:HD2	1.93	0.50
2:W:263:PHE:HB2	2:W:289:PHE:CE1	2.47	0.50
1:P:279:ASN:HB3	1:P:341:ILE:HD13	1.92	0.50
1:N:233:PRO:HG2	2:S:11:ALA:HB3	1.93	0.50
1:A:178:GLN:NE2	1:A:261:SER:HB2	2.26	0.50
1:M:202:ASN:ND2	1:M:202:ASN:N	2.58	0.50
1:P:145:VAL:O	1:P:149:ILE:HG12	2.12	0.50
1:D:263:ASP:O	2:K:9:MET:SD	2.69	0.50
1:P:54:ILE:HD11	1:P:88:ILE:HG12	1.93	0.50
2:W:175:TRP:CZ3	3:X:48:LEU:HD12	2.47	0.50
1:A:12:LEU:O	1:A:12:LEU:HD22	2.12	0.50
1:A:178:GLN:CA	1:A:229:GLN:HE22	2.24	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:O:54:ILE:HD11	1:O:88:ILE:HG12	1.93	0.50
2:S:20:PHE:CE1	2:S:32:ALA:HB1	2.47	0.50
1:P:7:PRO:HG2	1:P:337:GLU:HG2	1.94	0.50
1:C:184:SER:O	1:C:187:LEU:HB2	2.11	0.50
1:M:50:GLN:NE2	1:M:76:LYS:HE2	2.21	0.50
2:S:283:PHE:HE1	3:T:40:ASN:HD21	1.59	0.50
2:S:102:ILE:HG21	2:S:139:THR:HG22	1.93	0.50
1:N:198:GLY:HA2	1:N:200:MET:H	1.76	0.50
1:B:147:LYS:HA	1:B:150:LYS:HE3	1.94	0.50
1:O:62:LEU:HB2	1:O:87:GLU:OE1	2.12	0.50
1:A:52:LEU:HD12	1:A:163:VAL:HG13	1.93	0.50
1:B:279:ASN:HB3	1:B:341:ILE:HD13	1.93	0.50
3:H:35:LEU:HD12	3:H:38:VAL:CG2	2.40	0.49
1:B:202:ASN:ND2	1:B:202:ASN:N	2.55	0.49
2:E:278:LYS:HG3	2:E:295:LYS:HG2	1.94	0.49
1:C:6:GLU:O	1:C:310:HIS:HD2	1.95	0.49
1:N:6:GLU:O	1:N:310:HIS:HD2	1.94	0.49
2:U:263:PHE:HB2	2:U:289:PHE:CZ	2.47	0.49
2:S:90:VAL:HG21	2:S:123:SER:HA	1.93	0.49
1:A:32:THR:HB	1:A:61:ASN:HD22	1.77	0.49
1:D:246:PHE:CD2	1:C:27:GLY:HA2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:GLU:HG2	1:C:262:TYR:CE2	2.46	0.49
1:P:258:GLU:HG2	1:P:262:TYR:CE2	2.46	0.49
3:X:49:LYS:N	3:X:49:LYS:HD2	2.27	0.49
1:M:180:PRO:HA	1:M:183:LEU:HD21	1.94	0.49
2:Q:116:ILE:HA	2:Q:119:MET:HE2	1.95	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:D:278:GLU:OE1	1:D:292:TRP:HZ3	1.96	0.49
1:P:275:LEU:HB2	1:P:292:TRP:CD1	2.47	0.49
1:O:52:LEU:HD12	1:O:163:VAL:HG13	1.94	0.49
1:N:174:LEU:C	1:N:177:LEU:HG	2.31	0.49
2:E:202:SER:CB	3:F:33:LYS:HB2	2.38	0.49
1:A:147:LYS:HZ3	1:D:197:LEU:HD13	1.74	0.49
1:O:72:LYS:CE	1:O:151:ARG:HH12	2.23	0.49
2:I:256:GLN:HE22	3:J:29:LYS:HG3	1.77	0.49
2:W:208:HIS:NE2	3:X:29:LYS:HG2	2.27	0.49
2:U:229:ILE:HG21	3:V:14:SER:HA	1.93	0.49
2:K:61:LEU:HD22	2:K:100:ARG:NH2	2.27	0.49
1:O:153:GLU:O	1:O:158:GLU:HA	2.12	0.49
1:B:196:LYS:HG2	1:B:202:ASN:OD1	2.13	0.49
1:C:243:ILE:HG22	1:C:272:ASN:O	2.13	0.49
2:W:102:ILE:HG21	2:W:139:THR:HG22	1.93	0.49
1:D:6:GLU:O	1:D:310:HIS:HD2	1.96	0.49
1:P:274:LEU:HD12	1:P:313:LYS:HB3	1.95	0.49
1:O:5:VAL:HG11	1:O:309:PHE:O	2.12	0.49
1:N:32:THR:HG22	1:N:61:ASN:HD22	1.77	0.49
1:B:155:GLY:O	1:B:156:GLU:HB2	2.11	0.49
1:A:180:PRO:O	1:A:225:THR:HG21	2.12	0.49
1:C:135:GLY:HA3	1:C:179:LEU:CD2	2.36	0.49
1:D:141:SER:O	1:D:145:VAL:HG13	2.12	0.49
1:N:260:ILE:HD13	2:S:42:ARG:CG	2.43	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
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:N:143:MET:HB3	1:O:197:LEU:CB	2.35	0.49
2:K:102:ILE:HD11	2:K:119:MET:SD	2.53	0.49
1:B:12:LEU:HD22	1:B:12:LEU:O	2.12	0.49
1:A:134:PRO:O	1:A:179:LEU:HD22	2.12	0.49
1:M:174:LEU:C	1:M:177:LEU:HG	2.32	0.49
1:A:50:GLN:NE2	1:A:76:LYS:HE2	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:175:TRP:CE3	3:V:48:LEU:HD12	2.47	0.49
2:I:150:VAL:CG1	2:I:151:TYR:N	2.73	0.49
1:O:243:ILE:HG22	1:O:272:ASN:O	2.13	0.49
1:A:29:VAL:HG21	1:A:242:CYS:CA	2.39	0.49
1:N:32:THR:CG2	1:N:61:ASN:HD22	2.25	0.49
1:D:307:GLU:OE1	2:K:35:THR:HG22	2.12	0.49
1:P:15:SER:OG	1:P:18:HIS:HD2	1.96	0.49
3:F:49:LYS:N	3:F:49:LYS:HD2	2.28	0.49
1:C:178:GLN:CA	1:C:229:GLN:HE22	2.26	0.49
1:B:198:GLY:HA2	1:B:200:MET:H	1.78	0.49
1:M:16:THR:HG22	1:M:46:GLN:HE21	1.74	0.49
1:C:274:LEU:HD22	1:C:299:LEU:HD11	1.94	0.49
2:W:278:LYS:HG3	2:W:295:LYS:HG2	1.94	0.49
2:S:191:PHE:CZ	2:S:211:LYS:HG3	2.48	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
1:M:153:GLU:O	1:M:158:GLU:HA	2.12	0.49
2:U:124:ILE:HG12	2:U:132:GLY:N	2.27	0.49
1:D:260:ILE:HG21	2:K:46:SER:OG	2.13	0.49
1:B:177:LEU:N	1:B:177:LEU:HD23	2.28	0.49
1:N:134:PRO:O	1:N:179:LEU:HD22	2.13	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
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:A:141:SER:O	1:A:145:VAL:HG13	2.12	0.49
2:I:150:VAL:CG1	2:I:151:TYR:H	2.23	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
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:O:32:THR:CB	1:O:61:ASN:HD22	2.26	0.49
1:C:62:LEU:HB2	1:C:87:GLU:OE1	2.13	0.49
1:M:198:GLY:CA	1:M:200:MET:H	2.26	0.49
3:H:49:LYS:HD2	3:H:49:LYS:N	2.28	0.49
1:P:178:GLN:CA	1:P:229:GLN:HE22	2.26	0.49
1:O:184:SER:O	1:O:187:LEU:HB2	2.13	0.49
1:M:180:PRO:O	1:M:225:THR:HG21	2.13	0.49
1:A:187:LEU:HD21	1:D:190:PHE:CD1	2.48	0.49
1:M:201:LEU:HG	1:M:205:MET:CE	2.43	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)
2:E:283:PHE:HE1	3:F:40:ASN:HD21	1.60	0.49
2:I:204:ILE:HG22	2:I:208:HIS:HD2	1.77	0.49
2:G:236:ILE:HD11	2:G:253:ILE:HD12	1.95	0.49
1:O:32:THR:CG2	1:O:61:ASN:HD22	2.26	0.49
2:I:191:PHE:HZ	2:I:211:LYS:HG3	1.76	0.49
1:N:7:PRO:HG2	1:N:337:GLU:HG2	1.94	0.49
3:L:49:LYS:HD2	3:L:49:LYS:N	2.28	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:N:138:GLU:CB	1:N:176:PHE:HB3	2.36	0.48
1:O:174:LEU:HD13	1:O:177:LEU:CD1	2.44	0.48
1:M:174:LEU:HD13	1:M:177:LEU:CD1	2.43	0.48
1:P:243:ILE:HG22	1:P:272:ASN:O	2.12	0.48
1:M:29:VAL:HG21	1:M:242:CYS:CA	2.41	0.48
1:N:274:LEU:HD12	1:N:313:LYS:HB3	1.95	0.48
1:D:153:GLU:HB3	1:D:158:GLU:O	2.13	0.48
1:B:10:HIS:HD2	1:B:335:ASN:ND2	2.12	0.48
1:P:62:LEU:HB2	1:P:87:GLU:OE1	2.13	0.48
2:K:154:GLU:HG3	2:K:168:TYR:CE1	2.48	0.48
3:J:49:LYS:HD2	3:J:49:LYS:N	2.28	0.48
1:M:12:LEU:O	1:M:12:LEU:HD22	2.13	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
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:S:150:VAL:CG1	2:S:151:TYR:H	2.26	0.48
1:C:281:GLN:O	1:C:282:GLU:CB	2.61	0.48
1:D:54:ILE:HD12	1:D:86:MET:HB3	1.95	0.48
2:U:227:GLU:OE2	3:V:10:HIS:NE2	2.46	0.48
2:Q:52:ALA:O	2:Q:56:ILE:HG13	2.13	0.48
1:B:201:LEU:HD22	1:C:146:MET:CB	2.41	0.48
2:G:116:ILE:HA	2:G:119:MET:HE2	1.95	0.48
2:G:112:LEU:HD23	2:G:149:PHE:CE2	2.46	0.48
2:U:151:TYR:OH	3:V:47:THR:HG23	2.13	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:E:61:LEU:HD22	2:E:100:ARG:NH2	2.28	0.48
1:P:190:PHE:CD1	1:P:190:PHE:C	2.86	0.48
1:C:178:GLN:HA	1:C:229:GLN:NE2	2.26	0.48
1:M:177:LEU:N	1:M:177:LEU:HD23	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:39:THR:HG23	3:J:40:ASN:N	2.26	0.48
1:D:145:VAL:O	1:D:149:ILE:HG12	2.14	0.48
1:C:29:VAL:HG13	1:C:29:VAL:O	2.13	0.48
1:N:243:ILE:HG22	1:N:272:ASN:O	2.13	0.48
3:H:39:THR:HG23	3:H:40:ASN:N	2.26	0.48
2:Q:112:LEU:HD23	2:Q:149:PHE:CE2	2.47	0.48
2:I:263:PHE:HB2	2:I:289:PHE:CZ	2.48	0.48
1:P:32:THR:CG2	1:P:61:ASN:HD22	2.26	0.48
2:W:202:SER:HB2	3:X:33:LYS:CB	2.43	0.48
1:B:32:THR:HG22	1:B:61:ASN:HD22	1.77	0.48
2:K:218:PHE:HZ	2:K:242:TYR:CZ	2.32	0.48
1:B:145:VAL:O	1:B:149:ILE:HG12	2.13	0.48
1:C:145:VAL:O	1:C:149:ILE:HG12	2.14	0.48
1:M:72:LYS:CE	1:M:151:ARG:HH12	2.20	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:A:247:LEU:CB	1:B:247:LEU:HD13	2.43	0.48
2:K:282:GLU:O	2:K:286:GLN:HG3	2.13	0.48
1:D:275:LEU:HB2	1:D:292:TRP:CD1	2.48	0.48
1:M:7:PRO:HG2	1:M:337:GLU:HG2	1.94	0.48
1:C:276:PHE:HA	1:C:292:TRP:CZ2	2.49	0.48
1:B:143:MET:HG3	1:C:196:LYS:HG3	1.95	0.48
1:B:72:LYS:CE	1:B:151:ARG:HH12	2.25	0.48
1:P:260:ILE:HG22	2:W:46:SER:OG	2.13	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
1:A:174:LEU:CD1	1:A:177:LEU:HD11	2.42	0.48
2:G:115:VAL:HG12	2:G:119:MET:CE	2.43	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:275:LEU:HB2	1:A:292:TRP:CD1	2.49	0.48
1:B:143:MET:SD	1:C:201:LEU:CD2	2.94	0.48
1:C:196:LYS:O	1:C:197:LEU:C	2.52	0.48
1:N:180:PRO:HA	1:N:183:LEU:HD21	1.96	0.48
2:G:204:ILE:HG22	2:G:208:HIS:HD2	1.79	0.48
1:N:29:VAL:HG21	1:N:242:CYS:CA	2.44	0.48
1:A:274:LEU:HD12	1:A:313:LYS:HB3	1.96	0.48
2:K:194:LEU:HD22	2:K:210:SER:HB2	1.96	0.48
1:M:134:PRO:O	1:M:179:LEU:HD22	2.13	0.48
1:C:134:PRO:O	1:C:179:LEU:HD22	2.14	0.48
1:D:196:LYS:O	1:D:197:LEU:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:O	1:A:149:ILE:HG12	2.13	0.48
1:N:153:GLU:HB3	1:N:158:GLU:O	2.14	0.48
1:M:276:PHE:HA	1:M:292:TRP:CZ2	2.49	0.48
1:A:32:THR:HG22	1:A:61:ASN:HD22	1.79	0.48
2:G:52:ALA:O	2:G:56:ILE:HG13	2.14	0.48
1:B:52:LEU:HD12	1:B:163:VAL:HG13	1.95	0.48
2:I:61:LEU:HD22	2:I:100:ARG:NH2	2.29	0.48
1:O:190:PHE:CD1	1:O:190:PHE:C	2.87	0.47
1:C:174:LEU:C	1:C:177:LEU:HG	2.33	0.47
1:A:196:LYS:NZ	1:A:202:ASN:CG	2.67	0.47
2:W:112:LEU:HD23	2:W:149:PHE:CE2	2.47	0.47
1:P:276:PHE:HA	1:P:292:TRP:CZ2	2.49	0.47
2:I:172:LEU:HD21	2:I:193:ARG:HD3	1.95	0.47
1:C:202:ASN:N	1:C:202:ASN:ND2	2.60	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:N:184:SER:O	1:N:187:LEU:HB2	2.14	0.47
3:R:35:LEU:HD12	3:R:38:VAL:CG2	2.38	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:U:102:ILE:HD11	2:U:119:MET:SD	2.54	0.47
1:O:198:GLY:HA2	1:O:200:MET:H	1.79	0.47
2:K:52:ALA:O	2:K:56:ILE:HG13	2.15	0.47
1:B:138:GLU:HB3	1:B:176:PHE:HD1	1.78	0.47
1:N:147:LYS:NZ	1:O:197:LEU:HD22	2.29	0.47
2:I:42:ARG:HH21	1:C:305:LEU:HD22	1.76	0.47
1:C:174:LEU:HD22	1:C:177:LEU:CD1	2.34	0.47
2:I:102:ILE:HD11	2:I:119:MET:SD	2.55	0.47
1:M:259:LEU:CD1	1:M:266:VAL:HG11	2.45	0.47
2:I:218:PHE:HZ	2:I:242:TYR:CZ	2.32	0.47
1:D:195:ASN:ND2	1:D:195:ASN:N	2.62	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:U:150:VAL:CG1	2:U:151:TYR:N	2.78	0.47
2:I:204:ILE:HG12	3:J:31:TYR:HD2	1.80	0.47
2:W:94:SER:HB3	2:W:122:TRP:CZ2	2.49	0.47
2:S:263:PHE:HB2	2:S:289:PHE:CZ	2.49	0.47
1:A:6:GLU:O	1:A:310:HIS:HD2	1.96	0.47
1:C:77:VAL:HG22	1:C:80:MET:HB2	1.95	0.47
1:C:215:LYS:HA	1:C:218:GLU:HG2	1.96	0.47
2:S:204:ILE:HG22	2:S:208:HIS:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:VAL:HG13	1:B:29:VAL:O	2.13	0.47
2:S:150:VAL:CG1	2:S:151:TYR:N	2.75	0.47
1:D:5:VAL:N	2:K:19:ARG:NH1	2.63	0.47
1:B:283:HIS:O	1:B:284:ASN:HB2	2.15	0.47
1:P:231:THR:O	1:P:232:ASP:O	2.32	0.47
2:G:124:ILE:HG12	2:G:132:GLY:N	2.28	0.47
1:D:138:GLU:HB3	1:D:176:PHE:HD1	1.79	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:M:29:VAL:HG23	1:M:243:ILE:HG12	1.96	0.47
1:A:5:VAL:HG11	1:A:309:PHE:O	2.15	0.47
2:K:204:ILE:CG1	3:L:31:TYR:HD2	2.28	0.47
1:C:280:ASP:HB2	1:C:348:TYR:OH	2.14	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:A:194:THR:HG22	1:D:183:LEU:CD1	2.45	0.47
1:P:154:GLN:HG3	1:C:79:GLY:O	2.15	0.47
1:N:190:PHE:C	1:N:190:PHE:CD1	2.87	0.47
1:B:180:PRO:HA	1:B:183:LEU:HD21	1.96	0.47
1:C:146:MET:HE2	1:C:149:ILE:HG13	1.96	0.47
1:A:147:LYS:HA	1:A:150:LYS:HE3	1.97	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:M:281:GLN:O	1:M:282:GLU:CB	2.63	0.47
2:E:94:SER:HB3	2:E:122:TRP:CZ2	2.50	0.47
1:N:217:ASN:OD1	1:O:217:ASN:ND2	2.47	0.47
2:E:191:PHE:CZ	2:E:211:LYS:HG3	2.49	0.47
2:G:191:PHE:CZ	2:G:211:LYS:HG3	2.50	0.47
1:B:10:HIS:HD2	1:B:335:ASN:HD21	1.63	0.47
1:B:32:THR:CB	1:B:61:ASN:HD22	2.27	0.47
1:B:276:PHE:HA	1:B:292:TRP:CZ2	2.49	0.47
2:G:188:ALA:HB2	2:G:244:ASP:HB3	1.97	0.47
1:B:15:SER:OG	1:B:18:HIS:HD2	1.97	0.47
1:C:15:SER:OG	1:C:18:HIS:HD2	1.97	0.47
2:K:159:LEU:HD21	3:L:41:LEU:HD22	1.97	0.47
1:P:174:LEU:CG	1:P:177:LEU:HD11	2.45	0.47
1:M:178:GLN:NE2	1:M:261:SER:HB2	2.30	0.47
1:P:196:LYS:O	1:P:197:LEU:C	2.52	0.47
1:M:305:LEU:HD22	2:Q:42:ARG:HH22	1.73	0.47
2:Q:102:ILE:HD11	2:Q:119:MET:SD	2.55	0.47
2:U:102:ILE:HG21	2:U:139:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:17:LEU:CD1	2:U:58:GLN:HG2	2.44	0.47
2:U:204:ILE:HG22	2:U:208:HIS:HD2	1.79	0.47
1:P:32:THR:HG22	1:P:61:ASN:HD22	1.80	0.47
1:D:32:THR:CG2	1:D:61:ASN:HD22	2.27	0.47
1:D:276:PHE:HA	1:D:292:TRP:CZ2	2.50	0.47
1:B:32:THR:CG2	1:B:61:ASN:HD22	2.28	0.47
1:D:73:ASP:HA	1:D:152:GLN:CD	2.35	0.47
1:P:153:GLU:O	1:P:158:GLU:HA	2.15	0.47
1:M:195:ASN:ND2	1:M:195:ASN:N	2.63	0.47
1:O:178:GLN:HA	1:O:229:GLN:NE2	2.29	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:C:195:ASN:N	1:C:195:ASN:ND2	2.62	0.47
1:C:32:THR:HB	1:C:61:ASN:HD22	1.80	0.47
1:O:346:VAL:O	1:O:349:GLU:HB3	2.14	0.47
1:M:54:ILE:HD11	1:M:88:ILE:CD1	2.45	0.47
1:C:278:GLU:OE1	1:C:292:TRP:HZ3	1.98	0.47
1:C:73:ASP:HA	1:C:152:GLN:CD	2.34	0.47
3:X:39:THR:HG23	3:X:40:ASN:OD1	2.15	0.47
2:I:102:ILE:HG21	2:I:139:THR:HG22	1.97	0.47
2:G:94:SER:HB3	2:G:122:TRP:CZ2	2.49	0.47
1:A:32:THR:CG2	1:A:61:ASN:HD22	2.28	0.47
2:U:87:GLU:HA	2:U:126:PHE:CZ	2.50	0.47
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
2:U:202:SER:CB	3:V:33:LYS:HB2	2.42	0.46
2:K:102:ILE:HG21	2:K:139:THR:HG22	1.97	0.46
1:O:20:TRP:CB	1:O:236:THR:HG23	2.45	0.46
1:M:274:LEU:HD22	1:M:299:LEU:HD11	1.97	0.46
2:G:189:GLU:HB3	3:H:48:LEU:CD2	2.45	0.46
1:P:279:ASN:OD1	1:P:341:ILE:HD11	2.14	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
2:S:218:PHE:HZ	2:S:242:TYR:CZ	2.33	0.46
1:P:178:GLN:HA	1:P:229:GLN:NE2	2.28	0.46
1:M:190:PHE:CD1	1:P:187:LEU:HD21	2.50	0.46
3:V:35:LEU:HD12	3:V:38:VAL:CG2	2.37	0.46
1:D:73:ASP:HA	1:D:152:GLN:NE2	2.30	0.46
2:W:205:SER:HB2	3:X:32:THR:HG23	1.97	0.46
1:B:73:ASP:HA	1:B:152:GLN:CD	2.35	0.46
2:E:124:ILE:HG12	2:E:132:GLY:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:THR:HG22	1:D:231:THR:O	2.15	0.46
1:B:174:LEU:HD13	1:B:177:LEU:HD11	1.97	0.46
1:M:193:ILE:C	1:M:195:ASN:N	2.69	0.46
1:M:190:PHE:CE2	1:P:183:LEU:HB2	2.50	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:B:174:LEU:C	1:B:177:LEU:HG	2.32	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:C:177:LEU:HD23	1:C:177:LEU:N	2.31	0.46
1:P:191:GLY:O	1:P:195:ASN:ND2	2.48	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:N:281:GLN:O	1:N:282:GLU:CB	2.64	0.46
2:I:12:LYS:HE3	1:C:267:ASN:HB2	1.98	0.46
2:G:263:PHE:HB2	2:G:289:PHE:CZ	2.51	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:D:247:LEU:HD13	1:C:247:LEU:CB	2.46	0.46
1:C:54:ILE:HD11	1:C:88:ILE:HG12	1.98	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:M:138:GLU:HB3	1:M:176:PHE:HD1	1.79	0.46
1:P:174:LEU:HB3	1:P:177:LEU:HG	1.98	0.46
1:B:184:SER:O	1:B:187:LEU:HB2	2.14	0.46
1:N:201:LEU:HG	1:N:205:MET:CE	2.46	0.46
1:M:285:CYS:SG	1:M:288:CYS:HB2	2.55	0.46
2:K:94:SER:HB3	2:K:122:TRP:CZ2	2.50	0.46
1:B:32:THR:HB	1:B:61:ASN:HD22	1.81	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:O:174:LEU:HD22	1:O:177:LEU:CD1	2.32	0.46
1:D:281:GLN:O	1:D:282:GLU:CB	2.63	0.46
2:G:189:GLU:HB3	3:H:48:LEU:HD22	1.98	0.46
2:Q:218:PHE:HZ	2:Q:242:TYR:CZ	2.34	0.46
2:K:124:ILE:HG12	2:K:132:GLY:N	2.31	0.46
2:G:171:LEU:HD23	2:G:171:LEU:C	2.36	0.46
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:D:215:LYS:HA	1:D:218:GLU:HG2	1.97	0.46
2:K:115:VAL:HG12	2:K:119:MET:CE	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:347:ILE:C	1:P:349:GLU:N	2.69	0.46
2:G:154:GLU:HG3	2:G:168:TYR:CE1	2.51	0.46
1:N:10:HIS:HD2	1:N:335:ASN:HD21	1.64	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:O:180:PRO:HA	1:O:183:LEU:HD21	1.98	0.46
1:B:230:PHE:HA	2:G:9:MET:HE1	1.97	0.46
2:U:175:TRP:CH2	3:V:48:LEU:HD12	2.50	0.46
2:E:189:GLU:HB3	3:F:48:LEU:HD21	1.98	0.46
2:E:112:LEU:CD1	2:E:143:LYS:HD2	2.46	0.46
2:W:281:LEU:HB2	2:W:295:LYS:HE2	1.98	0.46
2:Q:94:SER:HB3	2:Q:122:TRP:CZ2	2.51	0.46
1:B:347:ILE:C	1:B:349:GLU:N	2.69	0.46
1:O:32:THR:HB	1:O:61:ASN:HD22	1.80	0.46
1:C:73:ASP:HA	1:C:152:GLN:NE2	2.31	0.46
2:Q:124:ILE:HG12	2:Q:132:GLY:N	2.30	0.46
2:E:232:ASN:HB2	3:F:21:THR:HB	1.98	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:N:236:THR:HG22	1:N:264:MET:HE3	1.97	0.46
1:C:259:LEU:CD1	1:C:266:VAL:HG11	2.46	0.46
1:P:260:ILE:CD1	2:W:42:ARG:HG2	2.47	0.46
1:N:5:VAL:HG11	1:N:309:PHE:O	2.16	0.46
2:W:124:ILE:HG12	2:W:132:GLY:N	2.31	0.46
1:C:10:HIS:HD2	1:C:335:ASN:ND2	2.14	0.46
1:D:15:SER:OG	1:D:18:HIS:HD2	1.99	0.46
2:W:171:LEU:C	2:W:171:LEU:HD23	2.36	0.46
2:G:227:GLU:HG3	2:G:227:GLU:O	2.16	0.46
3:X:19:LEU:HD12	3:X:19:LEU:O	2.14	0.46
1:A:138:GLU:HB3	1:A:176:PHE:HD1	1.80	0.45
1:P:215:LYS:HA	1:P:218:GLU:HG2	1.98	0.45
1:O:16:THR:HB	1:O:49:LYS:CE	2.46	0.45
2:U:278:LYS:HG3	2:U:295:LYS:HG2	1.98	0.45
1:M:278:GLU:OE1	1:M:292:TRP:HZ3	1.99	0.45
1:P:278:GLU:OE1	1:P:292:TRP:HZ3	1.98	0.45
1:A:233:PRO:HB3	2:E:9:MET:N	2.31	0.45
2:S:145:LEU:HG	3:T:54:GLN:HE22	1.80	0.45
1:D:180:PRO:O	1:D:225:THR:HG21	2.15	0.45
1:N:197:LEU:O	1:O:143:MET:CE	2.64	0.45
1:O:201:LEU:HG	1:O:205:MET:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:20:TRP:HE3	1:N:165:PHE:HE2	1.64	0.45
2:G:283:PHE:HE1	3:H:40:ASN:HD21	1.64	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
2:I:282:GLU:O	2:I:286:GLN:HG3	2.16	0.45
1:A:283:HIS:O	1:A:284:ASN:HB2	2.17	0.45
1:N:283:HIS:O	1:N:284:ASN:HB2	2.16	0.45
2:S:94:SER:HB3	2:S:122:TRP:CZ2	2.50	0.45
1:C:279:ASN:OD1	1:C:341:ILE:HD11	2.17	0.45
1:O:153:GLU:HB3	1:O:158:GLU:O	2.17	0.45
1:M:280:ASP:HB2	1:M:348:TYR:OH	2.16	0.45
2:U:188:ALA:HB2	2:U:244:ASP:HB3	1.97	0.45
2:Q:89:LYS:HA	2:Q:126:PHE:HB3	1.99	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
3:R:19:LEU:O	3:R:19:LEU:HD12	2.16	0.45
1:P:180:PRO:HA	1:P:183:LEU:HD21	1.98	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
2:W:91:ASP:O	2:W:95:VAL:HG23	2.17	0.45
1:P:155:GLY:O	1:P:156:GLU:HB2	2.16	0.45
1:B:280:ASP:HB2	1:B:348:TYR:OH	2.16	0.45
1:C:12:LEU:HD22	1:C:12:LEU:O	2.17	0.45
2:E:102:ILE:HD11	2:E:119:MET:SD	2.56	0.45
2:W:115:VAL:HG12	2:W:119:MET:CE	2.47	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:K:175:TRP:CH2	3:L:48:LEU:HD12	2.51	0.45
1:D:274:LEU:HD22	1:D:299:LEU:HD11	1.98	0.45
1:B:281:GLN:O	1:B:282:GLU:CB	2.64	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
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
1:M:190:PHE:CD1	1:M:190:PHE:C	2.89	0.45
1:B:201:LEU:HG	1:B:205:MET:CE	2.47	0.45
1:A:196:LYS:O	1:A:197:LEU:C	2.54	0.45
1:O:29:VAL:HG21	1:O:242:CYS:CA	2.42	0.45
2:E:111:ASN:O	2:E:112:LEU:C	2.55	0.45
2:Q:202:SER:HB2	3:R:33:LYS:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:204:ILE:HG22	2:Q:208:HIS:HD2	1.82	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
1:A:62:LEU:HB2	1:A:87:GLU:OE1	2.16	0.45
2:U:171:LEU:HD23	2:U:171:LEU:C	2.37	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
1:P:257:GLN:NE2	2:W:45:ARG:CB	2.79	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:A:274:LEU:HD22	1:A:299:LEU:HD11	1.99	0.45
1:N:276:PHE:HA	1:N:292:TRP:CZ2	2.51	0.45
2:I:87:GLU:HA	2:I:126:PHE:CZ	2.51	0.45
2:W:283:PHE:CE1	3:X:42:GLY:HA2	2.52	0.45
2:Q:279:SER:HB2	3:R:43:VAL:HG11	1.98	0.45
2:G:89:LYS:HA	2:G:126:PHE:HB3	1.98	0.45
2:W:227:GLU:O	2:W:227:GLU:HG3	2.17	0.45
1:C:138:GLU:HB3	1:C:176:PHE:HD1	1.81	0.45
1:A:205:MET:O	1:D:228:GLN:HG2	2.15	0.45
1:N:196:LYS:HG3	1:O:143:MET:HG3	1.99	0.45
2:W:150:VAL:CG1	2:W:151:TYR:N	2.78	0.45
2:U:111:ASN:O	2:U:112:LEU:C	2.55	0.45
2:I:111:ASN:O	2:I:112:LEU:C	2.55	0.45
2:U:236:ILE:HD11	2:U:253:ILE:HD12	1.98	0.45
1:C:274:LEU:HD12	1:C:313:LYS:HB3	1.99	0.45
1:P:153:GLU:HB3	1:P:158:GLU:O	2.16	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
2:E:89:LYS:HA	2:E:126:PHE:HB3	1.99	0.45
1:P:12:LEU:HD22	1:P:12:LEU:O	2.17	0.45
2:U:112:LEU:CD1	2:U:143:LYS:HD2	2.46	0.45
1:O:54:ILE:HG13	1:O:86:MET:O	2.17	0.45
1:C:275:LEU:HD11	1:C:291:ARG:HD3	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:C	2:K:171:LEU:HD23	2.38	0.45
1:N:286:LYS:HD3	1:N:286:LYS:H	1.81	0.45
1:A:190:PHE:CD1	1:D:187:LEU:HD21	2.52	0.45
1:M:187:LEU:CD1	1:P:190:PHE:CE1	2.94	0.45
1:B:16:THR:HB	1:B:49:LYS:CE	2.47	0.45
2:E:150:VAL:CG1	2:E:151:TYR:N	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:256:GLN:HE22	3:F:29:LYS:CG	2.27	0.45
2:U:225:LYS:HB2	2:U:240:GLU:HB2	1.98	0.45
2:K:17:LEU:CD1	2:K:58:GLN:HG2	2.46	0.45
2:W:111:ASN:O	2:W:112:LEU:C	2.55	0.45
1:O:279:ASN:OD1	1:O:341:ILE:HD11	2.17	0.45
1:P:198:GLY:HA2	1:P:200:MET:H	1.82	0.45
1:D:292:TRP:CZ3	1:D:296:LYS:HE2	2.51	0.45
2:G:194:LEU:HD22	2:G:210:SER:HB2	1.99	0.45
1:N:10:HIS:HD2	1:N:335:ASN:ND2	2.14	0.45
2:Q:154:GLU:HG3	2:Q:168:TYR:CE1	2.51	0.45
1:A:280:ASP:HB2	1:A:348:TYR:OH	2.17	0.45
1:P:73:ASP:HA	1:P:152:GLN:CD	2.38	0.45
1:M:256:ILE:O	1:M:260:ILE:HG13	2.17	0.45
1:N:29:VAL:HG23	1:N:243:ILE:HG12	1.98	0.45
1:P:257:GLN:NE2	2:W:45:ARG:HB2	2.31	0.45
2:E:204:ILE:HG22	2:E:208:HIS:HD2	1.81	0.45
1:P:20:TRP:HE3	1:P:165:PHE:HE2	1.65	0.45
1:B:150:LYS:HE2	1:C:200:MET:HG2	1.99	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
2:E:172:LEU:HD21	2:E:193:ARG:HD3	1.98	0.45
1:M:15:SER:OG	1:M:18:HIS:HD2	2.00	0.45
2:I:188:ALA:HB2	2:I:244:ASP:HB3	1.99	0.45
2:E:171:LEU:C	2:E:171:LEU:HD23	2.37	0.45
1:M:199:PRO:CG	1:C:156:GLU:CG	2.96	0.44
2:W:234:TYR:HB2	3:X:21:THR:HG21	1.99	0.44
1:P:29:VAL:HG23	1:P:243:ILE:HG12	1.99	0.44
1:N:141:SER:O	1:N:145:VAL:HG13	2.17	0.44
1:D:20:TRP:HE3	1:D:165:PHE:HE2	1.65	0.44
1:B:274:LEU:HD12	1:B:313:LYS:HB3	1.98	0.44
1:D:247:LEU:HB3	1:C:247:LEU:HB3	1.98	0.44
1:A:198:GLY:HA2	1:A:200:MET:H	1.81	0.44
1:N:292:TRP:CZ3	1:N:296:LYS:HE2	2.52	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
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:U:40:ALA:O	2:U:44:VAL:HG23	2.17	0.44
2:K:172:LEU:HD21	2:K:193:ARG:HD3	1.99	0.44
1:N:179:LEU:HG	1:N:183:LEU:HD13	2.00	0.44
1:O:196:LYS:NZ	1:O:202:ASN:CG	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:GLY:O	1:C:156:GLU:HB2	2.16	0.44
1:D:190:PHE:C	1:D:190:PHE:CD1	2.91	0.44
1:A:215:LYS:HA	1:A:218:GLU:HG2	1.97	0.44
1:N:274:LEU:HD22	1:N:299:LEU:HD11	1.98	0.44
1:M:20:TRP:HE3	1:M:165:PHE:HE2	1.65	0.44
1:P:281:GLN:O	1:P:282:GLU:CB	2.65	0.44
2:E:282:GLU:O	2:E:286:GLN:HG3	2.17	0.44
1:A:172:HIS:HB3	1:A:258:GLU:OE2	2.17	0.44
1:C:347:ILE:C	1:C:349:GLU:N	2.70	0.44
1:D:279:ASN:OD1	1:D:341:ILE:HD11	2.17	0.44
1:C:276:PHE:HA	1:C:292:TRP:CE2	2.52	0.44
2:W:188:ALA:HB2	2:W:244:ASP:HB3	1.99	0.44
1:B:307:GLU:CD	2:G:35:THR:HG22	2.38	0.44
2:S:89:LYS:HA	2:S:126:PHE:HB3	1.99	0.44
1:N:168:ALA:HB1	1:N:169:PRO:HD2	2.00	0.44
1:B:143:MET:CG	1:C:196:LYS:HD2	2.47	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:K:111:ASN:O	2:K:112:LEU:C	2.55	0.44
2:I:202:SER:HB2	3:J:33:LYS:CB	2.46	0.44
1:M:347:ILE:C	1:M:349:GLU:N	2.70	0.44
2:I:94:SER:HB3	2:I:122:TRP:CZ2	2.52	0.44
2:U:154:GLU:HG3	2:U:168:TYR:CE1	2.52	0.44
2:E:179:VAL:HB	2:E:182:ILE:HD13	2.00	0.44
2:W:168:TYR:CE2	2:W:194:LEU:HD23	2.52	0.44
2:S:52:ALA:O	2:S:56:ILE:HG13	2.17	0.44
2:I:9:MET:HE1	1:C:263:ASP:O	2.17	0.44
1:N:233:PRO:CG	2:S:11:ALA:HB3	2.48	0.44
1:M:147:LYS:HZ1	1:P:197:LEU:CD1	2.22	0.44
2:G:150:VAL:CG1	2:G:151:TYR:N	2.78	0.44
2:Q:111:ASN:O	2:Q:112:LEU:C	2.56	0.44
1:P:281:GLN:HA	1:P:281:GLN:NE2	2.31	0.44
1:D:347:ILE:C	1:D:349:GLU:N	2.71	0.44
1:D:346:VAL:O	1:D:349:GLU:HB3	2.17	0.44
2:Q:231:LYS:HB2	3:R:17:LEU:HG	1.99	0.44
2:U:89:LYS:HA	2:U:126:PHE:HB3	1.99	0.44
1:O:276:PHE:HA	1:O:292:TRP:CE2	2.53	0.44
1:A:155:GLY:O	1:A:156:GLU:HB2	2.18	0.44
1:C:312:VAL:HG21	1:C:334:LEU:HD23	1.99	0.44
1:B:153:GLU:O	1:B:158:GLU:HA	2.16	0.44
2:S:179:VAL:HB	2:S:182:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:168:TYR:CE2	2:E:194:LEU:HD23	2.53	0.44
1:B:259:LEU:CD1	1:B:266:VAL:HG11	2.47	0.44
1:M:178:GLN:CA	1:M:229:GLN:HE22	2.30	0.44
1:A:178:GLN:HA	1:A:229:GLN:NE2	2.30	0.44
1:B:230:PHE:CG	2:G:9:MET:HE3	2.52	0.44
2:G:208:HIS:NE2	3:H:29:LYS:HG2	2.32	0.44
2:U:115:VAL:HG12	2:U:119:MET:CE	2.48	0.44
2:G:112:LEU:CD1	2:G:143:LYS:HD2	2.47	0.44
1:N:260:ILE:HG22	2:S:46:SER:OG	2.18	0.44
2:K:236:ILE:HD11	2:K:253:ILE:HD12	2.00	0.44
1:C:254:ARG:HG3	1:C:255:LEU:H	1.82	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
1:A:230:PHE:HA	2:E:9:MET:HE1	2.00	0.44
1:A:168:ALA:HB1	1:A:169:PRO:HD2	1.99	0.44
2:E:231:LYS:HB2	3:F:17:LEU:HG	1.99	0.44
1:D:180:PRO:HB2	1:D:225:THR:CG2	2.48	0.44
1:N:180:PRO:O	1:N:225:THR:HG21	2.17	0.44
2:K:116:ILE:HD13	2:K:144:LEU:HG	1.99	0.44
2:E:281:LEU:HB2	2:E:295:LYS:HE2	1.98	0.44
1:A:247:LEU:HD13	1:B:247:LEU:CB	2.46	0.44
1:C:283:HIS:O	1:C:284:ASN:HB2	2.17	0.44
2:E:178:GLN:NE2	3:F:53:LYS:O	2.50	0.44
1:N:259:LEU:CD1	1:N:266:VAL:HG11	2.47	0.44
2:S:278:LYS:CG	2:S:295:LYS:HG2	2.48	0.44
1:N:244:SER:OG	1:N:299:LEU:HG	2.18	0.44
2:G:107:PRO:HB3	2:G:146:GLU:HB3	2.00	0.44
1:O:247:LEU:CB	1:P:247:LEU:HD13	2.48	0.44
2:S:227:GLU:O	2:S:227:GLU:HG3	2.18	0.44
2:K:227:GLU:HG3	2:K:227:GLU:O	2.18	0.44
1:D:178:GLN:NE2	1:D:261:SER:HB2	2.32	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
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:O:247:LEU:HD13	1:P:247:LEU:HB3	2.00	0.44
1:A:77:VAL:HG22	1:A:80:MET:HB2	2.00	0.44
2:U:9:MET:CG	2:U:10:GLY:N	2.81	0.44
1:P:147:LYS:HA	1:P:150:LYS:HE3	1.99	0.44
1:P:16:THR:HB	1:P:49:LYS:CE	2.48	0.44
1:O:76:LYS:HD3	1:O:84:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:LYS:HA	1:D:150:LYS:HE3	1.99	0.44
3:F:39:THR:HG23	3:F:40:ASN:OD1	2.18	0.44
2:U:275:GLN:HA	2:U:275:GLN:NE2	2.33	0.44
1:P:283:HIS:O	1:P:284:ASN:HB2	2.18	0.44
1:A:20:TRP:HE3	1:A:165:PHE:HE2	1.66	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:D:263:ASP:O	2:K:9:MET:HE1	2.17	0.44
2:U:238:PHE:CE2	3:V:10:HIS:HB2	2.53	0.44
2:E:52:ALA:O	2:E:56:ILE:HG13	2.17	0.44
1:O:280:ASP:HB2	1:O:348:TYR:OH	2.18	0.44
1:P:24:GLY:HA2	1:P:167:THR:OG1	2.17	0.44
1:N:231:THR:O	1:N:232:ASP:O	2.36	0.43
2:S:236:ILE:HD11	2:S:253:ILE:HD12	2.00	0.43
3:V:39:THR:HG23	3:V:40:ASN:OD1	2.18	0.43
2:E:116:ILE:HD13	2:E:144:LEU:HG	2.00	0.43
1:P:193:ILE:C	1:P:195:ASN:N	2.72	0.43
1:N:242:CYS:HB2	1:N:248:SER:OG	2.18	0.43
1:D:172:HIS:HB3	1:D:258:GLU:OE2	2.17	0.43
1:D:32:THR:CB	1:D:61:ASN:HD22	2.31	0.43
2:U:227:GLU:O	2:U:227:GLU:HG3	2.18	0.43
1:O:292:TRP:CZ3	1:O:296:LYS:HE2	2.53	0.43
2:Q:168:TYR:CE2	2:Q:194:LEU:HD23	2.53	0.43
2:E:194:LEU:HD22	2:E:210:SER:HB2	1.99	0.43
2:Q:172:LEU:HD21	2:Q:193:ARG:HD3	1.99	0.43
1:O:181:ASN:ND2	1:O:226:ILE:HG12	2.33	0.43
1:O:168:ALA:HB1	1:O:169:PRO:HD2	1.99	0.43
2:I:250:LEU:HD11	3:J:13:VAL:HG22	1.99	0.43
2:Q:171:LEU:HD23	2:Q:171:LEU:C	2.38	0.43
2:S:171:LEU:C	2:S:171:LEU:HD23	2.38	0.43
1:N:194:THR:C	1:N:195:ASN:HD22	2.22	0.43
1:M:135:GLY:HA3	1:M:179:LEU:CD2	2.39	0.43
2:I:231:LYS:HB2	3:J:17:LEU:HG	2.00	0.43
1:N:54:ILE:HD12	1:N:86:MET:HB3	2.00	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
2:G:87:GLU:HA	2:G:126:PHE:CZ	2.53	0.43
1:M:253:GLU:OE1	2:Q:45:ARG:NH2	2.51	0.43
2:E:40:ALA:O	2:E:44:VAL:HG23	2.17	0.43
1:A:199:PRO:O	1:A:203:SER:HB2	2.18	0.43

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:193:ILE:C	1:N:195:ASN:N	2.72	0.43
1:D:193:ILE:C	1:D: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
3:L:39:THR:HG23	3:L:40:ASN:OD1	2.18	0.43
2:Q:116:ILE:HD13	2:Q:144:LEU:HG	2.01	0.43
2:K:231:LYS:HB2	3:L:17:LEU:HG	2.01	0.43
1:M:32:THR:CG2	1:M:61:ASN:HD22	2.32	0.43
2:W:202:SER:CB	3:X:33:LYS:HB2	2.49	0.43
1:D:275:LEU:HD11	1:D:291:ARG:HD3	1.99	0.43
1:C:275:LEU:HB2	1:C:292:TRP:CD1	2.53	0.43
2:G:40:ALA:O	2:G:44:VAL:HG23	2.18	0.43
1:C:24:GLY:HA2	1:C:167:THR:OG1	2.18	0.43
1:D:10:HIS:HD2	1:D:335:ASN:ND2	2.17	0.43
1:M:193:ILE:O	1:M:195:ASN:N	2.52	0.43
1:O:174:LEU:CG	1:O:177:LEU:HD11	2.49	0.43
1:C:180:PRO:O	1:C:225:THR:HG21	2.19	0.43
2:G:9:MET:CG	2:G:10:GLY:N	2.82	0.43
1:D:27:GLY:HA2	1:C:246:PHE:CE2	2.53	0.43
1:O:347:ILE:C	1:O:349:GLU:N	2.71	0.43
1:N:275:LEU:HD11	1:N:291:ARG:HD3	2.00	0.43
1:A:278:GLU:OE1	1:A:292:TRP:HZ3	2.02	0.43
1:O:275:LEU:HD11	1:O:291:ARG:HD3	2.00	0.43
2:E:232:ASN:HB2	3:F:21:THR:CB	2.48	0.43
2:W:193:ARG:HA	3:X:45:LEU:HD13	2.01	0.43
1:P:179:LEU:N	1:P:180:PRO:CD	2.81	0.43
1:N:180:PRO:HA	1:N:183:LEU:CD2	2.49	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:M:143:MET:HE2	1:P:197:LEU:CB	2.45	0.43
2:G:150:VAL:CG1	2:G:151:TYR:H	2.31	0.43
1:A:347:ILE:C	1:A:349:GLU:N	2.71	0.43
1:B:292:TRP:CZ3	1:B:296:LYS:HE2	2.54	0.43
1:O:155:GLY:O	1:O:156:GLU:HB2	2.17	0.43
2:K:188:ALA:HB2	2:K:244:ASP:HB3	2.01	0.43
1:N:190:PHE:CZ	1:O:183:LEU:CG	2.96	0.43
1:B:198:GLY:CA	1:B:200:MET:N	2.82	0.43
1:C:29:VAL:HG23	1:C:243:ILE:HG12	2.00	0.43
1:O:260:ILE:HD13	2:U:42:ARG:HG2	2.01	0.43
2:E:150:VAL:CG1	2:E:151:TYR:H	2.29	0.43
2:S:281:LEU:HB2	2:S:295:LYS:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:204:ILE:HG12	3:V:31:TYR:HD2	1.83	0.43
1:O:254:ARG:HG3	1:O:255:LEU:H	1.83	0.43
1:P:276:PHE:HA	1:P:292:TRP:CE2	2.53	0.43
2:G:168:TYR:CE2	2:G:194:LEU:HD23	2.54	0.43
1:A:344:GLY:O	1:A:348:TYR:HD2	2.02	0.43
2:G:172:LEU:HD21	2:G:193:ARG:HD3	1.99	0.43
1:P:280:ASP:HB2	1:P:348:TYR:OH	2.19	0.43
1:P:174:LEU:CD1	1:P:177:LEU:HD11	2.45	0.42
1:A:29:VAL:O	1:A:29:VAL:HG13	2.19	0.42
2:I:16:THR:HG21	1:C:308:ASP:CG	2.39	0.42
1:M:283:HIS:O	1:M:284:ASN:HB2	2.19	0.42
1:B:236:THR:HG22	1:B:264:MET:HE3	2.00	0.42
1:M:276:PHE:HA	1:M:292:TRP:CE2	2.54	0.42
2:E:179:VAL:HB	2:E:182:ILE:CD1	2.49	0.42
1:P:10:HIS:HD2	1:P:335:ASN:ND2	2.17	0.42
2:I:179:VAL:HB	2:I:182:ILE:HD13	2.01	0.42
2:Q:188:ALA:HB2	2:Q:244:ASP:HB3	2.00	0.42
1:P:16:THR:CG2	1:P:46:GLN:NE2	2.75	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
2:S:116:ILE:HD13	2:S:144:LEU:HG	2.01	0.42
1:C:198:GLY:HA2	1:C:200:MET:H	1.82	0.42
1:B:54:ILE:HD12	1:B:86:MET:HB3	2.00	0.42
1:B:275:LEU:HB2	1:B:292:TRP:CD1	2.53	0.42
2:W:179:VAL:HB	2:W:182:ILE:HD13	2.01	0.42
1:O:10:HIS:HD2	1:O:335:ASN:ND2	2.17	0.42
1:C:168:ALA:HB1	1:C:169:PRO:HD2	1.99	0.42
1:D:344:GLY:O	1:D:348:TYR:HD2	2.01	0.42
1:D:168:ALA:HB1	1:D:169:PRO:HD2	1.99	0.42
2:Q:227:GLU:O	2:Q:227:GLU:HG3	2.18	0.42
1:N:190:PHE:CE2	1:O:183:LEU:CB	2.95	0.42
1:B:179:LEU:HG	1:B:183:LEU:HD13	2.01	0.42
1:A:174:LEU:HB3	1:A:177:LEU:HG	2.01	0.42
1:C:180:PRO:HB2	1:C:225:THR:CG2	2.49	0.42
2:S:102:ILE:HD11	2:S:119:MET:SD	2.60	0.42
2:W:102:ILE:HD11	2:W:119:MET:SD	2.59	0.42
2:U:116:ILE:HD13	2:U:144:LEU:HG	2.00	0.42
1:A:244:SER:OG	1:A:299:LEU:HG	2.19	0.42
1:O:274:LEU:HD22	1:O:299:LEU:HD11	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:LEU:HD22	1:D:53:LEU:N	2.34	0.42
1:A:73:ASP:HA	1:A:152:GLN:CD	2.40	0.42
2:S:231:LYS:HE2	3:T:18:THR:OG1	2.18	0.42
2:S:232:ASN:HB2	3:T:21:THR:HB	2.01	0.42
1:B:178:GLN:HE22	1:B:261:SER:HB2	1.83	0.42
1:D:194:THR:C	1:D:195:ASN:HD22	2.22	0.42
1:M:147:LYS:HZ2	1:P:197:LEU:HD13	1.78	0.42
2:W:98:LEU:O	2:W:102:ILE:HG13	2.19	0.42
2:Q:105:LEU:CB	2:Q:143:LYS:HE2	2.50	0.42
2:I:275:GLN:NE2	2:I:275:GLN:HA	2.34	0.42
1:B:274:LEU:HD22	1:B:299:LEU:HD11	2.00	0.42
3:V:52:TYR:O	3:V:53:LYS:HG3	2.20	0.42
2:I:194:LEU:HD22	2:I:210:SER:HB2	2.01	0.42
2:S:23:LYS:HD3	2:S:31:GLU:HB3	2.01	0.42
1:N:24:GLY:HA2	1:N:167:THR:OG1	2.19	0.42
2:E:188:ALA:HB2	2:E:244:ASP:HB3	2.01	0.42
1:D:179:LEU:N	1:D:180:PRO:CD	2.81	0.42
1:A:138:GLU:H	1:A:138:GLU:CD	2.22	0.42
1:P:154:GLN:OE1	1:C:79:GLY:HA3	2.19	0.42
1:M:179:LEU:N	1:M:180:PRO:CD	2.82	0.42
2:I:283:PHE:CZ	3:J:42:GLY:HA2	2.54	0.42
1:M:244:SER:OG	1:M:299:LEU:HG	2.18	0.42
1:C:172:HIS:HB3	1:C:258:GLU:OE2	2.19	0.42
1:M:279:ASN:OD1	1:M:341:ILE:HD11	2.19	0.42
2:I:216:GLU:O	2:I:220:GLU:HG3	2.20	0.42
2:E:91:ASP:O	2:E:95:VAL:HG23	2.19	0.42
1:O:22:PHE:CE1	1:O:174:LEU:HD21	2.54	0.42
1:A:201:LEU:HG	1:A:205:MET:CE	2.50	0.42
1:C:174:LEU:HD22	1:C:177:LEU:HD21	2.02	0.42
2:S:133:ASP:HA	2:S:134:PRO:HD3	1.90	0.42
1:B:200:MET:CE	1:C:150:LYS:HE2	2.49	0.42
3:J:39:THR:HG23	3:J:40:ASN:OD1	2.20	0.42
1:O:227:ARG:CZ	1:O:227:ARG:HB3	2.50	0.42
1:C:242:CYS:HB2	1:C:248:SER:OG	2.20	0.42
2:Q:115:VAL:HG12	2:Q:119:MET:CE	2.49	0.42
2:U:98:LEU:O	2:U:102:ILE:HG13	2.19	0.42
2:I:278:LYS:HG3	2:I:295:LYS:HG2	2.01	0.42
1:A:284:ASN:ND2	1:A:284:ASN:N	2.67	0.42
1:O:281:GLN:NE2	1:O:281:GLN:HA	2.34	0.42
1:B:20:TRP:CB	1:B:236:THR:HG23	2.50	0.42
1:N:198:GLY:CA	1:N:200:MET:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:254:THR:HG22	2:K:289:PHE:HZ	1.85	0.42
1:P:54:ILE:HD11	1:P:88:ILE:CD1	2.50	0.42
2:K:193:ARG:HA	3:L:45:LEU:HD13	2.01	0.42
1:A:253:GLU:OE1	2:E:45:ARG:NH2	2.52	0.42
2:S:221:LYS:HD3	2:S:222:PHE:CE2	2.55	0.42
2:S:172:LEU:HD21	2:S:193:ARG:HD3	2.01	0.42
2:W:133:ASP:HA	2:W:134:PRO:HD3	1.90	0.42
2:I:227:GLU:HG3	2:I:227:GLU:O	2.19	0.42
1:A:183:LEU:HG	1:D:190:PHE:CZ	2.54	0.42
2:U:9:MET:HG2	2:U:10:GLY:H	1.85	0.42
1:N:215:LYS:NZ	1:N:215:LYS:HB2	2.35	0.42
2:I:116:ILE:HD13	2:I:144:LEU:HG	2.02	0.42
2:Q:150:VAL:CG1	2:Q:151:TYR:H	2.29	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:U:179:VAL:HG22	3:V:50:TYR:CG	2.54	0.42
2:W:194:LEU:HD22	2:W:210:SER:HB2	2.00	0.42
2:I:9:MET:CE	1:C:263:ASP:O	2.68	0.42
1:A:23:VAL:HA	1:A:239:VAL:O	2.18	0.42
2:G:225:LYS:HB2	2:G:240:GLU:HB2	2.00	0.42
2:U:183:GLU:HG2	2:U:184:ASP:N	2.35	0.42
2:U:172:LEU:HD21	2:U:193:ARG:HD3	2.02	0.42
1:P:178:GLN:NE2	1:P:261:SER:HB2	2.35	0.42
1:N:147:LYS:HA	1:N:150:LYS:HE3	2.01	0.42
2:U:256:GLN:HE22	3:V:29:LYS:CG	2.32	0.42
1:D:231:THR:O	1:D:232:ASP:O	2.38	0.42
2:G:179:VAL:HB	2:G:182:ILE:CD1	2.50	0.42
1:M:73:ASP:HA	1:M:152:GLN:CD	2.40	0.42
1:M:62:LEU:HB2	1:M:87:GLU:OE1	2.19	0.42
2:S:183:GLU:CG	2:S:184:ASP:N	2.82	0.42
1:B:24:GLY:HA2	1:B:167:THR:OG1	2.19	0.42
1:D:312:VAL:HG21	1:D:334:LEU:HD23	2.02	0.42
2:E:227:GLU:O	2:E:227:GLU:HG3	2.18	0.42
1:P:22:PHE:CE1	1:P:174:LEU:HD21	2.55	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
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:B:194:THR:CG2	1:C:183:LEU:HD11	2.47	0.42
1:N:196:LYS:HE2	1:N:202:ASN:ND2	2.35	0.42
1:P:196:LYS:NZ	1:P:202:ASN:CG	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:35:LEU:HD12	3:X:35:LEU:HA	1.92	0.42
2:U:133:ASP:HA	2:U:134:PRO:HD3	1.90	0.42
1:B:16:THR:HB	1:B:49:LYS:HE2	2.01	0.42
2:I:236:ILE:HD11	2:I:253:ILE:HD12	2.02	0.42
2:W:283:PHE:CZ	3:X:42:GLY:HA2	2.55	0.42
1:C:231:THR:O	1:C:232:ASP:O	2.38	0.42
2:G:231:LYS:HB2	3:H:17:LEU:HG	2.02	0.42
1:O:57:ASP:OD1	1:O:58:PRO:HD2	2.20	0.42
1:A:190:PHE:CZ	1:D:183:LEU:HG	2.55	0.42
1:O:196:LYS:HG2	1:O:196:LYS:HZ3	1.67	0.42
2:K:133:ASP:HA	2:K:134:PRO:HD3	1.90	0.42
1:O:20:TRP:HE3	1:O:165:PHE:CE2	2.38	0.42
2:W:236:ILE:HD11	2:W:253:ILE:HD12	2.02	0.42
1:N:275:LEU:HB2	1:N:292:TRP:CD1	2.55	0.42
1:D:263:ASP:O	2:K:9:MET:CE	2.67	0.42
2:U:234:TYR:HB2	3:V:21:THR:HG21	2.02	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
1:A:57:ASP:OD1	1:A:58:PRO:HD2	2.19	0.42
1:B:146:MET:HE2	1:B:149:ILE:HG13	2.02	0.41
1:C:201:LEU:HG	1:C:205:MET:CE	2.51	0.41
1:B:178:GLN:CA	1:B:229:GLN:HE22	2.32	0.41
1:O:259:LEU:CD1	1:O:266:VAL:HG11	2.49	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:D:198:GLY:CA	1:D:200:MET:N	2.81	0.41
1:A:20:TRP:HE3	1:A:165:PHE:CE2	2.38	0.41
1:O:275:LEU:HB2	1:O:292:TRP:CD1	2.55	0.41
1:B:21:ILE:HB	1:B:164:ILE:HD13	2.02	0.41
1:O:193:ILE:C	1:O:195:ASN:N	2.73	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:O:233:PRO:HB3	2:U:9:MET:N	2.35	0.41
2:G:217:ARG:HE	1:M:154:GLN:NE2	2.17	0.41
2:Q:133:ASP:HA	2:Q:134:PRO:HD3	1.90	0.41
1:B:196:LYS:HG3	1:C:143:MET:HG3	2.01	0.41
1:C:16:THR:HB	1:C:49:LYS:CE	2.50	0.41
1:O:305:LEU:HD22	2:U:42:ARG:NH2	2.35	0.41
2:S:190:PHE:CE1	3:T:48:LEU:HD13	2.55	0.41
1:B:56:THR:HB	1:B:90:PRO:CG	2.48	0.41
1:D:198:GLY:C	1:D:200:MET:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:54:ILE:HD12	1:O:86:MET:HB3	2.02	0.41
1:M:57:ASP:OD1	1:M:58:PRO:HD2	2.20	0.41
2:I:183:GLU:CG	2:I:184:ASP:N	2.82	0.41
1:M:191:GLY:O	1:M:194:THR:OG1	2.36	0.41
1:M:147:LYS:HA	1:M:150:LYS:HE3	2.02	0.41
1:D:16:THR:HB	1:D:49:LYS:HE3	2.01	0.41
1:A:281:GLN:HA	1:A:281:GLN:NE2	2.36	0.41
2:I:35:THR:CG2	1:C:307:GLU:CD	2.89	0.41
1:N:198:GLY:C	1:N:200:MET:H	2.24	0.41
2:Q:61:LEU:HD22	2:Q:100:ARG:HH21	1.85	0.41
1:M:198:GLY:C	1:M:200:MET:H	2.23	0.41
2:U:232:ASN:HB2	3:V:21:THR:CB	2.51	0.41
1:O:77:VAL:HG22	1:O:80:MET:HB2	2.03	0.41
1:N:280:ASP:HB2	1:N:348:TYR:OH	2.20	0.41
2:U:52:ALA:O	2:U:56:ILE:HG13	2.20	0.41
1:M:312:VAL:HG21	1:M:334:LEU:HD23	2.00	0.41
2:W:225:LYS:HB2	2:W:240:GLU:HB2	2.01	0.41
1:M:187:LEU:CG	1:P:190:PHE:CZ	2.99	0.41
1:A:174:LEU:HD22	1:A:177:LEU:HD21	2.01	0.41
1:N:20:TRP:CB	1:N:236:THR:HG23	2.51	0.41
1:P:146:MET:HE2	1:P:149:ILE:HG13	2.03	0.41
1:B:29:VAL:HG21	1:B:242:CYS:CA	2.44	0.41
2:I:98:LEU:O	2:I:102:ILE:HG13	2.20	0.41
2:Q:150:VAL:CG1	2:Q:151:TYR:N	2.78	0.41
1:C:20:TRP:HE3	1:C:165:PHE:HE2	1.68	0.41
1:P:198:GLY:C	1:P:200:MET:H	2.24	0.41
2:Q:191:PHE:CZ	2:Q:211:LYS:HG3	2.54	0.41
1:P:73:ASP:HA	1:P:152:GLN:NE2	2.35	0.41
2:I:179:VAL:HB	2:I:182:ILE:CD1	2.50	0.41
2:I:168:TYR:CE2	2:I:194:LEU:HD23	2.55	0.41
2:E:183:GLU:CG	2:E:184:ASP:N	2.83	0.41
2:U:107:PRO:HB3	2:U:146:GLU:HB3	2.02	0.41
3:T:45:LEU:HB3	3:T:46:PRO:HD2	2.02	0.41
3:H:45:LEU:HB3	3:H:46:PRO:HD2	2.01	0.41
1:P:21:ILE:HB	1:P:164:ILE:HD13	2.02	0.41
1:B:146:MET:HG3	1:C:201:LEU:HD21	2.03	0.41
1:A:180:PRO:HB2	1:A:225:THR:CG2	2.50	0.41
3:F:35:LEU:HA	3:F:35:LEU:HD12	1.91	0.41
1:B:263:ASP:HB3	2:G:9:MET:CE	2.49	0.41
2:W:116:ILE:HD13	2:W:144:LEU:HG	2.02	0.41
2:E:283:PHE:CE1	3:F:42:GLY:HA2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:20:TRP:HE3	1:P:165:PHE:CE2	2.38	0.41
1:M:20:TRP:HE3	1:M:165:PHE:CE2	2.39	0.41
1:A:236:THR:HG22	1:A:264:MET:HE3	2.02	0.41
1:M:291:ARG:HD2	1:N:291:ARG:HD2	2.02	0.41
1:D:256:ILE:O	1:D:260:ILE:HG13	2.21	0.41
2:W:172:LEU:HD21	2:W:193:ARG:HD3	2.02	0.41
1:M:231:THR:O	1:M:232:ASP:O	2.37	0.41
1:B:62:LEU:HB2	1:B:87:GLU:OE1	2.21	0.41
1:C:273:GLN:C	1:C:316:LEU:HB2	2.40	0.41
1:B:57:ASP:OD1	1:B:58:PRO:HD2	2.20	0.41
3:V:35:LEU:HD12	3:V:35:LEU:HA	1.92	0.41
1:B:230:PHE:O	1:B:232:ASP:N	2.53	0.41
1:B:196:LYS:HG3	1:C:143:MET:CG	2.51	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
2:S:253:ILE:O	2:S:256:GLN:HB2	2.21	0.41
1:C:29:VAL:HG21	1:C:242:CYS:CA	2.47	0.41
2:Q:17:LEU:CD1	2:Q:58:GLN:HG2	2.48	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:B:281:GLN:NE2	1:B:281:GLN:HA	2.36	0.41
1:C:198:GLY:CA	1:C:200:MET:N	2.84	0.41
1:B:275:LEU:HD11	1:B:291:ARG:HD3	2.01	0.41
2:W:154:GLU:HG3	2:W:168:TYR:CE1	2.55	0.41
1:P:57:ASP:OD1	1:P:58:PRO:HD2	2.19	0.41
2:E:175:TRP:CG	3:F:52:TYR:HD1	2.38	0.41
2:Q:91:ASP:O	2:Q:95:VAL:HG23	2.20	0.41
1:A:314:MET:CE	1:A:333:PHE:HB2	2.51	0.41
1:M:178:GLN:HA	1:M:229:GLN:NE2	2.34	0.41
1:A:135:GLY:HA3	1:A:179:LEU:CD2	2.38	0.41
2:G:9:MET:HG2	2:G:10:GLY:H	1.85	0.41
2:Q:105:LEU:HB2	2:Q:143:LYS:HE2	2.03	0.41
2:S:175:TRP:CH2	3:T:48:LEU:HD12	2.55	0.41
2:G:275:GLN:HA	2:G:275:GLN:NE2	2.35	0.41
2:U:253:ILE:O	2:U:256:GLN:HB2	2.21	0.41
2:K:202:SER:HB2	3:L:33:LYS:CB	2.50	0.41
1:C:198:GLY:C	1:C:200:MET:H	2.24	0.41
1:M:254:ARG:HG3	1:M:255:LEU:H	1.84	0.41
2:E:193:ARG:HA	3:F:45:LEU:HD13	2.02	0.41
1:O:247:LEU:HB3	1:P:247:LEU:HB3	2.01	0.41
2:Q:193:ARG:HA	3:R:45:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:224:GLU:O	1:O:228:GLN:HG3	2.20	0.41
2:E:107:PRO:HB3	2:E:146:GLU:HB3	2.03	0.41
1:A:193:ILE:C	1:A:195:ASN:N	2.74	0.41
1:N:196:LYS:HZ3	1:N:202:ASN:CG	2.24	0.41
1:N:20:TRP:CE3	1:N:165:PHE:CE2	3.09	0.41
1:P:244:SER:OG	1:P:299:LEU:HG	2.21	0.41
1:M:20:TRP:CB	1:M:236:THR:HG23	2.48	0.41
1:D:20:TRP:HE3	1:D:165:PHE:CE2	2.39	0.41
1:C:281:GLN:NE2	1:C:281:GLN:HA	2.35	0.41
1:M:32:THR:HG22	1:M:61:ASN:HD22	1.86	0.41
1:A:198:GLY:C	1:A:200:MET:H	2.24	0.41
1:O:288:CYS:SG	1:P:287:ARG:HB3	2.61	0.41
1:A:21:ILE:HB	1:A:164:ILE:HD13	2.03	0.41
2:K:238:PHE:HA	2:K:246:ASN:OD1	2.21	0.41
1:B:286:LYS:HD3	1:B:286:LYS:H	1.84	0.41
1:D:135:GLY:HA3	1:D:179:LEU:CD2	2.40	0.41
1:P:177:LEU:HD23	1:P:177:LEU:N	2.35	0.41
1:B:22:PHE:CE1	1:B:174:LEU:HD21	2.55	0.41
1:N:230:PHE:CA	2:S:9:MET:CE	2.91	0.41
1:O:191:GLY:O	1:O:194:THR:OG1	2.31	0.41
1:A:180:PRO:HB2	1:A:225:THR:HG23	2.03	0.41
1:C:179:LEU:N	1:C:180:PRO:CD	2.83	0.41
1:M:205:MET:HG3	1:P:228:GLN:NE2	2.36	0.41
1:C:16:THR:CG2	1:C:46:GLN:NE2	2.79	0.41
1:B:40:ILE:HG21	1:B:328:THR:HG22	2.03	0.41
2:S:115:VAL:HG12	2:S:119:MET:CE	2.50	0.41
1:A:272:ASN:O	1:A:273:GLN:HB2	2.21	0.41
2:G:102:ILE:HD11	2:G:119:MET:SD	2.61	0.41
2:W:150:VAL:CG1	2:W:151:TYR:H	2.29	0.41
2:G:281:LEU:HB2	2:G:295:LYS:HE2	2.02	0.41
1:P:56:THR:HB	1:P:90:PRO:CG	2.49	0.41
1:D:267:ASN:CB	2:K:12:LYS:HZ1	2.31	0.41
1:P:20:TRP:CB	1:P:236:THR:HG23	2.48	0.41
1:A:198:GLY:CA	1:A:200:MET:N	2.83	0.41
2:W:205:SER:HB3	3:X:32:THR:CG2	2.51	0.41
1:O:10:HIS:HD2	1:O:335:ASN:HD21	1.69	0.41
2:I:154:GLU:HG3	2:I:168:TYR:CE1	2.55	0.41
1:M:307:GLU:CD	2:Q:35:THR:HG22	2.41	0.41
2:K:203:ASN:OD1	3:L:32:THR:HG22	2.20	0.41
2:I:40:ALA:O	2:I:44:VAL:HG23	2.21	0.41
1:A:153:GLU:HB3	1:A:158:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:MET:CE	1:C:333:PHE:HB2	2.51	0.41
2:Q:225:LYS:HB2	2:Q:240:GLU:HB2	2.02	0.41
1:P:174:LEU:HB3	1:P:177:LEU:HD11	2.02	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: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
2:W:231:LYS:HB2	3:X:17:LEU:HG	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:M:275:LEU:HD11	1:M:291:ARG:HD3	2.02	0.41
1:N:73:ASP:HA	1:N:152:GLN:CD	2.41	0.41
1:O:314:MET:CE	1:O:333:PHE:HB2	2.51	0.41
2:S:40:ALA:O	2:S:44:VAL:HG23	2.20	0.41
1:O:287:ARG:H	1:O:287:ARG:HG2	1.72	0.41
1:C:57:ASP:OD1	1:C:58:PRO:HD2	2.21	0.41
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
1:C:54:ILE:HD12	1:C:86:MET:HB3	2.03	0.40
3:L:45:LEU:HB3	3:L:46:PRO:HD2	2.03	0.40
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
3:J:45:LEU:HB3	3:J:46:PRO:HD2	2.02	0.40
2:I:189:GLU:HB3	3:J:48:LEU:HD22	2.03	0.40
1:O:73:ASP:HA	1:O:152:GLN:CD	2.41	0.40
2:S:240:GLU:HG2	3:T:6:SER:OG	2.21	0.40
2:S:198:TYR:HD1	2:S:201:ILE:HD11	1.86	0.40
1:P:168:ALA:HB1	1:P:169:PRO:HD2	2.02	0.40
1:P:180:PRO:HB2	1:P:225:THR:CG2	2.51	0.40
1:B:179:LEU:N	1:B:180:PRO:CD	2.82	0.40
1:M:187:LEU:HD21	1:P:190:PHE:CG	2.56	0.40
1:C:180:PRO:HB2	1:C:225:THR:HG23	2.03	0.40
2:S:98:LEU:O	2:S:102:ILE:HG13	2.20	0.40
1:A:273:GLN:C	1:A:316:LEU:HB2	2.42	0.40
1:P:5:VAL:HG11	1:P:309:PHE:O	2.22	0.40
1:M:6:GLU:O	1:M:8:ASN:N	2.49	0.40
1:P:10:HIS:HD2	1:P:335:ASN:HD21	1.70	0.40
2:W:183:GLU:HG2	2:W:184:ASP:N	2.37	0.40
1:A:231:THR:O	1:A:232:ASP:O	2.39	0.40
1:M:10:HIS:HD2	1:M:335:ASN:ND2	2.20	0.40
1:A:24:GLY:HA2	1:A:167:THR:OG1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:155:GLY:O	1:N:156:GLU:HB2	2.22	0.40
1:B:181:ASN:ND2	1:B:226:ILE:HG12	2.36	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
2:G:217:ARG:HE	1:M:154:GLN:HE22	1.63	0.40
1:A:146:MET:HE2	1:A:149:ILE:HG13	2.03	0.40
2:E:98:LEU:O	2:E:102:ILE:HG13	2.22	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:U:231:LYS:HB2	3:V:17:LEU:HG	2.03	0.40
2:Q:189:GLU:HB3	3:R:48:LEU:HD22	2.03	0.40
2:U:179:VAL:HB	2:U:182:ILE:HD13	2.03	0.40
1:D:260:ILE:CG2	2:K:46:SER:OG	2.70	0.40
2:U:227:GLU:CD	3:V:10:HIS:CD2	2.95	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:G:91:ASP:O	2:G:95:VAL:HG23	2.21	0.40
2:E:293:ALA:HA	2:E:294:PRO:HD3	1.98	0.40
1:C:157:GLY:O	1:C:159:THR:N	2.54	0.40
1:C:21:ILE:HB	1:C:164:ILE:HD13	2.03	0.40
1:P:259:LEU:CD1	1:P:266:VAL:HG11	2.51	0.40
1:M:224:GLU:O	1:M:228:GLN:HG3	2.21	0.40
1:B:198:GLY:C	1:B:200:MET:H	2.24	0.40
3:T:39:THR:HG23	3:T:40:ASN:OD1	2.21	0.40
2:E:115:VAL:HG12	2:E:119:MET:HE1	2.04	0.40
1:M:16:THR:HB	1:M:49:LYS:CE	2.50	0.40
1:N:256:ILE:O	1:N:260:ILE:HG13	2.21	0.40
1:C:20:TRP:HE3	1:C:165:PHE:CE2	2.40	0.40
1:P:198:GLY:CA	1:P:200:MET:N	2.83	0.40
2:G:61:LEU:HD22	2:G:100:ARG:HH21	1.85	0.40
2:Q:194:LEU:HD22	2:Q:210:SER:HB2	2.02	0.40
2:E:154:GLU:HG3	2:E:168:TYR:CE1	2.56	0.40
3:R:45:LEU:HB3	3:R:46:PRO:HD2	2.02	0.40
1:B:226:ILE:HG22	1:B:226:ILE:O	2.20	0.40
1:N:57:ASP:OD1	1:N:58:PRO:HD2	2.21	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
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:M:180:PRO:HB2	1:M:225:THR:CG2	2.51	0.40
3:H:35:LEU:HA	3:H:35:LEU:HD12	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:115:VAL:HG12	2:E:119:MET:CE	2.51	0.40
2:Q:98:LEU:O	2:Q:102:ILE:HG13	2.22	0.40
3:H:39:THR:HG23	3:H:40:ASN:OD1	2.22	0.40
2:Q:17:LEU:HA	2:Q:17:LEU:HD23	1.96	0.40
1:A:54:ILE:HD11	1:A:88:ILE:CD1	2.52	0.40
2:Q:253:ILE:O	2:Q:256:GLN:HB2	2.22	0.40
1:M:344:GLY:O	1:M:348:TYR:HD2	2.04	0.40
1:M:231:THR:HG22	1:M:231:THR:O	2.21	0.40
2:I:189:GLU:HB3	3:J:48:LEU:CD2	2.51	0.40
2:W:183:GLU:CG	2:W:184:ASP:N	2.85	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:G:183:GLU:CG	2:G:184:ASP:N	2.84	0.40
1:A:224:GLU:O	1:A:228:GLN:HG3	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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%)	4	35
1	B	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	4	35
1	C	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	4	35
1	D	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	4	35
1	M	298/373 (80%)	257 (86%)	32 (11%)	9 (3%)	5	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	N	298/373 (80%)	257 (86%)	30 (10%)	11 (4%)	4 37
1	O	298/373 (80%)	260 (87%)	26 (9%)	12 (4%)	4 35
1	P	298/373 (80%)	257 (86%)	29 (10%)	12 (4%)	4 35
2	E	289/319 (91%)	269 (93%)	19 (7%)	1 (0%)	46 83
2	G	289/319 (91%)	270 (93%)	18 (6%)	1 (0%)	46 83
2	I	289/319 (91%)	269 (93%)	19 (7%)	1 (0%)	46 83
2	K	289/319 (91%)	269 (93%)	18 (6%)	2 (1%)	26 71
2	Q	289/319 (91%)	268 (93%)	20 (7%)	1 (0%)	46 83
2	S	289/319 (91%)	271 (94%)	17 (6%)	1 (0%)	46 83
2	U	289/319 (91%)	271 (94%)	16 (6%)	2 (1%)	26 71
2	W	289/319 (91%)	268 (93%)	19 (7%)	2 (1%)	26 71
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%)	9 51

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%)	17	54
1	B	272/325 (84%)	251 (92%)	21 (8%)	16	53
1	C	272/325 (84%)	251 (92%)	21 (8%)	16	53
1	D	272/325 (84%)	252 (93%)	20 (7%)	17	54
1	M	272/325 (84%)	252 (93%)	20 (7%)	17	54
1	N	272/325 (84%)	251 (92%)	21 (8%)	16	53
1	O	272/325 (84%)	252 (93%)	20 (7%)	17	54
1	P	272/325 (84%)	253 (93%)	19 (7%)	19	56
2	E	260/284 (92%)	253 (97%)	7 (3%)	52	79
2	G	260/284 (92%)	254 (98%)	6 (2%)	58	83
2	I	260/284 (92%)	254 (98%)	6 (2%)	58	83
2	K	260/284 (92%)	254 (98%)	6 (2%)	58	83
2	Q	260/284 (92%)	253 (97%)	7 (3%)	52	79
2	S	260/284 (92%)	254 (98%)	6 (2%)	58	83
2	U	260/284 (92%)	253 (97%)	7 (3%)	52	79
2	W	260/284 (92%)	254 (98%)	6 (2%)	58	83
3	F	50/52 (96%)	48 (96%)	2 (4%)	38	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	H	50/52 (96%)	47 (94%)	3 (6%)	24 61
3	J	50/52 (96%)	48 (96%)	2 (4%)	38 71
3	L	50/52 (96%)	47 (94%)	3 (6%)	24 61
3	R	50/52 (96%)	47 (94%)	3 (6%)	24 61
3	T	50/52 (96%)	47 (94%)	3 (6%)	24 61
3	V	50/52 (96%)	47 (94%)	3 (6%)	24 61
3	X	50/52 (96%)	47 (94%)	3 (6%)	24 61
All	All	4656/5288 (88%)	4421 (95%)	235 (5%)	30 66

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

Some 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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	304/373 (81%)	0.39	35 (11%) 6 11	355, 355, 355, 355	0
1	B	304/373 (81%)	0.61	40 (13%) 4 10	362, 362, 362, 362	0
1	C	304/373 (81%)	0.48	40 (13%) 4 10	364, 364, 364, 364	0
1	D	304/373 (81%)	0.57	37 (12%) 5 11	347, 347, 347, 347	0
1	M	304/373 (81%)	0.34	28 (9%) 11 15	357, 357, 357, 357	0
1	N	304/373 (81%)	0.50	31 (10%) 9 13	350, 350, 350, 350	0
1	O	304/373 (81%)	0.47	35 (11%) 6 11	355, 355, 355, 355	0
1	P	304/373 (81%)	0.42	25 (8%) 14 18	353, 353, 353, 353	0
2	E	291/319 (91%)	0.58	26 (8%) 12 16	294, 363, 363, 363	1 (0%)
2	G	291/319 (91%)	0.38	19 (6%) 22 23	298, 367, 367, 367	1 (0%)
2	I	291/319 (91%)	0.30	17 (5%) 26 27	287, 354, 354, 354	1 (0%)
2	K	291/319 (91%)	0.58	29 (9%) 9 14	302, 372, 372, 372	1 (0%)
2	Q	291/319 (91%)	0.51	27 (9%) 11 15	291, 359, 359, 359	1 (0%)
2	S	291/319 (91%)	0.46	24 (8%) 14 18	295, 364, 364, 364	1 (0%)
2	U	291/319 (91%)	0.47	18 (6%) 24 24	298, 368, 368, 368	1 (0%)
2	W	291/319 (91%)	0.56	27 (9%) 11 15	303, 374, 374, 374	1 (0%)
3	F	54/56 (96%)	0.84	9 (16%) 2 8	373, 373, 373, 373	0
3	H	54/56 (96%)	0.47	5 (9%) 11 15	379, 379, 379, 379	0
3	J	54/56 (96%)	0.61	5 (9%) 11 15	370, 370, 370, 370	0
3	L	54/56 (96%)	1.22	12 (22%) 1 6	386, 386, 386, 386	0
3	R	54/56 (96%)	0.59	7 (12%) 5 10	371, 371, 371, 371	0
3	T	54/56 (96%)	0.58	7 (12%) 5 10	380, 380, 380, 380	0
3	V	54/56 (96%)	0.65	8 (14%) 3 9	384, 384, 384, 384	0
3	X	54/56 (96%)	0.84	8 (14%) 3 9	386, 386, 386, 386	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	5192/5984 (86%)	0.50	519 (9%)	9	14	287, 362, 379, 386	8 (0%)

All (519) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	30	GLY	8.2
1	D	24	GLY	7.8
1	D	30	GLY	7.2
1	B	317	CYS	7.1
1	N	26	LYS	6.8
1	B	131	GLY	6.8
3	L	51	LYS	6.8
1	B	30	GLY	6.6
3	T	55	ASN	6.6
1	N	27	GLY	6.5
1	N	30	GLY	6.3
1	P	30	GLY	6.1
3	F	50	TYR	6.0
1	M	30	GLY	5.8
1	M	26	LYS	5.8
1	A	24	GLY	5.8
1	O	152	GLN	5.7
1	C	74	ALA	5.6
1	C	279	ASN	5.5
1	O	30	GLY	5.5
1	M	29	VAL	5.4
3	L	50	TYR	5.4
3	L	40	ASN	5.4
1	D	351	GLU	5.3
1	O	26	LYS	5.3
1	B	206	GLY	5.2
3	F	51	LYS	5.2
2	E	296	GLN	5.2
2	S	179	VAL	5.2
1	C	317	CYS	5.1
1	P	26	LYS	5.1
3	F	40	ASN	5.0
2	K	293	ALA	5.0
1	P	29	VAL	4.9
3	F	42	GLY	4.9
1	D	26	LYS	4.9
1	M	25	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
2	S	292	VAL	4.8
2	G	293	ALA	4.8
2	I	128	GLU	4.8
2	K	294	PRO	4.7
3	F	56	ARG	4.7
1	B	26	LYS	4.6
2	E	181	ASP	4.6
1	D	25	GLY	4.6
1	B	58	PRO	4.6
2	W	180	ASP	4.6
3	V	43	VAL	4.5
1	N	28	GLY	4.5
1	C	28	GLY	4.5
3	X	51	LYS	4.5
1	B	132	SER	4.5
2	W	192	SER	4.5
2	E	179	VAL	4.4
2	G	128	GLU	4.4
1	M	27	GLY	4.3
2	E	295	LYS	4.3
1	N	32	THR	4.3
2	G	294	PRO	4.3
2	W	294	PRO	4.2
2	S	197	ASN	4.2
1	A	30	GLY	4.2
2	K	244	ASP	4.2
1	P	317	CYS	4.1
1	C	318	ALA	4.1
2	S	130	LYS	4.1
2	G	130	LYS	4.1
1	P	279	ASN	4.0
1	C	315	PRO	4.0
2	Q	192	SER	4.0
1	A	167	THR	4.0
2	I	294	PRO	4.0
2	K	298	ASN	4.0
1	A	28	GLY	4.0
1	D	28	GLY	4.0
1	B	280	ASP	4.0
1	N	34	SER	4.0
1	B	318	ALA	3.9
1	C	166	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	N	29	VAL	3.9
1	P	272	ASN	3.9
2	U	128	GLU	3.9
2	S	293	ALA	3.9
1	N	166	ASP	3.9
1	B	24	GLY	3.9
2	E	298	ASN	3.9
1	M	24	GLY	3.9
1	D	166	ASP	3.9
1	A	58	PRO	3.8
1	O	150	LYS	3.8
1	B	281	GLN	3.8
2	I	296	GLN	3.8
3	R	56	ARG	3.8
2	Q	295	LYS	3.8
2	K	243	SER	3.8
2	E	297	THR	3.7
2	I	295	LYS	3.8
1	A	346	VAL	3.7
1	D	318	ALA	3.7
1	N	35	SER	3.7
2	W	189	GLU	3.7
1	D	241	VAL	3.7
1	A	337	GLU	3.7
1	O	206	GLY	3.7
3	X	55	ASN	3.7
1	P	25	GLY	3.7
1	B	279	ASN	3.7
1	O	131	GLY	3.6
2	W	293	ALA	3.6
2	U	130	LYS	3.6
1	M	350	LEU	3.6
1	C	26	LYS	3.6
1	O	73	ASP	3.6
2	S	234	TYR	3.6
3	L	53	LYS	3.5
1	O	151	ARG	3.5
1	O	28	GLY	3.5
1	C	69	LYS	3.5
2	E	182	ILE	3.5
2	W	193	ARG	3.5
2	K	227	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	G	292	VAL	3.5
2	S	233	GLY	3.5
1	N	206	GLY	3.5
2	S	180	ASP	3.5
1	B	15	SER	3.5
1	M	86	MET	3.5
1	N	33	THR	3.4
1	A	317	CYS	3.4
2	I	130	LYS	3.4
3	L	6	SER	3.4
1	C	272	ASN	3.4
1	N	240	CYS	3.4
3	R	40	ASN	3.4
2	S	295	LYS	3.4
1	B	27	GLY	3.4
1	D	350	LEU	3.4
2	W	298	ASN	3.4
2	S	231	LYS	3.4
2	U	129	TYR	3.4
1	A	27	GLY	3.4
3	H	56	ARG	3.4
1	A	29	VAL	3.4
2	E	275	GLN	3.4
2	E	294	PRO	3.4
1	B	166	ASP	3.4
1	D	272	ASN	3.3
1	N	24	GLY	3.3
1	O	157	GLY	3.3
2	G	296	GLN	3.3
1	C	281	GLN	3.3
1	P	27	GLY	3.3
2	S	294	PRO	3.3
2	U	294	PRO	3.3
1	C	86	MET	3.3
1	M	347	ILE	3.3
1	C	158	GLU	3.3
2	Q	296	GLN	3.3
2	U	182	ILE	3.3
1	D	58	PRO	3.3
1	D	319	GLY	3.3
1	P	132	SER	3.3
2	S	232	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	166	ASP	3.3
2	K	197	ASN	3.3
1	D	280	ASP	3.3
3	F	55	ASN	3.3
1	O	279	ASN	3.2
3	R	55	ASN	3.2
1	C	85	CYS	3.2
3	L	39	THR	3.2
1	O	27	GLY	3.2
1	A	157	GLY	3.2
1	M	241	VAL	3.2
1	D	268	SER	3.2
1	P	69	LYS	3.2
1	O	166	ASP	3.2
2	U	194	LEU	3.2
3	T	54	GLN	3.2
1	N	74	ALA	3.2
1	O	58	PRO	3.2
2	Q	227	GLU	3.2
2	Q	109	GLU	3.1
2	E	180	ASP	3.1
1	D	29	VAL	3.1
1	P	315	PRO	3.1
1	M	349	GLU	3.1
1	P	319	GLY	3.1
3	T	56	ARG	3.1
3	X	45	LEU	3.1
1	B	315	PRO	3.1
2	E	197	ASN	3.1
1	M	346	VAL	3.1
1	N	279	ASN	3.1
2	K	226	TYR	3.1
1	C	152	GLN	3.1
2	Q	180	ASP	3.1
3	J	3	THR	3.1
1	D	278	GLU	3.1
1	O	37	SER	3.1
2	S	193	ARG	3.1
1	B	14	THR	3.0
2	U	296	GLN	3.0
1	M	351	GLU	3.0
1	C	29	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	Q	282	GLU	3.0
1	C	277	ALA	3.0
1	M	348	TYR	3.0
2	W	238	PHE	3.0
1	A	23	VAL	3.0
1	D	317	CYS	3.0
2	I	129	TYR	3.0
1	A	26	LYS	3.0
1	C	27	GLY	3.0
2	K	299	PHE	2.9
2	W	187	VAL	2.9
1	D	197	LEU	2.9
2	W	197	ASN	2.9
2	K	192	SER	2.9
1	A	344	GLY	2.9
2	U	192	SER	2.9
2	I	222	PHE	2.9
1	D	34	SER	2.9
3	V	42	GLY	2.9
1	B	205	MET	2.9
1	M	166	ASP	2.9
2	W	179	VAL	2.9
1	M	222	ASN	2.9
1	M	272	ASN	2.9
1	N	31	LYS	2.8
2	Q	298	ASN	2.9
1	B	34	SER	2.8
2	U	179	VAL	2.8
1	C	278	GLU	2.8
3	L	4	SER	2.8
1	B	25	GLY	2.8
2	E	224	PRO	2.8
1	A	319	GLY	2.8
2	K	240	GLU	2.8
3	X	56	ARG	2.8
2	E	128	GLU	2.8
2	K	179	VAL	2.8
3	L	56	ARG	2.8
1	N	23	VAL	2.8
2	Q	179	VAL	2.8
1	C	68	GLU	2.8
2	W	296	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	P	34	SER	2.8
1	B	156	GLU	2.8
2	K	104	GLU	2.7
2	S	192	SER	2.7
2	W	107	PRO	2.7
1	A	241	VAL	2.7
2	Q	244	ASP	2.7
3	T	21	THR	2.7
2	K	292	VAL	2.7
3	L	24	GLU	2.7
1	D	349	GLU	2.7
1	B	170	THR	2.7
3	T	4	SER	2.7
2	Q	133	ASP	2.7
2	I	221	LYS	2.7
1	P	89	ASP	2.7
1	C	153	GLU	2.7
2	S	181	ASP	2.7
2	E	127	SER	2.7
2	G	126	PHE	2.7
1	A	347	ILE	2.7
2	G	111	ASN	2.7
2	E	10	GLY	2.7
1	B	277	ALA	2.7
1	N	89	ASP	2.7
1	P	348	TYR	2.7
2	K	297	THR	2.7
1	B	155	GLY	2.7
1	D	32	THR	2.7
1	O	280	ASP	2.7
2	G	287	GLU	2.7
3	R	42	GLY	2.7
2	Q	181	ASP	2.7
3	V	39	THR	2.7
1	O	74	ALA	2.7
1	D	167	THR	2.7
1	O	155	GLY	2.6
3	X	5	ALA	2.6
2	E	193	ARG	2.6
1	C	280	ASP	2.6
1	O	315	PRO	2.6
2	G	131	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	131	GLY	2.6
3	X	4	SER	2.6
1	M	34	SER	2.6
1	O	33	THR	2.6
3	H	4	SER	2.6
1	A	34	SER	2.6
2	I	297	THR	2.6
2	Q	297	THR	2.6
2	Q	294	PRO	2.6
1	A	156	GLU	2.6
1	P	24	GLY	2.6
2	U	193	ARG	2.6
1	D	33	THR	2.6
2	U	131	PHE	2.6
2	G	127	SER	2.6
3	J	51	LYS	2.6
1	A	25	GLY	2.6
1	P	281	GLN	2.6
1	A	222	ASN	2.6
1	O	132	SER	2.6
2	K	180	ASP	2.6
1	M	315	PRO	2.6
1	C	286	LYS	2.6
2	E	226	TYR	2.6
1	B	278	GLU	2.6
2	W	297	THR	2.6
2	U	295	LYS	2.6
2	Q	125	LYS	2.6
1	D	335	ASN	2.6
3	X	28	PRO	2.6
3	J	4	SER	2.6
1	P	131	GLY	2.5
1	N	277	ALA	2.5
1	M	317	CYS	2.5
1	O	154	GLN	2.5
2	I	293	ALA	2.5
3	L	5	ALA	2.5
2	W	292	VAL	2.5
3	T	23	THR	2.5
1	C	351	GLU	2.5
1	O	59	ALA	2.5
2	W	57	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	W	182	ILE	2.5
2	K	224	PRO	2.5
2	K	238	PHE	2.5
1	D	240	CYS	2.5
1	A	315	PRO	2.5
2	I	131	PHE	2.5
2	K	11	ALA	2.5
2	S	282	GLU	2.5
1	C	132	SER	2.5
2	K	194	LEU	2.5
2	W	188	ALA	2.5
1	O	159	THR	2.5
1	A	36	CYS	2.5
1	A	158	GLU	2.5
2	K	189	GLU	2.5
2	E	192	SER	2.5
1	O	32	THR	2.5
3	R	39	THR	2.5
2	Q	228	LYS	2.5
1	P	32	THR	2.5
1	C	167	THR	2.5
2	W	239	PHE	2.5
2	G	181	ASP	2.5
1	O	317	CYS	2.4
2	W	194	LEU	2.5
2	G	295	LYS	2.4
1	N	268	SER	2.4
2	Q	193	ARG	2.4
1	B	234	ASP	2.4
1	B	276	PHE	2.4
2	S	128	GLU	2.4
1	B	158	GLU	2.4
2	E	104	GLU	2.4
1	B	59	ALA	2.4
1	O	72	LYS	2.4
1	N	265	ASP	2.4
1	P	166	ASP	2.4
2	I	180	ASP	2.4
1	D	35	SER	2.4
1	O	24	GLY	2.4
1	C	72	LYS	2.4
1	M	28	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	345	LYS	2.4
1	C	32	THR	2.4
1	C	33	THR	2.4
3	H	37	ASP	2.4
1	N	131	GLY	2.4
2	K	228	LYS	2.4
2	S	131	PHE	2.4
1	B	33	THR	2.4
3	V	3	THR	2.4
1	N	272	ASN	2.4
2	G	221	LYS	2.4
1	N	58	PRO	2.4
3	X	49	LYS	2.4
1	D	170	THR	2.4
1	P	280	ASP	2.4
2	U	186	THR	2.3
1	O	237	THR	2.3
1	D	31	LYS	2.3
2	K	241	ASP	2.3
1	D	329	LYS	2.3
1	N	280	ASP	2.3
3	F	53	LYS	2.3
1	C	5	VAL	2.3
2	G	192	SER	2.3
1	O	153	GLU	2.3
1	A	90	PRO	2.3
1	A	31	LYS	2.3
1	P	278	GLU	2.3
2	K	193	ARG	2.3
2	U	244	ASP	2.3
1	D	154	GLN	2.3
1	M	170	THR	2.3
1	N	315	PRO	2.3
1	C	340	PRO	2.3
2	I	234	TYR	2.3
3	V	44	PRO	2.3
1	B	319	GLY	2.3
1	C	73	ASP	2.3
2	S	291	ILE	2.3
1	P	68	GLU	2.3
2	I	229	ILE	2.3
2	K	181	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
3	T	3	THR	2.3
1	A	57	ASP	2.2
1	A	89	ASP	2.2
1	C	273	GLN	2.2
1	B	152	GLN	2.2
2	S	286	GLN	2.2
2	S	178	GLN	2.2
1	C	71	GLY	2.2
1	A	35	SER	2.2
1	P	36	CYS	2.2
1	D	37	SER	2.2
1	C	157	GLY	2.2
1	A	350	LEU	2.2
1	M	267	ASN	2.2
2	Q	188	ALA	2.2
2	Q	283	PHE	2.2
2	E	194	LEU	2.2
3	F	49	LYS	2.2
1	D	348	TYR	2.2
2	W	184	ASP	2.2
1	M	32	THR	2.2
3	V	55	ASN	2.2
1	C	131	GLY	2.2
1	B	347	ILE	2.2
1	O	240	CYS	2.2
1	C	308	ASP	2.2
1	C	338	TYR	2.2
2	G	112	LEU	2.2
1	O	34	SER	2.2
3	R	50	TYR	2.2
1	B	29	VAL	2.2
2	E	210	SER	2.2
2	Q	112	LEU	2.2
3	J	36	LYS	2.2
3	L	10	HIS	2.2
1	B	167	THR	2.2
2	G	110	PRO	2.2
1	O	205	MET	2.2
2	K	275	GLN	2.2
1	A	272	ASN	2.2
3	V	4	SER	2.2
2	E	168	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	293	ALA	2.1
1	M	268	SER	2.1
1	O	167	THR	2.1
2	I	230	ASP	2.1
2	U	249	GLN	2.1
2	G	297	THR	2.1
1	B	37	SER	2.1
1	B	240	CYS	2.1
1	D	347	ILE	2.1
2	I	224	PRO	2.1
2	W	30	TYR	2.1
2	Q	149	PHE	2.1
2	Q	293	ALA	2.1
2	E	125	LYS	2.1
2	Q	58	GLN	2.1
2	S	230	ASP	2.1
2	U	219	ILE	2.1
3	J	40	ASN	2.1
1	N	57	ASP	2.1
1	A	32	THR	2.1
1	N	239	VAL	2.1
1	B	157	GLY	2.1
1	N	278	GLU	2.1
3	H	3	THR	2.1
1	N	158	GLU	2.1
3	F	39	THR	2.1
1	D	81	ASN	2.1
3	H	5	ALA	2.1
2	W	181	ASP	2.1
2	Q	275	GLN	2.1
1	B	171	GLY	2.1
1	D	171	GLY	2.1
2	Q	285	GLY	2.1
2	E	227	GLU	2.1
2	K	239	PHE	2.1
1	N	237	THR	2.0
2	U	269	HIS	2.0
2	E	126	PHE	2.0
2	Q	197	ASN	2.0
2	W	155	ARG	2.0
2	S	278	LYS	2.0
1	B	338	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	O	268	SER	2.0
1	M	273	GLN	2.0
2	I	298	ASN	2.0
2	K	229	ILE	2.0
2	U	183	GLU	2.0
2	Q	189	GLU	2.0
2	S	182	ILE	2.0
1	D	27	GLY	2.0
1	M	344	GLY	2.0
1	C	168	ALA	2.0
2	G	129	TYR	2.0
1	A	318	ALA	2.0
3	L	52	TYR	2.0
3	R	53	LYS	2.0
1	P	33	THR	2.0
2	W	84	ASP	2.0
2	W	185	SER	2.0
3	V	6	SER	2.0
2	W	227	GLU	2.0
2	K	130	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	ZN	A	500	1/1	0.95	0.23	-0.55	354,354,354,354	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	ZN	D	501	1/1	0.88	0.09	-2.20	363,363,363,363	0
4	ZN	M	401	1/1	0.93	0.07	-2.59	356,356,356,356	0
4	ZN	O	401	1/1	0.93	0.14	-2.61	354,354,354,354	0

6.5 Other polymers (i)

There are no such residues in this entry.