



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:51 PM UTC

PDB ID : 6GEB / pdb_00006geb
Title : X-ray structure of the Legionella pneumophila ATPase DotB
Authors : Prevost, M.S.; Waksman, G.
Deposited on : 2018-04-26
Resolution : 3.19 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

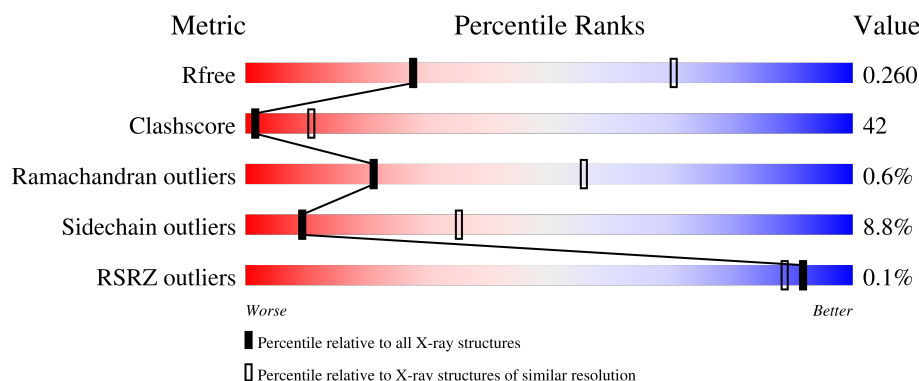
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 Å.

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



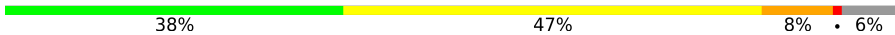
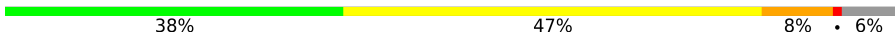
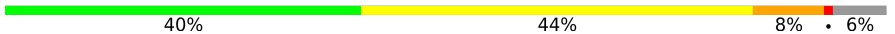
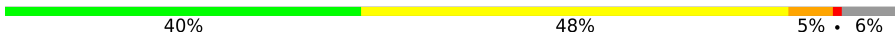
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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	391	
1	B	391	
1	C	391	
1	D	391	
1	E	391	

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Mol	Chain	Length	Quality of chain
1	F	391	
1	G	391	
1	H	391	
1	I	391	
1	J	391	
1	K	391	
1	L	391	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	J	401	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34658 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 DotB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2907	1826	512	558	11			
1	B	371	Total	C	N	O	S	0	0	0
			2906	1826	510	559	11			
1	C	369	Total	C	N	O	S	0	0	0
			2886	1814	503	558	11			
1	D	368	Total	C	N	O	S	0	0	0
			2874	1806	503	554	11			
1	E	367	Total	C	N	O	S	0	0	0
			2867	1805	498	553	11			
1	F	366	Total	C	N	O	S	0	0	0
			2859	1800	495	553	11			
1	G	369	Total	C	N	O	S	0	0	0
			2907	1826	512	558	11			
1	H	371	Total	C	N	O	S	0	0	0
			2906	1826	510	559	11			
1	I	369	Total	C	N	O	S	0	0	0
			2886	1814	503	558	11			
1	J	368	Total	C	N	O	S	0	0	0
			2874	1806	503	554	11			
1	K	367	Total	C	N	O	S	0	0	0
			2867	1805	498	553	11			
1	L	366	Total	C	N	O	S	0	0	0
			2859	1800	495	553	11			

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP O52185
A	-12	ALA	-	expression tag	UNP O52185
A	-11	SER	-	expression tag	UNP O52185
A	-10	TRP	-	expression tag	UNP O52185
A	-9	SER	-	expression tag	UNP O52185

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	expression tag	UNP O52185
A	-7	PRO	-	expression tag	UNP O52185
A	-6	GLN	-	expression tag	UNP O52185
A	-5	PHE	-	expression tag	UNP O52185
A	-4	GLU	-	expression tag	UNP O52185
A	-3	LYS	-	expression tag	UNP O52185
A	-2	ILE	-	expression tag	UNP O52185
A	-1	GLU	-	expression tag	UNP O52185
A	0	GLY	-	expression tag	UNP O52185
A	1	ARG	-	expression tag	UNP O52185
B	-13	MET	-	initiating methionine	UNP O52185
B	-12	ALA	-	expression tag	UNP O52185
B	-11	SER	-	expression tag	UNP O52185
B	-10	TRP	-	expression tag	UNP O52185
B	-9	SER	-	expression tag	UNP O52185
B	-8	HIS	-	expression tag	UNP O52185
B	-7	PRO	-	expression tag	UNP O52185
B	-6	GLN	-	expression tag	UNP O52185
B	-5	PHE	-	expression tag	UNP O52185
B	-4	GLU	-	expression tag	UNP O52185
B	-3	LYS	-	expression tag	UNP O52185
B	-2	ILE	-	expression tag	UNP O52185
B	-1	GLU	-	expression tag	UNP O52185
B	0	GLY	-	expression tag	UNP O52185
B	1	ARG	-	expression tag	UNP O52185
C	-13	MET	-	initiating methionine	UNP O52185
C	-12	ALA	-	expression tag	UNP O52185
C	-11	SER	-	expression tag	UNP O52185
C	-10	TRP	-	expression tag	UNP O52185
C	-9	SER	-	expression tag	UNP O52185
C	-8	HIS	-	expression tag	UNP O52185
C	-7	PRO	-	expression tag	UNP O52185
C	-6	GLN	-	expression tag	UNP O52185
C	-5	PHE	-	expression tag	UNP O52185
C	-4	GLU	-	expression tag	UNP O52185
C	-3	LYS	-	expression tag	UNP O52185
C	-2	ILE	-	expression tag	UNP O52185
C	-1	GLU	-	expression tag	UNP O52185
C	0	GLY	-	expression tag	UNP O52185
C	1	ARG	-	expression tag	UNP O52185
D	-13	MET	-	initiating methionine	UNP O52185
D	-12	ALA	-	expression tag	UNP O52185

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	SER	-	expression tag	UNP O52185
D	-10	TRP	-	expression tag	UNP O52185
D	-9	SER	-	expression tag	UNP O52185
D	-8	HIS	-	expression tag	UNP O52185
D	-7	PRO	-	expression tag	UNP O52185
D	-6	GLN	-	expression tag	UNP O52185
D	-5	PHE	-	expression tag	UNP O52185
D	-4	GLU	-	expression tag	UNP O52185
D	-3	LYS	-	expression tag	UNP O52185
D	-2	ILE	-	expression tag	UNP O52185
D	-1	GLU	-	expression tag	UNP O52185
D	0	GLY	-	expression tag	UNP O52185
D	1	ARG	-	expression tag	UNP O52185
E	-13	MET	-	initiating methionine	UNP O52185
E	-12	ALA	-	expression tag	UNP O52185
E	-11	SER	-	expression tag	UNP O52185
E	-10	TRP	-	expression tag	UNP O52185
E	-9	SER	-	expression tag	UNP O52185
E	-8	HIS	-	expression tag	UNP O52185
E	-7	PRO	-	expression tag	UNP O52185
E	-6	GLN	-	expression tag	UNP O52185
E	-5	PHE	-	expression tag	UNP O52185
E	-4	GLU	-	expression tag	UNP O52185
E	-3	LYS	-	expression tag	UNP O52185
E	-2	ILE	-	expression tag	UNP O52185
E	-1	GLU	-	expression tag	UNP O52185
E	0	GLY	-	expression tag	UNP O52185
E	1	ARG	-	expression tag	UNP O52185
F	-13	MET	-	initiating methionine	UNP O52185
F	-12	ALA	-	expression tag	UNP O52185
F	-11	SER	-	expression tag	UNP O52185
F	-10	TRP	-	expression tag	UNP O52185
F	-9	SER	-	expression tag	UNP O52185
F	-8	HIS	-	expression tag	UNP O52185
F	-7	PRO	-	expression tag	UNP O52185
F	-6	GLN	-	expression tag	UNP O52185
F	-5	PHE	-	expression tag	UNP O52185
F	-4	GLU	-	expression tag	UNP O52185
F	-3	LYS	-	expression tag	UNP O52185
F	-2	ILE	-	expression tag	UNP O52185
F	-1	GLU	-	expression tag	UNP O52185
F	0	GLY	-	expression tag	UNP O52185

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	ARG	-	expression tag	UNP O52185
G	-13	MET	-	initiating methionine	UNP O52185
G	-12	ALA	-	expression tag	UNP O52185
G	-11	SER	-	expression tag	UNP O52185
G	-10	TRP	-	expression tag	UNP O52185
G	-9	SER	-	expression tag	UNP O52185
G	-8	HIS	-	expression tag	UNP O52185
G	-7	PRO	-	expression tag	UNP O52185
G	-6	GLN	-	expression tag	UNP O52185
G	-5	PHE	-	expression tag	UNP O52185
G	-4	GLU	-	expression tag	UNP O52185
G	-3	LYS	-	expression tag	UNP O52185
G	-2	ILE	-	expression tag	UNP O52185
G	-1	GLU	-	expression tag	UNP O52185
G	0	GLY	-	expression tag	UNP O52185
G	1	ARG	-	expression tag	UNP O52185
H	-13	MET	-	initiating methionine	UNP O52185
H	-12	ALA	-	expression tag	UNP O52185
H	-11	SER	-	expression tag	UNP O52185
H	-10	TRP	-	expression tag	UNP O52185
H	-9	SER	-	expression tag	UNP O52185
H	-8	HIS	-	expression tag	UNP O52185
H	-7	PRO	-	expression tag	UNP O52185
H	-6	GLN	-	expression tag	UNP O52185
H	-5	PHE	-	expression tag	UNP O52185
H	-4	GLU	-	expression tag	UNP O52185
H	-3	LYS	-	expression tag	UNP O52185
H	-2	ILE	-	expression tag	UNP O52185
H	-1	GLU	-	expression tag	UNP O52185
H	0	GLY	-	expression tag	UNP O52185
H	1	ARG	-	expression tag	UNP O52185
I	-13	MET	-	initiating methionine	UNP O52185
I	-12	ALA	-	expression tag	UNP O52185
I	-11	SER	-	expression tag	UNP O52185
I	-10	TRP	-	expression tag	UNP O52185
I	-9	SER	-	expression tag	UNP O52185
I	-8	HIS	-	expression tag	UNP O52185
I	-7	PRO	-	expression tag	UNP O52185
I	-6	GLN	-	expression tag	UNP O52185
I	-5	PHE	-	expression tag	UNP O52185
I	-4	GLU	-	expression tag	UNP O52185
I	-3	LYS	-	expression tag	UNP O52185

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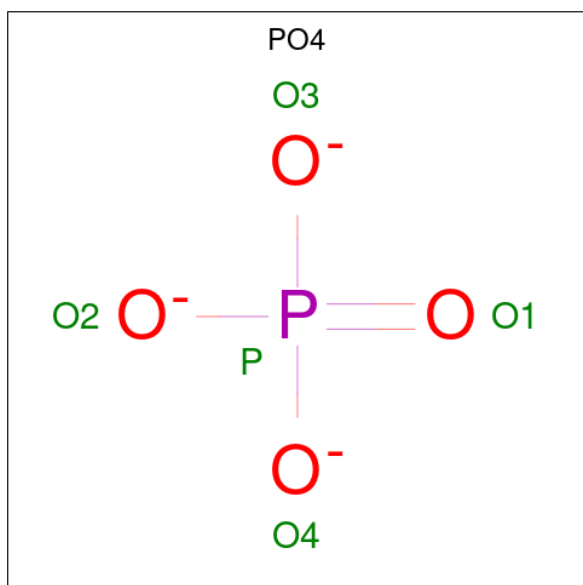
Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	ILE	-	expression tag	UNP O52185
I	-1	GLU	-	expression tag	UNP O52185
I	0	GLY	-	expression tag	UNP O52185
I	1	ARG	-	expression tag	UNP O52185
J	-13	MET	-	initiating methionine	UNP O52185
J	-12	ALA	-	expression tag	UNP O52185
J	-11	SER	-	expression tag	UNP O52185
J	-10	TRP	-	expression tag	UNP O52185
J	-9	SER	-	expression tag	UNP O52185
J	-8	HIS	-	expression tag	UNP O52185
J	-7	PRO	-	expression tag	UNP O52185
J	-6	GLN	-	expression tag	UNP O52185
J	-5	PHE	-	expression tag	UNP O52185
J	-4	GLU	-	expression tag	UNP O52185
J	-3	LYS	-	expression tag	UNP O52185
J	-2	ILE	-	expression tag	UNP O52185
J	-1	GLU	-	expression tag	UNP O52185
J	0	GLY	-	expression tag	UNP O52185
J	1	ARG	-	expression tag	UNP O52185
K	-13	MET	-	initiating methionine	UNP O52185
K	-12	ALA	-	expression tag	UNP O52185
K	-11	SER	-	expression tag	UNP O52185
K	-10	TRP	-	expression tag	UNP O52185
K	-9	SER	-	expression tag	UNP O52185
K	-8	HIS	-	expression tag	UNP O52185
K	-7	PRO	-	expression tag	UNP O52185
K	-6	GLN	-	expression tag	UNP O52185
K	-5	PHE	-	expression tag	UNP O52185
K	-4	GLU	-	expression tag	UNP O52185
K	-3	LYS	-	expression tag	UNP O52185
K	-2	ILE	-	expression tag	UNP O52185
K	-1	GLU	-	expression tag	UNP O52185
K	0	GLY	-	expression tag	UNP O52185
K	1	ARG	-	expression tag	UNP O52185
L	-13	MET	-	initiating methionine	UNP O52185
L	-12	ALA	-	expression tag	UNP O52185
L	-11	SER	-	expression tag	UNP O52185
L	-10	TRP	-	expression tag	UNP O52185
L	-9	SER	-	expression tag	UNP O52185
L	-8	HIS	-	expression tag	UNP O52185
L	-7	PRO	-	expression tag	UNP O52185
L	-6	GLN	-	expression tag	UNP O52185

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-5	PHE	-	expression tag	UNP O52185
L	-4	GLU	-	expression tag	UNP O52185
L	-3	LYS	-	expression tag	UNP O52185
L	-2	ILE	-	expression tag	UNP O52185
L	-1	GLU	-	expression tag	UNP O52185
L	0	GLY	-	expression tag	UNP O52185
L	1	ARG	-	expression tag	UNP O52185

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		

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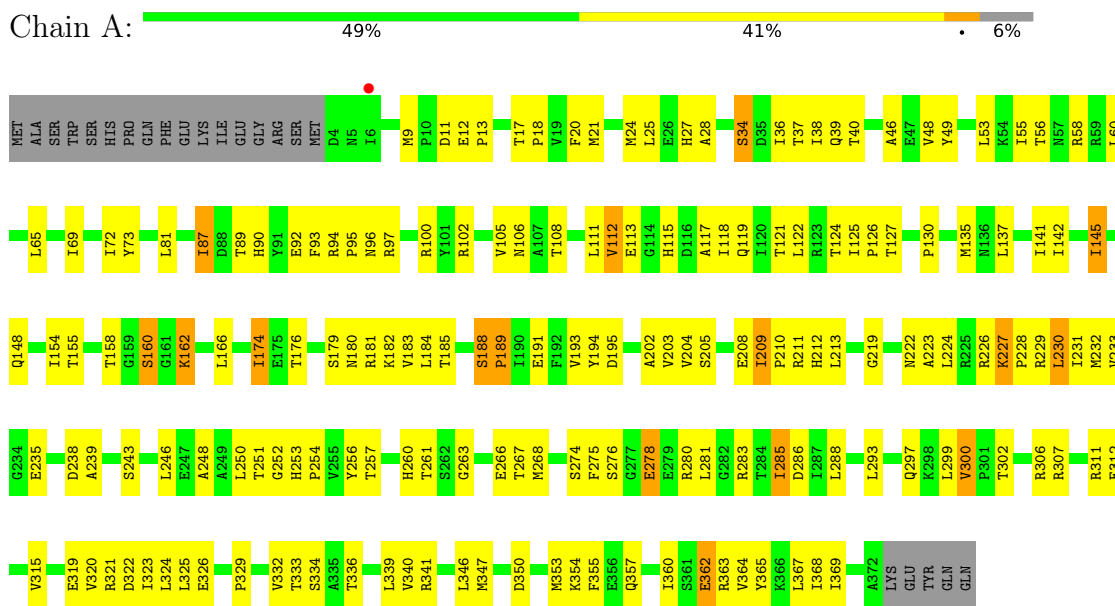
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		
2	K	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		

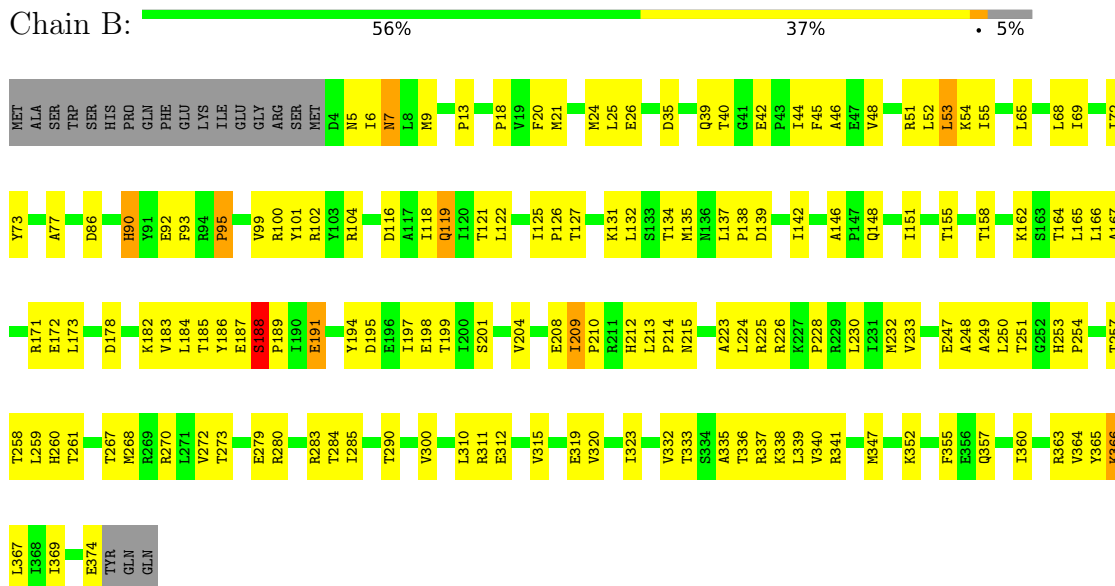
3 Residue-property plots

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

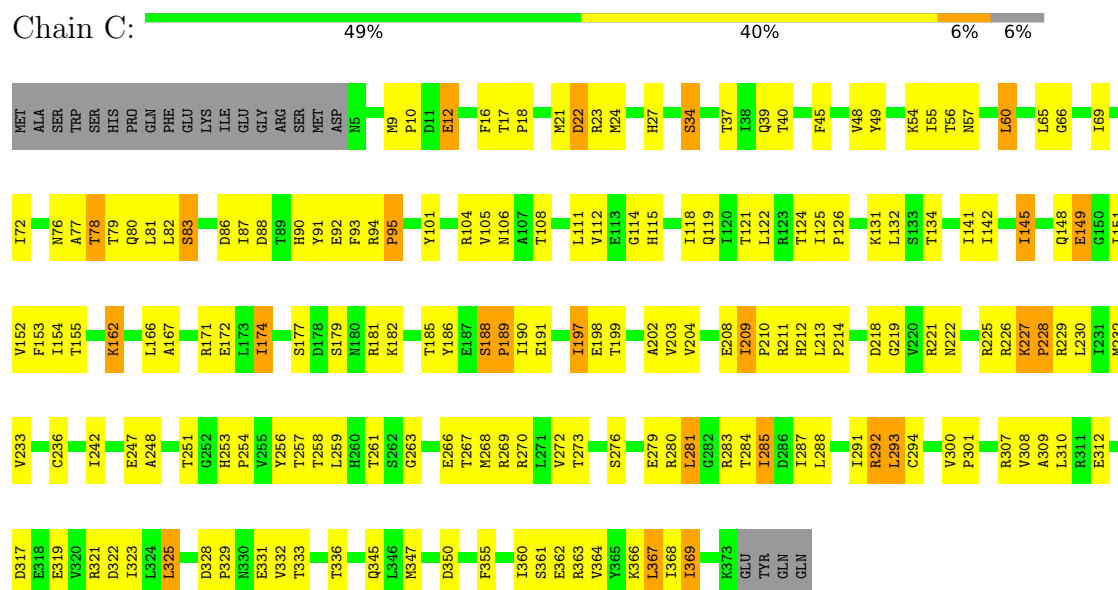
• Molecule 1: DotB



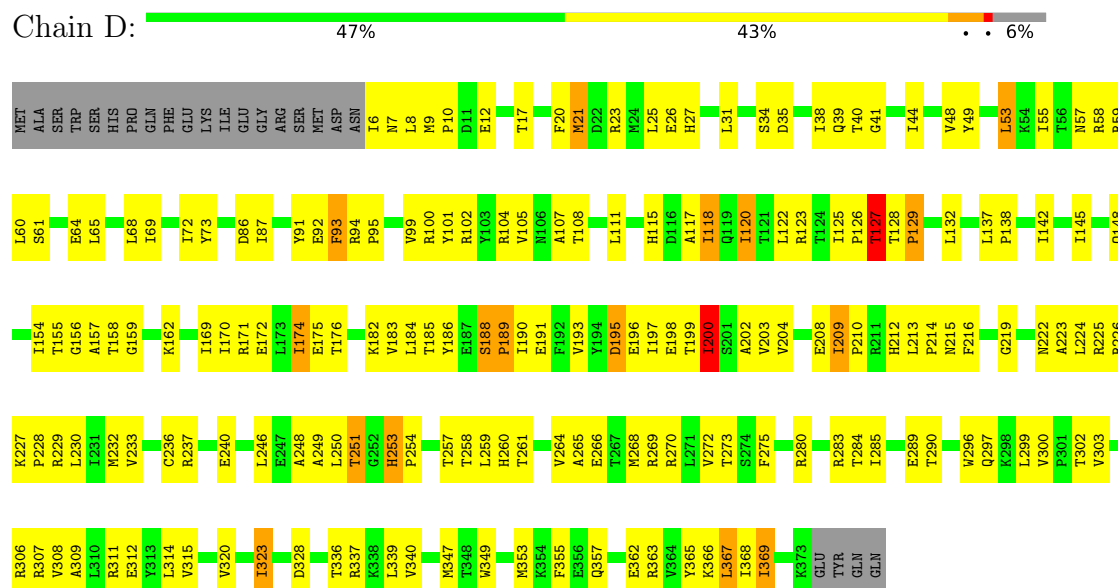
• Molecule 1: DotB



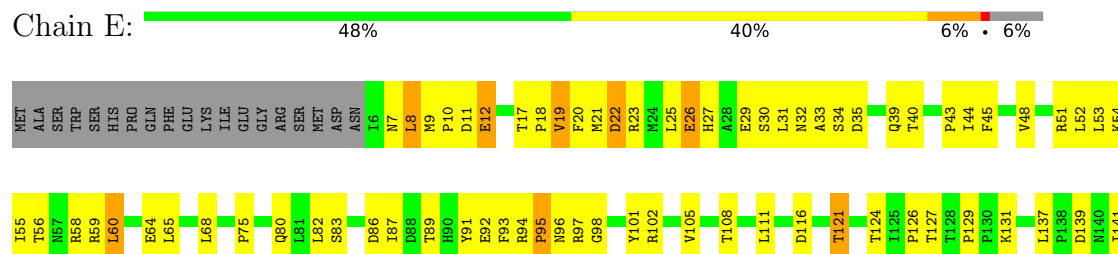
- Molecule 1: DotB

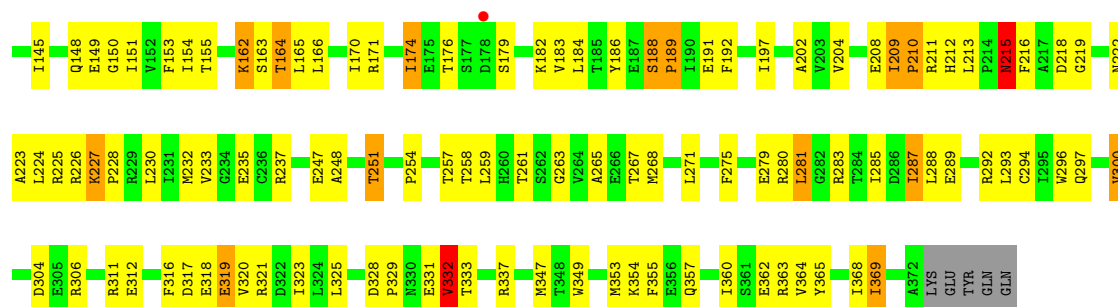


- Molecule 1: DotB



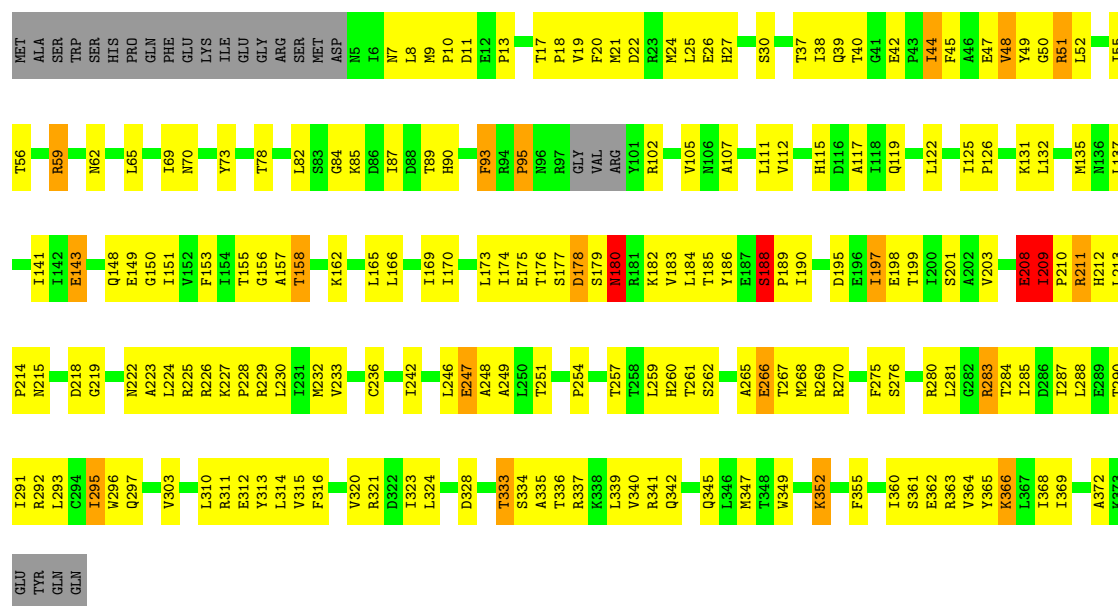
- Molecule 1: DotB





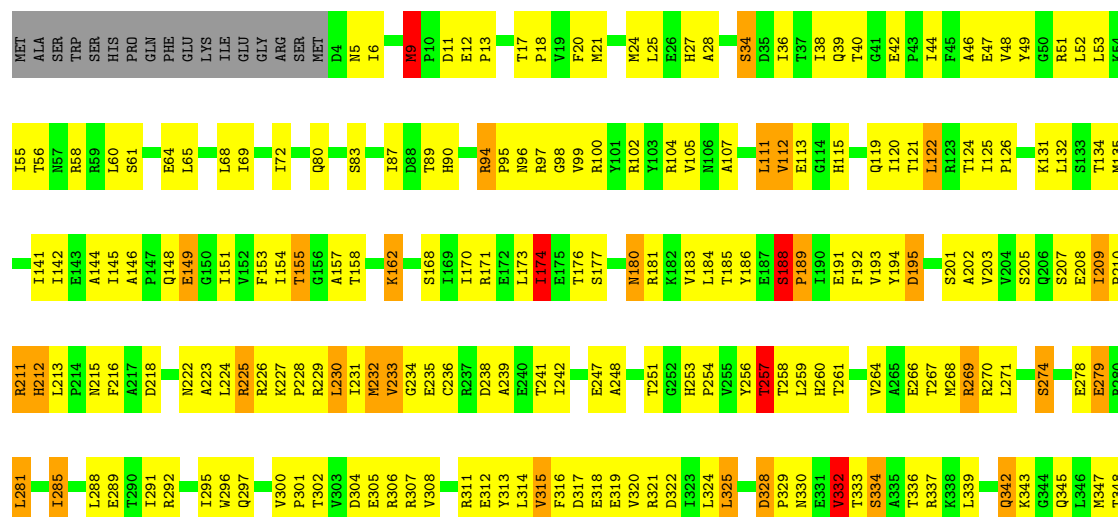
• Molecule 1: DotB

Chain F: 44% 44% 5% • 6%



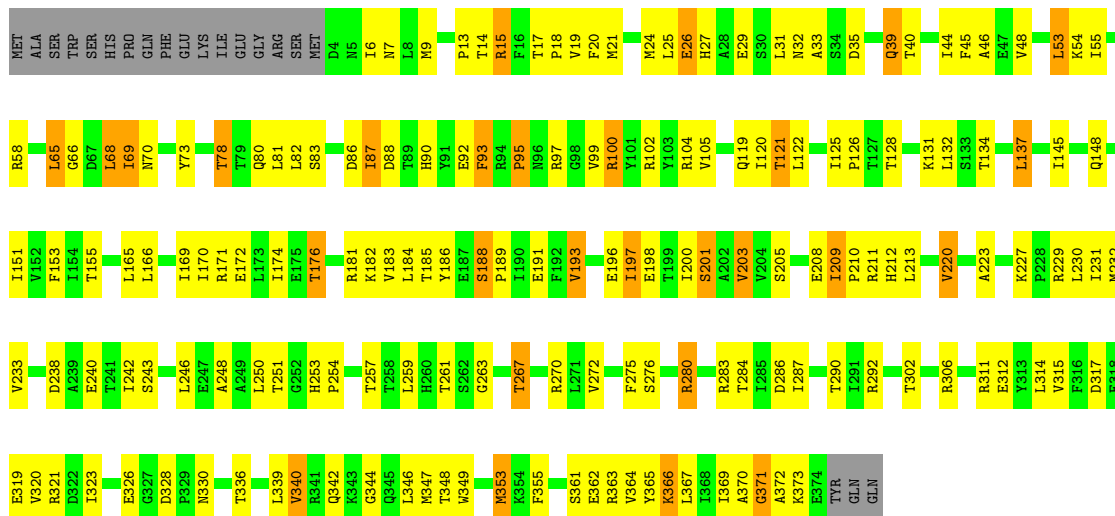
• Molecule 1: DotB

Chain G: 38% 46% 9% • 6%

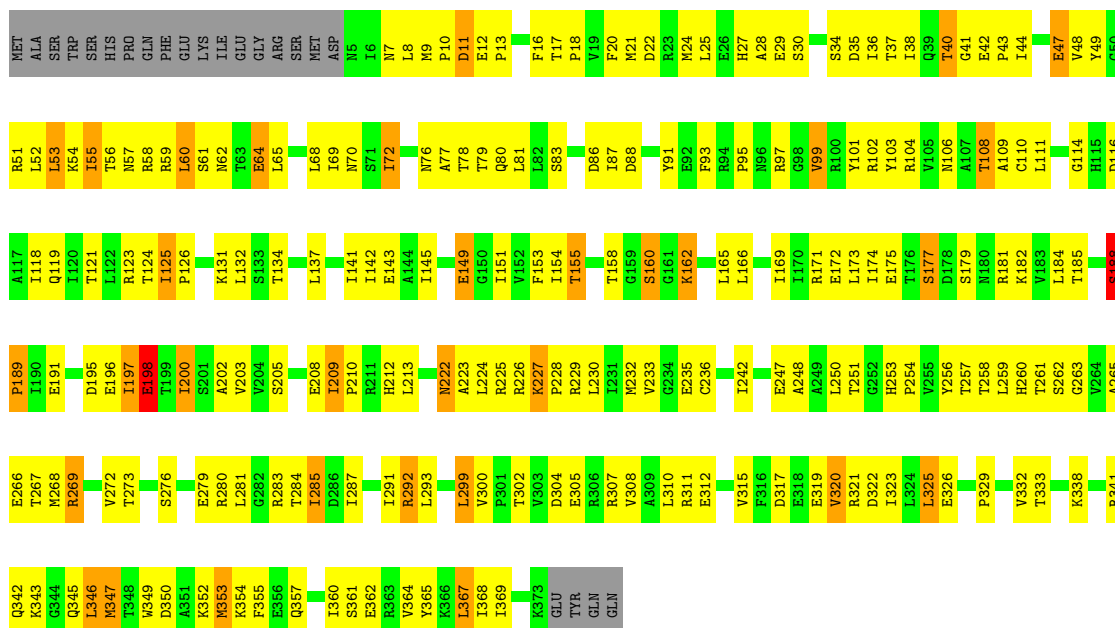




- Molecule 1: DotB

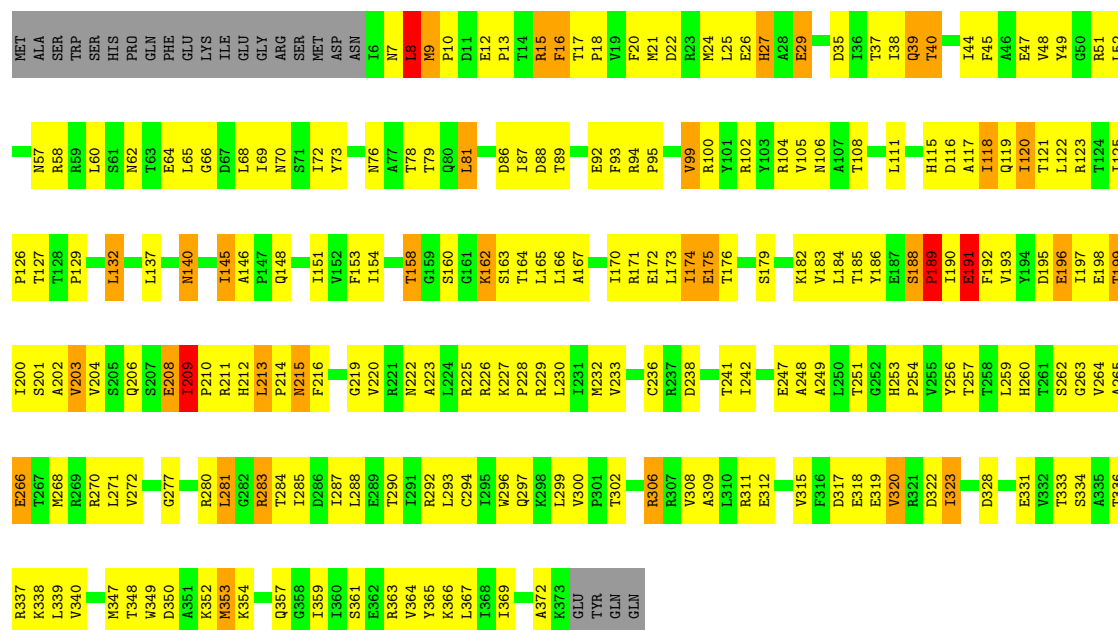


- Molecule 1: DotB



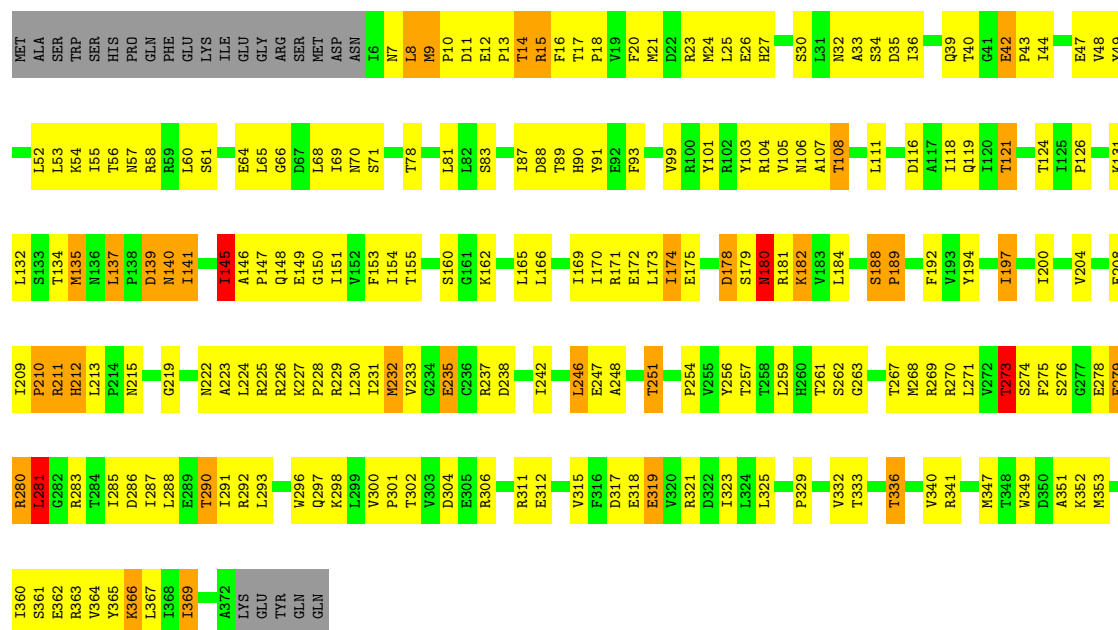
- Molecule 1: DotB





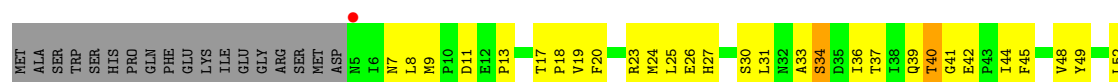
• Molecule 1: DotB

Chain K: 40% 44% 8% • 6%



• Molecule 1: DotB

Chain L: 40% 48% 5% • 6%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	109.20Å 109.30Å 119.80Å 83.70° 86.60° 60.70°	Depositor
Resolution (Å)	36.04 – 3.19 36.04 – 3.19	Depositor EDS
% Data completeness (in resolution range)	98.0 (36.04-3.19) 98.0 (36.04-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.233 , 0.261 0.234 , 0.260	Depositor DCC
R_{free} test set	3841 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	103.3	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.034 for h-k,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	34658	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.93	2/2954 (0.1%)	0.76	5/4009 (0.1%)
1	B	0.97	1/2953 (0.0%)	0.74	3/4009 (0.1%)
1	C	0.97	4/2933 (0.1%)	0.75	1/3984 (0.0%)
1	D	1.02	4/2920 (0.1%)	0.83	5/3965 (0.1%)
1	E	1.01	5/2914 (0.2%)	0.88	14/3958 (0.4%)
1	F	1.01	2/2904 (0.1%)	0.86	12/3943 (0.3%)
1	G	1.24	7/2954 (0.2%)	1.03	14/4009 (0.3%)
1	H	1.08	4/2953 (0.1%)	0.78	1/4009 (0.0%)
1	I	1.12	3/2933 (0.1%)	0.88	5/3984 (0.1%)
1	J	1.09	7/2920 (0.2%)	0.90	9/3965 (0.2%)
1	K	1.13	7/2914 (0.2%)	0.96	12/3958 (0.3%)
1	L	1.09	1/2904 (0.0%)	0.91	8/3943 (0.2%)
All	All	1.06	47/35156 (0.1%)	0.86	89/47736 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	K	0	1
1	L	0	1
All	All	0	3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	227	LYS	C-O	9.97	1.28	1.23
1	H	227	LYS	C-O	9.94	1.28	1.23
1	F	209	ILE	CA-CB	-8.79	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	369	ILE	N-CA	-8.15	1.36	1.46
1	C	190	ILE	C-O	-7.77	1.16	1.24
1	I	326	GLU	CA-C	7.47	1.62	1.52
1	H	227	LYS	CA-CB	7.26	1.57	1.52
1	K	281	LEU	C-O	-7.17	1.15	1.24
1	D	195	ASP	C-O	-7.11	1.15	1.24
1	E	281	LEU	C-O	-7.00	1.16	1.24
1	A	227	LYS	C-O	-6.95	1.20	1.23
1	J	188	SER	N-CA	-6.83	1.41	1.46
1	A	112	VAL	CA-C	-6.77	1.44	1.52
1	G	112	VAL	CA-C	-6.58	1.44	1.52
1	E	19	VAL	N-CA	-6.44	1.38	1.46
1	K	210	PRO	C-O	-6.42	1.16	1.24
1	B	357	GLN	C-O	-6.35	1.16	1.24
1	G	351	ALA	N-CA	-6.27	1.39	1.46
1	J	27	HIS	C-O	-6.17	1.17	1.24
1	C	225	ARG	C-O	-6.16	1.16	1.24
1	G	314	LEU	CA-C	-6.08	1.45	1.52
1	J	208	GLU	CA-C	-6.07	1.45	1.52
1	H	39	GLN	C-O	-6.06	1.16	1.23
1	G	359	ILE	N-CA	-6.05	1.38	1.46
1	J	191	GLU	C-O	-5.96	1.17	1.24
1	K	273	THR	C-O	-5.96	1.16	1.24
1	G	11	ASP	C-O	-5.84	1.15	1.23
1	I	304	ASP	C-O	-5.83	1.16	1.24
1	E	139	ASP	C-O	-5.80	1.16	1.24
1	D	250	LEU	C-O	-5.70	1.17	1.24
1	K	11	ASP	CA-C	-5.69	1.47	1.53
1	I	227	LYS	C-O	-5.68	1.21	1.23
1	K	179	SER	C-O	-5.67	1.16	1.23
1	F	48	VAL	CA-CB	-5.63	1.47	1.54
1	E	227	LYS	CA-C	5.55	1.57	1.53
1	D	57	ASN	C-O	5.47	1.30	1.24
1	J	9	MET	CA-C	-5.45	1.46	1.53
1	L	201	SER	C-O	-5.44	1.16	1.24
1	K	14	THR	C-O	-5.42	1.17	1.24
1	C	83	SER	C-O	-5.36	1.17	1.24
1	J	209	ILE	C-N	5.29	1.40	1.34
1	E	210	PRO	C-O	-5.29	1.17	1.24
1	G	257	THR	CB-OG1	-5.24	1.35	1.43
1	H	220	VAL	C-O	-5.21	1.18	1.24
1	J	16	PHE	C-O	-5.21	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	179	SER	CA-C	-5.03	1.46	1.52
1	D	154	ILE	C-O	-5.00	1.18	1.24

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	211	ARG	N-CA-C	11.65	126.02	111.69
1	K	211	ARG	N-CA-C	11.04	125.27	111.69
1	F	209	ILE	O-C-N	9.01	126.19	120.42
1	B	187	GLU	N-CA-C	8.97	124.28	113.16
1	L	188	SER	N-CA-C	-8.86	100.58	112.55
1	D	129	PRO	O-C-N	8.60	125.19	121.15
1	L	209	ILE	O-C-N	8.36	126.00	120.07
1	E	209	ILE	CA-C-N	-8.35	109.75	118.85
1	E	209	ILE	C-N-CA	-8.35	109.75	118.85
1	K	145	ILE	N-CA-C	8.27	121.42	111.09
1	G	188	SER	N-CA-C	-8.25	101.41	112.55
1	E	188	SER	N-CA-C	-8.24	101.43	112.55
1	F	188	SER	N-CA-C	-7.92	101.86	112.55
1	J	213	LEU	N-CA-C	7.80	120.71	108.55
1	A	188	SER	N-CA-C	-7.76	102.08	112.55
1	I	188	SER	N-CA-C	-7.40	102.56	112.55
1	J	209	ILE	CA-C-N	-7.32	110.87	118.85
1	J	209	ILE	C-N-CA	-7.32	110.87	118.85
1	G	234	GLY	N-CA-C	-7.26	101.41	112.51
1	K	209	ILE	CA-C-N	-7.18	111.02	118.85
1	K	209	ILE	C-N-CA	-7.18	111.02	118.85
1	L	209	ILE	CA-C-N	-6.93	111.17	119.84
1	L	209	ILE	C-N-CA	-6.93	111.17	119.84
1	C	227	LYS	O-C-N	6.89	124.70	121.53
1	E	332	VAL	N-CA-C	6.88	123.64	109.34
1	K	146	ALA	CA-C-N	-6.83	112.95	119.85
1	K	146	ALA	C-N-CA	-6.83	112.95	119.85
1	I	188	SER	O-C-N	6.83	125.77	120.38
1	D	188	SER	N-CA-C	-6.76	103.42	112.55
1	I	188	SER	CA-C-N	-6.74	111.42	119.84
1	I	188	SER	C-N-CA	-6.74	111.42	119.84
1	G	212	HIS	N-CA-C	6.60	118.56	111.36
1	J	175	GLU	N-CA-C	6.52	118.38	111.28
1	F	211	ARG	NE-CZ-NH2	6.44	125.00	119.20
1	D	200	ILE	N-CA-C	6.42	117.20	110.72
1	F	188	SER	O-C-N	6.36	125.41	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	182	LYS	N-CA-C	-6.24	97.53	108.20
1	F	188	SER	CA-C-N	-6.19	112.10	119.84
1	F	188	SER	C-N-CA	-6.19	112.10	119.84
1	G	332	VAL	N-CA-C	6.16	122.16	109.34
1	G	332	VAL	CB-CA-C	-6.10	101.29	111.29
1	L	211	ARG	N-CA-C	6.09	117.99	111.36
1	F	209	ILE	CA-C-N	-6.08	112.23	118.85
1	F	209	ILE	C-N-CA	-6.08	112.23	118.85
1	L	95	PRO	N-CA-CB	6.05	109.26	102.67
1	K	212	HIS	N-CA-C	6.03	120.76	113.41
1	G	188	SER	O-C-N	6.00	125.12	120.38
1	F	95	PRO	N-CA-CB	6.00	109.55	103.25
1	J	188	SER	N-CA-C	-5.94	104.54	112.55
1	G	355	PHE	N-CA-C	5.79	117.27	111.07
1	G	211	ARG	N-CA-C	5.76	120.81	113.55
1	J	16	PHE	N-CA-C	5.71	118.52	109.96
1	A	11	ASP	N-CA-C	5.69	119.09	111.24
1	D	127	THR	N-CA-C	5.67	118.40	111.82
1	F	209	ILE	CA-C-O	-5.65	114.90	118.69
1	F	208	GLU	N-CA-C	-5.56	101.62	109.96
1	E	188	SER	CA-C-N	-5.53	112.93	119.84
1	E	188	SER	C-N-CA	-5.53	112.93	119.84
1	K	180	ASN	N-CA-C	-5.53	101.33	109.62
1	E	188	SER	O-C-N	5.50	124.73	120.38
1	I	198	GLU	N-CA-C	-5.50	101.02	109.76
1	K	42	GLU	CA-C-N	-5.44	115.13	120.52
1	K	42	GLU	C-N-CA	-5.44	115.13	120.52
1	G	174	ILE	N-CA-C	5.44	116.93	111.00
1	J	189	PRO	CA-N-CD	-5.43	104.40	112.00
1	J	8	LEU	N-CA-C	5.43	117.64	109.23
1	E	209	ILE	N-CA-C	5.31	120.35	108.88
1	E	12	GLU	CA-C-N	-5.29	115.28	120.52
1	E	12	GLU	C-N-CA	-5.29	115.28	120.52
1	D	323	ILE	CB-CG1-CD1	5.28	124.89	113.80
1	L	188	SER	O-C-N	5.27	124.54	120.38
1	B	188	SER	CA-C-N	-5.27	114.37	119.90
1	B	188	SER	C-N-CA	-5.27	114.37	119.90
1	F	51	ARG	N-CA-C	5.21	117.85	110.50
1	E	215	ASN	N-CA-C	5.21	115.41	108.38
1	A	188	SER	CA-C-N	-5.19	113.35	119.84
1	A	188	SER	C-N-CA	-5.19	113.35	119.84
1	L	209	ILE	N-CA-C	5.18	120.12	112.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	332	VAL	CB-CA-C	-5.18	102.80	111.29
1	H	280	ARG	N-CA-C	5.17	117.32	111.11
1	A	286	ASP	N-CA-C	-5.17	105.54	111.07
1	G	9	MET	CA-C-N	-5.15	114.43	119.99
1	G	9	MET	C-N-CA	-5.15	114.43	119.99
1	E	26	GLU	N-CA-C	-5.09	105.73	111.28
1	J	208	GLU	N-CA-C	-5.07	100.89	108.96
1	G	325	LEU	N-CA-C	5.05	116.47	111.07
1	G	368	ILE	CB-CA-C	-5.04	105.34	112.14
1	G	209	ILE	N-CA-C	5.02	119.73	108.88
1	K	280	ARG	N-CA-C	5.02	121.49	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	180	ASN	Mainchain
1	K	246	LEU	Mainchain
1	L	372	ALA	Peptide

5.2 Too-close contacts

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	2907	0	2949	215	0
1	B	2906	0	2929	204	0
1	C	2886	0	2907	204	1
1	D	2874	0	2901	198	0
1	E	2867	0	2891	218	0
1	F	2859	0	2876	248	1
1	G	2907	0	2949	370	0
1	H	2906	0	2929	235	0
1	I	2886	0	2907	340	0
1	J	2874	0	2901	349	0
1	K	2867	0	2891	278	0
1	L	2859	0	2876	255	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	2	0
2	K	5	0	0	1	0
2	L	5	0	0	0	0
All	All	34658	0	34906	2932	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (2932) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:9:MET:CE	1:J:24:MET:HA	1.29	1.53
1:G:291:ILE:HD13	1:G:316:PHE:CE2	1.64	1.31
1:G:355:PHE:CZ	1:G:365:TYR:CD2	2.23	1.25
1:J:9:MET:CE	1:J:24:MET:CA	2.13	1.25
1:D:236:CYS:SG	1:D:259:LEU:HD21	1.79	1.23
1:E:29:GLU:HG2	1:E:101:TYR:CE2	1.74	1.22
1:G:355:PHE:CZ	1:G:365:TYR:HD2	1.55	1.22
1:K:40:THR:HG22	1:K:65:LEU:HD22	1.22	1.21
1:J:280:ARG:O	1:J:284:THR:HG23	1.40	1.20
1:L:215:ASN:OD1	1:L:218:ASP:HB2	1.40	1.20
1:C:280:ARG:O	1:C:284:THR:HG23	1.39	1.19
1:L:112:VAL:HG23	1:L:117:ALA:CB	1.73	1.17
1:I:280:ARG:O	1:I:284:THR:HG23	1.42	1.17
1:G:291:ILE:CG2	1:G:316:PHE:HD2	1.57	1.16
1:I:355:PHE:CE2	1:I:362:GLU:HA	1.80	1.15
1:D:8:LEU:HD13	1:D:9:MET:N	1.60	1.15
1:I:24:MET:HE2	1:I:44:ILE:CD1	1.76	1.15
1:K:16:PHE:HZ	1:K:24:MET:HE3	1.13	1.13
1:J:9:MET:HE1	1:J:24:MET:CA	1.75	1.13
1:D:261:THR:HG21	1:D:270:ARG:HG3	1.17	1.12
1:K:363:ARG:HA	1:K:366:LYS:CD	1.78	1.12
1:I:261:THR:HG23	1:I:267:THR:HG22	1.21	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:MET:CE	1:I:44:ILE:HD13	1.77	1.12
1:B:93:PHE:CZ	1:B:101:TYR:HD2	1.68	1.11
1:F:190:ILE:HG12	1:F:208:GLU:HG3	1.25	1.11
1:J:121:THR:HG21	1:K:182:LYS:HZ3	1.06	1.11
1:D:280:ARG:O	1:D:284:THR:HG23	1.46	1.11
1:G:363:ARG:HA	1:G:366:LYS:HD2	1.17	1.11
1:I:104:ARG:CG	1:I:125:ILE:HD11	1.80	1.11
1:H:48:VAL:HG21	1:H:53:LEU:HD11	1.32	1.11
1:E:162:LYS:HD3	1:E:258:THR:HB	1.32	1.10
1:G:356:GLU:N	1:G:356:GLU:OE2	1.83	1.10
1:L:112:VAL:HG23	1:L:117:ALA:HB2	1.33	1.10
1:B:280:ARG:O	1:B:284:THR:HG23	1.50	1.10
1:I:24:MET:HE2	1:I:44:ILE:HD13	1.14	1.10
1:G:291:ILE:HG12	1:G:316:PHE:CD2	1.87	1.09
1:I:108:THR:HG21	1:J:222:ASN:HD21	1.08	1.09
1:I:40:THR:HG22	1:I:65:LEU:HD12	1.21	1.09
1:J:15:ARG:HG2	1:J:64:GLU:OE2	1.53	1.09
1:F:48:VAL:HG12	1:F:49:TYR:HD2	1.17	1.09
1:D:102:ARG:HH21	1:D:127:THR:HG22	1.12	1.08
1:D:175:GLU:HA	1:D:199:THR:HG22	1.31	1.08
1:F:174:ILE:HG22	1:F:199:THR:HG21	1.34	1.08
1:K:353:MET:HA	1:K:353:MET:HE3	1.35	1.08
1:K:135:MET:HE3	1:K:135:MET:HA	1.34	1.08
1:C:104:ARG:HG3	1:C:125:ILE:HD11	1.33	1.07
1:J:60:LEU:HD13	1:J:64:GLU:OE1	1.55	1.07
1:H:365:TYR:CZ	1:H:369:ILE:HD11	1.90	1.07
1:I:321:ARG:O	1:I:325:LEU:HD12	1.55	1.07
1:J:174:ILE:HG12	1:J:199:THR:HG21	1.37	1.06
1:G:180:ASN:HB3	1:L:52:LEU:HB2	1.38	1.06
1:I:104:ARG:CG	1:I:125:ILE:CD1	2.34	1.06
1:J:9:MET:HE1	1:J:24:MET:CB	1.86	1.05
1:G:291:ILE:CD1	1:G:316:PHE:CE2	2.38	1.05
1:E:40:THR:HG22	1:E:65:LEU:HD22	1.36	1.05
1:I:261:THR:CG2	1:I:267:THR:HG22	1.86	1.04
1:K:288:LEU:HD13	1:K:325:LEU:HD23	1.39	1.04
1:A:355:PHE:HA	1:A:360:ILE:HG22	1.31	1.04
1:E:108:THR:HG21	1:F:226:ARG:NH2	1.72	1.04
1:G:119:GLN:HE22	1:H:182:LYS:NZ	1.56	1.04
1:C:321:ARG:O	1:C:325:LEU:HD12	1.57	1.03
1:E:21:MET:HE2	1:E:68:LEU:HG	1.40	1.03
1:I:104:ARG:HG2	1:I:125:ILE:HD11	1.32	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:261:THR:HG21	1:I:267:THR:HA	1.39	1.03
1:K:363:ARG:HA	1:K:366:LYS:HD3	1.03	1.03
1:B:155:THR:HG22	1:B:259:LEU:HB2	1.39	1.03
1:I:104:ARG:HG2	1:I:125:ILE:CD1	1.89	1.03
1:J:9:MET:HE1	1:J:24:MET:HA	1.33	1.03
1:J:353:MET:O	1:J:357:GLN:HG2	1.59	1.03
1:K:24:MET:HE1	1:K:44:ILE:HD12	1.35	1.03
1:L:9:MET:SD	1:L:56:THR:HG22	1.97	1.03
1:F:73:TYR:CD1	1:F:89:THR:HG21	1.93	1.03
1:F:9:MET:HG2	1:F:10:PRO:HD2	1.39	1.02
1:G:269:ARG:HG2	1:G:269:ARG:HH11	1.18	1.02
1:F:40:THR:HG23	1:F:65:LEU:HD22	1.40	1.02
1:G:355:PHE:CE2	1:G:365:TYR:CD2	2.48	1.02
1:E:261:THR:OG1	1:E:267:THR:HG22	1.59	1.02
1:F:125:ILE:HD12	1:F:126:PRO:HD2	1.42	1.02
1:F:155:THR:HG22	1:F:259:LEU:HB2	1.39	1.02
1:I:355:PHE:HE2	1:I:362:GLU:CA	1.70	1.02
1:I:355:PHE:HE2	1:I:362:GLU:HA	0.90	1.02
1:C:104:ARG:CG	1:C:125:ILE:HD11	1.89	1.01
1:J:9:MET:HE3	1:J:24:MET:CA	1.82	1.01
1:J:121:THR:HG21	1:K:182:LYS:NZ	1.74	1.01
1:C:79:THR:HA	1:C:82:LEU:HD12	1.04	1.01
1:K:261:THR:OG1	1:K:267:THR:HG22	1.60	1.00
1:D:261:THR:CG2	1:D:270:ARG:HG3	1.91	1.00
1:K:16:PHE:CZ	1:K:24:MET:HE3	1.96	1.00
1:G:291:ILE:CG2	1:G:316:PHE:CD2	2.44	1.00
1:B:212:HIS:O	1:B:213:LEU:HD12	1.62	1.00
1:G:21:MET:HE1	1:G:72:ILE:HD11	1.43	1.00
1:A:261:THR:HB	1:A:267:THR:HG22	1.44	0.99
1:J:365:TYR:CE2	1:J:369:ILE:HD11	1.96	0.99
1:F:48:VAL:HG12	1:F:49:TYR:CD2	1.97	0.99
1:C:79:THR:CA	1:C:82:LEU:HD12	1.91	0.99
1:F:24:MET:SD	1:F:44:ILE:HD12	2.03	0.99
1:K:170:ILE:O	1:K:174:ILE:HG22	1.61	0.98
1:L:24:MET:SD	1:L:44:ILE:HD13	2.02	0.98
1:L:183:VAL:HG13	1:L:230:LEU:HD22	1.45	0.98
1:D:40:THR:HG22	1:D:65:LEU:HD22	1.42	0.98
1:J:196:GLU:N	1:J:196:GLU:OE1	1.97	0.98
1:H:188:SER:OG	1:H:189:PRO:HD3	1.62	0.98
1:J:15:ARG:HA	1:J:58:ARG:NH1	1.78	0.98
1:A:285:ILE:H	1:A:285:ILE:HD12	1.25	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:MET:HE1	1:C:72:ILE:HD11	1.43	0.97
1:H:212:HIS:O	1:H:213:LEU:HD12	1.63	0.97
1:B:365:TYR:CZ	1:B:369:ILE:HD11	2.00	0.97
1:E:40:THR:CG2	1:E:65:LEU:HD22	1.94	0.97
1:E:164:THR:HG22	1:E:192:PHE:HZ	1.26	0.97
1:G:291:ILE:HG23	1:G:316:PHE:HD2	1.30	0.97
1:C:40:THR:HG22	1:C:65:LEU:HD22	1.47	0.97
1:F:13:PRO:HG3	1:F:20:PHE:CD2	2.00	0.97
1:J:272:VAL:HG13	1:J:284:THR:HG22	1.46	0.97
1:K:108:THR:HG21	1:L:222:ASN:HD21	1.27	0.97
1:L:233:VAL:HB	1:L:257:THR:HG22	1.47	0.96
1:G:239:ALA:HA	1:G:242:ILE:HD12	1.47	0.96
1:E:164:THR:HG22	1:E:192:PHE:CZ	2.00	0.96
1:I:13:PRO:HB3	1:I:20:PHE:CE2	1.99	0.96
1:I:272:VAL:HG13	1:I:284:THR:HG22	1.46	0.96
1:D:264:VAL:HG11	1:D:340:VAL:HG11	1.44	0.96
1:J:174:ILE:HG12	1:J:199:THR:CG2	1.94	0.96
1:I:355:PHE:CZ	1:I:362:GLU:HG2	2.00	0.96
1:L:112:VAL:CG2	1:L:117:ALA:CB	2.43	0.96
1:H:14:THR:O	1:H:15:ARG:NE	1.97	0.95
1:J:352:LYS:HG3	1:J:365:TYR:OH	1.65	0.95
1:D:40:THR:CG2	1:D:65:LEU:HD22	1.96	0.95
1:H:125:ILE:HD12	1:H:126:PRO:HD2	1.47	0.95
1:K:40:THR:CG2	1:K:65:LEU:HD22	1.95	0.95
1:E:353:MET:HA	1:E:353:MET:HE3	1.46	0.95
1:G:40:THR:HG22	1:G:65:LEU:HD22	1.45	0.95
1:F:233:VAL:HB	1:F:257:THR:HG22	1.49	0.95
1:G:363:ARG:CA	1:G:366:LYS:HD2	1.97	0.95
1:L:125:ILE:HD12	1:L:126:PRO:HD2	1.47	0.95
1:H:233:VAL:HB	1:H:257:THR:HG22	1.48	0.94
1:J:24:MET:HE1	1:J:25:LEU:HD23	1.48	0.94
1:I:233:VAL:HB	1:I:257:THR:HG22	1.49	0.94
1:J:60:LEU:CD1	1:J:64:GLU:OE1	2.14	0.94
1:G:119:GLN:HE22	1:H:182:LYS:HZ1	1.06	0.94
1:G:363:ARG:HA	1:G:366:LYS:CD	1.98	0.94
1:I:154:ILE:CG2	1:I:162:LYS:HB3	1.96	0.94
1:B:21:MET:HE1	1:B:72:ILE:HD11	1.45	0.94
1:C:154:ILE:CG2	1:C:162:LYS:HB3	1.97	0.94
1:G:216:PHE:HD2	1:G:233:VAL:HG12	1.30	0.94
1:I:25:LEU:HD13	1:I:103:TYR:CE2	2.02	0.94
1:J:121:THR:CG2	1:K:182:LYS:HZ3	1.80	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:233:VAL:HB	1:J:257:THR:HG22	1.46	0.94
1:K:135:MET:HA	1:K:135:MET:CE	1.96	0.94
1:G:365:TYR:HA	1:G:368:ILE:HD12	1.49	0.94
1:B:233:VAL:HB	1:B:257:THR:HG22	1.47	0.94
1:D:233:VAL:HB	1:D:257:THR:HG22	1.48	0.94
1:C:233:VAL:HB	1:C:257:THR:HG22	1.50	0.94
1:J:9:MET:HA	1:J:27:HIS:CD2	2.03	0.94
1:F:335:ALA:O	1:F:339:LEU:HD23	1.68	0.93
1:D:8:LEU:HD13	1:D:9:MET:H	1.18	0.93
1:J:9:MET:HE1	1:J:24:MET:HB2	1.50	0.93
1:L:24:MET:SD	1:L:44:ILE:CD1	2.57	0.93
1:E:208:GLU:H	1:E:212:HIS:HD2	1.09	0.93
1:K:332:VAL:O	1:K:336:THR:HG22	1.69	0.93
1:L:40:THR:HG22	1:L:65:LEU:HD23	1.49	0.93
1:G:149:GLU:OE1	1:G:149:GLU:N	2.01	0.93
1:J:262:SER:O	1:J:266:GLU:HG3	1.69	0.93
1:K:363:ARG:CA	1:K:366:LYS:HD3	1.98	0.93
1:F:183:VAL:HG13	1:F:230:LEU:HD22	1.49	0.93
1:I:287:ILE:O	1:I:291:ILE:HG13	1.69	0.93
1:G:135:MET:HE2	1:G:135:MET:HA	1.50	0.92
1:K:16:PHE:CZ	1:K:24:MET:CE	2.52	0.92
1:I:61:SER:HB3	1:I:64:GLU:HG3	1.51	0.92
1:I:154:ILE:HG22	1:I:162:LYS:HB3	1.52	0.92
1:I:108:THR:HG21	1:J:222:ASN:ND2	1.84	0.92
1:A:233:VAL:HB	1:A:257:THR:HG22	1.52	0.92
1:B:93:PHE:CZ	1:B:101:TYR:CD2	2.58	0.92
1:E:365:TYR:O	1:E:368:ILE:HG22	1.69	0.92
1:I:104:ARG:HG3	1:I:125:ILE:CD1	1.99	0.92
1:C:261:THR:HB	1:C:267:THR:HG22	1.50	0.92
1:A:12:GLU:OE1	1:A:56:THR:HG23	1.67	0.92
1:G:174:ILE:HD11	1:G:202:ALA:HB1	1.52	0.92
1:I:65:LEU:HA	1:I:68:LEU:HD12	1.51	0.92
1:A:155:THR:HG21	1:A:267:THR:HG21	1.50	0.91
1:A:278:GLU:OE2	1:F:269:ARG:NH2	2.03	0.91
1:D:23:ARG:NH1	1:D:26:GLU:OE2	2.02	0.91
1:E:108:THR:CB	1:F:226:ARG:NH2	2.33	0.91
1:G:291:ILE:CG1	1:G:316:PHE:CD2	2.52	0.91
1:D:129:PRO:O	1:D:171:ARG:NH1	2.03	0.91
1:D:175:GLU:HA	1:D:199:THR:CG2	1.99	0.91
1:G:155:THR:HG23	1:G:259:LEU:HB2	1.52	0.91
1:E:35:ASP:CG	1:F:227:LYS:HD2	1.96	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:LEU:HD12	1:G:112:VAL:N	1.84	0.91
1:C:287:ILE:O	1:C:291:ILE:HG13	1.69	0.91
1:L:48:VAL:HG12	1:L:49:TYR:CD2	2.05	0.91
1:I:40:THR:CG2	1:I:65:LEU:HD12	2.01	0.91
1:J:121:THR:CG2	1:K:182:LYS:NZ	2.32	0.91
1:A:355:PHE:HA	1:A:360:ILE:CG2	2.00	0.90
1:I:261:THR:HG21	1:I:267:THR:CA	2.00	0.90
1:C:293:LEU:HD22	1:C:294:CYS:N	1.86	0.90
1:B:247:GLU:O	1:B:251:THR:HG23	1.72	0.90
1:E:108:THR:CG2	1:F:226:ARG:NH2	2.35	0.90
1:B:119:GLN:NE2	1:C:226:ARG:HH21	1.69	0.90
1:A:94:ARG:HE	1:A:100:ARG:HG2	1.36	0.90
1:G:291:ILE:HD13	1:G:316:PHE:HE2	1.27	0.90
1:L:222:ASN:HA	1:L:225:ARG:HH21	1.37	0.90
1:A:40:THR:HG22	1:A:65:LEU:HD22	1.52	0.90
1:G:216:PHE:HD2	1:G:233:VAL:CG1	1.84	0.89
1:H:272:VAL:HG13	1:H:284:THR:HG22	1.54	0.89
1:I:184:LEU:HD12	1:I:228:PRO:HG3	1.51	0.89
1:H:188:SER:O	1:H:208:GLU:HG3	1.72	0.89
1:F:296:TRP:HE1	1:F:347:MET:HE2	1.35	0.89
1:B:337:ARG:O	1:B:340:VAL:HG22	1.72	0.89
1:D:353:MET:O	1:D:357:GLN:HG2	1.71	0.89
1:G:291:ILE:HG21	1:G:316:PHE:CD2	2.06	0.89
1:G:17:THR:HG23	1:G:18:PRO:HD2	1.55	0.89
1:H:280:ARG:O	1:H:284:THR:HG23	1.72	0.88
1:G:69:ILE:HD11	1:G:120:ILE:CG1	2.03	0.88
1:L:40:THR:CG2	1:L:65:LEU:HD23	2.02	0.88
1:D:236:CYS:SG	1:D:259:LEU:CD2	2.60	0.88
1:E:35:ASP:OD2	1:F:227:LYS:HD2	1.73	0.88
1:G:278:GLU:CD	1:L:337:ARG:NH1	2.31	0.88
1:H:48:VAL:HG21	1:H:53:LEU:CD1	2.02	0.88
1:I:266:GLU:OE1	1:I:266:GLU:N	2.06	0.88
1:G:230:LEU:HD13	1:G:231:ILE:N	1.89	0.88
1:J:94:ARG:CB	1:J:100:ARG:HD2	2.04	0.88
1:L:156:GLY:HA2	1:L:296:TRP:CZ3	2.08	0.88
1:I:175:GLU:O	1:I:200:ILE:HD11	1.74	0.88
1:G:238:ASP:OD1	1:G:239:ALA:N	2.06	0.88
1:H:349:TRP:CZ3	1:H:353:MET:HE2	2.09	0.88
1:J:81:LEU:HD21	1:J:87:ILE:HD12	1.56	0.88
1:H:238:ASP:HB3	1:H:240:GLU:OE1	1.74	0.87
1:A:285:ILE:HG23	1:A:325:LEU:HD11	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:MET:HE2	1:E:68:LEU:CG	2.03	0.87
1:H:188:SER:HB3	1:H:189:PRO:CD	2.05	0.87
1:H:188:SER:CB	1:H:189:PRO:CD	2.52	0.87
1:C:208:GLU:H	1:C:212:HIS:HD2	1.23	0.87
1:F:21:MET:O	1:F:25:LEU:HG	1.73	0.87
1:A:17:THR:HG23	1:A:18:PRO:HD2	1.55	0.87
1:B:151:ILE:HG13	1:B:290:THR:HG22	1.56	0.87
1:G:365:TYR:CA	1:G:368:ILE:HD12	2.05	0.87
1:J:24:MET:HE1	1:J:25:LEU:CD2	2.04	0.87
1:L:9:MET:HE3	1:L:24:MET:HB2	1.56	0.87
1:K:288:LEU:CD1	1:K:325:LEU:HD23	2.03	0.87
1:C:40:THR:CG2	1:C:65:LEU:HD22	2.04	0.87
1:F:17:THR:HG23	1:F:18:PRO:HD2	1.57	0.87
1:A:365:TYR:CZ	1:A:369:ILE:HD11	2.10	0.86
1:C:355:PHE:HE1	1:C:362:GLU:HG2	1.40	0.86
1:I:329:PRO:HA	1:I:332:VAL:HG23	1.54	0.86
1:A:94:ARG:HH21	1:A:100:ARG:HG3	1.38	0.86
1:D:102:ARG:NH2	1:D:127:THR:HG22	1.88	0.86
1:I:175:GLU:O	1:I:200:ILE:CD1	2.23	0.86
1:H:171:ARG:HG3	1:H:197:ILE:HD13	1.56	0.86
1:G:230:LEU:HD21	1:G:256:TYR:CE1	2.09	0.86
1:H:73:TYR:OH	1:H:210:PRO:HB2	1.76	0.86
1:D:258:THR:O	1:D:259:LEU:HD23	1.76	0.86
1:F:9:MET:HA	1:F:27:HIS:HD1	1.39	0.86
1:G:40:THR:CG2	1:G:65:LEU:HD22	2.05	0.85
1:J:125:ILE:CD1	1:J:126:PRO:HD2	2.06	0.85
1:A:355:PHE:CA	1:A:360:ILE:HG22	2.06	0.85
1:C:154:ILE:HG22	1:C:162:LYS:HB3	1.55	0.85
1:I:235:GLU:OE1	1:I:260:HIS:NE2	2.09	0.85
1:K:173:LEU:HD22	1:K:181:ARG:CZ	2.06	0.85
1:E:365:TYR:CE2	1:E:369:ILE:HD11	2.12	0.85
1:D:208:GLU:H	1:D:212:HIS:HD2	1.21	0.85
1:K:137:LEU:HG	1:K:141:ILE:HD11	1.59	0.85
1:D:349:TRP:CH2	1:D:353:MET:HE3	2.11	0.85
1:E:95:PRO:HG2	1:E:96:ASN:H	1.40	0.85
1:J:183:VAL:HG13	1:J:230:LEU:HD22	1.55	0.85
1:K:90:HIS:NE2	1:K:104:ARG:HG3	1.92	0.85
1:F:9:MET:CG	1:F:10:PRO:HD2	2.05	0.85
1:A:12:GLU:CD	1:A:56:THR:HG23	2.01	0.85
1:B:374:GLU:CB	1:C:281:LEU:HD22	2.06	0.85
1:G:216:PHE:CD2	1:G:233:VAL:HG12	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:102:ARG:NH1	1:J:127:THR:HG22	1.92	0.84
1:A:243:SER:OG	1:A:283:ARG:NH2	2.10	0.84
1:E:29:GLU:HG2	1:E:101:TYR:HE2	1.35	0.84
1:H:17:THR:HG1	1:H:20:PHE:HD2	1.20	0.84
1:A:208:GLU:H	1:A:212:HIS:HD2	1.22	0.84
1:J:8:LEU:O	1:J:27:HIS:NE2	2.11	0.84
1:J:9:MET:HE3	1:J:24:MET:HA	0.85	0.84
1:A:94:ARG:HH12	1:A:97:ARG:HD2	1.41	0.84
1:F:40:THR:CG2	1:F:65:LEU:HD22	2.06	0.84
1:I:24:MET:SD	1:I:25:LEU:HD23	2.18	0.84
1:K:16:PHE:HZ	1:K:24:MET:CE	1.87	0.84
1:F:296:TRP:NE1	1:F:347:MET:HE2	1.93	0.84
1:H:9:MET:HE3	1:H:24:MET:CA	2.08	0.84
1:J:92:GLU:HG3	1:J:102:ARG:HG2	1.59	0.84
1:J:102:ARG:CZ	1:J:193:VAL:HG21	2.07	0.84
1:G:288:LEU:O	1:G:291:ILE:HG22	1.77	0.83
1:J:81:LEU:HD21	1:J:87:ILE:CD1	2.07	0.83
1:K:108:THR:HG21	1:L:222:ASN:ND2	1.93	0.83
1:F:132:LEU:HD13	1:F:169:ILE:HD13	1.60	0.83
1:G:180:ASN:HA	1:G:201:SER:O	1.79	0.83
1:I:104:ARG:HG3	1:I:125:ILE:HD11	1.60	0.83
1:A:229:ARG:NH1	1:A:252:GLY:O	2.10	0.83
1:H:171:ARG:HG3	1:H:197:ILE:CD1	2.08	0.83
1:J:12:GLU:OE2	1:J:57:ASN:N	2.12	0.83
1:L:17:THR:HG23	1:L:18:PRO:HD2	1.58	0.83
1:H:188:SER:HB3	1:H:189:PRO:HD2	1.61	0.83
1:I:38:ILE:HG22	1:I:65:LEU:HD21	1.60	0.83
1:K:171:ARG:HA	1:K:174:ILE:CG2	2.08	0.83
1:A:40:THR:CG2	1:A:65:LEU:HD22	2.07	0.83
1:D:174:ILE:HG12	1:D:199:THR:HG21	1.58	0.83
1:G:69:ILE:CD1	1:G:120:ILE:HD13	2.08	0.83
1:J:39:GLN:HE21	1:J:119:GLN:HG3	1.44	0.83
1:B:46:ALA:HB2	1:B:55:ILE:HD11	1.61	0.83
1:D:272:VAL:HG13	1:D:284:THR:HG22	1.61	0.83
1:I:25:LEU:CD1	1:I:103:TYR:CE2	2.61	0.83
1:A:21:MET:HE1	1:A:72:ILE:HD11	1.59	0.83
1:L:190:ILE:HG12	1:L:208:GLU:CG	2.07	0.83
1:A:130:PRO:HB2	1:A:135:MET:HE3	1.58	0.82
1:L:13:PRO:HB3	1:L:20:PHE:CE2	2.13	0.82
1:C:79:THR:HA	1:C:82:LEU:CD1	2.00	0.82
1:H:208:GLU:H	1:H:212:HIS:HD2	1.26	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:ILE:CD1	1:G:295:ILE:HD12	2.09	0.82
1:G:233:VAL:HB	1:G:257:THR:CG2	2.09	0.82
1:I:47:GLU:HA	1:I:52:LEU:HD23	1.59	0.82
1:J:10:PRO:HD3	1:J:27:HIS:HD2	1.44	0.82
1:G:352:LYS:HG3	1:G:365:TYR:CE2	2.14	0.82
1:B:104:ARG:HD3	1:B:191:GLU:OE1	1.80	0.82
1:C:276:SER:O	1:C:280:ARG:HB2	1.80	0.82
1:F:222:ASN:HA	1:F:225:ARG:NH2	1.95	0.82
1:G:365:TYR:HA	1:G:368:ILE:CD1	2.09	0.82
1:J:13:PRO:HB3	1:J:20:PHE:CE1	2.15	0.82
1:L:156:GLY:HA2	1:L:296:TRP:HZ3	1.44	0.82
1:G:318:GLU:HG3	1:L:363:ARG:CZ	2.10	0.81
1:J:317:ASP:HB3	1:J:320:VAL:HG23	1.60	0.81
1:K:194:TYR:O	1:K:197:ILE:HG22	1.80	0.81
1:K:108:THR:CG2	1:L:222:ASN:HD21	1.93	0.81
1:K:276:SER:HA	1:K:280:ARG:HD2	1.60	0.81
1:C:328:ASP:HB3	1:C:331:GLU:HG3	1.60	0.81
1:F:8:LEU:O	1:F:27:HIS:HE1	1.64	0.81
1:F:44:ILE:HG13	1:F:56:THR:HG21	1.60	0.81
1:F:78:THR:O	1:F:82:LEU:HD12	1.81	0.81
1:F:174:ILE:CG2	1:F:199:THR:HG21	2.10	0.81
1:F:293:LEU:HD13	1:F:315:VAL:HG22	1.63	0.81
1:I:49:TYR:O	1:I:307:ARG:HD2	1.80	0.81
1:E:108:THR:HG21	1:F:226:ARG:HH22	1.45	0.81
1:K:230:LEU:HD23	1:K:231:ILE:N	1.95	0.81
1:B:249:ALA:HB1	1:B:290:THR:HG23	1.60	0.81
1:E:170:ILE:O	1:E:174:ILE:HG22	1.79	0.81
1:J:104:ARG:CZ	1:J:123:ARG:HH11	1.93	0.81
1:F:209:ILE:HD11	1:F:215:ASN:C	2.05	0.81
1:G:173:LEU:HG	1:G:181:ARG:NH1	1.95	0.81
1:L:132:LEU:HD13	1:L:169:ILE:HD13	1.61	0.81
1:I:24:MET:CE	1:I:44:ILE:CD1	2.47	0.81
1:J:352:LYS:HG3	1:J:365:TYR:CZ	2.14	0.81
1:L:89:THR:HG22	1:L:90:HIS:H	1.44	0.81
1:K:361:SER:HB2	1:K:364:VAL:HG23	1.61	0.81
1:G:312:GLU:HB2	1:G:347:MET:HB2	1.63	0.81
1:E:233:VAL:HB	1:E:257:THR:HG22	1.62	0.80
1:G:9:MET:CE	1:G:24:MET:HA	2.11	0.80
1:F:132:LEU:CD1	1:F:169:ILE:HD13	2.11	0.80
1:A:188:SER:O	1:A:208:GLU:HG3	1.80	0.80
1:G:342:GLN:HG2	1:G:343:LYS:HG2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:263:GLY:O	1:I:267:THR:HG23	1.81	0.80
1:H:92:GLU:OE1	1:H:100:ARG:HD2	1.80	0.80
1:L:222:ASN:HA	1:L:225:ARG:NH2	1.95	0.80
1:H:283:ARG:O	1:H:287:ILE:HG13	1.82	0.80
1:J:9:MET:CG	1:J:10:PRO:HD2	2.11	0.80
1:A:119:GLN:HE22	1:B:182:LYS:HE2	1.46	0.80
1:E:208:GLU:H	1:E:212:HIS:CD2	1.99	0.80
1:H:172:GLU:O	1:H:176:THR:HG23	1.80	0.80
1:K:233:VAL:HB	1:K:257:THR:HG22	1.63	0.80
1:A:365:TYR:CE2	1:A:369:ILE:HD11	2.17	0.80
1:G:69:ILE:HD11	1:G:120:ILE:HG12	1.64	0.80
1:C:361:SER:HB3	1:C:364:VAL:HG23	1.65	0.79
1:E:162:LYS:HD3	1:E:258:THR:CB	2.11	0.79
1:F:209:ILE:HG22	1:F:210:PRO:HD3	1.63	0.79
1:L:337:ARG:O	1:L:340:VAL:HG22	1.81	0.79
1:E:355:PHE:HB2	1:E:360:ILE:HD11	1.63	0.79
1:J:45:PHE:HD2	1:J:52:LEU:HG	1.45	0.79
1:E:316:PHE:HA	1:E:320:VAL:HG21	1.62	0.79
1:I:61:SER:HB3	1:I:64:GLU:CG	2.13	0.79
1:K:137:LEU:HD11	1:K:311:ARG:CZ	2.12	0.79
1:E:219:GLY:O	1:E:222:ASN:HB3	1.83	0.79
1:K:286:ASP:O	1:K:290:THR:OG1	2.00	0.79
1:L:25:LEU:HD13	1:L:93:PHE:CE2	2.16	0.79
1:E:164:THR:CG2	1:E:192:PHE:HZ	1.96	0.79
1:G:111:LEU:HD11	1:G:113:GLU:O	1.83	0.79
1:I:279:GLU:HG2	1:I:283:ARG:HG2	1.64	0.79
1:A:238:ASP:OD1	1:A:239:ALA:N	2.15	0.79
1:G:355:PHE:CE2	1:G:365:TYR:CG	2.71	0.79
1:H:9:MET:HE3	1:H:24:MET:HA	1.65	0.79
1:J:199:THR:CG2	1:J:202:ALA:HB3	2.13	0.79
1:K:12:GLU:OE2	1:K:57:ASN:N	2.16	0.79
1:L:365:TYR:CE2	1:L:369:ILE:HD11	2.18	0.79
1:A:89:THR:HG22	1:A:90:HIS:H	1.47	0.79
1:J:52:LEU:N	1:K:180:ASN:OD1	2.15	0.79
1:L:9:MET:CE	1:L:24:MET:HB2	2.11	0.79
1:C:77:ALA:O	1:C:81:LEU:HD13	1.82	0.79
1:G:318:GLU:HG3	1:L:363:ARG:NH2	1.98	0.79
1:J:10:PRO:HD3	1:J:27:HIS:CD2	2.18	0.79
1:F:149:GLU:HG2	1:F:150:GLY:N	1.96	0.78
1:D:183:VAL:HG13	1:D:230:LEU:HD22	1.65	0.78
1:I:166:LEU:HD23	1:I:169:ILE:HD12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ILE:HD11	1:C:199:THR:HG21	1.66	0.78
1:D:264:VAL:CG1	1:D:340:VAL:HG11	2.12	0.78
1:F:320:VAL:HA	1:F:323:ILE:HD12	1.65	0.78
1:G:188:SER:OG	1:G:189:PRO:HD3	1.83	0.78
1:G:235:GLU:HA	1:G:258:THR:O	1.83	0.78
1:I:160:SER:HA	1:I:299:LEU:HG	1.64	0.78
1:I:171:ARG:O	1:I:174:ILE:HG22	1.83	0.78
1:J:99:VAL:C	1:J:100:ARG:HD3	2.09	0.78
1:G:80:GLN:O	1:G:83:SER:OG	2.02	0.78
1:H:317:ASP:HB2	1:H:320:VAL:HG23	1.66	0.78
1:G:69:ILE:HG12	1:G:120:ILE:HD11	1.66	0.78
1:J:99:VAL:O	1:J:100:ARG:HD3	1.82	0.78
1:B:208:GLU:H	1:B:212:HIS:HD2	1.29	0.78
1:A:94:ARG:NH1	1:A:97:ARG:HA	1.99	0.78
1:D:72:ILE:HD11	1:D:105:VAL:HG21	1.63	0.78
1:J:9:MET:HG3	1:J:10:PRO:HD2	1.64	0.78
1:K:219:GLY:O	1:K:222:ASN:HB3	1.83	0.78
1:L:149:GLU:HG2	1:L:150:GLY:N	1.97	0.78
1:L:280:ARG:O	1:L:284:THR:OG1	2.01	0.78
1:C:17:THR:HG23	1:C:18:PRO:HD2	1.66	0.78
1:H:212:HIS:C	1:H:213:LEU:HD12	2.08	0.78
1:I:35:ASP:OD2	1:I:123:ARG:HG3	1.84	0.78
1:J:337:ARG:O	1:J:340:VAL:HG22	1.83	0.78
1:K:111:LEU:CD2	1:L:90:HIS:NE2	2.47	0.78
1:A:355:PHE:CA	1:A:360:ILE:CG2	2.62	0.78
1:F:9:MET:HG2	1:F:10:PRO:CD	2.14	0.77
1:B:365:TYR:OH	1:B:369:ILE:HD11	1.84	0.77
1:D:104:ARG:CZ	1:D:123:ARG:HH11	1.97	0.77
1:J:89:THR:HA	1:J:208:GLU:OE1	1.84	0.77
1:K:137:LEU:HD11	1:K:311:ARG:NE	2.00	0.77
1:C:80:GLN:O	1:C:83:SER:HB3	1.83	0.77
1:H:186:TYR:OH	1:H:223:ALA:HB2	1.84	0.77
1:J:92:GLU:OE2	1:J:102:ARG:NE	2.16	0.77
1:J:199:THR:HG23	1:J:202:ALA:HB3	1.65	0.77
1:K:208:GLU:H	1:K:212:HIS:HD2	1.31	0.77
1:K:321:ARG:O	1:K:325:LEU:HG	1.84	0.77
1:B:90:HIS:NE2	1:B:92:GLU:HG3	2.00	0.77
1:C:22:ASP:OD2	1:C:93:PHE:CD2	2.37	0.77
1:G:233:VAL:HB	1:G:257:THR:HG22	1.65	0.77
1:G:364:VAL:C	1:G:368:ILE:HD12	2.09	0.77
1:D:174:ILE:C	1:D:199:THR:HG21	2.10	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:ILE:HD12	1:D:200:ILE:O	1.85	0.77
1:F:190:ILE:CG1	1:F:208:GLU:HG3	2.11	0.77
1:G:345:GLN:HG3	1:G:349:TRP:CE3	2.20	0.77
1:B:186:TYR:OH	1:B:223:ALA:HB2	1.84	0.77
1:J:129:PRO:HG3	1:J:167:ALA:HB1	1.67	0.77
1:L:9:MET:HG3	1:L:55:ILE:O	1.84	0.77
1:J:13:PRO:HG3	1:J:20:PHE:CD1	2.20	0.77
1:J:209:ILE:HG22	1:J:210:PRO:HD3	1.68	0.76
1:K:8:LEU:N	1:K:8:LEU:HD23	2.00	0.76
1:C:366:LYS:O	1:C:369:ILE:HG22	1.84	0.76
1:H:320:VAL:HG13	1:H:339:LEU:HD13	1.68	0.76
1:I:52:LEU:O	1:I:53:LEU:HD23	1.85	0.76
1:I:258:THR:O	1:I:259:LEU:HD12	1.85	0.76
1:L:194:TYR:HA	1:L:197:ILE:HD13	1.67	0.76
1:I:173:LEU:O	1:I:181:ARG:NH2	2.18	0.76
1:G:258:THR:O	1:G:259:LEU:HD23	1.85	0.76
1:G:332:VAL:HG23	1:G:333:THR:H	1.49	0.76
1:F:195:ASP:O	1:F:198:GLU:OE2	2.03	0.76
1:E:7:ASN:C	1:E:8:LEU:HG	2.08	0.76
1:K:269:ARG:HB2	1:K:333:THR:CG2	2.16	0.76
1:E:17:THR:CG2	1:E:18:PRO:HD2	2.15	0.76
1:H:65:LEU:CD1	1:H:120:ILE:HD12	2.15	0.76
1:I:13:PRO:HG3	1:I:20:PHE:CD2	2.21	0.76
1:K:137:LEU:CG	1:K:141:ILE:HD11	2.16	0.76
1:B:212:HIS:C	1:B:213:LEU:HD12	2.11	0.76
1:G:12:GLU:CD	1:G:56:THR:HG23	2.11	0.76
1:I:17:THR:HG23	1:I:18:PRO:HD2	1.68	0.76
1:C:293:LEU:HD22	1:C:294:CYS:H	1.51	0.75
1:E:58:ARG:HH12	1:E:64:GLU:CD	1.94	0.75
1:G:180:ASN:HB3	1:L:52:LEU:CB	2.15	0.75
1:I:54:LYS:C	1:I:55:ILE:HD13	2.12	0.75
1:I:149:GLU:O	1:I:292:ARG:HD2	1.86	0.75
1:A:92:GLU:CG	1:A:102:ARG:HG2	2.16	0.75
1:B:125:ILE:HD12	1:B:126:PRO:HD2	1.69	0.75
1:J:92:GLU:OE2	1:J:102:ARG:CZ	2.34	0.75
1:L:190:ILE:HG12	1:L:208:GLU:HG2	1.66	0.75
1:C:132:LEU:HB2	1:C:172:GLU:HG3	1.68	0.75
1:F:261:THR:HG22	1:F:270:ARG:HE	1.49	0.75
1:I:52:LEU:C	1:I:53:LEU:HD23	2.10	0.75
1:F:183:VAL:HG13	1:F:230:LEU:CD2	2.16	0.75
1:G:135:MET:HE2	1:G:135:MET:CA	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:125:ILE:HD12	1:J:126:PRO:HD2	1.66	0.75
1:F:197:ILE:HD12	1:F:197:ILE:O	1.85	0.75
1:I:209:ILE:O	1:I:213:LEU:O	2.04	0.75
1:F:296:TRP:HE1	1:F:347:MET:CE	2.00	0.75
1:H:18:PRO:O	1:H:21:MET:HB3	1.87	0.75
1:J:219:GLY:O	1:J:222:ASN:HB3	1.87	0.75
1:L:333:THR:O	1:L:336:THR:OG1	2.02	0.75
1:C:88:ASP:OD1	1:C:106:ASN:ND2	2.19	0.75
1:D:38:ILE:HB	1:D:120:ILE:HG23	1.68	0.75
1:F:125:ILE:HD12	1:F:126:PRO:CD	2.17	0.75
1:G:174:ILE:CD1	1:G:202:ALA:HB1	2.15	0.75
1:G:302:THR:OG1	1:G:306:ARG:O	2.05	0.75
1:I:80:GLN:O	1:I:83:SER:HB3	1.87	0.75
1:J:10:PRO:CD	1:J:27:HIS:HD2	1.99	0.75
1:L:293:LEU:HD13	1:L:315:VAL:HG22	1.67	0.75
1:H:209:ILE:O	1:H:213:LEU:O	2.03	0.75
1:J:353:MET:HE2	1:J:353:MET:N	2.00	0.75
1:L:183:VAL:HG13	1:L:230:LEU:CD2	2.17	0.75
1:L:190:ILE:N	1:L:208:GLU:OE2	2.20	0.75
1:F:9:MET:HA	1:F:27:HIS:ND1	2.01	0.75
1:H:68:LEU:HD23	1:H:68:LEU:N	2.01	0.75
1:L:40:THR:HG21	1:L:62:ASN:OD1	1.87	0.75
1:B:100:ARG:HE	1:B:102:ARG:HH12	1.33	0.74
1:C:154:ILE:HG21	1:C:162:LYS:HB3	1.69	0.74
1:D:171:ARG:HG3	1:D:197:ILE:HD13	1.69	0.74
1:K:13:PRO:HB2	1:K:15:ARG:O	1.87	0.74
1:E:108:THR:CB	1:F:226:ARG:HH21	1.99	0.74
1:J:175:GLU:HG3	1:J:197:ILE:CG2	2.16	0.74
1:D:61:SER:OG	1:D:64:GLU:OE2	2.04	0.74
1:F:296:TRP:NE1	1:F:347:MET:CE	2.50	0.74
1:J:72:ILE:HD11	1:J:105:VAL:HG21	1.69	0.74
1:K:111:LEU:HD21	1:L:90:HIS:NE2	2.03	0.74
1:L:154:ILE:HG22	1:L:162:LYS:HG2	1.69	0.74
1:L:155:THR:OG1	1:L:261:THR:O	2.05	0.74
1:C:17:THR:CG2	1:C:18:PRO:HD2	2.17	0.74
1:C:155:THR:HG21	1:C:267:THR:HG21	1.70	0.74
1:G:17:THR:CG2	1:G:18:PRO:HD2	2.18	0.74
1:E:183:VAL:HG13	1:E:230:LEU:HD22	1.70	0.74
1:F:297:GLN:HB2	1:F:311:ARG:HG2	1.67	0.74
1:H:119:GLN:OE1	1:I:205:SER:HB2	1.87	0.74
1:G:279:GLU:OE1	1:G:279:GLU:HA	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:328:ASP:OD1	1:H:330:ASN:N	2.19	0.74
1:I:43:PRO:HD3	1:I:59:ARG:HG2	1.69	0.74
1:I:132:LEU:HB2	1:I:172:GLU:HG3	1.70	0.74
1:J:65:LEU:HD23	1:J:118:ILE:O	1.87	0.74
1:J:102:ARG:NH2	1:J:193:VAL:HG21	2.03	0.74
1:J:145:ILE:CD1	1:J:293:LEU:CD2	2.66	0.74
1:F:174:ILE:HG22	1:F:199:THR:CG2	2.16	0.74
1:K:25:LEU:HD13	1:K:93:PHE:CE2	2.23	0.74
1:K:35:ASP:C	1:K:36:ILE:HD12	2.13	0.74
1:B:102:ARG:HE	1:B:127:THR:HG22	1.53	0.73
1:E:108:THR:HG21	1:F:226:ARG:HH21	1.53	0.73
1:G:365:TYR:O	1:G:369:ILE:HG13	1.87	0.73
1:E:89:THR:HG23	1:E:105:VAL:CG1	2.18	0.73
1:F:156:GLY:HA2	1:F:296:TRP:CZ3	2.23	0.73
1:L:25:LEU:HD13	1:L:93:PHE:HE2	1.51	0.73
1:A:49:TYR:CZ	1:A:306:ARG:HG3	2.22	0.73
1:D:366:LYS:O	1:D:369:ILE:HG23	1.88	0.73
1:K:7:ASN:C	1:K:8:LEU:HD23	2.13	0.73
1:E:8:LEU:HD12	1:E:31:LEU:HD11	1.68	0.73
1:E:328:ASP:N	1:E:331:GLU:OE2	2.21	0.73
1:G:238:ASP:C	1:G:242:ILE:HD12	2.14	0.73
1:G:102:ARG:NH2	1:G:125:ILE:HG21	2.02	0.73
1:I:110:CYS:O	1:J:212:HIS:HE1	1.72	0.73
1:J:102:ARG:HE	1:J:193:VAL:HG11	1.54	0.73
1:J:352:LYS:HA	1:J:365:TYR:CE1	2.23	0.73
1:K:9:MET:SD	1:K:10:PRO:HD2	2.28	0.73
1:A:203:VAL:HG13	1:F:42:GLU:OE1	1.87	0.73
1:G:235:GLU:CA	1:G:258:THR:OG1	2.36	0.73
1:G:278:GLU:OE1	1:L:337:ARG:NH1	2.22	0.73
1:I:104:ARG:HG3	1:I:125:ILE:HD13	1.68	0.73
1:B:100:ARG:NE	1:B:102:ARG:HH12	1.86	0.73
1:E:17:THR:HG23	1:E:18:PRO:HD2	1.71	0.73
1:G:183:VAL:HG22	1:G:230:LEU:HB3	1.69	0.73
1:K:68:LEU:O	1:K:71:SER:OG	2.05	0.73
1:L:188:SER:HA	1:L:209:ILE:HG22	1.71	0.73
1:C:329:PRO:HA	1:C:332:VAL:HG23	1.70	0.72
1:G:89:THR:HG22	1:G:90:HIS:N	2.04	0.72
1:I:276:SER:O	1:I:280:ARG:HB2	1.88	0.72
1:E:354:LYS:HE2	1:E:354:LYS:HA	1.69	0.72
1:I:365:TYR:O	1:I:368:ILE:HG13	1.89	0.72
1:L:61:SER:OG	1:L:64:GLU:HG3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:THR:HG22	1:G:90:HIS:H	1.53	0.72
1:G:235:GLU:N	1:G:258:THR:OG1	2.21	0.72
1:I:353:MET:HG2	1:I:357:GLN:HE22	1.54	0.72
1:K:17:THR:HG23	1:K:18:PRO:HD2	1.71	0.72
1:K:171:ARG:HA	1:K:174:ILE:HG21	1.70	0.72
1:K:275:PHE:O	1:K:280:ARG:HD2	1.90	0.72
1:A:34:SER:O	1:A:124:THR:HG23	1.88	0.72
1:K:362:GLU:O	1:K:366:LYS:HG3	1.90	0.72
1:D:366:LYS:HA	1:D:369:ILE:CG2	2.20	0.72
1:F:188:SER:O	1:F:208:GLU:HG2	1.88	0.72
1:H:92:GLU:HG2	1:H:102:ARG:HG2	1.72	0.72
1:H:363:ARG:NH1	1:I:322:ASP:OD1	2.22	0.72
1:L:143:GLU:OE1	1:L:143:GLU:HA	1.89	0.72
1:G:155:THR:HG23	1:G:259:LEU:CB	2.20	0.72
1:I:197:ILE:HD12	1:I:197:ILE:N	2.04	0.72
1:J:7:ASN:O	1:J:8:LEU:HD12	1.89	0.72
1:I:24:MET:HE2	1:I:44:ILE:HG21	1.70	0.72
1:A:17:THR:CG2	1:A:18:PRO:HD2	2.19	0.72
1:C:279:GLU:HG2	1:C:283:ARG:HG2	1.72	0.72
1:G:42:GLU:OE2	1:H:198:GLU:OE2	2.07	0.72
1:H:97:ARG:NH2	1:H:99:VAL:HG21	2.04	0.72
1:J:39:GLN:C	1:J:65:LEU:HD21	2.14	0.72
1:K:9:MET:HB2	1:K:55:ILE:O	1.89	0.72
1:F:337:ARG:O	1:F:340:VAL:HG22	1.90	0.72
1:I:37:THR:HG21	1:J:182:LYS:HD2	1.72	0.72
1:F:173:LEU:O	1:F:179:SER:OG	2.07	0.71
1:G:69:ILE:HG12	1:G:120:ILE:CD1	2.19	0.71
1:G:291:ILE:O	1:G:292:ARG:NH1	2.23	0.71
1:G:300:VAL:HG13	1:G:301:PRO:HD2	1.70	0.71
1:K:88:ASP:OD1	1:K:106:ASN:ND2	2.21	0.71
1:K:363:ARG:O	1:K:367:LEU:HG	1.88	0.71
1:A:113:GLU:OE1	1:B:100:ARG:NH2	2.23	0.71
1:E:21:MET:CE	1:E:68:LEU:HG	2.18	0.71
1:G:230:LEU:HD13	1:G:230:LEU:C	2.15	0.71
1:G:317:ASP:C	1:G:321:ARG:NH1	2.48	0.71
1:H:155:THR:HG22	1:H:259:LEU:HB2	1.72	0.71
1:J:191:GLU:HB3	1:J:192:PHE:CD1	2.24	0.71
1:J:248:ALA:O	1:J:251:THR:OG1	2.08	0.71
1:L:248:ALA:O	1:L:251:THR:OG1	2.06	0.71
1:I:230:LEU:HD11	1:I:256:TYR:CD1	2.25	0.71
1:E:45:PHE:CE1	1:E:54:LYS:HG2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:GLU:O	1:C:292:ARG:HD2	1.90	0.71
1:E:9:MET:HB2	1:E:55:ILE:O	1.90	0.71
1:F:143:GLU:OE1	1:F:143:GLU:HA	1.90	0.71
1:I:17:THR:CG2	1:I:18:PRO:HD2	2.20	0.71
1:G:173:LEU:O	1:G:181:ARG:NH2	2.14	0.71
1:H:35:ASP:OD2	1:I:227:LYS:HD3	1.90	0.71
1:J:182:LYS:NZ	1:J:226:ARG:O	2.24	0.71
1:J:183:VAL:HB	1:J:204:VAL:HG22	1.72	0.71
1:K:40:THR:HG22	1:K:65:LEU:CD2	2.14	0.71
1:B:224:LEU:HD21	1:B:248:ALA:HA	1.72	0.71
1:B:249:ALA:CB	1:B:290:THR:CG2	2.68	0.71
1:E:328:ASP:O	1:E:331:GLU:HG2	1.89	0.71
1:E:332:VAL:HG23	1:E:333:THR:H	1.55	0.71
1:I:49:TYR:C	1:I:307:ARG:HD2	2.16	0.71
1:J:102:ARG:HH11	1:J:127:THR:HG22	1.53	0.71
1:K:44:ILE:HG22	1:K:55:ILE:HD11	1.73	0.71
1:K:269:ARG:O	1:K:273:THR:OG1	2.09	0.71
1:B:249:ALA:HB1	1:B:290:THR:CG2	2.20	0.71
1:E:43:PRO:HD3	1:E:59:ARG:HD3	1.73	0.70
1:F:209:ILE:HD11	1:F:215:ASN:O	1.91	0.70
1:H:208:GLU:H	1:H:212:HIS:CD2	2.09	0.70
1:I:34:SER:O	1:I:124:THR:HG23	1.91	0.70
1:I:88:ASP:OD1	1:I:106:ASN:ND2	2.24	0.70
1:K:353:MET:HA	1:K:353:MET:CE	2.19	0.70
1:E:129:PRO:HB2	1:E:171:ARG:HD3	1.73	0.70
1:H:188:SER:CB	1:H:189:PRO:HD3	2.19	0.70
1:I:208:GLU:H	1:I:212:HIS:HD2	1.37	0.70
1:K:111:LEU:HD13	1:L:90:HIS:CE1	2.27	0.70
1:K:288:LEU:HB3	1:K:325:LEU:HD21	1.73	0.70
1:E:108:THR:HB	1:F:226:ARG:NH2	2.07	0.70
1:K:263:GLY:O	1:K:267:THR:HG23	1.91	0.70
1:I:137:LEU:HD23	1:I:311:ARG:NH1	2.06	0.70
1:I:367:LEU:HD23	1:I:367:LEU:C	2.16	0.70
1:B:208:GLU:H	1:B:212:HIS:CD2	2.09	0.70
1:F:345:GLN:HG3	1:F:349:TRP:HE3	1.54	0.70
1:G:173:LEU:C	1:G:181:ARG:HH22	1.99	0.70
1:L:125:ILE:HD12	1:L:126:PRO:CD	2.20	0.70
1:I:174:ILE:HG13	1:I:202:ALA:HB1	1.74	0.70
1:J:40:THR:HG23	1:J:62:ASN:HA	1.74	0.70
1:J:58:ARG:NH1	1:J:64:GLU:OE2	2.23	0.70
1:L:112:VAL:HG23	1:L:117:ALA:HB3	1.68	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:15:ARG:CG	1:J:64:GLU:OE2	2.37	0.70
1:J:94:ARG:CB	1:J:100:ARG:CD	2.69	0.70
1:G:69:ILE:HD11	1:G:120:ILE:CD1	2.21	0.70
1:B:73:TYR:OH	1:B:210:PRO:HB2	1.92	0.70
1:D:155:THR:HG22	1:D:259:LEU:HB2	1.74	0.70
1:E:9:MET:CG	1:E:10:PRO:HD2	2.22	0.70
1:E:27:HIS:O	1:E:30:SER:OG	2.03	0.70
1:E:263:GLY:O	1:E:267:THR:HG23	1.91	0.70
1:G:235:GLU:HB3	1:G:258:THR:OG1	1.92	0.70
1:G:248:ALA:O	1:G:251:THR:OG1	2.10	0.70
1:I:25:LEU:CD1	1:I:103:TYR:HE2	2.05	0.70
1:I:48:VAL:N	1:I:51:ARG:O	2.20	0.70
1:I:365:TYR:CE2	1:I:369:ILE:HD11	2.27	0.70
1:G:306:ARG:HG2	1:G:307:ARG:N	2.07	0.69
1:G:354:LYS:HB3	1:G:360:ILE:CD1	2.21	0.69
1:J:186:TYR:OH	1:J:223:ALA:HB2	1.91	0.69
1:I:24:MET:HE1	1:I:38:ILE:HD11	1.73	0.69
1:K:302:THR:OG1	1:K:304:ASP:OD1	2.07	0.69
1:C:367:LEU:HD23	1:C:367:LEU:C	2.17	0.69
1:G:238:ASP:O	1:G:242:ILE:HD12	1.93	0.69
1:H:155:THR:HG21	1:H:267:THR:HG21	1.74	0.69
1:I:22:ASP:OD2	1:I:93:PHE:CE1	2.45	0.69
1:F:73:TYR:CD1	1:F:89:THR:CG2	2.73	0.69
1:G:322:ASP:HA	1:G:325:LEU:HD12	1.72	0.69
1:J:140:ASN:H	1:J:140:ASN:HD22	1.40	0.69
1:K:288:LEU:CB	1:K:325:LEU:HD21	2.23	0.69
1:L:24:MET:SD	1:L:44:ILE:HD12	2.31	0.69
1:D:224:LEU:HD21	1:D:248:ALA:HA	1.72	0.69
1:E:7:ASN:HA	1:E:54:LYS:O	1.92	0.69
1:G:318:GLU:O	1:G:322:ASP:OD2	2.09	0.69
1:D:94:ARG:CB	1:D:100:ARG:HE	2.05	0.69
1:G:21:MET:HE3	1:G:68:LEU:HD22	1.74	0.69
1:G:119:GLN:NE2	1:H:182:LYS:NZ	2.37	0.69
1:G:208:GLU:H	1:G:212:HIS:HD2	1.39	0.69
1:G:239:ALA:CA	1:G:242:ILE:HD12	2.20	0.69
1:I:95:PRO:HD2	1:I:99:VAL:O	1.92	0.69
1:I:184:LEU:CD1	1:I:228:PRO:HB3	2.23	0.69
1:K:24:MET:SD	1:K:44:ILE:HD13	2.32	0.69
1:B:197:ILE:HG22	1:B:199:THR:HG23	1.75	0.69
1:A:293:LEU:HD13	1:A:315:VAL:HG22	1.73	0.69
1:F:186:TYR:OH	1:F:223:ALA:HB2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:SER:OG	1:G:64:GLU:OE1	2.07	0.69
1:G:322:ASP:OD1	1:L:363:ARG:NH2	2.24	0.69
1:L:171:ARG:O	1:L:175:GLU:HG3	1.93	0.69
1:L:296:TRP:NE1	1:L:347:MET:CE	2.55	0.69
1:B:183:VAL:HG13	1:B:230:LEU:HD22	1.74	0.69
1:F:24:MET:SD	1:F:44:ILE:HG21	2.33	0.69
1:L:13:PRO:HB3	1:L:20:PHE:CD2	2.27	0.69
1:L:89:THR:HG22	1:L:90:HIS:N	2.08	0.69
1:C:272:VAL:HG13	1:C:284:THR:HG22	1.73	0.69
1:D:8:LEU:CD1	1:D:9:MET:N	2.49	0.69
1:H:19:VAL:HG23	1:H:20:PHE:N	2.07	0.69
1:G:132:LEU:O	1:G:132:LEU:HD23	1.92	0.68
1:G:317:ASP:HB3	1:G:320:VAL:HG23	1.75	0.68
1:K:137:LEU:CD1	1:K:311:ARG:CZ	2.71	0.68
1:I:41:GLY:O	1:I:59:ARG:HD2	1.93	0.68
1:I:95:PRO:CD	1:I:99:VAL:O	2.41	0.68
1:J:29:GLU:HA	1:J:29:GLU:OE2	1.93	0.68
1:L:312:GLU:HB2	1:L:347:MET:N	2.08	0.68
1:D:268:MET:HG3	1:D:336:THR:HG21	1.75	0.68
1:G:154:ILE:HD11	1:G:295:ILE:HD12	1.74	0.68
1:G:215:ASN:OD1	1:G:218:ASP:OD2	2.11	0.68
1:G:269:ARG:HH11	1:G:269:ARG:CG	2.03	0.68
1:J:72:ILE:HD13	1:J:105:VAL:HG11	1.75	0.68
1:J:337:ARG:NH1	1:K:278:GLU:OE1	2.26	0.68
1:L:9:MET:SD	1:L:56:THR:CG2	2.80	0.68
1:A:94:ARG:HH21	1:A:100:ARG:CG	2.06	0.68
1:A:285:ILE:HD12	1:A:285:ILE:N	2.06	0.68
1:D:186:TYR:OH	1:D:223:ALA:HB2	1.94	0.68
1:B:352:LYS:HA	1:B:365:TYR:CE1	2.27	0.68
1:C:208:GLU:H	1:C:212:HIS:CD2	2.08	0.68
1:K:24:MET:SD	1:K:44:ILE:HG21	2.34	0.68
1:G:9:MET:HE1	1:G:24:MET:HB2	1.74	0.68
1:H:21:MET:HE1	1:H:68:LEU:HB3	1.74	0.68
1:H:272:VAL:HG13	1:H:284:THR:CG2	2.22	0.68
1:I:61:SER:H	1:I:64:GLU:CD	2.01	0.68
1:I:341:ARG:HG2	1:I:346:LEU:HD11	1.75	0.68
1:J:209:ILE:HG22	1:J:210:PRO:CD	2.23	0.68
1:A:340:VAL:HG12	1:A:346:LEU:HD12	1.75	0.68
1:F:9:MET:CE	1:F:24:MET:HB2	2.23	0.68
1:H:119:GLN:HE22	1:I:182:LYS:HE3	1.59	0.68
1:I:248:ALA:O	1:I:251:THR:OG1	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:246:LEU:HD21	1:K:287:ILE:HD13	1.76	0.68
1:L:40:THR:HG22	1:L:65:LEU:CD2	2.24	0.68
1:L:296:TRP:CD1	1:L:347:MET:HE2	2.28	0.68
1:D:35:ASP:OD2	1:E:227:LYS:HD2	1.93	0.68
1:E:155:THR:HG22	1:E:259:LEU:HB2	1.76	0.68
1:F:17:THR:CG2	1:F:18:PRO:HD2	2.23	0.68
1:I:361:SER:HB3	1:I:364:VAL:HG23	1.75	0.68
1:L:197:ILE:HD12	1:L:197:ILE:N	2.08	0.68
1:K:155:THR:HG22	1:K:259:LEU:HB2	1.74	0.67
1:C:188:SER:O	1:C:208:GLU:HG3	1.94	0.67
1:D:296:TRP:CE3	1:D:347:MET:HE2	2.29	0.67
1:E:304:ASP:OD2	1:E:306:ARG:HD2	1.94	0.67
1:I:86:ASP:OD2	1:J:225:ARG:NH1	2.24	0.67
1:E:329:PRO:O	1:E:332:VAL:HG13	1.94	0.67
1:H:86:ASP:HB2	1:I:213:LEU:HD21	1.76	0.67
1:I:208:GLU:H	1:I:212:HIS:CD2	2.12	0.67
1:I:261:THR:CG2	1:I:267:THR:CG2	2.70	0.67
1:K:288:LEU:CB	1:K:325:LEU:CD2	2.73	0.67
1:L:215:ASN:OD1	1:L:218:ASP:CB	2.31	0.67
1:A:137:LEU:HD23	1:A:141:ILE:HG21	1.75	0.67
1:D:208:GLU:H	1:D:212:HIS:CD2	2.07	0.67
1:D:367:LEU:HD11	1:E:325:LEU:HD13	1.77	0.67
1:G:69:ILE:HD11	1:G:120:ILE:HD13	1.76	0.67
1:G:230:LEU:HD21	1:G:256:TYR:HE1	1.57	0.67
1:K:300:VAL:HG13	1:K:301:PRO:HD2	1.76	0.67
1:L:302:THR:OG1	1:L:306:ARG:O	2.08	0.67
1:G:69:ILE:CD1	1:G:120:ILE:CD1	2.71	0.67
1:C:287:ILE:HG22	1:C:291:ILE:HD11	1.75	0.67
1:I:184:LEU:HD12	1:I:228:PRO:CG	2.25	0.67
1:A:208:GLU:H	1:A:212:HIS:CD2	2.08	0.67
1:B:40:THR:OG1	1:B:65:LEU:HD22	1.95	0.67
1:C:363:ARG:HG3	1:C:364:VAL:N	2.08	0.67
1:E:164:THR:CG2	1:E:192:PHE:CZ	2.74	0.67
1:G:324:LEU:HD21	1:G:339:LEU:HD12	1.77	0.67
1:L:132:LEU:CD1	1:L:169:ILE:HD13	2.24	0.67
1:B:259:LEU:HD12	1:B:267:THR:HG23	1.76	0.67
1:G:355:PHE:HZ	1:G:365:TYR:HD2	1.31	0.67
1:J:40:THR:N	1:J:65:LEU:HD21	2.10	0.67
1:J:323:ILE:HD13	1:J:323:ILE:N	2.09	0.67
1:K:292:ARG:HH21	1:K:292:ARG:HG3	1.57	0.67
1:A:281:LEU:C	1:A:281:LEU:HD13	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:ARG:NH2	1:D:260:HIS:HB2	2.10	0.67
1:E:22:ASP:OD1	1:E:22:ASP:N	2.28	0.67
1:I:65:LEU:HA	1:I:68:LEU:CD1	2.24	0.67
1:J:38:ILE:HB	1:J:120:ILE:HG23	1.77	0.67
1:K:131:LYS:O	1:K:134:THR:OG1	2.10	0.67
1:C:119:GLN:HE22	1:D:182:LYS:HE2	1.58	0.67
1:F:184:LEU:HD13	1:F:226:ARG:HD2	1.75	0.67
1:L:319:GLU:O	1:L:323:ILE:HG13	1.95	0.67
1:A:297:GLN:HE21	1:A:311:ARG:NE	1.93	0.66
1:H:131:LYS:O	1:H:134:THR:OG1	2.14	0.66
1:C:76:ASN:O	1:C:79:THR:OG1	2.12	0.66
1:H:18:PRO:O	1:H:21:MET:N	2.28	0.66
1:J:24:MET:HE3	1:J:25:LEU:N	2.11	0.66
1:K:111:LEU:CD1	1:L:90:HIS:NE2	2.59	0.66
1:L:270:ARG:O	1:L:274:SER:OG	2.12	0.66
1:L:313:TYR:CE2	1:L:345:GLN:NE2	2.63	0.66
1:A:92:GLU:HG3	1:A:102:ARG:HG2	1.76	0.66
1:C:300:VAL:HG21	1:C:310:LEU:HD12	1.78	0.66
1:D:198:GLU:HA	1:D:198:GLU:OE2	1.95	0.66
1:G:321:ARG:HH11	1:G:321:ARG:HG3	1.61	0.66
1:H:349:TRP:HZ3	1:H:353:MET:HE2	1.59	0.66
1:I:109:ALA:C	1:J:212:HIS:ND1	2.54	0.66
1:L:313:TYR:HE2	1:L:345:GLN:NE2	1.93	0.66
1:B:65:LEU:HD23	1:B:118:ILE:O	1.95	0.66
1:F:209:ILE:HG22	1:F:210:PRO:CD	2.25	0.66
1:G:328:ASP:OD1	1:G:330:ASN:N	2.27	0.66
1:A:124:THR:O	1:A:125:ILE:HD13	1.96	0.66
1:F:78:THR:O	1:F:82:LEU:CD1	2.44	0.66
1:G:281:LEU:HD21	1:G:329:PRO:HG2	1.76	0.66
1:G:345:GLN:HG3	1:G:349:TRP:CZ3	2.31	0.66
1:H:46:ALA:HB2	1:H:55:ILE:HD11	1.75	0.66
1:K:27:HIS:O	1:K:30:SER:OG	2.10	0.66
1:A:188:SER:OG	1:A:189:PRO:HD3	1.96	0.66
1:G:69:ILE:HD11	1:G:120:ILE:CG2	2.25	0.66
1:G:247:GLU:O	1:G:251:THR:HG23	1.95	0.66
1:G:355:PHE:HZ	1:G:365:TYR:CD2	2.04	0.66
1:G:269:ARG:HG2	1:G:269:ARG:NH1	1.97	0.66
1:I:16:PHE:CE1	1:I:20:PHE:HB3	2.30	0.66
1:B:46:ALA:CB	1:B:55:ILE:HD11	2.25	0.66
1:E:188:SER:HB3	1:E:189:PRO:HD3	1.77	0.66
1:F:125:ILE:CD1	1:F:126:PRO:HD2	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:212:HIS:O	1:G:213:LEU:HD23	1.96	0.66
1:K:171:ARG:C	1:K:174:ILE:HG22	2.21	0.66
1:A:230:LEU:HD13	1:A:231:ILE:N	2.10	0.66
1:C:361:SER:OG	1:C:363:ARG:HG2	1.95	0.66
1:D:272:VAL:HG13	1:D:284:THR:CG2	2.25	0.66
1:I:365:TYR:HA	1:I:368:ILE:HD11	1.78	0.66
1:K:150:GLY:HA3	1:K:292:ARG:HD2	1.76	0.66
1:G:239:ALA:HA	1:G:242:ILE:CD1	2.24	0.65
1:G:366:LYS:O	1:G:369:ILE:HB	1.94	0.65
1:B:151:ILE:HG13	1:B:290:THR:CG2	2.26	0.65
1:E:33:ALA:HB2	1:E:48:VAL:HG22	1.79	0.65
1:G:317:ASP:OD1	1:G:319:GLU:N	2.25	0.65
1:G:364:VAL:O	1:G:368:ILE:HD12	1.96	0.65
1:G:318:GLU:O	1:G:322:ASP:CG	2.38	0.65
1:G:354:LYS:CB	1:G:360:ILE:HD11	2.26	0.65
1:I:110:CYS:C	1:J:212:HIS:CE1	2.75	0.65
1:I:321:ARG:O	1:I:325:LEU:CD1	2.38	0.65
1:K:24:MET:CE	1:K:44:ILE:HD12	2.20	0.65
1:K:171:ARG:CA	1:K:174:ILE:CG2	2.73	0.65
1:A:9:MET:HB3	1:A:55:ILE:HG23	1.78	0.65
1:C:174:ILE:CD1	1:C:199:THR:HG21	2.27	0.65
1:G:355:PHE:CZ	1:G:365:TYR:CG	2.84	0.65
1:I:236:CYS:SG	1:I:242:ILE:HG12	2.37	0.65
1:J:297:GLN:HG3	1:J:311:ARG:HG2	1.77	0.65
1:K:12:GLU:OE2	1:K:58:ARG:N	2.22	0.65
1:K:13:PRO:HG3	1:K:20:PHE:CD2	2.31	0.65
1:A:12:GLU:OE2	1:A:58:ARG:CB	2.44	0.65
1:E:9:MET:HG3	1:E:10:PRO:HD2	1.79	0.65
1:F:313:TYR:CE2	1:F:345:GLN:NE2	2.64	0.65
1:G:291:ILE:HG23	1:G:316:PHE:CD2	2.20	0.65
1:G:355:PHE:O	1:G:358:GLY:N	2.28	0.65
1:I:21:MET:CE	1:I:68:LEU:HD23	2.26	0.65
1:F:13:PRO:HG3	1:F:20:PHE:CE2	2.32	0.65
1:I:177:SER:N	1:I:200:ILE:HD13	2.12	0.65
1:J:17:THR:CG2	1:J:18:PRO:HD2	2.26	0.65
1:J:40:THR:N	1:J:65:LEU:CD2	2.59	0.65
1:F:40:THR:OG1	1:F:117:ALA:HB1	1.96	0.65
1:F:222:ASN:HA	1:F:225:ARG:HH21	1.60	0.65
1:G:216:PHE:CD2	1:G:233:VAL:CG1	2.75	0.65
1:H:243:SER:OG	1:H:283:ARG:NH2	2.30	0.65
1:I:77:ALA:O	1:I:81:LEU:HD13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:21:MET:O	1:J:24:MET:HE3	1.96	0.65
1:J:238:ASP:O	1:J:242:ILE:HG13	1.96	0.65
1:J:333:THR:O	1:J:336:THR:OG1	2.10	0.65
1:B:21:MET:HE1	1:B:72:ILE:CD1	2.25	0.65
1:B:45:PHE:CE2	1:C:203:VAL:HG22	2.32	0.65
1:E:176:THR:HG23	1:E:179:SER:HB3	1.79	0.65
1:F:281:LEU:O	1:F:285:ILE:HD13	1.96	0.65
1:G:329:PRO:O	1:G:332:VAL:HG13	1.97	0.65
1:H:261:THR:OG1	1:H:267:THR:HG23	1.97	0.65
1:I:174:ILE:HG13	1:I:202:ALA:CB	2.25	0.65
1:K:269:ARG:HB2	1:K:333:THR:HG22	1.78	0.65
1:K:304:ASP:CG	1:K:306:ARG:HG3	2.21	0.65
1:L:283:ARG:O	1:L:287:ILE:HG13	1.97	0.65
1:A:209:ILE:O	1:A:213:LEU:O	2.15	0.65
1:F:352:LYS:HB2	1:F:365:TYR:OH	1.97	0.65
1:G:317:ASP:OD1	1:G:318:GLU:N	2.30	0.65
1:J:17:THR:HG22	1:J:18:PRO:HD2	1.79	0.65
1:J:81:LEU:N	1:J:81:LEU:HD23	2.12	0.65
1:J:121:THR:HG22	1:K:182:LYS:HZ1	1.61	0.65
1:C:12:GLU:OE1	1:C:57:ASN:OD1	2.14	0.65
1:E:58:ARG:NH1	1:E:64:GLU:OE1	2.29	0.65
1:I:25:LEU:HD12	1:I:103:TYR:HE2	1.62	0.65
1:K:121:THR:HG21	1:L:182:LYS:HZ1	1.62	0.65
1:G:184:LEU:HG	1:G:228:PRO:HB3	1.78	0.64
1:J:92:GLU:HG3	1:J:102:ARG:CG	2.27	0.64
1:K:43:PRO:HG3	1:K:54:LYS:HD3	1.78	0.64
1:L:9:MET:HE3	1:L:24:MET:CB	2.27	0.64
1:L:275:PHE:CE2	1:L:283:ARG:HD3	2.31	0.64
1:G:111:LEU:HD12	1:G:111:LEU:C	2.22	0.64
1:I:65:LEU:CA	1:I:68:LEU:HD12	2.25	0.64
1:I:142:ILE:O	1:I:145:ILE:HG13	1.97	0.64
1:D:214:PRO:C	1:D:215:ASN:HD22	2.05	0.64
1:F:208:GLU:H	1:F:212:HIS:HD2	1.43	0.64
1:G:105:VAL:HG12	1:G:122:LEU:HG	1.79	0.64
1:I:329:PRO:HA	1:I:332:VAL:CG2	2.26	0.64
1:A:208:GLU:HG2	1:A:210:PRO:HD2	1.80	0.64
1:K:24:MET:HE1	1:K:44:ILE:CD1	2.20	0.64
1:H:21:MET:HE3	1:H:68:LEU:HD13	1.77	0.64
1:I:175:GLU:O	1:I:200:ILE:HD12	1.96	0.64
1:I:184:LEU:HG	1:I:228:PRO:HB3	1.77	0.64
1:L:141:ILE:HD11	1:L:313:TYR:CE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:THR:HG22	1:A:90:HIS:N	2.13	0.64
1:B:100:ARG:HE	1:B:102:ARG:NH1	1.95	0.64
1:I:261:THR:HG23	1:I:267:THR:CG2	2.14	0.64
1:J:15:ARG:HA	1:J:58:ARG:HH11	1.61	0.64
1:K:293:LEU:HD13	1:K:315:VAL:HG22	1.79	0.64
1:C:104:ARG:HG3	1:C:125:ILE:CD1	2.22	0.64
1:D:69:ILE:HA	1:D:72:ILE:HG22	1.79	0.64
1:E:137:LEU:HB3	1:E:141:ILE:HD11	1.78	0.64
1:G:278:GLU:CD	1:L:337:ARG:HH12	2.02	0.64
1:H:104:ARG:HH21	1:H:191:GLU:CD	2.05	0.64
1:I:48:VAL:O	1:I:51:ARG:N	2.27	0.64
1:D:261:THR:HG21	1:D:270:ARG:CG	2.11	0.64
1:D:264:VAL:HG11	1:D:340:VAL:CG1	2.25	0.64
1:F:9:MET:HE2	1:F:24:MET:HB2	1.79	0.64
1:F:352:LYS:HD2	1:F:365:TYR:OH	1.97	0.64
1:H:200:ILE:HG22	1:H:201:SER:HB3	1.79	0.64
1:J:125:ILE:CG1	1:J:126:PRO:HD2	2.27	0.64
1:L:25:LEU:HD23	1:L:36:ILE:HD13	1.79	0.64
1:D:69:ILE:HD12	1:D:72:ILE:CG2	2.28	0.64
1:E:186:TYR:OH	1:E:222:ASN:ND2	2.30	0.64
1:F:246:LEU:HD23	1:F:290:THR:HG21	1.77	0.64
1:G:94:ARG:HB3	1:G:99:VAL:O	1.98	0.64
1:L:131:LYS:HD3	1:L:171:ARG:NH2	2.12	0.64
1:L:197:ILE:HD12	1:L:197:ILE:H	1.63	0.64
1:J:70:ASN:OD1	1:J:78:THR:OG1	2.14	0.64
1:K:208:GLU:H	1:K:212:HIS:CD2	2.14	0.64
1:K:296:TRP:CE3	1:K:347:MET:HE2	2.33	0.64
1:A:97:ARG:HH11	1:A:97:ARG:HG3	1.62	0.63
1:B:166:LEU:HD11	1:B:258:THR:CG2	2.27	0.63
1:B:171:ARG:HG3	1:B:197:ILE:CD1	2.28	0.63
1:C:22:ASP:OD1	1:C:91:TYR:OH	2.16	0.63
1:G:180:ASN:CB	1:L:52:LEU:HB2	2.23	0.63
1:I:16:PHE:CZ	1:I:21:MET:HA	2.33	0.63
1:I:24:MET:HE2	1:I:44:ILE:HD12	1.75	0.63
1:L:261:THR:HG21	1:L:267:THR:HA	1.81	0.63
1:B:24:MET:HE2	1:B:44:ILE:HD13	1.79	0.63
1:C:166:LEU:HD13	1:C:232:MET:CE	2.28	0.63
1:E:9:MET:HA	1:E:27:HIS:CE1	2.33	0.63
1:J:121:THR:CG2	1:K:182:LYS:HZ1	2.11	0.63
1:K:7:ASN:HA	1:K:54:LYS:O	1.98	0.63
1:G:112:VAL:HG12	1:G:113:GLU:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:22:ASP:OD2	1:I:93:PHE:CD1	2.51	0.63
1:I:61:SER:CB	1:I:64:GLU:HG3	2.26	0.63
1:J:354:LYS:HG3	1:J:359:ILE:HD12	1.80	0.63
1:A:12:GLU:OE2	1:A:58:ARG:HB2	1.97	0.63
1:G:12:GLU:OE1	1:G:56:THR:HG23	1.98	0.63
1:G:122:LEU:N	1:G:122:LEU:HD12	2.14	0.63
1:I:182:LYS:HE2	1:I:184:LEU:HD21	1.81	0.63
1:K:171:ARG:CA	1:K:174:ILE:HG22	2.28	0.63
1:J:352:LYS:CA	1:J:365:TYR:CE1	2.80	0.63
1:L:275:PHE:CE2	1:L:283:ARG:HB3	2.32	0.63
1:F:111:LEU:HD12	1:F:115:HIS:C	2.23	0.63
1:C:111:LEU:C	1:C:111:LEU:HD13	2.23	0.63
1:C:166:LEU:CD2	1:C:232:MET:HE1	2.29	0.63
1:D:41:GLY:O	1:D:59:ARG:HD3	1.99	0.63
1:E:353:MET:HE3	1:E:353:MET:CA	2.26	0.63
1:G:46:ALA:HB2	1:G:55:ILE:HD12	1.78	0.63
1:I:141:ILE:O	1:I:145:ILE:HG23	1.99	0.63
1:K:137:LEU:HG	1:K:141:ILE:CD1	2.28	0.63
1:G:230:LEU:C	1:G:230:LEU:CD1	2.72	0.63
1:G:235:GLU:CB	1:G:258:THR:O	2.47	0.63
1:H:246:LEU:O	1:H:250:LEU:HD12	1.99	0.63
1:J:352:LYS:CA	1:J:365:TYR:HE1	2.12	0.63
1:B:48:VAL:HG23	1:B:48:VAL:O	1.98	0.63
1:B:48:VAL:CG2	1:B:53:LEU:HD11	2.29	0.63
1:B:209:ILE:O	1:B:213:LEU:O	2.15	0.63
1:G:155:THR:CG2	1:G:259:LEU:HB2	2.27	0.63
1:J:69:ILE:HA	1:J:72:ILE:CG2	2.29	0.63
1:K:17:THR:CG2	1:K:18:PRO:HD2	2.29	0.63
1:C:12:GLU:CD	1:C:56:THR:OG1	2.42	0.62
1:E:154:ILE:HG21	1:E:165:LEU:HD23	1.80	0.62
1:G:111:LEU:HD22	1:H:90:HIS:CE1	2.33	0.62
1:G:224:LEU:HD21	1:G:248:ALA:HA	1.81	0.62
1:J:13:PRO:HG3	1:J:20:PHE:HD1	1.63	0.62
1:E:349:TRP:CZ3	1:E:353:MET:HG3	2.35	0.62
1:F:361:SER:O	1:F:364:VAL:HG12	1.99	0.62
1:K:188:SER:O	1:K:208:GLU:HG3	1.98	0.62
1:G:367:LEU:O	1:G:367:LEU:HD23	1.99	0.62
1:I:131:LYS:O	1:I:134:THR:OG1	2.15	0.62
1:L:66:GLY:O	1:L:69:ILE:HG22	1.99	0.62
1:E:48:VAL:O	1:E:51:ARG:HG2	1.99	0.62
1:F:214:PRO:HB2	1:F:218:ASP:OD2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:14:THR:C	1:H:15:ARG:HE	2.03	0.62
1:J:125:ILE:HG13	1:J:126:PRO:HD2	1.82	0.62
1:K:269:ARG:HB2	1:K:333:THR:HG21	1.82	0.62
1:B:332:VAL:O	1:B:336:THR:HG23	1.99	0.62
1:D:209:ILE:O	1:D:213:LEU:O	2.16	0.62
1:E:44:ILE:H	1:E:56:THR:HG22	1.64	0.62
1:H:65:LEU:HD11	1:H:120:ILE:HD12	1.80	0.62
1:A:135:MET:HB3	1:A:137:LEU:CD1	2.29	0.62
1:F:236:CYS:SG	1:F:242:ILE:HG12	2.39	0.62
1:G:9:MET:HE1	1:G:24:MET:CB	2.30	0.62
1:G:348:THR:O	1:G:351:ALA:HB3	2.00	0.62
1:I:355:PHE:CE2	1:I:362:GLU:HG2	2.33	0.62
1:L:296:TRP:NE1	1:L:347:MET:HE3	2.14	0.62
1:B:102:ARG:NE	1:B:127:THR:HG22	2.14	0.62
1:B:249:ALA:CB	1:B:290:THR:HG21	2.29	0.62
1:C:81:LEU:HD11	1:C:87:ILE:CD1	2.30	0.62
1:E:7:ASN:O	1:E:8:LEU:HD23	2.00	0.62
1:G:230:LEU:CD2	1:G:256:TYR:HE1	2.13	0.62
1:G:352:LYS:O	1:G:355:PHE:HB2	1.98	0.62
1:K:171:ARG:O	1:K:174:ILE:CG2	2.48	0.62
1:G:268:MET:HG3	1:G:336:THR:HG21	1.80	0.62
1:H:230:LEU:HD23	1:H:230:LEU:C	2.24	0.62
1:J:172:GLU:O	1:J:176:THR:HG23	1.99	0.62
1:A:141:ILE:O	1:A:145:ILE:HG23	1.99	0.62
1:B:90:HIS:C	1:B:90:HIS:CD2	2.78	0.62
1:B:184:LEU:HD22	1:B:226:ARG:HH21	1.65	0.62
1:B:188:SER:HB3	1:B:189:PRO:HD2	1.82	0.62
1:D:69:ILE:HA	1:D:72:ILE:CG2	2.30	0.62
1:G:302:THR:OG1	1:G:304:ASP:OD1	2.07	0.62
1:H:81:LEU:HD21	1:H:87:ILE:HG13	1.81	0.62
1:I:230:LEU:CD1	1:I:256:TYR:CE1	2.82	0.62
1:I:354:LYS:O	1:I:357:GLN:N	2.33	0.62
1:L:264:VAL:HG22	1:L:294:CYS:SG	2.39	0.62
1:B:352:LYS:HA	1:B:365:TYR:HE1	1.64	0.61
1:C:236:CYS:SG	1:C:242:ILE:HG12	2.40	0.61
1:D:174:ILE:O	1:D:199:THR:HG21	2.00	0.61
1:D:307:ARG:NH2	1:E:251:THR:O	2.32	0.61
1:D:320:VAL:HG13	1:D:339:LEU:HD13	1.80	0.61
1:E:162:LYS:CD	1:E:258:THR:HB	2.21	0.61
1:E:317:ASP:OD1	1:E:318:GLU:N	2.31	0.61
1:F:22:ASP:O	1:F:26:GLU:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:ALA:HB2	1:G:315:VAL:CG1	2.30	0.61
1:I:197:ILE:HD12	1:I:197:ILE:H	1.65	0.61
1:I:355:PHE:CZ	1:I:362:GLU:CG	2.81	0.61
1:A:49:TYR:CE1	1:A:306:ARG:HG3	2.35	0.61
1:C:81:LEU:HD11	1:C:87:ILE:HD12	1.82	0.61
1:F:132:LEU:HD11	1:F:169:ILE:CD1	2.30	0.61
1:G:365:TYR:N	1:G:368:ILE:HD12	2.14	0.61
1:H:248:ALA:O	1:H:251:THR:HB	2.00	0.61
1:C:209:ILE:O	1:C:213:LEU:O	2.18	0.61
1:G:235:GLU:CA	1:G:258:THR:O	2.47	0.61
1:I:76:ASN:O	1:I:79:THR:OG1	2.15	0.61
1:L:27:HIS:O	1:L:30:SER:OG	2.17	0.61
1:D:249:ALA:HB1	1:D:290:THR:OG1	2.00	0.61
1:F:328:ASP:O	1:F:328:ASP:OD1	2.17	0.61
1:G:69:ILE:CG1	1:G:120:ILE:CD1	2.78	0.61
1:G:333:THR:O	1:G:336:THR:OG1	2.13	0.61
1:I:287:ILE:HG22	1:I:291:ILE:HD11	1.81	0.61
1:J:88:ASP:OD1	1:J:106:ASN:ND2	2.33	0.61
1:J:171:ARG:O	1:J:175:GLU:HB2	2.00	0.61
1:L:310:LEU:HD22	1:L:354:LYS:HG3	1.81	0.61
1:A:94:ARG:HH11	1:A:97:ARG:HA	1.66	0.61
1:C:132:LEU:HB2	1:C:172:GLU:CG	2.31	0.61
1:G:188:SER:O	1:G:208:GLU:HG3	2.00	0.61
1:J:37:THR:OG1	1:K:182:LYS:HE3	2.00	0.61
1:A:46:ALA:HB2	1:A:55:ILE:HD12	1.83	0.61
1:H:125:ILE:HD12	1:H:126:PRO:CD	2.25	0.61
1:J:174:ILE:HG23	1:J:175:GLU:N	2.16	0.61
1:A:224:LEU:HD21	1:A:248:ALA:HA	1.82	0.61
1:B:363:ARG:NH1	1:C:322:ASP:OD1	2.33	0.61
1:G:317:ASP:O	1:G:321:ARG:N	2.19	0.61
1:J:175:GLU:HG3	1:J:197:ILE:HG23	1.81	0.61
1:L:186:TYR:HB3	1:L:209:ILE:HD13	1.83	0.61
1:B:319:GLU:O	1:B:323:ILE:HG13	2.00	0.61
1:C:197:ILE:HD12	1:C:197:ILE:N	2.16	0.61
1:H:251:THR:HG22	1:H:253:HIS:CD2	2.35	0.61
1:I:21:MET:HE2	1:I:68:LEU:CD2	2.31	0.61
1:J:213:LEU:HD22	1:J:214:PRO:HD3	1.83	0.61
1:K:70:ASN:OD1	1:K:78:THR:HG23	2.00	0.61
1:A:261:THR:HG21	1:A:267:THR:N	2.16	0.61
1:I:86:ASP:CG	1:J:225:ARG:HH12	2.09	0.61
1:J:272:VAL:HG13	1:J:284:THR:CG2	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:208:GLU:HG2	1:K:210:PRO:HD2	1.83	0.61
1:K:262:SER:HB2	1:K:296:TRP:CZ2	2.35	0.61
1:L:355:PHE:CZ	1:L:362:GLU:HG3	2.36	0.61
1:A:365:TYR:CE1	1:A:369:ILE:HD11	2.35	0.60
1:C:188:SER:OG	1:C:189:PRO:HD3	2.01	0.60
1:C:188:SER:CB	1:C:189:PRO:HD3	2.30	0.60
1:D:99:VAL:HG12	1:D:100:ARG:N	2.16	0.60
1:E:188:SER:O	1:E:208:GLU:HG3	2.01	0.60
1:H:48:VAL:CG2	1:H:53:LEU:CD1	2.76	0.60
1:J:60:LEU:HD12	1:J:64:GLU:OE1	2.01	0.60
1:K:47:GLU:HG3	1:K:52:LEU:HD12	1.83	0.60
1:K:175:GLU:OE2	1:K:197:ILE:HD11	2.01	0.60
1:I:7:ASN:O	1:I:55:ILE:HA	2.01	0.60
1:I:34:SER:OG	1:I:35:ASP:OD1	2.12	0.60
1:I:116:ASP:OD1	1:J:211:ARG:NH2	2.34	0.60
1:A:119:GLN:HE22	1:B:182:LYS:CE	2.14	0.60
1:F:281:LEU:O	1:F:285:ILE:CD1	2.50	0.60
1:G:121:THR:C	1:G:122:LEU:HD12	2.26	0.60
1:I:132:LEU:CB	1:I:172:GLU:HG3	2.31	0.60
1:K:317:ASP:OD1	1:K:318:GLU:N	2.34	0.60
1:B:367:LEU:CD2	1:C:325:LEU:HD22	2.31	0.60
1:G:352:LYS:HG3	1:G:365:TYR:CZ	2.35	0.60
1:L:149:GLU:HG2	1:L:150:GLY:H	1.64	0.60
1:L:189:PRO:HA	1:L:208:GLU:OE2	2.01	0.60
1:E:34:SER:OG	1:E:35:ASP:OD1	2.12	0.60
1:E:188:SER:HA	1:E:210:PRO:HD3	1.83	0.60
1:F:212:HIS:O	1:F:213:LEU:HG	2.02	0.60
1:G:291:ILE:CG1	1:G:316:PHE:CE2	2.81	0.60
1:I:47:GLU:CA	1:I:52:LEU:HD23	2.31	0.60
1:I:174:ILE:CG1	1:I:202:ALA:CB	2.79	0.60
1:K:288:LEU:HB3	1:K:325:LEU:CD2	2.30	0.60
1:L:219:GLY:O	1:L:222:ASN:HB3	2.02	0.60
1:L:333:THR:HG23	1:L:334:SER:N	2.17	0.60
1:A:275:PHE:O	1:A:280:ARG:NE	2.31	0.60
1:B:116:ASP:OD2	1:C:211:ARG:NH1	2.34	0.60
1:B:209:ILE:N	1:B:210:PRO:HD2	2.17	0.60
1:K:270:ARG:O	1:K:274:SER:OG	2.20	0.60
1:I:132:LEU:HB2	1:I:172:GLU:CG	2.31	0.60
1:I:300:VAL:HG21	1:I:310:LEU:HD12	1.82	0.60
1:K:170:ILE:O	1:K:174:ILE:CG2	2.45	0.60
1:A:233:VAL:HB	1:A:257:THR:CG2	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:THR:OG1	1:A:253:HIS:HD2	1.84	0.60
1:A:268:MET:HG3	1:A:336:THR:HG21	1.84	0.60
1:E:275:PHE:O	1:E:280:ARG:HB2	2.02	0.60
1:F:236:CYS:SG	1:F:242:ILE:CG1	2.90	0.60
1:G:9:MET:HE1	1:G:24:MET:CA	2.31	0.60
1:G:119:GLN:NE2	1:H:182:LYS:HZ1	1.89	0.60
1:G:355:PHE:CZ	1:G:365:TYR:CB	2.84	0.60
1:G:355:PHE:CE2	1:G:365:TYR:HB2	2.36	0.60
1:J:191:GLU:HB3	1:J:192:PHE:CE1	2.36	0.60
1:J:264:VAL:CG1	1:J:340:VAL:HG11	2.32	0.60
1:F:111:LEU:HD12	1:F:115:HIS:O	2.02	0.60
1:F:208:GLU:N	1:F:212:HIS:HD2	2.00	0.60
1:H:230:LEU:HD23	1:H:231:ILE:N	2.17	0.60
1:I:188:SER:O	1:I:208:GLU:HG3	2.02	0.60
1:G:145:ILE:C	1:G:145:ILE:HD12	2.27	0.60
1:I:236:CYS:SG	1:I:242:ILE:CG1	2.90	0.60
1:A:341:ARG:HG2	1:A:346:LEU:HD21	1.84	0.59
1:C:300:VAL:HG11	1:C:368:ILE:HD11	1.84	0.59
1:D:170:ILE:O	1:D:174:ILE:HG22	2.02	0.59
1:D:355:PHE:HE1	1:D:362:GLU:HG3	1.67	0.59
1:E:40:THR:HG23	1:E:65:LEU:HD22	1.84	0.59
1:H:9:MET:HE3	1:H:24:MET:N	2.17	0.59
1:I:154:ILE:HG21	1:I:162:LYS:HB3	1.84	0.59
1:K:171:ARG:O	1:K:174:ILE:HG23	2.02	0.59
1:B:9:MET:HE3	1:B:24:MET:CA	2.32	0.59
1:C:236:CYS:SG	1:C:242:ILE:CG1	2.90	0.59
1:E:108:THR:CG2	1:F:226:ARG:HH21	2.05	0.59
1:F:314:LEU:HD23	1:F:315:VAL:C	2.27	0.59
1:G:235:GLU:HB2	1:G:258:THR:O	2.02	0.59
1:G:355:PHE:CE2	1:G:365:TYR:CB	2.85	0.59
1:J:146:ALA:HB2	1:J:173:LEU:HD21	1.85	0.59
1:K:352:LYS:HB2	1:K:365:TYR:OH	2.01	0.59
1:B:125:ILE:CD1	1:B:126:PRO:HD2	2.31	0.59
1:F:291:ILE:HD13	1:F:316:PHE:CZ	2.36	0.59
1:J:69:ILE:HA	1:J:72:ILE:HG22	1.85	0.59
1:J:238:ASP:OD1	1:J:241:THR:OG1	2.15	0.59
1:K:61:SER:HB3	1:K:64:GLU:OE1	2.02	0.59
1:C:78:THR:O	1:C:82:LEU:HG	2.02	0.59
1:F:259:LEU:HD13	1:F:267:THR:HG23	1.83	0.59
1:G:211:ARG:NH2	1:L:116:ASP:OD1	2.36	0.59
1:H:48:VAL:CG2	1:H:53:LEU:HD11	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:353:MET:CG	1:I:357:GLN:HE22	2.15	0.59
1:L:24:MET:SD	1:L:44:ILE:HG21	2.43	0.59
1:L:125:ILE:CD1	1:L:126:PRO:HD2	2.28	0.59
1:L:324:LEU:HD22	1:L:332:VAL:HG13	1.84	0.59
1:D:349:TRP:CZ2	1:D:353:MET:HE3	2.38	0.59
1:J:317:ASP:OD1	1:J:318:GLU:N	2.35	0.59
1:D:65:LEU:HB3	1:D:118:ILE:CG1	2.33	0.59
1:F:209:ILE:HD13	1:F:209:ILE:O	2.02	0.59
1:H:188:SER:OG	1:H:189:PRO:CD	2.42	0.59
1:C:171:ARG:O	1:C:174:ILE:HG22	2.03	0.59
1:I:155:THR:HG21	1:I:267:THR:HG21	1.84	0.59
1:I:365:TYR:O	1:I:368:ILE:CG1	2.51	0.59
1:J:216:PHE:O	1:J:220:VAL:HG23	2.02	0.59
1:L:73:TYR:CE1	1:L:87:ILE:HG23	2.38	0.59
1:B:272:VAL:HG13	1:B:284:THR:HG22	1.85	0.59
1:D:171:ARG:HG3	1:D:197:ILE:CD1	2.33	0.59
1:G:9:MET:HE1	1:G:24:MET:HA	1.84	0.59
1:I:319:GLU:OE2	1:I:343:LYS:NZ	2.35	0.59
1:B:365:TYR:CE2	1:B:369:ILE:HD11	2.38	0.59
1:E:44:ILE:H	1:E:56:THR:CG2	2.16	0.59
1:F:178:ASP:O	1:F:180:ASN:ND2	2.36	0.59
1:G:132:LEU:HD23	1:G:132:LEU:C	2.27	0.59
1:G:345:GLN:HB2	1:G:349:TRP:HZ3	1.68	0.59
1:H:27:HIS:HD2	1:H:55:ILE:CG2	2.16	0.59
1:K:16:PHE:CZ	1:K:24:MET:HE1	2.36	0.59
1:F:156:GLY:HA2	1:F:296:TRP:HZ3	1.66	0.58
1:I:81:LEU:HD11	1:I:87:ILE:CD1	2.33	0.58
1:K:12:GLU:CD	1:K:57:ASN:H	2.11	0.58
1:K:119:GLN:HE21	1:K:121:THR:HG23	1.67	0.58
1:A:9:MET:HA	1:A:27:HIS:CE1	2.38	0.58
1:A:350:ASP:OD1	1:A:354:LYS:NZ	2.28	0.58
1:B:46:ALA:HB2	1:B:55:ILE:CD1	2.31	0.58
1:E:21:MET:O	1:E:25:LEU:N	2.28	0.58
1:F:209:ILE:CG2	1:F:210:PRO:HD3	2.32	0.58
1:G:296:TRP:CH2	1:G:347:MET:HE1	2.38	0.58
1:H:92:GLU:CG	1:H:102:ARG:HG2	2.33	0.58
1:K:14:THR:OG1	1:K:15:ARG:N	2.32	0.58
1:L:314:LEU:HD23	1:L:315:VAL:C	2.28	0.58
1:F:180:ASN:HA	1:F:201:SER:O	2.03	0.58
1:J:40:THR:HG23	1:J:62:ASN:CA	2.33	0.58
1:J:145:ILE:HD12	1:J:293:LEU:CD2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:174:ILE:O	1:J:199:THR:HG21	2.03	0.58
1:E:353:MET:HA	1:E:353:MET:CE	2.22	0.58
1:J:9:MET:HG2	1:J:10:PRO:HD2	1.84	0.58
1:K:296:TRP:CZ3	1:K:347:MET:HE2	2.39	0.58
1:B:9:MET:CE	1:B:24:MET:HB2	2.34	0.58
1:D:92:GLU:OE2	1:D:102:ARG:NH1	2.37	0.58
1:E:166:LEU:HD13	1:E:232:MET:HE3	1.84	0.58
1:I:302:THR:HG21	1:I:308:VAL:HB	1.85	0.58
1:K:137:LEU:CD2	1:K:141:ILE:HD11	2.34	0.58
1:L:275:PHE:CE2	1:L:283:ARG:CD	2.87	0.58
1:B:365:TYR:CE2	1:B:369:ILE:CD1	2.87	0.58
1:F:73:TYR:CE1	1:F:89:THR:CG2	2.87	0.58
1:G:264:VAL:HG23	1:G:312:GLU:OE2	2.03	0.58
1:I:108:THR:CG2	1:J:222:ASN:HD21	2.00	0.58
1:J:26:GLU:OE1	1:J:95:PRO:HB2	2.02	0.58
1:J:353:MET:HE2	1:J:353:MET:H	1.67	0.58
1:K:44:ILE:CG2	1:K:55:ILE:HD11	2.33	0.58
1:K:222:ASN:O	1:K:225:ARG:N	2.35	0.58
1:B:102:ARG:HH21	1:B:127:THR:HB	1.68	0.58
1:D:10:PRO:HD3	1:D:27:HIS:ND1	2.18	0.58
1:E:209:ILE:HG13	1:E:216:PHE:CD1	2.38	0.58
1:G:170:ILE:HD12	1:G:194:TYR:OH	2.04	0.58
1:H:21:MET:CE	1:H:68:LEU:HB3	2.34	0.58
1:I:317:ASP:H	1:I:320:VAL:CG2	2.17	0.58
1:J:68:LEU:O	1:J:72:ILE:HG22	2.04	0.58
1:K:180:ASN:N	1:K:180:ASN:HD22	2.00	0.58
1:K:283:ARG:O	1:K:287:ILE:HG12	2.04	0.58
1:L:112:VAL:CG2	1:L:117:ALA:HB3	2.30	0.58
1:L:190:ILE:CG1	1:L:208:GLU:HG2	2.34	0.58
1:A:94:ARG:NE	1:A:100:ARG:HE	2.00	0.58
1:H:290:THR:O	1:H:292:ARG:NH2	2.37	0.58
1:H:370:ALA:O	1:H:371:GLY:C	2.47	0.58
1:I:104:ARG:CG	1:I:125:ILE:HD13	2.24	0.58
1:J:352:LYS:CG	1:J:365:TYR:OH	2.48	0.58
1:K:223:ALA:O	1:K:228:PRO:HD3	2.04	0.58
1:C:152:VAL:HG13	1:C:293:LEU:HD12	1.85	0.58
1:E:184:LEU:HG	1:E:228:PRO:HB3	1.86	0.58
1:K:184:LEU:HG	1:K:228:PRO:HB3	1.85	0.58
1:A:230:LEU:HD21	1:A:256:TYR:CE1	2.39	0.57
1:G:6:ILE:C	1:G:6:ILE:HD12	2.28	0.57
1:G:21:MET:CE	1:G:72:ILE:HD11	2.26	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:182:LYS:HZ1	1:J:226:ARG:HB3	1.69	0.57
1:L:173:LEU:HD22	1:L:181:ARG:NH2	2.19	0.57
1:E:355:PHE:HE2	1:E:362:GLU:HA	1.68	0.57
1:F:149:GLU:HG2	1:F:150:GLY:H	1.64	0.57
1:H:65:LEU:HD12	1:H:120:ILE:HD12	1.86	0.57
1:H:121:THR:HG21	1:I:182:LYS:HZ1	1.69	0.57
1:I:7:ASN:C	1:I:8:LEU:HD12	2.29	0.57
1:J:145:ILE:CD1	1:J:293:LEU:HD21	2.34	0.57
1:L:275:PHE:CD2	1:L:283:ARG:HB3	2.39	0.57
1:B:188:SER:O	1:B:208:GLU:HG3	2.04	0.57
1:E:80:GLN:O	1:E:83:SER:HB3	2.04	0.57
1:G:354:LYS:HB3	1:G:360:ILE:HD11	1.86	0.57
1:I:62:ASN:OD1	1:I:118:ILE:HD12	2.05	0.57
1:I:177:SER:CA	1:I:200:ILE:HD13	2.34	0.57
1:C:214:PRO:HG2	1:C:218:ASP:OD2	2.04	0.57
1:J:22:ASP:O	1:J:25:LEU:HB2	2.05	0.57
1:E:321:ARG:O	1:E:325:LEU:HG	2.05	0.57
1:F:219:GLY:O	1:F:222:ASN:HB3	2.04	0.57
1:K:194:TYR:CD2	1:K:204:VAL:HG11	2.40	0.57
1:A:46:ALA:HB2	1:A:55:ILE:CD1	2.35	0.57
1:C:209:ILE:N	1:C:210:PRO:HD2	2.19	0.57
1:E:93:PHE:HE2	1:E:95:PRO:HA	1.69	0.57
1:E:275:PHE:O	1:E:280:ARG:CB	2.52	0.57
1:G:21:MET:HE1	1:G:72:ILE:CD1	2.27	0.57
1:J:238:ASP:OD1	1:J:241:THR:HG23	2.04	0.57
1:L:27:HIS:CD2	1:L:31:LEU:HD13	2.39	0.57
1:L:40:THR:HG23	1:L:118:ILE:O	2.04	0.57
1:A:92:GLU:OE2	1:A:100:ARG:NH1	2.36	0.57
1:B:48:VAL:HG22	1:B:53:LEU:HD11	1.86	0.57
1:F:188:SER:HA	1:F:209:ILE:HG22	1.86	0.57
1:G:222:ASN:O	1:G:225:ARG:HG3	2.05	0.57
1:H:251:THR:CG2	1:H:253:HIS:CD2	2.87	0.57
1:I:110:CYS:O	1:J:212:HIS:CE1	2.55	0.57
1:K:171:ARG:O	1:K:175:GLU:HB2	2.04	0.57
1:A:119:GLN:NE2	1:B:182:LYS:HE2	2.16	0.57
1:A:184:LEU:HG	1:A:228:PRO:HB3	1.86	0.57
1:H:365:TYR:OH	1:H:369:ILE:HD11	2.04	0.57
1:I:81:LEU:HD11	1:I:87:ILE:HD12	1.85	0.57
1:I:111:LEU:HD12	1:J:190:ILE:HD12	1.85	0.57
1:K:25:LEU:CD1	1:K:93:PHE:CE2	2.88	0.57
1:K:111:LEU:HD11	1:L:90:HIS:NE2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:HG22	1:A:162:LYS:HB3	1.87	0.57
1:A:320:VAL:HG13	1:A:339:LEU:HD13	1.87	0.57
1:F:313:TYR:HE2	1:F:345:GLN:NE2	2.02	0.57
1:G:122:LEU:N	1:G:122:LEU:CD1	2.68	0.57
1:G:144:ALA:CB	1:G:315:VAL:HG13	2.35	0.57
1:G:235:GLU:CB	1:G:258:THR:OG1	2.52	0.57
1:I:13:PRO:CG	1:I:20:PHE:CD2	2.88	0.57
1:I:197:ILE:H	1:I:197:ILE:CD1	2.17	0.57
1:K:281:LEU:HD12	1:K:281:LEU:O	2.05	0.57
1:L:317:ASP:OD1	1:L:318:GLU:N	2.38	0.57
1:B:171:ARG:HG3	1:B:197:ILE:HD13	1.86	0.57
1:C:34:SER:O	1:C:124:THR:HG23	2.05	0.57
1:C:48:VAL:HG12	1:C:49:TYR:HD2	1.70	0.57
1:C:333:THR:O	1:C:336:THR:OG1	2.14	0.57
1:E:43:PRO:HG2	1:E:54:LYS:HD3	1.85	0.57
1:G:126:PRO:HB2	1:G:192:PHE:CE1	2.39	0.57
1:G:260:HIS:CD2	1:G:261:THR:CG2	2.88	0.57
1:I:179:SER:HB2	1:I:181:ARG:NH2	2.20	0.57
1:J:92:GLU:OE2	1:J:102:ARG:NH2	2.38	0.57
1:K:25:LEU:HD13	1:K:93:PHE:HE2	1.69	0.57
1:L:320:VAL:HG13	1:L:339:LEU:HD12	1.87	0.57
1:E:150:GLY:HA3	1:E:292:ARG:HD2	1.86	0.56
1:F:49:TYR:CD1	1:F:50:GLY:N	2.71	0.56
1:I:197:ILE:N	1:I:197:ILE:CD1	2.68	0.56
1:C:131:LYS:O	1:C:134:THR:OG1	2.22	0.56
1:D:111:LEU:HD22	1:D:115:HIS:O	2.05	0.56
1:H:185:THR:HG22	1:H:232:MET:HB3	1.86	0.56
1:H:229:ARG:HG2	1:H:229:ARG:HH21	1.68	0.56
1:H:276:SER:O	1:H:280:ARG:HB2	2.05	0.56
1:K:93:PHE:CE2	1:K:103:TYR:CE1	2.93	0.56
1:L:40:THR:HG23	1:L:65:LEU:HD23	1.86	0.56
1:A:297:GLN:HG3	1:A:311:ARG:HG2	1.86	0.56
1:B:21:MET:SD	1:B:68:LEU:HD22	2.45	0.56
1:C:104:ARG:CD	1:C:125:ILE:HD11	2.34	0.56
1:D:184:LEU:HG	1:D:228:PRO:HB3	1.87	0.56
1:D:246:LEU:HD23	1:D:290:THR:HG21	1.87	0.56
1:D:355:PHE:CE1	1:D:362:GLU:HG3	2.40	0.56
1:E:9:MET:HG2	1:E:10:PRO:HD2	1.86	0.56
1:E:17:THR:HG22	1:E:18:PRO:HD2	1.87	0.56
1:E:223:ALA:O	1:E:228:PRO:HD3	2.04	0.56
1:E:288:LEU:HB3	1:E:325:LEU:HD21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:ILE:HB	1:F:56:THR:HG23	1.87	0.56
1:G:208:GLU:H	1:G:212:HIS:CD2	2.21	0.56
1:I:22:ASP:HB3	1:I:93:PHE:CE2	2.40	0.56
1:K:89:THR:HG23	1:K:105:VAL:CG1	2.34	0.56
1:A:211:ARG:O	1:F:84:GLY:HA2	2.06	0.56
1:C:355:PHE:CE1	1:C:362:GLU:HG2	2.31	0.56
1:G:46:ALA:HB2	1:G:55:ILE:CD1	2.34	0.56
1:I:22:ASP:OD2	1:I:93:PHE:CZ	2.58	0.56
1:L:61:SER:O	1:L:64:GLU:N	2.38	0.56
1:L:365:TYR:CZ	1:L:369:ILE:HD11	2.40	0.56
1:A:25:LEU:HD23	1:A:36:ILE:CD1	2.36	0.56
1:A:306:ARG:HG2	1:A:307:ARG:H	1.71	0.56
1:B:279:GLU:O	1:B:283:ARG:HG2	2.05	0.56
1:C:166:LEU:HD12	1:C:167:ALA:N	2.20	0.56
1:D:86:ASP:OD1	1:D:87:ILE:N	2.39	0.56
1:I:174:ILE:HG12	1:I:202:ALA:HB3	1.87	0.56
1:I:367:LEU:HD23	1:I:368:ILE:N	2.19	0.56
1:J:102:ARG:NE	1:J:193:VAL:HG21	2.20	0.56
1:L:297:GLN:OE1	1:L:311:ARG:NH2	2.37	0.56
1:A:182:LYS:HD2	1:F:37:THR:HG21	1.88	0.56
1:A:340:VAL:HG12	1:A:346:LEU:CD1	2.36	0.56
1:C:361:SER:HB3	1:C:364:VAL:CG2	2.34	0.56
1:F:135:MET:HB3	1:F:137:LEU:HD13	1.88	0.56
1:G:5:ASN:C	1:G:6:ILE:HG23	2.31	0.56
1:G:291:ILE:HG21	1:G:316:PHE:CE2	2.41	0.56
1:H:209:ILE:N	1:H:210:PRO:HD2	2.21	0.56
1:J:171:ARG:C	1:J:174:ILE:HG22	2.31	0.56
1:L:333:THR:HG23	1:L:334:SER:H	1.70	0.56
1:L:337:ARG:O	1:L:340:VAL:CG2	2.53	0.56
1:B:132:LEU:HB2	1:B:172:GLU:HG3	1.88	0.56
1:B:367:LEU:HD23	1:C:325:LEU:HD22	1.88	0.56
1:E:8:LEU:CD1	1:E:31:LEU:HD11	2.36	0.56
1:E:23:ARG:NH1	1:E:26:GLU:OE1	2.39	0.56
1:F:283:ARG:O	1:F:287:ILE:HG13	2.06	0.56
1:G:89:THR:CG2	1:G:90:HIS:H	2.18	0.56
1:G:320:VAL:CG1	1:G:339:LEU:HD13	2.35	0.56
1:A:94:ARG:HD3	1:A:96:ASN:O	2.06	0.56
1:A:126:PRO:O	1:A:191:GLU:O	2.23	0.56
1:A:288:LEU:O	1:A:321:ARG:HD2	2.06	0.56
1:H:58:ARG:NH2	1:H:58:ARG:HB3	2.21	0.56
1:H:68:LEU:HD23	1:H:68:LEU:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:276:SER:O	1:H:280:ARG:N	2.37	0.56
1:J:174:ILE:C	1:J:199:THR:HG21	2.31	0.56
1:A:142:ILE:HA	1:A:145:ILE:HG12	1.87	0.56
1:C:166:LEU:HD22	1:C:232:MET:HE1	1.87	0.56
1:E:17:THR:CG2	1:E:18:PRO:CD	2.84	0.56
1:E:208:GLU:N	1:E:212:HIS:HD2	1.92	0.56
1:B:55:ILE:O	1:B:55:ILE:HG22	2.06	0.56
1:D:365:TYR:O	1:D:369:ILE:HG22	2.05	0.56
1:E:108:THR:CG2	1:F:226:ARG:HH22	2.11	0.56
1:I:68:LEU:O	1:I:72:ILE:HG13	2.06	0.56
1:J:185:THR:HG22	1:J:232:MET:HB3	1.88	0.56
1:K:21:MET:HE2	1:K:68:LEU:HG	1.88	0.56
1:K:329:PRO:O	1:K:332:VAL:HG13	2.06	0.56
1:A:37:THR:HG21	1:B:182:LYS:HD2	1.86	0.55
1:D:174:ILE:HG12	1:D:199:THR:CG2	2.31	0.55
1:D:188:SER:HB3	1:D:189:PRO:HD3	1.88	0.55
1:E:102:ARG:NH1	1:E:127:THR:HG21	2.21	0.55
1:E:275:PHE:O	1:E:280:ARG:HG3	2.06	0.55
1:H:355:PHE:CZ	1:H:362:GLU:HG3	2.41	0.55
1:J:299:LEU:HA	1:J:308:VAL:O	2.06	0.55
1:B:102:ARG:HE	1:B:127:THR:HA	1.70	0.55
1:E:10:PRO:HG2	1:E:11:ASP:OD1	2.05	0.55
1:H:81:LEU:CD2	1:H:87:ILE:HG13	2.36	0.55
1:K:93:PHE:CE2	1:K:103:TYR:HE1	2.23	0.55
1:K:169:ILE:O	1:K:172:GLU:HB3	2.06	0.55
1:C:149:GLU:O	1:C:292:ARG:CD	2.53	0.55
1:D:155:THR:HB	1:D:261:THR:O	2.06	0.55
1:G:144:ALA:HB2	1:G:315:VAL:HG11	1.89	0.55
1:G:355:PHE:HE2	1:G:365:TYR:CG	2.21	0.55
1:H:121:THR:HG21	1:I:182:LYS:NZ	2.20	0.55
1:H:240:GLU:H	1:H:240:GLU:CD	2.12	0.55
1:J:209:ILE:HD11	1:J:215:ASN:O	2.05	0.55
1:J:349:TRP:CE3	1:J:353:MET:HE3	2.42	0.55
1:K:173:LEU:HD22	1:K:181:ARG:NE	2.21	0.55
1:B:249:ALA:HB3	1:B:290:THR:HG21	1.88	0.55
1:F:93:PHE:O	1:F:93:PHE:CD1	2.60	0.55
1:F:132:LEU:CD1	1:F:169:ILE:CD1	2.83	0.55
1:G:34:SER:O	1:G:124:THR:HG23	2.07	0.55
1:G:288:LEU:CD1	1:G:325:LEU:HD23	2.36	0.55
1:G:367:LEU:HD23	1:G:367:LEU:C	2.32	0.55
1:B:259:LEU:HD12	1:B:267:THR:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:LEU:HD23	1:D:118:ILE:O	2.06	0.55
1:F:9:MET:HE2	1:F:24:MET:CB	2.36	0.55
1:G:25:LEU:HD23	1:G:36:ILE:CD1	2.37	0.55
1:J:10:PRO:CD	1:J:27:HIS:CD2	2.84	0.55
1:G:361:SER:HB3	1:G:364:VAL:HG23	1.88	0.55
1:H:104:ARG:HD3	1:H:191:GLU:CD	2.31	0.55
1:H:312:GLU:HB2	1:H:347:MET:N	2.22	0.55
1:I:171:ARG:HA	1:I:174:ILE:HG22	1.88	0.55
1:A:251:THR:OG1	1:A:253:HIS:CD2	2.60	0.55
1:G:365:TYR:CZ	1:G:369:ILE:HD11	2.41	0.55
1:I:230:LEU:CD1	1:I:256:TYR:CD1	2.90	0.55
1:J:45:PHE:CD2	1:J:52:LEU:HG	2.35	0.55
1:A:130:PRO:CB	1:A:135:MET:HE3	2.33	0.55
1:B:93:PHE:CD1	1:B:93:PHE:C	2.85	0.55
1:B:102:ARG:HB2	1:B:125:ILE:CG2	2.37	0.55
1:E:7:ASN:C	1:E:8:LEU:CG	2.79	0.55
1:F:166:LEU:HD13	1:F:232:MET:SD	2.47	0.55
1:I:247:GLU:O	1:I:251:THR:HG23	2.07	0.55
1:I:272:VAL:HG13	1:I:284:THR:CG2	2.31	0.55
1:J:140:ASN:H	1:J:140:ASN:ND2	2.05	0.55
1:L:73:TYR:CD1	1:L:87:ILE:HG23	2.42	0.55
1:A:203:VAL:CG1	1:F:42:GLU:OE1	2.55	0.55
1:E:43:PRO:CG	1:E:54:LYS:HD3	2.37	0.55
1:G:320:VAL:HG13	1:G:339:LEU:HD13	1.88	0.55
1:H:261:THR:CG2	1:H:270:ARG:HD2	2.36	0.55
1:A:230:LEU:HD13	1:A:230:LEU:C	2.31	0.55
1:B:92:GLU:HA	1:B:101:TYR:O	2.07	0.55
1:C:186:TYR:CE2	1:C:219:GLY:CA	2.90	0.55
1:F:27:HIS:O	1:F:30:SER:OG	2.20	0.55
1:F:102:ARG:C	1:F:125:ILE:HG22	2.32	0.55
1:F:291:ILE:CD1	1:F:316:PHE:CE1	2.90	0.55
1:I:352:LYS:HD2	1:I:365:TYR:OH	2.06	0.55
1:K:36:ILE:HD12	1:K:36:ILE:N	2.22	0.55
1:K:149:GLU:OE1	1:K:149:GLU:N	2.40	0.55
1:L:273:THR:O	1:L:275:PHE:N	2.40	0.55
1:B:280:ARG:O	1:B:284:THR:CG2	2.42	0.54
1:E:89:THR:HG23	1:E:105:VAL:HG13	1.87	0.54
1:G:94:ARG:CB	1:G:99:VAL:O	2.55	0.54
1:H:340:VAL:HG23	1:H:346:LEU:CD2	2.38	0.54
1:J:24:MET:CE	1:J:25:LEU:HD23	2.30	0.54
1:A:105:VAL:HG12	1:A:122:LEU:HG	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:THR:C	1:A:125:ILE:HD13	2.32	0.54
1:B:9:MET:HE3	1:B:24:MET:N	2.22	0.54
1:D:104:ARG:NE	1:D:123:ARG:HH11	2.05	0.54
1:D:172:GLU:O	1:D:176:THR:HG23	2.07	0.54
1:H:181:ARG:HG2	1:H:229:ARG:CG	2.37	0.54
1:I:209:ILE:N	1:I:210:PRO:HD2	2.22	0.54
1:J:69:ILE:HD12	1:J:72:ILE:CG2	2.37	0.54
1:J:170:ILE:O	1:J:174:ILE:HG22	2.08	0.54
1:A:135:MET:CB	1:A:137:LEU:CD1	2.85	0.54
1:H:70:ASN:OD1	1:H:78:THR:OG1	2.22	0.54
1:K:238:ASP:O	1:K:242:ILE:HG13	2.07	0.54
1:G:174:ILE:CD1	1:G:202:ALA:CB	2.85	0.54
1:G:230:LEU:CD2	1:G:256:TYR:CE1	2.86	0.54
1:G:288:LEU:HD13	1:G:325:LEU:HD23	1.90	0.54
1:K:298:LYS:HB2	1:K:347:MET:HE1	1.90	0.54
1:L:17:THR:HG23	1:L:18:PRO:CD	2.34	0.54
1:L:132:LEU:HD23	1:L:172:GLU:OE1	2.07	0.54
1:C:21:MET:HE1	1:C:72:ILE:CD1	2.28	0.54
1:D:296:TRP:CE3	1:D:347:MET:CE	2.91	0.54
1:E:116:ASP:OD1	1:F:211:ARG:NH1	2.37	0.54
1:E:319:GLU:O	1:E:323:ILE:HG13	2.07	0.54
1:F:8:LEU:O	1:F:27:HIS:CE1	2.54	0.54
1:G:184:LEU:HD22	1:G:226:ARG:HH21	1.73	0.54
1:H:13:PRO:HB2	1:H:15:ARG:O	2.08	0.54
1:B:9:MET:SD	1:B:24:MET:HB2	2.48	0.54
1:D:156:GLY:O	1:D:162:LYS:NZ	2.40	0.54
1:F:180:ASN:ND2	1:F:180:ASN:H	2.06	0.54
1:G:229:ARG:NE	1:G:229:ARG:HA	2.22	0.54
1:I:55:ILE:HD13	1:I:55:ILE:N	2.19	0.54
1:I:174:ILE:CG1	1:I:202:ALA:HB3	2.38	0.54
1:J:25:LEU:CD1	1:J:93:PHE:CE2	2.90	0.54
1:K:171:ARG:NE	1:K:197:ILE:HD11	2.23	0.54
1:B:95:PRO:HD2	1:B:99:VAL:O	2.08	0.54
1:E:174:ILE:HG13	1:E:202:ALA:CB	2.37	0.54
1:J:95:PRO:HD2	1:J:99:VAL:O	2.07	0.54
1:C:251:THR:OG1	1:C:253:HIS:HD2	1.91	0.54
1:C:261:THR:HG21	1:C:267:THR:N	2.23	0.54
1:G:296:TRP:CZ3	1:G:347:MET:SD	3.01	0.54
1:G:355:PHE:HE2	1:G:365:TYR:HB2	1.73	0.54
1:J:102:ARG:NH1	1:J:127:THR:CG2	2.70	0.54
1:J:116:ASP:OD1	1:K:211:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:141:ILE:HG22	1:L:145:ILE:HD13	1.89	0.54
1:L:291:ILE:CD1	1:L:316:PHE:CE1	2.90	0.54
1:A:155:THR:HG21	1:A:267:THR:CG2	2.31	0.54
1:B:26:GLU:OE1	1:B:95:PRO:HB3	2.08	0.54
1:E:320:VAL:HG23	1:E:321:ARG:N	2.23	0.54
1:G:345:GLN:CG	1:G:349:TRP:CZ3	2.90	0.54
1:L:304:ASP:OD1	1:L:304:ASP:N	2.41	0.54
1:B:366:LYS:HD3	1:B:366:LYS:C	2.33	0.54
1:C:9:MET:HA	1:C:27:HIS:CE1	2.43	0.54
1:D:17:THR:OG1	1:D:20:PHE:HD2	1.91	0.54
1:D:65:LEU:HB3	1:D:118:ILE:HG12	1.89	0.54
1:H:119:GLN:OE1	1:I:205:SER:CB	2.55	0.54
1:J:191:GLU:OE2	1:J:192:PHE:HE1	1.91	0.54
1:J:365:TYR:CE2	1:J:369:ILE:CD1	2.84	0.54
1:B:5:ASN:CB	1:B:51:ARG:NH2	2.71	0.53
1:C:108:THR:HG21	1:D:222:ASN:HD21	1.73	0.53
1:F:361:SER:O	1:F:364:VAL:CG1	2.56	0.53
1:G:260:HIS:CD2	1:G:261:THR:HG23	2.43	0.53
1:I:293:LEU:HD13	1:I:315:VAL:HG22	1.90	0.53
1:J:104:ARG:NE	1:J:123:ARG:HH11	2.07	0.53
1:L:105:VAL:HG22	1:L:122:LEU:HG	1.90	0.53
1:L:352:LYS:HA	1:L:365:TYR:CE1	2.43	0.53
1:D:171:ARG:O	1:D:174:ILE:HG22	2.08	0.53
1:H:86:ASP:OD2	1:I:225:ARG:NH1	2.38	0.53
1:H:348:THR:CG2	1:H:372:ALA:HB3	2.39	0.53
1:I:10:PRO:HG2	1:I:11:ASP:OD1	2.08	0.53
1:K:349:TRP:O	1:K:353:MET:HG2	2.09	0.53
1:K:361:SER:HB2	1:K:364:VAL:CG2	2.37	0.53
1:D:125:ILE:CD1	1:D:126:PRO:HD2	2.38	0.53
1:F:38:ILE:HG12	1:F:44:ILE:HD13	1.90	0.53
1:G:296:TRP:CH2	1:G:347:MET:CE	2.90	0.53
1:J:86:ASP:OD1	1:J:87:ILE:N	2.41	0.53
1:H:198:GLU:OE1	1:H:198:GLU:HA	2.07	0.53
1:I:184:LEU:CG	1:I:228:PRO:HB3	2.39	0.53
1:J:171:ARG:O	1:J:174:ILE:HG22	2.09	0.53
1:K:349:TRP:CZ3	1:K:353:MET:HG3	2.43	0.53
1:A:94:ARG:NH1	1:A:97:ARG:HD2	2.17	0.53
1:B:185:THR:HG22	1:B:232:MET:HB3	1.91	0.53
1:B:352:LYS:CA	1:B:365:TYR:HE1	2.22	0.53
1:D:302:THR:OG1	1:D:306:ARG:O	2.19	0.53
1:D:312:GLU:HB2	1:D:347:MET:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:GLU:OE1	1:E:149:GLU:N	2.41	0.53
1:J:132:LEU:CD2	1:J:137:LEU:HD12	2.39	0.53
1:K:40:THR:CG2	1:K:65:LEU:CD2	2.80	0.53
1:L:188:SER:HB2	1:L:189:PRO:HD3	1.91	0.53
1:A:179:SER:HB2	1:A:181:ARG:NH2	2.24	0.53
1:A:355:PHE:HB2	1:A:360:ILE:HG21	1.90	0.53
1:G:203:VAL:HG12	1:L:39:GLN:HE22	1.74	0.53
1:H:125:ILE:CD1	1:H:126:PRO:HD2	2.29	0.53
1:I:355:PHE:CE2	1:I:362:GLU:CA	2.61	0.53
1:J:25:LEU:HD13	1:J:93:PHE:HE2	1.74	0.53
1:K:39:GLN:C	1:K:65:LEU:HD21	2.33	0.53
1:D:72:ILE:HD13	1:D:105:VAL:HG11	1.90	0.53
1:D:222:ASN:OD1	1:D:226:ARG:NH1	2.42	0.53
1:F:276:SER:O	1:F:280:ARG:HB2	2.09	0.53
1:F:291:ILE:HD11	1:F:316:PHE:CE1	2.42	0.53
1:H:102:ARG:CZ	1:H:193:VAL:CG2	2.87	0.53
1:H:229:ARG:O	1:H:229:ARG:HD3	2.09	0.53
1:I:9:MET:HE3	1:I:12:GLU:HG3	1.91	0.53
1:J:349:TRP:CD2	1:J:353:MET:HE3	2.44	0.53
1:D:184:LEU:HD22	1:D:226:ARG:HH21	1.73	0.53
1:F:285:ILE:HD12	1:F:285:ILE:N	2.24	0.53
1:G:94:ARG:HB3	1:G:100:ARG:HG2	1.89	0.53
1:G:144:ALA:CB	1:G:315:VAL:CG1	2.86	0.53
1:G:271:LEU:O	1:G:274:SER:OG	2.20	0.53
1:K:288:LEU:HB2	1:K:325:LEU:CD2	2.38	0.53
1:A:97:ARG:HG3	1:A:97:ARG:NH1	2.24	0.53
1:B:132:LEU:HB2	1:B:172:GLU:CG	2.39	0.53
1:C:197:ILE:N	1:C:197:ILE:CD1	2.71	0.53
1:C:300:VAL:CG1	1:C:301:PRO:HD2	2.39	0.53
1:D:100:ARG:HH21	1:D:100:ARG:HG3	1.74	0.53
1:D:145:ILE:HG12	1:D:169:ILE:HD12	1.91	0.53
1:D:248:ALA:O	1:D:253:HIS:HD2	1.92	0.53
1:J:209:ILE:O	1:J:213:LEU:N	2.35	0.53
1:K:34:SER:OG	1:K:35:ASP:OD1	2.13	0.53
1:A:94:ARG:NE	1:A:100:ARG:HG2	2.17	0.53
1:B:319:GLU:HG2	1:B:320:VAL:N	2.23	0.53
1:C:88:ASP:OD2	1:D:225:ARG:HD2	2.09	0.53
1:C:186:TYR:CD2	1:C:219:GLY:HA3	2.43	0.53
1:G:28:ALA:CB	1:G:36:ILE:HD11	2.39	0.53
1:I:21:MET:HE2	1:I:68:LEU:HD23	1.88	0.53
1:L:90:HIS:CD2	1:L:102:ARG:NH2	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:276:SER:O	1:L:280:ARG:HB2	2.09	0.53
1:A:28:ALA:CB	1:A:36:ILE:HD11	2.39	0.52
1:C:270:ARG:NH1	1:D:289:GLU:OE2	2.42	0.52
1:D:35:ASP:OD2	1:E:227:LYS:CD	2.56	0.52
1:H:261:THR:CG2	1:H:270:ARG:CD	2.87	0.52
1:I:184:LEU:CD1	1:I:228:PRO:HG3	2.33	0.52
1:J:40:THR:OG1	1:J:117:ALA:HB1	2.09	0.52
1:J:264:VAL:HG23	1:J:294:CYS:SG	2.48	0.52
1:K:111:LEU:CD1	1:L:90:HIS:CE1	2.92	0.52
1:K:155:THR:O	1:K:296:TRP:HA	2.08	0.52
1:K:171:ARG:C	1:K:174:ILE:CG2	2.82	0.52
1:K:319:GLU:O	1:K:323:ILE:HG13	2.08	0.52
1:C:171:ARG:HA	1:C:174:ILE:HG22	1.92	0.52
1:C:185:THR:HG22	1:C:232:MET:HB3	1.90	0.52
1:D:40:THR:HG23	1:D:65:LEU:HD22	1.84	0.52
1:D:248:ALA:O	1:D:251:THR:OG1	2.28	0.52
1:E:93:PHE:CD2	1:E:94:ARG:N	2.78	0.52
1:F:11:ASP:O	1:F:13:PRO:HD3	2.09	0.52
1:H:119:GLN:NE2	1:I:182:LYS:HE3	2.23	0.52
1:I:16:PHE:CZ	1:I:21:MET:N	2.77	0.52
1:I:230:LEU:HD11	1:I:256:TYR:CE1	2.42	0.52
1:J:16:PHE:CD2	1:J:60:LEU:HD11	2.44	0.52
1:L:132:LEU:CD2	1:L:172:GLU:OE1	2.58	0.52
1:L:141:ILE:HD11	1:L:313:TYR:CD1	2.45	0.52
1:A:25:LEU:HD23	1:A:36:ILE:HD13	1.91	0.52
1:G:260:HIS:CD2	1:G:261:THR:N	2.77	0.52
1:G:352:LYS:HA	1:G:355:PHE:CD2	2.45	0.52
1:I:355:PHE:HZ	1:I:362:GLU:HG2	1.63	0.52
1:J:212:HIS:O	1:J:213:LEU:HD23	2.09	0.52
1:K:188:SER:OG	1:K:189:PRO:HD3	2.08	0.52
1:B:24:MET:SD	1:B:25:LEU:HD23	2.49	0.52
1:D:69:ILE:HD12	1:D:72:ILE:HG23	1.92	0.52
1:F:290:THR:O	1:F:292:ARG:NH2	2.43	0.52
1:G:155:THR:HG23	1:G:259:LEU:C	2.35	0.52
1:G:313:TYR:CE2	1:G:345:GLN:CD	2.87	0.52
1:H:19:VAL:HG23	1:H:20:PHE:H	1.73	0.52
1:H:68:LEU:N	1:H:68:LEU:CD2	2.73	0.52
1:H:183:VAL:HG13	1:H:230:LEU:HD22	1.91	0.52
1:I:302:THR:CG2	1:I:308:VAL:HB	2.39	0.52
1:J:263:GLY:HA3	1:J:266:GLU:HG2	1.92	0.52
1:A:185:THR:HG22	1:A:232:MET:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLU:CG	1:A:210:PRO:HD2	2.39	0.52
1:B:279:GLU:HG2	1:B:283:ARG:HG2	1.91	0.52
1:B:312:GLU:HB2	1:B:347:MET:N	2.25	0.52
1:B:365:TYR:C	1:B:365:TYR:CD2	2.87	0.52
1:C:17:THR:CG2	1:C:18:PRO:CD	2.87	0.52
1:G:180:ASN:HD22	1:G:180:ASN:H	1.57	0.52
1:H:99:VAL:HG12	1:H:100:ARG:N	2.24	0.52
1:H:137:LEU:HD11	1:H:311:ARG:CZ	2.39	0.52
1:K:23:ARG:NH1	1:K:26:GLU:OE2	2.42	0.52
1:K:230:LEU:HD23	1:K:230:LEU:C	2.35	0.52
1:L:186:TYR:HB3	1:L:209:ILE:CD1	2.40	0.52
1:G:131:LYS:CG	1:G:171:ARG:NH1	2.73	0.52
1:H:181:ARG:HG2	1:H:229:ARG:HG3	1.91	0.52
1:I:61:SER:N	1:I:64:GLU:OE1	2.41	0.52
1:J:302:THR:OG1	1:J:306:ARG:O	2.27	0.52
1:K:292:ARG:HG3	1:K:292:ARG:NH2	2.20	0.52
1:L:291:ILE:HD13	1:L:316:PHE:CZ	2.44	0.52
1:B:337:ARG:CZ	1:B:341:ARG:NH1	2.73	0.52
1:D:296:TRP:CH2	1:D:347:MET:HE3	2.45	0.52
1:F:9:MET:HA	1:F:27:HIS:CE1	2.45	0.52
1:A:17:THR:CG2	1:A:18:PRO:CD	2.88	0.52
1:A:263:GLY:O	1:A:267:THR:HG23	2.09	0.52
1:A:300:VAL:HG21	1:A:368:ILE:HD11	1.89	0.52
1:D:12:GLU:OE2	1:D:58:ARG:HB2	2.09	0.52
1:D:21:MET:O	1:D:25:LEU:HG	2.09	0.52
1:D:159:GLY:O	1:D:299:LEU:HD12	2.10	0.52
1:J:312:GLU:HB2	1:J:347:MET:N	2.25	0.52
1:K:90:HIS:CD2	1:K:104:ARG:HG3	2.45	0.52
1:D:40:THR:HG21	1:D:117:ALA:HB1	1.91	0.52
1:G:365:TYR:CE1	1:G:369:ILE:HD11	2.45	0.52
1:H:275:PHE:CD1	1:H:283:ARG:HG3	2.45	0.52
1:I:44:ILE:H	1:I:56:THR:CG2	2.23	0.52
1:I:119:GLN:HE22	1:J:182:LYS:HE2	1.74	0.52
1:J:263:GLY:HA3	1:J:266:GLU:CG	2.40	0.52
1:L:41:GLY:C	1:L:42:GLU:HG2	2.34	0.52
1:L:187:GLU:O	1:L:209:ILE:N	2.36	0.52
1:B:21:MET:CE	1:B:72:ILE:HD11	2.31	0.52
1:H:27:HIS:CD2	1:H:55:ILE:HG23	2.45	0.52
1:J:25:LEU:HD13	1:J:93:PHE:CE2	2.44	0.52
1:K:208:GLU:CG	1:K:210:PRO:HD2	2.39	0.52
1:K:333:THR:O	1:K:336:THR:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:SER:HB2	1:F:119:GLN:OE1	2.10	0.51
1:H:27:HIS:CD2	1:H:55:ILE:CG2	2.93	0.51
1:I:184:LEU:CD1	1:I:228:PRO:CG	2.88	0.51
1:J:21:MET:O	1:J:25:LEU:HG	2.10	0.51
1:A:223:ALA:O	1:A:228:PRO:CD	2.59	0.51
1:A:261:THR:HG21	1:A:266:GLU:C	2.35	0.51
1:C:319:GLU:O	1:C:323:ILE:HG13	2.10	0.51
1:D:44:ILE:HG22	1:D:55:ILE:HD11	1.91	0.51
1:D:349:TRP:CZ3	1:D:353:MET:HE3	2.45	0.51
1:E:154:ILE:CG2	1:E:165:LEU:HD23	2.39	0.51
1:E:297:GLN:NE2	1:E:311:ARG:NE	2.58	0.51
1:F:209:ILE:CG2	1:F:210:PRO:CD	2.87	0.51
1:G:25:LEU:HD23	1:G:36:ILE:HD13	1.91	0.51
1:G:270:ARG:NH2	1:H:286:ASP:OD1	2.38	0.51
1:H:119:GLN:HE22	1:I:182:LYS:CE	2.21	0.51
1:I:251:THR:OG1	1:I:253:HIS:HD2	1.92	0.51
1:K:365:TYR:HE1	1:K:369:ILE:HD11	1.76	0.51
1:L:70:ASN:OD1	1:L:78:THR:OG1	2.27	0.51
1:A:160:SER:O	1:A:299:LEU:HG	2.10	0.51
1:B:35:ASP:OD2	1:C:227:LYS:HD3	2.10	0.51
1:F:265:ALA:HB3	1:F:337:ARG:NH2	2.26	0.51
1:H:319:GLU:O	1:H:323:ILE:HG13	2.11	0.51
1:I:29:GLU:HG2	1:I:101:TYR:CZ	2.45	0.51
1:I:265:ALA:O	1:I:268:MET:HB2	2.11	0.51
1:I:345:GLN:HE21	1:I:350:ASP:HB2	1.76	0.51
1:L:40:THR:N	1:L:65:LEU:HD23	2.25	0.51
1:B:7:ASN:N	1:B:7:ASN:HD22	2.09	0.51
1:B:39:GLN:C	1:B:65:LEU:HD21	2.36	0.51
1:D:104:ARG:HD2	1:D:125:ILE:HD13	1.92	0.51
1:D:249:ALA:CB	1:D:290:THR:OG1	2.58	0.51
1:E:75:PRO:HD3	1:J:323:ILE:HD12	1.92	0.51
1:F:208:GLU:H	1:F:212:HIS:CD2	2.25	0.51
1:F:259:LEU:CD1	1:F:267:THR:HG23	2.40	0.51
1:F:314:LEU:HD11	1:F:339:LEU:HB3	1.92	0.51
1:F:336:THR:O	1:F:340:VAL:HG13	2.11	0.51
1:A:227:LYS:HE3	1:F:47:GLU:OE1	2.09	0.51
1:C:132:LEU:CB	1:C:172:GLU:HG3	2.39	0.51
1:D:125:ILE:HG13	1:D:126:PRO:HD2	1.93	0.51
1:F:360:ILE:HB	1:F:364:VAL:HG11	1.92	0.51
1:G:173:LEU:C	1:G:181:ARG:NH2	2.67	0.51
1:G:236:CYS:HB2	1:G:241:THR:OG1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ILE:CG2	1:A:60:LEU:HD22	2.41	0.51
1:B:99:VAL:HG12	1:B:100:ARG:H	1.75	0.51
1:B:194:TYR:CD2	1:B:204:VAL:HG11	2.46	0.51
1:C:273:THR:HG22	1:C:280:ARG:HH11	1.76	0.51
1:E:349:TRP:CH2	1:E:353:MET:HG3	2.45	0.51
1:G:174:ILE:CG1	1:G:202:ALA:HB1	2.40	0.51
1:G:352:LYS:HD2	1:G:365:TYR:OH	2.10	0.51
1:I:281:LEU:HD23	1:I:285:ILE:HD13	1.91	0.51
1:J:200:ILE:HG23	1:J:201:SER:N	2.25	0.51
1:J:233:VAL:HB	1:J:257:THR:CG2	2.32	0.51
1:K:55:ILE:HG13	1:K:56:THR:HG23	1.92	0.51
1:A:92:GLU:HG2	1:A:102:ARG:HG2	1.90	0.51
1:B:360:ILE:HD12	1:B:365:TYR:HB2	1.92	0.51
1:C:263:GLY:O	1:C:267:THR:HG23	2.11	0.51
1:G:351:ALA:O	1:G:354:LYS:HB2	2.10	0.51
1:J:21:MET:O	1:J:24:MET:HB3	2.11	0.51
1:J:145:ILE:HD12	1:J:293:LEU:HD23	1.92	0.51
1:J:208:GLU:HB3	1:J:211:ARG:HB3	1.93	0.51
1:B:18:PRO:O	1:B:21:MET:HB3	2.11	0.51
1:C:230:LEU:HD11	1:C:256:TYR:CD1	2.45	0.51
1:C:248:ALA:O	1:C:251:THR:OG1	2.25	0.51
1:I:102:ARG:O	1:I:103:TYR:CD1	2.64	0.51
1:J:352:LYS:N	1:J:365:TYR:HE1	2.09	0.51
1:L:296:TRP:CD1	1:L:347:MET:CE	2.94	0.51
1:A:142:ILE:O	1:A:145:ILE:HG13	2.11	0.51
1:B:6:ILE:HG23	1:B:54:LYS:HG3	1.91	0.51
1:B:272:VAL:HG13	1:B:284:THR:CG2	2.41	0.51
1:D:209:ILE:N	1:D:210:PRO:HD2	2.25	0.51
1:H:19:VAL:CG2	1:H:20:PHE:N	2.72	0.51
1:I:261:THR:HG21	1:I:267:THR:CB	2.41	0.51
1:J:132:LEU:HD21	1:J:137:LEU:HD12	1.92	0.51
1:K:288:LEU:HB2	1:K:325:LEU:HD21	1.92	0.51
1:L:87:ILE:HB	1:L:107:ALA:HB3	1.93	0.51
1:C:81:LEU:HD12	1:C:81:LEU:N	2.25	0.51
1:C:111:LEU:HD11	1:C:114:GLY:H	1.75	0.51
1:C:229:ARG:HG3	1:C:229:ARG:O	2.10	0.51
1:E:39:GLN:C	1:E:65:LEU:HD21	2.35	0.51
1:E:174:ILE:HD12	1:E:204:VAL:CG2	2.40	0.51
1:F:355:PHE:CZ	1:F:362:GLU:HG3	2.46	0.51
1:I:9:MET:CE	1:I:12:GLU:HG3	2.41	0.51
1:J:76:ASN:O	1:J:79:THR:OG1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:115:HIS:N	1:L:115:HIS:CD2	2.79	0.51
1:A:223:ALA:O	1:A:228:PRO:HD3	2.11	0.50
1:D:6:ILE:HA	1:D:53:LEU:HD13	1.93	0.50
1:D:125:ILE:HD12	1:D:126:PRO:HD2	1.93	0.50
1:G:21:MET:CE	1:G:68:LEU:HD22	2.40	0.50
1:H:9:MET:CE	1:H:24:MET:HB2	2.42	0.50
1:H:188:SER:HG	1:H:189:PRO:HD3	1.70	0.50
1:I:302:THR:CG2	1:I:308:VAL:CG1	2.89	0.50
1:I:353:MET:CG	1:I:357:GLN:NE2	2.74	0.50
1:A:363:ARG:HG3	1:A:364:VAL:N	2.26	0.50
1:D:248:ALA:HA	1:D:251:THR:OG1	2.11	0.50
1:G:355:PHE:HZ	1:G:365:TYR:HB3	1.76	0.50
1:H:229:ARG:CZ	1:H:229:ARG:HB2	2.41	0.50
1:J:123:ARG:NH2	1:K:225:ARG:O	2.44	0.50
1:J:264:VAL:HG23	1:J:294:CYS:CB	2.41	0.50
1:A:12:GLU:OE2	1:A:58:ARG:HB3	2.11	0.50
1:B:336:THR:O	1:B:340:VAL:HG13	2.12	0.50
1:D:105:VAL:HG22	1:D:122:LEU:HG	1.92	0.50
1:I:27:HIS:O	1:I:30:SER:HB3	2.12	0.50
1:L:73:TYR:CD1	1:L:87:ILE:CG2	2.94	0.50
1:L:291:ILE:HD11	1:L:316:PHE:CE1	2.47	0.50
1:A:158:THR:CG2	1:A:260:HIS:CE1	2.94	0.50
1:E:9:MET:HG2	1:E:10:PRO:CD	2.41	0.50
1:E:215:ASN:HD21	1:E:218:ASP:CG	2.19	0.50
1:E:332:VAL:HG23	1:E:333:THR:N	2.26	0.50
1:I:24:MET:SD	1:I:25:LEU:CD2	2.96	0.50
1:J:264:VAL:HG11	1:J:340:VAL:HG11	1.94	0.50
1:J:348:THR:CG2	1:J:372:ALA:CB	2.90	0.50
1:K:137:LEU:HD23	1:K:141:ILE:HD11	1.94	0.50
1:K:171:ARG:NE	1:K:197:ILE:CD1	2.74	0.50
1:A:261:THR:HG21	1:A:267:THR:HA	1.93	0.50
1:A:261:THR:HG21	1:A:267:THR:CA	2.41	0.50
1:B:9:MET:HE3	1:B:24:MET:HA	1.92	0.50
1:C:166:LEU:CD1	1:C:232:MET:HE1	2.41	0.50
1:C:363:ARG:HG3	1:C:364:VAL:H	1.75	0.50
1:E:288:LEU:HB3	1:E:325:LEU:CD2	2.41	0.50
1:F:364:VAL:HG13	1:F:365:TYR:H	1.76	0.50
1:G:17:THR:CG2	1:G:18:PRO:CD	2.88	0.50
1:G:345:GLN:CB	1:G:349:TRP:HZ3	2.24	0.50
1:H:251:THR:CG2	1:H:253:HIS:NE2	2.74	0.50
1:I:149:GLU:O	1:I:292:ARG:CD	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:180:ASN:N	1:K:180:ASN:ND2	2.60	0.50
1:L:296:TRP:HE1	1:L:347:MET:HE3	1.76	0.50
1:A:12:GLU:CD	1:A:56:THR:CG2	2.82	0.50
1:B:125:ILE:HG12	1:B:191:GLU:O	2.11	0.50
1:D:174:ILE:HG23	1:D:175:GLU:N	2.26	0.50
1:D:367:LEU:CD1	1:E:325:LEU:HD13	2.41	0.50
1:E:224:LEU:HD21	1:E:248:ALA:HA	1.94	0.50
1:G:291:ILE:CB	1:G:316:PHE:HD2	2.22	0.50
1:J:264:VAL:HG23	1:J:294:CYS:HB3	1.94	0.50
1:K:65:LEU:HD23	1:K:118:ILE:O	2.12	0.50
1:B:188:SER:CB	1:B:189:PRO:CD	2.90	0.50
1:F:87:ILE:HB	1:F:107:ALA:HB3	1.92	0.50
1:G:369:ILE:O	1:G:372:ALA:N	2.43	0.50
1:H:365:TYR:CE1	1:H:369:ILE:HD11	2.45	0.50
1:I:25:LEU:HD12	1:I:103:TYR:CE2	2.40	0.50
1:J:184:LEU:HD22	1:J:226:ARG:HH21	1.76	0.50
1:K:363:ARG:HA	1:K:366:LYS:HD2	1.85	0.50
1:B:158:THR:HG22	1:C:247:GLU:CD	2.36	0.50
1:B:360:ILE:CD1	1:B:365:TYR:HB2	2.41	0.50
1:C:230:LEU:CD1	1:C:256:TYR:CE1	2.95	0.50
1:D:367:LEU:HD21	1:E:289:GLU:CD	2.37	0.50
1:E:155:THR:HG21	1:E:267:THR:HG21	1.94	0.50
1:G:135:MET:CA	1:G:135:MET:CE	2.89	0.50
1:H:137:LEU:CD1	1:H:311:ARG:CZ	2.90	0.50
1:I:17:THR:CG2	1:I:18:PRO:CD	2.88	0.50
1:I:300:VAL:O	1:I:308:VAL:HG12	2.11	0.50
1:J:16:PHE:CZ	1:J:44:ILE:CD1	2.95	0.50
1:L:275:PHE:CD2	1:L:283:ARG:CB	2.95	0.50
1:A:312:GLU:HB2	1:A:347:MET:N	2.26	0.50
1:B:99:VAL:HG12	1:B:100:ARG:N	2.27	0.50
1:B:135:MET:HB3	1:B:137:LEU:HD13	1.92	0.50
1:C:40:THR:HG23	1:C:65:LEU:HD22	1.91	0.50
1:D:93:PHE:C	1:D:93:PHE:CD1	2.89	0.50
1:F:27:HIS:C	1:F:27:HIS:CD2	2.90	0.50
1:I:154:ILE:HD13	1:I:166:LEU:HD21	1.94	0.50
1:K:276:SER:HA	1:K:280:ARG:CD	2.35	0.50
1:L:310:LEU:CD2	1:L:354:LYS:HG3	2.41	0.50
1:A:324:LEU:HD21	1:A:336:THR:HG23	1.94	0.49
1:B:146:ALA:HB2	1:B:173:LEU:HD21	1.94	0.49
1:E:29:GLU:CG	1:E:101:TYR:HE2	2.16	0.49
1:F:17:THR:HG22	1:F:19:VAL:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:184:LEU:HD22	1:H:205:SER:OG	2.12	0.49
1:H:320:VAL:CG1	1:H:339:LEU:HD13	2.41	0.49
1:I:25:LEU:HD22	1:I:36:ILE:HD13	1.93	0.49
1:I:28:ALA:CB	1:I:36:ILE:HD11	2.42	0.49
1:I:81:LEU:HD23	1:I:118:ILE:HG12	1.94	0.49
1:J:17:THR:CG2	1:J:18:PRO:CD	2.90	0.49
1:J:17:THR:HG22	1:J:18:PRO:CD	2.41	0.49
1:J:264:VAL:HG11	1:J:340:VAL:CG1	2.42	0.49
1:A:17:THR:HG23	1:A:18:PRO:CD	2.35	0.49
1:A:184:LEU:HD22	1:A:226:ARG:HH21	1.77	0.49
1:A:319:GLU:O	1:A:323:ILE:HG13	2.12	0.49
1:C:258:THR:O	1:C:259:LEU:HD12	2.12	0.49
1:D:39:GLN:C	1:D:65:LEU:HD21	2.37	0.49
1:D:104:ARG:NE	1:D:123:ARG:NH1	2.60	0.49
1:E:288:LEU:HD23	1:E:325:LEU:HD23	1.94	0.49
1:E:354:LYS:HE2	1:E:357:GLN:HG3	1.93	0.49
1:G:56:THR:HG22	1:G:58:ARG:H	1.76	0.49
1:G:145:ILE:HD12	1:G:146:ALA:N	2.27	0.49
1:G:180:ASN:H	1:G:180:ASN:ND2	2.09	0.49
1:J:86:ASP:HB2	1:K:213:LEU:HD21	1.93	0.49
1:J:236:CYS:SG	1:J:259:LEU:HD11	2.53	0.49
1:K:116:ASP:N	1:K:116:ASP:OD1	2.43	0.49
1:K:269:ARG:HG3	1:K:333:THR:HG21	1.94	0.49
1:A:246:LEU:O	1:A:250:LEU:HG	2.12	0.49
1:C:111:LEU:HD21	1:C:114:GLY:C	2.37	0.49
1:C:188:SER:HB3	1:C:189:PRO:HD3	1.94	0.49
1:D:8:LEU:HD13	1:D:8:LEU:C	2.35	0.49
1:E:275:PHE:O	1:E:280:ARG:CG	2.60	0.49
1:G:42:GLU:OE1	1:H:203:VAL:HG13	2.11	0.49
1:G:89:THR:CG2	1:G:90:HIS:N	2.71	0.49
1:G:174:ILE:HG13	1:G:202:ALA:CB	2.43	0.49
1:G:269:ARG:CG	1:G:269:ARG:NH1	2.68	0.49
1:H:340:VAL:O	1:H:344:GLY:N	2.44	0.49
1:K:171:ARG:HE	1:K:197:ILE:HD11	1.78	0.49
1:K:173:LEU:CD2	1:K:181:ARG:NH1	2.75	0.49
1:A:12:GLU:OE1	1:A:56:THR:CG2	2.52	0.49
1:B:155:THR:CG2	1:B:259:LEU:HB2	2.26	0.49
1:C:152:VAL:HG13	1:C:293:LEU:CD1	2.41	0.49
1:D:92:GLU:OE2	1:D:102:ARG:NE	2.45	0.49
1:D:320:VAL:CG1	1:D:339:LEU:HD13	2.42	0.49
1:E:27:HIS:C	1:E:27:HIS:CD2	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:PRO:HG3	1:F:20:PHE:CG	2.45	0.49
1:F:248:ALA:O	1:F:251:THR:OG1	2.28	0.49
1:H:17:THR:OG1	1:H:20:PHE:CD2	2.65	0.49
1:K:312:GLU:HB2	1:K:347:MET:N	2.28	0.49
1:A:306:ARG:HG2	1:A:307:ARG:N	2.27	0.49
1:E:154:ILE:HG22	1:E:162:LYS:HB2	1.94	0.49
1:F:49:TYR:HD1	1:F:50:GLY:H	1.56	0.49
1:G:185:THR:HG22	1:G:232:MET:HB3	1.94	0.49
1:H:340:VAL:HG23	1:H:346:LEU:HD21	1.93	0.49
1:I:16:PHE:CE2	1:I:21:MET:HA	2.47	0.49
1:J:268:MET:HE1	1:J:288:LEU:CD1	2.42	0.49
1:L:209:ILE:HG21	1:L:216:PHE:CE1	2.47	0.49
1:C:312:GLU:HB2	1:C:347:MET:N	2.27	0.49
1:D:314:LEU:HB2	1:D:340:VAL:HG12	1.93	0.49
1:G:102:ARG:HH21	1:G:125:ILE:HG21	1.75	0.49
1:H:233:VAL:HB	1:H:257:THR:CG2	2.32	0.49
1:J:15:ARG:HB3	1:J:15:ARG:HH21	1.78	0.49
1:D:148:GLN:O	1:D:254:PRO:HD3	2.13	0.49
1:D:171:ARG:HA	1:D:174:ILE:HG22	1.94	0.49
1:G:38:ILE:CG2	1:G:60:LEU:HD22	2.42	0.49
1:G:291:ILE:CB	1:G:316:PHE:CD2	2.95	0.49
1:H:66:GLY:O	1:H:69:ILE:HG22	2.12	0.49
1:H:86:ASP:OD1	1:I:222:ASN:ND2	2.45	0.49
1:I:269:ARG:HG3	1:I:333:THR:HG21	1.93	0.49
1:J:105:VAL:HG22	1:J:122:LEU:HG	1.95	0.49
1:J:361:SER:HB3	1:J:364:VAL:HG23	1.94	0.49
1:L:90:HIS:CD2	1:L:102:ARG:HH22	2.31	0.49
1:L:197:ILE:HG22	1:L:197:ILE:O	2.12	0.49
1:A:97:ARG:HD2	1:A:97:ARG:O	2.12	0.49
1:D:156:GLY:C	1:D:162:LYS:HZ1	2.20	0.49
1:E:137:LEU:HD23	1:E:141:ILE:HD11	1.95	0.49
1:E:317:ASP:O	1:E:320:VAL:HG22	2.13	0.49
1:K:42:GLU:OE1	1:K:43:PRO:HD2	2.13	0.49
1:L:156:GLY:O	1:L:260:HIS:HA	2.12	0.49
1:L:170:ILE:HG22	1:L:174:ILE:CD1	2.43	0.49
1:A:55:ILE:O	1:A:55:ILE:CG2	2.60	0.49
1:B:73:TYR:O	1:B:77:ALA:HB2	2.12	0.49
1:F:335:ALA:O	1:F:339:LEU:CD2	2.54	0.49
1:G:47:GLU:HG3	1:G:52:LEU:CD2	2.42	0.49
1:G:354:LYS:HB3	1:G:360:ILE:HD12	1.93	0.49
1:H:95:PRO:HG2	1:H:97:ARG:HH11	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:224:LEU:HD21	1:K:248:ALA:HA	1.94	0.49
1:L:305:GLU:CG	1:L:305:GLU:O	2.61	0.49
1:A:154:ILE:CG2	1:A:162:LYS:HB3	2.42	0.49
1:B:259:LEU:CD1	1:B:267:THR:HG23	2.43	0.49
1:C:12:GLU:CD	1:C:56:THR:HG1	2.21	0.49
1:C:81:LEU:N	1:C:81:LEU:CD1	2.75	0.49
1:G:135:MET:HE2	1:G:135:MET:N	2.27	0.49
1:I:281:LEU:HD23	1:I:285:ILE:CD1	2.43	0.49
1:J:51:ARG:HA	1:K:180:ASN:OD1	2.12	0.49
1:J:148:GLN:O	1:J:254:PRO:HD3	2.13	0.49
1:K:155:THR:HG21	1:K:267:THR:HG21	1.94	0.49
1:L:335:ALA:O	1:L:339:LEU:HD23	2.12	0.49
1:A:108:THR:HG23	1:B:213:LEU:HD11	1.95	0.48
1:E:91:TYR:OH	1:J:338:LYS:NZ	2.46	0.48
1:E:162:LYS:HG2	1:E:163:SER:N	2.28	0.48
1:F:137:LEU:HD11	1:F:311:ARG:NH2	2.28	0.48
1:F:233:VAL:HB	1:F:257:THR:CG2	2.34	0.48
1:G:69:ILE:CD1	1:G:120:ILE:HG12	2.38	0.48
1:J:9:MET:CE	1:J:24:MET:CB	2.66	0.48
1:J:166:LEU:CD2	1:J:256:TYR:HB3	2.42	0.48
1:K:91:TYR:CE1	1:K:93:PHE:CD2	3.01	0.48
1:K:126:PRO:HB2	1:K:192:PHE:CE1	2.48	0.48
1:K:132:LEU:HD23	1:K:132:LEU:C	2.38	0.48
1:B:119:GLN:HE22	1:C:226:ARG:HD2	1.77	0.48
1:B:164:THR:OG1	1:B:165:LEU:N	2.46	0.48
1:B:337:ARG:NE	1:B:341:ARG:HH11	2.11	0.48
1:F:73:TYR:HD1	1:F:89:THR:HG21	1.65	0.48
1:G:201:SER:C	1:L:52:LEU:HD23	2.38	0.48
1:H:6:ILE:C	1:H:7:ASN:HD22	2.21	0.48
1:H:229:ARG:HH21	1:H:229:ARG:CG	2.25	0.48
1:I:109:ALA:CB	1:J:212:HIS:ND1	2.76	0.48
1:J:199:THR:CG2	1:J:202:ALA:CB	2.87	0.48
1:K:172:GLU:OE1	1:K:172:GLU:HA	2.13	0.48
1:L:170:ILE:HG22	1:L:174:ILE:HD12	1.94	0.48
1:A:111:LEU:HD12	1:A:115:HIS:O	2.13	0.48
1:A:297:GLN:HE21	1:A:311:ARG:CZ	2.25	0.48
1:B:214:PRO:C	1:B:215:ASN:HD22	2.21	0.48
1:C:119:GLN:HE22	1:D:182:LYS:CE	2.25	0.48
1:C:300:VAL:HG12	1:C:301:PRO:HD2	1.95	0.48
1:C:360:ILE:HG23	1:C:364:VAL:HB	1.95	0.48
1:E:64:GLU:O	1:E:68:LEU:HD13	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:345:GLN:HG3	1:F:349:TRP:CE3	2.43	0.48
1:G:203:VAL:CG1	1:L:39:GLN:NE2	2.76	0.48
1:H:33:ALA:HA	1:H:48:VAL:HA	1.96	0.48
1:H:45:PHE:CE2	1:I:203:VAL:HG22	2.48	0.48
1:H:188:SER:C	1:H:208:GLU:HG3	2.37	0.48
1:I:188:SER:HB3	1:I:189:PRO:HD3	1.95	0.48
1:L:17:THR:HG22	1:L:19:VAL:H	1.77	0.48
1:B:6:ILE:C	1:B:7:ASN:HD22	2.20	0.48
1:D:171:ARG:CA	1:D:174:ILE:HG22	2.44	0.48
1:E:300:VAL:HG13	1:E:364:VAL:HG11	1.95	0.48
1:G:145:ILE:C	1:G:145:ILE:CD1	2.86	0.48
1:H:128:THR:CG2	1:H:196:GLU:HG3	2.42	0.48
1:H:183:VAL:C	1:H:184:LEU:HD23	2.38	0.48
1:I:349:TRP:C	1:I:349:TRP:CD1	2.91	0.48
1:J:125:ILE:HD12	1:J:126:PRO:CD	2.42	0.48
1:K:262:SER:HB2	1:K:296:TRP:CE2	2.48	0.48
1:L:132:LEU:CD1	1:L:169:ILE:CD1	2.89	0.48
1:A:92:GLU:OE1	1:A:102:ARG:NH2	2.44	0.48
1:A:108:THR:HG21	1:B:226:ARG:HH12	1.78	0.48
1:D:44:ILE:CG2	1:D:55:ILE:HD11	2.43	0.48
1:F:284:THR:O	1:F:288:LEU:HD23	2.13	0.48
1:G:131:LYS:O	1:G:134:THR:HB	2.12	0.48
1:G:142:ILE:O	1:G:145:ILE:HG13	2.14	0.48
1:G:360:ILE:HG22	1:G:361:SER:N	2.28	0.48
1:H:6:ILE:O	1:H:7:ASN:ND2	2.46	0.48
1:H:93:PHE:CD1	1:H:93:PHE:C	2.91	0.48
1:I:355:PHE:HZ	1:I:362:GLU:CG	2.24	0.48
1:J:209:ILE:HG22	1:J:210:PRO:N	2.29	0.48
1:L:48:VAL:CG1	1:L:49:TYR:CD2	2.90	0.48
1:C:111:LEU:HD22	1:C:115:HIS:O	2.13	0.48
1:C:268:MET:SD	1:C:291:ILE:CD1	3.01	0.48
1:D:297:GLN:OE1	1:D:311:ARG:NE	2.46	0.48
1:E:312:GLU:HB2	1:E:347:MET:N	2.27	0.48
1:G:174:ILE:HD11	1:G:202:ALA:CB	2.32	0.48
1:J:40:THR:HG23	1:J:62:ASN:N	2.29	0.48
1:J:69:ILE:HD12	1:J:72:ILE:HG23	1.96	0.48
1:J:72:ILE:CD1	1:J:105:VAL:HG21	2.40	0.48
1:L:149:GLU:CG	1:L:150:GLY:N	2.73	0.48
1:F:158:THR:HB	1:F:260:HIS:HE1	1.78	0.48
1:F:365:TYR:CE2	1:F:369:ILE:HD11	2.49	0.48
1:G:157:ALA:O	1:G:162:LYS:NZ	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:21:MET:O	1:H:25:LEU:HG	2.14	0.48
1:H:251:THR:HG22	1:H:253:HIS:NE2	2.27	0.48
1:J:35:ASP:OD2	1:K:227:LYS:HD2	2.13	0.48
1:K:259:LEU:HD11	1:K:271:LEU:HD21	1.96	0.48
1:A:194:TYR:CD2	1:A:204:VAL:HG11	2.48	0.48
1:A:297:GLN:HG3	1:A:311:ARG:CG	2.44	0.48
1:D:366:LYS:HA	1:D:369:ILE:HG22	1.93	0.48
1:E:21:MET:HE2	1:E:68:LEU:CD2	2.42	0.48
1:E:182:LYS:NZ	1:E:226:ARG:O	2.46	0.48
1:E:247:GLU:O	1:E:251:THR:OG1	2.31	0.48
1:G:55:ILE:O	1:G:55:ILE:CG2	2.62	0.48
1:G:193:VAL:HG21	1:G:195:ASP:OD2	2.13	0.48
1:H:170:ILE:O	1:H:174:ILE:HG12	2.14	0.48
1:I:16:PHE:HZ	1:I:21:MET:HA	1.79	0.48
1:K:60:LEU:HB3	1:K:65:LEU:CD1	2.44	0.48
1:K:91:TYR:HE1	1:K:93:PHE:CD2	2.31	0.48
1:L:76:ASN:O	1:L:79:THR:OG1	2.25	0.48
1:L:112:VAL:CG2	1:L:117:ALA:HB2	2.19	0.48
1:A:9:MET:HE1	1:A:24:MET:HB2	1.96	0.48
1:A:94:ARG:HE	1:A:100:ARG:CG	2.19	0.48
1:B:223:ALA:O	1:B:228:PRO:HD3	2.13	0.48
1:C:188:SER:CB	1:C:189:PRO:CD	2.92	0.48
1:E:126:PRO:O	1:E:191:GLU:O	2.31	0.48
1:F:135:MET:CB	1:F:137:LEU:HD13	2.43	0.48
1:G:21:MET:SD	1:G:68:LEU:HD22	2.54	0.48
1:G:96:ASN:CG	1:G:98:GLY:H	2.20	0.48
1:J:40:THR:CG2	1:J:62:ASN:CA	2.92	0.48
1:J:209:ILE:HD13	1:J:209:ILE:HA	1.71	0.48
1:K:189:PRO:HD2	1:K:189:PRO:O	2.14	0.48
1:K:336:THR:O	1:K:340:VAL:HG23	2.14	0.48
1:L:93:PHE:CE2	1:L:103:TYR:HE2	2.32	0.48
1:A:353:MET:HG3	1:A:357:GLN:HE21	1.78	0.48
1:B:55:ILE:O	1:B:55:ILE:CG2	2.62	0.48
1:D:366:LYS:O	1:D:369:ILE:CG2	2.59	0.48
1:F:48:VAL:O	1:F:49:TYR:CD2	2.66	0.48
1:F:182:LYS:HG3	1:F:203:VAL:HG13	1.96	0.48
1:F:291:ILE:HD13	1:F:316:PHE:CE2	2.49	0.48
1:G:193:VAL:HG22	1:G:195:ASP:H	1.79	0.48
1:K:300:VAL:CG1	1:K:301:PRO:HD2	2.42	0.48
1:A:329:PRO:O	1:A:332:VAL:HG13	2.14	0.47
1:B:268:MET:HG3	1:B:336:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:GLN:O	1:E:254:PRO:HD3	2.14	0.47
1:E:215:ASN:HD22	1:E:218:ASP:HB2	1.78	0.47
1:G:296:TRP:CZ3	1:G:347:MET:CE	2.96	0.47
1:G:313:TYR:HE2	1:G:345:GLN:CD	2.22	0.47
1:I:174:ILE:HG23	1:I:175:GLU:N	2.28	0.47
1:I:365:TYR:CZ	1:I:369:ILE:HD11	2.49	0.47
1:J:158:THR:HA	1:J:162:LYS:HZ2	1.79	0.47
1:B:42:GLU:OE1	1:C:203:VAL:HG13	2.14	0.47
1:C:92:GLU:HG2	1:C:93:PHE:N	2.29	0.47
1:C:268:MET:HE1	1:C:288:LEU:HD23	1.96	0.47
1:D:94:ARG:CB	1:D:100:ARG:NE	2.74	0.47
1:G:329:PRO:O	1:G:332:VAL:HG22	2.14	0.47
1:G:365:TYR:HA	1:G:368:ILE:HD13	1.96	0.47
1:H:88:ASP:OD2	1:I:225:ARG:NE	2.47	0.47
1:H:240:GLU:CD	1:H:240:GLU:N	2.72	0.47
1:J:190:ILE:HG22	1:J:190:ILE:O	2.13	0.47
1:L:7:ASN:O	1:L:54:LYS:O	2.31	0.47
1:A:302:THR:OG1	1:A:306:ARG:O	2.29	0.47
1:B:100:ARG:NE	1:B:102:ARG:NH1	2.56	0.47
1:C:209:ILE:H	1:C:210:PRO:HD2	1.80	0.47
1:G:69:ILE:HD12	1:G:107:ALA:HB2	1.96	0.47
1:G:362:GLU:HG2	1:G:366:LYS:HE2	1.96	0.47
1:H:27:HIS:HD2	1:H:55:ILE:HG21	1.79	0.47
1:H:369:ILE:O	1:H:370:ALA:C	2.58	0.47
1:I:11:ASP:OD1	1:I:11:ASP:N	2.48	0.47
1:I:166:LEU:HD12	1:I:232:MET:HE1	1.97	0.47
1:J:40:THR:CG2	1:J:62:ASN:HA	2.43	0.47
1:J:184:LEU:HG	1:J:228:PRO:HB3	1.95	0.47
1:J:348:THR:CG2	1:J:372:ALA:HB2	2.45	0.47
1:A:278:GLU:OE2	1:F:266:GLU:HG3	2.14	0.47
1:A:365:TYR:CD2	1:A:369:ILE:HD11	2.49	0.47
1:E:288:LEU:CD2	1:E:325:LEU:HD23	2.45	0.47
1:F:44:ILE:HB	1:F:56:THR:CG2	2.45	0.47
1:K:160:SER:N	2:K:401:PO4:O1	2.36	0.47
1:K:285:ILE:HD12	1:K:285:ILE:N	2.28	0.47
1:A:81:LEU:HD12	1:A:118:ILE:HG12	1.95	0.47
1:C:281:LEU:HD23	1:C:285:ILE:CD1	2.44	0.47
1:H:211:ARG:HD2	1:H:212:HIS:CE1	2.48	0.47
1:H:314:LEU:HD13	1:H:340:VAL:HA	1.97	0.47
1:I:114:GLY:N	1:J:92:GLU:OE1	2.47	0.47
1:I:184:LEU:HD11	1:I:228:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:265:ALA:HB3	1:I:266:GLU:OE1	2.14	0.47
1:I:319:GLU:O	1:I:323:ILE:HG13	2.15	0.47
1:J:209:ILE:CD1	1:J:215:ASN:C	2.88	0.47
1:K:34:SER:O	1:K:124:THR:HG23	2.15	0.47
1:L:8:LEU:O	1:L:27:HIS:CE1	2.68	0.47
1:L:190:ILE:CG1	1:L:208:GLU:CG	2.86	0.47
1:A:332:VAL:HG23	1:A:333:THR:H	1.79	0.47
1:C:197:ILE:CD1	1:C:197:ILE:H	2.26	0.47
1:G:235:GLU:HG3	1:G:235:GLU:O	2.14	0.47
1:G:297:GLN:HE22	1:G:311:ARG:HH21	1.62	0.47
1:J:195:ASP:O	1:J:198:GLU:HG2	2.14	0.47
1:K:24:MET:SD	1:K:44:ILE:CD1	3.01	0.47
1:K:119:GLN:HE21	1:K:121:THR:CG2	2.26	0.47
1:A:40:THR:HG23	1:A:65:LEU:HD22	1.93	0.47
1:C:236:CYS:SG	1:C:242:ILE:HG13	2.55	0.47
1:F:24:MET:SD	1:F:44:ILE:CD1	2.90	0.47
1:F:102:ARG:HB3	1:F:125:ILE:CG2	2.45	0.47
1:F:105:VAL:HG22	1:F:122:LEU:HG	1.96	0.47
1:F:334:SER:HA	1:F:337:ARG:HG3	1.97	0.47
1:G:131:LYS:HG2	1:G:171:ARG:NH1	2.29	0.47
1:H:6:ILE:HD13	1:H:54:LYS:HD2	1.97	0.47
1:I:13:PRO:CB	1:I:20:PHE:CE2	2.86	0.47
1:I:224:LEU:HD21	1:I:248:ALA:HA	1.96	0.47
1:I:229:ARG:HG3	1:I:229:ARG:O	2.15	0.47
1:I:235:GLU:OE1	1:I:260:HIS:CE1	2.67	0.47
1:K:17:THR:CG2	1:K:18:PRO:CD	2.93	0.47
1:K:25:LEU:HD13	1:K:93:PHE:CZ	2.49	0.47
1:L:175:GLU:HA	1:L:199:THR:HG21	1.96	0.47
1:L:183:VAL:CG1	1:L:230:LEU:HD22	2.31	0.47
1:A:48:VAL:HG12	1:A:49:TYR:HD2	1.80	0.47
1:A:56:THR:HG22	1:A:58:ARG:H	1.80	0.47
1:A:112:VAL:HG23	1:A:117:ALA:HB3	1.96	0.47
1:B:374:GLU:CB	1:C:281:LEU:CD2	2.88	0.47
1:C:9:MET:HB2	1:C:10:PRO:HD2	1.97	0.47
1:F:310:LEU:CD1	1:F:368:ILE:CD1	2.92	0.47
1:G:135:MET:HA	1:G:135:MET:CE	2.34	0.47
1:G:362:GLU:OE1	1:G:366:LYS:HE3	2.15	0.47
1:H:166:LEU:HD13	1:H:232:MET:SD	2.54	0.47
1:K:333:THR:O	1:K:336:THR:CG2	2.62	0.47
1:K:363:ARG:CA	1:K:366:LYS:CD	2.71	0.47
1:L:135:MET:HB2	1:L:137:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:296:TRP:NE1	1:L:347:MET:HE2	2.26	0.47
1:B:337:ARG:HG2	1:B:341:ARG:NH1	2.30	0.47
1:C:141:ILE:O	1:C:145:ILE:HG23	2.15	0.47
1:C:329:PRO:O	1:C:332:VAL:HG23	2.15	0.47
1:F:209:ILE:C	1:F:209:ILE:CD1	2.88	0.47
1:H:302:THR:OG1	1:H:306:ARG:O	2.29	0.47
1:H:364:VAL:HA	1:H:367:LEU:HD12	1.97	0.47
1:I:222:ASN:C	1:I:222:ASN:OD1	2.57	0.47
1:I:329:PRO:CA	1:I:332:VAL:HG23	2.36	0.47
1:J:283:ARG:O	1:J:287:ILE:HG13	2.15	0.47
1:A:213:LEU:HD13	1:A:219:GLY:HA2	1.96	0.47
1:A:281:LEU:HD13	1:A:285:ILE:HD11	1.97	0.47
1:B:102:ARG:C	1:B:125:ILE:HG22	2.40	0.47
1:C:93:PHE:CE1	1:C:101:TYR:HB2	2.50	0.47
1:D:92:GLU:HA	1:D:101:TYR:O	2.15	0.47
1:G:238:ASP:O	1:G:242:ILE:CD1	2.63	0.47
1:I:21:MET:HE2	1:I:68:LEU:HD22	1.96	0.47
1:J:40:THR:N	1:J:65:LEU:HD22	2.30	0.47
1:K:148:GLN:HB3	1:K:149:GLU:OE1	2.15	0.47
1:B:119:GLN:HE22	1:C:226:ARG:CD	2.28	0.46
1:B:272:VAL:HG21	1:B:332:VAL:HG11	1.97	0.46
1:C:268:MET:HG3	1:C:336:THR:HG21	1.97	0.46
1:D:40:THR:O	1:D:60:LEU:O	2.31	0.46
1:F:17:THR:CG2	1:F:18:PRO:CD	2.92	0.46
1:H:220:VAL:O	1:H:223:ALA:N	2.49	0.46
1:J:104:ARG:NE	1:J:123:ARG:NH1	2.62	0.46
1:J:174:ILE:CG2	1:J:175:GLU:N	2.78	0.46
1:K:40:THR:N	1:K:65:LEU:CD2	2.78	0.46
1:K:223:ALA:O	1:K:228:PRO:CD	2.62	0.46
1:E:261:THR:OG1	1:E:267:THR:CG2	2.49	0.46
1:F:102:ARG:HB3	1:F:125:ILE:HG23	1.96	0.46
1:F:236:CYS:SG	1:F:242:ILE:HG13	2.54	0.46
1:G:94:ARG:HD3	1:G:97:ARG:HA	1.98	0.46
1:G:111:LEU:CD2	1:H:90:HIS:CE1	2.97	0.46
1:G:318:GLU:CG	1:L:363:ARG:NH2	2.74	0.46
1:H:270:ARG:HH11	1:H:270:ARG:HG3	1.79	0.46
1:I:64:GLU:O	1:I:68:LEU:HD12	2.15	0.46
1:I:137:LEU:CD2	1:I:311:ARG:NH1	2.76	0.46
1:I:273:THR:HG22	1:I:280:ARG:HH11	1.80	0.46
1:K:261:THR:OG1	1:K:267:THR:CG2	2.49	0.46
1:L:148:GLN:O	1:L:254:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:184:LEU:HD11	1:L:226:ARG:HB2	1.97	0.46
1:L:190:ILE:CD1	1:L:208:GLU:HG2	2.45	0.46
1:L:291:ILE:HD13	1:L:316:PHE:CE1	2.49	0.46
1:A:137:LEU:HD23	1:A:141:ILE:CG2	2.45	0.46
1:C:86:ASP:OD1	1:C:87:ILE:N	2.48	0.46
1:F:291:ILE:CD1	1:F:316:PHE:CZ	2.99	0.46
1:J:108:THR:HB	1:K:226:ARG:NH1	2.29	0.46
1:K:166:LEU:HD13	1:K:232:MET:HE3	1.96	0.46
1:K:173:LEU:HD22	1:K:181:ARG:NH1	2.29	0.46
1:L:90:HIS:H	1:L:90:HIS:HD1	1.62	0.46
1:L:238:ASP:C	1:L:238:ASP:OD1	2.57	0.46
1:B:48:VAL:O	1:B:48:VAL:CG2	2.63	0.46
1:C:182:LYS:HE2	1:C:226:ARG:O	2.16	0.46
1:D:171:ARG:C	1:D:174:ILE:HG22	2.40	0.46
1:D:264:VAL:HG13	1:D:265:ALA:N	2.31	0.46
1:F:182:LYS:HZ3	1:F:184:LEU:HD21	1.81	0.46
1:G:297:GLN:NE2	1:G:311:ARG:HE	2.13	0.46
1:G:369:ILE:HG22	1:G:370:ALA:N	2.30	0.46
1:H:19:VAL:CG2	1:H:20:PHE:H	2.29	0.46
1:H:39:GLN:HA	1:H:65:LEU:HD21	1.98	0.46
1:I:109:ALA:HB1	1:J:212:HIS:ND1	2.30	0.46
1:J:7:ASN:C	1:J:8:LEU:HD12	2.40	0.46
1:L:27:HIS:CD2	1:L:31:LEU:CD1	2.98	0.46
1:B:260:HIS:HE1	1:C:221:ARG:NH2	2.14	0.46
1:G:260:HIS:CD2	1:G:261:THR:HG22	2.49	0.46
1:H:40:THR:N	1:H:65:LEU:CD2	2.78	0.46
1:I:171:ARG:C	1:I:174:ILE:HG22	2.40	0.46
1:J:48:VAL:HG12	1:J:49:TYR:CD2	2.49	0.46
1:J:296:TRP:CH2	1:J:347:MET:HE3	2.50	0.46
1:K:21:MET:HE2	1:K:68:LEU:CG	2.46	0.46
1:K:139:ASP:O	1:K:140:ASN:C	2.59	0.46
1:C:60:LEU:HB3	1:C:65:LEU:CD1	2.46	0.46
1:C:261:THR:HG21	1:C:266:GLU:C	2.40	0.46
1:D:269:ARG:O	1:D:273:THR:HG23	2.16	0.46
1:D:337:ARG:O	1:D:340:VAL:HG22	2.15	0.46
1:E:316:PHE:HA	1:E:320:VAL:CG2	2.40	0.46
1:F:111:LEU:CD1	1:F:115:HIS:C	2.87	0.46
1:H:229:ARG:CG	1:H:229:ARG:NH2	2.79	0.46
1:H:366:LYS:HE3	1:H:366:LYS:HB3	1.72	0.46
1:I:43:PRO:CB	1:I:56:THR:HG23	2.45	0.46
1:I:47:GLU:HB2	1:I:52:LEU:CD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:16:PHE:CZ	1:J:44:ILE:HD12	2.50	0.46
1:J:39:GLN:NE2	1:J:119:GLN:HG3	2.20	0.46
1:J:72:ILE:CD1	1:J:105:VAL:HG11	2.43	0.46
1:K:173:LEU:CD2	1:K:181:ARG:CZ	2.87	0.46
1:A:89:THR:C	1:A:105:VAL:HG22	2.41	0.46
1:A:230:LEU:C	1:A:230:LEU:CD1	2.88	0.46
1:B:335:ALA:HA	1:B:338:LYS:HD3	1.98	0.46
1:D:240:GLU:HA	1:D:240:GLU:OE2	2.15	0.46
1:F:141:ILE:HD11	1:F:313:TYR:CE2	2.51	0.46
1:G:131:LYS:HG3	1:G:171:ARG:NH1	2.31	0.46
1:I:7:ASN:OD1	1:I:27:HIS:CE1	2.68	0.46
1:I:13:PRO:HD3	1:I:20:PHE:CD1	2.51	0.46
1:I:355:PHE:HE2	1:I:362:GLU:CB	2.27	0.46
1:J:13:PRO:CG	1:J:20:PHE:CD1	2.97	0.46
1:A:235:GLU:OE1	1:A:260:HIS:NE2	2.48	0.46
1:B:135:MET:CB	1:B:137:LEU:HD13	2.46	0.46
1:C:119:GLN:NE2	1:D:182:LYS:HE2	2.28	0.46
1:F:8:LEU:C	1:F:27:HIS:HE1	2.22	0.46
1:G:297:GLN:NE2	1:G:311:ARG:NE	2.64	0.46
1:J:175:GLU:HG3	1:J:197:ILE:HG21	1.95	0.46
1:J:296:TRP:CE3	1:J:347:MET:HE2	2.51	0.46
1:J:320:VAL:CG1	1:J:339:LEU:HD13	2.46	0.46
1:J:348:THR:HG22	1:J:372:ALA:HB2	1.97	0.46
1:L:251:THR:OG1	1:L:253:HIS:CD2	2.69	0.46
1:B:273:THR:O	1:B:273:THR:HG22	2.14	0.46
1:D:7:ASN:CB	1:D:31:LEU:HD21	2.45	0.46
1:E:137:LEU:CG	1:E:141:ILE:HD11	2.46	0.46
1:G:155:THR:HG23	1:G:259:LEU:CA	2.46	0.46
1:G:321:ARG:NH1	1:G:321:ARG:HG3	2.29	0.46
1:I:42:GLU:OE1	1:J:203:VAL:HG13	2.16	0.46
1:I:251:THR:OG1	1:I:253:HIS:CD2	2.69	0.46
1:J:281:LEU:O	1:J:284:THR:OG1	2.25	0.46
1:A:93:PHE:CD1	1:A:93:PHE:C	2.94	0.46
1:A:341:ARG:HA	1:A:346:LEU:HD11	1.98	0.46
1:B:102:ARG:HB2	1:B:125:ILE:HG22	1.98	0.46
1:C:142:ILE:O	1:C:145:ILE:HG13	2.16	0.46
1:D:99:VAL:CG1	1:D:100:ARG:N	2.78	0.46
1:E:293:LEU:HD12	1:E:294:CYS:N	2.31	0.46
1:F:262:SER:HA	1:F:296:TRP:CE3	2.51	0.46
1:G:13:PRO:HG3	1:G:20:PHE:CG	2.51	0.46
1:G:180:ASN:ND2	1:G:180:ASN:N	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:251:THR:OG1	1:G:253:HIS:CD2	2.69	0.46
1:G:352:LYS:HB2	1:G:365:TYR:CZ	2.51	0.46
1:I:355:PHE:CE2	1:I:362:GLU:CB	2.99	0.46
1:J:118:ILE:O	1:J:118:ILE:HG13	2.12	0.46
1:J:127:THR:O	1:J:193:VAL:HG22	2.15	0.46
1:J:192:PHE:CD1	1:J:192:PHE:N	2.84	0.46
1:K:64:GLU:O	1:K:68:LEU:HD13	2.16	0.46
1:C:166:LEU:CD1	1:C:232:MET:CE	2.94	0.45
1:E:18:PRO:O	1:E:21:MET:HB2	2.16	0.45
1:E:96:ASN:O	1:E:98:GLY:N	2.41	0.45
1:E:223:ALA:O	1:E:228:PRO:CD	2.64	0.45
1:F:364:VAL:HG13	1:F:365:TYR:N	2.31	0.45
1:I:185:THR:HG22	1:I:232:MET:HB3	1.99	0.45
1:K:7:ASN:C	1:K:8:LEU:CD2	2.87	0.45
1:K:148:GLN:O	1:K:254:PRO:HD3	2.16	0.45
1:K:247:GLU:O	1:K:251:THR:OG1	2.33	0.45
1:L:40:THR:H	1:L:65:LEU:HD23	1.81	0.45
1:A:281:LEU:C	1:A:281:LEU:CD1	2.89	0.45
1:B:333:THR:O	1:B:336:THR:OG1	2.30	0.45
1:F:93:PHE:CD1	1:F:93:PHE:C	2.94	0.45
1:G:40:THR:HG23	1:G:65:LEU:HD22	1.94	0.45
1:G:69:ILE:HD11	1:G:120:ILE:CB	2.46	0.45
1:G:174:ILE:HD12	1:G:174:ILE:HA	1.69	0.45
1:G:236:CYS:SG	1:G:259:LEU:HD21	2.55	0.45
1:H:148:GLN:O	1:H:254:PRO:HD3	2.16	0.45
1:J:145:ILE:HD13	1:J:293:LEU:HD21	1.97	0.45
1:K:268:MET:HE1	1:K:291:ILE:HG21	1.98	0.45
1:K:285:ILE:N	1:K:285:ILE:CD1	2.79	0.45
1:C:132:LEU:HD22	1:C:172:GLU:HG3	1.98	0.45
1:D:68:LEU:O	1:D:72:ILE:HG22	2.16	0.45
1:D:195:ASP:OD1	1:D:196:GLU:N	2.49	0.45
1:E:148:GLN:HB3	1:E:149:GLU:OE1	2.16	0.45
1:E:197:ILE:O	1:E:197:ILE:HG23	2.15	0.45
1:F:268:MET:HG2	1:F:336:THR:HG21	1.96	0.45
1:G:132:LEU:HA	1:G:168:SER:OG	2.17	0.45
1:H:104:ARG:HD3	1:H:191:GLU:HG2	1.98	0.45
1:J:48:VAL:HG12	1:J:49:TYR:HD2	1.81	0.45
1:J:52:LEU:H	1:K:180:ASN:CG	2.19	0.45
1:A:49:TYR:OH	1:A:306:ARG:HG3	2.15	0.45
1:A:95:PRO:HG2	1:A:96:ASN:ND2	2.31	0.45
1:B:40:THR:N	1:B:65:LEU:CD2	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:PRO:O	1:B:142:ILE:HG12	2.16	0.45
1:H:132:LEU:CB	1:H:172:GLU:HG3	2.46	0.45
1:H:340:VAL:CG2	1:H:346:LEU:HD21	2.46	0.45
1:I:40:THR:N	1:I:65:LEU:HD11	2.31	0.45
1:I:185:THR:HA	1:I:232:MET:HB3	1.99	0.45
1:J:199:THR:HG21	1:J:202:ALA:CB	2.47	0.45
1:J:229:ARG:O	1:J:229:ARG:HG3	2.17	0.45
1:K:174:ILE:HG23	1:K:175:GLU:N	2.32	0.45
1:L:25:LEU:CD1	1:L:93:PHE:CE2	2.93	0.45
1:B:148:GLN:O	1:B:254:PRO:HD3	2.16	0.45
1:B:261:THR:CG2	1:B:270:ARG:HD2	2.46	0.45
1:F:292:ARG:HD3	1:F:321:ARG:NH1	2.32	0.45
1:G:134:THR:HB	1:G:135:MET:HE3	1.98	0.45
1:I:17:THR:HG23	1:I:18:PRO:CD	2.44	0.45
1:I:353:MET:HG2	1:I:357:GLN:NE2	2.28	0.45
1:J:17:THR:HG23	1:J:18:PRO:HD2	1.97	0.45
1:K:111:LEU:HD22	1:L:90:HIS:NE2	2.30	0.45
1:L:34:SER:O	1:L:124:THR:HG23	2.17	0.45
1:L:89:THR:CG2	1:L:90:HIS:H	2.20	0.45
1:L:92:GLU:HB2	1:L:102:ARG:HG3	1.98	0.45
1:L:233:VAL:HB	1:L:257:THR:CG2	2.33	0.45
1:L:249:ALA:CB	1:L:290:THR:OG1	2.64	0.45
1:A:281:LEU:HD13	1:A:281:LEU:O	2.16	0.45
1:B:208:GLU:HG3	1:B:210:PRO:HD2	1.98	0.45
1:B:360:ILE:HB	1:B:364:VAL:CG1	2.47	0.45
1:B:366:LYS:C	1:B:366:LYS:CD	2.89	0.45
1:C:185:THR:HA	1:C:232:MET:HB3	1.99	0.45
1:E:162:LYS:CD	1:E:258:THR:CB	2.90	0.45
1:E:176:THR:HG23	1:E:179:SER:CB	2.46	0.45
1:G:188:SER:HA	1:G:210:PRO:HD3	1.97	0.45
1:G:239:ALA:N	1:G:242:ILE:HD12	2.31	0.45
1:G:355:PHE:HZ	1:G:365:TYR:CB	2.27	0.45
1:H:7:ASN:HB3	1:H:31:LEU:HD21	1.98	0.45
1:I:38:ILE:CG2	1:I:65:LEU:HD21	2.40	0.45
1:I:48:VAL:HG12	1:I:49:TYR:CD2	2.51	0.45
1:I:229:ARG:O	1:I:254:PRO:HD2	2.17	0.45
1:J:27:HIS:ND1	1:J:27:HIS:C	2.75	0.45
1:K:365:TYR:CE1	1:K:369:ILE:HD11	2.52	0.45
1:L:216:PHE:O	1:L:220:VAL:HG23	2.17	0.45
1:A:261:THR:CB	1:A:267:THR:HG22	2.30	0.45
1:A:278:GLU:HB3	1:F:269:ARG:HH22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ILE:C	1:B:7:ASN:ND2	2.75	0.45
1:B:21:MET:O	1:B:25:LEU:HG	2.15	0.45
1:C:21:MET:CE	1:C:72:ILE:HD11	2.29	0.45
1:C:81:LEU:HD23	1:C:118:ILE:HG12	1.99	0.45
1:D:157:ALA:O	1:D:162:LYS:NZ	2.50	0.45
1:F:27:HIS:O	1:F:27:HIS:HD2	1.99	0.45
1:H:78:THR:O	1:H:82:LEU:HD23	2.16	0.45
1:H:99:VAL:CG1	1:H:100:ARG:N	2.79	0.45
1:I:177:SER:OG	1:I:200:ILE:HG21	2.17	0.45
1:J:160:SER:N	2:J:401:PO4:O1	2.49	0.45
1:A:174:ILE:HG13	1:A:202:ALA:CB	2.46	0.45
1:B:54:LYS:HG3	1:B:54:LYS:O	2.16	0.45
1:B:261:THR:HG21	1:B:270:ARG:HD2	1.98	0.45
1:D:125:ILE:CG1	1:D:126:PRO:HD2	2.46	0.45
1:D:269:ARG:NH1	1:D:270:ARG:HH12	2.15	0.45
1:E:22:ASP:OD2	1:E:93:PHE:CD1	2.70	0.45
1:H:18:PRO:O	1:H:21:MET:CB	2.61	0.45
1:I:69:ILE:HG23	1:I:70:ASN:N	2.31	0.45
1:I:137:LEU:HD11	1:I:165:LEU:HD11	1.99	0.45
1:J:39:GLN:CA	1:J:65:LEU:HD21	2.46	0.45
1:J:73:TYR:CD2	1:J:73:TYR:O	2.70	0.45
1:J:81:LEU:HD23	1:J:81:LEU:H	1.80	0.45
1:J:238:ASP:OD1	1:J:241:THR:CG2	2.65	0.45
1:A:180:ASN:HB3	1:F:52:LEU:HB2	1.99	0.45
1:B:86:ASP:HB2	1:C:213:LEU:HD21	1.99	0.45
1:C:179:SER:HB2	1:C:181:ARG:NH2	2.31	0.45
1:C:345:GLN:NE2	1:C:350:ASP:OD1	2.49	0.45
1:F:249:ALA:HB1	1:F:290:THR:OG1	2.17	0.45
1:G:17:THR:HG23	1:G:18:PRO:CD	2.36	0.45
1:G:233:VAL:O	1:G:257:THR:HG22	2.17	0.45
1:I:223:ALA:O	1:I:228:PRO:CD	2.65	0.45
1:J:125:ILE:HG13	1:J:126:PRO:CD	2.45	0.45
1:J:247:GLU:O	1:J:251:THR:HG23	2.17	0.45
1:J:281:LEU:O	1:J:285:ILE:HD13	2.17	0.45
1:J:323:ILE:HD13	1:J:323:ILE:H	1.78	0.45
1:A:148:GLN:O	1:A:254:PRO:HD3	2.17	0.45
1:A:230:LEU:HD22	1:A:254:PRO:HB2	1.98	0.45
1:B:21:MET:HE3	1:B:122:LEU:HD21	1.99	0.45
1:C:17:THR:HG22	1:C:18:PRO:HD2	1.96	0.45
1:D:138:PRO:O	1:D:142:ILE:HG12	2.17	0.45
1:F:70:ASN:OD1	1:F:78:THR:OG1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:155:THR:HG21	1:H:267:THR:CG2	2.44	0.45
1:I:47:GLU:HB2	1:I:52:LEU:HD21	1.98	0.45
1:I:70:ASN:OD1	1:I:78:THR:OG1	2.34	0.45
1:I:104:ARG:N	1:I:125:ILE:HD11	2.32	0.45
1:J:102:ARG:NE	1:J:193:VAL:HG11	2.25	0.45
1:J:198:GLU:OE2	1:J:198:GLU:HA	2.16	0.45
1:J:300:VAL:O	1:J:308:VAL:HG12	2.17	0.45
1:K:188:SER:OG	1:K:189:PRO:CD	2.65	0.45
1:L:33:ALA:HA	1:L:48:VAL:HA	1.98	0.45
1:L:40:THR:N	1:L:65:LEU:CD2	2.80	0.45
1:A:227:LYS:CE	1:F:47:GLU:OE1	2.64	0.44
1:D:38:ILE:HB	1:D:120:ILE:CG2	2.42	0.44
1:D:73:TYR:CG	1:D:73:TYR:O	2.69	0.44
1:E:34:SER:O	1:E:124:THR:HG23	2.17	0.44
1:E:60:LEU:HB3	1:E:65:LEU:CD1	2.47	0.44
1:E:349:TRP:CZ3	1:E:353:MET:CG	2.99	0.44
1:G:322:ASP:O	1:G:325:LEU:HB2	2.17	0.44
1:G:355:PHE:HE2	1:G:365:TYR:CB	2.29	0.44
1:H:209:ILE:H	1:H:210:PRO:HD2	1.81	0.44
1:I:65:LEU:HD23	1:I:68:LEU:HD13	1.98	0.44
1:J:24:MET:SD	1:J:24:MET:C	3.01	0.44
1:J:65:LEU:HB3	1:J:118:ILE:HG12	1.98	0.44
1:L:78:THR:O	1:L:82:LEU:HD13	2.17	0.44
1:L:185:THR:HG22	1:L:232:MET:HB3	1.99	0.44
1:L:209:ILE:HD12	1:L:209:ILE:HA	1.73	0.44
1:C:142:ILE:HA	1:C:145:ILE:HG12	1.98	0.44
1:D:69:ILE:CA	1:D:72:ILE:HG22	2.47	0.44
1:H:6:ILE:HG23	1:H:54:LYS:HG3	1.99	0.44
1:H:261:THR:HG23	1:H:270:ARG:HD3	1.98	0.44
1:I:293:LEU:CD1	1:I:315:VAL:HG22	2.47	0.44
1:J:176:THR:O	1:J:179:SER:HB3	2.18	0.44
1:J:214:PRO:O	1:J:215:ASN:ND2	2.50	0.44
1:A:21:MET:HE1	1:A:72:ILE:CD1	2.40	0.44
1:B:102:ARG:HH21	1:B:127:THR:CG2	2.30	0.44
1:D:175:GLU:CA	1:D:199:THR:CG2	2.86	0.44
1:E:285:ILE:N	1:E:285:ILE:CD1	2.80	0.44
1:G:9:MET:CE	1:G:24:MET:CA	2.85	0.44
1:G:306:ARG:CG	1:G:307:ARG:N	2.78	0.44
1:I:16:PHE:CZ	1:I:21:MET:CA	3.00	0.44
1:I:17:THR:HG22	1:I:18:PRO:HD2	1.99	0.44
1:I:61:SER:HB2	1:I:64:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:209:ILE:H	1:I:210:PRO:HD2	1.81	0.44
1:L:273:THR:C	1:L:275:PHE:H	2.26	0.44
1:A:28:ALA:HB3	1:A:36:ILE:HD11	2.00	0.44
1:B:102:ARG:HH21	1:B:127:THR:CB	2.31	0.44
1:B:337:ARG:NE	1:B:341:ARG:NH1	2.65	0.44
1:B:365:TYR:CZ	1:B:369:ILE:CD1	2.86	0.44
1:C:126:PRO:O	1:C:191:GLU:O	2.35	0.44
1:H:364:VAL:HG13	1:H:365:TYR:N	2.33	0.44
1:I:97:ARG:CB	1:I:99:VAL:HG23	2.48	0.44
1:J:353:MET:HE2	1:J:353:MET:CA	2.47	0.44
1:K:304:ASP:OD2	1:K:306:ARG:HG3	2.18	0.44
1:A:350:ASP:OD1	1:A:354:LYS:HD3	2.17	0.44
1:C:55:ILE:O	1:C:55:ILE:HG22	2.17	0.44
1:C:148:GLN:O	1:C:254:PRO:HD3	2.18	0.44
1:E:285:ILE:N	1:E:285:ILE:HD12	2.31	0.44
1:G:193:VAL:HG22	1:G:194:TYR:N	2.31	0.44
1:H:88:ASP:OD2	1:I:225:ARG:CD	2.65	0.44
1:H:151:ILE:HG21	1:H:153:PHE:CZ	2.53	0.44
1:I:184:LEU:CD1	1:I:228:PRO:CB	2.92	0.44
1:I:195:ASP:OD1	1:I:196:GLU:N	2.50	0.44
1:J:264:VAL:HG13	1:J:265:ALA:N	2.33	0.44
1:K:135:MET:CE	1:K:135:MET:CA	2.77	0.44
1:L:40:THR:HG22	1:L:65:LEU:CB	2.48	0.44
1:L:288:LEU:CD1	1:L:324:LEU:HD13	2.48	0.44
1:A:106:ASN:HD22	1:B:225:ARG:HB3	1.82	0.44
1:B:249:ALA:CB	1:B:290:THR:HG23	2.32	0.44
1:B:251:THR:OG1	1:B:253:HIS:CD2	2.71	0.44
1:C:24:MET:C	1:C:24:MET:SD	3.01	0.44
1:D:108:THR:HB	1:E:226:ARG:NH1	2.33	0.44
1:D:171:ARG:HA	1:D:174:ILE:CG2	2.47	0.44
1:E:89:THR:CG2	1:E:105:VAL:HG13	2.47	0.44
1:E:259:LEU:HD11	1:E:271:LEU:HD21	2.00	0.44
1:F:285:ILE:HD12	1:F:285:ILE:H	1.82	0.44
1:G:111:LEU:HD22	1:H:90:HIS:NE2	2.33	0.44
1:H:92:GLU:OE2	1:H:102:ARG:NH1	2.49	0.44
1:J:13:PRO:HB3	1:J:20:PHE:CD1	2.52	0.44
1:J:111:LEU:HD22	1:J:115:HIS:O	2.18	0.44
1:J:166:LEU:HD13	1:J:232:MET:SD	2.57	0.44
1:L:129:PRO:O	1:L:171:ARG:NH1	2.48	0.44
1:L:365:TYR:O	1:L:369:ILE:HG13	2.18	0.44
1:C:39:GLN:C	1:C:65:LEU:HD21	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:LEU:HD22	1:C:293:LEU:C	2.39	0.44
1:E:162:LYS:CD	1:E:258:THR:CG2	2.96	0.44
1:G:334:SER:O	1:G:337:ARG:HB3	2.18	0.44
1:H:165:LEU:O	1:H:169:ILE:HG13	2.18	0.44
1:H:183:VAL:O	1:H:184:LEU:HD23	2.17	0.44
1:H:261:THR:HG23	1:H:270:ARG:CD	2.48	0.44
1:J:214:PRO:C	1:J:215:ASN:ND2	2.76	0.44
1:J:308:VAL:HG22	1:J:309:ALA:N	2.33	0.44
1:L:9:MET:HE3	1:L:24:MET:CA	2.48	0.44
1:L:89:THR:CG2	1:L:90:HIS:N	2.78	0.44
1:A:174:ILE:CD1	1:A:183:VAL:HG21	2.48	0.44
1:B:209:ILE:H	1:B:210:PRO:HD2	1.83	0.44
1:C:108:THR:HG21	1:D:222:ASN:ND2	2.32	0.44
1:C:108:THR:HG21	1:D:226:ARG:HH11	1.82	0.44
1:D:118:ILE:O	1:D:118:ILE:HG13	2.16	0.44
1:E:131:LYS:HB2	1:E:171:ARG:HH21	1.82	0.44
1:F:156:GLY:N	1:F:162:LYS:HD3	2.33	0.44
1:F:166:LEU:HD13	1:F:232:MET:HE1	2.00	0.44
1:F:288:LEU:CD1	1:F:324:LEU:HD13	2.47	0.44
1:H:229:ARG:HB2	1:H:229:ARG:NH2	2.33	0.44
1:I:166:LEU:HD13	1:I:232:MET:SD	2.58	0.44
1:I:365:TYR:HA	1:I:368:ILE:CD1	2.46	0.44
1:K:81:LEU:HD12	1:K:118:ILE:HG12	1.99	0.44
1:C:94:ARG:O	1:C:95:PRO:O	2.36	0.44
1:C:301:PRO:HA	1:C:307:ARG:HD3	2.00	0.44
1:D:128:THR:HG23	1:D:196:GLU:OE1	2.18	0.44
1:D:229:ARG:HG3	1:D:229:ARG:O	2.18	0.44
1:D:363:ARG:O	1:D:366:LYS:HG2	2.17	0.44
1:E:354:LYS:HE2	1:E:354:LYS:CA	2.42	0.44
1:G:186:TYR:HB3	1:G:209:ILE:HD11	2.00	0.44
1:H:24:MET:HE2	1:H:44:ILE:HD13	1.99	0.44
1:H:137:LEU:HD11	1:H:311:ARG:NE	2.33	0.44
1:K:145:ILE:O	1:K:147:PRO:HD2	2.17	0.44
1:K:366:LYS:HG3	1:K:366:LYS:H	1.57	0.44
1:A:332:VAL:HG23	1:A:333:THR:N	2.33	0.43
1:B:209:ILE:N	1:B:210:PRO:CD	2.80	0.43
1:C:111:LEU:C	1:C:111:LEU:CD1	2.90	0.43
1:C:209:ILE:HD13	1:C:209:ILE:HA	1.73	0.43
1:D:233:VAL:HB	1:D:257:THR:CG2	2.33	0.43
1:E:17:THR:HG23	1:E:18:PRO:CD	2.44	0.43
1:E:111:LEU:CD2	1:F:90:HIS:NE2	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:291:ILE:HD13	1:F:316:PHE:CE1	2.52	0.43
1:G:39:GLN:C	1:G:65:LEU:HD21	2.42	0.43
1:H:317:ASP:O	1:H:321:ARG:HG3	2.18	0.43
1:I:22:ASP:OD2	1:I:93:PHE:CG	2.71	0.43
1:I:126:PRO:O	1:I:191:GLU:O	2.35	0.43
1:J:145:ILE:HD13	1:J:293:LEU:CD2	2.47	0.43
1:K:111:LEU:HD21	1:L:90:HIS:CD2	2.52	0.43
1:K:302:THR:OG1	1:K:306:ARG:O	2.36	0.43
1:K:333:THR:HA	1:K:336:THR:CG2	2.49	0.43
1:L:331:GLU:HG3	1:L:334:SER:HB2	2.00	0.43
1:C:258:THR:C	1:C:259:LEU:HD12	2.44	0.43
1:D:300:VAL:HG11	1:D:368:ILE:HD11	1.99	0.43
1:E:353:MET:O	1:E:357:GLN:HG2	2.17	0.43
1:F:40:THR:CG2	1:F:62:ASN:HA	2.48	0.43
1:G:5:ASN:C	1:G:6:ILE:CG2	2.90	0.43
1:H:105:VAL:HG22	1:H:122:LEU:HG	2.00	0.43
1:H:246:LEU:C	1:H:250:LEU:HD12	2.43	0.43
1:I:47:GLU:CB	1:I:52:LEU:CD2	2.96	0.43
1:I:165:LEU:O	1:I:169:ILE:HG13	2.18	0.43
1:I:236:CYS:SG	1:I:242:ILE:HG13	2.58	0.43
1:I:283:ARG:HD3	1:I:283:ARG:HA	1.70	0.43
1:J:158:THR:HB	1:J:260:HIS:HE1	1.82	0.43
1:K:40:THR:N	1:K:65:LEU:HD21	2.33	0.43
1:L:222:ASN:CA	1:L:225:ARG:NH2	2.75	0.43
1:L:290:THR:O	1:L:292:ARG:NH2	2.52	0.43
1:A:222:ASN:OD1	1:A:226:ARG:NH1	2.52	0.43
1:A:355:PHE:CB	1:A:360:ILE:CG2	2.96	0.43
1:C:230:LEU:HD11	1:C:256:TYR:CE1	2.53	0.43
1:E:222:ASN:O	1:E:225:ARG:N	2.49	0.43
1:F:148:GLN:O	1:F:254:PRO:HD3	2.17	0.43
1:F:249:ALA:CB	1:F:290:THR:OG1	2.65	0.43
1:F:369:ILE:O	1:F:372:ALA:CB	2.66	0.43
1:H:361:SER:O	1:H:364:VAL:HG12	2.19	0.43
1:I:70:ASN:ND2	1:I:78:THR:OG1	2.52	0.43
1:J:151:ILE:HG21	1:J:153:PHE:CZ	2.53	0.43
1:A:333:THR:O	1:A:336:THR:OG1	2.35	0.43
1:A:355:PHE:N	1:A:360:ILE:HG22	2.33	0.43
1:B:40:THR:N	1:B:65:LEU:HD21	2.33	0.43
1:B:48:VAL:HG21	1:B:53:LEU:HD11	2.00	0.43
1:B:139:ASP:OD1	1:B:139:ASP:N	2.49	0.43
1:C:105:VAL:HG22	1:C:122:LEU:HG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ARG:HG3	1:C:333:THR:HG21	2.00	0.43
1:D:190:ILE:O	1:D:190:ILE:HG22	2.17	0.43
1:E:23:ARG:HD3	1:E:23:ARG:HA	1.75	0.43
1:F:333:THR:O	1:F:336:THR:OG1	2.28	0.43
1:H:55:ILE:HG22	1:H:55:ILE:O	2.18	0.43
1:I:60:LEU:HD23	1:I:60:LEU:N	2.33	0.43
1:K:178:ASP:OD1	1:K:178:ASP:N	2.50	0.43
1:B:102:ARG:HE	1:B:127:THR:CG2	2.27	0.43
1:C:363:ARG:CG	1:C:364:VAL:N	2.77	0.43
1:F:37:THR:OG1	1:F:45:PHE:HB2	2.18	0.43
1:F:135:MET:HB3	1:F:137:LEU:CD1	2.48	0.43
1:F:179:SER:OG	1:F:179:SER:O	2.37	0.43
1:G:28:ALA:HB3	1:G:36:ILE:HD11	1.99	0.43
1:G:223:ALA:O	1:G:228:PRO:HD3	2.19	0.43
1:J:183:VAL:HG13	1:J:230:LEU:CD2	2.37	0.43
1:A:13:PRO:HG3	1:A:20:PHE:CG	2.53	0.43
1:A:355:PHE:HB2	1:A:360:ILE:CG2	2.48	0.43
1:D:156:GLY:C	1:D:162:LYS:NZ	2.77	0.43
1:G:151:ILE:HG21	1:G:153:PHE:CZ	2.53	0.43
1:G:235:GLU:HA	1:G:258:THR:OG1	2.17	0.43
1:I:13:PRO:HG3	1:I:20:PHE:CG	2.53	0.43
1:I:360:ILE:HG23	1:I:364:VAL:HB	2.01	0.43
1:J:25:LEU:HD12	1:J:93:PHE:CE2	2.53	0.43
1:J:223:ALA:O	1:J:228:PRO:HD3	2.17	0.43
1:L:162:LYS:HE2	1:L:162:LYS:HB2	1.79	0.43
1:L:361:SER:HB2	1:L:364:VAL:HG23	2.00	0.43
1:C:16:PHE:HE1	1:C:21:MET:HA	1.83	0.43
1:D:69:ILE:HA	1:D:69:ILE:HD12	1.87	0.43
1:E:86:ASP:OD2	1:F:222:ASN:ND2	2.50	0.43
1:F:39:GLN:C	1:F:65:LEU:HD21	2.44	0.43
1:F:157:ALA:O	1:F:162:LYS:NZ	2.50	0.43
1:H:88:ASP:OD2	1:I:225:ARG:HD2	2.19	0.43
1:H:372:ALA:O	1:H:373:LYS:C	2.61	0.43
1:I:12:GLU:OE1	1:I:58:ARG:NE	2.52	0.43
1:I:48:VAL:HG12	1:I:49:TYR:HD2	1.84	0.43
1:I:230:LEU:HD13	1:I:256:TYR:CE1	2.53	0.43
1:J:174:ILE:O	1:J:199:THR:CG2	2.67	0.43
1:L:220:VAL:O	1:L:223:ALA:HB3	2.18	0.43
1:L:236:CYS:O	1:L:259:LEU:HD21	2.18	0.43
1:L:238:ASP:O	1:L:241:THR:HG22	2.18	0.43
1:B:73:TYR:O	1:B:73:TYR:CD2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:PHE:CE2	1:D:203:VAL:HG22	2.54	0.43
1:C:174:ILE:CD1	1:C:199:THR:CG2	2.96	0.43
1:C:174:ILE:HG13	1:C:202:ALA:HB1	2.01	0.43
1:C:268:MET:SD	1:C:291:ILE:HD13	2.59	0.43
1:D:73:TYR:O	1:D:73:TYR:CD2	2.72	0.43
1:H:65:LEU:HD12	1:H:120:ILE:CD1	2.49	0.43
1:H:104:ARG:NH2	1:H:191:GLU:CD	2.76	0.43
1:K:48:VAL:HG12	1:K:49:TYR:CD2	2.54	0.43
1:K:93:PHE:HE2	1:K:103:TYR:CE1	2.36	0.43
1:K:235:GLU:OE2	1:K:237:ARG:NE	2.51	0.43
1:K:317:ASP:O	1:K:321:ARG:HG3	2.18	0.43
1:L:60:LEU:N	1:L:60:LEU:HD12	2.33	0.43
1:A:37:THR:CG2	1:B:182:LYS:HE3	2.49	0.43
1:D:185:THR:HG22	1:D:232:MET:HB3	2.00	0.43
1:E:137:LEU:CB	1:E:141:ILE:HD11	2.46	0.43
1:E:155:THR:O	1:E:296:TRP:HA	2.18	0.43
1:F:362:GLU:O	1:F:366:LYS:HG3	2.19	0.43
1:H:261:THR:CG2	1:H:270:ARG:HD3	2.49	0.43
1:J:160:SER:O	1:J:297:GLN:NE2	2.52	0.43
1:J:249:ALA:HB1	1:J:290:THR:OG1	2.19	0.43
1:K:8:LEU:O	1:K:27:HIS:CE1	2.71	0.43
1:K:12:GLU:CD	1:K:57:ASN:N	2.72	0.43
1:K:21:MET:CE	1:K:68:LEU:HG	2.48	0.43
1:B:188:SER:CB	1:B:189:PRO:HD2	2.48	0.43
1:E:209:ILE:HG13	1:E:216:PHE:CE1	2.54	0.43
1:F:59:ARG:H	1:F:59:ARG:HG3	1.66	0.43
1:G:223:ALA:O	1:G:228:PRO:CD	2.66	0.43
1:H:9:MET:CE	1:H:24:MET:N	2.82	0.43
1:H:230:LEU:C	1:H:230:LEU:CD2	2.91	0.43
1:I:81:LEU:N	1:I:81:LEU:CD1	2.82	0.43
1:J:13:PRO:HB3	1:J:20:PHE:HE1	1.73	0.43
1:J:283:ARG:HA	1:J:283:ARG:HE	1.84	0.43
1:K:9:MET:SD	1:K:10:PRO:CD	3.03	0.43
1:K:171:ARG:O	1:K:174:ILE:HG22	2.14	0.43
1:L:305:GLU:O	1:L:306:ARG:HD3	2.19	0.43
1:A:39:GLN:C	1:A:65:LEU:HD21	2.44	0.42
1:B:195:ASP:O	1:B:198:GLU:HB2	2.19	0.42
1:C:37:THR:OG1	1:C:45:PHE:HB2	2.18	0.42
1:D:296:TRP:CZ3	1:D:347:MET:HE3	2.54	0.42
1:E:9:MET:CG	1:E:10:PRO:CD	2.96	0.42
1:E:17:THR:HB	1:E:20:PHE:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:ILE:HG21	1:E:153:PHE:CZ	2.54	0.42
1:E:162:LYS:HD3	1:E:258:THR:CG2	2.47	0.42
1:F:17:THR:HB	1:F:20:PHE:HD1	1.84	0.42
1:F:48:VAL:C	1:F:49:TYR:CD2	2.97	0.42
1:G:155:THR:CG2	1:G:259:LEU:O	2.67	0.42
1:G:354:LYS:CB	1:G:360:ILE:CD1	2.88	0.42
1:H:339:LEU:HD23	1:H:339:LEU:HA	1.81	0.42
1:I:312:GLU:HB2	1:I:347:MET:N	2.33	0.42
1:J:73:TYR:O	1:J:73:TYR:CG	2.71	0.42
1:K:181:ARG:HA	1:K:229:ARG:HB3	2.01	0.42
1:L:17:THR:HB	1:L:20:PHE:CD1	2.54	0.42
1:L:112:VAL:CG2	1:L:117:ALA:HB1	2.41	0.42
1:A:102:ARG:HH11	1:A:127:THR:HG21	1.85	0.42
1:A:306:ARG:CG	1:A:307:ARG:H	2.32	0.42
1:D:123:ARG:NH2	1:E:225:ARG:O	2.52	0.42
1:E:8:LEU:O	1:E:27:HIS:CE1	2.73	0.42
1:E:174:ILE:HG13	1:E:202:ALA:HB1	2.00	0.42
1:E:265:ALA:CB	1:E:337:ARG:HG3	2.49	0.42
1:F:175:GLU:HA	1:F:199:THR:HG22	2.00	0.42
1:G:355:PHE:HB2	1:G:356:GLU:OE2	2.18	0.42
1:J:171:ARG:HA	1:J:174:ILE:CG2	2.49	0.42
1:J:173:LEU:O	1:J:179:SER:HB2	2.18	0.42
1:J:251:THR:OG1	1:J:253:HIS:CD2	2.72	0.42
1:K:269:ARG:NH2	1:L:322:ASP:OD1	2.52	0.42
1:A:94:ARG:HH12	1:A:97:ARG:CD	2.22	0.42
1:A:333:THR:OG1	1:A:334:SER:N	2.52	0.42
1:A:355:PHE:CE1	1:A:362:GLU:HA	2.54	0.42
1:C:111:LEU:HD13	1:C:112:VAL:N	2.33	0.42
1:E:22:ASP:OD2	1:E:93:PHE:CE1	2.72	0.42
1:E:93:PHE:CD2	1:E:93:PHE:C	2.96	0.42
1:F:112:VAL:O	1:F:112:VAL:HG23	2.17	0.42
1:F:212:HIS:C	1:F:213:LEU:HG	2.44	0.42
1:G:155:THR:CG2	1:G:259:LEU:C	2.92	0.42
1:G:181:ARG:HD3	1:G:229:ARG:HG3	2.00	0.42
1:G:296:TRP:CE3	1:G:347:MET:SD	3.12	0.42
1:I:13:PRO:HB3	1:I:20:PHE:CD2	2.51	0.42
1:I:21:MET:HE3	1:I:68:LEU:HD23	1.99	0.42
1:L:194:TYR:HA	1:L:197:ILE:CD1	2.43	0.42
1:L:292:ARG:HD3	1:L:321:ARG:NH1	2.34	0.42
1:A:179:SER:HB2	1:A:181:ARG:HH21	1.83	0.42
1:A:281:LEU:O	1:A:285:ILE:CD1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:ILE:HG13	1:E:202:ALA:HB3	2.01	0.42
1:E:271:LEU:HB3	1:E:287:ILE:HD12	2.01	0.42
1:F:151:ILE:HG21	1:F:153:PHE:CZ	2.54	0.42
1:G:95:PRO:HD2	1:G:99:VAL:HG23	2.01	0.42
1:G:96:ASN:OD1	1:G:97:ARG:N	2.52	0.42
1:G:289:GLU:C	1:G:289:GLU:CD	2.87	0.42
1:H:40:THR:OG1	1:H:65:LEU:HD23	2.19	0.42
1:H:80:GLN:O	1:H:83:SER:HB2	2.18	0.42
1:H:263:GLY:O	1:H:267:THR:OG1	2.34	0.42
1:I:57:ASN:OD1	1:I:57:ASN:N	2.51	0.42
1:I:72:ILE:CG2	1:I:91:TYR:HB2	2.49	0.42
1:I:364:VAL:O	1:I:368:ILE:HG12	2.20	0.42
1:K:90:HIS:CD2	1:K:104:ARG:HA	2.54	0.42
1:K:91:TYR:CE1	1:K:93:PHE:HD2	2.37	0.42
1:L:299:LEU:HD23	1:L:299:LEU:HA	1.93	0.42
1:B:315:VAL:O	1:B:315:VAL:HG13	2.18	0.42
1:D:296:TRP:CZ3	1:D:347:MET:CE	3.02	0.42
1:E:95:PRO:CG	1:E:96:ASN:H	2.11	0.42
1:E:368:ILE:HD12	1:E:368:ILE:HA	1.91	0.42
1:F:184:LEU:CD1	1:F:228:PRO:HB3	2.49	0.42
1:G:203:VAL:CG1	1:L:39:GLN:HE22	2.32	0.42
1:H:119:GLN:NE2	1:I:182:LYS:CE	2.82	0.42
1:I:338:LYS:HE3	1:I:342:GLN:OE1	2.20	0.42
1:K:66:GLY:O	1:K:69:ILE:HG22	2.20	0.42
1:K:230:LEU:C	1:K:230:LEU:CD2	2.93	0.42
1:L:165:LEU:O	1:L:169:ILE:HG12	2.20	0.42
1:L:329:PRO:HA	1:L:332:VAL:HG23	2.01	0.42
1:A:188:SER:OG	1:A:189:PRO:CD	2.67	0.42
1:B:132:LEU:CB	1:B:172:GLU:HG3	2.49	0.42
1:B:250:LEU:HD23	1:B:250:LEU:HA	1.90	0.42
1:E:149:GLU:O	1:E:292:ARG:HD3	2.20	0.42
1:E:213:LEU:HD23	1:E:213:LEU:HA	1.82	0.42
1:E:215:ASN:N	1:E:215:ASN:ND2	2.66	0.42
1:F:170:ILE:HG22	1:F:174:ILE:HD12	2.00	0.42
1:G:317:ASP:CA	1:G:321:ARG:HH12	2.32	0.42
1:I:12:GLU:OE2	1:I:58:ARG:HG3	2.20	0.42
1:I:61:SER:CB	1:I:64:GLU:OE1	2.67	0.42
1:J:263:GLY:CA	1:J:266:GLU:HG2	2.50	0.42
1:J:268:MET:HG3	1:J:336:THR:HG21	2.00	0.42
1:K:151:ILE:HG21	1:K:153:PHE:CZ	2.54	0.42
1:L:149:GLU:CG	1:L:150:GLY:H	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:TYR:O	1:A:369:ILE:HD12	2.19	0.42
1:B:137:LEU:HD11	1:B:311:ARG:NH2	2.35	0.42
1:C:69:ILE:HD12	1:C:69:ILE:HA	1.90	0.42
1:C:155:THR:HG22	1:C:259:LEU:HB2	2.02	0.42
1:D:92:GLU:CD	1:D:102:ARG:HE	2.27	0.42
1:G:48:VAL:HG12	1:G:49:TYR:CD2	2.55	0.42
1:H:340:VAL:CG2	1:H:346:LEU:CD2	2.97	0.42
1:J:40:THR:HG21	1:J:62:ASN:HB2	2.01	0.42
1:K:25:LEU:CD1	1:K:93:PHE:CZ	3.03	0.42
1:K:293:LEU:CD1	1:K:315:VAL:HG22	2.46	0.42
1:L:7:ASN:C	1:L:8:LEU:HD22	2.45	0.42
1:C:48:VAL:HG12	1:C:49:TYR:CD2	2.51	0.42
1:F:132:LEU:HD11	1:F:169:ILE:HD11	2.02	0.42
1:G:104:ARG:HB2	1:G:125:ILE:HD11	2.01	0.42
1:H:26:GLU:OE1	1:H:95:PRO:HB3	2.19	0.42
1:H:145:ILE:HD12	1:H:145:ILE:HA	1.92	0.42
1:I:349:TRP:O	1:I:349:TRP:HD1	2.03	0.42
1:B:131:LYS:HB2	1:B:134:THR:HG23	2.01	0.42
1:D:65:LEU:HD23	1:D:118:ILE:HG13	2.01	0.42
1:D:186:TYR:CZ	1:D:219:GLY:O	2.72	0.42
1:F:73:TYR:CE1	1:F:89:THR:HG22	2.54	0.42
1:F:185:THR:HG22	1:F:232:MET:HB3	2.00	0.42
1:G:235:GLU:N	1:G:258:THR:HG1	2.18	0.42
1:G:306:ARG:HG2	1:G:307:ARG:H	1.83	0.42
1:G:362:GLU:O	1:G:366:LYS:HG3	2.20	0.42
1:I:64:GLU:C	1:I:68:LEU:HD12	2.44	0.42
1:J:163:SER:CB	1:J:191:GLU:OE2	2.68	0.42
1:J:263:GLY:C	1:J:266:GLU:HG2	2.44	0.42
1:K:91:TYR:CD1	1:K:93:PHE:HD2	2.37	0.42
1:K:288:LEU:CB	1:K:325:LEU:HD23	2.47	0.42
1:A:21:MET:CE	1:A:72:ILE:HD11	2.39	0.42
1:A:37:THR:HG21	1:B:182:LYS:HE3	2.02	0.42
1:E:19:VAL:HG21	1:J:331:GLU:HG3	2.01	0.42
1:G:205:SER:HB2	1:L:119:GLN:OE1	2.19	0.42
1:H:54:LYS:HG3	1:H:54:LYS:O	2.19	0.42
1:H:348:THR:HG22	1:H:372:ALA:HB3	2.02	0.42
1:J:9:MET:CE	1:J:24:MET:N	2.78	0.42
1:J:81:LEU:CD2	1:J:87:ILE:CD1	2.89	0.42
1:J:319:GLU:O	1:J:323:ILE:HG12	2.19	0.42
1:J:363:ARG:HG3	1:J:366:LYS:HE3	2.02	0.42
1:K:154:ILE:HG21	1:K:165:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:THR:O	1:B:167:ALA:N	2.53	0.41
1:C:174:ILE:HD12	1:C:204:VAL:CG2	2.50	0.41
1:D:87:ILE:HB	1:D:107:ALA:HB3	2.02	0.41
1:D:273:THR:C	1:D:275:PHE:H	2.28	0.41
1:D:308:VAL:HG22	1:D:309:ALA:N	2.35	0.41
1:G:148:GLN:O	1:G:254:PRO:HD3	2.20	0.41
1:G:279:GLU:OE1	1:G:279:GLU:CA	2.61	0.41
1:H:172:GLU:O	1:H:176:THR:CG2	2.62	0.41
1:I:16:PHE:CZ	1:I:20:PHE:C	2.98	0.41
1:I:198:GLU:H	1:I:198:GLU:HG2	1.55	0.41
1:J:69:ILE:CA	1:J:72:ILE:HG22	2.50	0.41
1:J:249:ALA:CB	1:J:290:THR:OG1	2.68	0.41
1:J:302:THR:HG1	1:J:306:ARG:C	2.24	0.41
1:K:242:ILE:HD13	1:K:271:LEU:CD2	2.49	0.41
1:K:297:GLN:HE21	1:K:311:ARG:NE	2.17	0.41
1:K:352:LYS:HA	1:K:365:TYR:CE2	2.56	0.41
1:L:135:MET:HE2	1:L:165:LEU:HD13	2.02	0.41
1:L:193:VAL:HA	1:L:206:GLN:HE22	1.84	0.41
1:A:158:THR:OG1	1:B:251:THR:O	2.27	0.41
1:A:278:GLU:OE2	1:F:337:ARG:NH1	2.52	0.41
1:A:320:VAL:CG1	1:A:339:LEU:HD13	2.50	0.41
1:B:119:GLN:NE2	1:C:226:ARG:NH2	2.53	0.41
1:B:125:ILE:HD12	1:B:125:ILE:HA	1.93	0.41
1:C:162:LYS:O	1:C:166:LEU:HG	2.20	0.41
1:C:251:THR:OG1	1:C:253:HIS:CD2	2.71	0.41
1:C:367:LEU:C	1:C:367:LEU:CD2	2.87	0.41
1:D:174:ILE:HD12	1:D:204:VAL:HG21	2.01	0.41
1:E:108:THR:OG1	1:F:226:ARG:NH2	2.47	0.41
1:E:237:ARG:CZ	1:F:247:GLU:OE1	2.68	0.41
1:F:183:VAL:CG1	1:F:230:LEU:HD22	2.36	0.41
1:F:340:VAL:HG23	1:F:341:ARG:N	2.35	0.41
1:G:126:PRO:O	1:G:191:GLU:O	2.38	0.41
1:G:300:VAL:O	1:G:308:VAL:HG12	2.20	0.41
1:G:318:GLU:CG	1:L:363:ARG:CZ	2.91	0.41
1:G:328:ASP:OD1	1:G:328:ASP:C	2.64	0.41
1:I:44:ILE:H	1:I:56:THR:HG22	1.84	0.41
1:J:315:VAL:O	1:J:315:VAL:HG13	2.19	0.41
1:K:351:ALA:O	1:K:360:ILE:HD11	2.20	0.41
1:L:73:TYR:CD2	1:L:73:TYR:C	2.98	0.41
1:L:102:ARG:C	1:L:125:ILE:HG22	2.45	0.41
1:L:182:LYS:HG3	1:L:203:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:TYR:CD2	1:A:87:ILE:HG12	2.54	0.41
1:A:209:ILE:N	1:A:210:PRO:CD	2.84	0.41
1:B:13:PRO:HG3	1:B:20:PHE:CG	2.55	0.41
1:C:171:ARG:C	1:C:174:ILE:HG22	2.45	0.41
1:C:209:ILE:N	1:C:210:PRO:CD	2.83	0.41
1:D:48:VAL:HG12	1:D:49:TYR:HD2	1.86	0.41
1:F:222:ASN:OD1	1:F:226:ARG:NE	2.53	0.41
1:G:158:THR:HA	1:G:162:LYS:NZ	2.34	0.41
1:G:352:LYS:CG	1:G:365:TYR:CZ	3.02	0.41
1:H:246:LEU:O	1:H:250:LEU:CD1	2.67	0.41
1:H:336:THR:O	1:H:340:VAL:HG13	2.20	0.41
1:H:367:LEU:HD23	1:I:325:LEU:HD22	2.02	0.41
1:J:209:ILE:HD12	1:J:215:ASN:C	2.45	0.41
1:J:302:THR:N	1:J:306:ARG:O	2.53	0.41
1:J:350:ASP:OD1	1:J:354:LYS:HD3	2.20	0.41
1:A:297:GLN:HE21	1:A:311:ARG:HE	1.65	0.41
1:B:69:ILE:HD12	1:B:69:ILE:HA	1.92	0.41
1:B:135:MET:HB3	1:B:137:LEU:CD1	2.49	0.41
1:E:296:TRP:CE3	1:E:347:MET:HE2	2.56	0.41
1:G:291:ILE:C	1:G:292:ARG:HG2	2.46	0.41
1:I:119:GLN:HE22	1:J:182:LYS:CE	2.32	0.41
1:I:355:PHE:CD1	1:I:355:PHE:C	2.98	0.41
1:J:100:ARG:HD3	1:J:100:ARG:N	2.30	0.41
1:J:166:LEU:HD21	1:J:256:TYR:HB3	2.02	0.41
1:J:212:HIS:O	1:J:213:LEU:HG	2.20	0.41
1:L:37:THR:OG1	1:L:45:PHE:HB2	2.21	0.41
1:L:305:GLU:C	1:L:306:ARG:HD3	2.45	0.41
1:L:314:LEU:HD11	1:L:339:LEU:HB3	2.03	0.41
1:A:60:LEU:HB3	1:A:65:LEU:CD1	2.50	0.41
1:D:95:PRO:HD2	1:D:99:VAL:O	2.21	0.41
1:D:315:VAL:HG13	1:D:315:VAL:O	2.20	0.41
1:F:9:MET:HE1	1:F:24:MET:HB2	1.98	0.41
1:F:141:ILE:HG23	1:F:295:ILE:HD11	2.01	0.41
1:F:275:PHE:CE1	1:F:283:ARG:HD3	2.56	0.41
1:G:132:LEU:C	1:G:132:LEU:CD2	2.94	0.41
1:H:58:ARG:HB3	1:H:58:ARG:CZ	2.51	0.41
1:J:162:LYS:HE3	2:J:401:PO4:O1	2.20	0.41
1:K:87:ILE:HB	1:K:107:ALA:HB3	2.02	0.41
1:A:37:THR:HG22	1:A:121:THR:HG23	2.02	0.41
1:A:183:VAL:HG13	1:A:230:LEU:HD12	2.02	0.41
1:A:322:ASP:OD1	1:F:363:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:MET:HE1	1:B:20:PHE:O	2.21	0.41
1:D:72:ILE:HG13	1:D:91:TYR:CD1	2.55	0.41
1:D:280:ARG:O	1:D:284:THR:CG2	2.40	0.41
1:E:116:ASP:CG	1:F:211:ARG:NH1	2.79	0.41
1:E:121:THR:CG2	1:F:182:LYS:HE3	2.51	0.41
1:E:288:LEU:CB	1:E:325:LEU:HD21	2.50	0.41
1:G:69:ILE:HD11	1:G:120:ILE:HG23	2.02	0.41
1:G:176:THR:CG2	1:G:177:SER:N	2.84	0.41
1:H:29:GLU:OE1	1:H:29:GLU:HA	2.19	0.41
1:H:208:GLU:HG2	1:H:210:PRO:HD2	2.03	0.41
1:I:54:LYS:O	1:I:55:ILE:HD13	2.18	0.41
1:I:110:CYS:HB2	1:J:206:GLN:O	2.20	0.41
1:I:166:LEU:CD1	1:I:232:MET:HE1	2.50	0.41
1:I:171:ARG:CA	1:I:174:ILE:HG22	2.50	0.41
1:I:174:ILE:HG12	1:I:202:ALA:CB	2.50	0.41
1:J:78:THR:H	1:J:78:THR:HG1	1.60	0.41
1:J:165:LEU:HD12	1:J:165:LEU:O	2.20	0.41
1:K:111:LEU:HD13	1:L:90:HIS:HE1	1.78	0.41
1:K:279:GLU:H	1:K:279:GLU:HG2	1.61	0.41
1:L:17:THR:CG2	1:L:18:PRO:HD2	2.41	0.41
1:L:188:SER:HA	1:L:209:ILE:CG2	2.45	0.41
1:C:281:LEU:HD23	1:C:285:ILE:HD13	2.02	0.41
1:C:308:VAL:HG22	1:C:309:ALA:N	2.36	0.41
1:D:158:THR:HG22	1:E:247:GLU:OE1	2.21	0.41
1:D:223:ALA:O	1:D:228:PRO:HD3	2.20	0.41
1:E:215:ASN:ND2	1:E:218:ASP:HB2	2.35	0.41
1:G:141:ILE:O	1:G:144:ALA:N	2.45	0.41
1:G:208:GLU:CG	1:G:210:PRO:HD2	2.51	0.41
1:H:132:LEU:HB2	1:H:172:GLU:CG	2.51	0.41
1:J:47:GLU:HA	1:J:51:ARG:O	2.21	0.41
1:K:283:ARG:HD2	1:K:283:ARG:N	2.35	0.41
1:L:332:VAL:O	1:L:336:THR:HG23	2.20	0.41
1:C:17:THR:HG23	1:C:18:PRO:CD	2.44	0.41
1:C:66:GLY:O	1:C:69:ILE:HG22	2.21	0.41
1:C:182:LYS:HB3	1:C:228:PRO:HA	2.02	0.41
1:E:86:ASP:OD1	1:E:87:ILE:N	2.53	0.41
1:F:69:ILE:HD12	1:F:69:ILE:HA	1.88	0.41
1:I:24:MET:HE3	1:I:44:ILE:CD1	2.47	0.41
1:I:151:ILE:CG2	1:I:153:PHE:CE1	3.04	0.41
1:J:60:LEU:HB3	1:J:65:LEU:CD1	2.50	0.41
1:K:33:ALA:HB2	1:K:48:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:93:PHE:HE2	1:L:103:TYR:HE2	1.67	0.41
1:L:247:GLU:O	1:L:251:THR:HG23	2.20	0.41
1:L:271:LEU:HD23	1:L:271:LEU:HA	1.92	0.41
1:L:287:ILE:O	1:L:290:THR:HG22	2.20	0.41
1:A:89:THR:CG2	1:A:90:HIS:H	2.25	0.41
1:A:166:LEU:HD13	1:A:232:MET:HE1	2.03	0.41
1:B:90:HIS:NE2	1:B:92:GLU:CG	2.79	0.41
1:B:223:ALA:O	1:B:228:PRO:CD	2.69	0.41
1:B:300:VAL:HG21	1:B:310:LEU:HD11	2.02	0.41
1:B:355:PHE:CD1	1:B:355:PHE:C	2.95	0.41
1:C:81:LEU:CD1	1:C:87:ILE:CD1	2.99	0.41
1:E:268:MET:CE	1:E:288:LEU:HD12	2.51	0.41
1:F:149:GLU:CG	1:F:150:GLY:N	2.73	0.41
1:F:269:ARG:HG3	1:F:333:THR:HB	2.03	0.41
1:F:288:LEU:HD11	1:F:324:LEU:HD13	2.03	0.41
1:G:24:MET:HE2	1:G:44:ILE:HD13	2.02	0.41
1:G:47:GLU:HG3	1:G:52:LEU:HD23	2.03	0.41
1:G:183:VAL:HG13	1:G:230:LEU:HD12	2.02	0.41
1:H:73:TYR:O	1:H:73:TYR:CG	2.73	0.41
1:H:242:ILE:O	1:H:246:LEU:HG	2.21	0.41
1:H:328:ASP:OD1	1:H:328:ASP:C	2.64	0.41
1:I:47:GLU:CB	1:I:52:LEU:HD23	2.50	0.41
1:J:188:SER:HB3	1:J:189:PRO:HD3	2.03	0.41
1:J:222:ASN:OD1	1:J:222:ASN:C	2.64	0.41
1:K:188:SER:HA	1:K:210:PRO:HD3	2.03	0.41
1:K:365:TYR:CD1	1:K:365:TYR:C	2.99	0.41
1:C:151:ILE:HG21	1:C:153:PHE:CZ	2.57	0.41
1:F:44:ILE:HG22	1:F:55:ILE:HD11	2.03	0.41
1:G:229:ARG:NE	1:G:229:ARG:CA	2.84	0.41
1:G:264:VAL:O	1:G:267:THR:HB	2.21	0.41
1:G:345:GLN:CB	1:G:349:TRP:CZ3	3.03	0.41
1:H:209:ILE:N	1:H:210:PRO:CD	2.83	0.41
1:H:212:HIS:C	1:H:213:LEU:CD1	2.87	0.41
1:I:353:MET:HG3	1:I:357:GLN:NE2	2.36	0.41
1:J:9:MET:CG	1:J:10:PRO:CD	2.93	0.41
1:J:183:VAL:O	1:J:204:VAL:HA	2.20	0.41
1:K:230:LEU:HD21	1:K:256:TYR:CD1	2.56	0.41
1:L:7:ASN:O	1:L:55:ILE:HA	2.21	0.41
1:L:262:SER:HA	1:L:296:TRP:CZ3	2.56	0.41
1:L:352:LYS:CA	1:L:365:TYR:CE1	3.04	0.41
1:B:7:ASN:N	1:B:7:ASN:ND2	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:PHE:CE1	1:B:101:TYR:CD2	3.06	0.40
1:B:260:HIS:CE1	1:C:221:ARG:NH2	2.89	0.40
1:B:320:VAL:HG13	1:B:339:LEU:HD13	2.04	0.40
1:D:199:THR:OG1	1:D:202:ALA:HB3	2.20	0.40
1:E:279:GLU:O	1:E:283:ARG:HG2	2.21	0.40
1:E:328:ASP:C	1:E:328:ASP:OD1	2.64	0.40
1:F:165:LEU:O	1:F:169:ILE:HG12	2.21	0.40
1:G:9:MET:HA	1:G:27:HIS:CE1	2.56	0.40
1:G:186:TYR:HA	1:G:207:SER:O	2.21	0.40
1:G:313:TYR:CE2	1:G:345:GLN:OE1	2.74	0.40
1:H:65:LEU:HA	1:H:68:LEU:HG	2.03	0.40
1:I:209:ILE:N	1:I:210:PRO:CD	2.84	0.40
1:I:317:ASP:H	1:I:320:VAL:HG23	1.86	0.40
1:J:35:ASP:OD2	1:K:227:LYS:CD	2.69	0.40
1:J:119:GLN:NE2	1:K:182:LYS:HE2	2.36	0.40
1:J:277:GLY:HA2	1:J:280:ARG:HB3	2.03	0.40
1:J:354:LYS:HG3	1:J:359:ILE:CD1	2.48	0.40
1:L:44:ILE:CG2	1:L:55:ILE:HD11	2.51	0.40
1:B:188:SER:OG	1:B:189:PRO:CD	2.69	0.40
1:D:367:LEU:HD12	1:D:367:LEU:HA	1.88	0.40
1:F:182:LYS:HG3	1:F:203:VAL:CG1	2.51	0.40
1:G:222:ASN:O	1:G:225:ARG:CG	2.69	0.40
1:G:260:HIS:CD2	1:G:260:HIS:C	2.99	0.40
1:H:186:TYR:HB3	1:H:209:ILE:HD11	2.02	0.40
1:H:211:ARG:CD	1:H:212:HIS:CE1	3.04	0.40
1:K:23:ARG:O	1:K:26:GLU:HB2	2.21	0.40
1:K:288:LEU:CD1	1:K:325:LEU:CD2	2.88	0.40
1:A:40:THR:HG23	1:A:118:ILE:O	2.22	0.40
1:B:92:GLU:OE1	1:B:100:ARG:HD2	2.21	0.40
1:D:208:GLU:HG2	1:D:210:PRO:HD2	2.03	0.40
1:D:209:ILE:HD13	1:D:209:ILE:HA	1.82	0.40
1:E:137:LEU:HD23	1:E:141:ILE:CD1	2.51	0.40
1:E:208:GLU:HB3	1:E:212:HIS:CD2	2.56	0.40
1:F:49:TYR:CG	1:F:50:GLY:N	2.89	0.40
1:F:229:ARG:O	1:F:229:ARG:HG3	2.21	0.40
1:F:342:GLN:NE2	1:F:342:GLN:HA	2.36	0.40
1:G:131:LYS:O	1:G:134:THR:CB	2.69	0.40
1:G:285:ILE:HD13	1:L:371:GLY:HA2	2.04	0.40
1:I:17:THR:O	1:I:20:PHE:N	2.55	0.40
1:I:69:ILE:CG2	1:I:70:ASN:N	2.84	0.40
1:I:80:GLN:HE21	1:I:80:GLN:HB2	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:110:CYS:CA	1:J:212:HIS:CE1	3.04	0.40
1:I:352:LYS:HA	1:I:365:TYR:CE1	2.57	0.40
1:J:65:LEU:CD2	1:J:118:ILE:O	2.62	0.40
1:J:271:LEU:HB3	1:J:287:ILE:HD13	2.03	0.40
1:K:101:TYR:N	1:K:101:TYR:CD1	2.90	0.40
1:L:8:LEU:C	1:L:27:HIS:CE1	2.99	0.40
1:L:128:THR:HG22	1:L:197:ILE:HD11	2.03	0.40
1:A:158:THR:HG23	1:A:260:HIS:CE1	2.57	0.40
1:B:355:PHE:CD1	1:B:355:PHE:O	2.75	0.40
1:C:37:THR:HG21	1:D:182:LYS:HD2	2.02	0.40
1:D:125:ILE:HG12	1:D:191:GLU:O	2.22	0.40
1:E:52:LEU:H	1:F:180:ASN:HB3	1.86	0.40
1:F:17:THR:OG1	1:H:362:GLU:OE2	2.31	0.40
1:F:51:ARG:HG3	1:F:52:LEU:N	2.36	0.40
1:I:151:ILE:HG21	1:I:153:PHE:CZ	2.57	0.40
1:I:166:LEU:HD23	1:I:166:LEU:HA	1.92	0.40
1:I:177:SER:HA	1:I:200:ILE:HD13	2.03	0.40
1:J:183:VAL:CG1	1:J:230:LEU:HD22	2.40	0.40
1:J:302:THR:HG23	1:J:306:ARG:O	2.21	0.40
1:K:17:THR:HG23	1:K:18:PRO:CD	2.44	0.40
1:K:145:ILE:HA	1:K:145:ILE:HD12	1.90	0.40
1:A:250:LEU:HD23	1:A:250:LEU:HA	1.77	0.40
1:B:184:LEU:HG	1:B:228:PRO:HB3	2.03	0.40
1:C:319:GLU:H	1:C:319:GLU:HG3	1.67	0.40
1:D:209:ILE:HG13	1:D:216:PHE:CD1	2.57	0.40
1:D:223:ALA:O	1:D:228:PRO:CD	2.69	0.40
1:D:248:ALA:C	1:D:251:THR:OG1	2.64	0.40
1:E:288:LEU:CB	1:E:325:LEU:CD2	2.99	0.40
1:E:368:ILE:HG23	1:E:369:ILE:N	2.36	0.40
1:F:13:PRO:CG	1:F:20:PHE:CG	3.04	0.40
1:F:112:VAL:HG13	1:F:117:ALA:HB3	2.02	0.40
1:F:288:LEU:HD12	1:F:324:LEU:CB	2.51	0.40
1:G:9:MET:CE	1:G:24:MET:CB	2.99	0.40
1:G:288:LEU:HD12	1:G:325:LEU:HD23	2.03	0.40
1:H:315:VAL:HG13	1:H:315:VAL:O	2.21	0.40
1:I:111:LEU:CD2	1:J:212:HIS:HE2	2.35	0.40
1:J:24:MET:CE	1:J:25:LEU:CD2	2.89	0.40
1:J:66:GLY:O	1:J:69:ILE:HG22	2.22	0.40
1:L:23:ARG:O	1:L:26:GLU:HB2	2.21	0.40
1:L:151:ILE:HG21	1:L:153:PHE:CZ	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:GLU:OE1	1:F:7:ASN:ND2[1_565]	2.18	0.02

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	367/391 (94%)	352 (96%)	14 (4%)	1 (0%)	36	68
1	B	369/391 (94%)	351 (95%)	16 (4%)	2 (0%)	24	59
1	C	367/391 (94%)	349 (95%)	15 (4%)	3 (1%)	16	50
1	D	366/391 (94%)	352 (96%)	13 (4%)	1 (0%)	36	68
1	E	365/391 (93%)	346 (95%)	15 (4%)	4 (1%)	11	43
1	F	362/391 (93%)	344 (95%)	16 (4%)	2 (1%)	21	56
1	G	367/391 (94%)	351 (96%)	13 (4%)	3 (1%)	16	50
1	H	369/391 (94%)	346 (94%)	19 (5%)	4 (1%)	11	43
1	I	367/391 (94%)	347 (95%)	19 (5%)	1 (0%)	36	68
1	J	366/391 (94%)	347 (95%)	18 (5%)	1 (0%)	36	68
1	K	365/391 (93%)	346 (95%)	18 (5%)	1 (0%)	36	68
1	L	362/391 (93%)	345 (95%)	14 (4%)	3 (1%)	16	50
All	All	4392/4692 (94%)	4176 (95%)	190 (4%)	26 (1%)	21	56

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	188	SER
1	E	332	VAL
1	G	332	VAL
1	H	188	SER
1	C	95	PRO

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Mol	Chain	Res	Type
1	E	97	ARG
1	G	189	PRO
1	I	189	PRO
1	L	274	SER
1	A	189	PRO
1	C	188	SER
1	C	189	PRO
1	E	189	PRO
1	F	189	PRO
1	G	369	ILE
1	H	95	PRO
1	H	201	SER
1	H	371	GLY
1	L	189	PRO
1	L	210	PRO
1	E	95	PRO
1	F	95	PRO
1	B	95	PRO
1	D	189	PRO
1	J	189	PRO
1	K	189	PRO

5.3.2 Protein sidechains ⓘ

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	322/343 (94%)	301 (94%)	21 (6%)	15	47
1	B	319/343 (93%)	306 (96%)	13 (4%)	27	60
1	C	318/343 (93%)	292 (92%)	26 (8%)	10	39
1	D	316/343 (92%)	292 (92%)	24 (8%)	12	42
1	E	315/343 (92%)	293 (93%)	22 (7%)	14	45
1	F	314/343 (92%)	289 (92%)	25 (8%)	11	40
1	G	322/343 (94%)	283 (88%)	39 (12%)	5	22
1	H	319/343 (93%)	295 (92%)	24 (8%)	12	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	318/343 (93%)	279 (88%)	39 (12%)	4	22
1	J	316/343 (92%)	279 (88%)	37 (12%)	5	23
1	K	315/343 (92%)	280 (89%)	35 (11%)	6	25
1	L	314/343 (92%)	284 (90%)	30 (10%)	8	32
All	All	3808/4116 (92%)	3473 (91%)	335 (9%)	9	35

All (335) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	53	LEU
1	A	69	ILE
1	A	87	ILE
1	A	145	ILE
1	A	160	SER
1	A	162	LYS
1	A	174	ILE
1	A	176	THR
1	A	193	VAL
1	A	195	ASP
1	A	209	ILE
1	A	230	LEU
1	A	274	SER
1	A	276	SER
1	A	278	GLU
1	A	285	ILE
1	A	300	VAL
1	A	326	GLU
1	A	362	GLU
1	A	367	LEU
1	B	7	ASN
1	B	52	LEU
1	B	53	LEU
1	B	90	HIS
1	B	119	GLN
1	B	121	THR
1	B	162	LYS
1	B	178	ASP
1	B	191	GLU
1	B	201	SER
1	B	209	ILE

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Mol	Chain	Res	Type
1	B	285	ILE
1	B	366	LYS
1	C	12	GLU
1	C	22	ASP
1	C	23	ARG
1	C	34	SER
1	C	54	LYS
1	C	60	LEU
1	C	78	THR
1	C	90	HIS
1	C	121	THR
1	C	145	ILE
1	C	149	GLU
1	C	162	LYS
1	C	174	ILE
1	C	177	SER
1	C	197	ILE
1	C	209	ILE
1	C	222	ASN
1	C	228	PRO
1	C	281	LEU
1	C	285	ILE
1	C	292	ARG
1	C	293	LEU
1	C	317	ASP
1	C	325	LEU
1	C	367	LEU
1	C	369	ILE
1	D	21	MET
1	D	34	SER
1	D	53	LEU
1	D	93	PHE
1	D	118	ILE
1	D	120	ILE
1	D	127	THR
1	D	132	LEU
1	D	137	LEU
1	D	174	ILE
1	D	193	VAL
1	D	200	ILE
1	D	209	ILE
1	D	227	LYS

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Mol	Chain	Res	Type
1	D	251	THR
1	D	253	HIS
1	D	266	GLU
1	D	283	ARG
1	D	285	ILE
1	D	303	VAL
1	D	323	ILE
1	D	328	ASP
1	D	367	LEU
1	D	369	ILE
1	E	8	LEU
1	E	12	GLU
1	E	22	ASP
1	E	32	ASN
1	E	53	LEU
1	E	60	LEU
1	E	82	LEU
1	E	92	GLU
1	E	121	THR
1	E	145	ILE
1	E	162	LYS
1	E	164	THR
1	E	174	ILE
1	E	215	ASN
1	E	235	GLU
1	E	251	THR
1	E	281	LEU
1	E	287	ILE
1	E	300	VAL
1	E	319	GLU
1	E	363	ARG
1	E	369	ILE
1	F	44	ILE
1	F	59	ARG
1	F	85	LYS
1	F	93	PHE
1	F	131	LYS
1	F	143	GLU
1	F	158	THR
1	F	176	THR
1	F	177	SER
1	F	178	ASP

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Mol	Chain	Res	Type
1	F	180	ASN
1	F	188	SER
1	F	197	ILE
1	F	208	GLU
1	F	209	ILE
1	F	224	LEU
1	F	247	GLU
1	F	266	GLU
1	F	283	ARG
1	F	295	ILE
1	F	303	VAL
1	F	312	GLU
1	F	333	THR
1	F	352	LYS
1	F	366	LYS
1	G	9	MET
1	G	34	SER
1	G	51	ARG
1	G	53	LEU
1	G	87	ILE
1	G	94	ARG
1	G	111	LEU
1	G	115	HIS
1	G	122	LEU
1	G	149	GLU
1	G	155	THR
1	G	162	LYS
1	G	174	ILE
1	G	180	ASN
1	G	188	SER
1	G	195	ASP
1	G	225	ARG
1	G	227	LYS
1	G	230	LEU
1	G	232	MET
1	G	233	VAL
1	G	257	THR
1	G	266	GLU
1	G	269	ARG
1	G	274	SER
1	G	279	GLU
1	G	281	LEU

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Mol	Chain	Res	Type
1	G	285	ILE
1	G	305	GLU
1	G	315	VAL
1	G	328	ASP
1	G	332	VAL
1	G	334	SER
1	G	342	GLN
1	G	356	GLU
1	G	360	ILE
1	G	361	SER
1	G	364	VAL
1	G	366	LYS
1	H	15	ARG
1	H	26	GLU
1	H	32	ASN
1	H	53	LEU
1	H	65	LEU
1	H	68	LEU
1	H	69	ILE
1	H	78	THR
1	H	87	ILE
1	H	93	PHE
1	H	100	ARG
1	H	121	THR
1	H	137	LEU
1	H	176	THR
1	H	193	VAL
1	H	197	ILE
1	H	203	VAL
1	H	209	ILE
1	H	267	THR
1	H	326	GLU
1	H	340	VAL
1	H	342	GLN
1	H	353	MET
1	H	366	LYS
1	I	11	ASP
1	I	40	THR
1	I	47	GLU
1	I	53	LEU
1	I	55	ILE
1	I	60	LEU

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Mol	Chain	Res	Type
1	I	64	GLU
1	I	72	ILE
1	I	99	VAL
1	I	108	THR
1	I	121	THR
1	I	125	ILE
1	I	143	GLU
1	I	149	GLU
1	I	155	THR
1	I	158	THR
1	I	160	SER
1	I	162	LYS
1	I	177	SER
1	I	188	SER
1	I	197	ILE
1	I	198	GLU
1	I	200	ILE
1	I	209	ILE
1	I	222	ASN
1	I	226	ARG
1	I	250	LEU
1	I	262	SER
1	I	269	ARG
1	I	285	ILE
1	I	292	ARG
1	I	299	LEU
1	I	305	GLU
1	I	320	VAL
1	I	325	LEU
1	I	346	LEU
1	I	347	MET
1	I	353	MET
1	I	367	LEU
1	J	8	LEU
1	J	15	ARG
1	J	29	GLU
1	J	39	GLN
1	J	40	THR
1	J	81	LEU
1	J	99	VAL
1	J	118	ILE
1	J	120	ILE

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Mol	Chain	Res	Type
1	J	132	LEU
1	J	140	ASN
1	J	145	ILE
1	J	154	ILE
1	J	158	THR
1	J	162	LYS
1	J	164	THR
1	J	174	ILE
1	J	191	GLU
1	J	196	GLU
1	J	199	THR
1	J	203	VAL
1	J	209	ILE
1	J	215	ASN
1	J	227	LYS
1	J	266	GLU
1	J	270	ARG
1	J	281	LEU
1	J	283	ARG
1	J	292	ARG
1	J	306	ARG
1	J	320	VAL
1	J	322	ASP
1	J	323	ILE
1	J	328	ASP
1	J	334	SER
1	J	353	MET
1	J	367	LEU
1	K	8	LEU
1	K	9	MET
1	K	15	ARG
1	K	32	ASN
1	K	53	LEU
1	K	83	SER
1	K	99	VAL
1	K	108	THR
1	K	121	THR
1	K	135	MET
1	K	137	LEU
1	K	139	ASP
1	K	140	ASN
1	K	141	ILE

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Mol	Chain	Res	Type
1	K	145	ILE
1	K	162	LYS
1	K	174	ILE
1	K	178	ASP
1	K	180	ASN
1	K	188	SER
1	K	197	ILE
1	K	200	ILE
1	K	215	ASN
1	K	232	MET
1	K	235	GLU
1	K	251	THR
1	K	273	THR
1	K	279	GLU
1	K	281	LEU
1	K	290	THR
1	K	319	GLU
1	K	336	THR
1	K	341	ARG
1	K	366	LYS
1	K	369	ILE
1	L	11	ASP
1	L	34	SER
1	L	40	THR
1	L	54	LYS
1	L	59	ARG
1	L	65	LEU
1	L	112	VAL
1	L	115	HIS
1	L	143	GLU
1	L	155	THR
1	L	158	THR
1	L	162	LYS
1	L	164	THR
1	L	176	THR
1	L	177	SER
1	L	187	GLU
1	L	188	SER
1	L	193	VAL
1	L	197	ILE
1	L	208	GLU
1	L	209	ILE

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Mol	Chain	Res	Type
1	L	218	ASP
1	L	224	LEU
1	L	226	ARG
1	L	227	LYS
1	L	274	SER
1	L	284	THR
1	L	285	ILE
1	L	304	ASP
1	L	337	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	27	HIS
1	A	80	GLN
1	A	119	GLN
1	A	212	HIS
1	A	253	HIS
1	A	297	GLN
1	A	345	GLN
1	A	357	GLN
1	B	7	ASN
1	B	119	GLN
1	B	212	HIS
1	B	215	ASN
1	B	253	HIS
1	B	260	HIS
1	B	330	ASN
1	B	345	GLN
1	C	80	GLN
1	C	119	GLN
1	C	212	HIS
1	C	215	ASN
1	C	253	HIS
1	C	345	GLN
1	D	39	GLN
1	D	80	GLN
1	D	96	ASN
1	D	136	ASN
1	D	212	HIS
1	D	215	ASN

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Mol	Chain	Res	Type
1	D	253	HIS
1	D	260	HIS
1	E	80	GLN
1	E	106	ASN
1	E	119	GLN
1	E	212	HIS
1	E	215	ASN
1	E	222	ASN
1	E	297	GLN
1	E	345	GLN
1	F	27	HIS
1	F	39	GLN
1	F	80	GLN
1	F	119	GLN
1	F	180	ASN
1	F	212	HIS
1	F	253	HIS
1	F	260	HIS
1	F	342	GLN
1	F	357	GLN
1	G	27	HIS
1	G	80	GLN
1	G	119	GLN
1	G	180	ASN
1	G	212	HIS
1	G	253	HIS
1	G	297	GLN
1	H	7	ASN
1	H	27	HIS
1	H	32	ASN
1	H	212	HIS
1	H	215	ASN
1	H	260	HIS
1	H	330	ASN
1	H	345	GLN
1	H	357	GLN
1	I	27	HIS
1	I	80	GLN
1	I	180	ASN
1	I	212	HIS
1	I	253	HIS
1	I	357	GLN

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Mol	Chain	Res	Type
1	J	39	GLN
1	J	80	GLN
1	J	140	ASN
1	J	215	ASN
1	J	253	HIS
1	J	260	HIS
1	K	27	HIS
1	K	62	ASN
1	K	80	GLN
1	K	119	GLN
1	K	212	HIS
1	K	297	GLN
1	K	345	GLN
1	L	39	GLN
1	L	80	GLN
1	L	115	HIS
1	L	206	GLN
1	L	222	ASN
1	L	253	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	D	401	-	4,4,4	0.94	0	6,6,6	1.41	2 (33%)
2	PO4	F	401	-	4,4,4	0.94	0	6,6,6	1.41	0
2	PO4	C	401	-	4,4,4	0.82	0	6,6,6	0.81	0
2	PO4	B	401	-	4,4,4	0.88	0	6,6,6	1.32	1 (16%)
2	PO4	L	401	-	4,4,4	0.87	0	6,6,6	0.67	0
2	PO4	G	401	-	4,4,4	0.85	0	6,6,6	1.29	1 (16%)
2	PO4	H	401	-	4,4,4	0.85	0	6,6,6	1.37	1 (16%)
2	PO4	K	401	-	4,4,4	0.90	0	6,6,6	1.18	0
2	PO4	A	401	-	4,4,4	0.66	0	6,6,6	0.93	0
2	PO4	I	401	-	4,4,4	0.82	0	6,6,6	1.40	0
2	PO4	E	401	-	4,4,4	1.08	0	6,6,6	0.95	0
2	PO4	J	401	-	4,4,4	0.71	0	6,6,6	1.37	0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	PO4	O4-P-O3	2.65	116.15	107.91
2	H	401	PO4	O4-P-O1	-2.54	101.98	110.95
2	G	401	PO4	O3-P-O1	-2.51	102.08	110.95
2	D	401	PO4	O4-P-O1	-2.14	103.37	110.95
2	B	401	PO4	O2-P-O1	-2.08	103.58	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	401	PO4	1	0
2	J	401	PO4	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	369/391 (94%)	-0.24	1 (0%) 90 81	60, 96, 130, 172	0
1	B	371/391 (94%)	-0.37	0 100 100	62, 86, 119, 162	0
1	C	369/391 (94%)	-0.31	0 100 100	57, 85, 115, 161	0
1	D	368/391 (94%)	-0.35	0 100 100	57, 90, 121, 160	0
1	E	367/391 (93%)	-0.28	1 (0%) 90 81	66, 96, 139, 164	0
1	F	366/391 (93%)	-0.29	0 100 100	64, 93, 122, 140	0
1	G	369/391 (94%)	-0.25	0 100 100	69, 101, 142, 165	0
1	H	371/391 (94%)	-0.29	0 100 100	58, 89, 118, 169	0
1	I	369/391 (94%)	-0.19	0 100 100	71, 111, 151, 170	0
1	J	368/391 (94%)	-0.18	0 100 100	75, 102, 125, 141	0
1	K	367/391 (93%)	-0.16	0 100 100	74, 112, 150, 168	0
1	L	366/391 (93%)	-0.14	1 (0%) 90 81	79, 110, 138, 162	0
All	All	4420/4692 (94%)	-0.25	3 (0%) 92 89	57, 98, 136, 172	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	5	ASN	2.8
1	E	178	ASP	2.7
1	A	6	ILE	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	PO4	L	401	5/5	0.86	0.07	100,104,115,124	0
2	PO4	H	401	5/5	0.88	0.08	72,73,74,75	0
2	PO4	J	401	5/5	0.91	0.06	86,89,99,104	0
2	PO4	K	401	5/5	0.91	0.06	93,97,98,101	0
2	PO4	D	401	5/5	0.91	0.05	75,77,83,88	0
2	PO4	I	401	5/5	0.92	0.06	88,91,104,105	0
2	PO4	G	401	5/5	0.92	0.07	65,71,78,82	0
2	PO4	B	401	5/5	0.94	0.07	66,67,72,74	0
2	PO4	E	401	5/5	0.94	0.05	82,82,85,88	0
2	PO4	F	401	5/5	0.94	0.05	73,74,78,84	0
2	PO4	C	401	5/5	0.95	0.05	69,71,73,77	0
2	PO4	A	401	5/5	0.95	0.04	65,68,71,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.