Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 08:53 PM EDT

PDB ID	:	1SXI
Title	:	Structure of apo transcription regulator B. megaterium
Authors	:	Schumacher, M.A.; Allen, G.S.; Diel, M.; Seidel, G.; Hillen, W.; Brennan, R.G.
Deposited on	:	2004-03-30
Resolution	:	3.00 Å(reported)

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

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

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

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

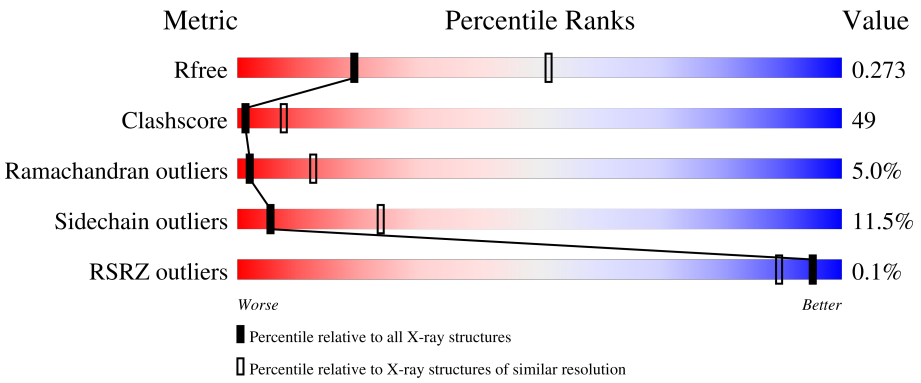
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	280	31% 55% 10% •
1	B	280	35% 52% 10% •
1	D	280	35% 53% 8% • •
1	G	280	27% 59% 11% •
1	I	280	42% 49% 7% •

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Mol	Chain	Length	Quality of chain
1	K	280	40% 48% 10%
1	L	280	29% 55% 14%
1	M	280	34% 53% 11%
1	N	280	34% 54% 9%
1	R	280	29% 57% 12%
1	T	280	40% 48% 10%
1	W	280	32% 53% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25483 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 Glucose-resistance amylase regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	273	2123	1337	352	426	8	0	0	0
1	D	273	2123	1337	352	426	8	0	0	0
1	B	273	2123	1337	352	426	8	0	0	0
1	I	273	2123	1337	352	426	8	0	0	0
1	R	273	2123	1337	352	426	8	0	0	0
1	T	273	2123	1337	352	426	8	0	0	0
1	L	273	2123	1337	352	426	8	0	0	0
1	K	273	2123	1337	352	426	8	0	0	0
1	W	273	2123	1337	352	426	8	0	0	0
1	G	273	2123	1337	352	426	8	0	0	0
1	N	273	2123	1337	352	426	8	0	0	0
1	M	273	2123	1337	352	426	8	0	0	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	MSE	MET	modified residue	UNP P46828
A	112	MSE	MET	modified residue	UNP P46828
A	123	MSE	MET	modified residue	UNP P46828
A	250	MSE	MET	modified residue	UNP P46828
A	282	MSE	MET	modified residue	UNP P46828

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Chain	Residue	Modelled	Actual	Comment	Reference
A	294	MSE	MET	modified residue	UNP P46828
A	302	MSE	MET	modified residue	UNP P46828
A	309	MSE	MET	modified residue	UNP P46828
B	88	MSE	MET	modified residue	UNP P46828
B	112	MSE	MET	modified residue	UNP P46828
B	123	MSE	MET	modified residue	UNP P46828
B	250	MSE	MET	modified residue	UNP P46828
B	282	MSE	MET	modified residue	UNP P46828
B	294	MSE	MET	modified residue	UNP P46828
B	302	MSE	MET	modified residue	UNP P46828
B	309	MSE	MET	modified residue	UNP P46828
R	88	MSE	MET	modified residue	UNP P46828
R	112	MSE	MET	modified residue	UNP P46828
R	123	MSE	MET	modified residue	UNP P46828
R	250	MSE	MET	modified residue	UNP P46828
R	282	MSE	MET	modified residue	UNP P46828
R	294	MSE	MET	modified residue	UNP P46828
R	302	MSE	MET	modified residue	UNP P46828
R	309	MSE	MET	modified residue	UNP P46828
L	88	MSE	MET	modified residue	UNP P46828
L	112	MSE	MET	modified residue	UNP P46828
L	123	MSE	MET	modified residue	UNP P46828
L	250	MSE	MET	modified residue	UNP P46828
L	282	MSE	MET	modified residue	UNP P46828
L	294	MSE	MET	modified residue	UNP P46828
L	302	MSE	MET	modified residue	UNP P46828
L	309	MSE	MET	modified residue	UNP P46828
W	88	MSE	MET	modified residue	UNP P46828
W	112	MSE	MET	modified residue	UNP P46828
W	123	MSE	MET	modified residue	UNP P46828
W	250	MSE	MET	modified residue	UNP P46828
W	282	MSE	MET	modified residue	UNP P46828
W	294	MSE	MET	modified residue	UNP P46828
W	302	MSE	MET	modified residue	UNP P46828
W	309	MSE	MET	modified residue	UNP P46828
M	88	MSE	MET	modified residue	UNP P46828
M	112	MSE	MET	modified residue	UNP P46828
M	123	MSE	MET	modified residue	UNP P46828
M	250	MSE	MET	modified residue	UNP P46828
M	282	MSE	MET	modified residue	UNP P46828
M	294	MSE	MET	modified residue	UNP P46828
M	302	MSE	MET	modified residue	UNP P46828

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Chain	Residue	Modelled	Actual	Comment	Reference
M	309	MSE	MET	modified residue	UNP P46828
D	88	MSE	MET	modified residue	UNP P46828
D	112	MSE	MET	modified residue	UNP P46828
D	123	MSE	MET	modified residue	UNP P46828
D	250	MSE	MET	modified residue	UNP P46828
D	282	MSE	MET	modified residue	UNP P46828
D	294	MSE	MET	modified residue	UNP P46828
D	302	MSE	MET	modified residue	UNP P46828
D	309	MSE	MET	modified residue	UNP P46828
I	88	MSE	MET	modified residue	UNP P46828
I	112	MSE	MET	modified residue	UNP P46828
I	123	MSE	MET	modified residue	UNP P46828
I	250	MSE	MET	modified residue	UNP P46828
I	282	MSE	MET	modified residue	UNP P46828
I	294	MSE	MET	modified residue	UNP P46828
I	302	MSE	MET	modified residue	UNP P46828
I	309	MSE	MET	modified residue	UNP P46828
T	88	MSE	MET	modified residue	UNP P46828
T	112	MSE	MET	modified residue	UNP P46828
T	123	MSE	MET	modified residue	UNP P46828
T	250	MSE	MET	modified residue	UNP P46828
T	282	MSE	MET	modified residue	UNP P46828
T	294	MSE	MET	modified residue	UNP P46828
T	302	MSE	MET	modified residue	UNP P46828
T	309	MSE	MET	modified residue	UNP P46828
K	88	MSE	MET	modified residue	UNP P46828
K	112	MSE	MET	modified residue	UNP P46828
K	123	MSE	MET	modified residue	UNP P46828
K	250	MSE	MET	modified residue	UNP P46828
K	282	MSE	MET	modified residue	UNP P46828
K	294	MSE	MET	modified residue	UNP P46828
K	302	MSE	MET	modified residue	UNP P46828
K	309	MSE	MET	modified residue	UNP P46828
G	88	MSE	MET	modified residue	UNP P46828
G	112	MSE	MET	modified residue	UNP P46828
G	123	MSE	MET	modified residue	UNP P46828
G	250	MSE	MET	modified residue	UNP P46828
G	282	MSE	MET	modified residue	UNP P46828
G	294	MSE	MET	modified residue	UNP P46828
G	302	MSE	MET	modified residue	UNP P46828
G	309	MSE	MET	modified residue	UNP P46828
N	88	MSE	MET	modified residue	UNP P46828

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Chain	Residue	Modelled	Actual	Comment	Reference
N	112	MSE	MET	modified residue	UNP P46828
N	123	MSE	MET	modified residue	UNP P46828
N	250	MSE	MET	modified residue	UNP P46828
N	282	MSE	MET	modified residue	UNP P46828
N	294	MSE	MET	modified residue	UNP P46828
N	302	MSE	MET	modified residue	UNP P46828
N	309	MSE	MET	modified residue	UNP P46828

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	T	2	2	2	0	0

- Molecule 3 is water.

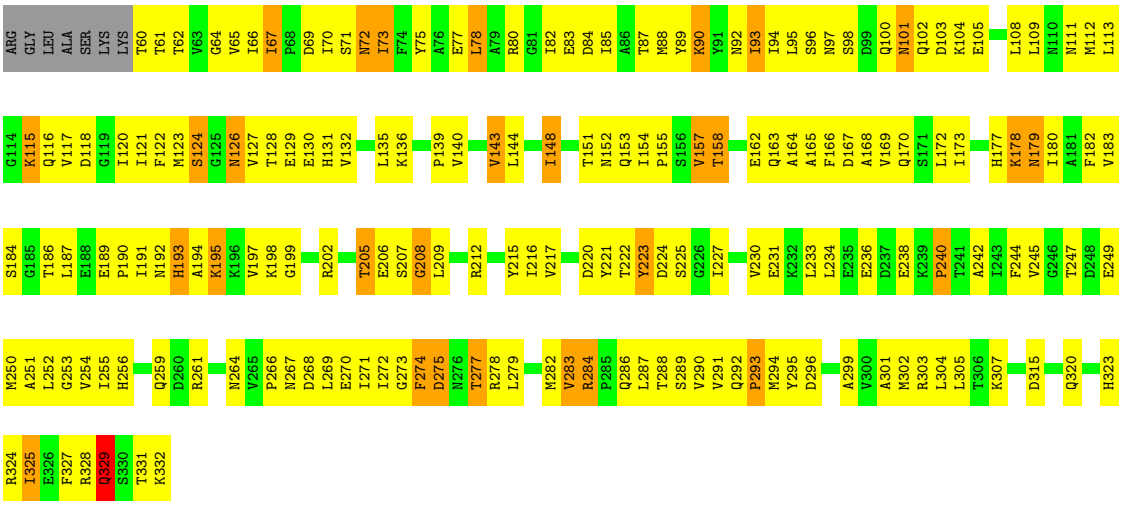
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	1	1	1	0	0
			Total	O		
3	D	3	3	3	0	0
			Total	O		
3	T	1	1	1	0	0

3 Residue-property plots (i)

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

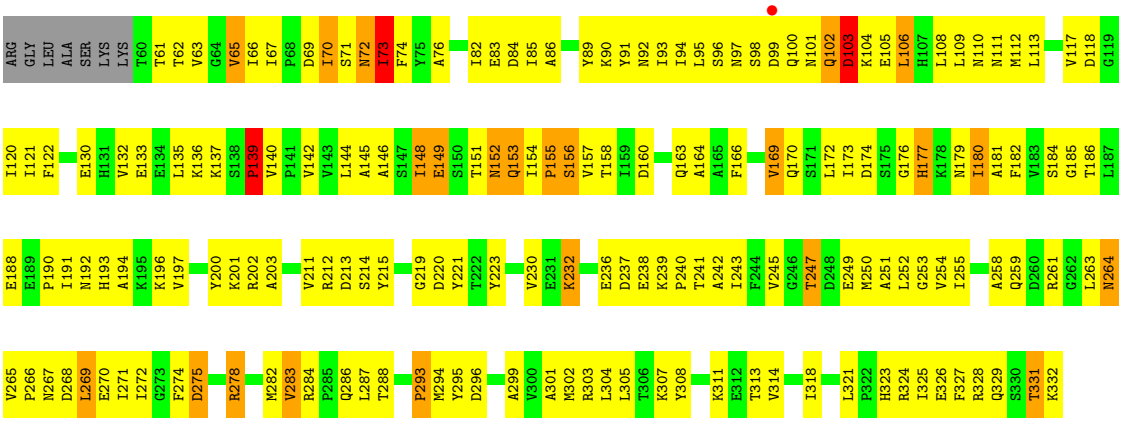
• Molecule 1: Glucose-resistance amylase regulator

Chain A: 31% 55% 10%



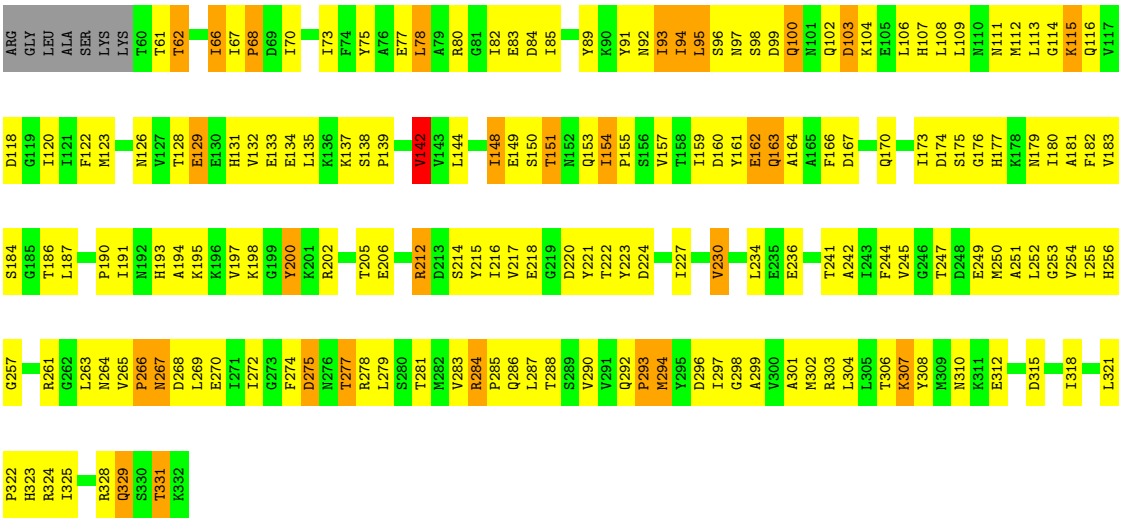
• Molecule 1: Glucose-resistance amylase regulator

Chain D: 35% 53% 8%



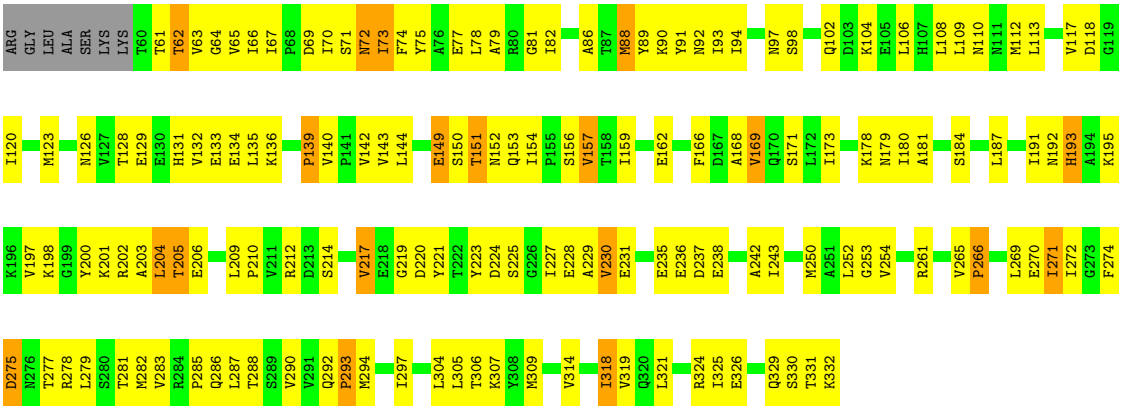
• Molecule 1: Glucose-resistance amylase regulator

Chain B: 35% 52% 10%



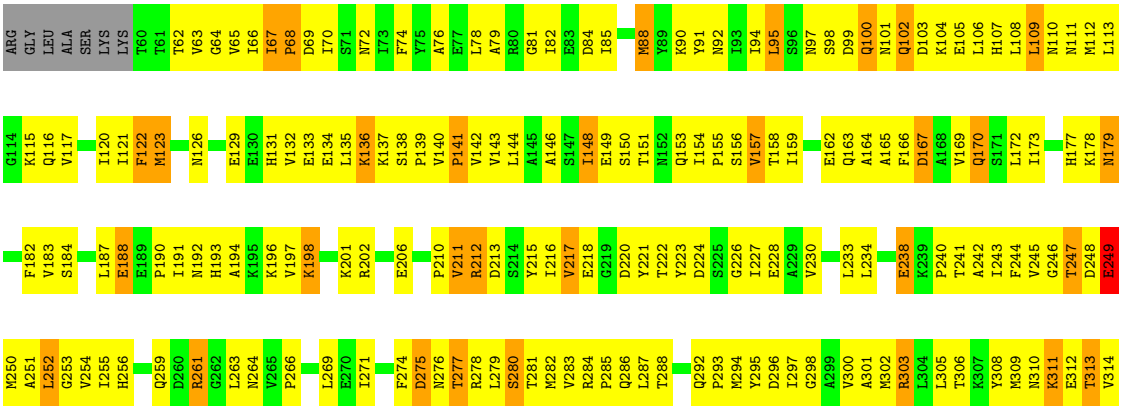
- Molecule 1: Glucose-resistance amylase regulator

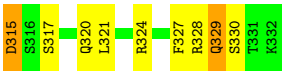
Chain I: 42% 49% 7%



- Molecule 1: Glucose-resistance amylase regulator

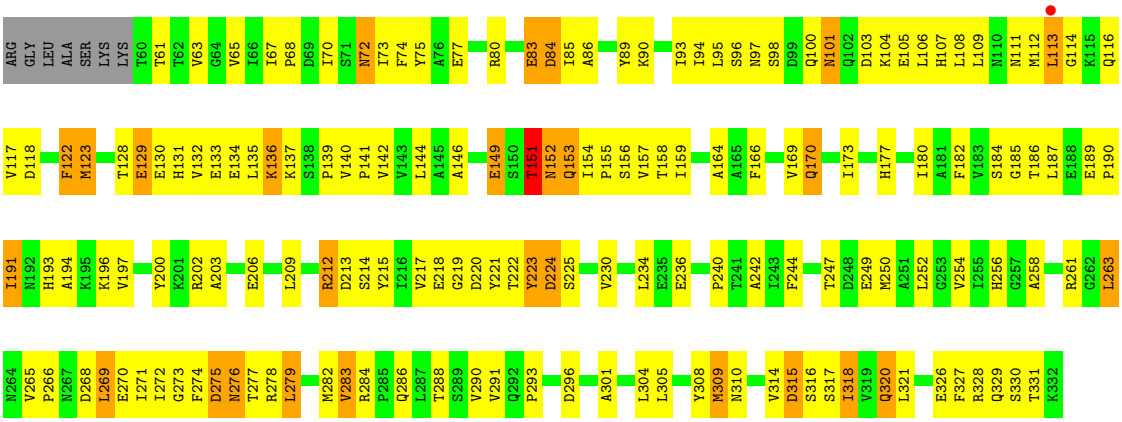
Chain R: 29% 57% 12%





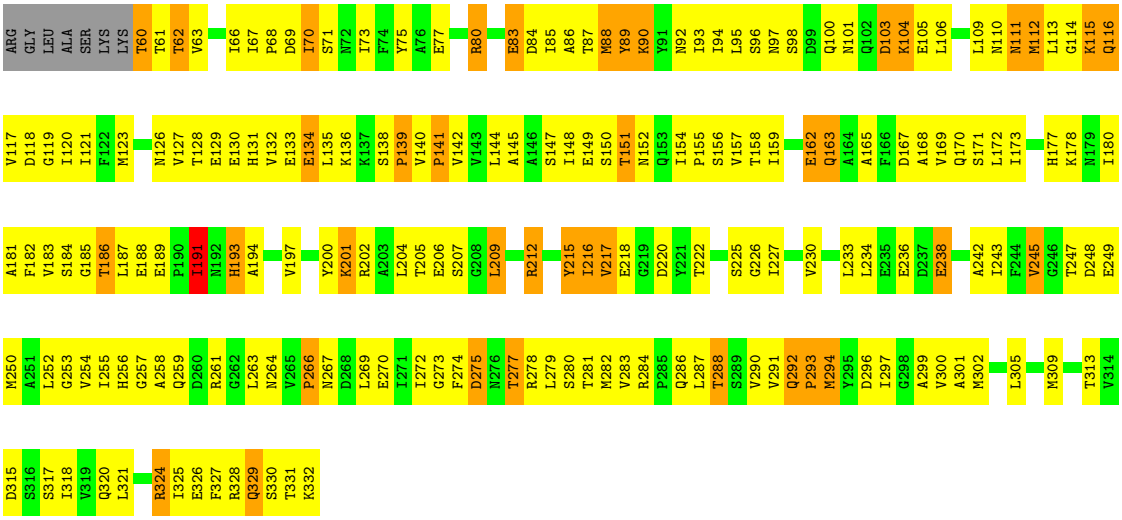
• Molecule 1: Glucose-resistance amylase regulator

Chain T:



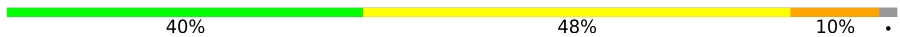
• Molecule 1: Glucose-resistance amylase regulator

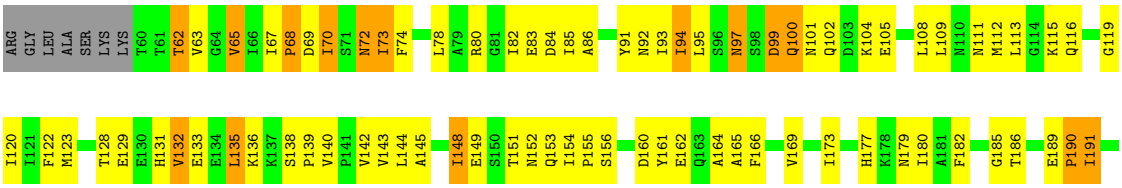
Chain L:

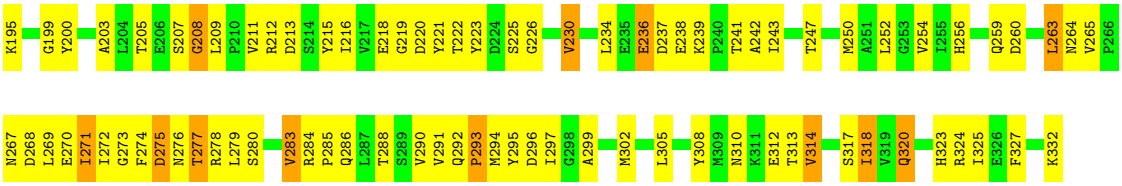


• Molecule 1: Glucose-resistance amylase regulator

Chain K:

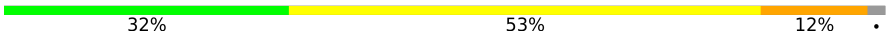


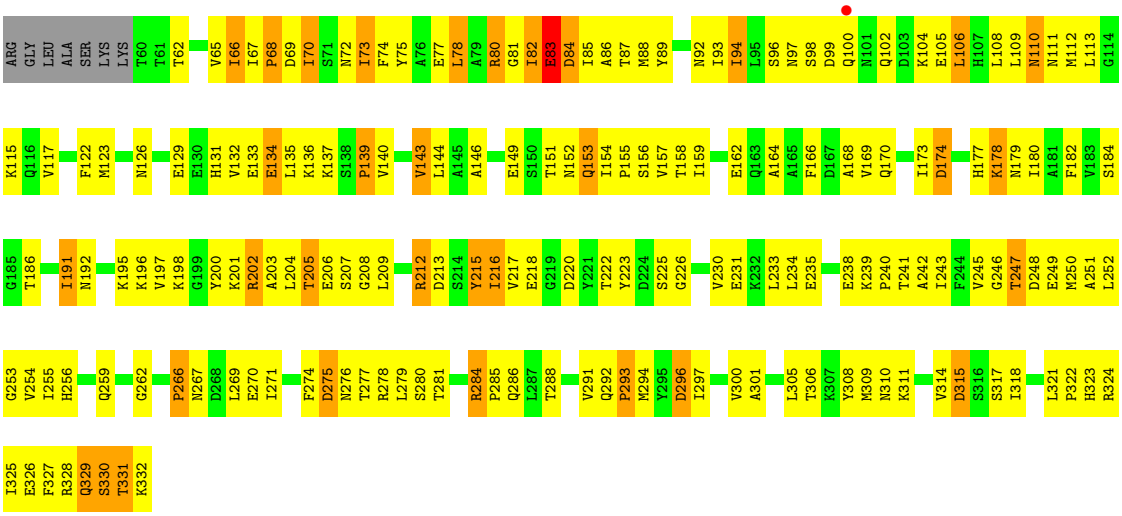




• Molecule 1: Glucose-resistance amylase regulator

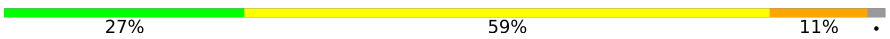
Chain W:

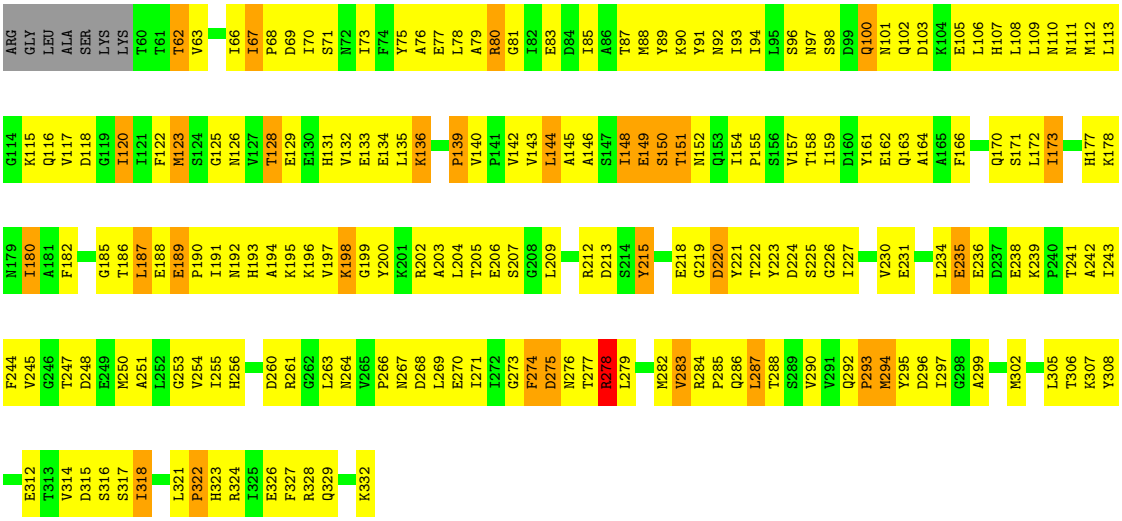




• Molecule 1: Glucose-resistance amylase regulator

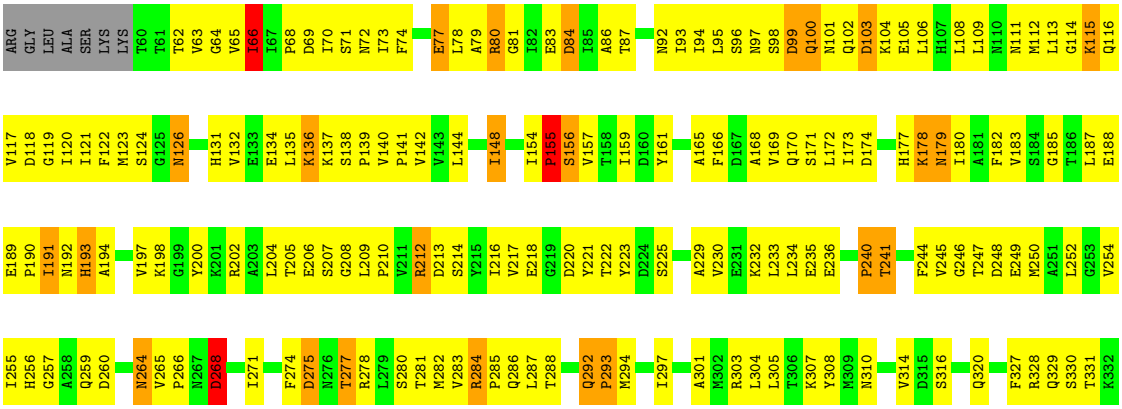
Chain G:





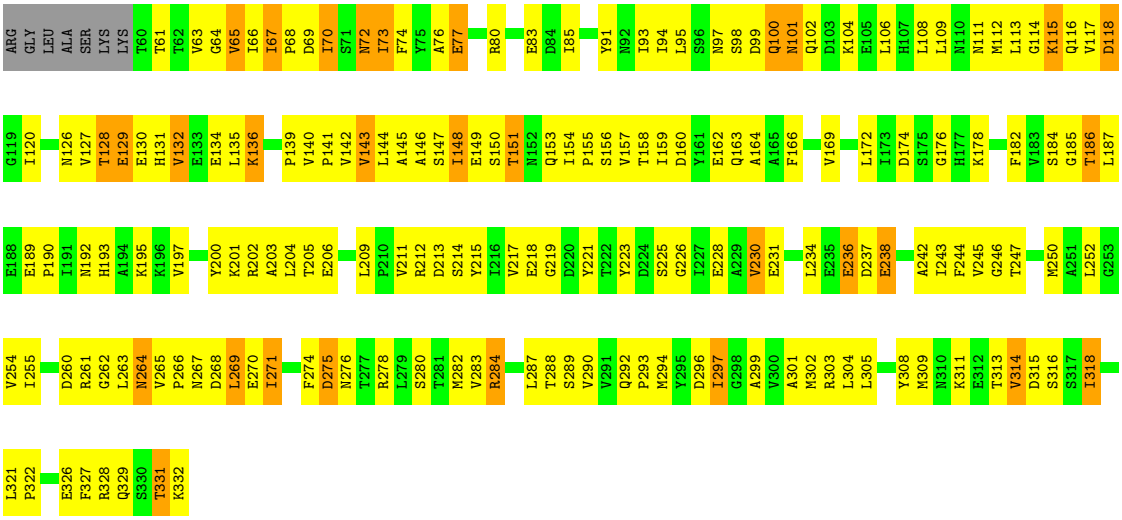
• Molecule 1: Glucose-resistance amylase regulator

Chain N:



- Molecule 1: Glucose-resistance amylase regulator

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	110.24Å 106.22Å 157.74Å 90.00° 108.20° 90.00°	Depositor
Resolution (Å)	74.58 – 3.00 74.57 – 2.99	Depositor EDS
% Data completeness (in resolution range)	95.5 (74.58-3.00) 94.9 (74.57-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 3.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.220 , 0.282 0.215 , 0.273	Depositor DCC
R_{free} test set	6726 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å^2)	61.6	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 62.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	25483	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.45	0/2148	0.70	0/2899
1	B	0.42	0/2148	0.69	0/2899
1	D	0.44	0/2148	0.69	0/2899
1	G	0.40	0/2148	0.67	0/2899
1	I	0.45	0/2148	0.73	0/2899
1	K	0.46	0/2148	0.71	0/2899
1	L	0.42	0/2148	0.69	0/2899
1	M	0.41	0/2148	0.70	0/2899
1	N	0.38	0/2148	0.66	0/2899
1	R	0.41	0/2148	0.68	0/2899
1	T	0.46	0/2148	0.72	1/2899 (0.0%)
1	W	0.46	0/2147	0.72	0/2896
All	All	0.43	0/25775	0.70	1/34785 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	151	THR	N-CA-C	5.54	125.96	111.00

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	2123	0	2121	239	0
1	B	2123	0	2121	189	0
1	D	2123	0	2121	198	0
1	G	2123	0	2121	241	0
1	I	2123	0	2121	162	0
1	K	2123	0	2121	201	0
1	L	2123	0	2121	238	0
1	M	2123	0	2121	204	0
1	N	2123	0	2121	249	0
1	R	2123	0	2121	234	0
1	T	2123	0	2121	191	0
1	W	2123	0	2120	254	0
2	T	2	0	0	0	0
3	A	1	0	0	0	0
3	D	3	0	0	0	0
3	T	1	0	0	0	0
All	All	25483	0	25451	2482	0

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 49.

All (2482) 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:W:115:LYS:HE2	1:G:94:ILE:HD11	1.25	1.17
1:D:121:ILE:HD11	1:D:302:MSE:HE3	1.20	1.16
1:G:234:LEU:HD13	1:G:261:ARG:HE	1.09	1.16
1:B:288:THR:HG22	1:B:328:ARG:H	1.07	1.15
1:B:70:ILE:HD11	1:I:70:ILE:HD11	1.20	1.15
1:I:219:GLY:HA3	1:I:250:MSE:HE1	1.27	1.12
1:A:223:TYR:HB2	1:D:282:MSE:HE3	1.31	1.11
1:N:62:THR:HG22	1:N:92:ASN:HB2	1.32	1.10
1:R:212:ARG:H	1:R:212:ARG:HD2	1.11	1.09
1:G:77:GLU:HB3	1:G:294:MSE:HE1	1.34	1.08
1:M:101:ASN:HD21	1:M:104:LYS:HB2	0.97	1.08
1:I:252:LEU:HG	1:I:283:VAL:HG11	1.32	1.08
1:R:277:THR:HG22	1:R:279:LEU:H	1.13	1.08
1:G:220:ASP:HB2	1:G:222:THR:HG23	1.34	1.07
1:W:98:SER:O	1:W:104:LYS:HD3	1.54	1.06
1:L:90:LYS:HA	1:L:90:LYS:HE2	1.31	1.06
1:W:285:PRO:HB2	1:W:329:GLN:HB3	1.33	1.05
1:B:223:TYR:HB2	1:I:282:MSE:HE3	1.38	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:318:ILE:H	1:K:318:ILE:HD13	1.17	1.04
1:W:288:THR:HG21	1:W:331:THR:HG23	1.39	1.04
1:W:112:MSE:HE2	1:W:112:MSE:HA	1.38	1.03
1:R:179:ASN:HB2	1:R:215:TYR:HE2	1.24	1.02
1:R:62:THR:HG22	1:R:92:ASN:HD21	1.26	1.01
1:L:70:ILE:H	1:L:97:ASN:HD21	1.09	1.00
1:B:277:THR:HG22	1:B:278:ARG:H	1.22	1.00
1:L:73:ILE:HD11	1:K:278:ARG:HH22	1.24	0.99
1:B:212:ARG:HB3	1:B:212:ARG:HH11	1.24	0.99
1:B:288:THR:HG22	1:B:328:ARG:N	1.78	0.99
1:A:62:THR:HG22	1:A:92:ASN:HB2	1.41	0.99
1:G:144:LEU:HD21	1:G:154:ILE:HD13	1.44	0.98
1:N:264:ASN:ND2	1:N:266:PRO:HD2	1.79	0.97
1:K:318:ILE:HD13	1:K:318:ILE:N	1.78	0.97
1:D:62:THR:HG22	1:D:92:ASN:HB2	1.43	0.96
1:K:70:ILE:HB	1:K:97:ASN:OD1	1.65	0.96
1:R:95:LEU:HD21	1:T:95:LEU:HD12	1.45	0.96
1:G:75:TYR:HD1	1:G:123:MSE:HE3	1.27	0.95
1:K:73:ILE:HD12	1:K:74:PHE:H	1.30	0.95
1:N:314:VAL:HG12	1:N:316:SER:H	1.30	0.95
1:B:70:ILE:HD11	1:I:70:ILE:CD1	1.97	0.95
1:M:101:ASN:ND2	1:M:104:LYS:HB2	1.82	0.95
1:D:120:ILE:HB	1:D:142:VAL:HG22	1.50	0.94
1:D:230:VAL:HG22	1:D:254:VAL:HG13	1.48	0.94
1:L:155:PRO:HB3	1:L:317:SER:HB3	1.50	0.94
1:N:274:PHE:O	1:N:275:ASP:HB2	1.66	0.94
1:I:219:GLY:HA3	1:I:250:MSE:CE	1.97	0.94
1:K:277:THR:HG22	1:K:279:LEU:H	1.30	0.93
1:B:212:ARG:HH12	1:B:214:SER:HB3	1.31	0.93
1:R:179:ASN:HB2	1:R:215:TYR:CE2	2.02	0.93
1:G:113:LEU:HD22	1:G:139:PRO:HD2	1.51	0.93
1:N:254:VAL:HG12	1:N:271:ILE:HD13	1.50	0.93
1:N:252:LEU:HG	1:N:283:VAL:HG11	1.49	0.93
1:M:101:ASN:HD21	1:M:104:LYS:CB	1.81	0.93
1:W:68:PRO:HD3	1:W:123:MSE:O	1.68	0.92
1:M:243:ILE:HB	1:M:271:ILE:HG22	1.52	0.92
1:D:144:LEU:HD11	1:D:154:ILE:HD11	1.51	0.92
1:R:148:ILE:HD12	1:R:191:ILE:HG12	1.51	0.92
1:A:252:LEU:HG	1:A:283:VAL:HG13	1.52	0.92
1:I:201:LYS:O	1:I:205:THR:HG22	1.69	0.91
1:K:73:ILE:CD1	1:K:74:PHE:H	1.82	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:THR:CG2	1:B:328:ARG:H	1.83	0.91
1:R:179:ASN:HD22	1:R:179:ASN:N	1.69	0.90
1:R:179:ASN:H	1:R:179:ASN:ND2	1.69	0.90
1:N:210:PRO:HB2	1:N:212:ARG:HE	1.34	0.90
1:T:151:THR:O	1:T:152:ASN:HB2	1.70	0.90
1:L:216:ILE:O	1:L:216:ILE:HG12	1.71	0.90
1:N:109:LEU:HD23	1:N:134:GLU:HG3	1.54	0.90
1:G:149:GLU:HG3	1:G:150:SER:N	1.85	0.90
1:N:70:ILE:HG13	1:M:70:ILE:HD11	1.52	0.90
1:A:93:ILE:H	1:A:93:ILE:HD12	1.35	0.89
1:W:86:ALA:CB	1:W:93:ILE:HD11	2.02	0.89
1:T:101:ASN:HD21	1:T:104:LYS:N	1.70	0.89
1:G:148:ILE:H	1:G:148:ILE:HD12	1.36	0.89
1:M:151:THR:HG22	1:M:153:GLN:HB2	1.55	0.89
1:T:187:LEU:HD12	1:T:218:GLU:OE2	1.72	0.89
1:B:274:PHE:O	1:B:275:ASP:HB2	1.73	0.89
1:M:230:VAL:HG13	1:M:254:VAL:HG13	1.54	0.89
1:A:148:ILE:HD12	1:A:191:ILE:HG23	1.51	0.88
1:A:73:ILE:HD12	1:A:279:LEU:HG	1.53	0.88
1:B:70:ILE:CD1	1:I:70:ILE:HD11	2.04	0.88
1:W:85:ILE:HG23	1:W:88:MSE:HE2	1.54	0.88
1:K:131:HIS:O	1:K:135:LEU:HB2	1.72	0.88
1:A:113:LEU:HD22	1:A:139:PRO:HB2	1.55	0.88
1:K:148:ILE:H	1:K:148:ILE:HD13	1.38	0.88
1:K:65:VAL:HG13	1:K:95:LEU:HD12	1.57	0.87
1:L:277:THR:HG23	1:L:279:LEU:H	1.38	0.87
1:A:288:THR:HG22	1:A:328:ARG:H	1.36	0.87
1:R:179:ASN:HD22	1:R:179:ASN:H	0.87	0.87
1:N:255:ILE:HG23	1:N:265:VAL:HG21	1.57	0.87
1:D:117:VAL:O	1:D:140:VAL:HG11	1.74	0.86
1:G:132:VAL:O	1:G:136:LYS:HG3	1.75	0.86
1:R:212:ARG:HD2	1:R:212:ARG:N	1.90	0.86
1:G:264:ASN:HB3	1:G:268:ASP:OD1	1.74	0.86
1:N:104:LYS:HE2	1:N:108:LEU:HD21	1.58	0.86
1:K:144:LEU:HG	1:K:154:ILE:HD11	1.55	0.86
1:R:183:VAL:HG12	1:R:250:MSE:HE3	1.56	0.86
1:G:111:ASN:O	1:G:115:LYS:HD3	1.76	0.85
1:G:234:LEU:HD13	1:G:261:ARG:NE	1.91	0.85
1:D:151:THR:OG1	1:D:153:GLN:HG2	1.76	0.85
1:A:70:ILE:HD11	1:D:70:ILE:HG13	1.57	0.85
1:G:288:THR:HG23	1:G:327:PHE:HA	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:THR:CG2	1:A:328:ARG:H	1.90	0.85
1:L:255:ILE:O	1:L:259:GLN:HG3	1.76	0.85
1:N:288:THR:HG21	1:N:331:THR:HG23	1.58	0.84
1:L:144:LEU:HB2	1:L:156:SER:HB3	1.59	0.84
1:W:297:ILE:HD13	1:W:321:LEU:HD12	1.58	0.84
1:A:113:LEU:HD13	1:A:139:PRO:HG2	1.60	0.84
1:A:66:ILE:HD11	1:A:122:PHE:CD2	2.12	0.84
1:K:144:LEU:CG	1:K:154:ILE:HD11	2.08	0.84
1:G:98:SER:HB2	1:G:105:GLU:HG2	1.59	0.84
1:T:276:ASN:ND2	1:T:291:VAL:HG22	1.93	0.84
1:W:178:LYS:HE3	1:W:179:ASN:HD22	1.40	0.84
1:R:62:THR:HG22	1:R:92:ASN:ND2	1.93	0.84
1:G:133:GLU:HA	1:G:136:LYS:HD2	1.60	0.83
1:B:120:ILE:HB	1:B:142:VAL:HB	1.60	0.83
1:I:243:ILE:HD13	1:I:269:LEU:HD11	1.58	0.83
1:B:277:THR:HG22	1:B:278:ARG:N	1.93	0.83
1:B:128:THR:O	1:B:132:VAL:HG23	1.77	0.83
1:I:271:ILE:HD11	1:I:330:SER:HB2	1.60	0.83
1:G:125:GLY:O	1:G:189:GLU:HG3	1.78	0.83
1:W:136:LYS:HZ3	1:W:153:GLN:HB3	1.44	0.82
1:L:284:ARG:NH1	1:K:256:HIS:HB3	1.93	0.82
1:W:115:LYS:CE	1:G:94:ILE:HD11	2.09	0.82
1:K:225:SER:OG	1:K:250:MSE:HE3	1.80	0.82
1:G:109:LEU:O	1:G:113:LEU:HG	1.79	0.82
1:M:288:THR:HG23	1:M:327:PHE:HA	1.60	0.82
1:I:72:ASN:ND2	1:I:74:PHE:H	1.77	0.82
1:R:182:PHE:CE1	1:R:184:SER:HB2	2.15	0.82
1:L:109:LEU:O	1:L:113:LEU:HG	1.80	0.82
1:G:170:GLN:HA	1:G:173:ILE:HG23	1.61	0.82
1:L:92:ASN:HD21	1:K:115:LYS:NZ	1.78	0.82
1:L:132:VAL:HG12	1:L:136:LYS:HD3	1.62	0.82
1:A:288:THR:HG22	1:A:328:ARG:N	1.94	0.81
1:G:77:GLU:O	1:G:80:ARG:HG3	1.80	0.81
1:N:117:VAL:O	1:N:140:VAL:HG11	1.80	0.81
1:T:101:ASN:HD21	1:T:104:LYS:H	1.25	0.81
1:L:172:LEU:HD13	1:L:242:ALA:HB1	1.63	0.81
1:K:230:VAL:HG21	1:K:254:VAL:HA	1.61	0.81
1:B:212:ARG:HB3	1:B:212:ARG:NH1	1.95	0.81
1:W:115:LYS:NZ	1:G:62:THR:HG21	1.95	0.81
1:A:183:VAL:HG22	1:A:217:VAL:CG1	2.11	0.80
1:M:305:LEU:HG	1:M:309:MSE:HE2	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:104:LYS:HB3	1:R:104:LYS:NZ	1.96	0.80
1:I:179:ASN:ND2	1:I:212:ARG:HH12	1.79	0.80
1:N:288:THR:CG2	1:N:328:ARG:H	1.94	0.80
1:W:113:LEU:HD22	1:W:139:PRO:HG2	1.63	0.80
1:W:243:ILE:HG13	1:W:269:LEU:HD11	1.64	0.80
1:B:77:GLU:OE1	1:B:278:ARG:HB2	1.81	0.80
1:L:139:PRO:HG2	1:L:140:VAL:H	1.46	0.80
1:A:85:ILE:HD13	1:A:299:ALA:HA	1.63	0.80
1:K:318:ILE:H	1:K:318:ILE:CD1	1.96	0.80
1:W:151:THR:HB	1:W:153:GLN:HE21	1.46	0.79
1:G:135:LEU:HD23	1:G:154:ILE:HG21	1.62	0.79
1:W:97:ASN:O	1:W:104:LYS:HE2	1.81	0.79
1:A:77:GLU:OE1	1:A:277:THR:HG23	1.82	0.79
1:A:329:GLN:CD	1:A:329:GLN:H	1.86	0.79
1:T:219:GLY:HA3	1:T:250:MSE:HE1	1.64	0.79
1:K:284:ARG:HH12	1:K:286:GLN:NE2	1.81	0.79
1:K:230:VAL:CG2	1:K:254:VAL:HA	2.11	0.79
1:R:112:MSE:HE2	1:R:117:VAL:HG11	1.63	0.79
1:T:128:THR:HG22	1:T:129:GLU:OE1	1.80	0.79
1:N:179:ASN:H	1:N:179:ASN:HD22	1.27	0.79
1:A:132:VAL:HA	1:A:154:ILE:HD11	1.63	0.79
1:B:293:PRO:O	1:B:297:ILE:HG12	1.83	0.79
1:T:234:LEU:HB3	1:T:261:ARG:HH21	1.46	0.79
1:M:112:MSE:HE2	1:M:117:VAL:HG11	1.64	0.79
1:G:149:GLU:HG2	1:G:152:ASN:H	1.46	0.79
1:G:220:ASP:O	1:G:221:TYR:HB2	1.81	0.79
1:G:297:ILE:HD13	1:G:321:LEU:HD12	1.63	0.79
1:T:104:LYS:NZ	1:T:108:LEU:HD11	1.98	0.78
1:K:252:LEU:HG	1:K:283:VAL:HG11	1.65	0.78
1:D:106:LEU:HD22	1:D:110:ASN:HD21	1.47	0.78
1:M:148:ILE:HD11	1:M:190:PRO:HB2	1.66	0.78
1:D:230:VAL:HG21	1:D:254:VAL:O	1.83	0.78
1:T:135:LEU:HD23	1:T:154:ILE:HD12	1.65	0.78
1:R:70:ILE:N	1:R:97:ASN:HD21	1.81	0.78
1:T:63:VAL:HG21	1:T:305:LEU:HD21	1.66	0.78
1:M:185:GLY:HA3	1:M:221:TYR:CE2	2.19	0.78
1:B:95:LEU:HD13	1:B:96:SER:H	1.47	0.78
1:G:105:GLU:O	1:G:109:LEU:HD13	1.83	0.78
1:I:181:ALA:HB3	1:I:243:ILE:HG13	1.64	0.77
1:L:315:ASP:OD1	1:W:315:ASP:HB2	1.82	0.77
1:A:66:ILE:HD11	1:A:122:PHE:HD2	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:THR:HG23	1:D:327:PHE:HA	1.66	0.77
1:G:225:SER:OG	1:G:250:MSE:HE3	1.85	0.77
1:G:230:VAL:O	1:G:234:LEU:HG	1.84	0.77
1:M:266:PRO:O	1:M:332:LYS:HD2	1.84	0.77
1:L:173:ILE:HD11	1:L:204:LEU:HD23	1.65	0.77
1:A:179:ASN:ND2	1:A:179:ASN:O	2.18	0.77
1:N:179:ASN:H	1:N:179:ASN:ND2	1.83	0.77
1:A:82:ILE:HG23	1:A:302:MSE:HE3	1.66	0.77
1:I:88:MSE:CE	1:R:296:ASP:HB3	2.15	0.77
1:G:148:ILE:HD13	1:G:190:PRO:HG2	1.66	0.77
1:K:219:GLY:HA3	1:K:250:MSE:HE1	1.65	0.77
1:A:135:LEU:HD23	1:A:154:ILE:HD13	1.65	0.77
1:R:70:ILE:H	1:R:97:ASN:HD21	1.31	0.77
1:M:73:ILE:HD12	1:M:74:PHE:N	1.99	0.77
1:N:288:THR:HG22	1:N:328:ARG:H	1.49	0.76
1:T:118:ASP:O	1:T:141:PRO:HD2	1.84	0.76
1:L:222:THR:O	1:L:225:SER:HB3	1.85	0.76
1:A:69:ASP:OD1	1:A:71:SER:HB3	1.86	0.76
1:R:247:THR:HG22	1:R:250:MSE:HB2	1.66	0.76
1:L:69:ASP:OD2	1:L:71:SER:HB2	1.85	0.76
1:M:151:THR:CG2	1:M:153:GLN:HB2	2.15	0.76
1:W:207:SER:O	1:W:209:LEU:HG	1.86	0.76
1:N:109:LEU:HD21	1:N:135:LEU:HA	1.67	0.76
1:R:256:HIS:HB3	1:T:284:ARG:HH21	1.50	0.76
1:G:212:ARG:HH12	1:G:238:GLU:CB	1.98	0.76
1:A:85:ILE:HG23	1:A:88:MSE:HE2	1.66	0.76
1:R:303:ARG:HG3	1:R:303:ARG:HH11	1.51	0.76
1:L:226:GLY:O	1:L:230:VAL:HG23	1.84	0.76
1:N:65:VAL:HG12	1:N:66:ILE:H	1.49	0.76
1:R:129:GLU:CD	1:R:129:GLU:H	1.86	0.76
1:R:286:GLN:HG3	1:R:329:GLN:HE21	1.51	0.76
1:W:112:MSE:HA	1:W:112:MSE:CE	2.16	0.76
1:A:80:ARG:HH22	1:D:99:ASP:HA	1.50	0.76
1:I:230:VAL:HG13	1:I:254:VAL:HG13	1.68	0.76
1:W:98:SER:HA	1:W:104:LYS:HG2	1.67	0.76
1:G:117:VAL:HG21	1:G:120:ILE:HD11	1.65	0.76
1:B:182:PHE:HE1	1:B:197:VAL:HG22	1.49	0.76
1:W:276:ASN:ND2	1:W:291:VAL:HG22	2.00	0.76
1:W:136:LYS:NZ	1:W:153:GLN:HB3	2.01	0.75
1:G:107:HIS:O	1:G:110:ASN:HB2	1.85	0.75
1:D:192:ASN:HA	1:D:196:LYS:HB2	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:182:PHE:HE1	1:T:197:VAL:HG22	1.52	0.75
1:L:274:PHE:O	1:L:275:ASP:HB2	1.85	0.75
1:A:223:TYR:CB	1:D:282:MSE:HE3	2.13	0.75
1:I:230:VAL:CG1	1:I:254:VAL:HG13	2.15	0.75
1:A:104:LYS:O	1:A:108:LEU:HG	1.87	0.75
1:R:201:LYS:HG2	1:R:211:VAL:HG11	1.68	0.75
1:K:97:ASN:O	1:K:108:LEU:HD11	1.87	0.75
1:B:80:ARG:HD2	1:B:83:GLU:HB3	1.68	0.75
1:B:286:GLN:HB2	1:B:329:GLN:HE22	1.51	0.75
1:I:252:LEU:CG	1:I:283:VAL:HG11	2.15	0.75
1:R:113:LEU:HD22	1:R:139:PRO:HD2	1.69	0.75
1:K:92:ASN:C	1:K:93:ILE:HD12	2.07	0.75
1:N:264:ASN:HD21	1:N:266:PRO:HD2	1.52	0.75
1:R:102:GLN:HG2	1:R:131:HIS:NE2	2.02	0.74
1:M:113:LEU:HD13	1:M:139:PRO:HD2	1.69	0.74
1:B:148:ILE:CD1	1:B:148:ILE:H	2.01	0.74
1:L:126:ASN:HB2	1:L:189:GLU:HG2	1.69	0.74
1:L:212:ARG:CB	1:L:212:ARG:HH11	1.98	0.74
1:W:109:LEU:HD21	1:W:135:LEU:CD1	2.18	0.74
1:G:149:GLU:HB2	1:G:154:ILE:HD11	1.68	0.74
1:D:73:ILE:HD13	1:D:73:ILE:N	2.02	0.74
1:I:178:LYS:HA	1:I:209:LEU:HD13	1.68	0.74
1:L:267:ASN:HA	1:L:332:LYS:HZ3	1.53	0.74
1:L:148:ILE:CG1	1:L:191:ILE:HG12	2.18	0.74
1:M:190:PRO:HA	1:M:193:HIS:CE1	2.22	0.74
1:A:177:HIS:NE2	1:A:270:GLU:HG3	2.03	0.74
1:B:98:SER:C	1:B:100:GLN:H	1.91	0.74
1:N:185:GLY:HA3	1:N:221:TYR:CE1	2.23	0.74
1:A:78:LEU:HD13	1:A:123:MSE:SE	2.38	0.74
1:A:82:ILE:HG23	1:A:302:MSE:CE	2.18	0.74
1:D:252:LEU:HG	1:D:283:VAL:HG11	1.70	0.74
1:B:70:ILE:H	1:B:97:ASN:ND2	1.85	0.74
1:I:66:ILE:HD11	1:I:112:MSE:HG3	1.70	0.74
1:G:77:GLU:CB	1:G:294:MSE:HE1	2.16	0.74
1:M:70:ILE:O	1:M:70:ILE:HD13	1.88	0.74
1:M:169:VAL:HG11	1:M:200:TYR:HA	1.70	0.74
1:B:212:ARG:HH11	1:B:212:ARG:CB	2.01	0.73
1:T:155:PRO:HG3	1:T:317:SER:HB3	1.68	0.73
1:G:85:ILE:H	1:G:85:ILE:HD12	1.53	0.73
1:T:182:PHE:CZ	1:T:184:SER:HB2	2.23	0.73
1:B:148:ILE:H	1:B:148:ILE:HD13	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:86:ALA:HB1	1:W:93:ILE:HD11	1.68	0.73
1:D:255:ILE:HG12	1:D:271:ILE:CD1	2.18	0.73
1:A:261:ARG:NH1	1:A:261:ARG:HB2	2.03	0.73
1:W:104:LYS:O	1:W:108:LEU:HG	1.89	0.73
1:M:104:LYS:O	1:M:108:LEU:HD13	1.87	0.73
1:D:255:ILE:HG23	1:D:265:VAL:HG21	1.70	0.73
1:I:219:GLY:CA	1:I:250:MSE:HE1	2.13	0.73
1:T:230:VAL:HG12	1:T:234:LEU:HG	1.71	0.73
1:K:265:VAL:HG12	1:K:285:PRO:HG3	1.71	0.73
1:W:285:PRO:HB2	1:W:329:GLN:CB	2.17	0.73
1:N:101:ASN:O	1:N:105:GLU:HG3	1.88	0.73
1:M:262:GLY:O	1:M:263:LEU:HD23	1.89	0.73
1:D:182:PHE:HE1	1:D:197:VAL:HG22	1.54	0.73
1:B:70:ILE:H	1:B:97:ASN:HD21	1.35	0.73
1:G:62:THR:HG22	1:G:92:ASN:OD1	1.88	0.73
1:M:201:LYS:O	1:M:205:THR:HG22	1.89	0.73
1:W:177:HIS:HB3	1:W:180:ILE:HD11	1.71	0.72
1:M:266:PRO:HB2	1:M:332:LYS:HG3	1.71	0.72
1:T:117:VAL:O	1:T:140:VAL:HG11	1.89	0.72
1:T:144:LEU:HB2	1:T:156:SER:HB3	1.69	0.72
1:W:178:LYS:CE	1:W:179:ASN:HD22	2.02	0.72
1:A:267:ASN:HA	1:A:332:LYS:HE3	1.70	0.72
1:B:277:THR:CG2	1:B:278:ARG:H	1.92	0.72
1:L:277:THR:CG2	1:L:279:LEU:H	2.02	0.72
1:N:78:LEU:HD12	1:N:123:MSE:SE	2.38	0.72
1:M:219:GLY:HA3	1:M:225:SER:HB3	1.71	0.72
1:A:230:VAL:CG2	1:A:254:VAL:HG13	2.19	0.72
1:W:179:ASN:HB2	1:W:215:TYR:HE2	1.54	0.72
1:K:113:LEU:HD13	1:K:139:PRO:HD2	1.71	0.72
1:G:230:VAL:HG21	1:G:254:VAL:HA	1.70	0.72
1:T:122:PHE:HB3	1:T:144:LEU:HD23	1.71	0.72
1:L:186:THR:HA	1:L:218:GLU:OE1	1.88	0.72
1:W:274:PHE:O	1:W:275:ASP:HB2	1.87	0.72
1:A:222:THR:HG22	1:A:224:ASP:H	1.55	0.72
1:B:212:ARG:NH1	1:B:214:SER:HB3	2.05	0.72
1:W:66:ILE:HG23	1:W:96:SER:HB2	1.71	0.72
1:L:92:ASN:HD21	1:K:115:LYS:HZ1	1.35	0.71
1:L:149:GLU:HG3	1:L:154:ILE:HG21	1.70	0.71
1:L:220:ASP:OD1	1:L:225:SER:HB2	1.89	0.71
1:M:80:ARG:HD2	1:M:80:ARG:O	1.90	0.71
1:L:83:GLU:OE2	1:K:104:LYS:NZ	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:95:LEU:HD13	1:L:96:SER:N	2.05	0.71
1:D:104:LYS:O	1:D:108:LEU:HG	1.88	0.71
1:B:157:VAL:HG11	1:B:301:ALA:HB2	1.70	0.71
1:T:212:ARG:N	1:T:212:ARG:HD2	2.05	0.71
1:G:293:PRO:O	1:G:297:ILE:HG12	1.90	0.71
1:B:93:ILE:H	1:B:93:ILE:HD12	1.55	0.71
1:B:133:GLU:O	1:B:137:LYS:HG3	1.90	0.71
1:G:149:GLU:HG3	1:G:150:SER:H	1.54	0.71
1:B:129:GLU:CD	1:B:129:GLU:H	1.92	0.71
1:I:173:ILE:HD12	1:I:209:LEU:HD12	1.72	0.71
1:I:297:ILE:HD13	1:I:321:LEU:HD12	1.71	0.71
1:R:153:GLN:O	1:R:154:ILE:HG12	1.91	0.71
1:W:305:LEU:HG	1:W:309:MSE:HE2	1.71	0.71
1:D:109:LEU:O	1:D:113:LEU:HG	1.91	0.71
1:L:90:LYS:HE2	1:L:90:LYS:CA	2.16	0.71
1:L:159:ILE:HD13	1:L:292:GLN:HB3	1.73	0.71
1:G:144:LEU:HD23	1:G:155:PRO:O	1.89	0.71
1:B:83:GLU:OE1	1:I:97:ASN:HB2	1.90	0.71
1:A:230:VAL:HG21	1:A:254:VAL:HG13	1.72	0.71
1:I:86:ALA:CB	1:I:93:ILE:HD11	2.21	0.71
1:K:144:LEU:HD12	1:K:149:GLU:HB2	1.72	0.71
1:W:216:ILE:HG13	1:W:216:ILE:O	1.90	0.71
1:A:148:ILE:HD13	1:A:148:ILE:H	1.56	0.71
1:K:113:LEU:HD22	1:K:139:PRO:HD2	1.73	0.71
1:K:99:ASP:HB2	1:K:101:ASN:HD22	1.57	0.70
1:W:179:ASN:HB2	1:W:215:TYR:CE2	2.26	0.70
1:D:186:THR:HG23	1:D:188:GLU:OE1	1.92	0.70
1:I:231:GLU:O	1:I:235:GLU:HG2	1.91	0.70
1:R:187:LEU:HD12	1:R:218:GLU:OE2	1.90	0.70
1:L:103:ASP:O	1:L:106:LEU:HB3	1.90	0.70
1:W:106:LEU:HG	1:W:134:GLU:OE2	1.90	0.70
1:N:177:HIS:ND1	1:N:241:THR:HB	2.06	0.70
1:R:226:GLY:O	1:R:230:VAL:HG23	1.92	0.70
1:M:109:LEU:O	1:M:113:LEU:HG	1.92	0.70
1:A:231:GLU:HG2	1:A:261:ARG:NH2	2.06	0.70
1:I:132:VAL:O	1:I:136:LYS:HG2	1.92	0.70
1:R:245:VAL:HG11	1:R:250:MSE:HB3	1.73	0.70
1:A:128:THR:HG22	1:A:129:GLU:H	1.54	0.70
1:I:231:GLU:HG2	1:I:261:ARG:HE	1.56	0.70
1:K:318:ILE:N	1:K:318:ILE:CD1	2.49	0.70
1:N:108:LEU:HA	1:N:111:ASN:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:255:ILE:HG12	1:N:271:ILE:HD12	1.74	0.70
1:A:288:THR:HG22	1:A:327:PHE:HA	1.74	0.70
1:I:88:MSE:HE2	1:R:296:ASP:HB3	1.73	0.70
1:W:135:LEU:HD23	1:W:154:ILE:HD11	1.74	0.70
1:N:223:TYR:CG	1:M:282:MSE:HG2	2.27	0.70
1:B:89:TYR:OH	1:B:303:ARG:HG2	1.91	0.70
1:K:264:ASN:HB3	1:K:268:ASP:HB2	1.74	0.70
1:W:151:THR:HB	1:W:153:GLN:NE2	2.06	0.70
1:A:72:ASN:HD22	1:A:75:TYR:HD2	1.40	0.69
1:A:222:THR:HG22	1:A:224:ASP:N	2.06	0.69
1:R:288:THR:H	1:R:330:SER:HB3	1.57	0.69
1:W:230:VAL:HA	1:W:233:LEU:HD12	1.74	0.69
1:B:157:VAL:O	1:B:157:VAL:HG13	1.93	0.69
1:L:73:ILE:HD11	1:K:278:ARG:NH2	2.05	0.69
1:A:67:ILE:H	1:A:67:ILE:HD13	1.57	0.69
1:R:286:GLN:HG3	1:R:329:GLN:NE2	2.06	0.69
1:N:136:LYS:HG2	1:N:137:LYS:NZ	2.08	0.69
1:A:70:ILE:CD1	1:D:70:ILE:HG13	2.22	0.69
1:B:95:LEU:HD13	1:B:96:SER:N	2.07	0.69
1:R:95:LEU:HD13	1:R:95:LEU:H	1.57	0.69
1:K:148:ILE:H	1:K:148:ILE:CD1	2.05	0.69
1:W:178:LYS:HE3	1:W:179:ASN:ND2	2.07	0.69
1:W:180:ILE:N	1:W:180:ILE:HD12	2.08	0.69
1:W:230:VAL:HG21	1:W:254:VAL:HA	1.73	0.69
1:M:73:ILE:HD12	1:M:74:PHE:H	1.57	0.69
1:A:148:ILE:H	1:A:148:ILE:CD1	2.05	0.69
1:L:98:SER:HA	1:L:104:LYS:HG2	1.74	0.69
1:K:277:THR:CG2	1:K:279:LEU:H	2.03	0.69
1:I:220:ASP:O	1:I:221:TYR:HB2	1.92	0.69
1:G:75:TYR:CD1	1:G:123:MSE:HE3	2.19	0.69
1:N:190:PRO:O	1:N:194:ALA:HB3	1.93	0.69
1:B:200:TYR:CE1	1:B:216:ILE:HD11	2.28	0.69
1:B:307:LYS:HE2	1:B:307:LYS:N	2.07	0.69
1:I:252:LEU:HG	1:I:283:VAL:CG1	2.18	0.69
1:R:277:THR:HG22	1:R:279:LEU:N	1.98	0.69
1:R:285:PRO:HB2	1:R:329:GLN:HB3	1.74	0.69
1:K:144:LEU:HG	1:K:154:ILE:CD1	2.22	0.69
1:G:247:THR:HB	1:G:250:MSE:HB2	1.75	0.69
1:N:135:LEU:HD12	1:N:142:VAL:HG11	1.74	0.69
1:T:109:LEU:HD21	1:T:135:LEU:HD13	1.72	0.69
1:K:82:ILE:O	1:K:85:ILE:HG22	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:94:ILE:HD13	1:K:94:ILE:H	1.56	0.69
1:W:70:ILE:O	1:W:70:ILE:HD13	1.92	0.69
1:G:255:ILE:HG12	1:G:271:ILE:HD12	1.74	0.69
1:M:63:VAL:HG13	1:M:93:ILE:HG12	1.75	0.69
1:B:285:PRO:HB2	1:B:329:GLN:O	1.93	0.69
1:G:234:LEU:HD22	1:G:261:ARG:HH21	1.57	0.69
1:G:277:THR:C	1:G:279:LEU:H	1.95	0.69
1:N:118:ASP:O	1:N:141:PRO:HD2	1.93	0.69
1:R:230:VAL:HG21	1:R:254:VAL:HA	1.76	0.68
1:D:230:VAL:CG2	1:D:254:VAL:HA	2.23	0.68
1:R:104:LYS:HB3	1:R:104:LYS:HZ3	1.57	0.68
1:R:230:VAL:CG2	1:R:254:VAL:HA	2.24	0.68
1:L:73:ILE:N	1:L:73:ILE:HD12	2.08	0.68
1:M:255:ILE:HG12	1:M:271:ILE:HD11	1.75	0.68
1:I:173:ILE:HD11	1:I:204:LEU:HD12	1.76	0.68
1:R:67:ILE:HA	1:R:123:MSE:HB2	1.74	0.68
1:A:71:SER:HA	1:D:76:ALA:HB1	1.74	0.68
1:A:100:GLN:HA	1:A:100:GLN:HE21	1.57	0.68
1:A:230:VAL:HG21	1:A:254:VAL:HA	1.73	0.68
1:W:92:ASN:HD21	1:G:111:ASN:ND2	1.92	0.68
1:M:157:VAL:HG11	1:M:301:ALA:HB2	1.75	0.68
1:B:286:GLN:HB2	1:B:329:GLN:NE2	2.08	0.68
1:R:255:ILE:HG12	1:R:271:ILE:HD12	1.75	0.68
1:I:293:PRO:O	1:I:297:ILE:HG12	1.94	0.68
1:L:168:ALA:O	1:L:171:SER:HB3	1.94	0.68
1:W:68:PRO:O	1:W:99:ASP:N	2.27	0.68
1:D:66:ILE:HD13	1:D:96:SER:HB3	1.75	0.68
1:B:148:ILE:HD12	1:B:191:ILE:HG12	1.74	0.68
1:T:101:ASN:ND2	1:T:101:ASN:C	2.46	0.68
1:L:67:ILE:HD11	1:L:70:ILE:HG13	1.75	0.68
1:G:102:GLN:NE2	1:G:128:THR:HG21	2.09	0.68
1:K:160:ASP:HB2	1:K:320:GLN:HE22	1.59	0.67
1:K:284:ARG:HH12	1:K:286:GLN:HE21	1.38	0.67
1:W:177:HIS:CD2	1:W:242:ALA:HB2	2.28	0.67
1:G:307:LYS:HZ2	1:G:312:GLU:HB3	1.59	0.67
1:N:99:ASP:O	1:N:100:GLN:HB3	1.92	0.67
1:N:62:THR:HG22	1:N:92:ASN:CB	2.19	0.67
1:A:252:LEU:HG	1:A:283:VAL:CG1	2.25	0.67
1:I:72:ASN:C	1:I:72:ASN:HD22	1.94	0.67
1:T:101:ASN:C	1:T:101:ASN:HD22	1.97	0.67
1:L:212:ARG:NH1	1:L:212:ARG:HB3	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:142:VAL:HG13	1:N:154:ILE:HD11	1.77	0.67
1:M:164:ALA:HB1	1:M:290:VAL:HG11	1.75	0.67
1:D:62:THR:HG22	1:D:92:ASN:CB	2.21	0.67
1:L:155:PRO:CB	1:L:317:SER:HB3	2.24	0.67
1:W:94:ILE:HG21	1:W:112:MSE:HE1	1.76	0.67
1:A:274:PHE:O	1:A:275:ASP:HB2	1.95	0.67
1:N:194:ALA:O	1:N:198:LYS:HD2	1.93	0.67
1:B:70:ILE:HB	1:B:97:ASN:HD21	1.60	0.67
1:I:271:ILE:CD1	1:I:330:SER:HB2	2.24	0.67
1:R:85:ILE:HA	1:R:88:MSE:HE2	1.74	0.67
1:N:144:LEU:HD21	1:N:154:ILE:HD13	1.74	0.67
1:N:246:GLY:O	1:N:274:PHE:HB3	1.94	0.67
1:M:128:THR:OG1	1:M:130:GLU:HB3	1.95	0.67
1:M:72:ASN:HD22	1:M:72:ASN:C	1.97	0.67
1:R:94:ILE:HG23	1:T:94:ILE:HG23	1.77	0.67
1:G:143:VAL:HG12	1:G:305:LEU:HD13	1.77	0.67
1:I:78:LEU:HB2	1:I:294:MSE:HE2	1.77	0.67
1:W:159:ILE:HG22	1:W:321:LEU:O	1.95	0.67
1:I:63:VAL:CG1	1:I:93:ILE:HG12	2.25	0.67
1:I:318:ILE:O	1:I:318:ILE:HD13	1.94	0.67
1:W:122:PHE:HB3	1:W:144:LEU:HD23	1.75	0.67
1:N:113:LEU:CD2	1:N:139:PRO:HD2	2.24	0.67
1:N:229:ALA:HA	1:N:232:LYS:HD2	1.77	0.67
1:A:62:THR:HG22	1:A:92:ASN:HD22	1.59	0.66
1:A:315:ASP:OD1	1:A:315:ASP:N	2.28	0.66
1:W:135:LEU:HD23	1:W:154:ILE:CD1	2.25	0.66
1:G:178:LYS:O	1:G:209:LEU:HD22	1.95	0.66
1:G:307:LYS:HG3	1:G:312:GLU:HB2	1.77	0.66
1:N:65:VAL:HG12	1:N:66:ILE:N	2.09	0.66
1:M:67:ILE:HD13	1:M:67:ILE:H	1.60	0.66
1:A:220:ASP:O	1:A:221:TYR:HB2	1.95	0.66
1:L:93:ILE:HD11	1:L:302:MSE:HE1	1.76	0.66
1:T:104:LYS:HZ2	1:T:108:LEU:HD11	1.61	0.66
1:K:93:ILE:HD12	1:K:93:ILE:N	2.10	0.66
1:W:73:ILE:HG22	1:W:74:PHE:N	2.11	0.66
1:M:230:VAL:CG1	1:M:254:VAL:HG13	2.24	0.66
1:M:326:GLU:HG2	1:M:328:ARG:NH2	2.10	0.66
1:L:152:ASN:HB3	1:L:318:ILE:HD11	1.78	0.66
1:G:113:LEU:CD2	1:G:139:PRO:HD2	2.24	0.66
1:B:180:ILE:HD12	1:B:180:ILE:N	2.10	0.66
1:T:68:PRO:HD3	1:T:123:MSE:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:234:LEU:CB	1:T:261:ARG:HH21	2.08	0.66
1:W:115:LYS:HZ3	1:G:62:THR:HG21	1.61	0.66
1:N:288:THR:HG22	1:N:328:ARG:N	2.10	0.66
1:R:82:ILE:CG2	1:R:302:MSE:HE2	2.25	0.66
1:L:63:VAL:HG13	1:L:93:ILE:HG12	1.76	0.66
1:L:86:ALA:HB2	1:L:93:ILE:CD1	2.26	0.66
1:L:288:THR:HG22	1:L:328:ARG:H	1.60	0.66
1:K:109:LEU:HD21	1:K:135:LEU:HD13	1.77	0.66
1:W:80:ARG:NH2	1:G:69:ASP:HA	2.11	0.66
1:N:73:ILE:HD12	1:N:73:ILE:H	1.59	0.66
1:N:118:ASP:O	1:N:140:VAL:HB	1.95	0.66
1:N:288:THR:CG2	1:N:331:THR:HG23	2.25	0.66
1:M:157:VAL:CG1	1:M:301:ALA:HB2	2.26	0.66
1:M:252:LEU:HG	1:M:283:VAL:HG13	1.76	0.66
1:T:131:HIS:O	1:T:135:LEU:HB2	1.95	0.66
1:T:318:ILE:HD13	1:T:318:ILE:N	2.09	0.66
1:L:77:GLU:HB3	1:L:294:MSE:HE3	1.77	0.66
1:M:293:PRO:O	1:M:297:ILE:HG12	1.96	0.66
1:A:329:GLN:N	1:A:329:GLN:OE1	2.29	0.66
1:B:212:ARG:HH12	1:B:214:SER:CB	2.08	0.66
1:B:272:ILE:HG12	1:B:288:THR:OG1	1.95	0.66
1:I:173:ILE:CD1	1:I:209:LEU:HD12	2.26	0.66
1:T:106:LEU:O	1:T:106:LEU:HD23	1.95	0.66
1:T:263:LEU:HD23	1:T:268:ASP:CB	2.26	0.66
1:G:324:ARG:NH2	1:G:326:GLU:OE1	2.25	0.66
1:N:247:THR:HG22	1:N:248:ASP:N	2.10	0.66
1:A:177:HIS:CE1	1:A:270:GLU:HG3	2.31	0.66
1:R:138:SER:HB2	1:R:139:PRO:HD2	1.78	0.66
1:L:288:THR:HB	1:L:327:PHE:HA	1.77	0.66
1:K:133:GLU:HA	1:K:136:LYS:CE	2.26	0.66
1:A:183:VAL:HG22	1:A:217:VAL:HG11	1.77	0.66
1:D:133:GLU:O	1:D:137:LYS:HE2	1.95	0.66
1:D:274:PHE:O	1:D:275:ASP:HB2	1.95	0.66
1:L:117:VAL:O	1:L:140:VAL:HG11	1.96	0.66
1:L:132:VAL:O	1:L:136:LYS:HB2	1.95	0.66
1:L:297:ILE:HA	1:L:321:LEU:HD11	1.77	0.66
1:W:70:ILE:HD11	1:G:70:ILE:CG1	2.26	0.66
1:G:230:VAL:CG2	1:G:254:VAL:HA	2.26	0.66
1:D:148:ILE:HD13	1:D:148:ILE:H	1.60	0.65
1:R:305:LEU:HG	1:R:309:MSE:HE2	1.77	0.65
1:W:73:ILE:HD11	1:G:73:ILE:HD11	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:151:THR:O	1:W:152:ASN:HB2	1.95	0.65
1:W:234:LEU:O	1:W:239:LYS:HE3	1.96	0.65
1:W:113:LEU:HD22	1:W:139:PRO:CG	2.26	0.65
1:W:146:ALA:HA	1:W:158:THR:HG22	1.78	0.65
1:W:254:VAL:HG12	1:W:271:ILE:HD13	1.79	0.65
1:L:121:ILE:HG22	1:L:123:MSE:HE2	1.77	0.65
1:L:230:VAL:HG22	1:L:254:VAL:HA	1.78	0.65
1:G:89:TYR:O	1:G:90:LYS:HB2	1.96	0.65
1:G:154:ILE:HD12	1:G:154:ILE:O	1.96	0.65
1:G:307:LYS:HG2	1:G:314:VAL:HG12	1.78	0.65
1:N:121:ILE:N	1:N:121:ILE:HD12	2.11	0.65
1:T:318:ILE:HD13	1:T:318:ILE:H	1.61	0.65
1:K:263:LEU:HD13	1:K:269:LEU:HD12	1.78	0.65
1:K:283:VAL:O	1:K:284:ARG:HD3	1.97	0.65
1:T:190:PRO:HA	1:T:193:HIS:CE1	2.32	0.65
1:K:112:MSE:HB3	1:K:120:ILE:HD11	1.77	0.65
1:K:112:MSE:HE2	1:K:112:MSE:HA	1.77	0.65
1:K:230:VAL:HG22	1:K:254:VAL:HG22	1.79	0.65
1:G:318:ILE:HD13	1:G:318:ILE:H	1.61	0.65
1:M:141:PRO:HG2	1:M:305:LEU:HD11	1.79	0.65
1:M:149:GLU:O	1:M:149:GLU:CD	2.35	0.65
1:D:255:ILE:HG12	1:D:271:ILE:HD13	1.79	0.65
1:D:307:LYS:HD2	1:D:314:VAL:HG12	1.79	0.65
1:I:265:VAL:HG12	1:I:285:PRO:HG3	1.79	0.65
1:L:328:ARG:HG2	1:L:328:ARG:HH11	1.61	0.65
1:A:191:ILE:HG13	1:A:192:ASN:OD1	1.96	0.65
1:D:149:GLU:O	1:D:149:GLU:HG3	1.96	0.65
1:T:65:VAL:HG13	1:T:95:LEU:HA	1.78	0.65
1:M:94:ILE:HG21	1:M:112:MSE:HE1	1.79	0.65
1:D:106:LEU:HD22	1:D:110:ASN:ND2	2.12	0.65
1:I:307:LYS:CD	1:I:314:VAL:HG12	2.27	0.65
1:K:70:ILE:O	1:K:70:ILE:HD13	1.96	0.65
1:M:263:LEU:O	1:M:268:ASP:HB2	1.96	0.65
1:W:212:ARG:O	1:W:215:TYR:HB2	1.97	0.65
1:R:252:LEU:HD22	1:T:282:MSE:CE	2.28	0.64
1:D:157:VAL:HG11	1:D:301:ALA:HB2	1.80	0.64
1:G:120:ILE:HB	1:G:142:VAL:HG22	1.80	0.64
1:B:151:THR:HG21	1:B:153:GLN:OE1	1.97	0.64
1:R:274:PHE:O	1:R:275:ASP:HB2	1.96	0.64
1:T:263:LEU:HD23	1:T:268:ASP:HB2	1.79	0.64
1:G:69:ASP:OD1	1:G:71:SER:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:245:VAL:HG21	1:R:251:ALA:HA	1.79	0.64
1:K:243:ILE:HB	1:K:271:ILE:HG22	1.80	0.64
1:N:113:LEU:HD22	1:N:139:PRO:HD2	1.78	0.64
1:N:168:ALA:O	1:N:171:SER:HB3	1.98	0.64
1:N:169:VAL:HG21	1:N:200:TYR:HA	1.78	0.64
1:N:252:LEU:HG	1:N:283:VAL:CG1	2.27	0.64
1:M:151:THR:HG22	1:M:153:GLN:CB	2.27	0.64
1:R:67:ILE:HG22	1:R:123:MSE:HG3	1.79	0.64
1:R:105:GLU:O	1:R:109:LEU:HB3	1.98	0.64
1:T:220:ASP:O	1:T:221:TYR:HB2	1.96	0.64
1:L:101:ASN:O	1:L:105:GLU:HG3	1.97	0.64
1:L:138:SER:OG	1:L:139:PRO:HD2	1.97	0.64
1:K:86:ALA:HB1	1:K:93:ILE:HD11	1.80	0.64
1:A:169:VAL:O	1:A:173:ILE:HG12	1.97	0.64
1:N:104:LYS:HE2	1:N:108:LEU:CD2	2.28	0.64
1:R:111:ASN:O	1:R:115:LYS:HG3	1.98	0.64
1:L:86:ALA:HB2	1:L:93:ILE:HD11	1.78	0.64
1:L:255:ILE:HD11	1:L:287:LEU:HD13	1.77	0.64
1:W:109:LEU:HD21	1:W:135:LEU:HD12	1.80	0.64
1:W:231:GLU:C	1:W:233:LEU:H	2.01	0.64
1:G:318:ILE:HD13	1:G:318:ILE:N	2.13	0.64
1:D:307:LYS:CD	1:D:314:VAL:HG12	2.28	0.64
1:I:169:VAL:O	1:I:173:ILE:HG12	1.98	0.64
1:K:128:THR:O	1:K:132:VAL:HG12	1.97	0.64
1:A:256:HIS:HE1	1:D:282:MSE:O	1.81	0.64
1:B:149:GLU:HG3	1:B:154:ILE:HG23	1.78	0.64
1:I:109:LEU:O	1:I:113:LEU:HG	1.97	0.64
1:W:202:ARG:O	1:W:206:GLU:HG3	1.98	0.64
1:G:144:LEU:HD23	1:G:144:LEU:H	1.63	0.64
1:B:144:LEU:HG	1:B:154:ILE:HD11	1.80	0.63
1:K:132:VAL:HG21	1:K:153:GLN:OE1	1.98	0.63
1:K:148:ILE:HD13	1:K:148:ILE:N	2.11	0.63
1:N:264:ASN:HD22	1:N:266:PRO:HD2	1.61	0.63
1:B:194:ALA:O	1:B:195:LYS:HD3	1.98	0.63
1:B:223:TYR:CB	1:I:282:MSE:HE3	2.24	0.63
1:B:292:GLN:O	1:B:294:MSE:N	2.32	0.63
1:T:186:THR:HB	1:T:189:GLU:HG3	1.80	0.63
1:A:272:ILE:HD12	1:A:272:ILE:N	2.14	0.63
1:D:160:ASP:OD1	1:D:163:GLN:HB2	1.98	0.63
1:L:115:LYS:HD3	1:K:94:ILE:HG21	1.80	0.63
1:M:109:LEU:HD11	1:M:113:LEU:HD21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ASN:C	1:A:126:ASN:HD22	2.01	0.63
1:L:149:GLU:OE1	1:L:154:ILE:HG22	1.98	0.63
1:K:166:PHE:CE2	1:K:203:ALA:HA	2.33	0.63
1:W:115:LYS:HZ1	1:G:62:THR:HG21	1.62	0.63
1:N:86:ALA:CB	1:N:93:ILE:HD11	2.29	0.63
1:M:68:PRO:HB3	1:M:100:GLN:HG3	1.80	0.63
1:T:223:TYR:HE1	1:T:256:HIS:HD2	1.45	0.63
1:W:97:ASN:HB3	1:G:83:GLU:CD	2.19	0.63
1:W:109:LEU:HD21	1:W:135:LEU:HD11	1.81	0.63
1:G:219:GLY:HA3	1:G:250:MSE:HE1	1.80	0.63
1:M:70:ILE:HB	1:M:97:ASN:HD21	1.64	0.63
1:A:72:ASN:ND2	1:A:75:TYR:CD2	2.67	0.63
1:A:129:GLU:O	1:A:132:VAL:HG12	1.99	0.63
1:I:274:PHE:O	1:I:275:ASP:HB2	1.97	0.63
1:T:83:GLU:HB2	1:T:93:ILE:HD13	1.81	0.63
1:T:108:LEU:O	1:T:112:MSE:HG3	1.99	0.63
1:K:132:VAL:O	1:K:136:LYS:HG3	1.98	0.63
1:K:213:ASP:O	1:K:216:ILE:HB	1.98	0.63
1:W:270:GLU:OE2	1:W:332:LYS:HB2	1.99	0.63
1:L:70:ILE:H	1:L:97:ASN:ND2	1.89	0.63
1:L:85:ILE:HD13	1:L:299:ALA:HA	1.80	0.63
1:L:326:GLU:HG3	1:L:328:ARG:NH1	2.14	0.63
1:N:304:LEU:O	1:N:307:LYS:HB2	1.99	0.63
1:B:82:ILE:HG23	1:B:302:MSE:HE2	1.79	0.63
1:B:163:GLN:OE1	1:B:163:GLN:HA	1.98	0.63
1:B:202:ARG:HA	1:B:205:THR:HG22	1.80	0.63
1:I:243:ILE:CD1	1:I:269:LEU:HD11	2.28	0.63
1:T:217:VAL:HG12	1:T:218:GLU:N	2.13	0.63
1:L:114:GLY:C	1:L:116:GLN:H	2.02	0.63
1:W:286:GLN:N	1:W:329:GLN:HB2	2.14	0.63
1:G:278:ARG:HB3	1:G:278:ARG:NH1	2.14	0.63
1:L:284:ARG:NH1	1:K:260:ASP:OD1	2.32	0.62
1:W:70:ILE:HD11	1:G:70:ILE:HG12	1.81	0.62
1:A:172:LEU:HD22	1:A:242:ALA:HB1	1.80	0.62
1:M:252:LEU:HD11	1:M:283:VAL:HG22	1.81	0.62
1:D:121:ILE:HD11	1:D:302:MSE:CE	2.13	0.62
1:I:153:GLN:O	1:I:154:ILE:HD13	1.99	0.62
1:R:230:VAL:HG22	1:R:254:VAL:HG13	1.81	0.62
1:R:287:LEU:HA	1:R:330:SER:HB2	1.81	0.62
1:W:78:LEU:O	1:W:78:LEU:HD22	1.99	0.62
1:G:191:ILE:O	1:G:195:LYS:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:131:HIS:O	1:M:135:LEU:HB2	2.00	0.62
1:W:278:ARG:HB3	1:W:278:ARG:NH1	2.14	0.62
1:A:67:ILE:HD12	1:A:95:LEU:HD12	1.81	0.62
1:I:139:PRO:HG2	1:I:140:VAL:H	1.64	0.62
1:R:305:LEU:O	1:R:309:MSE:HG3	2.00	0.62
1:L:288:THR:HG23	1:L:330:SER:OG	2.00	0.62
1:A:282:MSE:HE3	1:D:252:LEU:HD22	1.81	0.62
1:L:202:ARG:O	1:L:206:GLU:HG2	1.99	0.62
1:K:148:ILE:HD12	1:K:191:ILE:HB	1.80	0.62
1:W:288:THR:HG23	1:W:288:THR:O	1.98	0.62
1:G:321:LEU:HB3	1:G:322:PRO:HD2	1.82	0.62
1:A:80:ARG:NH2	1:D:97:ASN:HD21	1.98	0.62
1:A:190:PRO:HA	1:A:193:HIS:CD2	2.33	0.62
1:D:324:ARG:HG2	1:D:325:ILE:H	1.63	0.62
1:L:172:LEU:HG	1:L:272:ILE:HD12	1.82	0.62
1:W:98:SER:CA	1:W:108:LEU:HD11	2.30	0.62
1:I:169:VAL:HG11	1:I:200:TYR:HA	1.81	0.62
1:K:133:GLU:HA	1:K:136:LYS:HE2	1.82	0.62
1:D:97:ASN:O	1:D:108:LEU:HD11	2.00	0.62
1:D:302:MSE:HE2	1:D:302:MSE:HA	1.82	0.62
1:D:247:THR:HG22	1:D:250:MSE:H	1.65	0.61
1:G:251:ALA:HB1	1:G:287:LEU:HD11	1.81	0.61
1:A:93:ILE:HD12	1:A:93:ILE:N	2.13	0.61
1:A:157:VAL:HG11	1:A:301:ALA:HA	1.82	0.61
1:I:97:ASN:O	1:I:108:LEU:HG	2.00	0.61
1:L:94:ILE:HG23	1:K:94:ILE:HB	1.81	0.61
1:L:113:LEU:HD22	1:L:139:PRO:CG	2.30	0.61
1:D:65:VAL:HG22	1:D:95:LEU:HD23	1.82	0.61
1:B:187:LEU:HG	1:B:218:GLU:CD	2.19	0.61
1:R:74:PHE:CE2	1:R:294:MSE:HG2	2.34	0.61
1:K:73:ILE:HD12	1:K:74:PHE:N	2.09	0.61
1:K:219:GLY:HA3	1:K:250:MSE:CE	2.28	0.61
1:N:230:VAL:HG21	1:N:254:VAL:HA	1.82	0.61
1:D:85:ILE:HG21	1:D:302:MSE:HG3	1.82	0.61
1:I:77:GLU:HG2	1:I:294:MSE:SE	2.51	0.61
1:R:165:ALA:HB1	1:R:244:PHE:HE2	1.65	0.61
1:R:243:ILE:HG13	1:R:269:LEU:HD11	1.83	0.61
1:G:85:ILE:HD12	1:G:85:ILE:N	2.14	0.61
1:N:170:GLN:HA	1:N:173:ILE:HB	1.81	0.61
1:B:230:VAL:HG13	1:B:254:VAL:HG13	1.82	0.61
1:B:245:VAL:HG11	1:B:251:ALA:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:252:LEU:HG	1:T:283:VAL:CG1	2.30	0.61
1:G:161:TYR:CE2	1:G:191:ILE:HD11	2.35	0.61
1:B:220:ASP:OD1	1:B:222:THR:HB	1.99	0.61
1:L:247:THR:HG22	1:L:250:MSE:H	1.65	0.61
1:M:225:SER:HB3	1:M:250:MSE:HE3	1.81	0.61
1:A:62:THR:CG2	1:A:92:ASN:HB2	2.25	0.61
1:R:120:ILE:O	1:R:142:VAL:HG23	2.00	0.61
1:T:166:PHE:O	1:T:170:GLN:HB2	2.00	0.61
1:L:277:THR:HG23	1:L:278:ARG:N	2.15	0.61
1:W:73:ILE:HG22	1:W:74:PHE:H	1.65	0.61
1:G:149:GLU:CG	1:G:150:SER:H	2.13	0.61
1:N:274:PHE:O	1:N:275:ASP:CB	2.47	0.61
1:M:65:VAL:HG13	1:M:95:LEU:HG	1.83	0.61
1:R:170:GLN:HA	1:R:173:ILE:HD12	1.82	0.61
1:K:173:ILE:HD13	1:K:207:SER:HB2	1.81	0.61
1:N:264:ASN:HB3	1:N:268:ASP:OD2	2.00	0.61
1:R:217:VAL:HG11	1:R:233:LEU:HG	1.82	0.61
1:R:288:THR:HG23	1:R:327:PHE:HA	1.81	0.61
1:L:282:MSE:HG2	1:K:223:TYR:CG	2.35	0.61
1:G:149:GLU:OE2	1:G:154:ILE:HG13	2.00	0.61
1:N:79:ALA:HB2	1:N:123:MSE:HE1	1.82	0.61
1:N:148:ILE:HG23	1:N:191:ILE:HG12	1.83	0.61
1:L:187:LEU:HD12	1:L:218:GLU:OE2	2.01	0.60
1:W:284:ARG:NH1	1:G:256:HIS:HB3	2.15	0.60
1:G:148:ILE:HD11	1:G:191:ILE:HB	1.82	0.60
1:M:200:TYR:O	1:M:204:LEU:HD13	2.00	0.60
1:D:102:GLN:HE21	1:D:130:GLU:CD	2.03	0.60
1:D:255:ILE:HG12	1:D:271:ILE:HD11	1.82	0.60
1:I:242:ALA:C	1:I:243:ILE:HD12	2.20	0.60
1:R:252:LEU:HG	1:R:283:VAL:CG2	2.31	0.60
1:A:148:ILE:HG13	1:A:190:PRO:HB2	1.82	0.60
1:A:182:PHE:CZ	1:A:184:SER:HB3	2.36	0.60
1:D:113:LEU:HD22	1:D:139:PRO:HB2	1.83	0.60
1:D:160:ASP:CG	1:D:163:GLN:HB2	2.21	0.60
1:B:222:THR:HG22	1:B:224:ASP:N	2.16	0.60
1:T:252:LEU:HG	1:T:283:VAL:HG13	1.82	0.60
1:L:62:THR:CG2	1:L:92:ASN:HD22	2.13	0.60
1:G:248:ASP:HB2	1:G:275:ASP:HB2	1.84	0.60
1:N:230:VAL:O	1:N:234:LEU:HD13	2.02	0.60
1:M:283:VAL:HG12	1:M:284:ARG:H	1.65	0.60
1:L:267:ASN:OD1	1:L:332:LYS:NZ	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:67:ILE:HG22	1:W:123:MSE:SE	2.51	0.60
1:W:191:ILE:HD13	1:W:191:ILE:N	2.17	0.60
1:G:307:LYS:NZ	1:G:312:GLU:HB3	2.16	0.60
1:N:173:ILE:HD13	1:N:209:LEU:HD12	1.83	0.60
1:N:254:VAL:HG12	1:N:271:ILE:CD1	2.28	0.60
1:N:288:THR:HB	1:N:327:PHE:HA	1.82	0.60
1:M:283:VAL:O	1:M:284:ARG:HD3	2.00	0.60
1:T:134:GLU:HA	1:T:137:LYS:HE2	1.83	0.60
1:L:267:ASN:HA	1:L:332:LYS:NZ	2.16	0.60
1:W:288:THR:HG22	1:W:330:SER:OG	2.01	0.60
1:M:72:ASN:ND2	1:M:74:PHE:H	2.00	0.60
1:M:114:GLY:C	1:M:116:GLN:H	2.05	0.60
1:D:179:ASN:OD1	1:D:212:ARG:NH2	2.33	0.60
1:B:274:PHE:O	1:B:275:ASP:CB	2.49	0.60
1:T:112:MSE:C	1:T:114:GLY:H	2.04	0.60
1:L:252:LEU:HD11	1:L:283:VAL:HB	1.82	0.60
1:K:271:ILE:HD13	1:K:271:ILE:N	2.17	0.60
1:L:177:HIS:CD2	1:L:242:ALA:HB2	2.37	0.60
1:G:248:ASP:HB2	1:G:274:PHE:O	2.02	0.60
1:M:264:ASN:OD1	1:M:267:ASN:ND2	2.35	0.60
1:R:70:ILE:O	1:T:70:ILE:HD11	2.01	0.60
1:K:144:LEU:CD1	1:K:154:ILE:HD11	2.32	0.60
1:N:157:VAL:HG11	1:N:301:ALA:HB2	1.83	0.60
1:T:223:TYR:H	1:T:249:GLU:HG2	1.67	0.60
1:W:166:PHE:CE2	1:W:203:ALA:HA	2.37	0.60
1:M:219:GLY:HA3	1:M:250:MSE:CE	2.31	0.60
1:A:288:THR:HG21	1:A:331:THR:OG1	2.02	0.60
1:D:302:MSE:HE1	1:D:305:LEU:CD2	2.32	0.60
1:R:78:LEU:O	1:R:78:LEU:HD23	2.01	0.60
1:T:219:GLY:HA3	1:T:250:MSE:CE	2.32	0.60
1:L:145:ALA:C	1:L:147:SER:H	2.05	0.60
1:D:106:LEU:CD2	1:D:110:ASN:HD21	2.15	0.59
1:G:230:VAL:HG22	1:G:254:VAL:HG13	1.83	0.59
1:N:109:LEU:HD22	1:N:135:LEU:HD22	1.84	0.59
1:A:118:ASP:O	1:A:140:VAL:HB	2.01	0.59
1:I:69:ASP:OD2	1:I:71:SER:HB2	2.02	0.59
1:T:97:ASN:O	1:T:108:LEU:HD22	2.02	0.59
1:L:149:GLU:HG3	1:L:154:ILE:CG2	2.32	0.59
1:W:255:ILE:HG12	1:W:271:ILE:HD12	1.84	0.59
1:N:222:THR:HG23	1:N:225:SER:H	1.67	0.59
1:M:132:VAL:O	1:M:136:LYS:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:293:PRO:HB2	1:M:296:ASP:HB2	1.85	0.59
1:I:78:LEU:HD21	1:I:82:ILE:HD11	1.85	0.59
1:R:212:ARG:H	1:R:212:ARG:CD	2.01	0.59
1:T:304:LEU:HD11	1:T:314:VAL:HG11	1.84	0.59
1:L:73:ILE:HD13	1:L:249:GLU:OE2	2.02	0.59
1:W:133:GLU:O	1:W:137:LYS:HG2	2.02	0.59
1:N:179:ASN:ND2	1:N:179:ASN:N	2.48	0.59
1:N:192:ASN:C	1:N:194:ALA:H	2.05	0.59
1:B:174:ASP:O	1:B:175:SER:C	2.41	0.59
1:I:113:LEU:HD22	1:I:139:PRO:CG	2.32	0.59
1:R:297:ILE:HG12	1:R:321:LEU:HD12	1.84	0.59
1:L:212:ARG:HH11	1:L:212:ARG:HB2	1.67	0.59
1:K:162:GLU:OE2	1:K:199:GLY:HA2	2.01	0.59
1:D:163:GLN:NE2	1:D:202:ARG:HH22	2.00	0.59
1:R:135:LEU:O	1:R:137:LYS:N	2.35	0.59
1:R:277:THR:CG2	1:R:278:ARG:N	2.65	0.59
1:W:98:SER:HA	1:W:108:LEU:HD11	1.84	0.59
1:N:182:PHE:HE1	1:N:197:VAL:HG22	1.68	0.59
1:M:265:VAL:HG13	1:M:269:LEU:O	2.03	0.59
1:I:149:GLU:OE2	1:I:152:ASN:N	2.35	0.59
1:L:288:THR:CG2	1:L:328:ARG:H	2.16	0.59
1:W:67:ILE:CG2	1:W:123:MSE:SE	3.00	0.59
1:N:284:ARG:NH1	1:M:260:ASP:OD2	2.35	0.59
1:A:222:THR:HB	1:A:225:SER:HB3	1.84	0.59
1:B:103:ASP:OD2	1:B:103:ASP:N	2.35	0.59
1:R:149:GLU:OE2	1:R:151:THR:HG23	2.03	0.59
1:R:155:PRO:HA	1:R:317:SER:OG	2.02	0.59
1:R:197:VAL:HG13	1:R:198:LYS:N	2.17	0.59
1:R:303:ARG:HG3	1:R:303:ARG:NH1	2.18	0.59
1:L:286:GLN:HB2	1:L:329:GLN:NE2	2.18	0.59
1:W:132:VAL:O	1:W:136:LYS:HG3	2.03	0.59
1:W:286:GLN:HB3	1:W:328:ARG:HD2	1.83	0.59
1:D:155:PRO:O	1:D:156:SER:HB3	2.03	0.59
1:I:144:LEU:HB2	1:I:156:SER:HB3	1.84	0.59
1:L:144:LEU:HB2	1:L:156:SER:CB	2.32	0.59
1:K:149:GLU:HG3	1:K:152:ASN:H	1.68	0.59
1:N:131:HIS:O	1:N:135:LEU:HD23	2.03	0.59
1:M:234:LEU:HD12	1:M:261:ARG:HD3	1.84	0.59
1:B:98:SER:O	1:B:100:GLN:N	2.36	0.59
1:I:209:LEU:HB3	1:I:210:PRO:HD2	1.84	0.59
1:T:67:ILE:HG22	1:T:123:MSE:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:94:ILE:HG23	1:M:94:ILE:HG13	1.84	0.59
1:N:104:LYS:HG3	1:N:108:LEU:HG	1.84	0.59
1:A:128:THR:HG22	1:A:129:GLU:N	2.18	0.59
1:R:122:PHE:HB3	1:R:144:LEU:HD23	1.83	0.59
1:R:248:ASP:O	1:R:249:GLU:CB	2.51	0.59
1:T:275:ASP:O	1:T:276:ASN:HB3	2.03	0.59
1:L:149:GLU:OE2	1:L:151:THR:HG23	2.03	0.59
1:W:308:TYR:HE1	1:W:314:VAL:CG1	2.16	0.59
1:N:69:ASP:OD2	1:N:71:SER:HB2	2.03	0.59
1:R:146:ALA:H	1:R:158:THR:HG22	1.66	0.58
1:G:164:ALA:HA	1:G:323:HIS:CD2	2.36	0.58
1:N:265:VAL:HB	1:N:266:PRO:HD3	1.84	0.58
1:B:66:ILE:HG22	1:B:112:MSE:HE3	1.84	0.58
1:B:78:LEU:O	1:B:82:ILE:HD13	2.02	0.58
1:B:106:LEU:HD22	1:B:134:GLU:HG2	1.85	0.58
1:W:82:ILE:O	1:W:85:ILE:N	2.36	0.58
1:G:220:ASP:HB2	1:G:222:THR:CG2	2.21	0.58
1:A:73:ILE:HG22	1:A:277:THR:HG21	1.84	0.58
1:B:252:LEU:H	1:B:252:LEU:HD12	1.68	0.58
1:R:146:ALA:N	1:R:158:THR:HG22	2.18	0.58
1:W:62:THR:HG22	1:W:92:ASN:CB	2.34	0.58
1:W:285:PRO:CB	1:W:329:GLN:HB3	2.21	0.58
1:N:63:VAL:O	1:N:93:ILE:HA	2.04	0.58
1:N:230:VAL:CG2	1:N:254:VAL:HA	2.33	0.58
1:B:245:VAL:HG11	1:B:251:ALA:CA	2.34	0.58
1:R:98:SER:HB2	1:R:105:GLU:HG2	1.86	0.58
1:K:120:ILE:HB	1:K:142:VAL:HG22	1.85	0.58
1:W:94:ILE:HD11	1:G:115:LYS:HE2	1.85	0.58
1:N:255:ILE:O	1:N:259:GLN:HG3	2.03	0.58
1:A:89:TYR:O	1:A:90:LYS:HB3	2.03	0.58
1:D:112:MSE:HE2	1:D:112:MSE:HA	1.83	0.58
1:D:304:LEU:O	1:D:308:TYR:HD1	1.85	0.58
1:I:159:ILE:HD13	1:I:292:GLN:HG2	1.85	0.58
1:M:108:LEU:O	1:M:112:MSE:HB2	2.02	0.58
1:D:180:ILE:HG22	1:D:200:TYR:HE2	1.67	0.58
1:I:206:GLU:HG3	1:M:316:SER:OG	2.03	0.58
1:R:82:ILE:HG23	1:R:302:MSE:HB2	1.85	0.58
1:R:274:PHE:O	1:R:275:ASP:CB	2.51	0.58
1:L:101:ASN:ND2	1:L:104:LYS:H	2.02	0.58
1:L:104:LYS:HE2	1:L:104:LYS:HA	1.85	0.58
1:L:168:ALA:HA	1:L:325:ILE:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:172:LEU:HG	1:L:272:ILE:CD1	2.34	0.58
1:W:62:THR:HG22	1:W:92:ASN:HB2	1.85	0.58
1:W:191:ILE:O	1:W:195:LYS:HB2	2.03	0.58
1:G:67:ILE:HD13	1:G:67:ILE:H	1.69	0.58
1:I:329:GLN:CD	1:I:329:GLN:N	2.57	0.58
1:T:169:VAL:O	1:T:173:ILE:HG12	2.03	0.58
1:L:70:ILE:HG12	1:K:70:ILE:HD11	1.86	0.58
1:L:188:GLU:N	1:L:188:GLU:OE2	2.34	0.58
1:A:245:VAL:HG21	1:A:254:VAL:HG21	1.86	0.58
1:A:291:VAL:HB	1:A:324:ARG:HG3	1.85	0.58
1:A:325:ILE:H	1:A:325:ILE:HD12	1.69	0.58
1:D:73:ILE:N	1:D:73:ILE:CD1	2.67	0.58
1:B:170:GLN:OE1	1:B:173:ILE:HG13	2.04	0.58
1:I:77:GLU:HB3	1:I:294:MSE:HE1	1.85	0.58
1:I:88:MSE:HE3	1:R:296:ASP:HB3	1.85	0.58
1:K:108:LEU:O	1:K:112:MSE:HG2	2.03	0.58
1:W:86:ALA:HB3	1:W:93:ILE:HD11	1.83	0.58
1:W:178:LYS:NZ	1:W:179:ASN:HB3	2.19	0.58
1:W:231:GLU:C	1:W:233:LEU:N	2.57	0.58
1:B:82:ILE:HG23	1:B:302:MSE:CE	2.34	0.58
1:N:102:GLN:O	1:N:106:LEU:HG	2.04	0.58
1:R:106:LEU:O	1:R:110:ASN:HB2	2.04	0.58
1:R:220:ASP:OD1	1:R:222:THR:HB	2.03	0.58
1:L:230:VAL:CG2	1:L:254:VAL:HA	2.33	0.58
1:W:88:MSE:HE3	1:W:89:TYR:HE2	1.68	0.58
1:G:62:THR:HB	1:G:92:ASN:HB2	1.85	0.58
1:N:206:GLU:C	1:N:208:GLY:H	2.06	0.58
1:M:143:VAL:HG11	1:M:305:LEU:HB2	1.86	0.58
1:B:283:VAL:HG12	1:B:284:ARG:H	1.68	0.57
1:R:224:ASP:O	1:R:227:ILE:HB	2.04	0.57
1:T:202:ARG:O	1:T:206:GLU:HB2	2.03	0.57
1:W:177:HIS:CB	1:W:180:ILE:HD11	2.33	0.57
1:G:266:PRO:CG	1:G:332:LYS:HB2	2.34	0.57
1:M:162:GLU:HA	1:M:195:LYS:O	2.04	0.57
1:G:102:GLN:HG2	1:G:131:HIS:CE1	2.39	0.57
1:G:177:HIS:CE1	1:G:270:GLU:HG3	2.39	0.57
1:N:223:TYR:CD2	1:M:282:MSE:HE3	2.38	0.57
1:B:68:PRO:HB3	1:B:100:GLN:HG2	1.86	0.57
1:G:78:LEU:O	1:G:78:LEU:HD23	2.04	0.57
1:D:190:PRO:O	1:D:194:ALA:HB3	2.04	0.57
1:G:149:GLU:CG	1:G:152:ASN:H	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:128:THR:O	1:M:131:HIS:HB2	2.04	0.57
1:D:232:LYS:HB2	1:D:232:LYS:NZ	2.18	0.57
1:L:157:VAL:HG21	1:L:301:ALA:HB2	1.86	0.57
1:I:72:ASN:ND2	1:I:72:ASN:C	2.58	0.57
1:I:73:ILE:HG12	1:I:279:LEU:HD11	1.87	0.57
1:I:113:LEU:HD22	1:I:139:PRO:HG2	1.87	0.57
1:R:95:LEU:HD13	1:R:95:LEU:N	2.20	0.57
1:T:67:ILE:HA	1:T:123:MSE:HB2	1.87	0.57
1:T:315:ASP:CG	1:T:316:SER:N	2.58	0.57
1:G:125:GLY:O	1:G:189:GLU:CG	2.52	0.57
1:G:226:GLY:O	1:G:230:VAL:HG23	2.04	0.57
1:G:274:PHE:O	1:G:275:ASP:HB2	2.04	0.57
1:M:67:ILE:HD12	1:M:95:LEU:HD23	1.85	0.57
1:M:72:ASN:O	1:M:74:PHE:N	2.37	0.57
1:A:192:ASN:O	1:A:197:VAL:HG23	2.05	0.57
1:B:245:VAL:HG21	1:B:254:VAL:HG21	1.87	0.57
1:R:63:VAL:HG11	1:R:302:MSE:HE1	1.86	0.57
1:R:187:LEU:O	1:R:188:GLU:HB2	2.04	0.57
1:W:67:ILE:HG22	1:W:123:MSE:HB2	1.86	0.57
1:A:183:VAL:HB	1:A:245:VAL:HG22	1.87	0.57
1:I:63:VAL:HG12	1:I:93:ILE:HG12	1.87	0.57
1:I:86:ALA:HB2	1:I:93:ILE:HD11	1.87	0.57
1:I:287:LEU:HA	1:I:330:SER:HB3	1.85	0.57
1:K:169:VAL:HG23	1:K:180:ILE:HG21	1.86	0.57
1:G:212:ARG:HH12	1:G:238:GLU:HB2	1.69	0.57
1:N:112:MSE:O	1:N:117:VAL:HG22	2.04	0.57
1:B:247:THR:HB	1:B:250:MSE:HE3	1.86	0.57
1:I:131:HIS:O	1:I:135:LEU:HB2	2.05	0.57
1:R:192:ASN:O	1:R:197:VAL:HG12	2.05	0.57
1:G:220:ASP:OD2	1:G:220:ASP:N	2.36	0.57
1:N:66:ILE:HD12	1:N:122:PHE:HD2	1.70	0.57
1:A:109:LEU:O	1:A:113:LEU:HG	2.04	0.57
1:D:98:SER:HB2	1:D:105:GLU:HG2	1.86	0.57
1:D:201:LYS:HG2	1:D:211:VAL:HG11	1.87	0.57
1:D:245:VAL:HG21	1:D:251:ALA:HA	1.87	0.57
1:D:302:MSE:HE1	1:D:305:LEU:HD23	1.86	0.57
1:R:78:LEU:HD22	1:R:123:MSE:CE	2.35	0.57
1:R:216:ILE:O	1:R:216:ILE:HG22	2.03	0.57
1:M:111:ASN:O	1:M:115:LYS:HG3	2.05	0.57
1:M:225:SER:CB	1:M:250:MSE:HE3	2.35	0.57
1:D:104:LYS:O	1:D:104:LYS:HG2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ASN:HD22	1:A:127:VAL:N	2.02	0.56
1:A:261:ARG:HB2	1:A:261:ARG:HH11	1.69	0.56
1:D:98:SER:HA	1:D:108:LEU:HD11	1.86	0.56
1:I:98:SER:HA	1:I:104:LYS:HG2	1.87	0.56
1:L:157:VAL:HG11	1:L:300:VAL:HG12	1.87	0.56
1:K:265:VAL:CG1	1:K:285:PRO:HG3	2.34	0.56
1:A:148:ILE:HD13	1:A:148:ILE:N	2.18	0.56
1:A:329:GLN:CD	1:A:329:GLN:N	2.57	0.56
1:B:183:VAL:HG22	1:B:217:VAL:CG1	2.34	0.56
1:K:102:GLN:HG3	1:K:131:HIS:CE1	2.40	0.56
1:W:278:ARG:HB3	1:W:278:ARG:HH11	1.69	0.56
1:W:286:GLN:H	1:W:329:GLN:HB2	1.71	0.56
1:W:308:TYR:CE1	1:W:314:VAL:HG11	2.40	0.56
1:N:117:VAL:HG21	1:N:120:ILE:HD11	1.86	0.56
1:M:63:VAL:CG1	1:M:93:ILE:HG12	2.35	0.56
1:M:118:ASP:OD1	1:M:118:ASP:N	2.38	0.56
1:M:304:LEU:HD11	1:M:314:VAL:HG11	1.87	0.56
1:A:100:GLN:HA	1:A:100:GLN:NE2	2.20	0.56
1:A:100:GLN:HE21	1:A:100:GLN:CA	2.16	0.56
1:A:255:ILE:O	1:A:259:GLN:HG3	2.04	0.56
1:R:252:LEU:HD22	1:T:282:MSE:HE3	1.86	0.56
1:T:63:VAL:CG2	1:T:305:LEU:HD21	2.34	0.56
1:L:248:ASP:OD1	1:L:277:THR:HG22	2.05	0.56
1:W:81:GLY:O	1:W:85:ILE:HG13	2.05	0.56
1:W:92:ASN:ND2	1:G:111:ASN:ND2	2.53	0.56
1:G:100:GLN:OE1	1:G:125:GLY:HA3	2.06	0.56
1:G:102:GLN:HG2	1:G:131:HIS:HE1	1.71	0.56
1:G:223:TYR:CE2	1:G:227:ILE:HD11	2.41	0.56
1:L:230:VAL:HG21	1:L:257:GLY:HA3	1.87	0.56
1:G:182:PHE:HZ	1:G:196:LYS:HG2	1.69	0.56
1:A:73:ILE:CG2	1:A:277:THR:HG21	2.35	0.56
1:A:93:ILE:O	1:A:94:ILE:HD13	2.06	0.56
1:D:89:TYR:OH	1:D:303:ARG:HD3	2.05	0.56
1:B:114:GLY:C	1:B:116:GLN:H	2.08	0.56
1:B:134:GLU:OE1	1:B:134:GLU:HA	2.05	0.56
1:R:70:ILE:HB	1:R:97:ASN:OD1	2.06	0.56
1:L:230:VAL:HG11	1:L:258:ALA:N	2.20	0.56
1:K:179:ASN:ND2	1:K:212:ARG:HH22	2.03	0.56
1:K:264:ASN:H	1:K:268:ASP:CB	2.19	0.56
1:K:271:ILE:O	1:K:271:ILE:HG12	2.04	0.56
1:B:98:SER:C	1:B:100:GLN:N	2.57	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:307:LYS:HD3	1:I:314:VAL:HG12	1.86	0.56
1:R:148:ILE:HD12	1:R:191:ILE:CG1	2.29	0.56
1:R:178:LYS:HG2	1:R:179:ASN:N	2.19	0.56
1:T:68:PRO:HG2	1:T:75:TYR:CZ	2.41	0.56
1:T:329:GLN:O	1:T:331:THR:N	2.38	0.56
1:W:182:PHE:HB2	1:W:200:TYR:CE2	2.40	0.56
1:N:191:ILE:O	1:N:191:ILE:HG22	2.06	0.56
1:T:132:VAL:O	1:T:136:LYS:HB2	2.06	0.56
1:N:307:LYS:CE	1:N:314:VAL:HG21	2.35	0.56
1:A:271:ILE:C	1:A:272:ILE:HD12	2.26	0.56
1:B:318:ILE:HG13	1:B:318:ILE:O	2.06	0.56
1:T:135:LEU:HD21	1:T:142:VAL:HG11	1.88	0.56
1:W:308:TYR:OH	1:W:314:VAL:HG11	2.05	0.56
1:M:72:ASN:C	1:M:72:ASN:ND2	2.59	0.56
1:M:182:PHE:HD2	1:M:244:PHE:O	1.88	0.56
1:D:151:THR:O	1:D:152:ASN:HB2	2.06	0.56
1:D:270:GLU:HG2	1:D:331:THR:OG1	2.06	0.56
1:B:183:VAL:HA	1:B:217:VAL:HG13	1.86	0.56
1:B:222:THR:HG22	1:B:224:ASP:H	1.69	0.56
1:B:252:LEU:CD2	1:B:283:VAL:HG22	2.36	0.56
1:R:78:LEU:HD22	1:R:123:MSE:HE1	1.87	0.56
1:N:221:TYR:HD1	1:N:250:MSE:HE2	1.70	0.56
1:N:259:GLN:HG2	1:N:265:VAL:HG23	1.87	0.56
1:M:66:ILE:O	1:M:66:ILE:HG22	2.05	0.56
1:R:135:LEU:C	1:R:137:LYS:H	2.08	0.55
1:R:187:LEU:O	1:R:188:GLU:CB	2.54	0.55
1:T:149:GLU:HG2	1:T:154:ILE:HG23	1.87	0.55
1:L:93:ILE:HD11	1:L:302:MSE:CE	2.37	0.55
1:N:98:SER:C	1:N:100:GLN:H	2.09	0.55
1:N:247:THR:HG22	1:N:249:GLU:H	1.71	0.55
1:A:169:VAL:HG12	1:A:180:ILE:HD12	1.87	0.55
1:D:299:ALA:HB1	1:D:303:ARG:NH2	2.22	0.55
1:R:94:ILE:HD12	1:T:94:ILE:CG2	2.36	0.55
1:L:300:VAL:HG21	1:L:321:LEU:HD21	1.87	0.55
1:L:305:LEU:O	1:L:309:MSE:HG3	2.07	0.55
1:W:177:HIS:HB3	1:W:180:ILE:CD1	2.36	0.55
1:N:288:THR:HG21	1:N:331:THR:CG2	2.33	0.55
1:A:169:VAL:CG1	1:A:180:ILE:HD12	2.37	0.55
1:A:178:LYS:CD	1:A:179:ASN:H	2.20	0.55
1:B:186:THR:HA	1:B:218:GLU:OE1	2.05	0.55
1:I:151:THR:HB	1:I:153:GLN:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:68:PRO:CB	1:W:100:GLN:HG3	2.36	0.55
1:W:292:GLN:O	1:W:294:MSE:N	2.40	0.55
1:G:68:PRO:HD3	1:G:123:MSE:O	2.07	0.55
1:G:135:LEU:O	1:G:136:LYS:C	2.45	0.55
1:G:255:ILE:HG12	1:G:271:ILE:CD1	2.37	0.55
1:N:81:GLY:O	1:N:84:ASP:HB2	2.07	0.55
1:N:114:GLY:C	1:N:116:GLN:H	2.09	0.55
1:N:223:TYR:CD1	1:M:282:MSE:HG2	2.42	0.55
1:M:132:VAL:HB	1:M:136:LYS:HE3	1.87	0.55
1:M:219:GLY:HA3	1:M:250:MSE:HE3	1.87	0.55
1:D:74:PHE:CE2	1:D:294:MSE:HE1	2.41	0.55
1:W:70:ILE:HB	1:W:97:ASN:OD1	2.06	0.55
1:N:92:ASN:HD22	1:M:115:LYS:CE	2.20	0.55
1:N:278:ARG:O	1:N:282:MSE:HG3	2.06	0.55
1:D:308:TYR:CE1	1:D:314:VAL:HG11	2.41	0.55
1:R:113:LEU:HD22	1:R:139:PRO:CD	2.37	0.55
1:N:92:ASN:HD22	1:M:115:LYS:HE3	1.70	0.55
1:M:64:GLY:O	1:M:120:ILE:HG23	2.07	0.55
1:L:286:GLN:HB2	1:L:329:GLN:HE22	1.72	0.55
1:K:277:THR:HG23	1:K:278:ARG:N	2.22	0.55
1:N:198:LYS:O	1:N:202:ARG:HB2	2.07	0.55
1:A:221:TYR:HA	1:A:250:MSE:HE2	1.89	0.55
1:B:182:PHE:CE1	1:B:184:SER:HB3	2.42	0.55
1:B:242:ALA:HA	1:B:269:LEU:HD12	1.89	0.55
1:W:230:VAL:CG2	1:W:254:VAL:HG13	2.37	0.55
1:N:86:ALA:HB3	1:N:93:ILE:HD11	1.88	0.55
1:A:66:ILE:HD11	1:A:122:PHE:CE2	2.42	0.55
1:D:242:ALA:HA	1:D:270:GLU:O	2.07	0.55
1:B:83:GLU:OE1	1:B:93:ILE:HD13	2.06	0.55
1:B:190:PRO:HA	1:B:193:HIS:CE1	2.41	0.55
1:I:179:ASN:HD21	1:I:212:ARG:HH12	1.51	0.55
1:R:63:VAL:HG12	1:R:64:GLY:N	2.22	0.55
1:T:182:PHE:HE1	1:T:197:VAL:CG2	2.19	0.55
1:T:182:PHE:CE1	1:T:197:VAL:HG22	2.37	0.55
1:G:308:TYR:CE2	1:G:314:VAL:HG11	2.42	0.55
1:M:318:ILE:O	1:M:318:ILE:HD13	2.07	0.55
1:A:173:ILE:HD13	1:A:180:ILE:HD11	1.88	0.55
1:D:223:TYR:CE1	1:D:253:GLY:HA2	2.42	0.55
1:I:112:MSE:HB3	1:I:120:ILE:HD11	1.89	0.55
1:K:310:ASN:HB2	1:K:312:GLU:HG3	1.88	0.55
1:G:285:PRO:HB2	1:G:329:GLN:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:148:ILE:CG2	1:N:191:ILE:HG12	2.37	0.55
1:D:61:THR:HA	1:D:118:ASP:OD1	2.07	0.55
1:D:264:ASN:O	1:D:268:ASP:HB2	2.07	0.55
1:T:63:VAL:HG21	1:T:305:LEU:CD2	2.35	0.55
1:T:72:ASN:C	1:T:72:ASN:HD22	2.10	0.55
1:L:70:ILE:HD11	1:K:70:ILE:HD11	1.89	0.55
1:L:238:GLU:HA	1:L:238:GLU:OE1	2.06	0.55
1:K:165:ALA:O	1:K:169:VAL:HG12	2.07	0.55
1:W:68:PRO:HB2	1:W:100:GLN:HG3	1.87	0.55
1:W:88:MSE:HE3	1:W:89:TYR:CE2	2.41	0.55
1:G:274:PHE:O	1:G:275:ASP:CB	2.55	0.55
1:N:293:PRO:HG2	1:N:297:ILE:HG13	1.89	0.55
1:A:162:GLU:HA	1:A:195:LYS:O	2.06	0.54
1:D:97:ASN:C	1:D:108:LEU:HD11	2.28	0.54
1:D:274:PHE:O	1:D:275:ASP:CB	2.55	0.54
1:B:67:ILE:HG22	1:B:123:MSE:HE3	1.88	0.54
1:B:180:ILE:HD12	1:B:180:ILE:H	1.72	0.54
1:R:227:ILE:HG22	1:R:228:GLU:N	2.21	0.54
1:T:144:LEU:HB2	1:T:156:SER:CB	2.36	0.54
1:T:152:ASN:OD1	1:T:318:ILE:HG21	2.06	0.54
1:L:70:ILE:CG1	1:K:70:ILE:HD11	2.36	0.54
1:W:318:ILE:N	1:W:318:ILE:HD12	2.22	0.54
1:N:73:ILE:HD12	1:N:73:ILE:N	2.21	0.54
1:A:73:ILE:HG22	1:A:277:THR:CG2	2.37	0.54
1:A:112:MSE:HB3	1:A:120:ILE:HD11	1.88	0.54
1:B:323:HIS:O	1:B:324:ARG:HB3	2.07	0.54
1:I:225:SER:OG	1:I:250:MSE:HE3	2.07	0.54
1:R:245:VAL:CG1	1:R:250:MSE:HB3	2.36	0.54
1:L:113:LEU:HD22	1:L:139:PRO:HG2	1.89	0.54
1:R:135:LEU:HD11	1:R:142:VAL:HG11	1.89	0.54
1:R:187:LEU:HB2	1:R:218:GLU:OE2	2.07	0.54
1:T:133:GLU:O	1:T:137:LYS:HG3	2.07	0.54
1:G:149:GLU:O	1:G:150:SER:CB	2.56	0.54
1:N:148:ILE:HD12	1:N:191:ILE:CG1	2.37	0.54
1:N:148:ILE:HD12	1:N:191:ILE:HG13	1.89	0.54
1:A:245:VAL:O	1:A:273:GLY:HA2	2.07	0.54
1:B:109:LEU:HD11	1:B:135:LEU:HD13	1.89	0.54
1:L:126:ASN:CB	1:L:189:GLU:HG2	2.37	0.54
1:L:157:VAL:CG2	1:L:301:ALA:HB2	2.37	0.54
1:L:193:HIS:CE1	1:L:194:ALA:HB2	2.42	0.54
1:L:212:ARG:O	1:L:215:TYR:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:212:ARG:HB3	1:W:212:ARG:HH11	1.72	0.54
1:G:193:HIS:O	1:G:198:LYS:HD3	2.07	0.54
1:A:62:THR:HG22	1:A:92:ASN:CB	2.26	0.54
1:A:148:ILE:CG1	1:A:190:PRO:HB2	2.37	0.54
1:D:111:ASN:HD22	1:D:111:ASN:N	2.03	0.54
1:B:66:ILE:HG13	1:B:66:ILE:O	2.07	0.54
1:B:142:VAL:O	1:B:142:VAL:HG22	2.08	0.54
1:R:132:VAL:O	1:R:136:LYS:HG3	2.07	0.54
1:K:264:ASN:H	1:K:268:ASP:HB3	1.71	0.54
1:W:284:ARG:NH2	1:G:223:TYR:OH	2.41	0.54
1:M:106:LEU:HD22	1:M:134:GLU:OE2	2.08	0.54
1:M:245:VAL:HG12	1:M:247:THR:H	1.72	0.54
1:A:85:ILE:HD13	1:A:299:ALA:CA	2.35	0.54
1:T:68:PRO:HD3	1:T:123:MSE:CB	2.38	0.54
1:T:215:TYR:CZ	1:T:240:PRO:HG3	2.42	0.54
1:L:112:MSE:HE3	1:L:112:MSE:HA	1.88	0.54
1:K:288:THR:HG23	1:K:327:PHE:HA	1.89	0.54
1:N:264:ASN:ND2	1:N:266:PRO:CD	2.65	0.54
1:M:113:LEU:HD13	1:M:139:PRO:CD	2.36	0.54
1:R:201:LYS:HG2	1:R:211:VAL:CG1	2.36	0.54
1:K:97:ASN:O	1:K:104:LYS:HE2	2.08	0.54
1:G:193:HIS:HA	1:G:197:VAL:CG1	2.38	0.54
1:G:243:ILE:HG13	1:G:269:LEU:HD11	1.90	0.54
1:A:207:SER:O	1:A:208:GLY:C	2.46	0.54
1:R:230:VAL:O	1:R:234:LEU:HG	2.07	0.54
1:L:329:GLN:C	1:L:331:THR:H	2.10	0.54
1:W:98:SER:HB3	1:W:108:LEU:HD12	1.90	0.54
1:W:149:GLU:OE2	1:W:152:ASN:N	2.41	0.54
1:G:157:VAL:O	1:G:158:THR:HG23	2.06	0.54
1:G:159:ILE:HD13	1:G:292:GLN:HG3	1.90	0.54
1:N:284:ARG:HD3	1:M:260:ASP:OD1	2.08	0.54
1:M:296:ASP:O	1:M:297:ILE:C	2.46	0.54
1:A:247:THR:HG22	1:A:250:MSE:H	1.72	0.54
1:D:66:ILE:HB	1:D:122:PHE:HD2	1.72	0.54
1:D:324:ARG:HG2	1:D:325:ILE:N	2.23	0.54
1:L:297:ILE:CG1	1:L:321:LEU:HD12	2.38	0.54
1:W:177:HIS:NE2	1:W:242:ALA:HB2	2.23	0.54
1:W:246:GLY:HA2	1:W:274:PHE:HB2	1.89	0.54
1:G:263:LEU:HD12	1:G:263:LEU:N	2.23	0.54
1:A:143:VAL:CG1	1:A:305:LEU:HD13	2.37	0.54
1:D:98:SER:CA	1:D:108:LEU:HD11	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:131:HIS:O	1:L:135:LEU:HB2	2.07	0.54
1:K:186:THR:HA	1:K:218:GLU:OE1	2.07	0.54
1:W:132:VAL:CG1	1:W:149:GLU:HG3	2.38	0.54
1:W:266:PRO:HB3	1:W:330:SER:O	2.08	0.54
1:N:66:ILE:CD1	1:N:122:PHE:HD2	2.21	0.54
1:N:307:LYS:HE3	1:N:314:VAL:HG21	1.90	0.54
1:A:115:LYS:HB2	1:A:115:LYS:NZ	2.23	0.53
1:I:129:GLU:O	1:I:132:VAL:HG22	2.08	0.53
1:I:231:GLU:HG2	1:I:261:ARG:NE	2.23	0.53
1:N:109:LEU:HD22	1:N:135:LEU:HD13	1.90	0.53
1:N:120:ILE:HB	1:N:142:VAL:HG23	1.90	0.53
1:M:68:PRO:HA	1:M:98:SER:OG	2.08	0.53
1:M:101:ASN:HD22	1:M:101:ASN:N	2.04	0.53
1:A:238:GLU:O	1:A:240:PRO:HD3	2.07	0.53
1:I:86:ALA:HB3	1:I:93:ILE:HD11	1.90	0.53
1:I:307:LYS:HD2	1:I:314:VAL:HG12	1.89	0.53
1:G:187:LEU:N	1:G:218:GLU:OE1	2.41	0.53
1:A:94:ILE:CG2	1:A:112:MSE:HE1	2.38	0.53
1:B:182:PHE:CE1	1:B:197:VAL:HG22	2.37	0.53
1:R:81:GLY:HA2	1:R:295:TYR:CE1	2.44	0.53
1:R:222:THR:HG22	1:R:224:ASP:N	2.24	0.53
1:R:246:GLY:C	1:R:274:PHE:HB3	2.28	0.53
1:R:324:ARG:HG2	1:R:324:ARG:HH11	1.72	0.53
1:K:78:LEU:O	1:K:82:ILE:HG13	2.07	0.53
1:K:160:ASP:N	1:K:320:GLN:HE22	2.06	0.53
1:G:180:ILE:O	1:G:200:TYR:OH	2.23	0.53
1:G:329:GLN:NE2	1:G:329:GLN:N	2.57	0.53
1:D:252:LEU:HG	1:D:283:VAL:CG1	2.38	0.53
1:L:88:MSE:C	1:L:90:LYS:H	2.12	0.53
1:G:85:ILE:HA	1:G:88:MSE:HE3	1.91	0.53
1:M:190:PRO:HA	1:M:193:HIS:ND1	2.22	0.53
1:M:252:LEU:HD11	1:M:283:VAL:CG2	2.38	0.53
1:T:104:LYS:HZ1	1:T:108:LEU:HD11	1.70	0.53
1:T:305:LEU:O	1:T:309:MSE:HG3	2.08	0.53
1:L:62:THR:HA	1:L:92:ASN:O	2.07	0.53
1:G:77:GLU:HA	1:G:80:ARG:HG2	1.90	0.53
1:N:136:LYS:HG2	1:N:137:LYS:HZ1	1.74	0.53
1:M:246:GLY:O	1:M:274:PHE:HB3	2.08	0.53
1:I:149:GLU:O	1:I:150:SER:HB2	2.09	0.53
1:W:69:ASP:O	1:W:72:ASN:HB3	2.07	0.53
1:W:317:SER:C	1:W:318:ILE:HD12	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:GLU:O	1:G:150:SER:HB2	2.08	0.53
1:N:282:MSE:HE3	1:M:223:TYR:HB2	1.90	0.53
1:M:178:LYS:HA	1:M:209:LEU:CD1	2.39	0.53
1:I:64:GLY:O	1:I:120:ILE:HG23	2.08	0.53
1:T:274:PHE:O	1:T:275:ASP:CB	2.55	0.53
1:K:160:ASP:CA	1:K:320:GLN:HE22	2.22	0.53
1:K:173:ILE:HD13	1:K:207:SER:CB	2.38	0.53
1:G:161:TYR:CZ	1:G:191:ILE:HD11	2.43	0.53
1:N:83:GLU:HA	1:N:93:ILE:CD1	2.38	0.53
1:N:220:ASP:OD2	1:N:225:SER:HB3	2.08	0.53
1:B:70:ILE:CB	1:B:97:ASN:HD21	2.22	0.53
1:B:129:GLU:N	1:B:129:GLU:OE2	2.39	0.53
1:R:255:ILE:O	1:R:259:GLN:HG3	2.09	0.53
1:T:252:LEU:HD11	1:T:283:VAL:HG22	1.91	0.53
1:T:274:PHE:O	1:T:275:ASP:HB2	2.08	0.53
1:L:129:GLU:O	1:L:133:GLU:HG2	2.08	0.53
1:W:73:ILE:CG2	1:W:74:PHE:H	2.22	0.53
1:I:271:ILE:HD13	1:I:271:ILE:H	1.74	0.53
1:R:250:MSE:O	1:R:254:VAL:HG23	2.09	0.53
1:W:97:ASN:C	1:W:108:LEU:HD11	2.29	0.53
1:G:286:GLN:HB3	1:G:328:ARG:HD3	1.91	0.53
1:N:69:ASP:C	1:N:71:SER:N	2.62	0.53
1:L:61:THR:HA	1:L:118:ASP:OD2	2.09	0.53
1:L:297:ILE:HG13	1:L:321:LEU:HD12	1.91	0.53
1:K:144:LEU:HB2	1:K:156:SER:HB3	1.90	0.53
1:K:277:THR:CG2	1:K:278:ARG:N	2.72	0.53
1:M:255:ILE:HG12	1:M:271:ILE:CD1	2.38	0.53
1:K:80:ARG:O	1:K:80:ARG:HD2	2.09	0.52
1:N:173:ILE:HD13	1:N:209:LEU:CD1	2.39	0.52
1:N:202:ARG:O	1:N:206:GLU:HG2	2.09	0.52
1:N:288:THR:HG22	1:N:328:ARG:HB2	1.91	0.52
1:A:94:ILE:HG23	1:D:94:ILE:HG23	1.92	0.52
1:B:77:GLU:OE2	1:B:294:MSE:CE	2.57	0.52
1:W:132:VAL:HG11	1:W:149:GLU:HG3	1.91	0.52
1:W:169:VAL:HG23	1:W:170:GLN:N	2.24	0.52
1:W:291:VAL:CG2	1:W:326:GLU:HB2	2.39	0.52
1:G:323:HIS:O	1:G:324:ARG:HG2	2.09	0.52
1:A:157:VAL:HG11	1:A:301:ALA:CA	2.38	0.52
1:R:182:PHE:HD2	1:R:244:PHE:CD2	2.26	0.52
1:T:77:GLU:O	1:T:80:ARG:HB3	2.09	0.52
1:L:243:ILE:HG12	1:L:269:LEU:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:160:ASP:CB	1:K:320:GLN:HE22	2.21	0.52
1:K:186:THR:H	1:K:221:TYR:HE1	1.57	0.52
1:N:221:TYR:HA	1:N:250:MSE:HG3	1.90	0.52
1:M:94:ILE:CG2	1:M:112:MSE:HE1	2.40	0.52
1:A:80:ARG:O	1:A:83:GLU:HB2	2.10	0.52
1:B:73:ILE:HD12	1:B:279:LEU:HD21	1.92	0.52
1:R:64:GLY:O	1:R:120:ILE:HG23	2.10	0.52
1:R:252:LEU:HG	1:R:283:VAL:HG21	1.90	0.52
1:T:230:VAL:CG2	1:T:254:VAL:HG13	2.40	0.52
1:W:164:ALA:HA	1:W:323:HIS:CD2	2.44	0.52
1:G:108:LEU:O	1:G:112:MSE:HG2	2.09	0.52
1:N:66:ILE:HG23	1:N:112:MSE:CE	2.40	0.52
1:N:78:LEU:HD13	1:N:78:LEU:O	2.09	0.52
1:A:72:ASN:ND2	1:A:75:TYR:HD2	2.06	0.52
1:B:144:LEU:HG	1:B:154:ILE:CD1	2.39	0.52
1:I:117:VAL:O	1:I:140:VAL:HG11	2.09	0.52
1:I:166:PHE:CE2	1:I:203:ALA:HA	2.45	0.52
1:R:190:PRO:HA	1:R:193:HIS:CE1	2.45	0.52
1:T:217:VAL:CG1	1:T:218:GLU:N	2.73	0.52
1:T:272:ILE:HG22	1:T:273:GLY:N	2.23	0.52
1:L:67:ILE:CD1	1:L:70:ILE:HG13	2.40	0.52
1:L:101:ASN:ND2	1:L:104:LYS:N	2.56	0.52
1:W:328:ARG:HG2	1:W:328:ARG:HH11	1.74	0.52
1:N:202:ARG:HA	1:N:205:THR:HG22	1.92	0.52
1:M:129:GLU:O	1:M:132:VAL:HG23	2.09	0.52
1:A:69:ASP:HB3	1:A:72:ASN:HB3	1.91	0.52
1:A:230:VAL:HG22	1:A:254:VAL:HG13	1.91	0.52
1:D:66:ILE:HB	1:D:122:PHE:CD2	2.45	0.52
1:B:252:LEU:HG	1:B:283:VAL:CG2	2.39	0.52
1:R:82:ILE:HG22	1:R:302:MSE:HE2	1.90	0.52
1:R:248:ASP:O	1:R:249:GLU:HB3	2.08	0.52
1:L:67:ILE:HG22	1:L:123:MSE:SE	2.60	0.52
1:L:180:ILE:HG12	1:L:242:ALA:HB3	1.92	0.52
1:G:278:ARG:HB3	1:G:278:ARG:CZ	2.40	0.52
1:G:305:LEU:O	1:G:308:TYR:N	2.43	0.52
1:N:247:THR:HG22	1:N:248:ASP:H	1.72	0.52
1:A:205:THR:CG2	1:A:206:GLU:N	2.73	0.52
1:A:287:LEU:HD12	1:A:288:THR:H	1.74	0.52
1:R:247:THR:HG22	1:R:250:MSE:H	1.74	0.52
1:T:263:LEU:HD23	1:T:268:ASP:HB3	1.92	0.52
1:L:148:ILE:HG13	1:L:191:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:146:ALA:CA	1:W:158:THR:HG22	2.39	0.52
1:W:247:THR:O	1:W:247:THR:HG22	2.09	0.52
1:G:294:MSE:O	1:G:295:TYR:C	2.47	0.52
1:M:102:GLN:O	1:M:106:LEU:HG	2.09	0.52
1:D:63:VAL:HG21	1:D:302:MSE:HE1	1.91	0.52
1:G:85:ILE:H	1:G:85:ILE:CD1	2.20	0.52
1:N:132:VAL:O	1:N:136:LYS:HB2	2.09	0.52
1:A:274:PHE:CE2	1:A:290:VAL:HG21	2.45	0.52
1:B:245:VAL:CG2	1:B:254:VAL:HG21	2.40	0.52
1:T:252:LEU:HD11	1:T:283:VAL:CG2	2.39	0.52
1:L:103:ASP:OD1	1:L:106:LEU:HD13	2.10	0.52
1:K:164:ALA:HA	1:K:323:HIS:CD2	2.45	0.52
1:W:184:SER:HA	1:W:250:MSE:HE1	1.92	0.52
1:D:97:ASN:O	1:D:104:LYS:HE2	2.09	0.52
1:B:77:GLU:OE2	1:B:294:MSE:HE3	2.09	0.52
1:B:230:VAL:HG13	1:B:254:VAL:CG1	2.40	0.52
1:I:78:LEU:HB2	1:I:294:MSE:CE	2.40	0.52
1:R:246:GLY:HA2	1:R:274:PHE:HB2	1.91	0.52
1:T:149:GLU:HG3	1:T:149:GLU:O	2.10	0.52
1:L:73:ILE:N	1:L:73:ILE:CD1	2.73	0.52
1:L:85:ILE:HD13	1:L:299:ALA:CA	2.40	0.52
1:K:144:LEU:HD11	1:K:154:ILE:HD11	1.92	0.52
1:K:252:LEU:HD21	1:K:279:LEU:HB3	1.91	0.52
1:N:136:LYS:HG2	1:N:137:LYS:HZ2	1.75	0.52
1:M:129:GLU:HA	1:M:132:VAL:CG2	2.40	0.52
1:A:60:THR:HG22	1:A:61:THR:N	2.25	0.51
1:R:144:LEU:HB2	1:R:156:SER:HB3	1.90	0.51
1:L:230:VAL:HG11	1:L:257:GLY:C	2.30	0.51
1:L:296:ASP:O	1:L:297:ILE:C	2.48	0.51
1:K:205:THR:HG22	1:K:211:VAL:HG21	1.91	0.51
1:W:291:VAL:HB	1:W:324:ARG:HG2	1.90	0.51
1:N:165:ALA:O	1:N:169:VAL:HG23	2.10	0.51
1:D:255:ILE:O	1:D:259:GLN:HG3	2.10	0.51
1:I:106:LEU:HD23	1:I:110:ASN:HD21	1.76	0.51
1:T:272:ILE:CG2	1:T:273:GLY:N	2.73	0.51
1:K:129:GLU:HA	1:K:132:VAL:CG1	2.40	0.51
1:W:67:ILE:HD12	1:W:67:ILE:O	2.10	0.51
1:G:266:PRO:HG2	1:G:332:LYS:HB2	1.93	0.51
1:N:115:LYS:H	1:N:115:LYS:HD2	1.75	0.51
1:M:126:ASN:HD22	1:M:189:GLU:HA	1.76	0.51
1:M:292:GLN:O	1:M:294:MSE:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:82:ILE:HG12	1:R:298:GLY:O	2.10	0.51
1:R:109:LEU:O	1:R:113:LEU:HG	2.11	0.51
1:T:326:GLU:HG3	1:T:328:ARG:HE	1.75	0.51
1:K:113:LEU:HD22	1:K:139:PRO:CD	2.40	0.51
1:W:73:ILE:CG2	1:W:74:PHE:N	2.74	0.51
1:W:291:VAL:HB	1:W:324:ARG:CG	2.41	0.51
1:G:85:ILE:HG12	1:G:299:ALA:HA	1.91	0.51
1:B:236:GLU:OE1	1:B:236:GLU:HA	2.10	0.51
1:T:83:GLU:OE2	1:T:84:ASP:OD2	2.27	0.51
1:G:162:GLU:OE2	1:G:199:GLY:N	2.43	0.51
1:G:307:LYS:HZ2	1:G:312:GLU:CB	2.22	0.51
1:K:226:GLY:O	1:K:230:VAL:HG23	2.11	0.51
1:W:178:LYS:HZ1	1:W:179:ASN:HB3	1.75	0.51
1:W:216:ILE:O	1:W:216:ILE:CG1	2.57	0.51
1:G:202:ARG:NH1	1:G:206:GLU:OE2	2.44	0.51
1:M:151:THR:HG21	1:M:153:GLN:OE1	2.09	0.51
1:D:85:ILE:HD11	1:D:295:TYR:CZ	2.45	0.51
1:D:148:ILE:H	1:D:148:ILE:CD1	2.24	0.51
1:I:288:THR:OG1	1:I:331:THR:HG22	2.10	0.51
1:T:70:ILE:H	1:T:97:ASN:HD21	1.59	0.51
1:T:286:GLN:O	1:T:328:ARG:HB2	2.11	0.51
1:L:113:LEU:HD13	1:L:139:PRO:CD	2.41	0.51
1:L:120:ILE:HG22	1:L:121:ILE:N	2.25	0.51
1:L:274:PHE:O	1:L:275:ASP:CB	2.58	0.51
1:K:80:ARG:NH1	1:K:84:ASP:OD2	2.39	0.51
1:K:274:PHE:O	1:K:275:ASP:HB2	2.10	0.51
1:W:201:LYS:O	1:W:204:LEU:N	2.44	0.51
1:W:201:LYS:O	1:W:203:ALA:N	2.44	0.51
1:W:226:GLY:O	1:W:230:VAL:HG23	2.11	0.51
1:W:252:LEU:HD22	1:G:282:MSE:CE	2.41	0.51
1:W:278:ARG:HH11	1:W:278:ARG:CB	2.23	0.51
1:G:273:GLY:O	1:G:290:VAL:HG23	2.11	0.51
1:N:69:ASP:C	1:N:71:SER:H	2.13	0.51
1:N:155:PRO:O	1:N:156:SER:HB3	2.11	0.51
1:D:164:ALA:HA	1:D:323:HIS:CE1	2.46	0.51
1:B:62:THR:HB	1:B:92:ASN:HB2	1.93	0.51
1:B:234:LEU:HD22	1:B:261:ARG:HG3	1.92	0.51
1:T:329:GLN:C	1:T:331:THR:H	2.14	0.51
1:K:86:ALA:HB1	1:K:93:ILE:CD1	2.39	0.51
1:W:180:ILE:N	1:W:180:ILE:CD1	2.73	0.51
1:D:153:GLN:HA	1:D:153:GLN:HE21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:70:ILE:O	1:I:70:ILE:HG12	2.10	0.51
1:R:135:LEU:HD23	1:R:154:ILE:HD12	1.92	0.51
1:T:328:ARG:HH11	1:T:328:ARG:HG3	1.75	0.51
1:L:112:MSE:C	1:L:114:GLY:H	2.12	0.51
1:G:172:LEU:O	1:G:177:HIS:HB2	2.11	0.51
1:N:157:VAL:CG1	1:N:301:ALA:HB2	2.41	0.51
1:B:85:ILE:HD11	1:B:299:ALA:HB2	1.93	0.51
1:L:62:THR:HG22	1:L:92:ASN:HB3	1.93	0.51
1:L:141:PRO:HB2	1:L:305:LEU:CD1	2.41	0.51
1:G:148:ILE:H	1:G:148:ILE:CD1	2.05	0.51
1:N:288:THR:HG22	1:N:328:ARG:CA	2.41	0.51
1:I:220:ASP:O	1:I:221:TYR:CB	2.58	0.51
1:K:104:LYS:O	1:K:108:LEU:HG	2.11	0.51
1:W:310:ASN:O	1:W:311:LYS:HG2	2.11	0.51
1:G:113:LEU:HB3	1:G:139:PRO:HG2	1.93	0.51
1:G:133:GLU:HA	1:G:136:LYS:CD	2.38	0.51
1:N:70:ILE:HG13	1:M:70:ILE:CD1	2.36	0.51
1:D:293:PRO:HB2	1:D:296:ASP:HB2	1.93	0.50
1:I:126:ASN:OD1	1:I:128:THR:HG23	2.11	0.50
1:I:242:ALA:HA	1:I:270:GLU:O	2.12	0.50
1:R:104:LYS:HB3	1:R:104:LYS:HZ2	1.76	0.50
1:T:129:GLU:HA	1:T:132:VAL:HG22	1.92	0.50
1:L:163:GLN:NE2	1:L:167:ASP:OD1	2.44	0.50
1:L:172:LEU:CD1	1:L:242:ALA:HB1	2.36	0.50
1:N:187:LEU:O	1:N:189:GLU:N	2.45	0.50
1:D:122:PHE:HB3	1:D:144:LEU:HD23	1.93	0.50
1:I:180:ILE:N	1:I:180:ILE:HD12	2.25	0.50
1:R:278:ARG:HB3	1:R:278:ARG:NH1	2.26	0.50
1:T:308:TYR:C	1:T:310:ASN:H	2.14	0.50
1:L:139:PRO:CG	1:L:140:VAL:H	2.22	0.50
1:N:172:LEU:O	1:N:177:HIS:HB2	2.11	0.50
1:N:217:VAL:HG21	1:N:232:LYS:CD	2.42	0.50
1:A:148:ILE:CD1	1:A:148:ILE:N	2.75	0.50
1:D:61:THR:HG23	1:D:118:ASP:OD1	2.12	0.50
1:B:114:GLY:C	1:B:116:GLN:N	2.65	0.50
1:L:70:ILE:CD1	1:K:70:ILE:HD11	2.42	0.50
1:G:288:THR:CG2	1:G:327:PHE:HA	2.37	0.50
1:N:217:VAL:HG21	1:N:232:LYS:HD2	1.94	0.50
1:A:105:GLU:O	1:A:109:LEU:HD23	2.11	0.50
1:D:172:LEU:HD21	1:D:272:ILE:HD13	1.93	0.50
1:I:202:ARG:HA	1:I:205:THR:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:136:LYS:HZ2	1:R:153:GLN:HB3	1.76	0.50
1:T:89:TYR:O	1:T:90:LYS:HB2	2.12	0.50
1:L:66:ILE:HG13	1:L:66:ILE:O	2.12	0.50
1:L:104:LYS:HA	1:L:104:LYS:CE	2.41	0.50
1:K:164:ALA:HA	1:K:323:HIS:NE2	2.27	0.50
1:K:230:VAL:HG22	1:K:254:VAL:HA	1.93	0.50
1:G:278:ARG:HD2	1:G:278:ARG:O	2.11	0.50
1:N:144:LEU:HD11	1:N:154:ILE:HG23	1.93	0.50
1:M:159:ILE:HD13	1:M:292:GLN:HG3	1.91	0.50
1:R:68:PRO:HG2	1:R:69:ASP:H	1.77	0.50
1:T:223:TYR:N	1:T:249:GLU:HG2	2.27	0.50
1:G:77:GLU:HA	1:G:80:ARG:CG	2.41	0.50
1:A:112:MSE:O	1:A:117:VAL:HG22	2.10	0.50
1:A:202:ARG:O	1:A:206:GLU:HB3	2.11	0.50
1:A:278:ARG:O	1:A:282:MSE:HG3	2.12	0.50
1:B:149:GLU:HG3	1:B:154:ILE:CG2	2.42	0.50
1:B:182:PHE:CZ	1:B:184:SER:HB3	2.47	0.50
1:I:67:ILE:HG22	1:I:123:MSE:SE	2.61	0.50
1:I:290:VAL:HG22	1:I:325:ILE:HG12	1.93	0.50
1:R:286:GLN:HB3	1:R:328:ARG:HD3	1.93	0.50
1:L:148:ILE:O	1:L:148:ILE:HD12	2.12	0.50
1:K:73:ILE:CD1	1:K:74:PHE:N	2.65	0.50
1:W:73:ILE:O	1:W:74:PHE:HB3	2.11	0.50
1:A:173:ILE:CD1	1:A:180:ILE:HD11	2.42	0.50
1:A:231:GLU:HG2	1:A:261:ARG:HH22	1.76	0.50
1:D:135:LEU:N	1:D:135:LEU:HD12	2.26	0.50
1:B:66:ILE:HG13	1:B:122:PHE:HD2	1.77	0.50
1:B:164:ALA:HB1	1:B:290:VAL:HG11	1.92	0.50
1:I:120:ILE:HB	1:I:142:VAL:HG22	1.94	0.50
1:I:166:PHE:C	1:I:166:PHE:CD1	2.85	0.50
1:T:234:LEU:HB3	1:T:261:ARG:NH2	2.23	0.50
1:K:113:LEU:CD1	1:K:139:PRO:HD2	2.41	0.50
1:K:119:GLY:HA2	1:K:140:VAL:HG13	1.94	0.50
1:G:128:THR:O	1:G:132:VAL:HG23	2.12	0.50
1:G:308:TYR:HE2	1:G:314:VAL:HG21	1.77	0.50
1:N:66:ILE:HD12	1:N:122:PHE:CD2	2.46	0.50
1:M:157:VAL:O	1:M:158:THR:HG23	2.11	0.50
1:A:121:ILE:HD11	1:A:305:LEU:HD22	1.94	0.50
1:B:68:PRO:HA	1:B:98:SER:OG	2.11	0.50
1:I:72:ASN:HB3	1:I:75:TYR:HB2	1.92	0.50
1:R:68:PRO:HA	1:R:99:ASP:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:THR:HG22	1:A:153:GLN:HG3	1.94	0.50
1:A:215:TYR:CZ	1:A:240:PRO:HG3	2.47	0.50
1:I:118:ASP:O	1:I:309:MSE:SE	2.80	0.50
1:L:162:GLU:HG3	1:L:163:GLN:N	2.27	0.50
1:G:193:HIS:HA	1:G:197:VAL:HG12	1.93	0.50
1:G:212:ARG:O	1:G:215:TYR:HB2	2.12	0.50
1:B:120:ILE:O	1:B:142:VAL:HA	2.12	0.49
1:B:183:VAL:HG22	1:B:217:VAL:HG11	1.94	0.49
1:I:135:LEU:HD23	1:I:154:ILE:HG13	1.93	0.49
1:R:280:SER:OG	1:R:328:ARG:NH1	2.45	0.49
1:T:132:VAL:HG23	1:T:133:GLU:N	2.27	0.49
1:L:73:ILE:CD1	1:K:278:ARG:HH22	2.11	0.49
1:K:263:LEU:HD23	1:K:268:ASP:OD1	2.12	0.49
1:G:113:LEU:HD13	1:G:139:PRO:CD	2.42	0.49
1:G:255:ILE:HD11	1:G:287:LEU:HD12	1.94	0.49
1:N:148:ILE:HG13	1:N:190:PRO:HB2	1.94	0.49
1:M:77:GLU:OE1	1:M:77:GLU:HA	2.12	0.49
1:M:143:VAL:CG1	1:M:305:LEU:HB2	2.42	0.49
1:I:132:VAL:HG11	1:I:149:GLU:OE1	2.12	0.49
1:I:220:ASP:H	1:I:250:MSE:HE3	1.77	0.49
1:T:151:THR:O	1:T:152:ASN:CB	2.50	0.49
1:K:205:THR:HG22	1:K:211:VAL:CG2	2.42	0.49
1:A:168:ALA:HB1	1:A:244:PHE:CE1	2.47	0.49
1:B:148:ILE:CD1	1:B:148:ILE:N	2.72	0.49
1:B:304:LEU:O	1:B:307:LYS:HB2	2.11	0.49
1:R:135:LEU:C	1:R:137:LYS:N	2.66	0.49
1:R:190:PRO:O	1:R:194:ALA:HB3	2.12	0.49
1:L:234:LEU:HD11	1:L:263:LEU:HD12	1.94	0.49
1:K:169:VAL:HG11	1:K:200:TYR:HA	1.93	0.49
1:N:73:ILE:O	1:N:77:GLU:HB2	2.12	0.49
1:N:204:LEU:C	1:N:206:GLU:H	2.14	0.49
1:A:178:LYS:HD3	1:A:179:ASN:N	2.27	0.49
1:L:110:ASN:O	1:L:112:MSE:N	2.45	0.49
1:L:193:HIS:ND1	1:L:194:ALA:N	2.61	0.49
1:G:277:THR:C	1:G:279:LEU:N	2.64	0.49
1:N:170:GLN:HA	1:N:173:ILE:CG1	2.42	0.49
1:N:173:ILE:CD1	1:N:209:LEU:HD12	2.42	0.49
1:I:179:ASN:ND2	1:I:212:ARG:NH1	2.54	0.49
1:I:274:PHE:O	1:I:275:ASP:CB	2.60	0.49
1:R:155:PRO:HG2	1:R:308:TYR:HE1	1.77	0.49
1:R:277:THR:HG23	1:R:278:ARG:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:135:LEU:HD23	1:T:154:ILE:CD1	2.39	0.49
1:T:288:THR:HG23	1:T:327:PHE:HA	1.93	0.49
1:W:170:GLN:O	1:W:174:ASP:OD1	2.31	0.49
1:N:65:VAL:CG1	1:N:66:ILE:H	2.24	0.49
1:N:179:ASN:HD22	1:N:179:ASN:N	1.95	0.49
1:N:264:ASN:HD22	1:N:264:ASN:C	2.15	0.49
1:A:101:ASN:OD1	1:A:103:ASP:HB2	2.13	0.49
1:A:180:ILE:HG23	1:A:242:ALA:O	2.12	0.49
1:R:117:VAL:O	1:R:140:VAL:HG11	2.13	0.49
1:L:80:ARG:HA	1:L:80:ARG:HH11	1.77	0.49
1:K:313:THR:HG23	1:K:313:THR:O	2.12	0.49
1:K:317:SER:H	1:K:318:ILE:HD13	1.78	0.49
1:W:139:PRO:HG2	1:W:140:VAL:H	1.76	0.49
1:N:182:PHE:CE1	1:N:197:VAL:HG22	2.48	0.49
1:A:223:TYR:H	1:D:278:ARG:HH22	1.59	0.49
1:D:113:LEU:HD22	1:D:139:PRO:HD2	1.94	0.49
1:D:113:LEU:CD2	1:D:139:PRO:HD2	2.43	0.49
1:B:205:THR:HG23	1:B:206:GLU:N	2.27	0.49
1:R:169:VAL:O	1:R:172:LEU:N	2.46	0.49
1:L:201:LYS:O	1:L:204:LEU:N	2.40	0.49
1:G:98:SER:CB	1:G:105:GLU:HG2	2.38	0.49
1:G:182:PHE:HD2	1:G:244:PHE:O	1.96	0.49
1:A:327:PHE:O	1:A:328:ARG:HG3	2.13	0.49
1:D:109:LEU:HD21	1:D:135:LEU:HG	1.93	0.49
1:D:136:LYS:HE3	1:D:153:GLN:HG3	1.94	0.49
1:D:215:TYR:HE1	1:D:236:GLU:HG2	1.78	0.49
1:B:264:ASN:OD1	1:B:267:ASN:HB2	2.11	0.49
1:T:169:VAL:HG11	1:T:200:TYR:HD2	1.76	0.49
1:T:177:HIS:HB3	1:T:180:ILE:CD1	2.43	0.49
1:W:201:LYS:O	1:W:202:ARG:C	2.51	0.49
1:G:163:GLN:HA	1:G:163:GLN:OE1	2.12	0.49
1:G:285:PRO:HB2	1:G:329:GLN:CB	2.42	0.49
1:N:137:LYS:N	1:N:137:LYS:HD2	2.27	0.49
1:A:113:LEU:HD11	1:A:139:PRO:HD2	1.94	0.49
1:B:265:VAL:CG1	1:B:285:PRO:HG3	2.43	0.49
1:T:187:LEU:HD12	1:T:218:GLU:CD	2.33	0.49
1:L:158:THR:O	1:L:321:LEU:N	2.45	0.49
1:W:155:PRO:O	1:W:156:SER:HB2	2.13	0.49
1:W:274:PHE:O	1:W:275:ASP:CB	2.59	0.49
1:G:219:GLY:HA3	1:G:250:MSE:CE	2.43	0.49
1:G:266:PRO:HG3	1:G:332:LYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:98:SER:O	1:N:100:GLN:N	2.45	0.49
1:M:127:VAL:HA	1:M:131:HIS:ND1	2.28	0.49
1:B:148:ILE:HD13	1:B:148:ILE:N	2.21	0.49
1:R:99:ASP:O	1:R:100:GLN:C	2.51	0.49
1:R:178:LYS:HZ3	1:R:179:ASN:HB3	1.78	0.49
1:T:184:SER:OG	1:T:185:GLY:N	2.46	0.49
1:K:144:LEU:CD1	1:K:149:GLU:HB2	2.39	0.49
1:G:263:LEU:HD12	1:G:263:LEU:H	1.78	0.49
1:N:80:ARG:O	1:N:80:ARG:HD3	2.13	0.49
1:N:126:ASN:HD22	1:N:126:ASN:C	2.16	0.49
1:A:93:ILE:H	1:A:93:ILE:CD1	2.14	0.48
1:A:98:SER:C	1:A:100:GLN:N	2.66	0.48
1:A:163:GLN:O	1:A:166:PHE:HB3	2.13	0.48
1:D:67:ILE:HD12	1:D:70:ILE:HA	1.94	0.48
1:D:89:TYR:O	1:D:90:LYS:HB2	2.13	0.48
1:D:181:ALA:HB3	1:D:243:ILE:HG12	1.94	0.48
1:I:106:LEU:HG	1:I:134:GLU:OE2	2.13	0.48
1:R:178:LYS:HD3	1:R:179:ASN:ND2	2.28	0.48
1:R:179:ASN:OD1	1:R:215:TYR:OH	2.27	0.48
1:R:247:THR:CG2	1:R:250:MSE:HB2	2.40	0.48
1:W:143:VAL:CG1	1:W:305:LEU:HB2	2.42	0.48
1:W:230:VAL:HG21	1:W:254:VAL:HG13	1.95	0.48
1:M:135:LEU:HD11	1:M:142:VAL:HG11	1.95	0.48
1:M:236:GLU:O	1:M:238:GLU:N	2.46	0.48
1:M:274:PHE:O	1:M:275:ASP:CB	2.60	0.48
1:D:247:THR:HG22	1:D:250:MSE:N	2.28	0.48
1:D:255:ILE:CG1	1:D:271:ILE:HD11	2.42	0.48
1:B:115:LYS:HE3	1:I:94:ILE:HD11	1.95	0.48
1:B:245:VAL:HG11	1:B:251:ALA:N	2.28	0.48
1:I:305:LEU:O	1:I:306:THR:C	2.52	0.48
1:K:113:LEU:CD2	1:K:139:PRO:HD2	2.42	0.48
1:W:80:ARG:O	1:W:81:GLY:C	2.51	0.48
1:G:101:ASN:O	1:G:105:GLU:HG3	2.13	0.48
1:N:159:ILE:HD11	1:N:161:TYR:CD2	2.48	0.48
1:A:122:PHE:HD1	1:A:144:LEU:HD22	1.78	0.48
1:B:265:VAL:HG12	1:B:285:PRO:HG3	1.94	0.48
1:R:192:ASN:HA	1:R:196:LYS:HB2	1.93	0.48
1:K:83:GLU:O	1:K:86:ALA:HB3	2.12	0.48
1:K:85:ILE:HD13	1:K:299:ALA:HA	1.96	0.48
1:K:252:LEU:HG	1:K:283:VAL:CG1	2.39	0.48
1:W:77:GLU:O	1:W:80:ARG:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:173:ILE:HD11	1:N:204:LEU:HD23	1.95	0.48
1:A:296:ASP:O	1:A:299:ALA:HB3	2.14	0.48
1:R:70:ILE:N	1:R:97:ASN:ND2	2.56	0.48
1:L:89:TYR:CD1	1:W:322:PRO:HG3	2.48	0.48
1:W:98:SER:O	1:W:99:ASP:HB3	2.13	0.48
1:G:149:GLU:HG3	1:G:151:THR:H	1.78	0.48
1:M:293:PRO:O	1:M:296:ASP:HB2	2.14	0.48
1:A:66:ILE:CD1	1:A:122:PHE:HD2	2.22	0.48
1:A:80:ARG:NH1	1:D:99:ASP:OD2	2.46	0.48
1:A:178:LYS:CD	1:A:179:ASN:N	2.76	0.48
1:B:109:LEU:O	1:B:113:LEU:HG	2.13	0.48
1:I:198:LYS:NZ	1:M:313:THR:HG21	2.28	0.48
1:I:202:ARG:HA	1:I:205:THR:HG23	1.96	0.48
1:I:281:THR:HB	1:I:286:GLN:HE22	1.78	0.48
1:T:157:VAL:HG13	1:T:157:VAL:O	2.12	0.48
1:G:166:PHE:CE1	1:G:170:GLN:HG3	2.49	0.48
1:B:91:TYR:OH	1:B:306:THR:HG23	2.13	0.48
1:B:308:TYR:C	1:B:310:ASN:N	2.67	0.48
1:I:304:LEU:C	1:I:304:LEU:HD23	2.33	0.48
1:R:132:VAL:HG12	1:R:136:LYS:HD2	1.94	0.48
1:L:148:ILE:HD11	1:L:191:ILE:HG12	1.96	0.48
1:K:164:ALA:HB1	1:K:290:VAL:HG11	1.94	0.48
1:W:105:GLU:OE1	1:W:131:HIS:CE1	2.66	0.48
1:W:192:ASN:O	1:W:197:VAL:HG23	2.13	0.48
1:G:192:ASN:O	1:G:197:VAL:HG12	2.12	0.48
1:N:98:SER:HA	1:N:104:LYS:HG2	1.95	0.48
1:M:267:ASN:H	1:M:267:ASN:HD22	1.61	0.48
1:D:66:ILE:CD1	1:D:96:SER:HB3	2.41	0.48
1:I:72:ASN:HD22	1:I:74:PHE:H	1.59	0.48
1:I:88:MSE:CE	1:R:296:ASP:CB	2.89	0.48
1:R:211:VAL:O	1:R:211:VAL:HG12	2.14	0.48
1:R:223:TYR:HA	1:R:249:GLU:O	2.14	0.48
1:R:300:VAL:HA	1:R:303:ARG:HB2	1.96	0.48
1:L:85:ILE:HG23	1:L:88:MSE:HE3	1.96	0.48
1:K:111:ASN:HB3	1:K:115:LYS:HZ1	1.78	0.48
1:K:284:ARG:NH1	1:K:286:GLN:HE21	2.07	0.48
1:W:247:THR:HB	1:W:250:MSE:HE2	1.94	0.48
1:G:83:GLU:OE2	1:G:93:ILE:HG21	2.14	0.48
1:G:91:TYR:HD2	1:G:302:MSE:HE1	1.78	0.48
1:M:85:ILE:HG22	1:M:302:MSE:HG3	1.95	0.48
1:M:192:ASN:O	1:M:197:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ASN:O	1:A:268:ASP:HB2	2.14	0.48
1:A:295:TYR:O	1:A:299:ALA:HB2	2.13	0.48
1:T:149:GLU:CD	1:T:152:ASN:H	2.17	0.48
1:L:98:SER:HB2	1:L:105:GLU:HG2	1.96	0.48
1:K:105:GLU:OE1	1:K:131:HIS:CE1	2.66	0.48
1:K:179:ASN:ND2	1:K:212:ARG:NH2	2.61	0.48
1:K:269:LEU:CD2	1:K:271:ILE:HG23	2.43	0.48
1:W:98:SER:N	1:W:108:LEU:HD11	2.28	0.48
1:M:114:GLY:O	1:M:116:GLN:N	2.45	0.48
1:A:98:SER:C	1:A:100:GLN:H	2.17	0.48
1:A:293:PRO:HB2	1:A:296:ASP:HB2	1.94	0.48
1:B:164:ALA:HB2	1:B:323:HIS:CD2	2.49	0.48
1:L:264:ASN:OD1	1:L:267:ASN:HB2	2.13	0.48
1:L:287:LEU:HA	1:L:330:SER:HB3	1.96	0.48
1:K:274:PHE:O	1:K:275:ASP:CB	2.61	0.48
1:W:230:VAL:CG2	1:W:254:VAL:HG22	2.44	0.48
1:G:236:GLU:HG3	1:G:238:GLU:O	2.14	0.48
1:N:260:ASP:CG	1:M:284:ARG:HH21	2.17	0.48
1:M:275:ASP:O	1:M:276:ASN:HB3	2.14	0.48
1:D:220:ASP:O	1:D:221:TYR:HB2	2.13	0.48
1:B:159:ILE:HG22	1:B:321:LEU:O	2.14	0.48
1:B:250:MSE:O	1:B:254:VAL:HG23	2.13	0.48
1:B:252:LEU:HD12	1:B:252:LEU:N	2.28	0.48
1:R:148:ILE:CD1	1:R:148:ILE:H	2.26	0.48
1:R:255:ILE:HD11	1:R:287:LEU:HD13	1.96	0.48
1:T:94:ILE:HB	1:T:112:MSE:HE1	1.95	0.48
1:L:67:ILE:O	1:L:97:ASN:HA	2.14	0.48
1:L:212:ARG:CB	1:L:212:ARG:NH1	2.65	0.48
1:K:191:ILE:HA	1:K:195:LYS:HG3	1.96	0.48
1:G:67:ILE:HD13	1:G:96:SER:O	2.13	0.48
1:N:144:LEU:HB2	1:N:156:SER:CB	2.43	0.48
1:N:264:ASN:ND2	1:N:264:ASN:C	2.67	0.48
1:M:144:LEU:HB2	1:M:156:SER:CB	2.44	0.48
1:B:70:ILE:N	1:B:97:ASN:HD21	2.05	0.47
1:I:149:GLU:CD	1:I:151:THR:HG1	2.16	0.47
1:R:136:LYS:NZ	1:R:153:GLN:HB3	2.29	0.47
1:T:101:ASN:ND2	1:T:104:LYS:N	2.51	0.47
1:T:159:ILE:HG22	1:T:321:LEU:O	2.13	0.47
1:T:169:VAL:HG23	1:T:203:ALA:CB	2.44	0.47
1:L:169:VAL:O	1:L:172:LEU:N	2.47	0.47
1:L:193:HIS:ND1	1:L:193:HIS:C	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:293:PRO:HB2	1:L:296:ASP:HB2	1.96	0.47
1:G:69:ASP:OD1	1:G:71:SER:N	2.43	0.47
1:N:119:GLY:HA3	1:N:305:LEU:HD21	1.96	0.47
1:M:187:LEU:O	1:M:193:HIS:HB3	2.14	0.47
1:M:283:VAL:O	1:M:284:ARG:CD	2.62	0.47
1:A:166:PHE:O	1:A:167:ASP:C	2.50	0.47
1:A:193:HIS:CD2	1:A:194:ALA:N	2.82	0.47
1:I:88:MSE:CE	1:R:321:LEU:HD22	2.44	0.47
1:I:192:ASN:O	1:I:197:VAL:HG23	2.14	0.47
1:R:94:ILE:CG2	1:T:94:ILE:HG23	2.44	0.47
1:L:139:PRO:HG2	1:L:140:VAL:N	2.22	0.47
1:L:145:ALA:C	1:L:147:SER:N	2.68	0.47
1:L:256:HIS:HE1	1:K:283:VAL:HA	1.79	0.47
1:G:231:GLU:O	1:G:235:GLU:HG2	2.14	0.47
1:D:148:ILE:HD12	1:D:191:ILE:HB	1.97	0.47
1:I:157:VAL:HA	1:I:319:VAL:O	2.13	0.47
1:T:277:THR:C	1:T:279:LEU:N	2.68	0.47
1:L:110:ASN:C	1:L:112:MSE:H	2.18	0.47
1:L:266:PRO:HA	1:L:269:LEU:O	2.14	0.47
1:L:329:GLN:NE2	1:L:329:GLN:N	2.62	0.47
1:K:111:ASN:HB3	1:K:115:LYS:NZ	2.28	0.47
1:W:77:GLU:HB3	1:W:294:MSE:HE3	1.96	0.47
1:W:83:GLU:HG2	1:W:93:ILE:HD13	1.95	0.47
1:G:148:ILE:HD12	1:G:148:ILE:N	2.17	0.47
1:G:155:PRO:HG2	1:G:308:TYR:CE1	2.49	0.47
1:N:220:ASP:CG	1:N:222:THR:HG22	2.34	0.47
1:D:284:ARG:HH21	1:D:286:GLN:HG2	1.79	0.47
1:B:70:ILE:HD11	1:I:70:ILE:CG1	2.42	0.47
1:R:182:PHE:CD2	1:R:244:PHE:CD2	3.02	0.47
1:R:278:ARG:CB	1:R:278:ARG:HH11	2.26	0.47
1:T:328:ARG:HG3	1:T:328:ARG:NH1	2.29	0.47
1:L:266:PRO:HB2	1:L:270:GLU:HG2	1.96	0.47
1:L:328:ARG:HH11	1:L:328:ARG:CG	2.25	0.47
1:W:169:VAL:CG2	1:W:170:GLN:N	2.77	0.47
1:N:170:GLN:HA	1:N:173:ILE:HG13	1.97	0.47
1:M:245:VAL:CG2	1:M:254:VAL:HG21	2.44	0.47
1:A:67:ILE:HD13	1:A:67:ILE:N	2.27	0.47
1:A:96:SER:OG	1:A:108:LEU:HD22	2.14	0.47
1:A:177:HIS:CE1	1:A:270:GLU:CG	2.96	0.47
1:R:222:THR:HG22	1:R:224:ASP:H	1.79	0.47
1:T:146:ALA:CA	1:T:158:THR:HG22	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:69:ASP:HB3	1:K:72:ASN:HB3	1.96	0.47
1:W:254:VAL:HG12	1:W:271:ILE:CD1	2.44	0.47
1:W:306:THR:HA	1:W:309:MSE:HE3	1.96	0.47
1:N:280:SER:HA	1:N:287:LEU:HB3	1.97	0.47
1:K:68:PRO:HB3	1:K:100:GLN:HG2	1.95	0.47
1:K:109:LEU:O	1:K:113:LEU:HG	2.15	0.47
1:G:180:ILE:HD13	1:G:180:ILE:N	2.29	0.47
1:N:114:GLY:C	1:N:116:GLN:N	2.68	0.47
1:M:267:ASN:ND2	1:M:267:ASN:H	2.13	0.47
1:A:115:LYS:HE2	1:D:94:ILE:HG13	1.96	0.47
1:A:199:GLY:O	1:A:202:ARG:HB2	2.15	0.47
1:A:325:ILE:HD12	1:A:325:ILE:N	2.29	0.47
1:D:145:ALA:O	1:D:146:ALA:C	2.53	0.47
1:D:185:GLY:O	1:D:186:THR:C	2.53	0.47
1:B:227:ILE:HG23	1:B:257:GLY:HA3	1.97	0.47
1:I:88:MSE:HE1	1:R:321:LEU:HD22	1.95	0.47
1:I:179:ASN:HD22	1:I:212:ARG:NH1	2.11	0.47
1:R:261:ARG:HB3	1:R:263:LEU:HD13	1.95	0.47
1:R:292:GLN:O	1:R:294:MSE:HG3	2.15	0.47
1:T:95:LEU:HD13	1:T:96:SER:N	2.29	0.47
1:T:109:LEU:CD2	1:T:135:LEU:HD13	2.41	0.47
1:T:182:PHE:HD2	1:T:244:PHE:O	1.98	0.47
1:T:284:ARG:NH1	1:T:286:GLN:HG2	2.29	0.47
1:L:97:ASN:HB2	1:K:83:GLU:OE2	2.15	0.47
1:W:97:ASN:HB3	1:G:83:GLU:OE2	2.14	0.47
1:W:162:GLU:OE2	1:W:202:ARG:HD3	2.14	0.47
1:G:123:MSE:HB3	1:G:145:ALA:O	2.15	0.47
1:N:112:MSE:HG3	1:N:117:VAL:HG21	1.96	0.47
1:N:115:LYS:HD2	1:N:115:LYS:N	2.29	0.47
1:A:67:ILE:CD1	1:A:95:LEU:HD12	2.45	0.47
1:A:80:ARG:NH2	1:D:99:ASP:HA	2.24	0.47
1:B:308:TYR:C	1:B:310:ASN:H	2.17	0.47
1:T:146:ALA:HA	1:T:158:THR:HG22	1.96	0.47
1:L:297:ILE:HA	1:L:321:LEU:CD1	2.44	0.47
1:K:151:THR:HG21	1:K:153:GLN:OE1	2.14	0.47
1:W:223:TYR:OH	1:G:284:ARG:NH2	2.48	0.47
1:N:210:PRO:HB2	1:N:212:ARG:NE	2.16	0.47
1:M:126:ASN:ND2	1:M:190:PRO:HD3	2.29	0.47
1:L:68:PRO:HG2	1:L:75:TYR:CE2	2.50	0.47
1:L:94:ILE:CG2	1:K:94:ILE:HB	2.44	0.47
1:L:329:GLN:C	1:L:331:THR:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:HD13	1:A:109:LEU:HA	1.74	0.47
1:A:223:TYR:CD1	1:A:223:TYR:C	2.87	0.47
1:B:223:TYR:OH	1:B:256:HIS:HD2	1.98	0.47
1:I:106:LEU:HD23	1:I:106:LEU:C	2.35	0.47
1:L:181:ALA:CB	1:L:233:LEU:HD13	2.45	0.47
1:M:202:ARG:O	1:M:206:GLU:HB2	2.14	0.47
1:D:186:THR:CG2	1:D:188:GLU:OE1	2.60	0.46
1:B:277:THR:CG2	1:B:278:ARG:N	2.60	0.46
1:R:300:VAL:O	1:R:300:VAL:HG12	2.15	0.46
1:T:109:LEU:HD21	1:T:135:LEU:CD1	2.44	0.46
1:L:80:ARG:HD3	1:L:84:ASP:OD2	2.15	0.46
1:W:83:GLU:OE1	1:W:83:GLU:O	2.33	0.46
1:W:201:LYS:C	1:W:203:ALA:N	2.69	0.46
1:G:144:LEU:HD23	1:G:144:LEU:N	2.28	0.46
1:G:245:VAL:HG12	1:G:247:THR:H	1.80	0.46
1:N:234:LEU:HD12	1:N:234:LEU:N	2.29	0.46
1:M:149:GLU:O	1:M:151:THR:N	2.48	0.46
1:A:97:ASN:O	1:A:108:LEU:HD11	2.15	0.46
1:D:86:ALA:HB1	1:D:93:ILE:HD13	1.96	0.46
1:D:166:PHE:CE2	1:D:203:ALA:HA	2.51	0.46
1:R:135:LEU:HD23	1:R:154:ILE:CD1	2.45	0.46
1:L:68:PRO:CG	1:L:75:TYR:CE2	2.98	0.46
1:K:113:LEU:HD13	1:K:139:PRO:CD	2.44	0.46
1:W:220:ASP:OD2	1:W:225:SER:OG	2.33	0.46
1:W:230:VAL:O	1:W:233:LEU:HB2	2.15	0.46
1:W:256:HIS:HE1	1:G:283:VAL:HA	1.80	0.46
1:W:297:ILE:CD1	1:W:321:LEU:HD12	2.39	0.46
1:N:192:ASN:C	1:N:194:ALA:N	2.68	0.46
1:M:185:GLY:O	1:M:186:THR:C	2.53	0.46
1:B:163:GLN:NE2	1:B:167:ASP:OD1	2.49	0.46
1:B:296:ASP:O	1:B:297:ILE:C	2.54	0.46
1:I:326:GLU:HA	1:I:326:GLU:OE2	2.16	0.46
1:R:95:LEU:HD22	1:T:95:LEU:HB3	1.98	0.46
1:R:279:LEU:C	1:R:281:THR:H	2.19	0.46
1:K:177:HIS:HB3	1:K:241:THR:HG1	1.80	0.46
1:N:275:ASP:HB3	1:N:277:THR:HG23	1.96	0.46
1:M:73:ILE:HG22	1:M:278:ARG:HH21	1.80	0.46
1:D:69:ASP:OD1	1:D:71:SER:HB3	2.16	0.46
1:R:103:ASP:O	1:R:107:HIS:HB2	2.14	0.46
1:K:222:THR:OG1	1:K:225:SER:HB3	2.15	0.46
1:W:70:ILE:HG12	1:G:70:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:GLN:O	1:G:106:LEU:HG	2.15	0.46
1:G:117:VAL:HG23	1:G:117:VAL:O	2.15	0.46
1:N:170:GLN:O	1:N:174:ASP:OD2	2.33	0.46
1:N:204:LEU:HD23	1:N:209:LEU:HD12	1.97	0.46
1:N:282:MSE:HG2	1:M:223:TYR:CD2	2.50	0.46
1:M:70:ILE:H	1:M:97:ASN:ND2	2.13	0.46
1:M:225:SER:O	1:M:228:GLU:HB2	2.14	0.46
1:A:287:LEU:HD12	1:A:288:THR:N	2.30	0.46
1:D:201:LYS:HG2	1:D:211:VAL:CG1	2.45	0.46
1:R:131:HIS:O	1:R:132:VAL:C	2.53	0.46
1:R:157:VAL:HG11	1:R:301:ALA:HB2	1.98	0.46
1:K:122:PHE:O	1:K:144:LEU:HA	2.16	0.46
1:K:186:THR:OG1	1:K:189:GLU:HG3	2.14	0.46
1:K:242:ALA:HA	1:K:270:GLU:O	2.16	0.46
1:K:278:ARG:HH11	1:K:278:ARG:HG2	1.80	0.46
1:W:98:SER:C	1:W:99:ASP:N	2.69	0.46
1:W:328:ARG:HH11	1:W:328:ARG:CG	2.28	0.46
1:N:80:ARG:HG2	1:M:97:ASN:OD1	2.15	0.46
1:A:274:PHE:O	1:A:275:ASP:CB	2.63	0.46
1:D:61:THR:HB	1:D:91:TYR:CD1	2.51	0.46
1:B:252:LEU:HD21	1:B:283:VAL:HG22	1.97	0.46
1:W:80:ARG:HH21	1:G:69:ASP:HA	1.81	0.46
1:M:205:THR:HG23	1:M:205:THR:O	2.16	0.46
1:A:158:THR:O	1:A:320:GLN:HA	2.15	0.46
1:A:164:ALA:HA	1:A:323:HIS:NE2	2.30	0.46
1:A:284:ARG:HH21	1:A:286:GLN:HG2	1.79	0.46
1:D:85:ILE:CG2	1:D:302:MSE:HG3	2.46	0.46
1:R:66:ILE:HB	1:R:122:PHE:HD2	1.80	0.46
1:T:118:ASP:O	1:T:140:VAL:HB	2.15	0.46
1:G:275:ASP:O	1:G:276:ASN:HB3	2.16	0.46
1:N:135:LEU:O	1:N:137:LYS:N	2.49	0.46
1:D:172:LEU:HD22	1:D:242:ALA:HB1	1.97	0.46
1:B:174:ASP:O	1:B:176:GLY:N	2.49	0.46
1:B:315:ASP:N	1:B:315:ASP:OD1	2.48	0.46
1:I:72:ASN:HD22	1:I:73:ILE:N	2.13	0.46
1:R:72:ASN:OD1	1:R:74:PHE:HB3	2.16	0.46
1:L:88:MSE:O	1:L:90:LYS:N	2.48	0.46
1:K:133:GLU:HA	1:K:136:LYS:HE3	1.96	0.46
1:G:76:ALA:O	1:G:79:ALA:HB3	2.15	0.46
1:N:166:PHE:CD2	1:N:202:ARG:CZ	2.98	0.46
1:M:131:HIS:O	1:M:135:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:141:PRO:HG2	1:M:305:LEU:CD1	2.44	0.46
1:M:187:LEU:N	1:M:218:GLU:OE2	2.45	0.46
1:M:226:GLY:O	1:M:230:VAL:HG22	2.16	0.46
1:M:234:LEU:CD1	1:M:261:ARG:HD3	2.45	0.46
1:A:178:LYS:O	1:A:209:LEU:HD13	2.15	0.46
1:I:193:HIS:C	1:I:193:HIS:CD2	2.90	0.46
1:R:106:LEU:HB3	1:R:134:GLU:OE1	2.16	0.46
1:R:197:VAL:CG1	1:R:198:LYS:N	2.78	0.46
1:R:292:GLN:O	1:R:294:MSE:N	2.49	0.46
1:T:72:ASN:ND2	1:T:74:PHE:H	2.14	0.46
1:T:212:ARG:HD2	1:T:212:ARG:H	1.76	0.46
1:N:232:LYS:O	1:N:235:GLU:HB3	2.15	0.46
1:A:64:GLY:HA3	1:A:112:MSE:HE2	1.97	0.46
1:D:66:ILE:HD11	1:D:112:MSE:HG3	1.96	0.46
1:D:98:SER:CB	1:D:105:GLU:HG2	2.45	0.46
1:B:227:ILE:HG12	1:B:253:GLY:O	2.16	0.46
1:L:324:ARG:HG3	1:L:324:ARG:HH11	1.80	0.46
1:W:291:VAL:HG23	1:W:326:GLU:HB2	1.97	0.46
1:G:117:VAL:CG2	1:G:120:ILE:HD11	2.42	0.46
1:G:177:HIS:HB3	1:G:180:ILE:CD1	2.47	0.46
1:G:205:THR:C	1:G:207:SER:H	2.19	0.46
1:N:83:GLU:OE2	1:M:97:ASN:HB2	2.16	0.46
1:N:180:ILE:HD12	1:N:180:ILE:N	2.31	0.46
1:A:89:TYR:O	1:A:90:LYS:CB	2.64	0.45
1:D:86:ALA:CB	1:D:93:ILE:HD13	2.46	0.45
1:D:182:PHE:CE1	1:D:197:VAL:HG22	2.42	0.45
1:D:299:ALA:HB1	1:D:303:ARG:HH21	1.80	0.45
1:B:252:LEU:HG	1:B:283:VAL:HG21	1.98	0.45
1:R:70:ILE:H	1:R:97:ASN:ND2	2.07	0.45
1:R:215:TYR:CE1	1:R:240:PRO:HG3	2.51	0.45
1:T:177:HIS:HB3	1:T:180:ILE:HD11	1.98	0.45
1:T:191:ILE:HD11	1:T:196:LYS:NZ	2.31	0.45
1:T:230:VAL:O	1:T:234:LEU:HG	2.16	0.45
1:L:127:VAL:HA	1:L:131:HIS:ND1	2.31	0.45
1:L:148:ILE:HG12	1:L:191:ILE:HG12	1.97	0.45
1:G:296:ASP:O	1:G:297:ILE:C	2.53	0.45
1:G:296:ASP:HA	1:G:299:ALA:HB3	1.97	0.45
1:N:64:GLY:O	1:N:120:ILE:HA	2.17	0.45
1:A:90:LYS:O	1:A:90:LYS:HG2	2.16	0.45
1:W:65:VAL:HG13	1:W:123:MSE:HE3	1.99	0.45
1:N:93:ILE:HG22	1:N:94:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:178:LYS:O	1:N:209:LEU:HD22	2.15	0.45
1:N:212:ARG:NH1	1:N:212:ARG:HG2	2.30	0.45
1:D:188:GLU:H	1:D:188:GLU:CD	2.19	0.45
1:I:168:ALA:O	1:I:171:SER:HB3	2.16	0.45
1:R:285:PRO:HB2	1:R:329:GLN:CB	2.46	0.45
1:T:157:VAL:O	1:T:158:THR:CG2	2.64	0.45
1:T:318:ILE:N	1:T:318:ILE:CD1	2.79	0.45
1:A:65:VAL:CG1	1:A:123:MSE:HE3	2.46	0.45
1:D:74:PHE:CD2	1:D:294:MSE:HE1	2.52	0.45
1:R:70:ILE:HG12	1:T:70:ILE:HD13	1.99	0.45
1:R:308:TYR:HE2	1:R:314:VAL:CG2	2.29	0.45
1:R:310:ASN:O	1:R:311:LYS:C	2.55	0.45
1:L:62:THR:HG21	1:L:92:ASN:HD22	1.81	0.45
1:L:126:ASN:OD1	1:L:128:THR:HG23	2.16	0.45
1:L:178:LYS:HA	1:L:209:LEU:HD21	1.98	0.45
1:L:282:MSE:HG2	1:K:223:TYR:CD2	2.52	0.45
1:K:236:GLU:OE2	1:K:237:ASP:N	2.49	0.45
1:W:80:ARG:O	1:W:82:ILE:N	2.50	0.45
1:W:296:ASP:OD2	1:W:296:ASP:N	2.49	0.45
1:D:66:ILE:HG21	1:D:122:PHE:HE2	1.82	0.45
1:R:252:LEU:HG	1:R:283:VAL:HG22	1.99	0.45
1:R:261:ARG:HB3	1:R:263:LEU:CD1	2.46	0.45
1:R:312:GLU:O	1:R:313:THR:O	2.34	0.45
1:T:265:VAL:HG13	1:T:269:LEU:O	2.16	0.45
1:L:130:GLU:O	1:L:133:GLU:HB2	2.17	0.45
1:L:216:ILE:O	1:L:216:ILE:CG1	2.52	0.45
1:K:143:VAL:HG22	1:K:155:PRO:HB2	1.98	0.45
1:W:129:GLU:O	1:W:132:VAL:HG22	2.17	0.45
1:W:144:LEU:HB2	1:W:156:SER:OG	2.16	0.45
1:N:70:ILE:O	1:N:70:ILE:HG12	2.16	0.45
1:N:104:LYS:O	1:N:108:LEU:HG	2.17	0.45
1:M:331:THR:HG23	1:M:332:LYS:N	2.31	0.45
1:D:153:GLN:HE21	1:D:153:GLN:CA	2.29	0.45
1:D:245:VAL:HB	1:D:251:ALA:HB2	1.99	0.45
1:B:308:TYR:O	1:B:310:ASN:N	2.50	0.45
1:I:102:GLN:HG3	1:I:131:HIS:NE2	2.31	0.45
1:R:165:ALA:HB1	1:R:244:PHE:CE2	2.48	0.45
1:R:324:ARG:HH11	1:R:324:ARG:CG	2.29	0.45
1:T:275:ASP:O	1:T:276:ASN:CB	2.65	0.45
1:G:329:GLN:N	1:G:329:GLN:CD	2.70	0.45
1:N:101:ASN:OD1	1:N:103:ASP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:223:TYR:CZ	1:M:282:MSE:HA	2.52	0.45
1:M:243:ILE:HB	1:M:271:ILE:CG2	2.35	0.45
1:I:78:LEU:C	1:I:78:LEU:HD23	2.37	0.45
1:R:109:LEU:C	1:R:109:LEU:HD23	2.37	0.45
1:R:143:VAL:HG22	1:R:155:PRO:HB2	1.98	0.45
1:K:212:ARG:NH1	1:K:238:GLU:OE1	2.50	0.45
1:W:80:ARG:HG2	1:W:80:ARG:NH1	2.32	0.45
1:W:230:VAL:HG21	1:W:254:VAL:CA	2.45	0.45
1:W:230:VAL:CG2	1:W:254:VAL:HA	2.42	0.45
1:N:97:ASN:ND2	1:N:99:ASP:H	2.15	0.45
1:M:76:ALA:O	1:M:80:ARG:HB2	2.17	0.45
1:M:178:LYS:HA	1:M:209:LEU:HD11	1.98	0.45
1:M:185:GLY:HA3	1:M:221:TYR:HE2	1.80	0.45
1:M:201:LYS:HG2	1:M:211:VAL:HG11	1.98	0.45
1:M:202:ARG:HG2	1:M:202:ARG:HH11	1.82	0.45
1:T:128:THR:C	1:T:130:GLU:H	2.18	0.45
1:T:214:SER:HB2	1:T:236:GLU:OE1	2.17	0.45
1:T:276:ASN:CG	1:T:291:VAL:HG22	2.35	0.45
1:K:220:ASP:C	1:K:221:TYR:HD1	2.20	0.45
1:W:62:THR:HB	1:W:92:ASN:HB3	1.98	0.45
1:W:247:THR:O	1:W:248:ASP:C	2.55	0.45
1:A:89:TYR:OH	1:A:303:ARG:HB3	2.17	0.45
1:A:304:LEU:O	1:A:307:LYS:HB2	2.16	0.45
1:D:323:HIS:CD2	1:D:323:HIS:C	2.90	0.45
1:B:202:ARG:O	1:B:206:GLU:HG3	2.17	0.45
1:T:149:GLU:O	1:T:149:GLU:CG	2.65	0.45
1:T:173:ILE:HD12	1:T:209:LEU:HD12	1.99	0.45
1:T:230:VAL:HG21	1:T:254:VAL:HG13	1.98	0.45
1:L:148:ILE:CD1	1:L:191:ILE:HG12	2.46	0.45
1:W:159:ILE:HG21	1:W:293:PRO:HD2	1.97	0.45
1:W:293:PRO:O	1:W:297:ILE:HG12	2.17	0.45
1:N:63:VAL:N	1:N:92:ASN:O	2.50	0.45
1:N:183:VAL:HB	1:N:245:VAL:HG13	1.98	0.45
1:M:109:LEU:CD1	1:M:113:LEU:HD21	2.44	0.45
1:D:318:ILE:HG13	1:D:318:ILE:O	2.17	0.45
1:D:329:GLN:CD	1:D:329:GLN:N	2.70	0.45
1:B:266:PRO:O	1:B:268:ASP:N	2.50	0.45
1:T:77:GLU:OE1	1:T:278:ARG:HG2	2.17	0.45
1:T:329:GLN:C	1:T:331:THR:N	2.70	0.45
1:L:183:VAL:HB	1:L:245:VAL:HG13	1.99	0.45
1:K:62:THR:HB	1:K:92:ASN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:93:ILE:N	1:K:93:ILE:CD1	2.79	0.45
1:W:80:ARG:NH1	1:G:97:ASN:OD1	2.49	0.45
1:N:197:VAL:O	1:N:200:TYR:HB3	2.17	0.45
1:B:202:ARG:HA	1:B:205:THR:CG2	2.47	0.44
1:B:205:THR:CG2	1:B:206:GLU:N	2.80	0.44
1:B:307:LYS:HE2	1:B:307:LYS:CA	2.47	0.44
1:I:94:ILE:HG21	1:I:112:MSE:HE1	1.99	0.44
1:R:99:ASP:O	1:R:101:ASN:N	2.50	0.44
1:R:148:ILE:CG1	1:R:190:PRO:HB2	2.47	0.44
1:R:212:ARG:HH11	1:R:212:ARG:HG3	1.82	0.44
1:L:180:ILE:HA	1:L:242:ALA:O	2.17	0.44
1:K:161:TYR:CE2	1:K:191:ILE:HD11	2.52	0.44
1:K:271:ILE:HD13	1:K:271:ILE:H	1.82	0.44
1:W:308:TYR:CE1	1:W:314:VAL:CG1	2.96	0.44
1:N:105:GLU:OE1	1:N:131:HIS:NE2	2.42	0.44
1:M:263:LEU:O	1:M:264:ASN:C	2.55	0.44
1:D:249:GLU:O	1:D:252:LEU:HB3	2.17	0.44
1:R:220:ASP:O	1:R:221:TYR:HB2	2.17	0.44
1:T:190:PRO:O	1:T:194:ALA:HB3	2.16	0.44
1:L:263:LEU:HA	1:L:263:LEU:HD23	1.79	0.44
1:W:70:ILE:C	1:W:72:ASN:H	2.20	0.44
1:W:308:TYR:CZ	1:W:314:VAL:HG11	2.53	0.44
1:G:129:GLU:CD	1:G:129:GLU:H	2.19	0.44
1:G:149:GLU:CD	1:G:154:ILE:HD11	2.38	0.44
1:G:162:GLU:OE2	1:G:198:LYS:HB3	2.17	0.44
1:G:279:LEU:O	1:G:279:LEU:HD22	2.17	0.44
1:N:109:LEU:HD23	1:N:134:GLU:CG	2.37	0.44
1:M:263:LEU:O	1:M:264:ASN:O	2.33	0.44
1:M:304:LEU:CD1	1:M:314:VAL:HG11	2.46	0.44
1:A:122:PHE:HE1	1:A:127:VAL:HG22	1.82	0.44
1:A:220:ASP:O	1:A:221:TYR:CB	2.65	0.44
1:D:302:MSE:CE	1:D:305:LEU:CD2	2.95	0.44
1:B:82:ILE:HD12	1:B:82:ILE:N	2.32	0.44
1:I:72:ASN:O	1:I:74:PHE:N	2.49	0.44
1:I:88:MSE:HE3	1:R:296:ASP:CB	2.47	0.44
1:I:266:PRO:HB2	1:I:332:LYS:HG3	1.99	0.44
1:R:148:ILE:N	1:R:148:ILE:HD13	2.33	0.44
1:T:242:ALA:HA	1:T:270:GLU:O	2.16	0.44
1:K:129:GLU:O	1:K:132:VAL:HG13	2.16	0.44
1:N:260:ASP:OD2	1:M:284:ARG:NH2	2.48	0.44
1:N:303:ARG:HG2	1:N:303:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:329:GLN:C	1:M:331:THR:H	2.21	0.44
1:A:73:ILE:CG2	1:A:277:THR:CG2	2.95	0.44
1:L:120:ILE:CG2	1:L:121:ILE:N	2.80	0.44
1:W:94:ILE:HG23	1:G:94:ILE:HG23	1.99	0.44
1:W:276:ASN:CG	1:W:291:VAL:HG22	2.37	0.44
1:G:293:PRO:HG2	1:G:297:ILE:HD11	1.99	0.44
1:A:233:LEU:HD22	1:A:240:PRO:HG2	1.98	0.44
1:A:273:GLY:O	1:A:289:SER:HA	2.17	0.44
1:D:307:LYS:HD3	1:D:314:VAL:HG12	1.99	0.44
1:T:157:VAL:C	1:T:158:THR:HG23	2.38	0.44
1:L:281:THR:HB	1:L:286:GLN:HE22	1.83	0.44
1:K:139:PRO:HG2	1:K:140:VAL:H	1.83	0.44
1:W:70:ILE:CG1	1:G:70:ILE:HD11	2.47	0.44
1:W:250:MSE:O	1:W:253:GLY:N	2.50	0.44
1:W:279:LEU:O	1:W:281:THR:N	2.50	0.44
1:N:206:GLU:O	1:N:208:GLY:N	2.48	0.44
1:N:217:VAL:HG22	1:N:218:GLU:N	2.32	0.44
1:N:266:PRO:HD3	1:N:285:PRO:HG3	1.98	0.44
1:A:121:ILE:CD1	1:A:305:LEU:HD22	2.48	0.44
1:B:114:GLY:O	1:B:116:GLN:N	2.51	0.44
1:I:94:ILE:CG2	1:I:112:MSE:HE1	2.46	0.44
1:L:60:THR:HB	1:L:61:THR:H	1.51	0.44
1:L:144:LEU:CD1	1:L:149:GLU:HB2	2.48	0.44
1:N:256:HIS:O	1:N:259:GLN:N	2.51	0.44
1:A:259:GLN:C	1:A:261:ARG:N	2.70	0.44
1:D:83:GLU:HA	1:D:86:ALA:CB	2.48	0.44
1:B:167:ASP:O	1:B:325:ILE:HD11	2.18	0.44
1:I:78:LEU:CB	1:I:294:MSE:HE2	2.47	0.44
1:R:67:ILE:O	1:R:97:ASN:HA	2.18	0.44
1:R:277:THR:HG21	1:R:279:LEU:HG	1.99	0.44
1:T:225:SER:OG	1:T:250:MSE:HE3	2.18	0.44
1:L:119:GLY:HA3	1:L:305:LEU:HD21	1.99	0.44
1:L:182:PHE:CZ	1:L:184:SER:HB2	2.53	0.44
1:L:217:VAL:HG12	1:L:233:LEU:HD21	1.99	0.44
1:K:129:GLU:HA	1:K:132:VAL:HG13	1.99	0.44
1:G:200:TYR:O	1:G:204:LEU:HD13	2.17	0.44
1:A:62:THR:HG22	1:A:92:ASN:ND2	2.29	0.44
1:I:133:GLU:HA	1:I:136:LYS:NZ	2.33	0.44
1:L:88:MSE:C	1:L:90:LYS:N	2.71	0.44
1:L:180:ILE:O	1:L:200:TYR:OH	2.28	0.44
1:K:123:MSE:HG2	1:K:145:ALA:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:234:LEU:O	1:K:239:LYS:HE3	2.18	0.44
1:K:291:VAL:N	1:K:324:ARG:O	2.47	0.44
1:W:247:THR:O	1:W:250:MSE:N	2.47	0.44
1:G:194:ALA:HA	1:G:198:LYS:NZ	2.33	0.44
1:G:239:LYS:HE2	1:G:239:LYS:HB2	1.89	0.44
1:N:144:LEU:HB2	1:N:156:SER:HB2	1.99	0.44
1:N:223:TYR:CD2	1:M:282:MSE:HG2	2.53	0.44
1:N:233:LEU:C	1:N:235:GLU:H	2.21	0.44
1:N:286:GLN:HB2	1:N:329:GLN:HG2	2.00	0.44
1:M:236:GLU:C	1:M:238:GLU:N	2.72	0.44
1:D:158:THR:O	1:D:321:LEU:N	2.45	0.44
1:D:230:VAL:HG11	1:D:258:ALA:HB2	2.00	0.44
1:R:90:LYS:C	1:R:91:TYR:HD2	2.21	0.44
1:R:278:ARG:NH1	1:R:278:ARG:CB	2.81	0.44
1:T:83:GLU:O	1:T:86:ALA:HB3	2.17	0.44
1:T:213:ASP:C	1:T:215:TYR:N	2.69	0.44
1:G:164:ALA:HA	1:G:323:HIS:NE2	2.33	0.44
1:G:264:ASN:OD1	1:G:267:ASN:HB2	2.17	0.44
1:D:271:ILE:O	1:D:271:ILE:HG13	2.16	0.43
1:I:78:LEU:N	1:I:294:MSE:HE2	2.33	0.43
1:R:238:GLU:OE1	1:R:238:GLU:HA	2.18	0.43
1:T:185:GLY:HA3	1:T:221:TYR:CE2	2.52	0.43
1:T:191:ILE:HD11	1:T:196:LYS:HZ2	1.82	0.43
1:L:131:HIS:C	1:L:133:GLU:N	2.69	0.43
1:K:151:THR:HG22	1:K:153:GLN:HG3	2.00	0.43
1:W:196:LYS:HE2	1:W:274:PHE:CE1	2.53	0.43
1:N:100:GLN:HG2	1:N:100:GLN:O	2.17	0.43
1:M:65:VAL:CG1	1:M:95:LEU:HG	2.47	0.43
1:A:251:ALA:C	1:A:253:GLY:N	2.72	0.43
1:D:326:GLU:HG2	1:D:328:ARG:NH2	2.33	0.43
1:B:70:ILE:HB	1:B:97:ASN:ND2	2.31	0.43
1:B:177:HIS:ND1	1:B:241:THR:OG1	2.49	0.43
1:L:114:GLY:O	1:L:116:GLN:N	2.50	0.43
1:L:184:SER:OG	1:L:185:GLY:N	2.50	0.43
1:W:144:LEU:HB2	1:W:156:SER:CB	2.48	0.43
1:G:180:ILE:HG23	1:G:242:ALA:HB3	2.00	0.43
1:N:72:ASN:OD1	1:N:74:PHE:HB3	2.19	0.43
1:N:205:THR:HG23	1:N:205:THR:O	2.18	0.43
1:N:217:VAL:HG11	1:N:229:ALA:HB1	2.00	0.43
1:N:234:LEU:N	1:N:234:LEU:CD1	2.81	0.43
1:A:77:GLU:OE2	1:A:278:ARG:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLN:HG3	1:A:100:GLN:O	2.18	0.43
1:A:230:VAL:O	1:A:234:LEU:HG	2.18	0.43
1:D:169:VAL:O	1:D:173:ILE:HG12	2.19	0.43
1:D:170:GLN:O	1:D:173:ILE:HB	2.18	0.43
1:R:101:ASN:OD1	1:R:104:LYS:HG3	2.18	0.43
1:R:212:ARG:HG3	1:R:212:ARG:NH1	2.32	0.43
1:R:306:THR:HA	1:R:309:MSE:HE3	1.99	0.43
1:L:256:HIS:CE1	1:K:283:VAL:HA	2.52	0.43
1:G:98:SER:C	1:G:100:GLN:N	2.70	0.43
1:G:113:LEU:HD22	1:G:139:PRO:CD	2.33	0.43
1:N:68:PRO:HA	1:N:98:SER:OG	2.18	0.43
1:N:69:ASP:CG	1:N:71:SER:HB2	2.38	0.43
1:M:276:ASN:HA	1:M:289:SER:OG	2.19	0.43
1:B:270:GLU:HG2	1:B:331:THR:HA	1.98	0.43
1:K:63:VAL:O	1:K:94:ILE:HD13	2.16	0.43
1:N:113:LEU:HD21	1:N:138:SER:OG	2.19	0.43
1:M:160:ASP:OD1	1:M:163:GLN:HB2	2.17	0.43
1:A:178:LYS:HD2	1:A:179:ASN:H	1.84	0.43
1:A:251:ALA:CB	1:A:287:LEU:HD22	2.48	0.43
1:D:264:ASN:H	1:D:268:ASP:HB2	1.84	0.43
1:I:89:TYR:HB3	1:I:91:TYR:CD2	2.53	0.43
1:T:112:MSE:C	1:T:114:GLY:N	2.70	0.43
1:L:101:ASN:HD22	1:L:104:LYS:HB2	1.82	0.43
1:K:119:GLY:HA2	1:K:140:VAL:CG1	2.48	0.43
1:A:169:VAL:O	1:A:169:VAL:HG12	2.18	0.43
1:A:170:GLN:OE1	1:A:170:GLN:HA	2.19	0.43
1:D:264:ASN:HB3	1:D:268:ASP:OD1	2.17	0.43
1:I:223:TYR:O	1:I:253:GLY:HA3	2.19	0.43
1:I:272:ILE:HG23	1:I:288:THR:HG22	2.01	0.43
1:T:314:VAL:HG12	1:T:316:SER:O	2.19	0.43
1:L:151:THR:O	1:L:152:ASN:HB2	2.18	0.43
1:K:293:PRO:HB2	1:K:296:ASP:HB2	2.00	0.43
1:W:129:GLU:HA	1:W:132:VAL:HG22	2.01	0.43
1:W:205:THR:C	1:W:207:SER:N	2.71	0.43
1:W:296:ASP:O	1:W:300:VAL:HG23	2.18	0.43
1:G:88:MSE:HE1	1:G:295:TYR:OH	2.18	0.43
1:G:91:TYR:CD2	1:G:302:MSE:HE1	2.52	0.43
1:G:149:GLU:HG3	1:G:151:THR:N	2.33	0.43
1:N:159:ILE:HD11	1:N:161:TYR:CE2	2.53	0.43
1:N:266:PRO:HG3	1:N:285:PRO:HB3	2.01	0.43
1:M:132:VAL:HG12	1:M:154:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:230:VAL:O	1:M:234:LEU:HG	2.19	0.43
1:M:299:ALA:O	1:M:303:ARG:HG3	2.18	0.43
1:A:102:GLN:HG2	1:A:131:HIS:HE1	1.84	0.43
1:A:111:ASN:HD21	1:D:94:ILE:HD11	1.83	0.43
1:D:82:ILE:O	1:D:85:ILE:HB	2.19	0.43
1:D:215:TYR:CZ	1:D:240:PRO:HG3	2.54	0.43
1:I:191:ILE:O	1:I:195:LYS:HB2	2.19	0.43
1:I:217:VAL:HG21	1:I:229:ALA:HB1	2.01	0.43
1:T:128:THR:C	1:T:130:GLU:N	2.72	0.43
1:L:111:ASN:O	1:L:115:LYS:HD2	2.18	0.43
1:L:204:LEU:O	1:L:205:THR:C	2.57	0.43
1:K:208:GLY:O	1:K:209:LEU:HG	2.19	0.43
1:K:292:GLN:O	1:K:294:MSE:N	2.52	0.43
1:W:288:THR:OG1	1:W:327:PHE:HA	2.19	0.43
1:G:270:GLU:C	1:G:271:ILE:HG13	2.39	0.43
1:M:74:PHE:HE2	1:M:294:MSE:HG2	1.83	0.43
1:M:231:GLU:HG2	1:M:261:ARG:HD2	2.00	0.43
1:M:274:PHE:O	1:M:275:ASP:HB2	2.17	0.43
1:A:288:THR:HG22	1:A:327:PHE:CA	2.46	0.43
1:B:148:ILE:HD12	1:B:191:ILE:CG1	2.46	0.43
1:R:76:ALA:O	1:R:79:ALA:HB3	2.19	0.43
1:R:102:GLN:HE21	1:R:102:GLN:HB3	1.57	0.43
1:R:221:TYR:H	1:R:250:MSE:SE	2.52	0.43
1:R:264:ASN:OD1	1:R:264:ASN:C	2.56	0.43
1:T:230:VAL:HG12	1:T:234:LEU:CG	2.43	0.43
1:L:73:ILE:CD1	1:L:73:ILE:H	2.31	0.43
1:L:227:ILE:HG12	1:L:253:GLY:O	2.19	0.43
1:G:157:VAL:O	1:G:158:THR:CG2	2.67	0.43
1:N:190:PRO:HA	1:N:193:HIS:CE1	2.54	0.43
1:M:321:LEU:HB3	1:M:322:PRO:HD2	2.01	0.43
1:A:73:ILE:HD12	1:A:279:LEU:CG	2.37	0.43
1:A:82:ILE:HG23	1:A:302:MSE:HE1	1.96	0.43
1:A:296:ASP:HA	1:A:299:ALA:HB3	2.01	0.43
1:B:135:LEU:HG	1:B:154:ILE:HD12	2.00	0.43
1:B:157:VAL:O	1:B:157:VAL:CG1	2.63	0.43
1:R:256:HIS:CB	1:T:284:ARG:HH21	2.26	0.43
1:T:223:TYR:HE1	1:T:256:HIS:CD2	2.29	0.43
1:L:128:THR:OG1	1:L:130:GLU:HB3	2.19	0.43
1:K:65:VAL:HG13	1:K:95:LEU:CD1	2.36	0.43
1:W:109:LEU:O	1:W:113:LEU:HG	2.18	0.43
1:W:286:GLN:H	1:W:329:GLN:CB	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:114:GLY:O	1:N:116:GLN:N	2.52	0.43
1:A:222:THR:O	1:A:223:TYR:C	2.57	0.43
1:D:102:GLN:HB3	1:D:103:ASP:H	1.73	0.43
1:D:230:VAL:HG22	1:D:254:VAL:CG1	2.34	0.43
1:B:265:VAL:HA	1:B:266:PRO:HA	1.83	0.43
1:I:243:ILE:HD12	1:I:243:ILE:N	2.34	0.43
1:R:277:THR:CG2	1:R:279:LEU:HG	2.48	0.43
1:R:282:MSE:HG2	1:T:223:TYR:CG	2.54	0.43
1:L:291:VAL:HG21	1:L:326:GLU:HB2	2.00	0.43
1:K:85:ILE:CG2	1:K:302:MSE:HG3	2.49	0.43
1:K:113:LEU:HD21	1:K:138:SER:HB2	2.00	0.43
1:W:78:LEU:O	1:W:82:ILE:HG12	2.19	0.43
1:W:286:GLN:HB3	1:W:328:ARG:CD	2.49	0.43
1:N:108:LEU:O	1:N:111:ASN:N	2.51	0.43
1:N:214:SER:HB2	1:N:236:GLU:OE2	2.18	0.43
1:M:114:GLY:C	1:M:116:GLN:N	2.72	0.43
1:A:77:GLU:OE1	1:A:277:THR:CG2	2.60	0.42
1:D:113:LEU:HD22	1:D:139:PRO:CD	2.49	0.42
1:D:287:LEU:HD12	1:D:288:THR:N	2.34	0.42
1:I:151:THR:O	1:I:153:GLN:HG3	2.19	0.42
1:R:104:LYS:O	1:R:108:LEU:HG	2.18	0.42
1:R:144:LEU:HB2	1:R:156:SER:CB	2.48	0.42
1:T:258:ALA:O	1:T:263:LEU:HB2	2.19	0.42
1:L:227:ILE:HA	1:L:230:VAL:HG23	1.99	0.42
1:L:249:GLU:OE1	1:K:278:ARG:NH1	2.51	0.42
1:L:286:GLN:HB2	1:L:328:ARG:HB3	2.01	0.42
1:K:94:ILE:HD13	1:K:94:ILE:N	2.30	0.42
1:K:133:GLU:C	1:K:135:LEU:H	2.22	0.42
1:K:272:ILE:HG22	1:K:273:GLY:N	2.33	0.42
1:W:173:ILE:HG23	1:W:209:LEU:HD11	2.02	0.42
1:W:247:THR:CG2	1:W:249:GLU:HB3	2.49	0.42
1:G:318:ILE:O	1:G:318:ILE:HG12	2.19	0.42
1:N:233:LEU:HB3	1:N:240:PRO:HG2	2.00	0.42
1:M:69:ASP:C	1:M:69:ASP:OD1	2.57	0.42
1:M:101:ASN:OD1	1:M:104:LYS:HG3	2.18	0.42
1:M:166:PHE:CE2	1:M:203:ALA:HA	2.54	0.42
1:M:234:LEU:HD12	1:M:261:ARG:CD	2.48	0.42
1:A:123:MSE:O	1:A:124:SER:HB3	2.19	0.42
1:A:165:ALA:O	1:A:169:VAL:HG23	2.19	0.42
1:D:113:LEU:HD22	1:D:139:PRO:CB	2.48	0.42
1:B:70:ILE:N	1:B:97:ASN:ND2	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:78:LEU:CA	1:I:294:MSE:HE2	2.49	0.42
1:R:146:ALA:CA	1:R:158:THR:HG22	2.49	0.42
1:L:181:ALA:HB1	1:L:215:TYR:O	2.18	0.42
1:K:273:GLY:N	1:K:288:THR:O	2.50	0.42
1:G:116:GLN:O	1:G:117:VAL:C	2.57	0.42
1:N:66:ILE:HG13	1:N:122:PHE:HA	2.00	0.42
1:N:121:ILE:N	1:N:121:ILE:CD1	2.80	0.42
1:N:212:ARG:HG2	1:N:212:ARG:HH11	1.84	0.42
1:M:280:SER:HA	1:M:287:LEU:HB3	2.02	0.42
1:A:62:THR:CG2	1:A:92:ASN:HD22	2.28	0.42
1:D:176:GLY:O	1:D:177:HIS:C	2.57	0.42
1:R:245:VAL:CG1	1:R:250:MSE:HE2	2.49	0.42
1:T:83:GLU:HB2	1:T:93:ILE:CD1	2.47	0.42
1:L:109:LEU:HD22	1:L:134:GLU:HB3	2.02	0.42
1:L:288:THR:HG22	1:L:328:ARG:N	2.31	0.42
1:K:91:TYR:CD1	1:K:302:MSE:HE1	2.54	0.42
1:K:185:GLY:HA3	1:K:221:TYR:CE1	2.54	0.42
1:G:247:THR:HB	1:G:250:MSE:CB	2.46	0.42
1:G:277:THR:O	1:G:279:LEU:N	2.51	0.42
1:M:61:THR:HG21	1:M:91:TYR:CE1	2.54	0.42
1:A:222:THR:CG2	1:A:224:ASP:HB2	2.49	0.42
1:A:266:PRO:HD3	1:A:329:GLN:O	2.19	0.42
1:D:69:ASP:HB3	1:D:72:ASN:HB2	2.01	0.42
1:D:232:LYS:HB2	1:D:232:LYS:HZ2	1.84	0.42
1:D:238:GLU:H	1:D:238:GLU:HG2	1.60	0.42
1:D:247:THR:HG23	1:D:249:GLU:H	1.84	0.42
1:B:94:ILE:O	1:B:94:ILE:HG22	2.18	0.42
1:B:191:ILE:H	1:B:191:ILE:HG13	1.66	0.42
1:B:223:TYR:CE1	1:B:227:ILE:HD11	2.53	0.42
1:R:146:ALA:HA	1:R:158:THR:HG22	2.01	0.42
1:T:111:ASN:HD22	1:T:111:ASN:N	2.17	0.42
1:T:129:GLU:C	1:T:132:VAL:HG22	2.39	0.42
1:T:193:HIS:CD2	1:T:194:ALA:N	2.88	0.42
1:K:128:THR:O	1:K:131:HIS:HB2	2.19	0.42
1:W:191:ILE:N	1:W:191:ILE:CD1	2.80	0.42
1:W:212:ARG:H	1:W:212:ARG:HG2	1.57	0.42
1:G:186:THR:O	1:G:187:LEU:C	2.58	0.42
1:G:327:PHE:CD1	1:G:327:PHE:N	2.87	0.42
1:N:170:GLN:HA	1:N:173:ILE:CB	2.47	0.42
1:N:236:GLU:OE1	1:N:236:GLU:HA	2.20	0.42
1:D:98:SER:HB3	1:D:108:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:184:SER:HB2	1:I:192:ASN:ND2	2.34	0.42
1:K:277:THR:HG22	1:K:279:LEU:N	2.14	0.42
1:W:255:ILE:O	1:W:259:GLN:HG3	2.19	0.42
1:N:96:SER:HB3	1:N:112:MSE:HE1	2.01	0.42
1:N:292:GLN:O	1:N:294:MSE:N	2.46	0.42
1:A:208:GLY:O	1:A:209:LEU:HG	2.20	0.42
1:R:202:ARG:O	1:R:206:GLU:HB3	2.20	0.42
1:T:108:LEU:HD12	1:T:108:LEU:N	2.35	0.42
1:T:149:GLU:OE2	1:T:153:GLN:N	2.45	0.42
1:L:114:GLY:C	1:L:116:GLN:N	2.71	0.42
1:L:123:MSE:HA	1:L:147:SER:OG	2.20	0.42
1:K:85:ILE:CD1	1:K:299:ALA:HA	2.50	0.42
1:W:98:SER:C	1:W:99:ASP:HB3	2.39	0.42
1:W:247:THR:HG22	1:W:250:MSE:H	1.84	0.42
1:W:286:GLN:O	1:W:328:ARG:HB2	2.19	0.42
1:G:144:LEU:CD2	1:G:154:ILE:HD13	2.33	0.42
1:G:230:VAL:CG2	1:G:254:VAL:HG13	2.48	0.42
1:G:279:LEU:O	1:G:279:LEU:HD13	2.19	0.42
1:M:72:ASN:HD22	1:M:73:ILE:N	2.17	0.42
1:A:80:ARG:CZ	1:D:97:ASN:HD21	2.33	0.42
1:A:130:GLU:N	1:A:130:GLU:CD	2.73	0.42
1:D:102:GLN:O	1:D:105:GLU:N	2.53	0.42
1:D:170:GLN:O	1:D:174:ASP:OD1	2.37	0.42
1:B:244:PHE:HZ	1:B:274:PHE:HD2	1.67	0.42
1:I:62:THR:HB	1:I:92:ASN:HD22	1.84	0.42
1:T:157:VAL:HG11	1:T:301:ALA:HB2	2.02	0.42
1:K:276:ASN:HB2	1:K:291:VAL:HA	2.00	0.42
1:W:110:ASN:ND2	1:W:111:ASN:ND2	2.68	0.42
1:W:217:VAL:HG23	1:W:218:GLU:N	2.35	0.42
1:G:308:TYR:CE2	1:G:314:VAL:HG21	2.54	0.42
1:N:117:VAL:CG2	1:N:120:ILE:HD11	2.50	0.42
1:N:210:PRO:CB	1:N:212:ARG:HE	2.19	0.42
1:N:230:VAL:HG22	1:N:254:VAL:HG13	2.02	0.42
1:M:270:GLU:OE1	1:M:332:LYS:HB2	2.20	0.42
1:D:72:ASN:O	1:D:73:ILE:C	2.58	0.42
1:D:120:ILE:O	1:D:142:VAL:HA	2.20	0.42
1:B:163:GLN:O	1:B:166:PHE:N	2.53	0.42
1:T:104:LYS:HA	1:T:107:HIS:HB3	2.01	0.42
1:K:293:PRO:O	1:K:297:ILE:HG13	2.19	0.42
1:W:80:ARG:HH12	1:G:70:ILE:HG22	1.85	0.42
1:M:98:SER:O	1:M:99:ASP:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:329:GLN:N	1:M:329:GLN:CD	2.73	0.42
1:A:292:GLN:O	1:A:294:MSE:N	2.52	0.42
1:D:82:ILE:HG22	1:D:83:GLU:N	2.34	0.42
1:D:219:GLY:HA3	1:D:250:MSE:HE1	2.01	0.42
1:D:328:ARG:HH11	1:D:328:ARG:HG3	1.83	0.42
1:I:149:GLU:O	1:I:150:SER:CB	2.68	0.42
1:R:70:ILE:O	1:R:70:ILE:HG12	2.20	0.42
1:R:303:ARG:NH1	1:R:303:ARG:CG	2.83	0.42
1:T:223:TYR:CE1	1:T:256:HIS:HD2	2.32	0.42
1:K:182:PHE:HB3	1:K:216:ILE:HD13	2.02	0.42
1:W:62:THR:HG22	1:W:92:ASN:HB3	2.02	0.42
1:W:80:ARG:HG2	1:W:80:ARG:HH11	1.84	0.42
1:W:144:LEU:HD12	1:W:156:SER:HB2	2.02	0.42
1:W:157:VAL:HG11	1:W:301:ALA:HB2	2.00	0.42
1:W:267:ASN:HA	1:W:332:LYS:HE3	2.02	0.42
1:N:284:ARG:NH2	1:M:223:TYR:OH	2.53	0.42
1:N:308:TYR:C	1:N:310:ASN:H	2.24	0.42
1:M:154:ILE:O	1:M:155:PRO:C	2.58	0.42
1:M:172:LEU:HD13	1:M:242:ALA:HB1	2.01	0.42
1:M:309:MSE:C	1:M:311:LYS:H	2.22	0.42
1:A:227:ILE:HD13	1:A:253:GLY:O	2.19	0.42
1:A:230:VAL:CG2	1:A:254:VAL:HA	2.45	0.42
1:D:286:GLN:HE21	1:D:328:ARG:HD3	1.85	0.42
1:B:93:ILE:HD12	1:B:93:ILE:N	2.31	0.42
1:R:308:TYR:HE2	1:R:314:VAL:HG21	1.85	0.42
1:T:67:ILE:HG22	1:T:123:MSE:CE	2.50	0.42
1:T:252:LEU:CD1	1:T:283:VAL:HG21	2.50	0.42
1:L:106:LEU:C	1:L:106:LEU:HD23	2.40	0.42
1:W:186:THR:HA	1:W:218:GLU:OE1	2.19	0.42
1:W:207:SER:O	1:W:208:GLY:C	2.58	0.42
1:W:230:VAL:HG22	1:W:254:VAL:HG13	2.01	0.42
1:G:277:THR:OG1	1:G:279:LEU:HB3	2.19	0.42
1:N:185:GLY:N	1:N:250:MSE:HE1	2.34	0.42
1:M:178:LYS:HA	1:M:209:LEU:HD13	2.01	0.42
1:A:165:ALA:O	1:A:168:ALA:HB3	2.20	0.41
1:A:212:ARG:H	1:A:212:ARG:HG2	1.65	0.41
1:A:261:ARG:HH11	1:A:261:ARG:CB	2.32	0.41
1:A:272:ILE:N	1:A:272:ILE:CD1	2.81	0.41
1:D:74:PHE:HE2	1:D:294:MSE:CE	2.33	0.41
1:D:92:ASN:C	1:D:93:ILE:HD12	2.41	0.41
1:B:78:LEU:O	1:B:82:ILE:CD1	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LEU:HD21	1:B:263:LEU:CD1	2.50	0.41
1:B:321:LEU:HB3	1:B:322:PRO:HD2	2.02	0.41
1:R:177:HIS:CE1	1:R:242:ALA:HB2	2.55	0.41
1:T:222:THR:O	1:T:224:ASP:N	2.53	0.41
1:L:73:ILE:HD12	1:L:73:ILE:H	1.81	0.41
1:L:197:VAL:O	1:L:200:TYR:HB3	2.20	0.41
1:W:93:ILE:HD12	1:W:93:ILE:N	2.35	0.41
1:G:85:ILE:N	1:G:85:ILE:CD1	2.83	0.41
1:N:99:ASP:O	1:N:100:GLN:CB	2.63	0.41
1:A:60:THR:CG2	1:A:61:THR:N	2.83	0.41
1:D:148:ILE:HD13	1:D:148:ILE:N	2.31	0.41
1:I:79:ALA:C	1:I:81:GLY:H	2.23	0.41
1:I:169:VAL:HG21	1:I:204:LEU:HD13	2.01	0.41
1:T:98:SER:C	1:T:100:GLN:H	2.22	0.41
1:K:220:ASP:O	1:K:221:TYR:HB2	2.20	0.41
1:K:264:ASN:OD1	1:K:267:ASN:HB2	2.19	0.41
1:W:68:PRO:HG3	1:W:75:TYR:CE2	2.55	0.41
1:W:284:ARG:HD3	1:W:284:ARG:HA	1.79	0.41
1:A:215:TYR:OH	1:A:238:GLU:HB2	2.20	0.41
1:D:69:ASP:O	1:D:71:SER:N	2.53	0.41
1:B:159:ILE:HG12	1:B:161:TYR:CZ	2.55	0.41
1:B:162:GLU:OE1	1:B:202:ARG:NH2	2.39	0.41
1:R:121:ILE:HD11	1:R:305:LEU:HD22	2.02	0.41
1:R:297:ILE:CG1	1:R:321:LEU:HD12	2.50	0.41
1:T:68:PRO:HD3	1:T:123:MSE:O	2.20	0.41
1:T:101:ASN:O	1:T:105:GLU:HB2	2.20	0.41
1:W:117:VAL:O	1:W:140:VAL:HG11	2.20	0.41
1:N:329:GLN:N	1:N:329:GLN:CD	2.74	0.41
1:M:145:ALA:C	1:M:147:SER:H	2.23	0.41
1:M:297:ILE:HD13	1:M:321:LEU:HD12	2.01	0.41
1:A:282:MSE:CE	1:D:252:LEU:HD22	2.48	0.41
1:D:101:ASN:O	1:D:105:GLU:HG3	2.20	0.41
1:D:137:LYS:HB2	1:D:137:LYS:HE3	1.84	0.41
1:B:102:GLN:HG2	1:B:131:HIS:HE1	1.84	0.41
1:R:324:ARG:CG	1:R:324:ARG:NH1	2.82	0.41
1:T:158:THR:O	1:T:320:GLN:HA	2.19	0.41
1:K:291:VAL:HG21	1:K:324:ARG:NH1	2.33	0.41
1:K:308:TYR:CE2	1:K:314:VAL:HG11	2.56	0.41
1:W:82:ILE:O	1:W:84:ASP:N	2.53	0.41
1:N:109:LEU:CD2	1:N:135:LEU:HD13	2.50	0.41
1:M:212:ARG:O	1:M:215:TYR:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:PRO:HA	1:A:193:HIS:NE2	2.35	0.41
1:D:65:VAL:CG2	1:D:95:LEU:HD23	2.50	0.41
1:D:99:ASP:O	1:D:100:GLN:HB3	2.21	0.41
1:D:245:VAL:HG11	1:D:251:ALA:N	2.35	0.41
1:B:307:LYS:HG3	1:B:312:GLU:OE1	2.21	0.41
1:I:63:VAL:N	1:I:92:ASN:O	2.54	0.41
1:I:132:VAL:CG1	1:I:149:GLU:OE1	2.69	0.41
1:R:177:HIS:ND1	1:R:242:ALA:HB2	2.36	0.41
1:T:223:TYR:CE1	1:T:256:HIS:CD2	3.09	0.41
1:L:131:HIS:C	1:L:133:GLU:H	2.24	0.41
1:W:62:THR:CG2	1:W:92:ASN:HB3	2.50	0.41
1:W:245:VAL:HG21	1:W:251:ALA:HA	2.01	0.41
1:G:241:THR:O	1:G:269:LEU:HA	2.20	0.41
1:N:221:TYR:CD1	1:N:250:MSE:HE2	2.53	0.41
1:A:66:ILE:O	1:A:66:ILE:HG13	2.20	0.41
1:A:154:ILE:HG23	1:A:155:PRO:HD2	2.01	0.41
1:A:187:LEU:O	1:A:193:HIS:HB3	2.20	0.41
1:A:252:LEU:HD11	1:A:283:VAL:HG22	2.03	0.41
1:D:182:PHE:HE1	1:D:197:VAL:CG2	2.30	0.41
1:D:266:PRO:HA	1:D:269:LEU:O	2.21	0.41
1:B:223:TYR:OH	1:B:256:HIS:CD2	2.73	0.41
1:R:66:ILE:O	1:R:123:MSE:HB2	2.20	0.41
1:R:106:LEU:HD21	1:R:131:HIS:CD2	2.56	0.41
1:T:136:LYS:NZ	1:T:136:LYS:CB	2.84	0.41
1:T:277:THR:C	1:T:279:LEU:H	2.23	0.41
1:L:204:LEU:HD22	1:L:209:LEU:HB2	2.01	0.41
1:L:288:THR:CB	1:L:328:ARG:H	2.34	0.41
1:K:189:GLU:HA	1:K:190:PRO:HD3	1.92	0.41
1:W:179:ASN:C	1:W:180:ILE:HD12	2.40	0.41
1:N:144:LEU:HD11	1:N:154:ILE:CG2	2.51	0.41
1:M:214:SER:HB2	1:M:236:GLU:OE2	2.21	0.41
1:B:80:ARG:HD2	1:B:80:ARG:O	2.20	0.41
1:B:221:TYR:HA	1:B:250:MSE:HE2	2.02	0.41
1:R:95:LEU:CD2	1:T:95:LEU:HB3	2.50	0.41
1:L:201:LYS:O	1:L:202:ARG:C	2.59	0.41
1:K:270:GLU:OE2	1:K:332:LYS:N	2.50	0.41
1:W:239:LYS:HA	1:W:240:PRO:HD3	1.88	0.41
1:G:66:ILE:HB	1:G:122:PHE:CD2	2.56	0.41
1:G:250:MSE:O	1:G:253:GLY:N	2.51	0.41
1:N:247:THR:CG2	1:N:248:ASP:N	2.79	0.41
1:M:117:VAL:O	1:M:140:VAL:HG11	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:PRO:HG2	1:D:332:LYS:HE2	2.03	0.41
1:I:90:LYS:HD2	1:R:324:ARG:HD2	2.03	0.41
1:I:133:GLU:HA	1:I:136:LYS:HZ1	1.85	0.41
1:T:131:HIS:O	1:T:135:LEU:CB	2.68	0.41
1:T:296:ASP:HB3	1:T:321:LEU:HD13	2.01	0.41
1:K:73:ILE:HD13	1:K:74:PHE:H	1.78	0.41
1:G:81:GLY:O	1:G:85:ILE:CD1	2.68	0.41
1:N:209:LEU:HA	1:N:210:PRO:HD3	1.82	0.41
1:A:77:GLU:O	1:A:80:ARG:HB3	2.21	0.41
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.89	0.41
1:A:247:THR:CG2	1:A:249:GLU:HB2	2.51	0.41
1:D:132:VAL:O	1:D:136:LYS:HB2	2.20	0.41
1:I:78:LEU:O	1:I:82:ILE:HG12	2.21	0.41
1:R:121:ILE:CD1	1:R:305:LEU:HD22	2.50	0.41
1:R:252:LEU:HD22	1:T:282:MSE:HE2	2.02	0.41
1:R:288:THR:H	1:R:330:SER:CB	2.30	0.41
1:T:318:ILE:O	1:T:318:ILE:HG12	2.21	0.41
1:L:128:THR:C	1:L:130:GLU:H	2.24	0.41
1:L:165:ALA:O	1:L:169:VAL:HG23	2.21	0.41
1:K:68:PRO:HB2	1:K:69:ASP:H	1.72	0.41
1:K:294:MSE:O	1:K:295:TYR:C	2.58	0.41
1:W:222:THR:OG1	1:W:225:SER:OG	2.30	0.41
1:G:170:GLN:CD	1:G:203:ALA:HB1	2.41	0.41
1:G:177:HIS:NE2	1:G:270:GLU:HG3	2.35	0.41
1:G:234:LEU:O	1:G:236:GLU:N	2.54	0.41
1:G:292:GLN:O	1:G:294:MSE:N	2.53	0.41
1:N:121:ILE:HD11	1:N:305:LEU:HD22	2.03	0.41
1:N:182:PHE:HD2	1:N:244:PHE:O	2.03	0.41
1:M:95:LEU:HD12	1:M:95:LEU:N	2.35	0.41
1:M:128:THR:HG1	1:M:130:GLU:HB3	1.85	0.41
1:M:155:PRO:HG3	1:M:308:TYR:OH	2.20	0.41
1:M:174:ASP:C	1:M:176:GLY:H	2.23	0.41
1:A:94:ILE:HG21	1:A:112:MSE:HE1	2.01	0.41
1:A:240:PRO:O	1:A:269:LEU:HD13	2.20	0.41
1:B:160:ASP:OD1	1:B:163:GLN:HB2	2.21	0.41
1:B:292:GLN:HE21	1:B:292:GLN:HB2	1.66	0.41
1:L:172:LEU:HD22	1:L:242:ALA:HB1	2.03	0.41
1:K:252:LEU:CD2	1:K:279:LEU:HB3	2.50	0.41
1:W:231:GLU:O	1:W:233:LEU:N	2.53	0.41
1:G:112:MSE:HB3	1:G:120:ILE:HD11	2.02	0.41
1:G:139:PRO:HB2	1:G:140:VAL:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:190:PRO:C	1:N:192:ASN:H	2.24	0.41
1:M:70:ILE:HG22	1:M:97:ASN:OD1	2.21	0.41
1:A:87:THR:HG22	1:A:87:THR:O	2.21	0.40
1:A:113:LEU:HD13	1:A:139:PRO:CG	2.42	0.40
1:A:230:VAL:HG21	1:A:254:VAL:CG1	2.47	0.40
1:D:85:ILE:HD13	1:D:85:ILE:HA	1.94	0.40
1:B:135:LEU:O	1:B:138:SER:HB3	2.20	0.40
1:I:89:TYR:O	1:I:90:LYS:CG	2.69	0.40
1:I:318:ILE:HD13	1:I:318:ILE:C	2.42	0.40
1:R:314:VAL:HG12	1:R:315:ASP:N	2.36	0.40
1:T:65:VAL:CG1	1:T:95:LEU:HD23	2.51	0.40
1:L:328:ARG:NH1	1:L:328:ARG:CG	2.82	0.40
1:W:68:PRO:HB3	1:W:100:GLN:HG3	2.02	0.40
1:W:168:ALA:HA	1:W:325:ILE:HD11	2.03	0.40
1:W:201:LYS:O	1:W:205:THR:HG23	2.21	0.40
1:W:231:GLU:HG2	1:W:235:GLU:HG3	2.04	0.40
1:N:84:ASP:O	1:N:87:THR:N	2.41	0.40
1:M:113:LEU:HD22	1:M:140:VAL:HG22	2.04	0.40
1:M:287:LEU:O	1:M:328:ARG:HD2	2.21	0.40
1:A:189:GLU:HA	1:A:190:PRO:HD3	1.84	0.40
1:D:120:ILE:HB	1:D:142:VAL:CG2	2.34	0.40
1:D:261:ARG:HH11	1:D:261:ARG:HG3	1.87	0.40
1:D:263:LEU:N	1:D:263:LEU:HD12	2.36	0.40
1:D:287:LEU:HD12	1:D:288:THR:H	1.85	0.40
1:B:181:ALA:HA	1:B:215:TYR:HB3	2.04	0.40
1:B:190:PRO:O	1:B:191:ILE:C	2.59	0.40
1:I:74:PHE:HB2	1:I:277:THR:HG21	2.03	0.40
1:I:277:THR:HB	1:I:278:ARG:H	1.57	0.40
1:R:227:ILE:HD12	1:R:253:GLY:CA	2.51	0.40
1:R:245:VAL:HG12	1:R:250:MSE:HE2	2.03	0.40
1:T:164:ALA:HB1	1:T:290:VAL:HG11	2.04	0.40
1:L:98:SER:CB	1:L:105:GLU:HG2	2.51	0.40
1:L:273:GLY:O	1:L:290:VAL:HG23	2.20	0.40
1:K:119:GLY:HA3	1:K:305:LEU:HD21	2.03	0.40
1:K:160:ASP:N	1:K:320:GLN:NE2	2.68	0.40
1:K:180:ILE:O	1:K:215:TYR:HD2	2.04	0.40
1:W:80:ARG:C	1:W:82:ILE:N	2.75	0.40
1:W:143:VAL:HG11	1:W:305:LEU:HB2	2.03	0.40
1:W:213:ASP:HA	1:W:216:ILE:HG23	2.03	0.40
1:W:326:GLU:HG3	1:W:328:ARG:NH1	2.35	0.40
1:G:145:ALA:O	1:G:146:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:316:SER:O	1:G:317:SER:C	2.58	0.40
1:N:142:VAL:HG13	1:N:154:ILE:CD1	2.49	0.40
1:M:72:ASN:O	1:M:73:ILE:C	2.57	0.40
1:A:126:ASN:C	1:A:126:ASN:ND2	2.73	0.40
1:A:157:VAL:HG11	1:A:301:ALA:CB	2.51	0.40
1:B:68:PRO:HB3	1:B:100:GLN:HE21	1.86	0.40
1:B:174:ASP:C	1:B:176:GLY:N	2.71	0.40
1:I:162:GLU:HA	1:I:195:LYS:O	2.21	0.40
1:I:198:LYS:NZ	1:M:313:THR:CG2	2.84	0.40
1:R:65:VAL:O	1:R:95:LEU:HA	2.20	0.40
1:R:166:PHE:HD1	1:R:167:ASP:N	2.19	0.40
1:G:149:GLU:HG2	1:G:152:ASN:N	2.25	0.40
1:G:187:LEU:HG	1:G:218:GLU:CG	2.52	0.40
1:N:212:ARG:N	1:N:212:ARG:HD2	2.36	0.40
1:A:136:LYS:NZ	1:A:153:GLN:HE22	2.18	0.40
1:A:252:LEU:HD22	1:A:279:LEU:HD22	2.03	0.40
1:D:177:HIS:ND1	1:D:241:THR:HB	2.36	0.40
1:D:190:PRO:HA	1:D:193:HIS:CE1	2.57	0.40
1:B:103:ASP:O	1:B:107:HIS:HB2	2.20	0.40
1:B:298:GLY:O	1:B:301:ALA:N	2.54	0.40
1:I:79:ALA:C	1:I:81:GLY:N	2.75	0.40
1:I:112:MSE:HA	1:I:112:MSE:HE2	2.03	0.40
1:T:113:LEU:HD11	1:T:140:VAL:HG22	2.02	0.40
1:T:189:GLU:HA	1:T:190:PRO:HD3	1.94	0.40
1:L:169:VAL:O	1:L:170:GLN:C	2.59	0.40
1:K:284:ARG:NH1	1:K:286:GLN:CG	2.85	0.40
1:W:275:ASP:HB3	1:W:277:THR:HG23	2.03	0.40
1:G:155:PRO:HA	1:G:317:SER:O	2.21	0.40
1:N:98:SER:C	1:N:100:GLN:N	2.75	0.40
1:N:108:LEU:O	1:N:111:ASN:HB3	2.21	0.40
1:N:281:THR:O	1:M:223:TYR:HE2	2.05	0.40
1:N:288:THR:HG23	1:N:330:SER:OG	2.22	0.40
1:M:182:PHE:CZ	1:M:184:SER:HB3	2.56	0.40
1:A:102:GLN:HE21	1:A:102:GLN:HB3	1.67	0.40
1:A:177:HIS:ND1	1:A:242:ALA:HB2	2.37	0.40
1:D:74:PHE:HE2	1:D:294:MSE:HE1	1.83	0.40
1:B:67:ILE:HD12	1:B:75:TYR:HB3	2.04	0.40
1:B:108:LEU:O	1:B:112:MSE:HB2	2.21	0.40
1:I:109:LEU:O	1:I:109:LEU:HG	2.20	0.40
1:T:98:SER:C	1:T:100:GLN:N	2.75	0.40
1:T:129:GLU:CA	1:T:132:VAL:HG22	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:77:GLU:CB	1:L:294:MSE:HE3	2.50	0.40
1:L:173:ILE:HD13	1:L:207:SER:OG	2.21	0.40
1:N:65:VAL:C	1:N:66:ILE:HG12	2.41	0.40
1:N:68:PRO:HG3	1:N:124:SER:HA	2.02	0.40

There are no symmetry-related clashes.

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	271/280 (97%)	217 (80%)	43 (16%)	11 (4%)	3 16
1	B	271/280 (97%)	218 (80%)	39 (14%)	14 (5%)	2 12
1	D	271/280 (97%)	224 (83%)	33 (12%)	14 (5%)	2 12
1	G	271/280 (97%)	199 (73%)	56 (21%)	16 (6%)	1 9
1	I	271/280 (97%)	226 (83%)	39 (14%)	6 (2%)	6 31
1	K	271/280 (97%)	233 (86%)	30 (11%)	8 (3%)	4 24
1	L	271/280 (97%)	212 (78%)	42 (16%)	17 (6%)	1 7
1	M	271/280 (97%)	222 (82%)	38 (14%)	11 (4%)	3 16
1	N	271/280 (97%)	204 (75%)	47 (17%)	20 (7%)	1 5
1	R	271/280 (97%)	209 (77%)	41 (15%)	21 (8%)	1 5
1	T	271/280 (97%)	231 (85%)	29 (11%)	11 (4%)	3 16
1	W	269/280 (96%)	219 (81%)	38 (14%)	12 (4%)	2 14
All	All	3250/3360 (97%)	2614 (80%)	475 (15%)	161 (5%)	2 12

All (161) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	GLY
1	D	102	GLN
1	B	275	ASP
1	R	275	ASP
1	R	313	THR
1	T	275	ASP
1	L	111	ASN
1	L	275	ASP
1	W	68	PRO
1	G	128	THR
1	G	139	PRO
1	G	275	ASP
1	N	66	ILE
1	N	103	ASP
1	N	136	LYS
1	N	178	LYS
1	M	100	GLN
1	M	150	SER
1	M	264	ASN
1	M	275	ASP
1	A	90	LYS
1	A	116	GLN
1	A	329	GLN
1	D	72	ASN
1	D	103	ASP
1	D	139	PRO
1	D	267	ASN
1	D	275	ASP
1	B	99	ASP
1	B	150	SER
1	B	255	ILE
1	B	267	ASN
1	B	293	PRO
1	B	294	MSE
1	I	275	ASP
1	R	100	GLN
1	R	116	GLN
1	R	136	LYS
1	R	150	SER
1	R	188	GLU
1	R	249	GLU
1	R	276	ASN
1	T	103	ASP

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Mol	Chain	Res	Type
1	T	152	ASN
1	T	223	TYR
1	T	330	SER
1	L	89	TYR
1	L	116	GLN
1	K	68	PRO
1	K	263	LEU
1	K	275	ASP
1	W	82	ILE
1	W	83	GLU
1	W	139	PRO
1	W	247	THR
1	W	262	GLY
1	W	280	SER
1	W	330	SER
1	G	150	SER
1	G	235	GLU
1	G	294	MSE
1	N	100	GLN
1	N	188	GLU
1	N	268	ASP
1	N	275	ASP
1	M	73	ILE
1	M	115	LYS
1	M	186	THR
1	M	237	ASP
1	A	72	ASN
1	D	70	ILE
1	D	73	ILE
1	D	177	HIS
1	D	293	PRO
1	B	68	PRO
1	B	142	VAL
1	I	187	LEU
1	R	164	ALA
1	R	311	LYS
1	T	276	ASN
1	L	88	MSE
1	L	100	GLN
1	L	115	LYS
1	K	191	ILE
1	W	275	ASP

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Mol	Chain	Res	Type
1	G	100	GLN
1	G	185	GLY
1	G	278	ARG
1	N	99	ASP
1	N	155	PRO
1	N	207	SER
1	N	277	THR
1	M	146	ALA
1	A	124	SER
1	A	275	ASP
1	A	293	PRO
1	D	311	LYS
1	B	100	GLN
1	B	277	THR
1	I	236	GLU
1	R	141	PRO
1	R	280	SER
1	T	116	GLN
1	L	162	GLU
1	L	280	SER
1	L	293	PRO
1	K	73	ILE
1	G	136	LYS
1	G	187	LEU
1	G	188	GLU
1	G	224	ASP
1	G	293	PRO
1	N	115	LYS
1	N	156	SER
1	N	193	HIS
1	D	155	PRO
1	D	156	SER
1	I	73	ILE
1	R	133	GLU
1	R	170	GLN
1	R	211	VAL
1	T	113	LEU
1	T	309	MSE
1	L	139	PRO
1	L	141	PRO
1	L	191	ILE
1	L	201	LYS

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Mol	Chain	Res	Type
1	L	209	LEU
1	K	190	PRO
1	K	293	PRO
1	W	202	ARG
1	W	293	PRO
1	G	306	THR
1	N	213	ASP
1	D	213	ASP
1	B	115	LYS
1	I	139	PRO
1	R	162	GLU
1	R	167	ASP
1	R	210	PRO
1	R	293	PRO
1	L	150	SER
1	K	208	GLY
1	G	213	ASP
1	A	73	ILE
1	A	216	ILE
1	R	68	PRO
1	T	139	PRO
1	W	73	ILE
1	N	240	PRO
1	M	217	VAL
1	A	240	PRO
1	T	293	PRO
1	N	191	ILE
1	N	257	GLY
1	N	293	PRO
1	M	297	ILE
1	I	293	PRO
1	L	142	VAL
1	B	139	PRO
1	B	155	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	239/236 (101%)	212 (89%)	27 (11%)	6	24
1	B	239/236 (101%)	206 (86%)	33 (14%)	3	17
1	D	239/236 (101%)	215 (90%)	24 (10%)	7	29
1	G	239/236 (101%)	209 (87%)	30 (13%)	4	20
1	I	239/236 (101%)	214 (90%)	25 (10%)	7	27
1	K	239/236 (101%)	214 (90%)	25 (10%)	7	27
1	L	239/236 (101%)	206 (86%)	33 (14%)	3	17
1	M	239/236 (101%)	213 (89%)	26 (11%)	6	25
1	N	239/236 (101%)	222 (93%)	17 (7%)	14	46
1	R	239/236 (101%)	207 (87%)	32 (13%)	4	17
1	T	239/236 (101%)	211 (88%)	28 (12%)	5	22
1	W	239/236 (101%)	208 (87%)	31 (13%)	4	19
All	All	2868/2832 (101%)	2537 (88%)	331 (12%)	5	24

All (331) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ILE
1	A	78	LEU
1	A	84	ASP
1	A	93	ILE
1	A	101	ASN
1	A	115	LYS
1	A	126	ASN
1	A	143	VAL
1	A	148	ILE
1	A	152	ASN
1	A	157	VAL
1	A	158	THR
1	A	178	LYS
1	A	179	ASN
1	A	186	THR
1	A	193	HIS
1	A	195	LYS
1	A	198	LYS
1	A	205	THR
1	A	223	TYR
1	A	236	GLU
1	A	274	PHE

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Mol	Chain	Res	Type
1	A	277	THR
1	A	283	VAL
1	A	284	ARG
1	A	325	ILE
1	A	329	GLN
1	D	65	VAL
1	D	73	ILE
1	D	84	ASP
1	D	103	ASP
1	D	106	LEU
1	D	139	PRO
1	D	148	ILE
1	D	149	GLU
1	D	152	ASN
1	D	153	GLN
1	D	169	VAL
1	D	180	ILE
1	D	184	SER
1	D	214	SER
1	D	232	LYS
1	D	237	ASP
1	D	239	LYS
1	D	247	THR
1	D	264	ASN
1	D	269	LEU
1	D	278	ARG
1	D	283	VAL
1	D	313	THR
1	D	331	THR
1	B	61	THR
1	B	62	THR
1	B	66	ILE
1	B	78	LEU
1	B	84	ASP
1	B	93	ILE
1	B	94	ILE
1	B	95	LEU
1	B	103	ASP
1	B	104	LYS
1	B	111	ASN
1	B	118	ASP
1	B	126	ASN

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Mol	Chain	Res	Type
1	B	129	GLU
1	B	142	VAL
1	B	148	ILE
1	B	151	THR
1	B	154	ILE
1	B	162	GLU
1	B	163	GLN
1	B	179	ASN
1	B	198	LYS
1	B	200	TYR
1	B	212	ARG
1	B	230	VAL
1	B	249	GLU
1	B	266	PRO
1	B	281	THR
1	B	284	ARG
1	B	287	LEU
1	B	307	LYS
1	B	329	GLN
1	B	331	THR
1	I	61	THR
1	I	62	THR
1	I	65	VAL
1	I	72	ASN
1	I	88	MSE
1	I	143	VAL
1	I	149	GLU
1	I	151	THR
1	I	157	VAL
1	I	169	VAL
1	I	193	HIS
1	I	204	LEU
1	I	205	THR
1	I	214	SER
1	I	217	VAL
1	I	224	ASP
1	I	227	ILE
1	I	228	GLU
1	I	230	VAL
1	I	237	ASP
1	I	238	GLU
1	I	266	PRO

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Mol	Chain	Res	Type
1	I	271	ILE
1	I	318	ILE
1	I	324	ARG
1	R	67	ILE
1	R	84	ASP
1	R	88	MSE
1	R	95	LEU
1	R	102	GLN
1	R	109	LEU
1	R	122	PHE
1	R	123	MSE
1	R	126	ASN
1	R	141	PRO
1	R	148	ILE
1	R	157	VAL
1	R	159	ILE
1	R	163	GLN
1	R	179	ASN
1	R	198	LYS
1	R	212	ARG
1	R	213	ASP
1	R	217	VAL
1	R	238	GLU
1	R	241	THR
1	R	247	THR
1	R	249	GLU
1	R	252	LEU
1	R	261	ARG
1	R	266	PRO
1	R	277	THR
1	R	284	ARG
1	R	303	ARG
1	R	315	ASP
1	R	320	GLN
1	R	329	GLN
1	T	61	THR
1	T	72	ASN
1	T	73	ILE
1	T	83	GLU
1	T	84	ASP
1	T	85	ILE
1	T	101	ASN

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Mol	Chain	Res	Type
1	T	122	PHE
1	T	123	MSE
1	T	129	GLU
1	T	136	LYS
1	T	149	GLU
1	T	151	THR
1	T	153	GLN
1	T	170	GLN
1	T	191	ILE
1	T	212	ARG
1	T	224	ASP
1	T	247	THR
1	T	263	LEU
1	T	266	PRO
1	T	269	LEU
1	T	271	ILE
1	T	279	LEU
1	T	283	VAL
1	T	315	ASP
1	T	318	ILE
1	T	320	GLN
1	L	60	THR
1	L	62	THR
1	L	70	ILE
1	L	80	ARG
1	L	83	GLU
1	L	87	THR
1	L	90	LYS
1	L	103	ASP
1	L	104	LYS
1	L	112	MSE
1	L	134	GLU
1	L	151	THR
1	L	163	GLN
1	L	186	THR
1	L	191	ILE
1	L	193	HIS
1	L	212	ARG
1	L	215	TYR
1	L	216	ILE
1	L	217	VAL
1	L	236	GLU

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Mol	Chain	Res	Type
1	L	238	GLU
1	L	245	VAL
1	L	261	ARG
1	L	266	PRO
1	L	277	THR
1	L	288	THR
1	L	292	GLN
1	L	294	MSE
1	L	313	THR
1	L	320	GLN
1	L	324	ARG
1	L	329	GLN
1	K	62	THR
1	K	65	VAL
1	K	67	ILE
1	K	70	ILE
1	K	72	ASN
1	K	94	ILE
1	K	97	ASN
1	K	99	ASP
1	K	100	GLN
1	K	116	GLN
1	K	132	VAL
1	K	135	LEU
1	K	148	ILE
1	K	230	VAL
1	K	236	GLU
1	K	247	THR
1	K	259	GLN
1	K	271	ILE
1	K	277	THR
1	K	280	SER
1	K	283	VAL
1	K	314	VAL
1	K	318	ILE
1	K	320	GLN
1	K	325	ILE
1	W	66	ILE
1	W	70	ILE
1	W	78	LEU
1	W	80	ARG
1	W	83	GLU

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Mol	Chain	Res	Type
1	W	84	ASP
1	W	87	THR
1	W	94	ILE
1	W	102	GLN
1	W	106	LEU
1	W	110	ASN
1	W	126	ASN
1	W	134	GLU
1	W	143	VAL
1	W	153	GLN
1	W	174	ASP
1	W	178	LYS
1	W	191	ILE
1	W	198	LYS
1	W	205	THR
1	W	212	ARG
1	W	215	TYR
1	W	216	ILE
1	W	238	GLU
1	W	241	THR
1	W	266	PRO
1	W	284	ARG
1	W	296	ASP
1	W	315	ASP
1	W	329	GLN
1	W	331	THR
1	G	62	THR
1	G	63	VAL
1	G	67	ILE
1	G	80	ARG
1	G	87	THR
1	G	103	ASP
1	G	118	ASP
1	G	120	ILE
1	G	123	MSE
1	G	126	ASN
1	G	134	GLU
1	G	144	LEU
1	G	148	ILE
1	G	149	GLU
1	G	151	THR
1	G	171	SER

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Mol	Chain	Res	Type
1	G	173	ILE
1	G	180	ILE
1	G	189	GLU
1	G	198	LYS
1	G	215	TYR
1	G	220	ASP
1	G	260	ASP
1	G	274	PHE
1	G	278	ARG
1	G	283	VAL
1	G	287	LEU
1	G	315	ASP
1	G	318	ILE
1	G	322	PRO
1	N	66	ILE
1	N	77	GLU
1	N	80	ARG
1	N	84	ASP
1	N	95	LEU
1	N	126	ASN
1	N	148	ILE
1	N	155	PRO
1	N	179	ASN
1	N	212	ARG
1	N	216	ILE
1	N	241	THR
1	N	264	ASN
1	N	268	ASP
1	N	284	ARG
1	N	292	GLN
1	N	320	GLN
1	M	65	VAL
1	M	67	ILE
1	M	70	ILE
1	M	72	ASN
1	M	77	GLU
1	M	83	GLU
1	M	101	ASN
1	M	118	ASP
1	M	128	THR
1	M	129	GLU
1	M	132	VAL

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Mol	Chain	Res	Type
1	M	136	LYS
1	M	143	VAL
1	M	148	ILE
1	M	151	THR
1	M	213	ASP
1	M	230	VAL
1	M	236	GLU
1	M	238	GLU
1	M	269	LEU
1	M	271	ILE
1	M	284	ARG
1	M	314	VAL
1	M	315	ASP
1	M	318	ILE
1	M	331	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	92	ASN
1	A	100	GLN
1	A	111	ASN
1	A	116	GLN
1	A	126	ASN
1	A	152	ASN
1	A	153	GLN
1	A	193	HIS
1	A	292	GLN
1	A	310	ASN
1	D	100	GLN
1	D	102	GLN
1	D	110	ASN
1	D	111	ASN
1	D	152	ASN
1	D	163	GLN
1	D	192	ASN
1	D	256	HIS
1	D	286	GLN
1	D	292	GLN
1	D	323	HIS
1	B	92	ASN

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Mol	Chain	Res	Type
1	B	97	ASN
1	B	100	GLN
1	B	126	ASN
1	B	152	ASN
1	B	153	GLN
1	B	256	HIS
1	B	329	GLN
1	I	72	ASN
1	I	92	ASN
1	I	100	GLN
1	I	110	ASN
1	I	111	ASN
1	I	152	ASN
1	I	153	GLN
1	I	179	ASN
1	I	192	ASN
1	I	193	HIS
1	I	286	GLN
1	I	292	GLN
1	R	97	ASN
1	R	102	GLN
1	R	116	GLN
1	R	126	ASN
1	R	163	GLN
1	R	179	ASN
1	R	192	ASN
1	R	292	GLN
1	T	72	ASN
1	T	101	ASN
1	T	163	GLN
1	T	192	ASN
1	T	193	HIS
1	T	256	HIS
1	T	276	ASN
1	T	286	GLN
1	T	292	GLN
1	T	320	GLN
1	L	92	ASN
1	L	97	ASN
1	L	101	ASN
1	L	153	GLN
1	L	163	GLN

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Mol	Chain	Res	Type
1	L	177	HIS
1	L	286	GLN
1	L	292	GLN
1	L	329	GLN
1	K	100	GLN
1	K	101	ASN
1	K	111	ASN
1	K	170	GLN
1	K	179	ASN
1	K	256	HIS
1	K	286	GLN
1	K	292	GLN
1	K	320	GLN
1	K	329	GLN
1	W	100	GLN
1	W	110	ASN
1	W	126	ASN
1	W	131	HIS
1	W	152	ASN
1	W	153	GLN
1	W	163	GLN
1	W	177	HIS
1	W	179	ASN
1	W	192	ASN
1	W	286	GLN
1	W	292	GLN
1	G	101	ASN
1	G	102	GLN
1	G	111	ASN
1	G	126	ASN
1	G	286	GLN
1	G	310	ASN
1	N	92	ASN
1	N	100	GLN
1	N	126	ASN
1	N	179	ASN
1	N	264	ASN
1	N	267	ASN
1	N	310	ASN
1	M	72	ASN
1	M	101	ASN
1	M	110	ASN

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Mol	Chain	Res	Type
1	M	111	ASN
1	M	126	ASN
1	M	179	ASN
1	M	192	ASN
1	M	256	HIS
1	M	267	ASN
1	M	286	GLN
1	M	292	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	98:SER	C	99:ASP	N	2.69

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	265/280 (94%)	-0.37	0	100	100	29, 57, 81, 98	0
1	B	265/280 (94%)	-0.53	0	100	100	22, 50, 73, 83	0
1	D	265/280 (94%)	-0.57	1 (0%)	92	79	17, 37, 93, 108	0
1	G	265/280 (94%)	-0.39	0	100	100	27, 57, 84, 91	0
1	I	265/280 (94%)	-0.58	0	100	100	13, 36, 89, 102	0
1	K	265/280 (94%)	-0.52	0	100	100	12, 42, 66, 83	0
1	L	265/280 (94%)	-0.51	0	100	100	22, 49, 74, 91	0
1	M	265/280 (94%)	-0.49	0	100	100	14, 49, 82, 94	0
1	N	265/280 (94%)	-0.26	0	100	100	33, 63, 103, 116	0
1	R	265/280 (94%)	-0.40	0	100	100	18, 50, 93, 100	0
1	T	265/280 (94%)	-0.49	1 (0%)	92	79	16, 37, 86, 112	0
1	W	265/280 (94%)	-0.43	1 (0%)	92	79	26, 49, 71, 85	0
All	All	3180/3360 (94%)	-0.46	3 (0%)	95	89	12, 49, 85, 116	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	100	GLN	3.4
1	D	99	ASP	3.2
1	T	113	LEU	2.2

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
2	MG	T	764	1/1	0.78	0.17	30,30,30,30	0
2	MG	T	754	1/1	0.90	0.40	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.