



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 02:40 am BST

PDB ID : 2JJM  
Title : Crystal Structure of a family GT4 glycosyltransferase from Bacillus anthracis ORF BA1558.  
Authors : Ruane, K.M.; Davies, G.J.; Martinez-Fleites, C.  
Deposited on : 2008-04-15  
Resolution : 3.10 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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

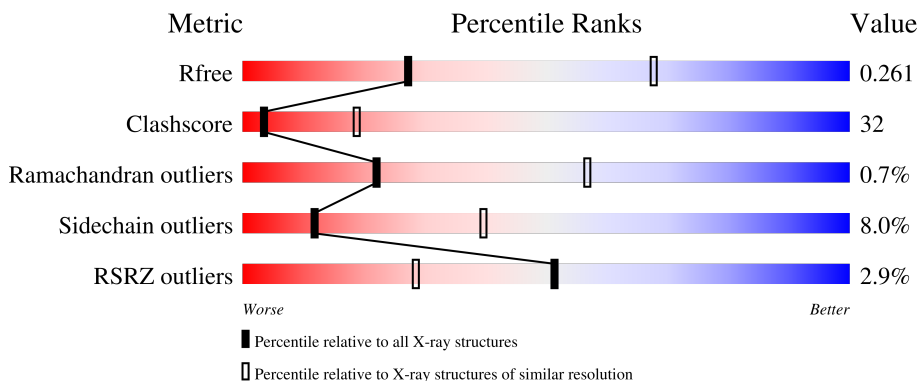
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 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	394	 % 51% 34% 6% • 9%
1	B	394	 4% 51% 34% 5% • 9%
1	C	394	 2% 52% 33% 6% • 9%
1	D	394	 % 53% 32% 6% • 9%
1	E	394	 2% 52% 34% 6% • 9%

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Mol	Chain	Length	Quality of chain
1	F	394	<p>2% 52% 33% 5% • 9%</p>
1	G	394	<p>% 52% 34% 6% • 9%</p>
1	H	394	<p>13% 51% 34% 5% • 9%</p>
1	I	394	<p>2% 52% 33% 6% • 9%</p>
1	J	394	<p>% 52% 33% 5% • 9%</p>
1	K	394	<p>2% 53% 33% 6% • 9%</p>
1	L	394	<p>% 52% 33% 6% • 9%</p>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 33924 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.

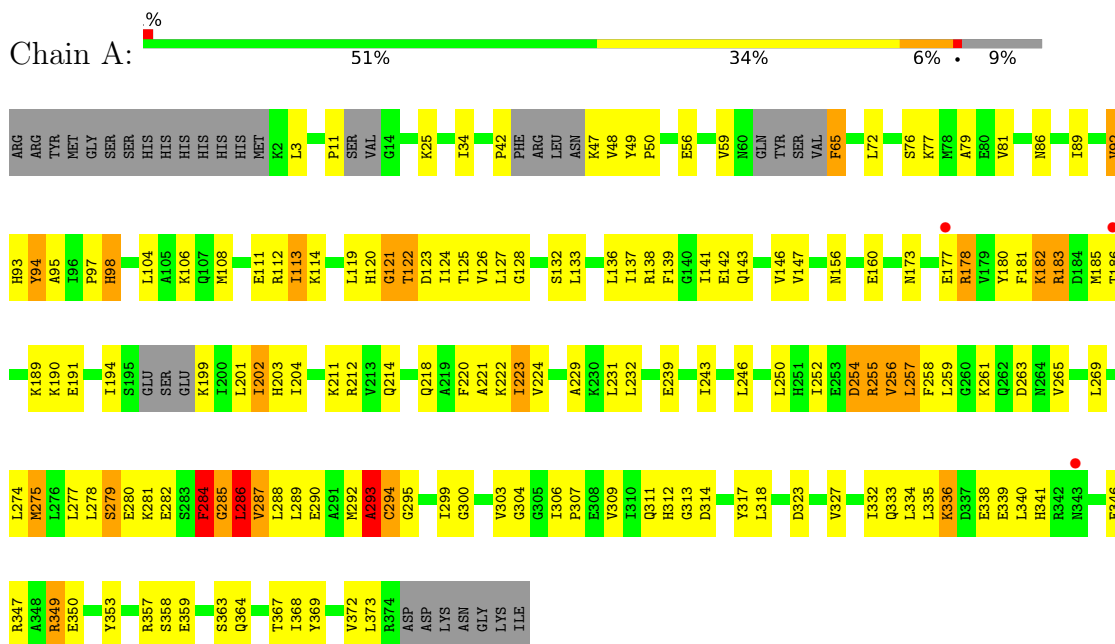
- Molecule 1 is a protein called GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	360	2827	1806	477	531	13	0	0	1
1	B	360	2827	1806	477	531	13	0	0	1
1	C	360	2827	1806	477	531	13	0	0	1
1	D	360	2827	1806	477	531	13	0	0	1
1	E	360	2827	1806	477	531	13	0	0	1
1	F	360	2827	1806	477	531	13	0	0	1
1	G	360	2827	1806	477	531	13	0	0	1
1	H	360	2827	1806	477	531	13	0	0	1
1	I	360	2827	1806	477	531	13	0	0	1
1	J	360	2827	1806	477	531	13	0	0	1
1	K	360	2827	1806	477	531	13	0	0	1
1	L	360	2827	1806	477	531	13	0	0	1

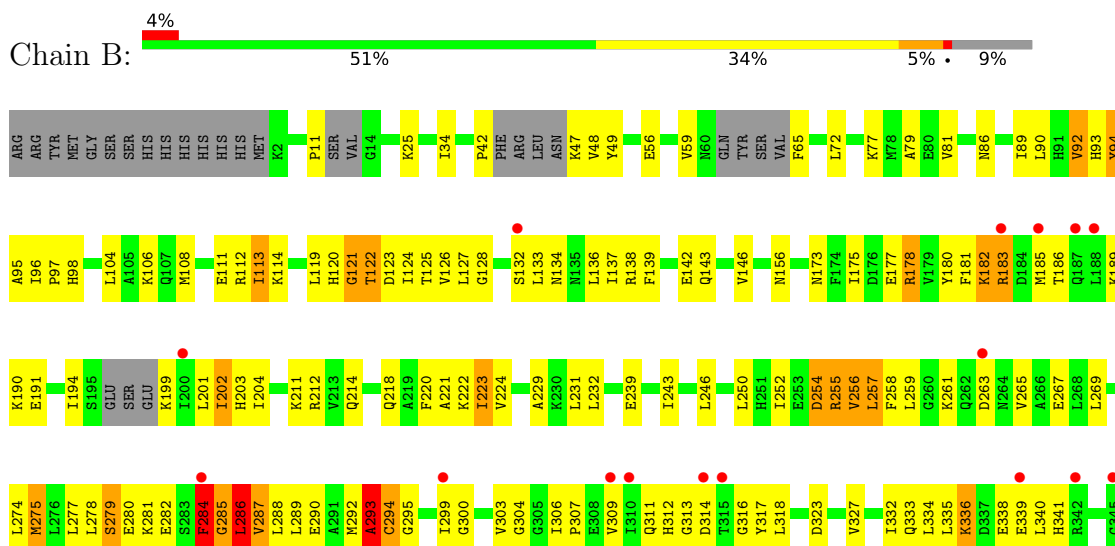
### 3 Residue-property plots i

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

- Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

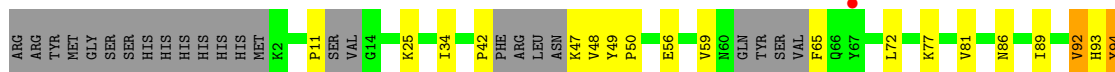


- Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

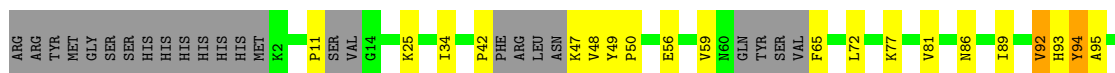




• Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

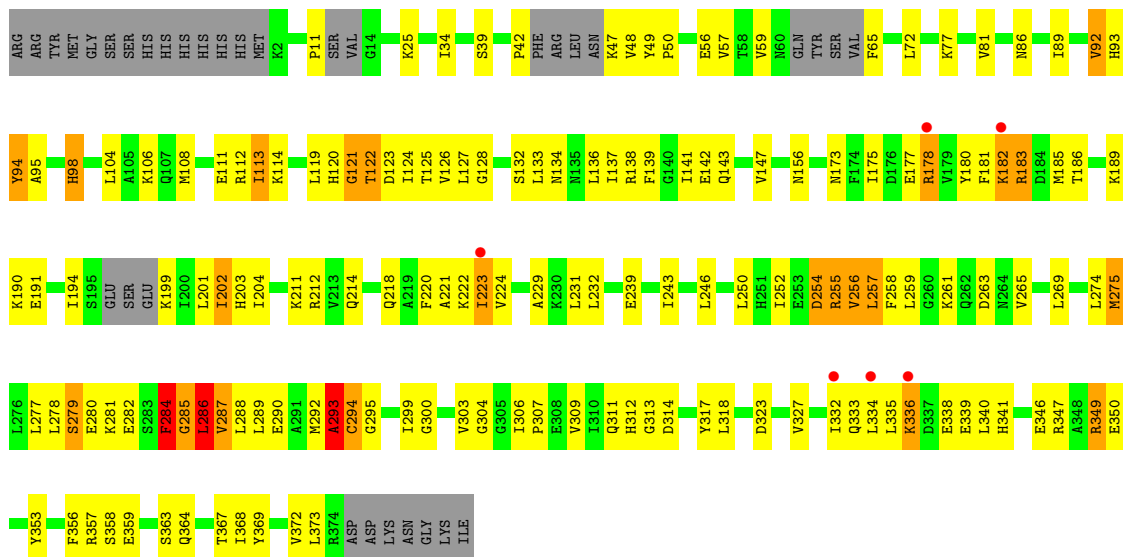


• Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

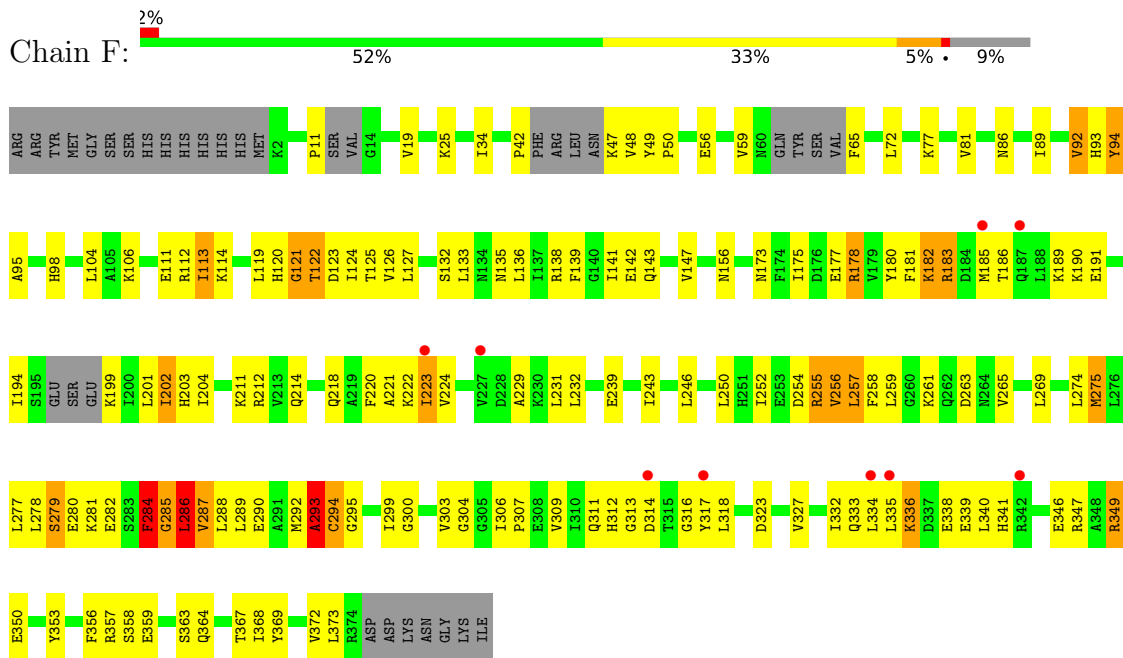


• Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

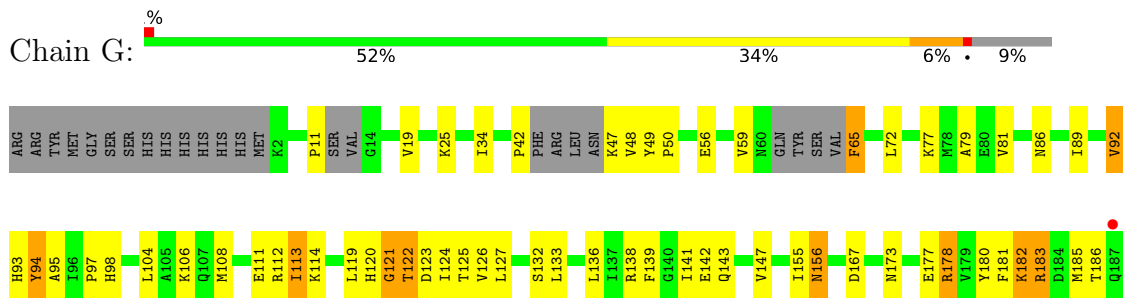


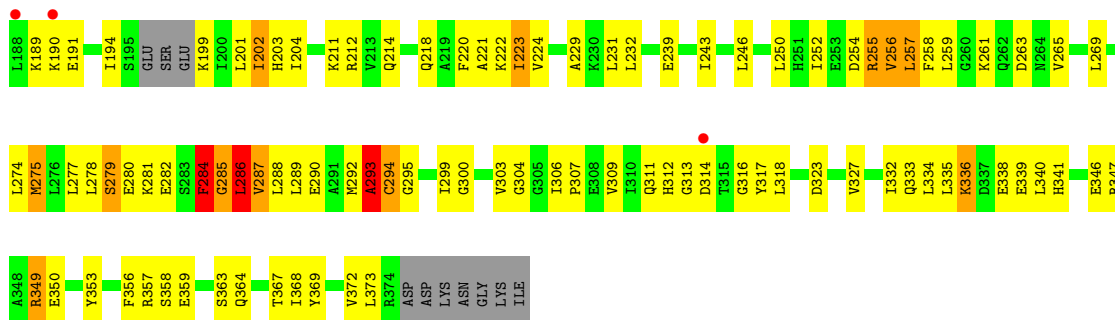


● Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

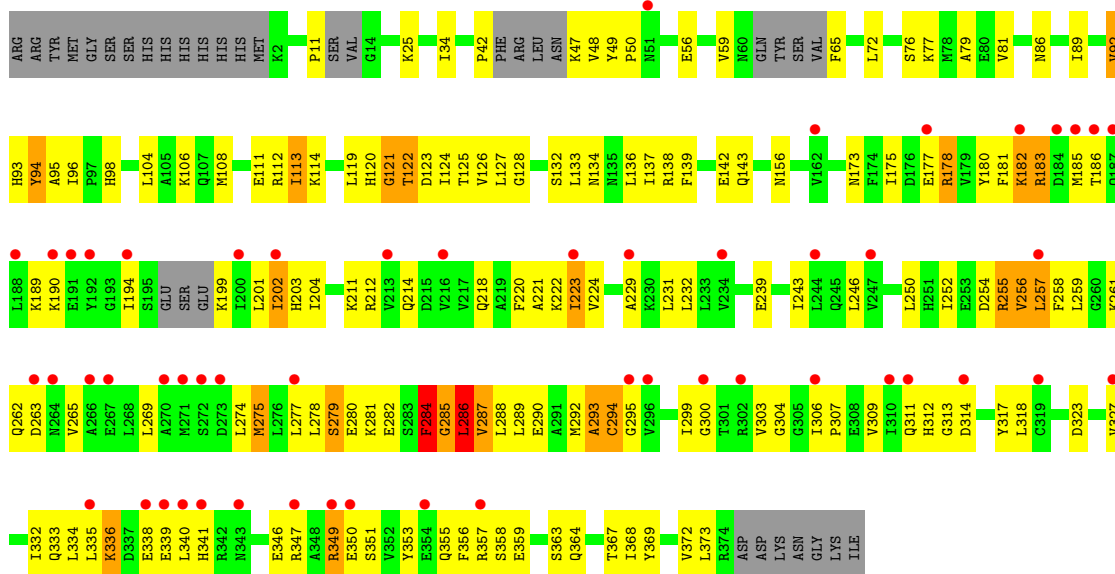


● Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

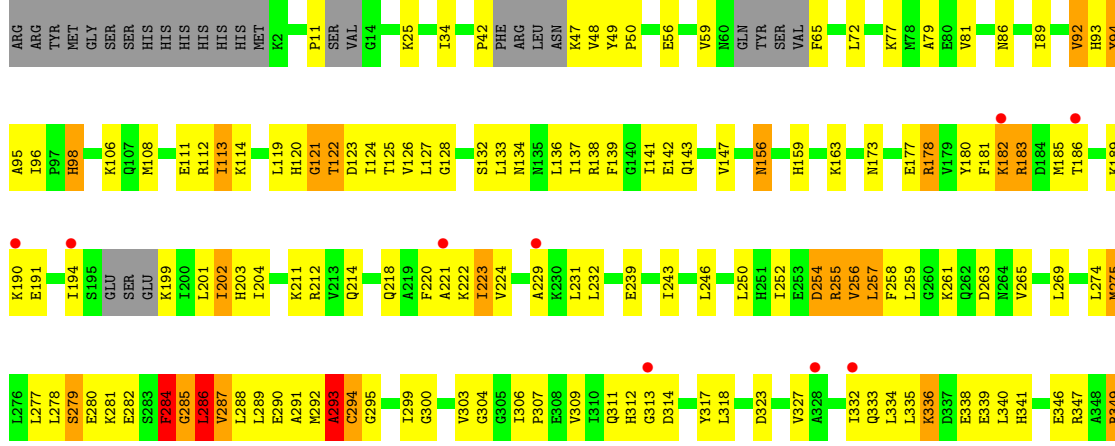




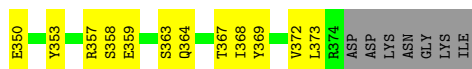
● Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN



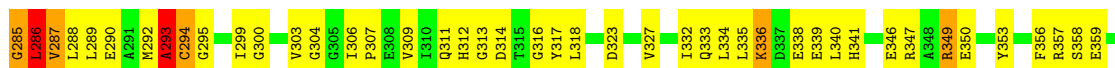
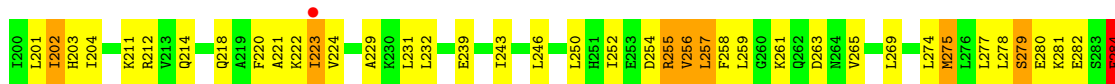
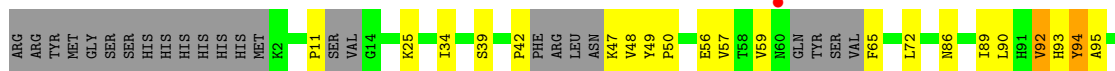
● Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN



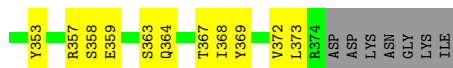
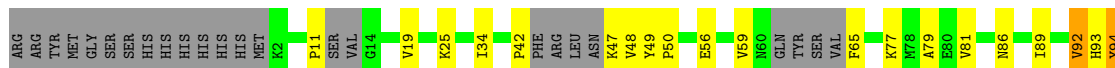




• Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN

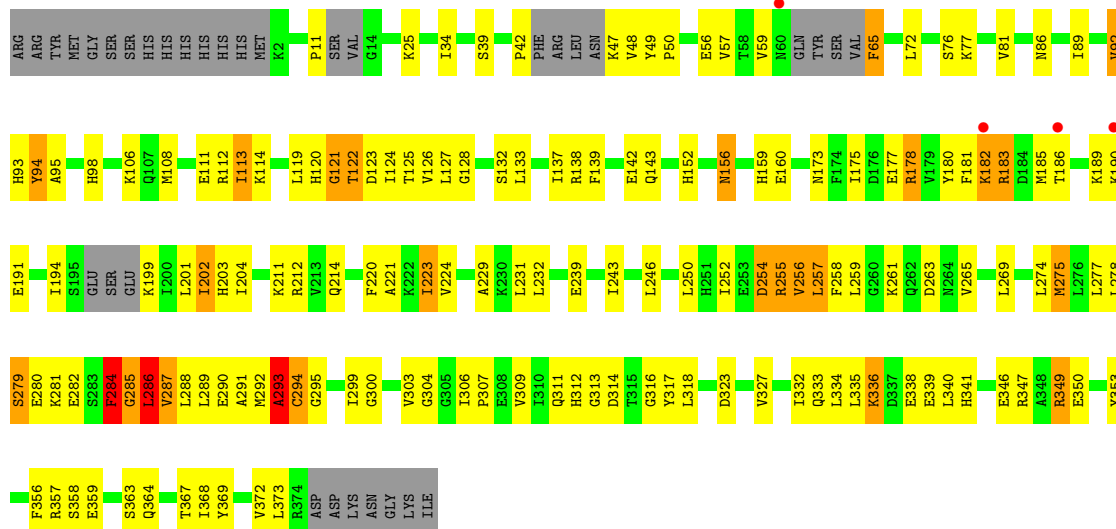


• Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN



• Molecule 1: GLYCOSYL TRANSFERASE, GROUP 1 FAMILY PROTEIN





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.60Å 204.67Å 135.33Å 90.00° 115.49° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 78.27 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-3.10) 89.5 (78.27-2.70)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 2.69Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.254 , 0.262 0.249 , 0.261	Depositor DCC
$R_{free}$ test set	5915 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	88.0	Xtrriage
Anisotropy	0.099	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 63.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.022 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	33924	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

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	0.86	8/2873 (0.3%)	0.89	10/3884 (0.3%)
1	B	0.86	7/2873 (0.2%)	0.90	10/3884 (0.3%)
1	C	0.87	8/2873 (0.3%)	0.89	10/3884 (0.3%)
1	D	0.86	8/2873 (0.3%)	0.89	10/3884 (0.3%)
1	E	0.87	8/2873 (0.3%)	0.89	10/3884 (0.3%)
1	F	0.86	8/2873 (0.3%)	0.89	9/3884 (0.2%)
1	G	0.87	8/2873 (0.3%)	0.90	9/3884 (0.2%)
1	H	0.86	6/2873 (0.2%)	0.90	9/3884 (0.2%)
1	I	0.87	8/2873 (0.3%)	0.90	10/3884 (0.3%)
1	J	0.89	8/2873 (0.3%)	0.89	8/3884 (0.2%)
1	K	0.87	7/2873 (0.2%)	0.89	10/3884 (0.3%)
1	L	0.87	7/2873 (0.2%)	0.89	10/3884 (0.3%)
All	All	0.87	91/34476 (0.3%)	0.89	115/46608 (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	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	3
1	J	0	2
1	K	0	2
1	L	0	2
All	All	0	25

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	287	VAL	CA-CB	-7.51	1.39	1.54
1	F	287	VAL	CA-CB	-7.43	1.39	1.54
1	D	287	VAL	CA-CB	-7.41	1.39	1.54
1	I	287	VAL	CA-CB	-7.41	1.39	1.54
1	G	287	VAL	CA-CB	-7.39	1.39	1.54
1	A	287	VAL	CA-CB	-7.34	1.39	1.54
1	B	287	VAL	CA-CB	-7.32	1.39	1.54
1	E	287	VAL	CA-CB	-7.32	1.39	1.54
1	L	287	VAL	CA-CB	-7.30	1.39	1.54
1	C	287	VAL	CA-CB	-7.30	1.39	1.54
1	K	287	VAL	CA-CB	-7.26	1.39	1.54
1	H	287	VAL	CA-CB	-7.17	1.39	1.54
1	F	92	VAL	CA-CB	-7.15	1.39	1.54
1	K	92	VAL	CA-CB	-7.12	1.39	1.54
1	G	92	VAL	CA-CB	-7.09	1.39	1.54
1	L	92	VAL	CA-CB	-7.06	1.40	1.54
1	A	92	VAL	CA-CB	-7.01	1.40	1.54
1	B	92	VAL	CA-CB	-7.01	1.40	1.54
1	G	256	VAL	CA-CB	-7.00	1.40	1.54
1	E	256	VAL	CA-CB	-6.97	1.40	1.54
1	H	256	VAL	CA-CB	-6.96	1.40	1.54
1	L	256	VAL	CA-CB	-6.95	1.40	1.54
1	E	92	VAL	CA-CB	-6.94	1.40	1.54
1	A	256	VAL	CA-CB	-6.92	1.40	1.54
1	D	92	VAL	CA-CB	-6.91	1.40	1.54
1	B	256	VAL	CA-CB	-6.90	1.40	1.54
1	I	92	VAL	CA-CB	-6.89	1.40	1.54
1	D	256	VAL	CA-CB	-6.89	1.40	1.54
1	H	92	VAL	CA-CB	-6.89	1.40	1.54
1	J	256	VAL	CA-CB	-6.87	1.40	1.54
1	C	256	VAL	CA-CB	-6.86	1.40	1.54
1	C	92	VAL	CA-CB	-6.84	1.40	1.54
1	F	256	VAL	CA-CB	-6.83	1.40	1.54
1	K	256	VAL	CA-CB	-6.80	1.40	1.54
1	I	256	VAL	CA-CB	-6.79	1.40	1.54
1	J	92	VAL	CA-CB	-6.62	1.40	1.54
1	K	92	VAL	CB-CG2	-6.36	1.39	1.52
1	F	92	VAL	CB-CG2	-6.36	1.39	1.52
1	L	92	VAL	CB-CG2	-6.28	1.39	1.52
1	G	92	VAL	CB-CG2	-6.28	1.39	1.52
1	B	92	VAL	CB-CG2	-6.25	1.39	1.52
1	C	92	VAL	CB-CG2	-6.21	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	92	VAL	CB-CG2	-6.20	1.39	1.52
1	D	92	VAL	CB-CG2	-6.17	1.39	1.52
1	A	92	VAL	CB-CG2	-6.16	1.40	1.52
1	F	294	CYS	CB-SG	-6.13	1.71	1.82
1	J	294	CYS	CB-SG	-6.12	1.71	1.82
1	J	92	VAL	CB-CG2	-6.12	1.40	1.52
1	K	294	CYS	CB-SG	-6.11	1.71	1.82
1	G	294	CYS	CB-SG	-6.11	1.71	1.82
1	E	92	VAL	CB-CG2	-6.10	1.40	1.52
1	A	294	CYS	CB-SG	-6.10	1.71	1.82
1	E	294	CYS	CB-SG	-6.07	1.72	1.82
1	H	92	VAL	CB-CG2	-6.06	1.40	1.52
1	H	294	CYS	CB-SG	-5.96	1.72	1.81
1	L	294	CYS	CB-SG	-5.92	1.72	1.81
1	B	294	CYS	CB-SG	-5.84	1.72	1.81
1	D	294	CYS	CB-SG	-5.79	1.72	1.81
1	K	95	ALA	CA-CB	-5.74	1.40	1.52
1	C	294	CYS	CB-SG	-5.71	1.72	1.81
1	I	294	CYS	CB-SG	-5.62	1.72	1.81
1	L	95	ALA	CA-CB	-5.52	1.40	1.52
1	J	95	ALA	CA-CB	-5.45	1.41	1.52
1	G	95	ALA	CA-CB	-5.44	1.41	1.52
1	K	92	VAL	CB-CG1	-5.44	1.41	1.52
1	J	92	VAL	CB-CG1	-5.37	1.41	1.52
1	I	95	ALA	CA-CB	-5.37	1.41	1.52
1	B	95	ALA	CA-CB	-5.35	1.41	1.52
1	C	92	VAL	CB-CG1	-5.32	1.41	1.52
1	E	95	ALA	CA-CB	-5.30	1.41	1.52
1	C	95	ALA	CA-CB	-5.29	1.41	1.52
1	D	95	ALA	CA-CB	-5.28	1.41	1.52
1	E	92	VAL	CB-CG1	-5.23	1.41	1.52
1	H	95	ALA	CA-CB	-5.21	1.41	1.52
1	F	95	ALA	CA-CB	-5.21	1.41	1.52
1	L	293	ALA	CA-CB	-5.21	1.41	1.52
1	F	92	VAL	CB-CG1	-5.20	1.42	1.52
1	A	95	ALA	CA-CB	-5.15	1.41	1.52
1	I	92	VAL	CB-CG1	-5.15	1.42	1.52
1	J	293	ALA	CA-CB	-5.14	1.41	1.52
1	G	293	ALA	CA-CB	-5.12	1.41	1.52
1	D	293	ALA	CA-CB	-5.12	1.41	1.52
1	C	293	ALA	CA-CB	-5.10	1.41	1.52
1	A	293	ALA	CA-CB	-5.07	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	92	VAL	CB-CG1	-5.07	1.42	1.52
1	F	293	ALA	CA-CB	-5.06	1.41	1.52
1	A	92	VAL	CB-CG1	-5.05	1.42	1.52
1	E	293	ALA	CA-CB	-5.04	1.41	1.52
1	I	293	ALA	CA-CB	-5.04	1.41	1.52
1	D	92	VAL	CB-CG1	-5.03	1.42	1.52
1	B	293	ALA	CA-CB	-5.02	1.42	1.52

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	121	GLY	N-CA-C	9.49	136.84	113.10
1	J	121	GLY	N-CA-C	9.48	136.80	113.10
1	H	121	GLY	N-CA-C	9.46	136.74	113.10
1	B	121	GLY	N-CA-C	9.45	136.72	113.10
1	D	121	GLY	N-CA-C	9.44	136.70	113.10
1	I	121	GLY	N-CA-C	9.44	136.69	113.10
1	K	121	GLY	N-CA-C	9.43	136.66	113.10
1	E	121	GLY	N-CA-C	9.42	136.66	113.10
1	A	121	GLY	N-CA-C	9.41	136.62	113.10
1	C	121	GLY	N-CA-C	9.39	136.59	113.10
1	G	121	GLY	N-CA-C	9.39	136.58	113.10
1	F	121	GLY	N-CA-C	9.35	136.48	113.10
1	G	284	PHE	N-CA-C	9.18	135.78	111.00
1	E	284	PHE	N-CA-C	9.14	135.69	111.00
1	E	285	GLY	N-CA-C	-9.13	90.27	113.10
1	K	284	PHE	N-CA-C	9.10	135.57	111.00
1	K	285	GLY	N-CA-C	-9.10	90.35	113.10
1	C	285	GLY	N-CA-C	-9.05	90.47	113.10
1	F	284	PHE	N-CA-C	9.05	135.44	111.00
1	B	284	PHE	N-CA-C	9.02	135.36	111.00
1	J	284	PHE	N-CA-C	9.02	135.35	111.00
1	C	284	PHE	N-CA-C	9.01	135.33	111.00
1	F	285	GLY	N-CA-C	-9.01	90.58	113.10
1	A	285	GLY	N-CA-C	-9.00	90.59	113.10
1	I	284	PHE	N-CA-C	9.00	135.30	111.00
1	L	284	PHE	N-CA-C	9.00	135.30	111.00
1	D	284	PHE	N-CA-C	8.99	135.28	111.00
1	I	285	GLY	N-CA-C	-8.96	90.71	113.10
1	D	285	GLY	N-CA-C	-8.95	90.73	113.10
1	G	285	GLY	N-CA-C	-8.95	90.72	113.10
1	A	284	PHE	N-CA-C	8.93	135.11	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	285	GLY	N-CA-C	-8.92	90.81	113.10
1	H	284	PHE	N-CA-C	8.89	135.01	111.00
1	B	285	GLY	N-CA-C	-8.89	90.87	113.10
1	H	285	GLY	N-CA-C	-8.89	90.87	113.10
1	J	285	GLY	N-CA-C	-8.45	91.97	113.10
1	H	286	LEU	C-N-CA	-7.71	102.41	121.70
1	B	286	LEU	C-N-CA	-7.69	102.47	121.70
1	D	286	LEU	C-N-CA	-7.64	102.59	121.70
1	J	286	LEU	C-N-CA	-7.63	102.61	121.70
1	E	286	LEU	C-N-CA	-7.63	102.64	121.70
1	I	286	LEU	C-N-CA	-7.61	102.67	121.70
1	G	286	LEU	C-N-CA	-7.61	102.68	121.70
1	A	286	LEU	C-N-CA	-7.60	102.69	121.70
1	L	286	LEU	C-N-CA	-7.60	102.69	121.70
1	K	286	LEU	C-N-CA	-7.60	102.69	121.70
1	C	286	LEU	C-N-CA	-7.58	102.76	121.70
1	F	286	LEU	C-N-CA	-7.55	102.82	121.70
1	H	257	LEU	CA-CB-CG	-7.13	98.90	115.30
1	B	257	LEU	CA-CB-CG	-7.13	98.91	115.30
1	F	257	LEU	CA-CB-CG	-7.10	98.96	115.30
1	C	257	LEU	CA-CB-CG	-7.08	99.00	115.30
1	I	257	LEU	CA-CB-CG	-7.07	99.04	115.30
1	E	257	LEU	CA-CB-CG	-7.05	99.09	115.30
1	D	257	LEU	CA-CB-CG	-7.04	99.11	115.30
1	A	257	LEU	CA-CB-CG	-7.02	99.15	115.30
1	G	257	LEU	CA-CB-CG	-7.01	99.17	115.30
1	J	257	LEU	CA-CB-CG	-7.01	99.17	115.30
1	L	257	LEU	CA-CB-CG	-7.00	99.19	115.30
1	K	257	LEU	CA-CB-CG	-6.98	99.25	115.30
1	L	93	HIS	N-CA-C	6.05	127.33	111.00
1	I	93	HIS	N-CA-C	6.03	127.29	111.00
1	F	93	HIS	N-CA-C	6.03	127.28	111.00
1	G	93	HIS	N-CA-C	6.03	127.28	111.00
1	D	93	HIS	N-CA-C	6.03	127.27	111.00
1	E	93	HIS	N-CA-C	6.02	127.25	111.00
1	B	93	HIS	N-CA-C	6.00	127.21	111.00
1	H	93	HIS	N-CA-C	6.00	127.20	111.00
1	A	93	HIS	N-CA-C	6.00	127.19	111.00
1	C	93	HIS	N-CA-C	5.94	127.03	111.00
1	K	93	HIS	N-CA-C	5.92	126.97	111.00
1	J	93	HIS	N-CA-C	5.81	126.69	111.00
1	C	284	PHE	CB-CA-C	-5.54	99.32	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	93	HIS	C-N-CA	-5.53	107.87	121.70
1	A	93	HIS	C-N-CA	-5.51	107.92	121.70
1	G	93	HIS	C-N-CA	-5.51	107.92	121.70
1	H	93	HIS	C-N-CA	-5.46	108.05	121.70
1	D	93	HIS	C-N-CA	-5.43	108.13	121.70
1	I	93	HIS	C-N-CA	-5.43	108.13	121.70
1	K	93	HIS	C-N-CA	-5.42	108.14	121.70
1	B	93	HIS	C-N-CA	-5.42	108.14	121.70
1	C	93	HIS	C-N-CA	-5.41	108.17	121.70
1	L	284	PHE	CB-CA-C	-5.41	99.58	110.40
1	F	93	HIS	C-N-CA	-5.41	108.19	121.70
1	E	93	HIS	C-N-CA	-5.40	108.19	121.70
1	J	93	HIS	C-N-CA	-5.38	108.24	121.70
1	I	284	PHE	CB-CA-C	-5.37	99.67	110.40
1	K	284	PHE	CB-CA-C	-5.30	99.79	110.40
1	B	284	PHE	CB-CA-C	-5.29	99.83	110.40
1	J	94	TYR	N-CA-C	-5.25	96.84	111.00
1	A	284	PHE	CB-CA-C	-5.24	99.92	110.40
1	G	284	PHE	CB-CA-C	-5.24	99.93	110.40
1	K	254	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	B	94	TYR	N-CA-C	-5.23	96.88	111.00
1	G	94	TYR	N-CA-C	-5.21	96.93	111.00
1	C	254	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	K	94	TYR	N-CA-C	-5.19	97.00	111.00
1	H	284	PHE	CB-CA-C	-5.18	100.03	110.40
1	E	284	PHE	CB-CA-C	-5.17	100.06	110.40
1	A	94	TYR	N-CA-C	-5.17	97.04	111.00
1	D	284	PHE	CB-CA-C	-5.17	100.06	110.40
1	D	94	TYR	N-CA-C	-5.15	97.10	111.00
1	F	284	PHE	CB-CA-C	-5.14	100.12	110.40
1	H	94	TYR	N-CA-C	-5.14	97.11	111.00
1	C	94	TYR	N-CA-C	-5.13	97.14	111.00
1	E	94	TYR	N-CA-C	-5.13	97.16	111.00
1	F	94	TYR	N-CA-C	-5.12	97.19	111.00
1	I	94	TYR	N-CA-C	-5.12	97.19	111.00
1	L	94	TYR	N-CA-C	-5.10	97.22	111.00
1	D	254	ASP	CB-CG-OD1	-5.07	113.73	118.30
1	B	254	ASP	CB-CG-OD1	-5.06	113.74	118.30
1	E	254	ASP	CB-CG-OD1	-5.02	113.78	118.30
1	L	254	ASP	CB-CG-OD1	-5.01	113.79	118.30
1	A	254	ASP	CB-CG-OD1	-5.00	113.80	118.30
1	I	254	ASP	CB-CG-OD1	-5.00	113.80	118.30

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	PHE	Peptide,Mainchain
1	B	284	PHE	Peptide,Mainchain
1	C	284	PHE	Peptide,Mainchain
1	D	284	PHE	Peptide,Mainchain
1	E	284	PHE	Peptide,Mainchain
1	F	284	PHE	Peptide,Mainchain
1	G	284	PHE	Peptide,Mainchain
1	H	284	PHE	Peptide,Mainchain
1	I	284	PHE	Peptide,Mainchain
1	I	96	ILE	Mainchain
1	J	284	PHE	Peptide,Mainchain
1	K	284	PHE	Peptide,Mainchain
1	L	284	PHE	Peptide,Mainchain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2827	0	2856	182	1
1	B	2827	0	2856	191	0
1	C	2827	0	2856	188	0
1	D	2827	0	2856	182	0
1	E	2827	0	2856	182	0
1	F	2827	0	2856	185	0
1	G	2827	0	2856	195	0
1	H	2827	0	2856	187	0
1	I	2827	0	2856	189	0
1	J	2827	0	2856	183	0
1	K	2827	0	2856	186	1
1	L	2827	0	2856	190	0
All	All	33924	0	34272	2180	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 32.

All (2180) 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:G:167:ASP:OD2	1:L:160:GLU:HA	1.15	1.27
1:A:286:LEU:HD12	1:A:286:LEU:N	1.55	1.17
1:B:286:LEU:H	1:B:286:LEU:CD1	1.54	1.16
1:K:280:GLU:O	1:K:281:LYS:HG2	1.46	1.16
1:G:280:GLU:O	1:G:281:LYS:HG2	1.47	1.15
1:A:280:GLU:O	1:A:281:LYS:HG2	1.46	1.15
1:E:280:GLU:O	1:E:281:LYS:HG2	1.46	1.15
1:I:280:GLU:O	1:I:281:LYS:HG2	1.47	1.15
1:C:280:GLU:O	1:C:281:LYS:HG2	1.47	1.14
1:L:280:GLU:O	1:L:281:LYS:HG2	1.47	1.14
1:I:286:LEU:HD12	1:I:286:LEU:N	1.54	1.14
1:B:280:GLU:O	1:B:281:LYS:HG2	1.46	1.13
1:F:286:LEU:H	1:F:286:LEU:CD1	1.54	1.13
1:D:286:LEU:HD12	1:D:286:LEU:N	1.55	1.13
1:H:280:GLU:O	1:H:281:LYS:HG2	1.46	1.12
1:J:280:GLU:O	1:J:281:LYS:HG2	1.47	1.12
1:F:280:GLU:O	1:F:281:LYS:HG2	1.47	1.10
1:C:286:LEU:HD12	1:C:286:LEU:N	1.55	1.10
1:D:280:GLU:O	1:D:281:LYS:HG2	1.47	1.10
1:C:286:LEU:H	1:C:286:LEU:CD1	1.54	1.09
1:I:286:LEU:H	1:I:286:LEU:CD1	1.53	1.09
1:K:286:LEU:HD12	1:K:286:LEU:N	1.54	1.08
1:J:286:LEU:HD12	1:J:286:LEU:N	1.56	1.08
1:D:286:LEU:H	1:D:286:LEU:CD1	1.55	1.08
1:E:286:LEU:H	1:E:286:LEU:CD1	1.54	1.08
1:E:286:LEU:HD12	1:E:286:LEU:N	1.55	1.08
1:L:286:LEU:H	1:L:286:LEU:CD1	1.54	1.08
1:J:286:LEU:H	1:J:286:LEU:CD1	1.56	1.07
1:B:286:LEU:HD12	1:B:286:LEU:N	1.55	1.07
1:H:286:LEU:HD12	1:H:286:LEU:N	1.55	1.07
1:H:286:LEU:H	1:H:286:LEU:CD1	1.55	1.06
1:G:286:LEU:H	1:G:286:LEU:CD1	1.54	1.06
1:L:286:LEU:HD12	1:L:286:LEU:N	1.55	1.06
1:A:286:LEU:O	1:A:287:VAL:C	1.91	1.05
1:G:286:LEU:HD12	1:G:286:LEU:N	1.55	1.05
1:F:286:LEU:HD12	1:F:286:LEU:N	1.55	1.04
1:K:286:LEU:H	1:K:286:LEU:CD1	1.54	1.04
1:F:256:VAL:C	1:F:257:LEU:HD12	1.78	1.04
1:K:256:VAL:C	1:K:257:LEU:HD12	1.78	1.04
1:G:256:VAL:C	1:G:257:LEU:HD12	1.78	1.03
1:L:256:VAL:C	1:L:257:LEU:HD12	1.78	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:VAL:C	1:A:257:LEU:HD12	1.78	1.03
1:L:286:LEU:O	1:L:287:VAL:C	1.90	1.03
1:C:256:VAL:C	1:C:257:LEU:HD12	1.78	1.03
1:F:286:LEU:O	1:F:287:VAL:C	1.90	1.03
1:H:256:VAL:C	1:H:257:LEU:HD12	1.78	1.03
1:A:286:LEU:H	1:A:286:LEU:CD1	1.54	1.03
1:B:256:VAL:C	1:B:257:LEU:HD12	1.78	1.03
1:E:256:VAL:C	1:E:257:LEU:HD12	1.78	1.03
1:I:256:VAL:C	1:I:257:LEU:HD12	1.78	1.03
1:G:286:LEU:O	1:G:287:VAL:C	1.91	1.03
1:D:256:VAL:C	1:D:257:LEU:HD12	1.78	1.02
1:J:256:VAL:C	1:J:257:LEU:HD12	1.78	1.02
1:K:220:PHE:HA	1:K:223:ILE:HG22	1.42	1.02
1:E:286:LEU:O	1:E:287:VAL:C	1.91	1.02
1:A:220:PHE:HA	1:A:223:ILE:HG22	1.42	1.01
1:I:220:PHE:HA	1:I:223:ILE:HG22	1.42	1.01
1:B:220:PHE:HA	1:B:223:ILE:HG22	1.42	1.01
1:H:220:PHE:HA	1:H:223:ILE:HG22	1.41	1.01
1:L:220:PHE:HA	1:L:223:ILE:HG22	1.42	1.01
1:G:167:ASP:OD2	1:L:160:GLU:CA	2.07	1.01
1:C:220:PHE:HA	1:C:223:ILE:HG22	1.41	1.01
1:F:220:PHE:HA	1:F:223:ILE:HG22	1.41	1.00
1:E:220:PHE:HA	1:E:223:ILE:HG22	1.42	1.00
1:B:281:LYS:HA	1:B:303:VAL:HG11	1.44	0.99
1:C:281:LYS:HA	1:C:303:VAL:HG11	1.44	0.99
1:E:281:LYS:HA	1:E:303:VAL:HG11	1.44	0.99
1:I:281:LYS:HA	1:I:303:VAL:HG11	1.44	0.99
1:G:281:LYS:HA	1:G:303:VAL:HG11	1.44	0.99
1:I:286:LEU:O	1:I:287:VAL:C	1.91	0.99
1:H:281:LYS:HA	1:H:303:VAL:HG11	1.44	0.99
1:D:220:PHE:HA	1:D:223:ILE:HG22	1.41	0.99
1:J:281:LYS:HA	1:J:303:VAL:HG11	1.44	0.98
1:G:220:PHE:HA	1:G:223:ILE:HG22	1.42	0.98
1:E:284:PHE:HB3	1:E:285:GLY:HA2	1.46	0.98
1:F:281:LYS:HA	1:F:303:VAL:HG11	1.44	0.98
1:H:257:LEU:HD12	1:H:257:LEU:N	1.79	0.98
1:J:286:LEU:O	1:J:287:VAL:C	1.90	0.98
1:A:257:LEU:HD12	1:A:257:LEU:N	1.79	0.98
1:J:220:PHE:HA	1:J:223:ILE:HG22	1.42	0.98
1:H:284:PHE:HB3	1:H:285:GLY:HA2	1.46	0.97
1:H:286:LEU:O	1:H:287:VAL:C	1.91	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:LYS:HA	1:D:303:VAL:HG11	1.44	0.97
1:I:284:PHE:HB3	1:I:285:GLY:HA2	1.46	0.97
1:K:257:LEU:HD12	1:K:257:LEU:N	1.79	0.97
1:G:284:PHE:HB3	1:G:285:GLY:HA2	1.45	0.97
1:I:257:LEU:HD12	1:I:257:LEU:N	1.79	0.97
1:L:281:LYS:HA	1:L:303:VAL:HG11	1.44	0.97
1:B:284:PHE:HB3	1:B:285:GLY:HA2	1.46	0.97
1:J:257:LEU:HD12	1:J:257:LEU:N	1.78	0.97
1:G:257:LEU:HD12	1:G:257:LEU:N	1.79	0.97
1:K:281:LYS:HA	1:K:303:VAL:HG11	1.45	0.97
1:A:284:PHE:HB3	1:A:285:GLY:HA2	1.46	0.96
1:C:284:PHE:HB3	1:C:285:GLY:HA2	1.45	0.96
1:D:257:LEU:HD12	1:D:257:LEU:N	1.79	0.96
1:D:286:LEU:O	1:D:287:VAL:C	1.91	0.96
1:C:286:LEU:O	1:C:287:VAL:C	1.91	0.96
1:A:281:LYS:HA	1:A:303:VAL:HG11	1.44	0.96
1:J:284:PHE:HB3	1:J:285:GLY:HA2	1.44	0.96
1:K:284:PHE:HB3	1:K:285:GLY:HA2	1.47	0.96
1:B:286:LEU:O	1:B:287:VAL:C	1.91	0.96
1:D:284:PHE:HB3	1:D:285:GLY:HA2	1.46	0.95
1:F:284:PHE:HB3	1:F:285:GLY:HA2	1.46	0.95
1:E:191:GLU:HG2	1:H:50:PRO:HG2	1.47	0.95
1:F:11:PRO:HG3	1:F:42:PRO:HG3	1.49	0.95
1:K:286:LEU:O	1:K:287:VAL:C	1.90	0.95
1:C:11:PRO:HG3	1:C:42:PRO:HG3	1.49	0.95
1:L:284:PHE:HB3	1:L:285:GLY:HA2	1.46	0.95
1:I:50:PRO:HG2	1:K:191:GLU:HG2	1.48	0.94
1:B:11:PRO:HG3	1:B:42:PRO:HG3	1.49	0.94
1:I:11:PRO:HG3	1:I:42:PRO:HG3	1.49	0.94
1:H:11:PRO:HG3	1:H:42:PRO:HG3	1.49	0.94
1:L:11:PRO:HG3	1:L:42:PRO:HG3	1.48	0.94
1:E:11:PRO:HG3	1:E:42:PRO:HG3	1.49	0.94
1:K:11:PRO:HG3	1:K:42:PRO:HG3	1.48	0.94
1:G:11:PRO:HG3	1:G:42:PRO:HG3	1.49	0.94
1:D:286:LEU:O	1:D:288:LEU:N	2.01	0.93
1:G:286:LEU:O	1:G:288:LEU:N	2.01	0.93
1:J:11:PRO:HG3	1:J:42:PRO:HG3	1.49	0.93
1:F:286:LEU:O	1:F:288:LEU:N	2.01	0.93
1:L:286:LEU:O	1:L:288:LEU:N	2.01	0.93
1:E:257:LEU:HD12	1:E:257:LEU:N	1.79	0.93
1:E:286:LEU:O	1:E:288:LEU:N	2.01	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:286:LEU:O	1:K:288:LEU:N	2.00	0.93
1:A:286:LEU:O	1:A:288:LEU:N	2.01	0.92
1:J:286:LEU:O	1:J:288:LEU:N	2.02	0.92
1:C:286:LEU:O	1:C:288:LEU:N	2.02	0.92
1:D:11:PRO:HG3	1:D:42:PRO:HG3	1.49	0.92
1:B:286:LEU:O	1:B:288:LEU:N	2.02	0.92
1:K:199:LYS:HB2	1:K:229:ALA:HB2	1.52	0.92
1:A:11:PRO:HG3	1:A:42:PRO:HG3	1.49	0.92
1:F:199:LYS:HB2	1:F:229:ALA:HB2	1.52	0.92
1:I:286:LEU:O	1:I:288:LEU:N	2.02	0.92
1:J:199:LYS:HB2	1:J:229:ALA:HB2	1.51	0.92
1:A:199:LYS:HB2	1:A:229:ALA:HB2	1.52	0.92
1:G:199:LYS:HB2	1:G:229:ALA:HB2	1.52	0.91
1:H:286:LEU:O	1:H:288:LEU:N	2.02	0.91
1:E:199:LYS:HB2	1:E:229:ALA:HB2	1.52	0.90
1:I:199:LYS:HB2	1:I:229:ALA:HB2	1.52	0.90
1:K:280:GLU:C	1:K:281:LYS:HG2	1.92	0.90
1:D:199:LYS:HB2	1:D:229:ALA:HB2	1.52	0.90
1:C:47:LYS:HG2	1:C:48:VAL:H	1.37	0.89
1:H:199:LYS:HB2	1:H:229:ALA:HB2	1.52	0.89
1:I:257:LEU:N	1:I:257:LEU:CD1	2.35	0.89
1:J:257:LEU:N	1:J:257:LEU:CD1	2.35	0.89
1:B:199:LYS:HB2	1:B:229:ALA:HB2	1.52	0.89
1:I:47:LYS:HG2	1:I:48:VAL:H	1.37	0.89
1:C:199:LYS:HB2	1:C:229:ALA:HB2	1.52	0.89
1:H:257:LEU:N	1:H:257:LEU:CD1	2.36	0.89
1:I:280:GLU:C	1:I:281:LYS:HG2	1.93	0.89
1:A:257:LEU:N	1:A:257:LEU:CD1	2.36	0.89
1:D:280:GLU:C	1:D:281:LYS:HG2	1.93	0.89
1:G:156:ASN:OD1	1:L:152:HIS:CG	2.26	0.89
1:C:257:LEU:CD1	1:C:257:LEU:N	2.36	0.89
1:E:257:LEU:N	1:E:257:LEU:CD1	2.36	0.89
1:F:280:GLU:C	1:F:281:LYS:HG2	1.93	0.89
1:K:257:LEU:N	1:K:257:LEU:CD1	2.35	0.89
1:J:286:LEU:HD12	1:J:286:LEU:H	0.72	0.88
1:E:47:LYS:HG2	1:E:48:VAL:H	1.37	0.88
1:D:257:LEU:N	1:D:257:LEU:CD1	2.36	0.88
1:H:280:GLU:C	1:H:281:LYS:HG2	1.93	0.88
1:L:199:LYS:HB2	1:L:229:ALA:HB2	1.52	0.88
1:D:47:LYS:HG2	1:D:48:VAL:H	1.37	0.88
1:G:257:LEU:N	1:G:257:LEU:CD1	2.35	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:LYS:HG2	1:H:48:VAL:H	1.38	0.88
1:B:257:LEU:N	1:B:257:LEU:CD1	2.35	0.88
1:A:280:GLU:C	1:A:281:LYS:HG2	1.93	0.88
1:G:47:LYS:HG2	1:G:48:VAL:H	1.37	0.88
1:J:47:LYS:HG2	1:J:48:VAL:H	1.36	0.88
1:F:47:LYS:HG2	1:F:48:VAL:H	1.37	0.88
1:B:280:GLU:C	1:B:281:LYS:HG2	1.93	0.87
1:L:257:LEU:N	1:L:257:LEU:CD1	2.35	0.87
1:L:280:GLU:C	1:L:281:LYS:HG2	1.93	0.87
1:E:286:LEU:H	1:E:286:LEU:HD12	0.70	0.87
1:F:257:LEU:HD12	1:F:257:LEU:N	1.79	0.87
1:F:257:LEU:N	1:F:257:LEU:CD1	2.36	0.87
1:B:286:LEU:H	1:B:286:LEU:HD12	0.71	0.86
1:A:47:LYS:HG2	1:A:48:VAL:H	1.37	0.86
1:L:47:LYS:HG2	1:L:48:VAL:H	1.38	0.86
1:L:286:LEU:H	1:L:286:LEU:HD12	0.71	0.86
1:B:47:LYS:HG2	1:B:48:VAL:H	1.37	0.86
1:E:280:GLU:C	1:E:281:LYS:HG2	1.93	0.86
1:G:286:LEU:H	1:G:286:LEU:HD12	0.71	0.86
1:H:286:LEU:HD12	1:H:286:LEU:H	0.71	0.86
1:K:47:LYS:HG2	1:K:48:VAL:H	1.39	0.85
1:L:257:LEU:HD12	1:L:257:LEU:N	1.79	0.85
1:A:286:LEU:HD12	1:A:286:LEU:H	0.71	0.85
1:C:286:LEU:HD12	1:C:286:LEU:H	0.70	0.85
1:C:257:LEU:HD12	1:C:257:LEU:N	1.79	0.85
1:I:286:LEU:HD12	1:I:286:LEU:H	0.70	0.85
1:K:286:LEU:HD12	1:K:286:LEU:H	0.70	0.84
1:J:280:GLU:C	1:J:281:LYS:HG2	1.94	0.84
1:G:280:GLU:C	1:G:281:LYS:HG2	1.93	0.84
1:D:286:LEU:HD12	1:D:286:LEU:H	0.71	0.83
1:H:211:LYS:HA	1:H:279:SER:HB3	1.61	0.83
1:B:257:LEU:HD12	1:B:257:LEU:N	1.79	0.83
1:D:220:PHE:HA	1:D:223:ILE:CG2	2.09	0.82
1:F:211:LYS:HA	1:F:279:SER:HB3	1.62	0.82
1:G:167:ASP:CG	1:L:160:GLU:HA	1.98	0.82
1:A:220:PHE:HA	1:A:223:ILE:CG2	2.10	0.82
1:B:211:LYS:HA	1:B:279:SER:HB3	1.61	0.82
1:G:72:LEU:HB3	1:H:136:LEU:HD21	1.61	0.82
1:C:280:GLU:C	1:C:281:LYS:HG2	1.93	0.82
1:G:167:ASP:OD1	1:L:159:HIS:C	2.18	0.82
1:L:211:LYS:HA	1:L:279:SER:HB3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:220:PHE:HA	1:J:223:ILE:CG2	2.10	0.82
1:B:220:PHE:HA	1:B:223:ILE:CG2	2.10	0.82
1:C:211:LYS:HA	1:C:279:SER:HB3	1.62	0.82
1:C:220:PHE:HA	1:C:223:ILE:CG2	2.10	0.82
1:K:220:PHE:HA	1:K:223:ILE:CG2	2.10	0.82
1:L:220:PHE:HA	1:L:223:ILE:CG2	2.10	0.81
1:F:286:LEU:H	1:F:286:LEU:HD12	0.71	0.81
1:I:211:LYS:HA	1:I:279:SER:HB3	1.61	0.81
1:I:220:PHE:HA	1:I:223:ILE:CG2	2.10	0.81
1:E:220:PHE:HA	1:E:223:ILE:CG2	2.10	0.81
1:H:256:VAL:HG11	1:H:258:PHE:CE2	2.16	0.81
1:E:256:VAL:HG11	1:E:258:PHE:CE2	2.16	0.81
1:F:220:PHE:HA	1:F:223:ILE:CG2	2.09	0.81
1:G:349:ARG:HB2	1:G:349:ARG:HH11	1.46	0.81
1:H:220:PHE:HA	1:H:223:ILE:CG2	2.10	0.81
1:D:211:LYS:HA	1:D:279:SER:HB3	1.61	0.80
1:J:211:LYS:HA	1:J:279:SER:HB3	1.61	0.80
1:A:211:LYS:HA	1:A:279:SER:HB3	1.62	0.80
1:C:256:VAL:HG11	1:C:258:PHE:CE2	2.17	0.80
1:F:256:VAL:HG11	1:F:258:PHE:CE2	2.16	0.80
1:G:211:LYS:HA	1:G:279:SER:HB3	1.62	0.80
1:G:220:PHE:HA	1:G:223:ILE:CG2	2.10	0.80
1:E:211:LYS:HA	1:E:279:SER:HB3	1.62	0.80
1:H:94:TYR:CE2	1:H:123:ASP:HB3	2.17	0.80
1:H:349:ARG:HB2	1:H:349:ARG:HH11	1.47	0.80
1:B:256:VAL:HG11	1:B:258:PHE:CE2	2.17	0.80
1:C:94:TYR:CE2	1:C:123:ASP:HB3	2.17	0.80
1:G:256:VAL:HG11	1:G:258:PHE:CE2	2.17	0.80
1:D:256:VAL:HG11	1:D:258:PHE:CE2	2.17	0.80
1:J:306:ILE:HB	1:J:307:PRO:HD3	1.64	0.80
1:L:94:TYR:CE2	1:L:123:ASP:HB3	2.17	0.80
1:D:94:TYR:CE2	1:D:123:ASP:HB3	2.17	0.79
1:I:349:ARG:HH11	1:I:349:ARG:HB2	1.47	0.79
1:C:349:ARG:HH11	1:C:349:ARG:HB2	1.47	0.79
1:J:349:ARG:HB2	1:J:349:ARG:HH11	1.47	0.79
1:K:211:LYS:HA	1:K:279:SER:HB3	1.62	0.79
1:L:256:VAL:HG11	1:L:258:PHE:CE2	2.17	0.79
1:F:349:ARG:HH11	1:F:349:ARG:HB2	1.47	0.79
1:E:94:TYR:CE2	1:E:123:ASP:HB3	2.18	0.79
1:I:256:VAL:HG11	1:I:258:PHE:CE2	2.17	0.79
1:A:306:ILE:HB	1:A:307:PRO:HD3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:TYR:CE2	1:A:123:ASP:HB3	2.18	0.79
1:H:306:ILE:HB	1:H:307:PRO:HD3	1.65	0.79
1:I:94:TYR:CE2	1:I:123:ASP:HB3	2.18	0.79
1:J:94:TYR:CE2	1:J:123:ASP:HB3	2.17	0.79
1:A:256:VAL:HG11	1:A:258:PHE:CE2	2.17	0.79
1:F:306:ILE:HB	1:F:307:PRO:HD3	1.64	0.79
1:G:94:TYR:CE2	1:G:123:ASP:HB3	2.17	0.79
1:B:306:ILE:HB	1:B:307:PRO:HD3	1.65	0.78
1:B:349:ARG:HB2	1:B:349:ARG:HH11	1.47	0.78
1:K:94:TYR:CE2	1:K:123:ASP:HB3	2.18	0.78
1:K:256:VAL:HG11	1:K:258:PHE:CE2	2.17	0.78
1:C:306:ILE:HB	1:C:307:PRO:HD3	1.65	0.78
1:J:256:VAL:HG11	1:J:258:PHE:CE2	2.17	0.78
1:D:349:ARG:HH11	1:D:349:ARG:HB2	1.47	0.78
1:K:306:ILE:HB	1:K:307:PRO:HD3	1.65	0.78
1:L:306:ILE:HB	1:L:307:PRO:HD3	1.65	0.78
1:B:94:TYR:CE2	1:B:123:ASP:HB3	2.17	0.78
1:E:349:ARG:HB2	1:E:349:ARG:HH11	1.47	0.78
1:I:306:ILE:HB	1:I:307:PRO:HD3	1.65	0.78
1:F:94:TYR:CE2	1:F:123:ASP:HB3	2.17	0.78
1:A:191:GLU:HG2	1:C:50:PRO:HG2	1.66	0.78
1:K:349:ARG:HB2	1:K:349:ARG:HH11	1.47	0.78
1:K:136:LEU:HD21	1:L:72:LEU:HB3	1.66	0.78
1:F:50:PRO:HG2	1:G:191:GLU:HG2	1.65	0.77
1:G:306:ILE:HB	1:G:307:PRO:HD3	1.65	0.77
1:H:286:LEU:O	1:H:289:LEU:N	2.18	0.77
1:L:349:ARG:HH11	1:L:349:ARG:HB2	1.47	0.77
1:D:306:ILE:HB	1:D:307:PRO:HD3	1.65	0.77
1:A:286:LEU:O	1:A:289:LEU:N	2.18	0.77
1:D:286:LEU:O	1:D:289:LEU:N	2.18	0.77
1:E:306:ILE:HB	1:E:307:PRO:HD3	1.65	0.77
1:K:94:TYR:OH	1:K:123:ASP:N	2.18	0.77
1:A:349:ARG:HH11	1:A:349:ARG:HB2	1.47	0.76
1:C:286:LEU:O	1:C:289:LEU:N	2.19	0.76
1:I:286:LEU:O	1:I:289:LEU:N	2.18	0.76
1:F:286:LEU:O	1:F:289:LEU:N	2.18	0.76
1:J:94:TYR:OH	1:J:123:ASP:N	2.19	0.76
1:B:286:LEU:O	1:B:289:LEU:N	2.18	0.76
1:G:286:LEU:O	1:G:289:LEU:N	2.18	0.76
1:L:94:TYR:OH	1:L:123:ASP:N	2.19	0.76
1:C:136:LEU:HD21	1:D:72:LEU:HB3	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:TYR:OH	1:B:123:ASP:N	2.19	0.76
1:F:94:TYR:OH	1:F:123:ASP:N	2.19	0.76
1:C:94:TYR:OH	1:C:123:ASP:N	2.19	0.75
1:K:286:LEU:O	1:K:289:LEU:N	2.19	0.75
1:H:94:TYR:OH	1:H:123:ASP:N	2.19	0.75
1:B:191:GLU:HG2	1:D:50:PRO:HG2	1.69	0.75
1:G:94:TYR:OH	1:G:123:ASP:N	2.19	0.75
1:J:47:LYS:HG2	1:J:48:VAL:N	2.02	0.75
1:J:286:LEU:O	1:J:289:LEU:N	2.20	0.75
1:A:94:TYR:OH	1:A:123:ASP:N	2.20	0.75
1:D:94:TYR:OH	1:D:123:ASP:N	2.19	0.75
1:E:186:THR:HA	1:E:189:LYS:HD2	1.69	0.75
1:H:369:TYR:O	1:H:372:VAL:HG12	1.87	0.75
1:H:186:THR:HA	1:H:189:LYS:HD2	1.69	0.75
1:I:94:TYR:OH	1:I:123:ASP:N	2.20	0.75
1:L:286:LEU:O	1:L:289:LEU:N	2.18	0.75
1:E:286:LEU:O	1:E:289:LEU:N	2.19	0.75
1:K:186:THR:HA	1:K:189:LYS:HD2	1.68	0.75
1:E:136:LEU:HD21	1:F:72:LEU:HB3	1.69	0.75
1:D:47:LYS:HG2	1:D:48:VAL:N	2.02	0.74
1:E:94:TYR:OH	1:E:123:ASP:N	2.19	0.74
1:E:369:TYR:O	1:E:372:VAL:HG12	1.87	0.74
1:A:186:THR:HA	1:A:189:LYS:HD2	1.69	0.74
1:D:186:THR:HA	1:D:189:LYS:HD2	1.69	0.74
1:D:369:TYR:O	1:D:372:VAL:HG12	1.87	0.74
1:G:186:THR:HA	1:G:189:LYS:HD2	1.69	0.74
1:B:186:THR:HA	1:B:189:LYS:HD2	1.69	0.74
1:C:186:THR:HA	1:C:189:LYS:HD2	1.69	0.74
1:G:369:TYR:O	1:G:372:VAL:HG12	1.88	0.74
1:I:186:THR:HA	1:I:189:LYS:HD2	1.69	0.74
1:J:186:THR:HA	1:J:189:LYS:HD2	1.70	0.74
1:L:186:THR:HA	1:L:189:LYS:HD2	1.69	0.74
1:L:369:TYR:O	1:L:372:VAL:HG12	1.87	0.74
1:F:369:TYR:O	1:F:372:VAL:HG12	1.88	0.74
1:B:369:TYR:O	1:B:372:VAL:HG12	1.88	0.74
1:B:47:LYS:HG2	1:B:48:VAL:N	2.03	0.74
1:E:47:LYS:HG2	1:E:48:VAL:N	2.03	0.74
1:F:186:THR:HA	1:F:189:LYS:HD2	1.69	0.74
1:F:47:LYS:HG2	1:F:48:VAL:N	2.03	0.74
1:I:369:TYR:O	1:I:372:VAL:HG12	1.88	0.73
1:A:369:TYR:O	1:A:372:VAL:HG12	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:LYS:HG2	1:H:48:VAL:N	2.03	0.73
1:G:47:LYS:HG2	1:G:48:VAL:N	2.03	0.73
1:J:191:GLU:HG2	1:L:50:PRO:HG2	1.71	0.73
1:C:47:LYS:HG2	1:C:48:VAL:N	2.03	0.73
1:K:47:LYS:HG2	1:K:48:VAL:N	2.04	0.73
1:A:47:LYS:HG2	1:A:48:VAL:N	2.03	0.73
1:C:369:TYR:O	1:C:372:VAL:HG12	1.88	0.73
1:L:47:LYS:HG2	1:L:48:VAL:N	2.03	0.73
1:K:280:GLU:C	1:K:281:LYS:CG	2.57	0.72
1:I:47:LYS:HG2	1:I:48:VAL:N	2.03	0.72
1:K:369:TYR:O	1:K:372:VAL:HG12	1.88	0.72
1:K:11:PRO:CG	1:K:42:PRO:HG3	2.20	0.72
1:A:11:PRO:CG	1:A:42:PRO:HG3	2.20	0.72
1:F:280:GLU:C	1:F:281:LYS:CG	2.58	0.72
1:A:257:LEU:O	1:A:258:PHE:C	2.27	0.72
1:A:280:GLU:C	1:A:281:LYS:CG	2.58	0.72
1:D:280:GLU:C	1:D:281:LYS:CG	2.58	0.72
1:G:257:LEU:O	1:G:258:PHE:C	2.27	0.72
1:I:257:LEU:O	1:I:258:PHE:C	2.27	0.72
1:K:256:VAL:C	1:K:257:LEU:CD1	2.58	0.71
1:G:280:GLU:C	1:G:281:LYS:CG	2.58	0.71
1:J:280:GLU:C	1:J:281:LYS:CG	2.58	0.71
1:J:369:TYR:O	1:J:372:VAL:HG12	1.89	0.71
1:L:11:PRO:CG	1:L:42:PRO:HG3	2.20	0.71
1:E:11:PRO:CG	1:E:42:PRO:HG3	2.20	0.71
1:H:280:GLU:C	1:H:281:LYS:CG	2.58	0.71
1:B:212:ARG:HA	1:B:214:GLN:HE22	1.56	0.71
1:B:280:GLU:C	1:B:281:LYS:CG	2.58	0.71
1:D:11:PRO:CG	1:D:42:PRO:HG3	2.20	0.71
1:J:212:ARG:HA	1:J:214:GLN:HE22	1.56	0.71
1:B:11:PRO:CG	1:B:42:PRO:HG3	2.20	0.71
1:D:212:ARG:HA	1:D:214:GLN:HE22	1.56	0.71
1:H:11:PRO:CG	1:H:42:PRO:HG3	2.20	0.71
1:I:280:GLU:C	1:I:281:LYS:CG	2.58	0.71
1:L:280:GLU:C	1:L:281:LYS:CG	2.58	0.71
1:C:286:LEU:C	1:C:288:LEU:N	2.43	0.71
1:E:280:GLU:C	1:E:281:LYS:CG	2.58	0.71
1:K:212:ARG:HA	1:K:214:GLN:HE22	1.56	0.71
1:B:257:LEU:O	1:B:258:PHE:C	2.27	0.70
1:H:212:ARG:HA	1:H:214:GLN:HE22	1.56	0.70
1:J:257:LEU:O	1:J:258:PHE:C	2.28	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:LEU:O	1:D:258:PHE:C	2.28	0.70
1:C:11:PRO:CG	1:C:42:PRO:HG3	2.20	0.70
1:C:280:GLU:C	1:C:281:LYS:CG	2.58	0.70
1:F:212:ARG:HA	1:F:214:GLN:HE22	1.56	0.70
1:G:256:VAL:C	1:G:257:LEU:CD1	2.59	0.70
1:L:212:ARG:HA	1:L:214:GLN:HE22	1.56	0.70
1:A:212:ARG:HA	1:A:214:GLN:HE22	1.56	0.70
1:F:11:PRO:CG	1:F:42:PRO:HG3	2.20	0.70
1:H:256:VAL:C	1:H:257:LEU:CD1	2.59	0.70
1:G:11:PRO:CG	1:G:42:PRO:HG3	2.20	0.70
1:I:212:ARG:HA	1:I:214:GLN:HE22	1.56	0.70
1:A:50:PRO:HG2	1:C:191:GLU:HG2	1.72	0.70
1:C:212:ARG:HA	1:C:214:GLN:HE22	1.56	0.70
1:I:11:PRO:CG	1:I:42:PRO:HG3	2.20	0.70
1:G:220:PHE:CA	1:G:223:ILE:HG22	2.21	0.69
1:I:72:LEU:HB3	1:J:136:LEU:HD21	1.73	0.69
1:C:220:PHE:CA	1:C:223:ILE:HG22	2.21	0.69
1:H:180:TYR:CE2	1:H:290:GLU:HB3	2.28	0.69
1:I:256:VAL:C	1:I:257:LEU:CD1	2.59	0.69
1:K:180:TYR:CE2	1:K:290:GLU:HB3	2.27	0.69
1:D:220:PHE:CA	1:D:223:ILE:HG22	2.20	0.69
1:G:212:ARG:HA	1:G:214:GLN:HE22	1.56	0.69
1:H:286:LEU:C	1:H:288:LEU:N	2.43	0.69
1:B:180:TYR:CE2	1:B:290:GLU:HB3	2.28	0.69
1:I:286:LEU:C	1:I:288:LEU:N	2.43	0.69
1:J:11:PRO:CG	1:J:42:PRO:HG3	2.20	0.69
1:K:220:PHE:CA	1:K:223:ILE:HG22	2.21	0.69
1:E:357:ARG:HG3	1:E:359:GLU:HG3	1.75	0.69
1:L:357:ARG:HG3	1:L:359:GLU:HG3	1.75	0.69
1:A:180:TYR:CE2	1:A:290:GLU:HB3	2.28	0.69
1:A:220:PHE:CA	1:A:223:ILE:HG22	2.21	0.69
1:B:357:ARG:HG3	1:B:359:GLU:HG3	1.75	0.69
1:C:357:ARG:HG3	1:C:359:GLU:HG3	1.75	0.69
1:D:180:TYR:CE2	1:D:290:GLU:HB3	2.28	0.69
1:F:257:LEU:O	1:F:258:PHE:C	2.27	0.69
1:H:220:PHE:CA	1:H:223:ILE:HG22	2.21	0.69
1:I:220:PHE:CA	1:I:223:ILE:HG22	2.21	0.69
1:J:180:TYR:CE2	1:J:290:GLU:HB3	2.28	0.69
1:F:180:TYR:CE2	1:F:290:GLU:HB3	2.28	0.69
1:A:256:VAL:C	1:A:257:LEU:CD1	2.59	0.69
1:E:212:ARG:HA	1:E:214:GLN:HE22	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:180:TYR:CE2	1:L:290:GLU:HB3	2.28	0.68
1:G:357:ARG:HG3	1:G:359:GLU:HG3	1.75	0.68
1:J:286:LEU:C	1:J:288:LEU:N	2.43	0.68
1:I:136:LEU:HD21	1:J:72:LEU:HB3	1.75	0.68
1:I:180:TYR:CE2	1:I:290:GLU:HB3	2.28	0.68
1:A:94:TYR:H	1:A:98:HIS:HD2	1.41	0.68
1:A:357:ARG:HG3	1:A:359:GLU:HG3	1.75	0.68
1:C:180:TYR:CE2	1:C:290:GLU:HB3	2.28	0.68
1:H:357:ARG:HG3	1:H:359:GLU:HG3	1.75	0.68
1:J:220:PHE:CA	1:J:223:ILE:HG22	2.21	0.68
1:K:357:ARG:HG3	1:K:359:GLU:HG3	1.75	0.68
1:B:220:PHE:CA	1:B:223:ILE:HG22	2.21	0.68
1:D:286:LEU:C	1:D:288:LEU:N	2.43	0.68
1:K:286:LEU:C	1:K:288:LEU:N	2.42	0.68
1:C:257:LEU:O	1:C:258:PHE:C	2.28	0.68
1:E:94:TYR:H	1:E:98:HIS:HD2	1.42	0.68
1:J:94:TYR:H	1:J:98:HIS:HD2	1.42	0.68
1:D:357:ARG:HG3	1:D:359:GLU:HG3	1.75	0.68
1:F:357:ARG:HG3	1:F:359:GLU:HG3	1.75	0.68
1:G:180:TYR:CE2	1:G:290:GLU:HB3	2.28	0.68
1:J:357:ARG:HG3	1:J:359:GLU:HG3	1.75	0.68
1:D:94:TYR:H	1:D:98:HIS:HD2	1.42	0.68
1:J:256:VAL:C	1:J:257:LEU:CD1	2.59	0.68
1:I:357:ARG:HG3	1:I:359:GLU:HG3	1.75	0.67
1:E:180:TYR:CE2	1:E:290:GLU:HB3	2.28	0.67
1:G:94:TYR:H	1:G:98:HIS:HD2	1.42	0.67
1:F:286:LEU:C	1:F:288:LEU:N	2.43	0.67
1:C:256:VAL:C	1:C:257:LEU:CD1	2.59	0.67
1:E:220:PHE:CA	1:E:223:ILE:HG22	2.21	0.67
1:I:94:TYR:H	1:I:98:HIS:HD2	1.43	0.67
1:C:94:TYR:H	1:C:98:HIS:HD2	1.42	0.67
1:D:256:VAL:C	1:D:257:LEU:CD1	2.59	0.67
1:D:257:LEU:HB3	1:D:259:LEU:CD1	2.25	0.67
1:F:220:PHE:CA	1:F:223:ILE:HG22	2.20	0.67
1:H:257:LEU:HB3	1:H:259:LEU:CD1	2.25	0.67
1:B:256:VAL:C	1:B:257:LEU:CD1	2.59	0.66
1:B:286:LEU:C	1:B:288:LEU:N	2.43	0.66
1:E:257:LEU:O	1:E:258:PHE:C	2.28	0.66
1:E:257:LEU:HB3	1:E:259:LEU:CD1	2.25	0.66
1:K:94:TYR:H	1:K:98:HIS:HD2	1.42	0.66
1:A:286:LEU:C	1:A:288:LEU:N	2.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:LEU:HB3	1:B:259:LEU:CD1	2.25	0.66
1:C:257:LEU:HB3	1:C:259:LEU:CD1	2.25	0.66
1:E:286:LEU:C	1:E:288:LEU:N	2.43	0.66
1:J:257:LEU:HB3	1:J:259:LEU:CD1	2.25	0.66
1:K:257:LEU:O	1:K:258:PHE:C	2.27	0.66
1:L:94:TYR:H	1:L:98:HIS:HD2	1.42	0.66
1:F:256:VAL:C	1:F:257:LEU:CD1	2.59	0.66
1:A:257:LEU:HB3	1:A:259:LEU:CD1	2.25	0.66
1:K:257:LEU:HB3	1:K:259:LEU:CD1	2.26	0.66
1:L:220:PHE:CA	1:L:223:ILE:HG22	2.21	0.66
1:F:333:GLN:HE22	1:F:340:LEU:HD23	1.61	0.66
1:F:94:TYR:H	1:F:98:HIS:HD2	1.42	0.66
1:F:223:ILE:HD11	1:F:335:LEU:HD12	1.78	0.66
1:I:257:LEU:HB3	1:I:259:LEU:CD1	2.25	0.66
1:C:333:GLN:HE22	1:C:340:LEU:HD23	1.61	0.66
1:E:223:ILE:HD11	1:E:335:LEU:HD12	1.78	0.66
1:L:257:LEU:O	1:L:258:PHE:C	2.28	0.66
1:L:257:LEU:HB3	1:L:259:LEU:CD1	2.25	0.66
1:G:333:GLN:HE22	1:G:340:LEU:HD23	1.61	0.66
1:H:94:TYR:H	1:H:98:HIS:HD2	1.43	0.66
1:B:94:TYR:H	1:B:98:HIS:HD2	1.42	0.66
1:H:223:ILE:HD11	1:H:335:LEU:HD12	1.78	0.66
1:I:223:ILE:HD11	1:I:335:LEU:HD12	1.78	0.66
1:F:257:LEU:HB3	1:F:259:LEU:CD1	2.25	0.66
1:G:223:ILE:HD11	1:G:335:LEU:HD12	1.78	0.66
1:C:223:ILE:HD11	1:C:335:LEU:HD12	1.78	0.65
1:G:257:LEU:HB3	1:G:259:LEU:CD1	2.26	0.65
1:A:333:GLN:HE22	1:A:340:LEU:HD23	1.61	0.65
1:B:223:ILE:HD11	1:B:335:LEU:HD12	1.78	0.65
1:K:333:GLN:HE22	1:K:340:LEU:HD23	1.61	0.65
1:I:333:GLN:HE22	1:I:340:LEU:HD23	1.61	0.65
1:K:353:TYR:O	1:K:357:ARG:HB2	1.97	0.65
1:L:223:ILE:HD11	1:L:335:LEU:HD12	1.78	0.65
1:L:333:GLN:HE22	1:L:340:LEU:HD23	1.61	0.65
1:B:221:ALA:O	1:B:224:VAL:HG12	1.97	0.65
1:D:223:ILE:HD11	1:D:335:LEU:HD12	1.78	0.65
1:D:333:GLN:HE22	1:D:340:LEU:HD23	1.61	0.65
1:E:256:VAL:C	1:E:257:LEU:CD1	2.59	0.65
1:J:333:GLN:HE22	1:J:340:LEU:HD23	1.61	0.65
1:J:353:TYR:O	1:J:357:ARG:HB2	1.97	0.65
1:K:223:ILE:HD11	1:K:335:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:GLN:HE22	1:E:340:LEU:HD23	1.61	0.65
1:G:353:TYR:O	1:G:357:ARG:HB2	1.97	0.65
1:I:221:ALA:O	1:I:224:VAL:HG12	1.97	0.65
1:B:323:ASP:O	1:B:327:VAL:HG23	1.98	0.64
1:B:353:TYR:O	1:B:357:ARG:HB2	1.97	0.64
1:C:353:TYR:O	1:C:357:ARG:HB2	1.97	0.64
1:I:353:TYR:O	1:I:357:ARG:HB2	1.97	0.64
1:K:221:ALA:O	1:K:224:VAL:HG12	1.98	0.64
1:A:223:ILE:HD11	1:A:335:LEU:HD12	1.78	0.64
1:F:353:TYR:O	1:F:357:ARG:HB2	1.97	0.64
1:I:284:PHE:HB3	1:I:285:GLY:CA	2.26	0.64
1:B:333:GLN:HE22	1:B:340:LEU:HD23	1.61	0.64
1:H:257:LEU:O	1:H:258:PHE:C	2.28	0.64
1:H:333:GLN:HE22	1:H:340:LEU:HD23	1.61	0.64
1:K:256:VAL:O	1:K:257:LEU:HD12	1.97	0.64
1:L:221:ALA:O	1:L:224:VAL:HG12	1.97	0.64
1:A:306:ILE:N	1:A:307:PRO:CD	2.61	0.64
1:H:349:ARG:HB2	1:H:349:ARG:NH1	2.13	0.64
1:H:353:TYR:O	1:H:357:ARG:HB2	1.97	0.64
1:E:349:ARG:HB2	1:E:349:ARG:NH1	2.13	0.64
1:I:323:ASP:O	1:I:327:VAL:HG23	1.98	0.64
1:K:257:LEU:O	1:K:259:LEU:CD1	2.46	0.64
1:B:306:ILE:N	1:B:307:PRO:CD	2.61	0.64
1:C:221:ALA:O	1:C:224:VAL:HG12	1.98	0.64
1:D:221:ALA:O	1:D:224:VAL:HG12	1.97	0.64
1:D:353:TYR:O	1:D:357:ARG:HB2	1.97	0.64
1:E:221:ALA:O	1:E:224:VAL:HG12	1.98	0.64
1:E:323:ASP:O	1:E:327:VAL:HG23	1.98	0.64
1:A:353:TYR:O	1:A:357:ARG:HB2	1.97	0.64
1:C:323:ASP:O	1:C:327:VAL:HG23	1.98	0.64
1:F:323:ASP:O	1:F:327:VAL:HG23	1.98	0.64
1:G:221:ALA:O	1:G:224:VAL:HG12	1.98	0.64
1:G:306:ILE:N	1:G:307:PRO:CD	2.61	0.64
1:J:221:ALA:O	1:J:224:VAL:HG12	1.98	0.64
1:L:256:VAL:C	1:L:257:LEU:CD1	2.59	0.64
1:E:353:TYR:O	1:E:357:ARG:HB2	1.97	0.63
1:H:323:ASP:O	1:H:327:VAL:HG23	1.98	0.63
1:J:223:ILE:HD11	1:J:335:LEU:HD12	1.79	0.63
1:A:323:ASP:O	1:A:327:VAL:HG23	1.98	0.63
1:B:256:VAL:O	1:B:257:LEU:HD12	1.97	0.63
1:C:257:LEU:O	1:C:259:LEU:CD1	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:LEU:HB3	1:F:136:LEU:HD21	1.79	0.63
1:F:254:ASP:C	1:F:254:ASP:OD1	2.34	0.63
1:L:289:LEU:O	1:L:290:GLU:C	2.36	0.63
1:L:306:ILE:N	1:L:307:PRO:CD	2.62	0.63
1:L:353:TYR:O	1:L:357:ARG:HB2	1.97	0.63
1:A:221:ALA:O	1:A:224:VAL:HG12	1.98	0.63
1:A:349:ARG:HB2	1:A:349:ARG:NH1	2.13	0.63
1:A:257:LEU:O	1:A:259:LEU:CD1	2.46	0.63
1:E:256:VAL:O	1:E:257:LEU:HD12	1.98	0.63
1:L:323:ASP:O	1:L:327:VAL:HG23	1.98	0.63
1:C:349:ARG:HB2	1:C:349:ARG:NH1	2.13	0.63
1:E:257:LEU:O	1:E:259:LEU:CD1	2.47	0.63
1:E:306:ILE:N	1:E:307:PRO:CD	2.62	0.63
1:F:221:ALA:O	1:F:224:VAL:HG12	1.97	0.63
1:K:254:ASP:OD1	1:K:254:ASP:C	2.33	0.63
1:K:306:ILE:N	1:K:307:PRO:CD	2.62	0.63
1:D:256:VAL:O	1:D:257:LEU:HD12	1.98	0.63
1:J:257:LEU:O	1:J:259:LEU:CD1	2.46	0.63
1:L:257:LEU:O	1:L:259:LEU:CD1	2.47	0.63
1:B:349:ARG:HB2	1:B:349:ARG:NH1	2.13	0.63
1:C:306:ILE:N	1:C:307:PRO:CD	2.62	0.63
1:G:132:SER:O	1:G:133:LEU:HD23	1.99	0.63
1:C:256:VAL:O	1:C:257:LEU:HD12	1.98	0.63
1:D:306:ILE:N	1:D:307:PRO:CD	2.62	0.63
1:G:254:ASP:C	1:G:254:ASP:OD1	2.34	0.63
1:H:221:ALA:O	1:H:224:VAL:HG12	1.98	0.63
1:A:256:VAL:O	1:A:257:LEU:HD12	1.98	0.63
1:H:306:ILE:N	1:H:307:PRO:CD	2.61	0.63
1:I:306:ILE:N	1:I:307:PRO:CD	2.62	0.63
1:K:323:ASP:O	1:K:327:VAL:HG23	1.98	0.63
1:L:256:VAL:O	1:L:257:LEU:HD12	1.98	0.63
1:B:257:LEU:O	1:B:259:LEU:CD1	2.46	0.62
1:E:256:VAL:O	1:E:256:VAL:HG12	1.97	0.62
1:F:257:LEU:O	1:F:259:LEU:CD1	2.46	0.62
1:G:257:LEU:O	1:G:259:LEU:CD1	2.47	0.62
1:H:256:VAL:O	1:H:257:LEU:HD12	1.98	0.62
1:J:323:ASP:O	1:J:327:VAL:HG23	1.98	0.62
1:C:284:PHE:HB3	1:C:285:GLY:CA	2.26	0.62
1:I:256:VAL:O	1:I:257:LEU:HD12	1.98	0.62
1:J:132:SER:O	1:J:133:LEU:HD23	1.98	0.62
1:F:256:VAL:O	1:F:257:LEU:HD12	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:286:LEU:C	1:G:288:LEU:N	2.43	0.62
1:G:323:ASP:O	1:G:327:VAL:HG23	1.98	0.62
1:I:349:ARG:HB2	1:I:349:ARG:NH1	2.13	0.62
1:B:204:ILE:HD13	1:B:265:VAL:HG21	1.82	0.62
1:D:323:ASP:O	1:D:327:VAL:HG23	1.98	0.62
1:E:132:SER:O	1:E:133:LEU:HD23	1.99	0.62
1:H:257:LEU:O	1:H:259:LEU:CD1	2.47	0.62
1:I:257:LEU:O	1:I:259:LEU:CD1	2.47	0.62
1:J:306:ILE:N	1:J:307:PRO:CD	2.62	0.62
1:L:286:LEU:C	1:L:288:LEU:N	2.42	0.62
1:C:204:ILE:HD13	1:C:265:VAL:HG21	1.82	0.62
1:D:257:LEU:O	1:D:259:LEU:CD1	2.47	0.62
1:J:256:VAL:O	1:J:256:VAL:HG12	1.97	0.62
1:J:256:VAL:O	1:J:257:LEU:HD12	1.99	0.62
1:A:132:SER:O	1:A:133:LEU:HD23	2.00	0.62
1:G:349:ARG:HB2	1:G:349:ARG:NH1	2.13	0.62
1:K:204:ILE:HD13	1:K:265:VAL:HG21	1.82	0.62
1:B:132:SER:O	1:B:133:LEU:HD23	1.99	0.62
1:E:204:ILE:HD13	1:E:265:VAL:HG21	1.82	0.62
1:I:204:ILE:HD13	1:I:265:VAL:HG21	1.82	0.62
1:L:132:SER:O	1:L:133:LEU:HD23	2.00	0.62
1:L:204:ILE:HD13	1:L:265:VAL:HG21	1.82	0.62
1:B:284:PHE:HB3	1:B:285:GLY:CA	2.27	0.62
1:D:204:ILE:HD13	1:D:265:VAL:HG21	1.82	0.62
1:F:132:SER:O	1:F:133:LEU:HD23	1.99	0.62
1:G:204:ILE:HD13	1:G:265:VAL:HG21	1.82	0.62
1:G:289:LEU:O	1:G:290:GLU:C	2.36	0.62
1:I:132:SER:O	1:I:133:LEU:HD23	1.99	0.62
1:J:349:ARG:HB2	1:J:349:ARG:NH1	2.13	0.62
1:L:256:VAL:O	1:L:256:VAL:HG12	1.97	0.62
1:C:132:SER:O	1:C:133:LEU:HD23	1.99	0.62
1:L:349:ARG:HB2	1:L:349:ARG:NH1	2.13	0.62
1:C:72:LEU:HB3	1:D:136:LEU:HD21	1.80	0.61
1:D:349:ARG:HB2	1:D:349:ARG:NH1	2.13	0.61
1:F:123:ASP:HA	1:F:127:LEU:HD12	1.82	0.61
1:F:306:ILE:N	1:F:307:PRO:CD	2.61	0.61
1:J:50:PRO:HG2	1:L:191:GLU:HG2	1.81	0.61
1:A:72:LEU:HB3	1:B:136:LEU:HD21	1.82	0.61
1:D:256:VAL:O	1:D:256:VAL:HG12	1.97	0.61
1:G:256:VAL:O	1:G:257:LEU:HD12	1.98	0.61
1:J:289:LEU:O	1:J:290:GLU:C	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:289:LEU:O	1:K:290:GLU:C	2.36	0.61
1:B:122:THR:HG22	1:B:126:VAL:CG1	2.31	0.61
1:H:281:LYS:NZ	1:H:281:LYS:CB	2.63	0.61
1:H:289:LEU:O	1:H:290:GLU:C	2.36	0.61
1:K:123:ASP:HA	1:K:127:LEU:HD12	1.82	0.61
1:E:123:ASP:HA	1:E:127:LEU:HD12	1.82	0.61
1:G:123:ASP:HA	1:G:127:LEU:HD12	1.82	0.61
1:H:204:ILE:HD13	1:H:265:VAL:HG21	1.82	0.61
1:L:281:LYS:NZ	1:L:281:LYS:CB	2.64	0.61
1:A:254:ASP:C	1:A:254:ASP:OD1	2.33	0.61
1:G:256:VAL:O	1:G:256:VAL:HG12	1.97	0.61
1:H:122:THR:HG22	1:H:126:VAL:CG1	2.31	0.61
1:H:132:SER:O	1:H:133:LEU:HD23	2.00	0.61
1:J:122:THR:HG22	1:J:126:VAL:CG1	2.31	0.61
1:J:204:ILE:HD13	1:J:265:VAL:HG21	1.82	0.61
1:K:132:SER:O	1:K:133:LEU:HD23	1.99	0.61
1:A:204:ILE:HD13	1:A:265:VAL:HG21	1.82	0.61
1:D:122:THR:HG22	1:D:126:VAL:CG1	2.31	0.61
1:D:132:SER:O	1:D:133:LEU:HD23	2.00	0.61
1:H:123:ASP:HA	1:H:127:LEU:HD12	1.82	0.61
1:E:281:LYS:NZ	1:E:281:LYS:CB	2.64	0.61
1:F:122:THR:HG22	1:F:126:VAL:CG1	2.31	0.61
1:G:281:LYS:CB	1:G:281:LYS:NZ	2.64	0.61
1:J:123:ASP:HA	1:J:127:LEU:HD12	1.81	0.61
1:J:254:ASP:C	1:J:254:ASP:OD1	2.33	0.61
1:J:284:PHE:HB3	1:J:285:GLY:CA	2.26	0.61
1:K:292:MET:O	1:K:294:CYS:N	2.34	0.61
1:B:292:MET:O	1:B:294:CYS:N	2.34	0.61
1:C:281:LYS:NZ	1:C:281:LYS:CB	2.64	0.61
1:L:123:ASP:HA	1:L:127:LEU:HD12	1.82	0.61
1:B:256:VAL:O	1:B:256:VAL:HG12	1.97	0.61
1:C:122:THR:HG22	1:C:126:VAL:CG1	2.30	0.61
1:D:254:ASP:C	1:D:254:ASP:OD1	2.34	0.61
1:G:167:ASP:OD1	1:L:160:GLU:N	2.34	0.61
1:L:122:THR:HG22	1:L:126:VAL:CG1	2.31	0.61
1:L:292:MET:O	1:L:294:CYS:N	2.34	0.61
1:A:123:ASP:HA	1:A:127:LEU:HD12	1.83	0.61
1:C:123:ASP:HA	1:C:127:LEU:HD12	1.82	0.61
1:F:281:LYS:NZ	1:F:281:LYS:CB	2.64	0.61
1:F:349:ARG:HB2	1:F:349:ARG:NH1	2.13	0.61
1:C:254:ASP:OD1	1:C:254:ASP:C	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:MET:O	1:C:294:CYS:N	2.34	0.60
1:D:284:PHE:HB3	1:D:285:GLY:CA	2.27	0.60
1:D:292:MET:O	1:D:294:CYS:N	2.34	0.60
1:H:254:ASP:C	1:H:254:ASP:OD1	2.34	0.60
1:I:281:LYS:O	1:I:282:GLU:HB2	2.01	0.60
1:D:281:LYS:NZ	1:D:281:LYS:CB	2.64	0.60
1:E:122:THR:HG22	1:E:126:VAL:CG1	2.31	0.60
1:E:292:MET:O	1:E:294:CYS:N	2.34	0.60
1:I:123:ASP:HA	1:I:127:LEU:HD12	1.82	0.60
1:K:349:ARG:HB2	1:K:349:ARG:NH1	2.13	0.60
1:A:122:THR:HG22	1:A:126:VAL:CG1	2.31	0.60
1:D:281:LYS:O	1:D:282:GLU:HB2	2.01	0.60
1:H:182:LYS:HZ1	1:H:349:ARG:HD3	1.66	0.60
1:I:122:THR:HG22	1:I:126:VAL:CG1	2.31	0.60
1:I:254:ASP:C	1:I:254:ASP:OD1	2.34	0.60
1:A:281:LYS:NZ	1:A:281:LYS:CB	2.64	0.60
1:D:123:ASP:HA	1:D:127:LEU:HD12	1.83	0.60
1:F:204:ILE:HD13	1:F:265:VAL:HG21	1.82	0.60
1:G:292:MET:O	1:G:294:CYS:N	2.34	0.60
1:K:212:ARG:HA	1:K:214:GLN:NE2	2.17	0.60
1:B:123:ASP:HA	1:B:127:LEU:HD12	1.82	0.60
1:H:284:PHE:HB3	1:H:285:GLY:CA	2.27	0.60
1:I:281:LYS:NZ	1:I:281:LYS:CB	2.64	0.60
1:K:281:LYS:NZ	1:K:281:LYS:CB	2.64	0.60
1:A:281:LYS:O	1:A:282:GLU:HB2	2.01	0.60
1:E:289:LEU:O	1:E:290:GLU:C	2.36	0.60
1:I:292:MET:O	1:I:294:CYS:N	2.34	0.60
1:J:281:LYS:O	1:J:282:GLU:HB2	2.01	0.60
1:A:292:MET:O	1:A:294:CYS:N	2.34	0.60
1:F:292:MET:O	1:F:294:CYS:N	2.34	0.60
1:K:281:LYS:O	1:K:282:GLU:HB2	2.01	0.60
1:A:289:LEU:O	1:A:290:GLU:C	2.36	0.60
1:D:289:LEU:O	1:D:290:GLU:C	2.36	0.60
1:F:191:GLU:HG2	1:G:50:PRO:HG2	1.83	0.60
1:G:281:LYS:O	1:G:282:GLU:HB2	2.01	0.60
1:K:256:VAL:O	1:K:256:VAL:HG12	1.98	0.60
1:D:113:ILE:HD13	1:D:114:LYS:H	1.67	0.60
1:F:289:LEU:O	1:F:290:GLU:C	2.36	0.60
1:K:122:THR:HG22	1:K:126:VAL:CG1	2.32	0.60
1:C:256:VAL:O	1:C:256:VAL:HG12	1.97	0.60
1:I:113:ILE:HD13	1:I:114:LYS:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:292:MET:O	1:J:294:CYS:N	2.35	0.60
1:L:281:LYS:O	1:L:282:GLU:HB2	2.01	0.60
1:A:212:ARG:HA	1:A:214:GLN:NE2	2.17	0.59
1:H:212:ARG:HA	1:H:214:GLN:NE2	2.17	0.59
1:J:287:VAL:HG23	1:J:287:VAL:O	2.02	0.59
1:B:281:LYS:CB	1:B:281:LYS:NZ	2.64	0.59
1:E:94:TYR:CD2	1:E:123:ASP:HB3	2.37	0.59
1:J:94:TYR:CD2	1:J:123:ASP:HB3	2.37	0.59
1:J:173:ASN:OD1	1:J:284:PHE:CD1	2.55	0.59
1:L:106:LYS:HG2	1:L:111:GLU:HA	1.84	0.59
1:A:173:ASN:OD1	1:A:284:PHE:CD1	2.55	0.59
1:C:281:LYS:O	1:C:282:GLU:HB2	2.01	0.59
1:E:212:ARG:HA	1:E:214:GLN:NE2	2.17	0.59
1:G:122:THR:HG22	1:G:126:VAL:CG1	2.31	0.59
1:G:173:ASN:OD1	1:G:284:PHE:CD1	2.56	0.59
1:H:292:MET:O	1:H:294:CYS:N	2.35	0.59
1:L:254:ASP:C	1:L:254:ASP:OD1	2.33	0.59
1:A:256:VAL:O	1:A:256:VAL:HG12	1.97	0.59
1:B:106:LYS:HG2	1:B:111:GLU:HA	1.84	0.59
1:B:173:ASN:OD1	1:B:284:PHE:CD1	2.56	0.59
1:B:212:ARG:HA	1:B:214:GLN:NE2	2.17	0.59
1:D:173:ASN:OD1	1:D:284:PHE:CD1	2.56	0.59
1:E:254:ASP:C	1:E:254:ASP:OD1	2.33	0.59
1:F:281:LYS:O	1:F:282:GLU:HB2	2.01	0.59
1:H:281:LYS:O	1:H:282:GLU:HB2	2.01	0.59
1:B:113:ILE:HD13	1:B:114:LYS:H	1.67	0.59
1:H:106:LYS:HG2	1:H:111:GLU:HA	1.84	0.59
1:J:281:LYS:CB	1:J:281:LYS:NZ	2.64	0.59
1:B:204:ILE:CD1	1:B:265:VAL:HG21	2.33	0.59
1:C:182:LYS:HZ1	1:C:349:ARG:HD3	1.66	0.59
1:G:250:LEU:HD23	1:G:252:ILE:HD11	1.85	0.59
1:H:94:TYR:CD2	1:H:123:ASP:HB3	2.37	0.59
1:J:212:ARG:HA	1:J:214:GLN:NE2	2.17	0.59
1:L:173:ASN:OD1	1:L:284:PHE:CD1	2.55	0.59
1:C:204:ILE:CD1	1:C:265:VAL:HG21	2.33	0.59
1:G:284:PHE:HB3	1:G:285:GLY:CA	2.26	0.59
1:I:250:LEU:HD23	1:I:252:ILE:HD11	1.85	0.59
1:L:113:ILE:HD13	1:L:114:LYS:H	1.68	0.59
1:L:284:PHE:HB3	1:L:285:GLY:CA	2.27	0.59
1:L:333:GLN:HE22	1:L:340:LEU:CD2	2.16	0.59
1:A:204:ILE:CD1	1:A:265:VAL:HG21	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:LYS:O	1:B:282:GLU:HB2	2.01	0.59
1:C:113:ILE:HD13	1:C:114:LYS:H	1.68	0.59
1:C:250:LEU:HD23	1:C:252:ILE:HD11	1.85	0.59
1:E:281:LYS:O	1:E:282:GLU:HB2	2.01	0.59
1:F:113:ILE:HD13	1:F:114:LYS:H	1.67	0.59
1:F:204:ILE:CD1	1:F:265:VAL:HG21	2.33	0.59
1:G:204:ILE:CD1	1:G:265:VAL:HG21	2.33	0.59
1:H:173:ASN:OD1	1:H:284:PHE:CD1	2.56	0.59
1:J:106:LYS:HG2	1:J:111:GLU:HA	1.84	0.59
1:L:121:GLY:O	1:L:125:THR:OG1	2.20	0.59
1:A:94:TYR:CD2	1:A:123:ASP:HB3	2.38	0.59
1:D:106:LYS:HG2	1:D:111:GLU:HA	1.84	0.59
1:F:212:ARG:HA	1:F:214:GLN:NE2	2.17	0.59
1:F:284:PHE:HB3	1:F:285:GLY:CA	2.27	0.59
1:I:204:ILE:CD1	1:I:265:VAL:HG21	2.33	0.59
1:A:250:LEU:HD23	1:A:252:ILE:HD11	1.85	0.59
1:B:254:ASP:C	1:B:254:ASP:OD1	2.34	0.59
1:C:212:ARG:HA	1:C:214:GLN:NE2	2.17	0.59
1:C:289:LEU:O	1:C:290:GLU:C	2.36	0.59
1:E:113:ILE:HD13	1:E:114:LYS:H	1.67	0.59
1:F:94:TYR:CD2	1:F:123:ASP:HB3	2.38	0.59
1:F:333:GLN:HE22	1:F:340:LEU:CD2	2.16	0.59
1:G:113:ILE:HD13	1:G:114:LYS:H	1.67	0.59
1:G:281:LYS:CB	1:G:281:LYS:HZ3	2.15	0.59
1:I:281:LYS:CB	1:I:281:LYS:HZ3	2.15	0.59
1:I:289:LEU:O	1:I:290:GLU:C	2.36	0.59
1:K:204:ILE:CD1	1:K:265:VAL:HG21	2.33	0.59
1:K:250:LEU:HD23	1:K:252:ILE:HD11	1.85	0.59
1:B:333:GLN:HE22	1:B:340:LEU:CD2	2.16	0.58
1:D:94:TYR:CD2	1:D:123:ASP:HB3	2.38	0.58
1:F:173:ASN:OD1	1:F:284:PHE:CD1	2.55	0.58
1:G:106:LYS:HG2	1:G:111:GLU:HA	1.84	0.58
1:G:333:GLN:HE22	1:G:340:LEU:CD2	2.16	0.58
1:L:212:ARG:HA	1:L:214:GLN:NE2	2.17	0.58
1:D:287:VAL:HG23	1:D:287:VAL:O	2.03	0.58
1:D:333:GLN:HE22	1:D:340:LEU:CD2	2.16	0.58
1:E:256:VAL:CG1	1:E:258:PHE:CE2	2.86	0.58
1:F:250:LEU:HD23	1:F:252:ILE:HD11	1.85	0.58
1:G:94:TYR:CD2	1:G:123:ASP:HB3	2.38	0.58
1:G:212:ARG:HA	1:G:214:GLN:NE2	2.17	0.58
1:I:94:TYR:CD2	1:I:123:ASP:HB3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:250:LEU:HD23	1:J:252:ILE:HD11	1.85	0.58
1:K:113:ILE:HD13	1:K:114:LYS:H	1.68	0.58
1:K:257:LEU:O	1:K:259:LEU:HD13	2.04	0.58
1:L:250:LEU:HD23	1:L:252:ILE:HD11	1.85	0.58
1:B:94:TYR:CD2	1:B:123:ASP:HB3	2.38	0.58
1:D:204:ILE:CD1	1:D:265:VAL:HG21	2.33	0.58
1:I:212:ARG:HA	1:I:214:GLN:NE2	2.17	0.58
1:E:173:ASN:OD1	1:E:284:PHE:CD1	2.56	0.58
1:F:182:LYS:HZ1	1:F:349:ARG:HD3	1.67	0.58
1:F:290:GLU:O	1:F:293:ALA:HB3	2.04	0.58
1:J:257:LEU:O	1:J:259:LEU:HD13	2.04	0.58
1:K:96:ILE:CG2	1:L:65:PHE:HZ	2.17	0.58
1:L:94:TYR:CD2	1:L:123:ASP:HB3	2.38	0.58
1:A:290:GLU:O	1:A:293:ALA:HB3	2.04	0.58
1:C:106:LYS:HG2	1:C:111:GLU:HA	1.84	0.58
1:D:212:ARG:HA	1:D:214:GLN:NE2	2.17	0.58
1:E:333:GLN:HE22	1:E:340:LEU:CD2	2.16	0.58
1:F:106:LYS:HG2	1:F:111:GLU:HA	1.84	0.58
1:H:113:ILE:HD13	1:H:114:LYS:H	1.67	0.58
1:I:173:ASN:OD1	1:I:284:PHE:CD1	2.56	0.58
1:J:204:ILE:CD1	1:J:265:VAL:HG21	2.34	0.58
1:A:257:LEU:O	1:A:259:LEU:HD13	2.04	0.58
1:D:250:LEU:HD23	1:D:252:ILE:HD11	1.85	0.58
1:C:290:GLU:O	1:C:293:ALA:HB3	2.04	0.58
1:E:106:LYS:HG2	1:E:111:GLU:HA	1.84	0.58
1:H:333:GLN:HE22	1:H:340:LEU:CD2	2.16	0.58
1:A:113:ILE:HD13	1:A:114:LYS:H	1.67	0.58
1:C:287:VAL:O	1:C:287:VAL:HG23	2.04	0.58
1:I:333:GLN:HE22	1:I:340:LEU:CD2	2.16	0.58
1:A:256:VAL:CG1	1:A:258:PHE:CE2	2.87	0.58
1:B:257:LEU:O	1:B:259:LEU:HD13	2.04	0.58
1:C:333:GLN:HE22	1:C:340:LEU:CD2	2.16	0.58
1:E:204:ILE:CD1	1:E:265:VAL:HG21	2.33	0.58
1:G:257:LEU:O	1:G:259:LEU:HD13	2.04	0.58
1:H:204:ILE:CD1	1:H:265:VAL:HG21	2.33	0.58
1:H:250:LEU:HD23	1:H:252:ILE:HD11	1.85	0.58
1:K:333:GLN:HE22	1:K:340:LEU:CD2	2.17	0.58
1:L:204:ILE:CD1	1:L:265:VAL:HG21	2.33	0.58
1:A:333:GLN:HE22	1:A:340:LEU:CD2	2.16	0.58
1:B:250:LEU:HD23	1:B:252:ILE:HD11	1.85	0.58
1:C:257:LEU:O	1:C:259:LEU:HD13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:287:VAL:O	1:I:287:VAL:HG23	2.03	0.58
1:K:106:LYS:HG2	1:K:111:GLU:HA	1.84	0.58
1:C:317:TYR:HE1	1:C:334:LEU:HD22	1.69	0.57
1:K:290:GLU:O	1:K:293:ALA:HB3	2.04	0.57
1:A:106:LYS:HG2	1:A:111:GLU:HA	1.84	0.57
1:C:94:TYR:CD2	1:C:123:ASP:HB3	2.38	0.57
1:D:257:LEU:O	1:D:259:LEU:HD13	2.05	0.57
1:G:287:VAL:HG23	1:G:287:VAL:O	2.03	0.57
1:J:290:GLU:O	1:J:293:ALA:HB3	2.04	0.57
1:C:256:VAL:CG1	1:C:258:PHE:CE2	2.87	0.57
1:I:256:VAL:O	1:I:256:VAL:HG12	1.97	0.57
1:B:289:LEU:O	1:B:290:GLU:C	2.36	0.57
1:B:306:ILE:H	1:B:307:PRO:CD	2.18	0.57
1:D:292:MET:O	1:D:293:ALA:C	2.42	0.57
1:E:257:LEU:O	1:E:259:LEU:HD13	2.04	0.57
1:J:113:ILE:HD13	1:J:114:LYS:H	1.68	0.57
1:J:182:LYS:NZ	1:J:349:ARG:HD3	2.19	0.57
1:K:256:VAL:CG1	1:K:258:PHE:CE2	2.87	0.57
1:E:250:LEU:HD23	1:E:252:ILE:HD11	1.85	0.57
1:F:256:VAL:CG1	1:F:258:PHE:CE2	2.87	0.57
1:G:182:LYS:NZ	1:G:349:ARG:HD3	2.20	0.57
1:H:94:TYR:CZ	1:H:123:ASP:HB3	2.40	0.57
1:H:290:GLU:O	1:H:293:ALA:HB3	2.04	0.57
1:H:317:TYR:HE1	1:H:334:LEU:HD22	1.69	0.57
1:I:290:GLU:O	1:I:293:ALA:HB3	2.04	0.57
1:K:94:TYR:CD2	1:K:123:ASP:HB3	2.39	0.57
1:K:332:ILE:HD12	1:K:333:GLN:N	2.20	0.57
1:L:256:VAL:CG1	1:L:258:PHE:CE2	2.88	0.57
1:A:306:ILE:H	1:A:307:PRO:CD	2.17	0.57
1:A:317:TYR:HE1	1:A:334:LEU:HD22	1.69	0.57
1:B:256:VAL:CG1	1:B:258:PHE:CE2	2.87	0.57
1:D:256:VAL:CG1	1:D:258:PHE:CE2	2.87	0.57
1:G:332:ILE:HD12	1:G:333:GLN:N	2.20	0.57
1:H:306:ILE:H	1:H:307:PRO:CD	2.18	0.57
1:J:317:TYR:HE1	1:J:334:LEU:HD22	1.69	0.57
1:J:332:ILE:HD12	1:J:333:GLN:N	2.20	0.57
1:K:173:ASN:OD1	1:K:284:PHE:CD1	2.58	0.57
1:A:275:MET:SD	1:A:287:VAL:CG2	2.93	0.57
1:F:317:TYR:HE1	1:F:334:LEU:HD22	1.69	0.57
1:G:167:ASP:CG	1:L:160:GLU:CA	2.67	0.57
1:H:275:MET:SD	1:H:287:VAL:CG2	2.93	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:257:LEU:O	1:L:259:LEU:HD13	2.05	0.57
1:L:275:MET:SD	1:L:287:VAL:CG2	2.93	0.57
1:B:182:LYS:NZ	1:B:349:ARG:HD3	2.20	0.57
1:G:256:VAL:CG1	1:G:258:PHE:CE2	2.87	0.57
1:H:284:PHE:C	1:H:284:PHE:CD2	2.75	0.57
1:J:333:GLN:HE22	1:J:340:LEU:CD2	2.17	0.57
1:L:290:GLU:O	1:L:293:ALA:HB3	2.04	0.57
1:C:182:LYS:NZ	1:C:349:ARG:HD3	2.20	0.57
1:E:290:GLU:O	1:E:293:ALA:HB3	2.04	0.57
1:H:257:LEU:O	1:H:259:LEU:HD13	2.04	0.57
1:K:284:PHE:HB3	1:K:285:GLY:CA	2.28	0.57
1:L:182:LYS:NZ	1:L:349:ARG:HD3	2.20	0.57
1:A:284:PHE:HB3	1:A:285:GLY:CA	2.27	0.57
1:A:332:ILE:HD12	1:A:333:GLN:N	2.20	0.57
1:B:290:GLU:O	1:B:293:ALA:HB3	2.04	0.57
1:B:317:TYR:HE1	1:B:334:LEU:HD22	1.69	0.57
1:D:332:ILE:HD12	1:D:333:GLN:N	2.20	0.57
1:I:106:LYS:HG2	1:I:111:GLU:HA	1.85	0.57
1:I:332:ILE:HD12	1:I:333:GLN:N	2.20	0.57
1:K:182:LYS:NZ	1:K:349:ARG:HD3	2.19	0.57
1:L:332:ILE:HD12	1:L:333:GLN:N	2.20	0.57
1:F:182:LYS:NZ	1:F:349:ARG:HD3	2.20	0.56
1:F:332:ILE:HD12	1:F:333:GLN:N	2.20	0.56
1:G:290:GLU:O	1:G:293:ALA:HB3	2.04	0.56
1:G:306:ILE:H	1:G:307:PRO:CD	2.17	0.56
1:H:256:VAL:CG1	1:H:258:PHE:CE2	2.87	0.56
1:H:332:ILE:HD12	1:H:333:GLN:N	2.20	0.56
1:I:306:ILE:H	1:I:307:PRO:CD	2.18	0.56
1:J:292:MET:O	1:J:293:ALA:C	2.43	0.56
1:B:332:ILE:HD12	1:B:333:GLN:N	2.20	0.56
1:D:317:TYR:HE1	1:D:334:LEU:HD22	1.69	0.56
1:E:173:ASN:HB2	1:E:284:PHE:HE1	1.71	0.56
1:E:292:MET:O	1:E:293:ALA:C	2.42	0.56
1:I:292:MET:O	1:I:293:ALA:C	2.42	0.56
1:I:312:HIS:NE2	1:I:317:TYR:HD2	2.03	0.56
1:A:182:LYS:NZ	1:A:349:ARG:HD3	2.20	0.56
1:C:312:HIS:NE2	1:C:317:TYR:HD2	2.04	0.56
1:D:182:LYS:NZ	1:D:349:ARG:HD3	2.20	0.56
1:E:317:TYR:HE1	1:E:334:LEU:HD22	1.69	0.56
1:F:287:VAL:O	1:F:287:VAL:HG23	2.03	0.56
1:F:306:ILE:H	1:F:307:PRO:CD	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:317:TYR:HE1	1:G:334:LEU:HD22	1.69	0.56
1:H:119:LEU:HD22	1:H:124:ILE:HD11	1.88	0.56
1:I:317:TYR:HE1	1:I:334:LEU:HD22	1.69	0.56
1:K:177:GLU:HG3	1:K:357:ARG:NH1	2.20	0.56
1:L:306:ILE:H	1:L:307:PRO:CD	2.18	0.56
1:C:292:MET:O	1:C:293:ALA:C	2.42	0.56
1:D:254:ASP:OD1	1:D:254:ASP:N	2.36	0.56
1:E:182:LYS:NZ	1:E:349:ARG:HD3	2.20	0.56
1:E:275:MET:SD	1:E:287:VAL:CG2	2.94	0.56
1:E:292:MET:O	1:E:295:GLY:N	2.37	0.56
1:G:275:MET:SD	1:G:287:VAL:CG2	2.93	0.56
1:H:312:HIS:NE2	1:H:317:TYR:HD2	2.03	0.56
1:I:182:LYS:NZ	1:I:349:ARG:HD3	2.20	0.56
1:L:317:TYR:HE1	1:L:334:LEU:HD22	1.69	0.56
1:B:254:ASP:OD1	1:B:254:ASP:N	2.36	0.56
1:G:119:LEU:HD22	1:G:124:ILE:HD11	1.88	0.56
1:I:257:LEU:O	1:I:259:LEU:HD13	2.04	0.56
1:I:317:TYR:OH	1:I:340:LEU:HD21	2.06	0.56
1:A:317:TYR:OH	1:A:340:LEU:HD21	2.06	0.56
1:D:290:GLU:O	1:D:293:ALA:HB3	2.04	0.56
1:E:332:ILE:HD12	1:E:333:GLN:N	2.20	0.56
1:F:257:LEU:O	1:F:259:LEU:HD13	2.04	0.56
1:H:173:ASN:HB2	1:H:284:PHE:HE1	1.71	0.56
1:L:317:TYR:OH	1:L:340:LEU:HD21	2.06	0.56
1:C:173:ASN:OD1	1:C:284:PHE:CD1	2.58	0.56
1:C:332:ILE:HD12	1:C:333:GLN:N	2.20	0.56
1:D:275:MET:SD	1:D:287:VAL:CG2	2.93	0.56
1:E:119:LEU:HD22	1:E:124:ILE:HD11	1.87	0.56
1:F:275:MET:SD	1:F:287:VAL:CG2	2.93	0.56
1:H:182:LYS:NZ	1:H:349:ARG:HD3	2.20	0.56
1:K:286:LEU:N	1:K:286:LEU:CD1	2.31	0.56
1:B:317:TYR:OH	1:B:340:LEU:HD21	2.06	0.56
1:C:317:TYR:OH	1:C:340:LEU:HD21	2.06	0.56
1:D:119:LEU:HD22	1:D:124:ILE:HD11	1.88	0.56
1:G:94:TYR:CZ	1:G:123:ASP:HB3	2.41	0.56
1:J:256:VAL:CG1	1:J:258:PHE:CE2	2.87	0.56
1:J:306:ILE:H	1:J:307:PRO:CD	2.18	0.56
1:B:275:MET:SD	1:B:287:VAL:CG2	2.93	0.56
1:C:286:LEU:N	1:C:286:LEU:CD1	2.31	0.56
1:E:306:ILE:H	1:E:307:PRO:CD	2.18	0.56
1:I:121:GLY:O	1:I:125:THR:OG1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:202:ILE:HD13	1:J:203:HIS:N	2.21	0.56
1:J:312:HIS:NE2	1:J:317:TYR:HD2	2.04	0.56
1:B:202:ILE:HD13	1:B:203:HIS:N	2.21	0.56
1:C:284:PHE:CD2	1:C:284:PHE:C	2.74	0.56
1:E:287:VAL:HG23	1:E:287:VAL:O	2.03	0.56
1:F:312:HIS:NE2	1:F:317:TYR:HD2	2.04	0.56
1:F:317:TYR:OH	1:F:340:LEU:HD21	2.06	0.56
1:H:292:MET:O	1:H:293:ALA:C	2.43	0.56
1:I:94:TYR:CZ	1:I:123:ASP:HB3	2.41	0.56
1:A:292:MET:O	1:A:293:ALA:C	2.42	0.55
1:B:177:GLU:HG3	1:B:357:ARG:NH1	2.22	0.55
1:B:312:HIS:NE2	1:B:317:TYR:HD2	2.04	0.55
1:E:121:GLY:O	1:E:125:THR:OG1	2.20	0.55
1:L:312:HIS:NE2	1:L:317:TYR:HD2	2.04	0.55
1:A:177:GLU:HG3	1:A:357:ARG:NH1	2.22	0.55
1:F:94:TYR:CZ	1:F:123:ASP:HB3	2.41	0.55
1:G:173:ASN:HB2	1:G:284:PHE:HE1	1.71	0.55
1:I:173:ASN:HB2	1:I:284:PHE:HE1	1.71	0.55
1:D:202:ILE:HD13	1:D:203:HIS:N	2.22	0.55
1:E:94:TYR:CZ	1:E:123:ASP:HB3	2.40	0.55
1:K:317:TYR:HE1	1:K:334:LEU:HD22	1.70	0.55
1:L:94:TYR:CZ	1:L:123:ASP:HB3	2.41	0.55
1:L:202:ILE:HD13	1:L:203:HIS:N	2.22	0.55
1:B:292:MET:O	1:B:293:ALA:C	2.42	0.55
1:C:94:TYR:CZ	1:C:123:ASP:HB3	2.41	0.55
1:C:177:GLU:HG3	1:C:357:ARG:NH1	2.22	0.55
1:C:275:MET:SD	1:C:287:VAL:CG2	2.94	0.55
1:F:119:LEU:HD22	1:F:124:ILE:HD11	1.88	0.55
1:F:177:GLU:HG3	1:F:357:ARG:NH1	2.22	0.55
1:G:317:TYR:OH	1:G:340:LEU:HD21	2.06	0.55
1:H:202:ILE:HD13	1:H:203:HIS:N	2.22	0.55
1:I:177:GLU:HG3	1:I:357:ARG:NH1	2.22	0.55
1:J:122:THR:HG22	1:J:126:VAL:HG11	1.89	0.55
1:K:275:MET:SD	1:K:287:VAL:CG2	2.94	0.55
1:K:287:VAL:O	1:K:287:VAL:HG23	2.04	0.55
1:A:173:ASN:HB2	1:A:284:PHE:HE1	1.72	0.55
1:A:202:ILE:HD13	1:A:203:HIS:N	2.22	0.55
1:C:306:ILE:H	1:C:307:PRO:CD	2.18	0.55
1:D:177:GLU:HG3	1:D:357:ARG:NH1	2.22	0.55
1:E:317:TYR:OH	1:E:340:LEU:HD21	2.06	0.55
1:F:292:MET:O	1:F:293:ALA:C	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:312:HIS:NE2	1:G:317:TYR:HD2	2.04	0.55
1:J:177:GLU:HG3	1:J:357:ARG:NH1	2.22	0.55
1:K:292:MET:O	1:K:293:ALA:C	2.42	0.55
1:A:94:TYR:CZ	1:A:123:ASP:HB3	2.41	0.55
1:B:121:GLY:O	1:B:125:THR:OG1	2.20	0.55
1:B:173:ASN:HB2	1:B:284:PHE:HE1	1.71	0.55
1:B:178:ARG:HA	1:B:178:ARG:NE	2.22	0.55
1:C:156:ASN:OD1	1:I:163:LYS:HA	2.06	0.55
1:D:122:THR:HG22	1:D:126:VAL:HG11	1.89	0.55
1:I:275:MET:SD	1:I:287:VAL:CG2	2.94	0.55
1:B:94:TYR:CZ	1:B:123:ASP:HB3	2.41	0.55
1:B:292:MET:O	1:B:295:GLY:N	2.36	0.55
1:D:317:TYR:OH	1:D:340:LEU:HD21	2.06	0.55
1:E:122:THR:HG22	1:E:126:VAL:HG11	1.89	0.55
1:H:122:THR:HG22	1:H:126:VAL:HG11	1.89	0.55
1:H:287:VAL:HG23	1:H:287:VAL:O	2.04	0.55
1:I:256:VAL:CG1	1:I:258:PHE:CE2	2.88	0.55
1:K:306:ILE:H	1:K:307:PRO:CD	2.19	0.55
1:L:177:GLU:HG3	1:L:357:ARG:NH1	2.22	0.55
1:L:312:HIS:C	1:L:312:HIS:CD2	2.80	0.55
1:A:119:LEU:HD22	1:A:124:ILE:HD11	1.88	0.55
1:D:94:TYR:CZ	1:D:123:ASP:HB3	2.41	0.55
1:E:284:PHE:HB3	1:E:285:GLY:CA	2.27	0.55
1:E:312:HIS:NE2	1:E:317:TYR:HD2	2.04	0.55
1:F:178:ARG:NE	1:F:178:ARG:HA	2.22	0.55
1:G:202:ILE:HD13	1:G:203:HIS:N	2.22	0.55
1:G:284:PHE:C	1:G:284:PHE:CD2	2.75	0.55
1:J:317:TYR:OH	1:J:340:LEU:HD21	2.07	0.55
1:B:119:LEU:HD22	1:B:124:ILE:HD11	1.88	0.55
1:C:178:ARG:NE	1:C:178:ARG:HA	2.22	0.55
1:E:177:GLU:HG3	1:E:357:ARG:NH1	2.22	0.55
1:H:178:ARG:NE	1:H:178:ARG:HA	2.22	0.55
1:L:178:ARG:NE	1:L:178:ARG:HA	2.22	0.55
1:A:173:ASN:OD1	1:A:284:PHE:HD1	1.91	0.54
1:D:312:HIS:NE2	1:D:317:TYR:HD2	2.04	0.54
1:E:202:ILE:HD13	1:E:203:HIS:N	2.22	0.54
1:G:254:ASP:OD1	1:G:254:ASP:N	2.36	0.54
1:I:119:LEU:HD22	1:I:124:ILE:HD11	1.88	0.54
1:I:178:ARG:NE	1:I:178:ARG:HA	2.23	0.54
1:I:202:ILE:HD13	1:I:203:HIS:N	2.22	0.54
1:K:312:HIS:NE2	1:K:317:TYR:HD2	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ASN:HB2	1:D:284:PHE:HE1	1.72	0.54
1:D:306:ILE:H	1:D:307:PRO:CD	2.19	0.54
1:F:173:ASN:HB2	1:F:284:PHE:HE1	1.72	0.54
1:J:178:ARG:HA	1:J:178:ARG:NE	2.22	0.54
1:K:281:LYS:CB	1:K:281:LYS:HZ3	2.19	0.54
1:K:284:PHE:C	1:K:284:PHE:CD2	2.75	0.54
1:L:119:LEU:HD22	1:L:124:ILE:HD11	1.88	0.54
1:L:292:MET:O	1:L:293:ALA:C	2.42	0.54
1:C:122:THR:HG22	1:C:126:VAL:HG11	1.89	0.54
1:C:173:ASN:HB2	1:C:284:PHE:HE1	1.71	0.54
1:G:122:THR:HG22	1:G:126:VAL:HG11	1.89	0.54
1:G:177:GLU:HG3	1:G:357:ARG:NH1	2.22	0.54
1:G:292:MET:O	1:G:293:ALA:C	2.42	0.54
1:L:173:ASN:HB2	1:L:284:PHE:HE1	1.73	0.54
1:C:119:LEU:HD22	1:C:124:ILE:HD11	1.88	0.54
1:C:202:ILE:HD13	1:C:203:HIS:N	2.22	0.54
1:G:178:ARG:NE	1:G:178:ARG:HA	2.22	0.54
1:H:177:GLU:HG3	1:H:357:ARG:NH1	2.22	0.54
1:I:284:PHE:C	1:I:284:PHE:CD2	2.76	0.54
1:A:287:VAL:O	1:A:287:VAL:HG23	2.03	0.54
1:D:178:ARG:NE	1:D:178:ARG:HA	2.22	0.54
1:E:178:ARG:HA	1:E:178:ARG:NE	2.22	0.54
1:F:122:THR:HG22	1:F:126:VAL:HG11	1.89	0.54
1:H:317:TYR:OH	1:H:340:LEU:HD21	2.06	0.54
1:J:275:MET:SD	1:J:287:VAL:CG2	2.96	0.54
1:J:284:PHE:C	1:J:284:PHE:CD2	2.77	0.54
1:L:254:ASP:OD1	1:L:254:ASP:N	2.36	0.54
1:B:287:VAL:HG23	1:B:287:VAL:O	2.04	0.54
1:D:286:LEU:N	1:D:286:LEU:CD1	2.31	0.54
1:I:349:ARG:HH11	1:I:349:ARG:CB	2.19	0.54
1:J:94:TYR:CZ	1:J:123:ASP:HB3	2.41	0.54
1:K:306:ILE:O	1:K:309:VAL:HG22	2.08	0.54
1:A:349:ARG:HH11	1:A:349:ARG:CB	2.19	0.54
1:F:256:VAL:O	1:F:256:VAL:HG12	1.97	0.54
1:K:119:LEU:HD22	1:K:124:ILE:HD11	1.88	0.54
1:L:122:THR:HG22	1:L:126:VAL:HG11	1.89	0.54
1:A:312:HIS:NE2	1:A:317:TYR:HD2	2.05	0.54
1:G:156:ASN:OD1	1:L:152:HIS:ND1	2.41	0.54
1:H:121:GLY:O	1:H:125:THR:OG1	2.19	0.54
1:H:223:ILE:O	1:H:223:ILE:HD13	2.08	0.54
1:J:173:ASN:HB2	1:J:284:PHE:HE1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:254:ASP:OD1	1:J:254:ASP:N	2.37	0.54
1:B:284:PHE:C	1:B:284:PHE:CD2	2.76	0.54
1:D:223:ILE:HD13	1:D:223:ILE:O	2.08	0.54
1:F:202:ILE:HD13	1:F:203:HIS:N	2.22	0.54
1:F:223:ILE:O	1:F:223:ILE:HD13	2.08	0.54
1:G:292:MET:O	1:G:295:GLY:N	2.36	0.54
1:K:139:PHE:O	1:K:143:GLN:HG2	2.08	0.54
1:K:178:ARG:NE	1:K:178:ARG:HA	2.22	0.54
1:A:223:ILE:O	1:A:223:ILE:HD13	2.08	0.54
1:D:121:GLY:O	1:D:125:THR:OG1	2.20	0.54
1:I:223:ILE:O	1:I:223:ILE:HD13	2.08	0.54
1:K:317:TYR:OH	1:K:340:LEU:HD21	2.08	0.54
1:L:284:PHE:C	1:L:284:PHE:CD2	2.76	0.54
1:A:178:ARG:NE	1:A:178:ARG:HA	2.22	0.53
1:C:292:MET:O	1:C:295:GLY:N	2.37	0.53
1:J:119:LEU:HD22	1:J:124:ILE:HD11	1.89	0.53
1:K:94:TYR:CZ	1:K:123:ASP:HB3	2.42	0.53
1:L:173:ASN:OD1	1:L:284:PHE:HD1	1.90	0.53
1:L:223:ILE:HD13	1:L:223:ILE:O	2.08	0.53
1:F:292:MET:O	1:F:295:GLY:N	2.37	0.53
1:G:223:ILE:HD13	1:G:223:ILE:O	2.08	0.53
1:H:312:HIS:CD2	1:H:312:HIS:C	2.81	0.53
1:K:173:ASN:HB2	1:K:284:PHE:HE1	1.74	0.53
1:K:364:GLN:O	1:K:368:ILE:HG13	2.09	0.53
1:A:312:HIS:C	1:A:312:HIS:CD2	2.80	0.53
1:C:223:ILE:O	1:C:223:ILE:HD13	2.08	0.53
1:J:246:LEU:O	1:J:250:LEU:HB2	2.09	0.53
1:K:202:ILE:HD13	1:K:203:HIS:N	2.22	0.53
1:B:122:THR:HG22	1:B:126:VAL:HG11	1.89	0.53
1:B:223:ILE:O	1:B:223:ILE:HD13	2.08	0.53
1:E:312:HIS:C	1:E:312:HIS:CD2	2.81	0.53
1:J:223:ILE:O	1:J:223:ILE:HD13	2.09	0.53
1:I:312:HIS:C	1:I:312:HIS:CD2	2.81	0.53
1:J:312:HIS:C	1:J:312:HIS:CD2	2.81	0.53
1:L:292:MET:O	1:L:295:GLY:N	2.37	0.53
1:A:182:LYS:HZ1	1:A:349:ARG:HD3	1.73	0.53
1:C:312:HIS:C	1:C:312:HIS:CD2	2.81	0.53
1:C:349:ARG:HH11	1:C:349:ARG:CB	2.19	0.53
1:F:284:PHE:C	1:F:284:PHE:CD2	2.75	0.53
1:F:349:ARG:HH11	1:F:349:ARG:CB	2.19	0.53
1:J:349:ARG:HH11	1:J:349:ARG:CB	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:LEU:O	1:C:259:LEU:HD12	2.09	0.53
1:D:292:MET:O	1:D:295:GLY:N	2.37	0.53
1:G:286:LEU:CD1	1:G:286:LEU:N	2.31	0.53
1:K:122:THR:HG22	1:K:126:VAL:HG11	1.90	0.53
1:K:257:LEU:O	1:K:259:LEU:HD12	2.09	0.53
1:L:182:LYS:HZ1	1:L:349:ARG:HD3	1.73	0.53
1:L:287:VAL:HG23	1:L:287:VAL:O	2.04	0.53
1:A:139:PHE:O	1:A:143:GLN:HG2	2.09	0.53
1:B:246:LEU:O	1:B:250:LEU:HB2	2.09	0.53
1:B:312:HIS:C	1:B:312:HIS:CD2	2.81	0.53
1:H:257:LEU:O	1:H:259:LEU:HD12	2.09	0.53
1:B:281:LYS:CB	1:B:281:LYS:HZ3	2.22	0.53
1:C:306:ILE:O	1:C:309:VAL:HG22	2.09	0.53
1:D:312:HIS:C	1:D:312:HIS:CD2	2.81	0.53
1:F:246:LEU:O	1:F:250:LEU:HB2	2.09	0.53
1:H:256:VAL:O	1:H:256:VAL:HG12	1.97	0.53
1:H:364:GLN:O	1:H:368:ILE:HG13	2.09	0.53
1:A:189:LYS:O	1:A:194:ILE:HG22	2.09	0.53
1:E:189:LYS:O	1:E:194:ILE:HG22	2.09	0.53
1:E:364:GLN:O	1:E:368:ILE:HG13	2.09	0.53
1:F:173:ASN:OD1	1:F:284:PHE:HD1	1.91	0.53
1:J:306:ILE:O	1:J:309:VAL:HG22	2.09	0.53
1:A:364:GLN:O	1:A:368:ILE:HG13	2.09	0.52
1:E:257:LEU:O	1:E:259:LEU:HD12	2.09	0.52
1:H:139:PHE:O	1:H:143:GLN:HG2	2.10	0.52
1:A:284:PHE:C	1:A:284:PHE:CD2	2.76	0.52
1:B:257:LEU:O	1:B:259:LEU:HD12	2.09	0.52
1:D:306:ILE:O	1:D:309:VAL:HG22	2.10	0.52
1:E:338:GLU:HG2	1:E:338:GLU:O	2.10	0.52
1:G:189:LYS:O	1:G:194:ILE:HG22	2.09	0.52
1:I:246:LEU:O	1:I:250:LEU:HB2	2.09	0.52
1:I:281:LYS:NZ	1:I:281:LYS:HB2	2.25	0.52
1:I:306:ILE:O	1:I:309:VAL:HG22	2.10	0.52
1:C:189:LYS:O	1:C:194:ILE:HG22	2.09	0.52
1:E:246:LEU:O	1:E:250:LEU:HB2	2.09	0.52
1:G:139:PHE:O	1:G:143:GLN:HG2	2.10	0.52
1:G:312:HIS:C	1:G:312:HIS:CD2	2.82	0.52
1:G:338:GLU:HG2	1:G:338:GLU:O	2.09	0.52
1:H:254:ASP:OD1	1:H:254:ASP:N	2.36	0.52
1:J:199:LYS:HB2	1:J:229:ALA:CB	2.34	0.52
1:J:257:LEU:O	1:J:259:LEU:HD12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:364:GLN:O	1:J:368:ILE:HG13	2.10	0.52
1:K:223:ILE:O	1:K:223:ILE:HD13	2.08	0.52
1:A:122:THR:HG22	1:A:126:VAL:HG11	1.90	0.52
1:A:246:LEU:O	1:A:250:LEU:HB2	2.09	0.52
1:A:254:ASP:OD1	1:A:254:ASP:N	2.36	0.52
1:B:139:PHE:O	1:B:143:GLN:HG2	2.09	0.52
1:D:281:LYS:NZ	1:D:281:LYS:HB2	2.25	0.52
1:F:364:GLN:O	1:F:368:ILE:HG13	2.10	0.52
1:G:364:GLN:O	1:G:368:ILE:HG13	2.09	0.52
1:H:292:MET:O	1:H:295:GLY:N	2.37	0.52
1:I:257:LEU:O	1:I:259:LEU:HD12	2.09	0.52
1:J:338:GLU:HG2	1:J:338:GLU:O	2.09	0.52
1:K:189:LYS:O	1:K:194:ILE:HG22	2.10	0.52
1:A:292:MET:O	1:A:295:GLY:N	2.37	0.52
1:E:281:LYS:NZ	1:E:281:LYS:HB2	2.25	0.52
1:F:189:LYS:O	1:F:194:ILE:HG22	2.09	0.52
1:G:246:LEU:O	1:G:250:LEU:HB2	2.09	0.52
1:G:306:ILE:O	1:G:309:VAL:HG22	2.10	0.52
1:H:94:TYR:CZ	1:H:123:ASP:N	2.78	0.52
1:H:120:HIS:O	1:H:123:ASP:OD1	2.28	0.52
1:L:349:ARG:HH11	1:L:349:ARG:CB	2.19	0.52
1:B:199:LYS:HB2	1:B:229:ALA:CB	2.35	0.52
1:C:246:LEU:O	1:C:250:LEU:HB2	2.10	0.52
1:C:281:LYS:NZ	1:C:281:LYS:HB2	2.25	0.52
1:E:139:PHE:O	1:E:143:GLN:HG2	2.09	0.52
1:E:349:ARG:HH11	1:E:349:ARG:CB	2.19	0.52
1:F:254:ASP:OD1	1:F:254:ASP:N	2.36	0.52
1:H:189:LYS:O	1:H:194:ILE:HG22	2.09	0.52
1:H:281:LYS:CB	1:H:281:LYS:HZ3	2.22	0.52
1:I:122:THR:HG22	1:I:126:VAL:HG11	1.89	0.52
1:J:254:ASP:OD1	1:J:255:ARG:HG3	2.10	0.52
1:L:139:PHE:O	1:L:143:GLN:HG2	2.10	0.52
1:C:120:HIS:O	1:C:123:ASP:OD1	2.28	0.52
1:C:254:ASP:OD1	1:C:254:ASP:N	2.36	0.52
1:C:338:GLU:O	1:C:338:GLU:HG2	2.09	0.52
1:D:246:LEU:O	1:D:250:LEU:HB2	2.09	0.52
1:F:257:LEU:O	1:F:259:LEU:HD12	2.09	0.52
1:G:94:TYR:CZ	1:G:123:ASP:N	2.78	0.52
1:H:25:LYS:HE2	1:H:49:TYR:OH	2.10	0.52
1:H:349:ARG:HH11	1:H:349:ARG:CB	2.19	0.52
1:K:281:LYS:NZ	1:K:281:LYS:HB2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:312:HIS:C	1:K:312:HIS:CD2	2.81	0.52
1:L:246:LEU:O	1:L:250:LEU:HB2	2.09	0.52
1:L:364:GLN:O	1:L:368:ILE:HG13	2.09	0.52
1:A:25:LYS:HE2	1:A:49:TYR:OH	2.10	0.52
1:C:223:ILE:HD11	1:C:335:LEU:CD1	2.40	0.52
1:D:139:PHE:O	1:D:143:GLN:HG2	2.09	0.52
1:E:94:TYR:CZ	1:E:123:ASP:N	2.78	0.52
1:I:139:PHE:O	1:I:143:GLN:HG2	2.10	0.52
1:K:223:ILE:HD11	1:K:335:LEU:CD1	2.40	0.52
1:K:246:LEU:O	1:K:250:LEU:HB2	2.10	0.52
1:L:189:LYS:O	1:L:194:ILE:HG22	2.09	0.52
1:A:120:HIS:O	1:A:123:ASP:OD1	2.28	0.52
1:D:94:TYR:CZ	1:D:123:ASP:N	2.78	0.52
1:D:364:GLN:O	1:D:368:ILE:HG13	2.10	0.52
1:E:120:HIS:O	1:E:123:ASP:OD1	2.28	0.52
1:E:223:ILE:O	1:E:223:ILE:HD13	2.09	0.52
1:F:120:HIS:O	1:F:123:ASP:OD1	2.28	0.52
1:G:120:HIS:O	1:G:123:ASP:OD1	2.28	0.52
1:H:246:LEU:O	1:H:250:LEU:HB2	2.09	0.52
1:K:338:GLU:O	1:K:338:GLU:HG2	2.10	0.52
1:L:306:ILE:O	1:L:309:VAL:HG22	2.10	0.52
1:A:212:ARG:HH11	1:A:212:ARG:HG3	1.75	0.52
1:A:257:LEU:O	1:A:259:LEU:HD12	2.09	0.52
1:B:25:LYS:HE2	1:B:49:TYR:OH	2.10	0.52
1:C:212:ARG:HH11	1:C:212:ARG:HG3	1.75	0.52
1:C:364:GLN:O	1:C:368:ILE:HG13	2.10	0.52
1:D:257:LEU:O	1:D:259:LEU:HD12	2.10	0.52
1:D:349:ARG:HH11	1:D:349:ARG:CB	2.19	0.52
1:E:212:ARG:HH11	1:E:212:ARG:HG3	1.75	0.52
1:E:281:LYS:CB	1:E:281:LYS:HZ3	2.23	0.52
1:F:139:PHE:O	1:F:143:GLN:HG2	2.10	0.52
1:L:281:LYS:NZ	1:L:281:LYS:HB2	2.25	0.52
1:A:223:ILE:HD11	1:A:335:LEU:CD1	2.40	0.51
1:B:338:GLU:HG2	1:B:338:GLU:O	2.09	0.51
1:D:189:LYS:O	1:D:194:ILE:HG22	2.09	0.51
1:F:121:GLY:O	1:F:125:THR:OG1	2.21	0.51
1:F:338:GLU:O	1:F:338:GLU:HG2	2.09	0.51
1:G:281:LYS:NZ	1:G:281:LYS:HB2	2.25	0.51
1:H:338:GLU:HG2	1:H:338:GLU:O	2.09	0.51
1:J:182:LYS:HZ1	1:J:349:ARG:HD3	1.75	0.51
1:J:292:MET:O	1:J:295:GLY:N	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:NZ	1:A:281:LYS:HB2	2.25	0.51
1:A:306:ILE:O	1:A:309:VAL:HG22	2.10	0.51
1:B:94:TYR:CZ	1:B:123:ASP:N	2.78	0.51
1:B:349:ARG:HH11	1:B:349:ARG:CB	2.19	0.51
1:C:94:TYR:CZ	1:C:123:ASP:N	2.79	0.51
1:D:284:PHE:C	1:D:284:PHE:CD2	2.75	0.51
1:G:25:LYS:HE2	1:G:49:TYR:OH	2.10	0.51
1:I:94:TYR:CZ	1:I:123:ASP:N	2.79	0.51
1:A:338:GLU:O	1:A:338:GLU:HG2	2.10	0.51
1:F:25:LYS:HE2	1:F:49:TYR:OH	2.10	0.51
1:F:281:LYS:NZ	1:F:281:LYS:HB2	2.25	0.51
1:G:257:LEU:O	1:G:259:LEU:HD12	2.10	0.51
1:H:212:ARG:HH11	1:H:212:ARG:HG3	1.76	0.51
1:I:120:HIS:O	1:I:123:ASP:OD1	2.28	0.51
1:J:94:TYR:CZ	1:J:123:ASP:N	2.78	0.51
1:K:94:TYR:CZ	1:K:123:ASP:N	2.78	0.51
1:L:94:TYR:CZ	1:L:123:ASP:N	2.78	0.51
1:L:223:ILE:HD11	1:L:335:LEU:CD1	2.41	0.51
1:L:338:GLU:O	1:L:338:GLU:HG2	2.09	0.51
1:A:281:LYS:CB	1:A:281:LYS:HZ3	2.21	0.51
1:B:120:HIS:O	1:B:123:ASP:OD1	2.28	0.51
1:B:223:ILE:HD11	1:B:335:LEU:CD1	2.40	0.51
1:B:306:ILE:O	1:B:309:VAL:HG22	2.09	0.51
1:G:212:ARG:HG3	1:G:212:ARG:HH11	1.76	0.51
1:J:281:LYS:NZ	1:J:281:LYS:HB2	2.25	0.51
1:B:281:LYS:NZ	1:B:281:LYS:HB2	2.25	0.51
1:B:364:GLN:O	1:B:368:ILE:HG13	2.09	0.51
1:E:223:ILE:HD11	1:E:335:LEU:CD1	2.40	0.51
1:F:94:TYR:CZ	1:F:123:ASP:N	2.78	0.51
1:I:50:PRO:CG	1:K:191:GLU:HG2	2.32	0.51
1:I:223:ILE:HD11	1:I:335:LEU:CD1	2.40	0.51
1:J:189:LYS:O	1:J:194:ILE:HG22	2.10	0.51
1:J:223:ILE:HD11	1:J:335:LEU:CD1	2.41	0.51
1:K:349:ARG:HH11	1:K:349:ARG:CB	2.19	0.51
1:L:281:LYS:CB	1:L:281:LYS:HZ3	2.22	0.51
1:B:189:LYS:O	1:B:194:ILE:HG22	2.09	0.51
1:E:284:PHE:C	1:E:284:PHE:CD2	2.74	0.51
1:H:306:ILE:O	1:H:309:VAL:HG22	2.09	0.51
1:I:25:LYS:HE2	1:I:49:TYR:OH	2.10	0.51
1:I:189:LYS:O	1:I:194:ILE:HG22	2.09	0.51
1:K:292:MET:O	1:K:295:GLY:N	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:25:LYS:HE2	1:L:49:TYR:OH	2.10	0.51
1:D:25:LYS:HE2	1:D:49:TYR:OH	2.10	0.51
1:D:199:LYS:HB2	1:D:229:ALA:CB	2.35	0.51
1:D:338:GLU:O	1:D:338:GLU:HG2	2.09	0.51
1:E:25:LYS:HE2	1:E:49:TYR:OH	2.10	0.51
1:F:306:ILE:O	1:F:309:VAL:HG22	2.10	0.51
1:F:312:HIS:C	1:F:312:HIS:CD2	2.81	0.51
1:I:183:ARG:NH1	1:I:185:MET:SD	2.84	0.51
1:I:338:GLU:O	1:I:338:GLU:HG2	2.09	0.51
1:I:364:GLN:O	1:I:368:ILE:HG13	2.10	0.51
1:J:139:PHE:O	1:J:143:GLN:HG2	2.10	0.51
1:G:121:GLY:O	1:G:125:THR:OG1	2.19	0.51
1:I:292:MET:O	1:I:295:GLY:N	2.37	0.51
1:K:121:GLY:O	1:K:125:THR:OG1	2.18	0.51
1:K:212:ARG:HH11	1:K:212:ARG:HG3	1.76	0.51
1:L:257:LEU:O	1:L:259:LEU:HD12	2.10	0.51
1:C:25:LYS:HE2	1:C:49:TYR:OH	2.10	0.51
1:C:254:ASP:OD1	1:C:255:ARG:HG3	2.11	0.51
1:F:202:ILE:HG21	1:F:269:LEU:HD23	1.93	0.51
1:F:281:LYS:CB	1:F:281:LYS:HZ3	2.24	0.51
1:H:281:LYS:NZ	1:H:281:LYS:HB2	2.24	0.51
1:K:25:LYS:HE2	1:K:49:TYR:OH	2.11	0.51
1:B:267:GLU:OE1	1:D:48:VAL:HG12	2.11	0.51
1:F:223:ILE:HD11	1:F:335:LEU:CD1	2.40	0.51
1:H:202:ILE:HG21	1:H:269:LEU:HD23	1.93	0.51
1:I:199:LYS:HB2	1:I:229:ALA:CB	2.35	0.51
1:C:183:ARG:NH1	1:C:185:MET:SD	2.84	0.50
1:E:306:ILE:O	1:E:309:VAL:HG22	2.10	0.50
1:F:254:ASP:OD1	1:F:255:ARG:HG3	2.11	0.50
1:G:182:LYS:HZ1	1:G:349:ARG:HD3	1.77	0.50
1:G:183:ARG:NH1	1:G:185:MET:SD	2.85	0.50
1:G:202:ILE:HG21	1:G:269:LEU:HD23	1.93	0.50
1:H:223:ILE:HD11	1:H:335:LEU:CD1	2.40	0.50
1:K:120:HIS:O	1:K:123:ASP:OD1	2.29	0.50
1:K:254:ASP:OD1	1:K:254:ASP:N	2.36	0.50
1:F:212:ARG:HH11	1:F:212:ARG:HG3	1.76	0.50
1:G:254:ASP:OD1	1:G:255:ARG:HG3	2.11	0.50
1:H:183:ARG:NH1	1:H:185:MET:SD	2.84	0.50
1:J:120:HIS:O	1:J:123:ASP:OD1	2.29	0.50
1:J:281:LYS:O	1:J:282:GLU:CB	2.58	0.50
1:L:254:ASP:OD1	1:L:255:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:TYR:CZ	1:A:123:ASP:N	2.78	0.50
1:D:212:ARG:HG3	1:D:212:ARG:HH11	1.76	0.50
1:E:254:ASP:OD1	1:E:255:ARG:HG3	2.11	0.50
1:G:136:LEU:HD21	1:H:72:LEU:HB3	1.93	0.50
1:I:254:ASP:OD1	1:I:254:ASP:N	2.36	0.50
1:L:183:ARG:NH1	1:L:185:MET:SD	2.84	0.50
1:B:254:ASP:OD1	1:B:255:ARG:HG3	2.11	0.50
1:G:223:ILE:HD11	1:G:335:LEU:CD1	2.41	0.50
1:I:50:PRO:HG2	1:K:191:GLU:CG	2.30	0.50
1:L:284:PHE:CB	1:L:285:GLY:HA2	2.32	0.50
1:C:139:PHE:O	1:C:143:GLN:HG2	2.10	0.50
1:C:202:ILE:HG21	1:C:269:LEU:HD23	1.93	0.50
1:D:183:ARG:NH1	1:D:185:MET:SD	2.85	0.50
1:D:254:ASP:OD1	1:D:255:ARG:HG3	2.11	0.50
1:I:202:ILE:HG21	1:I:269:LEU:HD23	1.93	0.50
1:K:254:ASP:OD1	1:K:255:ARG:HG3	2.11	0.50
1:A:254:ASP:OD1	1:A:255:ARG:HG3	2.11	0.50
1:B:202:ILE:HG21	1:B:269:LEU:HD23	1.93	0.50
1:B:212:ARG:HH11	1:B:212:ARG:HG3	1.75	0.50
1:D:173:ASN:OD1	1:D:284:PHE:HD1	1.93	0.50
1:H:254:ASP:OD1	1:H:255:ARG:HG3	2.11	0.50
1:I:191:GLU:HG2	1:K:50:PRO:HG2	1.94	0.50
1:K:183:ARG:NH1	1:K:185:MET:SD	2.84	0.50
1:A:183:ARG:NH1	1:A:185:MET:SD	2.85	0.50
1:E:183:ARG:NH1	1:E:185:MET:SD	2.85	0.50
1:K:202:ILE:HG21	1:K:269:LEU:HD23	1.93	0.50
1:L:120:HIS:O	1:L:123:ASP:OD1	2.29	0.50
1:G:97:PRO:HB3	1:H:72:LEU:CD2	2.42	0.50
1:K:284:PHE:CB	1:K:285:GLY:HA2	2.33	0.50
1:A:202:ILE:HG21	1:A:269:LEU:HD23	1.93	0.49
1:D:202:ILE:HG21	1:D:269:LEU:HD23	1.93	0.49
1:E:254:ASP:OD1	1:E:254:ASP:N	2.36	0.49
1:D:120:HIS:O	1:D:123:ASP:OD1	2.29	0.49
1:K:182:LYS:HZ2	1:K:349:ARG:CD	2.25	0.49
1:B:183:ARG:NH1	1:B:185:MET:SD	2.84	0.49
1:D:182:LYS:HZ1	1:D:349:ARG:HD3	1.78	0.49
1:E:202:ILE:HG21	1:E:269:LEU:HD23	1.93	0.49
1:I:212:ARG:HH11	1:I:212:ARG:HG3	1.76	0.49
1:I:254:ASP:OD1	1:I:255:ARG:HG3	2.11	0.49
1:J:173:ASN:OD1	1:J:284:PHE:HD1	1.94	0.49
1:J:183:ARG:NH1	1:J:185:MET:SD	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:212:ARG:HH11	1:J:212:ARG:HG3	1.76	0.49
1:K:223:ILE:HG12	1:K:332:ILE:HG23	1.94	0.49
1:B:173:ASN:OD1	1:B:284:PHE:HD1	1.93	0.49
1:K:123:ASP:O	1:K:127:LEU:HB2	2.12	0.49
1:L:202:ILE:HG21	1:L:269:LEU:HD23	1.93	0.49
1:L:212:ARG:HG3	1:L:212:ARG:HH11	1.75	0.49
1:G:349:ARG:HH11	1:G:349:ARG:CB	2.18	0.49
1:F:223:ILE:HG12	1:F:332:ILE:HG23	1.95	0.49
1:H:123:ASP:O	1:H:127:LEU:HB2	2.12	0.49
1:J:202:ILE:HG21	1:J:269:LEU:HD23	1.94	0.49
1:J:286:LEU:N	1:J:286:LEU:CD1	2.32	0.49
1:D:223:ILE:HD11	1:D:335:LEU:CD1	2.40	0.49
1:F:183:ARG:NH1	1:F:185:MET:SD	2.85	0.49
1:G:123:ASP:O	1:G:127:LEU:HB2	2.13	0.49
1:J:25:LYS:HE2	1:J:49:TYR:OH	2.11	0.49
1:J:123:ASP:O	1:J:127:LEU:HB2	2.13	0.49
1:L:281:LYS:O	1:L:282:GLU:CB	2.57	0.49
1:B:201:LEU:O	1:B:231:LEU:HD12	2.13	0.49
1:C:163:LYS:HA	1:I:156:ASN:OD1	2.12	0.49
1:G:223:ILE:HG12	1:G:332:ILE:HG23	1.95	0.49
1:H:173:ASN:OD1	1:H:284:PHE:HD1	1.96	0.49
1:A:312:HIS:HD2	1:A:313:GLY:N	2.11	0.49
1:C:201:LEU:O	1:C:231:LEU:HD12	2.13	0.49
1:C:363:SER:O	1:C:367:THR:HG23	2.13	0.49
1:D:312:HIS:HD2	1:D:313:GLY:N	2.11	0.49
1:E:123:ASP:O	1:E:127:LEU:HB2	2.13	0.49
1:E:223:ILE:HG12	1:E:332:ILE:HG23	1.95	0.49
1:I:173:ASN:OD1	1:I:284:PHE:HD1	1.95	0.49
1:J:281:LYS:CB	1:J:281:LYS:HZ3	2.25	0.49
1:B:363:SER:O	1:B:367:THR:HG23	2.13	0.49
1:C:123:ASP:O	1:C:127:LEU:HB2	2.13	0.49
1:D:281:LYS:CB	1:D:281:LYS:HZ3	2.26	0.49
1:I:312:HIS:HD2	1:I:313:GLY:N	2.11	0.49
1:J:121:GLY:O	1:J:125:THR:OG1	2.19	0.49
1:A:201:LEU:O	1:A:231:LEU:HD12	2.13	0.48
1:B:223:ILE:HG12	1:B:332:ILE:HG23	1.94	0.48
1:D:123:ASP:O	1:D:127:LEU:HB2	2.13	0.48
1:D:223:ILE:HG12	1:D:332:ILE:HG23	1.94	0.48
1:H:113:ILE:HD13	1:H:114:LYS:N	2.28	0.48
1:I:123:ASP:O	1:I:127:LEU:HB2	2.13	0.48
1:L:201:LEU:O	1:L:231:LEU:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:281:LYS:HA	1:L:303:VAL:CG1	2.32	0.48
1:L:312:HIS:HD2	1:L:313:GLY:N	2.10	0.48
1:A:123:ASP:O	1:A:127:LEU:HB2	2.13	0.48
1:B:123:ASP:O	1:B:127:LEU:HB2	2.13	0.48
1:C:312:HIS:HD2	1:C:313:GLY:N	2.11	0.48
1:G:363:SER:O	1:G:367:THR:HG23	2.13	0.48
1:H:363:SER:O	1:H:367:THR:HG23	2.13	0.48
1:I:122:THR:HG22	1:I:126:VAL:HG12	1.95	0.48
1:J:281:LYS:HA	1:J:303:VAL:CG1	2.32	0.48
1:K:173:ASN:OD1	1:K:284:PHE:HD1	1.96	0.48
1:A:65:PHE:HZ	1:B:96:ILE:CG2	2.26	0.48
1:B:182:LYS:HZ2	1:B:349:ARG:CD	2.26	0.48
1:E:363:SER:O	1:E:367:THR:HG23	2.13	0.48
1:H:223:ILE:HG12	1:H:332:ILE:HG23	1.95	0.48
1:I:201:LEU:O	1:I:231:LEU:HD12	2.14	0.48
1:J:89:ILE:HD11	1:J:373:LEU:HD11	1.95	0.48
1:D:122:THR:HG22	1:D:126:VAL:HG12	1.95	0.48
1:F:122:THR:HG22	1:F:126:VAL:HG12	1.95	0.48
1:I:182:LYS:HZ1	1:I:349:ARG:HD3	1.78	0.48
1:E:122:THR:HG22	1:E:126:VAL:HG12	1.95	0.48
1:H:201:LEU:O	1:H:231:LEU:HD12	2.13	0.48
1:I:223:ILE:HG12	1:I:332:ILE:HG23	1.95	0.48
1:I:363:SER:O	1:I:367:THR:HG23	2.14	0.48
1:K:89:ILE:HD11	1:K:373:LEU:HD11	1.95	0.48
1:B:312:HIS:HD2	1:B:313:GLY:N	2.11	0.48
1:D:113:ILE:HD13	1:D:114:LYS:N	2.29	0.48
1:H:312:HIS:HD2	1:H:313:GLY:N	2.11	0.48
1:J:223:ILE:HG12	1:J:332:ILE:HG23	1.95	0.48
1:J:312:HIS:HD2	1:J:313:GLY:N	2.12	0.48
1:L:363:SER:O	1:L:367:THR:HG23	2.14	0.48
1:A:199:LYS:HB2	1:A:229:ALA:CB	2.35	0.48
1:C:223:ILE:HG12	1:C:332:ILE:HG23	1.95	0.48
1:K:139:PHE:CG	1:L:108:MET:HG2	2.49	0.48
1:K:257:LEU:N	1:K:257:LEU:HD13	2.28	0.48
1:K:261:LYS:HG3	1:K:261:LYS:O	2.14	0.48
1:L:199:LYS:HB2	1:L:229:ALA:CB	2.35	0.48
1:B:89:ILE:HD11	1:B:373:LEU:HD11	1.96	0.48
1:C:113:ILE:HD13	1:C:114:LYS:N	2.29	0.48
1:G:312:HIS:HD2	1:G:313:GLY:N	2.12	0.48
1:I:89:ILE:HD11	1:I:373:LEU:HD11	1.96	0.48
1:K:201:LEU:O	1:K:231:LEU:HD12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HG12	1:A:332:ILE:HG23	1.95	0.48
1:B:281:LYS:O	1:B:282:GLU:CB	2.57	0.48
1:C:287:VAL:HG22	1:C:288:LEU:N	2.29	0.48
1:E:288:LEU:HA	1:E:288:LEU:HD23	1.62	0.48
1:F:123:ASP:O	1:F:127:LEU:HB2	2.13	0.48
1:F:201:LEU:O	1:F:231:LEU:HD12	2.13	0.48
1:I:113:ILE:HD13	1:I:114:LYS:N	2.29	0.48
1:L:122:THR:HG22	1:L:126:VAL:HG12	1.95	0.48
1:L:123:ASP:O	1:L:127:LEU:HB2	2.13	0.48
1:C:122:THR:HG22	1:C:126:VAL:HG12	1.95	0.48
1:D:89:ILE:HD11	1:D:373:LEU:HD11	1.96	0.48
1:D:201:LEU:O	1:D:231:LEU:HD12	2.14	0.48
1:F:113:ILE:HD13	1:F:114:LYS:N	2.29	0.48
1:G:122:THR:HG22	1:G:126:VAL:HG12	1.95	0.48
1:G:173:ASN:HB2	1:G:284:PHE:CE1	2.49	0.48
1:G:284:PHE:CB	1:G:285:GLY:HA2	2.31	0.48
1:J:363:SER:O	1:J:367:THR:HG23	2.14	0.48
1:B:173:ASN:HB2	1:B:284:PHE:CE1	2.49	0.47
1:G:173:ASN:OD1	1:G:284:PHE:HD1	1.95	0.47
1:I:173:ASN:HB2	1:I:284:PHE:CE1	2.49	0.47
1:J:122:THR:HG22	1:J:126:VAL:HG12	1.95	0.47
1:L:89:ILE:HD11	1:L:373:LEU:HD11	1.96	0.47
1:A:113:ILE:HD13	1:A:114:LYS:N	2.29	0.47
1:E:89:ILE:HD11	1:E:373:LEU:HD11	1.96	0.47
1:L:223:ILE:HG12	1:L:332:ILE:HG23	1.95	0.47
1:A:287:VAL:HG22	1:A:288:LEU:N	2.29	0.47
1:B:122:THR:HG22	1:B:126:VAL:HG12	1.95	0.47
1:E:199:LYS:HB2	1:E:229:ALA:CB	2.34	0.47
1:E:257:LEU:N	1:E:257:LEU:HD13	2.28	0.47
1:E:312:HIS:HD2	1:E:313:GLY:N	2.11	0.47
1:G:89:ILE:HD11	1:G:373:LEU:HD11	1.96	0.47
1:A:261:LYS:O	1:A:261:LYS:HG3	2.15	0.47
1:G:287:VAL:HG22	1:G:288:LEU:N	2.29	0.47
1:I:281:LYS:HA	1:I:303:VAL:CG1	2.31	0.47
1:A:89:ILE:HD11	1:A:373:LEU:HD11	1.96	0.47
1:A:363:SER:O	1:A:367:THR:HG23	2.13	0.47
1:E:113:ILE:HD13	1:E:114:LYS:N	2.29	0.47
1:B:113:ILE:HD13	1:B:114:LYS:N	2.28	0.47
1:C:199:LYS:HB2	1:C:229:ALA:CB	2.35	0.47
1:D:363:SER:O	1:D:367:THR:HG23	2.13	0.47
1:F:173:ASN:HB2	1:F:284:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:LYS:HG3	1:G:261:LYS:O	2.15	0.47
1:H:199:LYS:HB2	1:H:229:ALA:CB	2.34	0.47
1:H:281:LYS:O	1:H:282:GLU:CB	2.57	0.47
1:C:173:ASN:HB2	1:C:284:PHE:CE1	2.49	0.47
1:C:257:LEU:N	1:C:257:LEU:HD13	2.28	0.47
1:E:201:LEU:O	1:E:231:LEU:HD12	2.13	0.47
1:F:89:ILE:HD11	1:F:373:LEU:HD11	1.96	0.47
1:F:312:HIS:HD2	1:F:313:GLY:N	2.12	0.47
1:G:201:LEU:O	1:G:231:LEU:HD12	2.14	0.47
1:J:201:LEU:O	1:J:231:LEU:HD12	2.14	0.47
1:D:281:LYS:HA	1:D:303:VAL:CG1	2.31	0.47
1:F:281:LYS:HA	1:F:303:VAL:CG1	2.31	0.47
1:F:363:SER:O	1:F:367:THR:HG23	2.14	0.47
1:G:139:PHE:CG	1:H:108:MET:HG2	2.49	0.47
1:I:261:LYS:O	1:I:261:LYS:HG3	2.15	0.47
1:J:261:LYS:HG3	1:J:261:LYS:O	2.14	0.47
1:K:312:HIS:HD2	1:K:313:GLY:N	2.12	0.47
1:A:122:THR:HG22	1:A:126:VAL:HG12	1.95	0.47
1:C:156:ASN:OD1	1:I:159:HIS:O	2.33	0.47
1:H:173:ASN:HB2	1:H:284:PHE:CE1	2.49	0.47
1:L:261:LYS:HG3	1:L:261:LYS:O	2.15	0.47
1:A:121:GLY:O	1:A:125:THR:OG1	2.20	0.47
1:C:89:ILE:HD11	1:C:373:LEU:HD11	1.96	0.47
1:C:121:GLY:O	1:C:125:THR:OG1	2.20	0.47
1:G:113:ILE:HD13	1:G:114:LYS:N	2.29	0.47
1:G:199:LYS:HB2	1:G:229:ALA:CB	2.34	0.47
1:H:122:THR:HG22	1:H:126:VAL:HG12	1.95	0.47
1:K:339:GLU:OE1	1:K:339:GLU:HA	2.15	0.47
1:E:136:LEU:HD21	1:F:72:LEU:CB	2.42	0.46
1:H:89:ILE:HD11	1:H:373:LEU:HD11	1.97	0.46
1:K:177:GLU:HG3	1:K:357:ARG:HH11	1.80	0.46
1:K:363:SER:O	1:K:367:THR:HG23	2.15	0.46
1:A:173:ASN:HB2	1:A:284:PHE:CE1	2.49	0.46
1:E:136:LEU:CD2	1:F:72:LEU:HB3	2.43	0.46
1:F:261:LYS:O	1:F:261:LYS:HG3	2.14	0.46
1:J:173:ASN:HB2	1:J:284:PHE:CE1	2.50	0.46
1:K:113:ILE:HD13	1:K:114:LYS:N	2.29	0.46
1:L:113:ILE:HD13	1:L:114:LYS:N	2.29	0.46
1:B:261:LYS:HG3	1:B:261:LYS:O	2.15	0.46
1:C:339:GLU:OE1	1:C:339:GLU:HA	2.16	0.46
1:D:261:LYS:HG3	1:D:261:LYS:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:ASN:HB2	1:E:284:PHE:CE1	2.49	0.46
1:H:281:LYS:HA	1:H:303:VAL:CG1	2.31	0.46
1:K:287:VAL:HG22	1:K:288:LEU:N	2.29	0.46
1:C:261:LYS:HG3	1:C:261:LYS:O	2.15	0.46
1:E:48:VAL:HG23	1:H:262:GLN:OE1	2.16	0.46
1:E:261:LYS:HG3	1:E:261:LYS:O	2.14	0.46
1:K:175:ILE:HD13	1:K:175:ILE:HA	1.79	0.46
1:J:287:VAL:HG22	1:J:288:LEU:N	2.28	0.46
1:K:281:LYS:O	1:K:282:GLU:CB	2.57	0.46
1:L:173:ASN:HB2	1:L:284:PHE:CE1	2.50	0.46
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.62	0.46
1:C:281:LYS:CB	1:C:281:LYS:HZ3	2.28	0.46
1:D:173:ASN:HB2	1:D:284:PHE:CE1	2.50	0.46
1:K:122:THR:HG22	1:K:126:VAL:HG12	1.97	0.46
1:C:282:GLU:HG3	1:C:284:PHE:H	1.81	0.46
1:F:287:VAL:HG22	1:F:288:LEU:N	2.29	0.46
1:H:212:ARG:HG3	1:H:212:ARG:NH1	2.31	0.46
1:I:339:GLU:OE1	1:I:339:GLU:HA	2.16	0.46
1:J:113:ILE:HD13	1:J:114:LYS:N	2.30	0.46
1:A:257:LEU:N	1:A:257:LEU:HD13	2.28	0.46
1:D:287:VAL:HG22	1:D:288:LEU:N	2.29	0.46
1:E:173:ASN:OD1	1:E:284:PHE:HD1	1.96	0.46
1:E:182:LYS:HZ1	1:E:349:ARG:HD3	1.80	0.46
1:L:332:ILE:O	1:L:336:LYS:HG2	2.16	0.46
1:A:332:ILE:O	1:A:336:LYS:HG2	2.16	0.46
1:F:281:LYS:O	1:F:282:GLU:CB	2.58	0.46
1:H:282:GLU:HG3	1:H:284:PHE:H	1.81	0.46
1:A:76:SER:HB2	1:B:136:LEU:HD22	1.98	0.45
1:C:212:ARG:HG3	1:C:212:ARG:NH1	2.31	0.45
1:E:212:ARG:HG3	1:E:212:ARG:NH1	2.31	0.45
1:F:212:ARG:HG3	1:F:212:ARG:NH1	2.31	0.45
1:F:284:PHE:CB	1:F:285:GLY:HA2	2.32	0.45
1:I:287:VAL:HG22	1:I:288:LEU:N	2.29	0.45
1:L:282:GLU:HG3	1:L:284:PHE:H	1.81	0.45
1:B:282:GLU:HG3	1:B:284:PHE:H	1.81	0.45
1:C:175:ILE:HD13	1:C:175:ILE:HA	1.79	0.45
1:F:332:ILE:O	1:F:336:LYS:HG2	2.16	0.45
1:K:212:ARG:HG3	1:K:212:ARG:NH1	2.31	0.45
1:K:282:GLU:HG3	1:K:284:PHE:H	1.81	0.45
1:A:339:GLU:OE1	1:A:339:GLU:HA	2.16	0.45
1:D:339:GLU:HA	1:D:339:GLU:OE1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:GLU:OE1	1:E:339:GLU:HA	2.16	0.45
1:H:175:ILE:HD13	1:H:175:ILE:HA	1.79	0.45
1:K:199:LYS:O	1:K:229:ALA:HB1	2.17	0.45
1:B:212:ARG:HG3	1:B:212:ARG:NH1	2.31	0.45
1:B:332:ILE:O	1:B:336:LYS:HG2	2.16	0.45
1:D:212:ARG:HG3	1:D:212:ARG:NH1	2.32	0.45
1:E:281:LYS:O	1:E:282:GLU:CB	2.58	0.45
1:F:177:GLU:HG3	1:F:357:ARG:HH11	1.81	0.45
1:F:282:GLU:HG3	1:F:284:PHE:H	1.82	0.45
1:H:275:MET:SD	1:H:287:VAL:HG23	2.57	0.45
1:H:339:GLU:OE1	1:H:339:GLU:HA	2.16	0.45
1:A:212:ARG:HG3	1:A:212:ARG:NH1	2.31	0.45
1:A:275:MET:SD	1:A:287:VAL:HG23	2.57	0.45
1:B:112:ARG:NH2	1:B:112:ARG:HB3	2.32	0.45
1:C:332:ILE:O	1:C:336:LYS:HG2	2.16	0.45
1:H:112:ARG:NH2	1:H:112:ARG:HB3	2.32	0.45
1:H:287:VAL:HG22	1:H:288:LEU:N	2.30	0.45
1:K:112:ARG:NH2	1:K:112:ARG:HB3	2.32	0.45
1:C:112:ARG:NH2	1:C:112:ARG:HB3	2.32	0.45
1:D:112:ARG:NH2	1:D:112:ARG:HB3	2.32	0.45
1:D:175:ILE:HD13	1:D:175:ILE:HA	1.79	0.45
1:D:282:GLU:HG3	1:D:284:PHE:H	1.82	0.45
1:J:112:ARG:NH2	1:J:112:ARG:HB3	2.32	0.45
1:J:336:LYS:HE2	1:J:336:LYS:HB3	1.86	0.45
1:L:275:MET:SD	1:L:287:VAL:HG23	2.57	0.45
1:A:177:GLU:HG3	1:A:357:ARG:HH11	1.81	0.45
1:B:339:GLU:OE1	1:B:339:GLU:HA	2.16	0.45
1:C:136:LEU:CD2	1:D:72:LEU:HB3	2.43	0.45
1:F:112:ARG:HB3	1:F:112:ARG:NH2	2.32	0.45
1:G:332:ILE:O	1:G:336:LYS:HG2	2.16	0.45
1:H:261:LYS:HG3	1:H:261:LYS:O	2.15	0.45
1:H:332:ILE:O	1:H:336:LYS:HG2	2.16	0.45
1:J:339:GLU:OE1	1:J:339:GLU:HA	2.16	0.45
1:L:112:ARG:NH2	1:L:112:ARG:HB3	2.32	0.45
1:D:177:GLU:HG3	1:D:357:ARG:HH11	1.81	0.45
1:F:288:LEU:HA	1:F:288:LEU:HD23	1.62	0.45
1:G:212:ARG:HG3	1:G:212:ARG:NH1	2.31	0.45
1:G:339:GLU:HA	1:G:339:GLU:OE1	2.16	0.45
1:J:332:ILE:O	1:J:336:LYS:HG2	2.17	0.45
1:L:212:ARG:HG3	1:L:212:ARG:NH1	2.31	0.45
1:A:79:ALA:CB	1:A:108:MET:HE2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:LEU:HD11	1:B:341:HIS:HA	1.99	0.45
1:E:287:VAL:HG22	1:E:288:LEU:N	2.29	0.45
1:F:277:LEU:O	1:F:300:GLY:HA2	2.17	0.45
1:G:199:LYS:O	1:G:229:ALA:HB1	2.17	0.45
1:D:275:MET:SD	1:D:287:VAL:HG23	2.57	0.45
1:F:339:GLU:OE1	1:F:339:GLU:HA	2.16	0.45
1:G:104:LEU:HD23	1:G:104:LEU:HA	1.84	0.45
1:G:112:ARG:NH2	1:G:112:ARG:HB3	2.32	0.45
1:G:155:ILE:HG22	1:L:156:ASN:HD21	1.82	0.45
1:I:112:ARG:NH2	1:I:112:ARG:HB3	2.32	0.45
1:I:212:ARG:HG3	1:I:212:ARG:NH1	2.32	0.45
1:J:199:LYS:O	1:J:229:ALA:HB1	2.17	0.45
1:L:339:GLU:HA	1:L:339:GLU:OE1	2.16	0.45
1:C:277:LEU:O	1:C:300:GLY:HA2	2.17	0.44
1:D:199:LYS:O	1:D:229:ALA:HB1	2.18	0.44
1:E:112:ARG:NH2	1:E:112:ARG:HB3	2.32	0.44
1:E:177:GLU:HG3	1:E:357:ARG:HH11	1.82	0.44
1:E:277:LEU:O	1:E:300:GLY:HA2	2.17	0.44
1:G:282:GLU:HG3	1:G:284:PHE:H	1.82	0.44
1:I:177:GLU:HG3	1:I:357:ARG:HH11	1.81	0.44
1:I:282:GLU:HG3	1:I:284:PHE:H	1.82	0.44
1:I:284:PHE:CB	1:I:285:GLY:HA2	2.32	0.44
1:J:212:ARG:HG3	1:J:212:ARG:NH1	2.32	0.44
1:J:284:PHE:CB	1:J:285:GLY:HA2	2.30	0.44
1:B:275:MET:SD	1:B:287:VAL:HG23	2.57	0.44
1:D:332:ILE:O	1:D:336:LYS:HG2	2.16	0.44
1:E:332:ILE:O	1:E:336:LYS:HG2	2.16	0.44
1:F:199:LYS:O	1:F:229:ALA:HB1	2.17	0.44
1:F:252:ILE:HG22	1:F:255:ARG:HB2	1.99	0.44
1:F:275:MET:SD	1:F:287:VAL:HG23	2.57	0.44
1:I:277:LEU:O	1:I:300:GLY:HA2	2.17	0.44
1:I:332:ILE:O	1:I:336:LYS:HG2	2.16	0.44
1:K:332:ILE:O	1:K:336:LYS:HG2	2.17	0.44
1:L:257:LEU:N	1:L:257:LEU:HD13	2.28	0.44
1:A:277:LEU:O	1:A:300:GLY:HA2	2.17	0.44
1:A:281:LYS:O	1:A:282:GLU:CB	2.57	0.44
1:B:114:LYS:HG3	1:B:373:LEU:HD23	2.00	0.44
1:E:108:MET:CE	1:F:135:ASN:ND2	2.80	0.44
1:F:239:GLU:O	1:F:243:ILE:HG12	2.18	0.44
1:G:65:PHE:HZ	1:H:96:ILE:HG21	1.83	0.44
1:I:334:LEU:HD11	1:I:341:HIS:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:199:LYS:O	1:L:229:ALA:HB1	2.18	0.44
1:A:112:ARG:NH2	1:A:112:ARG:HB3	2.32	0.44
1:A:199:LYS:O	1:A:229:ALA:HB1	2.17	0.44
1:E:250:LEU:HB3	1:E:252:ILE:HG13	2.00	0.44
1:G:177:GLU:HG3	1:G:357:ARG:HH11	1.81	0.44
1:K:275:MET:SD	1:K:287:VAL:HG23	2.58	0.44
1:L:177:GLU:HG3	1:L:357:ARG:HH11	1.81	0.44
1:A:306:ILE:H	1:A:307:PRO:HD2	1.83	0.44
1:B:177:GLU:HG3	1:B:357:ARG:HH11	1.81	0.44
1:B:199:LYS:O	1:B:229:ALA:HB1	2.18	0.44
1:C:284:PHE:CB	1:C:285:GLY:HA2	2.32	0.44
1:E:275:MET:SD	1:E:287:VAL:HG23	2.57	0.44
1:F:250:LEU:HB3	1:F:252:ILE:HG13	2.00	0.44
1:G:275:MET:SD	1:G:287:VAL:HG23	2.57	0.44
1:I:288:LEU:HD23	1:I:288:LEU:HA	1.62	0.44
1:B:252:ILE:HG22	1:B:255:ARG:HB2	1.99	0.44
1:C:127:LEU:HD23	1:C:127:LEU:HA	1.81	0.44
1:C:186:THR:HA	1:C:189:LYS:CD	2.44	0.44
1:E:199:LYS:O	1:E:229:ALA:HB1	2.18	0.44
1:E:239:GLU:O	1:E:243:ILE:HG12	2.18	0.44
1:G:122:THR:HA	1:G:126:VAL:HG12	2.00	0.44
1:G:250:LEU:HB3	1:G:252:ILE:HG13	2.00	0.44
1:K:34:ILE:HD12	1:K:34:ILE:N	2.33	0.44
1:L:252:ILE:HG22	1:L:255:ARG:HB2	2.00	0.44
1:A:72:LEU:CD2	1:B:97:PRO:HB3	2.47	0.44
1:A:250:LEU:HB3	1:A:252:ILE:HG13	2.00	0.44
1:A:281:LYS:HA	1:A:303:VAL:CG1	2.32	0.44
1:A:282:GLU:HG3	1:A:284:PHE:H	1.82	0.44
1:B:175:ILE:HD13	1:B:175:ILE:HA	1.80	0.44
1:D:250:LEU:HB3	1:D:252:ILE:HG13	2.00	0.44
1:D:252:ILE:HG22	1:D:255:ARG:HB2	2.00	0.44
1:E:282:GLU:HG3	1:E:284:PHE:H	1.82	0.44
1:F:114:LYS:HG3	1:F:373:LEU:HD23	2.00	0.44
1:G:277:LEU:O	1:G:300:GLY:HA2	2.17	0.44
1:G:300:GLY:O	1:G:318:LEU:HA	2.18	0.44
1:H:186:THR:HA	1:H:189:LYS:CD	2.45	0.44
1:H:277:LEU:O	1:H:300:GLY:HA2	2.17	0.44
1:J:175:ILE:HD13	1:J:175:ILE:HA	1.78	0.44
1:J:177:GLU:HG3	1:J:357:ARG:HH11	1.82	0.44
1:L:334:LEU:HD11	1:L:341:HIS:HA	2.00	0.44
1:C:239:GLU:O	1:C:243:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:MET:SD	1:C:287:VAL:HG23	2.57	0.44
1:D:104:LEU:HA	1:D:104:LEU:HD23	1.84	0.44
1:E:252:ILE:HG22	1:E:255:ARG:HB2	2.00	0.44
1:F:122:THR:HA	1:F:126:VAL:HG12	2.00	0.44
1:G:97:PRO:HB3	1:H:72:LEU:HD21	2.00	0.44
1:G:257:LEU:N	1:G:257:LEU:HD13	2.28	0.44
1:I:239:GLU:O	1:I:243:ILE:HG12	2.18	0.44
1:J:250:LEU:HB3	1:J:252:ILE:HG13	2.00	0.44
1:K:104:LEU:HA	1:K:104:LEU:HD23	1.83	0.44
1:K:122:THR:HA	1:K:126:VAL:HG12	2.00	0.44
1:A:252:ILE:HG22	1:A:255:ARG:HB2	2.00	0.44
1:A:312:HIS:CD2	1:A:313:GLY:N	2.86	0.44
1:B:277:LEU:O	1:B:300:GLY:HA2	2.17	0.44
1:F:199:LYS:HB2	1:F:229:ALA:CB	2.35	0.44
1:G:281:LYS:O	1:G:282:GLU:CB	2.57	0.44
1:H:250:LEU:HB3	1:H:252:ILE:HG13	2.00	0.44
1:H:289:LEU:N	1:H:289:LEU:HD12	2.33	0.44
1:B:77:LYS:O	1:B:81:VAL:HG23	2.18	0.43
1:C:114:LYS:HG3	1:C:373:LEU:HD23	2.00	0.43
1:D:334:LEU:HD11	1:D:341:HIS:HA	1.99	0.43
1:G:79:ALA:CB	1:G:108:MET:HE2	2.48	0.43
1:G:239:GLU:O	1:G:243:ILE:HG12	2.18	0.43
1:I:250:LEU:HB3	1:I:252:ILE:HG13	2.00	0.43
1:J:239:GLU:O	1:J:243:ILE:HG12	2.17	0.43
1:K:277:LEU:O	1:K:300:GLY:HA2	2.17	0.43
1:L:114:LYS:HG3	1:L:373:LEU:HD23	2.00	0.43
1:L:250:LEU:HB3	1:L:252:ILE:HG13	2.00	0.43
1:L:312:HIS:CD2	1:L:313:GLY:N	2.86	0.43
1:A:97:PRO:HB3	1:B:72:LEU:CD2	2.48	0.43
1:B:250:LEU:HB3	1:B:252:ILE:HG13	2.00	0.43
1:C:300:GLY:O	1:C:318:LEU:HA	2.18	0.43
1:C:334:LEU:HD11	1:C:341:HIS:HA	1.99	0.43
1:D:239:GLU:O	1:D:243:ILE:HG12	2.18	0.43
1:D:277:LEU:O	1:D:300:GLY:HA2	2.17	0.43
1:F:306:ILE:H	1:F:307:PRO:HD2	1.83	0.43
1:G:77:LYS:O	1:G:81:VAL:HG23	2.19	0.43
1:G:252:ILE:HG22	1:G:255:ARG:HB2	1.99	0.43
1:L:287:VAL:HG22	1:L:288:LEU:N	2.29	0.43
1:B:312:HIS:CD2	1:B:313:GLY:N	2.86	0.43
1:C:173:ASN:OD1	1:C:284:PHE:HD1	2.00	0.43
1:D:77:LYS:O	1:D:81:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:177:GLU:HG3	1:H:357:ARG:HH11	1.81	0.43
1:I:275:MET:SD	1:I:287:VAL:HG23	2.58	0.43
1:J:252:ILE:HG22	1:J:255:ARG:HB2	2.00	0.43
1:L:277:LEU:O	1:L:300:GLY:HA2	2.17	0.43
1:L:300:GLY:O	1:L:318:LEU:HA	2.19	0.43
1:A:77:LYS:O	1:A:81:VAL:HG23	2.19	0.43
1:A:114:LYS:HG3	1:A:373:LEU:HD23	2.00	0.43
1:B:239:GLU:O	1:B:243:ILE:HG12	2.18	0.43
1:C:288:LEU:HD23	1:C:288:LEU:HA	1.62	0.43
1:F:34:ILE:HD12	1:F:34:ILE:N	2.34	0.43
1:G:136:LEU:HD22	1:H:76:SER:HB2	1.99	0.43
1:H:257:LEU:HD12	1:H:257:LEU:HA	1.63	0.43
1:I:257:LEU:N	1:I:257:LEU:HD13	2.28	0.43
1:J:212:ARG:HD3	1:J:280:GLU:OE1	2.18	0.43
1:B:182:LYS:HZ2	1:B:349:ARG:HD3	1.81	0.43
1:B:300:GLY:O	1:B:318:LEU:HA	2.19	0.43
1:C:306:ILE:H	1:C:307:PRO:HD2	1.83	0.43
1:C:311:GLN:HG3	1:C:314:ASP:HB3	2.01	0.43
1:C:312:HIS:CD2	1:C:313:GLY:N	2.87	0.43
1:D:114:LYS:HG3	1:D:373:LEU:HD23	2.00	0.43
1:D:312:HIS:CD2	1:D:313:GLY:N	2.86	0.43
1:E:122:THR:HA	1:E:126:VAL:HG12	2.00	0.43
1:F:257:LEU:N	1:F:257:LEU:HD13	2.28	0.43
1:F:334:LEU:HD11	1:F:341:HIS:HA	1.99	0.43
1:F:346:GLU:O	1:F:350:GLU:HG3	2.19	0.43
1:H:199:LYS:O	1:H:229:ALA:HB1	2.18	0.43
1:I:122:THR:HA	1:I:126:VAL:HG12	2.00	0.43
1:I:306:ILE:H	1:I:307:PRO:HD2	1.84	0.43
1:K:173:ASN:HB2	1:K:284:PHE:CE1	2.52	0.43
1:K:250:LEU:HB3	1:K:252:ILE:HG13	2.01	0.43
1:K:257:LEU:O	1:K:259:LEU:N	2.52	0.43
1:K:346:GLU:O	1:K:350:GLU:HG3	2.18	0.43
1:L:77:LYS:O	1:L:81:VAL:HG23	2.19	0.43
1:A:239:GLU:O	1:A:243:ILE:HG12	2.18	0.43
1:B:311:GLN:HG3	1:B:314:ASP:HB3	2.01	0.43
1:E:300:GLY:O	1:E:318:LEU:HA	2.19	0.43
1:E:334:LEU:HD11	1:E:341:HIS:HA	1.99	0.43
1:H:312:HIS:CD2	1:H:313:GLY:N	2.86	0.43
1:I:312:HIS:CD2	1:I:313:GLY:N	2.87	0.43
1:J:186:THR:HA	1:J:189:LYS:CD	2.45	0.43
1:L:289:LEU:N	1:L:289:LEU:HD12	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ILE:N	1:B:34:ILE:HD12	2.34	0.43
1:B:287:VAL:HG22	1:B:288:LEU:N	2.29	0.43
1:B:289:LEU:N	1:B:289:LEU:HD12	2.33	0.43
1:C:34:ILE:HD12	1:C:34:ILE:N	2.34	0.43
1:C:122:THR:HA	1:C:126:VAL:HG12	2.00	0.43
1:C:281:LYS:HB2	1:C:281:LYS:HZ2	1.83	0.43
1:D:281:LYS:O	1:D:282:GLU:CB	2.58	0.43
1:D:300:GLY:O	1:D:318:LEU:HA	2.18	0.43
1:G:257:LEU:O	1:G:259:LEU:N	2.52	0.43
1:G:313:GLY:N	1:G:316:GLY:O	2.38	0.43
1:H:122:THR:HA	1:H:126:VAL:HG12	2.00	0.43
1:H:252:ILE:HG22	1:H:255:ARG:HB2	2.00	0.43
1:H:300:GLY:O	1:H:318:LEU:HA	2.18	0.43
1:I:311:GLN:HG3	1:I:314:ASP:HB3	2.01	0.43
1:J:277:LEU:O	1:J:300:GLY:HA2	2.18	0.43
1:K:239:GLU:O	1:K:243:ILE:HG12	2.18	0.43
1:K:334:LEU:HD11	1:K:341:HIS:HA	1.99	0.43
1:A:34:ILE:HD12	1:A:34:ILE:N	2.34	0.43
1:A:311:GLN:HG3	1:A:314:ASP:HB3	2.01	0.43
1:B:257:LEU:N	1:B:257:LEU:HD13	2.28	0.43
1:C:257:LEU:O	1:C:259:LEU:N	2.52	0.43
1:D:122:THR:HA	1:D:126:VAL:HG12	2.00	0.43
1:E:77:LYS:O	1:E:81:VAL:HG23	2.19	0.43
1:E:119:LEU:HD22	1:E:124:ILE:CD1	2.49	0.43
1:E:312:HIS:CD2	1:E:313:GLY:N	2.87	0.43
1:F:312:HIS:CD2	1:F:313:GLY:N	2.87	0.43
1:G:288:LEU:HA	1:G:288:LEU:HD23	1.62	0.43
1:H:239:GLU:O	1:H:243:ILE:HG12	2.18	0.43
1:I:114:LYS:HG3	1:I:373:LEU:HD23	2.00	0.43
1:I:252:ILE:HG22	1:I:255:ARG:HB2	2.00	0.43
1:I:257:LEU:O	1:I:259:LEU:N	2.52	0.43
1:I:289:LEU:N	1:I:289:LEU:HD12	2.34	0.43
1:K:96:ILE:HG22	1:L:65:PHE:CZ	2.54	0.43
1:K:252:ILE:HG22	1:K:255:ARG:HB2	2.00	0.43
1:B:186:THR:HA	1:B:189:LYS:CD	2.45	0.43
1:B:281:LYS:HA	1:B:303:VAL:CG1	2.32	0.43
1:C:199:LYS:O	1:C:229:ALA:HB1	2.18	0.43
1:D:313:GLY:N	1:D:316:GLY:O	2.38	0.43
1:E:182:LYS:HZ2	1:E:349:ARG:CD	2.31	0.43
1:F:77:LYS:O	1:F:81:VAL:HG23	2.18	0.43
1:F:300:GLY:O	1:F:318:LEU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:346:GLU:O	1:G:350:GLU:HG3	2.19	0.43
1:J:34:ILE:N	1:J:34:ILE:HD12	2.34	0.43
1:J:114:LYS:HG3	1:J:373:LEU:HD23	2.01	0.43
1:J:275:MET:SD	1:J:287:VAL:HG23	2.59	0.43
1:J:311:GLN:HG3	1:J:314:ASP:HB3	2.00	0.43
1:J:312:HIS:CD2	1:J:313:GLY:N	2.87	0.43
1:J:334:LEU:HD11	1:J:341:HIS:HA	2.00	0.43
1:K:136:LEU:HD22	1:L:76:SER:HB2	1.99	0.43
1:K:274:LEU:HD11	1:K:299:ILE:HG13	2.01	0.43
1:L:311:GLN:HG3	1:L:314:ASP:HB3	2.01	0.43
1:A:274:LEU:HD11	1:A:299:ILE:HG13	2.01	0.43
1:B:346:GLU:O	1:B:350:GLU:HG3	2.19	0.43
1:D:127:LEU:HD23	1:D:127:LEU:HA	1.81	0.43
1:E:289:LEU:N	1:E:289:LEU:HD12	2.34	0.43
1:F:138:ARG:O	1:F:142:GLU:HG3	2.19	0.43
1:H:346:GLU:O	1:H:350:GLU:HG3	2.18	0.43
1:I:186:THR:HA	1:I:189:LYS:CD	2.45	0.43
1:K:121:GLY:O	1:K:125:THR:CB	2.66	0.43
1:L:119:LEU:HD22	1:L:124:ILE:CD1	2.49	0.43
1:A:122:THR:HA	1:A:126:VAL:HG12	2.00	0.42
1:A:138:ARG:O	1:A:142:GLU:HG3	2.19	0.42
1:B:104:LEU:HD23	1:B:104:LEU:HA	1.83	0.42
1:C:177:GLU:HG3	1:C:357:ARG:HH11	1.81	0.42
1:C:250:LEU:HB3	1:C:252:ILE:HG13	2.00	0.42
1:E:34:ILE:N	1:E:34:ILE:HD12	2.34	0.42
1:E:114:LYS:HG3	1:E:373:LEU:HD23	2.00	0.42
1:F:275:MET:SD	1:F:287:VAL:HG21	2.59	0.42
1:G:121:GLY:O	1:G:125:THR:CB	2.67	0.42
1:H:336:LYS:HE2	1:H:336:LYS:HB3	1.85	0.42
1:J:300:GLY:O	1:J:318:LEU:HA	2.18	0.42
1:J:306:ILE:H	1:J:307:PRO:HD2	1.84	0.42
1:K:114:LYS:HG3	1:K:373:LEU:HD23	2.01	0.42
1:K:311:GLN:HG3	1:K:314:ASP:HB3	2.01	0.42
1:A:275:MET:SD	1:A:287:VAL:HG21	2.59	0.42
1:A:300:GLY:O	1:A:318:LEU:HA	2.18	0.42
1:A:334:LEU:HD11	1:A:341:HIS:HA	1.99	0.42
1:C:77:LYS:O	1:C:81:VAL:HG23	2.19	0.42
1:E:286:LEU:CD1	1:E:286:LEU:N	2.31	0.42
1:G:275:MET:SD	1:G:287:VAL:HG21	2.59	0.42
1:H:34:ILE:N	1:H:34:ILE:HD12	2.34	0.42
1:I:34:ILE:HD12	1:I:34:ILE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:212:ARG:HD3	1:I:280:GLU:OE1	2.20	0.42
1:J:313:GLY:N	1:J:316:GLY:O	2.38	0.42
1:A:289:LEU:N	1:A:289:LEU:HD12	2.34	0.42
1:B:119:LEU:HD22	1:B:124:ILE:CD1	2.50	0.42
1:B:122:THR:HA	1:B:126:VAL:HG12	2.00	0.42
1:B:267:GLU:OE1	1:D:48:VAL:CG1	2.67	0.42
1:C:119:LEU:HD22	1:C:124:ILE:CD1	2.50	0.42
1:D:346:GLU:O	1:D:350:GLU:HG3	2.19	0.42
1:G:155:ILE:CG2	1:L:156:ASN:HD21	2.32	0.42
1:G:334:LEU:HD11	1:G:341:HIS:HA	1.99	0.42
1:H:114:LYS:HG3	1:H:373:LEU:HD23	2.00	0.42
1:H:138:ARG:O	1:H:142:GLU:HG3	2.20	0.42
1:I:300:GLY:O	1:I:318:LEU:HA	2.19	0.42
1:J:257:LEU:O	1:J:259:LEU:N	2.52	0.42
1:A:119:LEU:HD22	1:A:124:ILE:CD1	2.50	0.42
1:A:136:LEU:HD21	1:B:72:LEU:HB3	2.01	0.42
1:C:252:ILE:HG22	1:C:255:ARG:HB2	2.00	0.42
1:C:274:LEU:HD11	1:C:299:ILE:HG13	2.02	0.42
1:C:284:PHE:CD2	1:C:284:PHE:O	2.72	0.42
1:D:212:ARG:HD3	1:D:280:GLU:OE1	2.20	0.42
1:E:104:LEU:HA	1:E:104:LEU:HD23	1.84	0.42
1:E:138:ARG:O	1:E:142:GLU:HG3	2.20	0.42
1:F:257:LEU:O	1:F:259:LEU:N	2.52	0.42
1:F:336:LYS:HE2	1:F:336:LYS:HB3	1.85	0.42
1:I:199:LYS:O	1:I:229:ALA:HB1	2.17	0.42
1:I:257:LEU:HD12	1:I:257:LEU:HA	1.63	0.42
1:J:90:LEU:HD12	1:J:90:LEU:HA	1.86	0.42
1:K:138:ARG:O	1:K:142:GLU:HG3	2.19	0.42
1:L:212:ARG:HD3	1:L:280:GLU:OE1	2.20	0.42
1:A:257:LEU:O	1:A:259:LEU:N	2.52	0.42
1:B:212:ARG:HD3	1:B:280:GLU:OE1	2.20	0.42
1:F:313:GLY:N	1:F:316:GLY:O	2.38	0.42
1:G:114:LYS:HG3	1:G:373:LEU:HD23	2.00	0.42
1:G:284:PHE:CD2	1:G:284:PHE:O	2.73	0.42
1:G:311:GLN:HG3	1:G:314:ASP:HB3	2.01	0.42
1:H:104:LEU:HD23	1:H:104:LEU:HA	1.83	0.42
1:H:275:MET:SD	1:H:287:VAL:HG21	2.59	0.42
1:H:334:LEU:HD11	1:H:341:HIS:HA	2.00	0.42
1:J:122:THR:HA	1:J:126:VAL:HG12	2.00	0.42
1:K:119:LEU:HD22	1:K:124:ILE:CD1	2.49	0.42
1:K:313:GLY:N	1:K:316:GLY:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:122:THR:HA	1:L:126:VAL:HG12	2.00	0.42
1:A:346:GLU:O	1:A:350:GLU:HG3	2.19	0.42
1:B:90:LEU:HD12	1:B:90:LEU:HA	1.87	0.42
1:B:275:MET:SD	1:B:287:VAL:HG21	2.60	0.42
1:C:289:LEU:N	1:C:289:LEU:HD12	2.34	0.42
1:D:34:ILE:HD12	1:D:34:ILE:N	2.34	0.42
1:D:284:PHE:CD2	1:D:284:PHE:O	2.73	0.42
1:G:312:HIS:CD2	1:G:313:GLY:N	2.87	0.42
1:H:77:LYS:O	1:H:81:VAL:HG23	2.19	0.42
1:H:274:LEU:HD11	1:H:299:ILE:HG13	2.01	0.42
1:H:284:PHE:CD2	1:H:284:PHE:O	2.72	0.42
1:K:49:TYR:HA	1:K:50:PRO:HD3	1.86	0.42
1:K:274:LEU:HD21	1:K:299:ILE:HD12	2.01	0.42
1:L:239:GLU:O	1:L:243:ILE:HG12	2.18	0.42
1:L:346:GLU:O	1:L:350:GLU:HG3	2.19	0.42
1:B:127:LEU:HA	1:B:127:LEU:HD23	1.81	0.42
1:B:286:LEU:CD1	1:B:286:LEU:N	2.31	0.42
1:B:306:ILE:H	1:B:307:PRO:HD2	1.83	0.42
1:C:212:ARG:HD3	1:C:280:GLU:OE1	2.19	0.42
1:C:218:GLN:O	1:C:222:LYS:HG3	2.20	0.42
1:C:292:MET:C	1:C:294:CYS:N	2.73	0.42
1:D:138:ARG:O	1:D:142:GLU:HG3	2.19	0.42
1:D:281:LYS:HB2	1:D:281:LYS:HZ2	1.84	0.42
1:F:289:LEU:N	1:F:289:LEU:HD12	2.34	0.42
1:G:186:THR:HA	1:G:189:LYS:CD	2.45	0.42
1:L:127:LEU:HD23	1:L:127:LEU:HA	1.82	0.42
1:C:275:MET:SD	1:C:287:VAL:HG21	2.60	0.42
1:C:281:LYS:HA	1:C:303:VAL:CG1	2.32	0.42
1:D:121:GLY:O	1:D:125:THR:CB	2.68	0.42
1:D:182:LYS:HZ2	1:D:349:ARG:CD	2.33	0.42
1:D:275:MET:SD	1:D:287:VAL:HG21	2.59	0.42
1:E:346:GLU:O	1:E:350:GLU:HG3	2.19	0.42
1:F:311:GLN:HG3	1:F:314:ASP:HB3	2.01	0.42
1:G:212:ARG:HD3	1:G:280:GLU:OE1	2.20	0.42
1:H:218:GLN:O	1:H:222:LYS:HG3	2.20	0.42
1:H:257:LEU:N	1:H:257:LEU:HD13	2.28	0.42
1:I:274:LEU:HD11	1:I:299:ILE:HG13	2.01	0.42
1:K:182:LYS:HZ2	1:K:349:ARG:HD3	1.81	0.42
1:A:336:LYS:HE2	1:A:336:LYS:HB3	1.85	0.42
1:B:138:ARG:O	1:B:142:GLU:HG3	2.20	0.42
1:B:313:GLY:N	1:B:316:GLY:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:GLN:HG3	1:E:314:ASP:HB3	2.01	0.42
1:F:314:ASP:CG	1:F:347:ARG:HE	2.23	0.42
1:G:218:GLN:O	1:G:222:LYS:HG3	2.20	0.42
1:G:292:MET:C	1:G:294:CYS:N	2.73	0.42
1:I:79:ALA:CB	1:I:108:MET:HE2	2.49	0.42
1:J:104:LEU:HA	1:J:104:LEU:HD23	1.85	0.42
1:K:186:THR:HA	1:K:189:LYS:CD	2.45	0.42
1:K:312:HIS:CD2	1:K:313:GLY:N	2.87	0.42
1:L:275:MET:SD	1:L:287:VAL:HG21	2.59	0.42
1:L:288:LEU:HA	1:L:288:LEU:HD23	1.62	0.42
1:B:257:LEU:O	1:B:259:LEU:N	2.52	0.42
1:C:336:LYS:HG2	1:C:336:LYS:H	1.64	0.42
1:D:119:LEU:HD22	1:D:124:ILE:CD1	2.49	0.42
1:D:292:MET:C	1:D:294:CYS:N	2.73	0.42
1:J:121:GLY:O	1:J:125:THR:CB	2.68	0.42
1:J:202:ILE:HG12	1:J:232:LEU:HB2	2.02	0.42
1:C:128:GLY:HA2	1:C:137:ILE:HD12	2.02	0.41
1:C:189:LYS:HB3	1:C:194:ILE:HG23	2.02	0.41
1:D:218:GLN:O	1:D:222:LYS:HG3	2.20	0.41
1:D:314:ASP:CG	1:D:347:ARG:HE	2.24	0.41
1:E:189:LYS:HB3	1:E:194:ILE:HG23	2.02	0.41
1:E:212:ARG:HD3	1:E:280:GLU:OE1	2.20	0.41
1:F:212:ARG:HD3	1:F:280:GLU:OE1	2.20	0.41
1:G:138:ARG:O	1:G:142:GLU:HG3	2.20	0.41
1:G:189:LYS:HB3	1:G:194:ILE:HG23	2.02	0.41
1:G:306:ILE:H	1:G:307:PRO:HD2	1.83	0.41
1:H:128:GLY:HA2	1:H:137:ILE:HD12	2.02	0.41
1:I:182:LYS:HZ2	1:I:349:ARG:CD	2.33	0.41
1:I:218:GLN:O	1:I:222:LYS:HG3	2.20	0.41
1:I:284:PHE:CD2	1:I:284:PHE:O	2.73	0.41
1:K:127:LEU:HD23	1:K:127:LEU:HA	1.83	0.41
1:L:34:ILE:HD12	1:L:34:ILE:N	2.35	0.41
1:A:212:ARG:HD3	1:A:280:GLU:OE1	2.19	0.41
1:A:218:GLN:O	1:A:222:LYS:HG3	2.21	0.41
1:B:79:ALA:CB	1:B:108:MET:HE2	2.50	0.41
1:B:314:ASP:CG	1:B:347:ARG:HE	2.24	0.41
1:E:257:LEU:O	1:E:259:LEU:N	2.52	0.41
1:E:274:LEU:HD11	1:E:299:ILE:HG13	2.02	0.41
1:F:336:LYS:HG2	1:F:336:LYS:H	1.64	0.41
1:G:274:LEU:HD21	1:G:299:ILE:HD12	2.03	0.41
1:H:212:ARG:HD3	1:H:280:GLU:OE1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:257:LEU:O	1:H:259:LEU:N	2.52	0.41
1:I:127:LEU:HD23	1:I:127:LEU:HA	1.81	0.41
1:I:274:LEU:HD21	1:I:299:ILE:HD12	2.03	0.41
1:I:292:MET:C	1:I:294:CYS:N	2.73	0.41
1:J:314:ASP:CG	1:J:347:ARG:HE	2.24	0.41
1:K:275:MET:SD	1:K:287:VAL:HG21	2.60	0.41
1:K:284:PHE:CD2	1:K:284:PHE:O	2.72	0.41
1:A:121:GLY:O	1:A:125:THR:CB	2.68	0.41
1:A:306:ILE:N	1:A:307:PRO:HD2	2.35	0.41
1:B:128:GLY:HA2	1:B:137:ILE:HD12	2.02	0.41
1:B:189:LYS:HB3	1:B:194:ILE:HG23	2.02	0.41
1:C:121:GLY:O	1:C:125:THR:CB	2.68	0.41
1:C:159:HIS:CD2	1:I:159:HIS:CD2	3.08	0.41
1:C:346:GLU:O	1:C:350:GLU:HG3	2.19	0.41
1:F:104:LEU:HA	1:F:104:LEU:HD23	1.84	0.41
1:G:119:LEU:HD22	1:G:124:ILE:CD1	2.50	0.41
1:H:49:TYR:HA	1:H:50:PRO:HD3	1.85	0.41
1:H:292:MET:C	1:H:294:CYS:N	2.74	0.41
1:I:119:LEU:HD22	1:I:124:ILE:CD1	2.50	0.41
1:I:189:LYS:HB3	1:I:194:ILE:HG23	2.02	0.41
1:J:281:LYS:HB2	1:J:281:LYS:HZ2	1.85	0.41
1:J:282:GLU:HG3	1:J:284:PHE:H	1.85	0.41
1:J:288:LEU:HA	1:J:288:LEU:HD23	1.62	0.41
1:J:289:LEU:N	1:J:289:LEU:HD12	2.34	0.41
1:L:314:ASP:CG	1:L:347:ARG:HE	2.23	0.41
1:A:314:ASP:CG	1:A:347:ARG:HE	2.24	0.41
1:B:274:LEU:HD11	1:B:299:ILE:HG13	2.01	0.41
1:B:274:LEU:HD21	1:B:299:ILE:HD12	2.02	0.41
1:B:306:ILE:N	1:B:307:PRO:HD2	2.35	0.41
1:C:138:ARG:O	1:C:142:GLU:HG3	2.19	0.41
1:D:274:LEU:HD21	1:D:299:ILE:HD12	2.03	0.41
1:D:311:GLN:HG3	1:D:314:ASP:HB3	2.01	0.41
1:F:202:ILE:HG12	1:F:232:LEU:HB2	2.03	0.41
1:F:274:LEU:HD11	1:F:299:ILE:HG13	2.02	0.41
1:G:182:LYS:HZ2	1:G:349:ARG:CD	2.34	0.41
1:G:202:ILE:HG12	1:G:232:LEU:HB2	2.02	0.41
1:H:121:GLY:O	1:H:125:THR:CB	2.68	0.41
1:H:311:GLN:HG3	1:H:314:ASP:HB3	2.01	0.41
1:H:336:LYS:HG2	1:H:336:LYS:H	1.64	0.41
1:I:77:LYS:O	1:I:81:VAL:HG23	2.19	0.41
1:L:257:LEU:O	1:L:259:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:274:LEU:HD11	1:L:299:ILE:HG13	2.01	0.41
1:B:309:VAL:HG12	1:B:356:PHE:CZ	2.56	0.41
1:C:136:LEU:HD21	1:D:72:LEU:CB	2.42	0.41
1:C:306:ILE:N	1:C:307:PRO:HD2	2.36	0.41
1:E:121:GLY:O	1:E:125:THR:CB	2.68	0.41
1:E:314:ASP:CG	1:E:347:ARG:HE	2.24	0.41
1:F:175:ILE:HA	1:F:175:ILE:HD13	1.79	0.41
1:H:189:LYS:HB3	1:H:194:ILE:HG23	2.03	0.41
1:J:309:VAL:HG12	1:J:356:PHE:CZ	2.56	0.41
1:K:289:LEU:N	1:K:289:LEU:HD12	2.34	0.41
1:L:189:LYS:HB3	1:L:194:ILE:HG23	2.02	0.41
1:L:274:LEU:HD21	1:L:299:ILE:HD12	2.03	0.41
1:B:284:PHE:CD2	1:B:284:PHE:O	2.74	0.41
1:C:202:ILE:HG12	1:C:232:LEU:HB2	2.03	0.41
1:D:257:LEU:O	1:D:259:LEU:N	2.52	0.41
1:F:189:LYS:HB3	1:F:194:ILE:HG23	2.02	0.41
1:F:218:GLN:O	1:F:222:LYS:HG3	2.20	0.41
1:G:274:LEU:HD11	1:G:299:ILE:HG13	2.01	0.41
1:I:128:GLY:HA2	1:I:137:ILE:HD12	2.03	0.41
1:I:138:ARG:O	1:I:142:GLU:HG3	2.20	0.41
1:I:306:ILE:N	1:I:307:PRO:HD2	2.36	0.41
1:K:300:GLY:O	1:K:318:LEU:HA	2.19	0.41
1:E:128:GLY:HA2	1:E:137:ILE:HD12	2.03	0.41
1:H:314:ASP:CG	1:H:347:ARG:HE	2.24	0.41
1:I:275:MET:SD	1:I:287:VAL:HG21	2.60	0.41
1:I:346:GLU:O	1:I:350:GLU:HG3	2.19	0.41
1:J:138:ARG:O	1:J:142:GLU:HG3	2.20	0.41
1:J:218:GLN:O	1:J:222:LYS:HG3	2.20	0.41
1:J:250:LEU:HB3	1:J:252:ILE:CD1	2.51	0.41
1:K:77:LYS:O	1:K:81:VAL:HG23	2.20	0.41
1:K:287:VAL:O	1:K:288:LEU:C	2.55	0.41
1:L:175:ILE:HD13	1:L:175:ILE:HA	1.80	0.41
1:A:128:GLY:HA2	1:A:137:ILE:HD12	2.03	0.41
1:B:250:LEU:HB3	1:B:252:ILE:CD1	2.51	0.41
1:D:274:LEU:HD11	1:D:299:ILE:HG13	2.01	0.41
1:D:289:LEU:N	1:D:289:LEU:HD12	2.34	0.41
1:F:127:LEU:HA	1:F:127:LEU:HD23	1.81	0.41
1:H:202:ILE:HG12	1:H:232:LEU:HB2	2.02	0.41
1:H:250:LEU:HB3	1:H:252:ILE:CD1	2.51	0.41
1:K:79:ALA:CB	1:K:108:MET:HE2	2.51	0.41
1:L:49:TYR:HA	1:L:50:PRO:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HD12	1:A:3:LEU:HA	1.94	0.41
1:A:104:LEU:HA	1:A:104:LEU:HD23	1.84	0.41
1:A:189:LYS:HB3	1:A:194:ILE:HG23	2.02	0.41
1:A:202:ILE:HG12	1:A:232:LEU:HB2	2.03	0.41
1:A:250:LEU:HB3	1:A:252:ILE:CD1	2.51	0.41
1:A:287:VAL:O	1:A:288:LEU:C	2.56	0.41
1:B:121:GLY:O	1:B:125:THR:CB	2.68	0.41
1:D:250:LEU:HB3	1:D:252:ILE:CD1	2.51	0.41
1:D:309:VAL:HG12	1:D:356:PHE:CZ	2.56	0.41
1:E:218:GLN:O	1:E:222:LYS:HG3	2.20	0.41
1:E:250:LEU:HB3	1:E:252:ILE:CD1	2.51	0.41
1:E:284:PHE:CD2	1:E:284:PHE:O	2.73	0.41
1:E:309:VAL:HG12	1:E:356:PHE:CZ	2.56	0.41
1:E:347:ARG:O	1:E:350:GLU:HB2	2.21	0.41
1:F:121:GLY:O	1:F:125:THR:CB	2.68	0.41
1:F:141:ILE:HG23	1:F:147:VAL:HG21	2.03	0.41
1:F:284:PHE:CD2	1:F:284:PHE:O	2.73	0.41
1:G:72:LEU:CB	1:H:136:LEU:HD21	2.43	0.41
1:G:289:LEU:N	1:G:289:LEU:HD12	2.33	0.41
1:G:314:ASP:CG	1:G:347:ARG:HE	2.24	0.41
1:H:286:LEU:N	1:H:286:LEU:CD1	2.31	0.41
1:H:309:VAL:HG12	1:H:356:PHE:CZ	2.56	0.41
1:I:250:LEU:HB3	1:I:252:ILE:CD1	2.51	0.41
1:I:281:LYS:HZ3	1:I:281:LYS:HB2	1.83	0.41
1:J:257:LEU:N	1:J:257:LEU:HD13	2.28	0.41
1:J:292:MET:C	1:J:294:CYS:N	2.74	0.41
1:J:346:GLU:O	1:J:350:GLU:HG3	2.20	0.41
1:K:19:VAL:HG11	1:K:173:ASN:HD22	1.86	0.41
1:K:128:GLY:HA2	1:K:137:ILE:HD12	2.02	0.41
1:K:212:ARG:HD3	1:K:280:GLU:OE1	2.19	0.41
1:L:250:LEU:HB3	1:L:252:ILE:CD1	2.51	0.41
1:B:218:GLN:O	1:B:222:LYS:HG3	2.20	0.41
1:B:288:LEU:HA	1:B:288:LEU:HD23	1.61	0.41
1:D:202:ILE:HG12	1:D:232:LEU:HB2	2.03	0.41
1:E:141:ILE:HG23	1:E:147:VAL:HG21	2.03	0.41
1:E:175:ILE:HD13	1:E:175:ILE:HA	1.79	0.41
1:E:186:THR:HA	1:E:189:LYS:CD	2.45	0.41
1:E:275:MET:SD	1:E:287:VAL:HG21	2.60	0.41
1:F:119:LEU:HD22	1:F:124:ILE:CD1	2.49	0.41
1:F:306:ILE:N	1:F:307:PRO:HD2	2.36	0.41
1:G:34:ILE:HD12	1:G:34:ILE:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:347:ARG:O	1:H:350:GLU:HB2	2.21	0.41
1:I:281:LYS:O	1:I:282:GLU:CB	2.57	0.41
1:J:128:GLY:HA2	1:J:137:ILE:HD12	2.02	0.41
1:J:306:ILE:N	1:J:307:PRO:HD2	2.36	0.41
1:K:182:LYS:HZ1	1:K:349:ARG:HD3	1.86	0.41
1:K:336:LYS:HE2	1:K:336:LYS:HB3	1.85	0.41
1:L:39:SER:HB3	1:L:57:VAL:HB	2.03	0.41
1:L:121:GLY:O	1:L:125:THR:CB	2.68	0.41
1:L:138:ARG:O	1:L:142:GLU:HG3	2.20	0.41
1:L:313:GLY:N	1:L:316:GLY:O	2.39	0.41
1:B:134:ASN:ND2	1:B:138:ARG:NH2	2.69	0.40
1:D:141:ILE:HG23	1:D:147:VAL:HG21	2.03	0.40
1:D:336:LYS:HG2	1:D:336:LYS:H	1.64	0.40
1:D:336:LYS:HE2	1:D:336:LYS:HB3	1.85	0.40
1:E:49:TYR:HA	1:E:50:PRO:HD3	1.85	0.40
1:E:134:ASN:ND2	1:E:138:ARG:NH2	2.69	0.40
1:E:292:MET:C	1:E:294:CYS:N	2.73	0.40
1:F:274:LEU:HD21	1:F:299:ILE:HD12	2.03	0.40
1:F:292:MET:C	1:F:294:CYS:N	2.73	0.40
1:F:309:VAL:HG12	1:F:356:PHE:CZ	2.56	0.40
1:G:309:VAL:HG12	1:G:356:PHE:CZ	2.55	0.40
1:H:79:ALA:CB	1:H:108:MET:HE2	2.51	0.40
1:J:274:LEU:HD11	1:J:299:ILE:HG13	2.02	0.40
1:J:274:LEU:HD21	1:J:299:ILE:HD12	2.03	0.40
1:J:275:MET:SD	1:J:287:VAL:HG21	2.61	0.40
1:K:288:LEU:HA	1:K:288:LEU:HD23	1.60	0.40
1:K:292:MET:C	1:K:294:CYS:N	2.73	0.40
1:L:202:ILE:HG12	1:L:232:LEU:HB2	2.02	0.40
1:A:141:ILE:HG23	1:A:147:VAL:HG21	2.03	0.40
1:A:284:PHE:CD2	1:A:284:PHE:O	2.74	0.40
1:B:336:LYS:HE2	1:B:336:LYS:HB3	1.85	0.40
1:B:347:ARG:O	1:B:350:GLU:HB2	2.21	0.40
1:C:141:ILE:HG23	1:C:147:VAL:HG21	2.03	0.40
1:C:159:HIS:O	1:I:156:ASN:OD1	2.38	0.40
1:C:250:LEU:HB3	1:C:252:ILE:CD1	2.51	0.40
1:C:274:LEU:HD21	1:C:299:ILE:HD12	2.03	0.40
1:C:281:LYS:O	1:C:282:GLU:CB	2.58	0.40
1:C:287:VAL:O	1:C:288:LEU:C	2.56	0.40
1:C:309:VAL:HG12	1:C:356:PHE:CZ	2.56	0.40
1:I:121:GLY:O	1:I:125:THR:CB	2.68	0.40
1:I:134:ASN:ND2	1:I:138:ARG:NH2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:141:ILE:HG23	1:I:147:VAL:HG21	2.03	0.40
1:I:291:ALA:O	1:I:292:MET:C	2.60	0.40
1:J:39:SER:HB3	1:J:57:VAL:HB	2.04	0.40
1:K:250:LEU:HB3	1:K:252:ILE:CD1	2.51	0.40
1:L:306:ILE:N	1:L:307:PRO:HD2	2.36	0.40
1:A:274:LEU:HD21	1:A:299:ILE:HD12	2.03	0.40
1:B:106:LYS:HG3	1:B:113:ILE:HG22	2.03	0.40
1:B:202:ILE:HG12	1:B:232:LEU:HB2	2.02	0.40
1:E:202:ILE:HG12	1:E:232:LEU:HB2	2.03	0.40
1:F:347:ARG:O	1:F:350:GLU:HB2	2.21	0.40
1:G:141:ILE:HG23	1:G:147:VAL:HG21	2.03	0.40
1:H:351:SER:O	1:H:355:GLN:HG2	2.21	0.40
1:I:202:ILE:HG12	1:I:232:LEU:HB2	2.03	0.40
1:I:347:ARG:O	1:I:350:GLU:HB2	2.22	0.40
1:J:182:LYS:HZ2	1:J:349:ARG:CD	2.34	0.40
1:K:106:LYS:HG3	1:K:113:ILE:HG22	2.03	0.40
1:L:291:ALA:O	1:L:292:MET:C	2.60	0.40
1:L:306:ILE:H	1:L:307:PRO:HD2	1.83	0.40
1:L:347:ARG:O	1:L:350:GLU:HB2	2.21	0.40
1:A:146:VAL:HG11	1:A:368:ILE:CG2	2.52	0.40
1:B:292:MET:C	1:B:294:CYS:N	2.73	0.40
1:D:128:GLY:HA2	1:D:137:ILE:HD12	2.03	0.40
1:F:19:VAL:HG11	1:F:173:ASN:HD22	1.87	0.40
1:G:19:VAL:HG11	1:G:173:ASN:HD22	1.87	0.40
1:G:250:LEU:HB3	1:G:252:ILE:CD1	2.51	0.40
1:H:134:ASN:ND2	1:H:138:ARG:NH2	2.70	0.40
1:H:306:ILE:H	1:H:307:PRO:HD2	1.83	0.40
1:I:286:LEU:N	1:I:286:LEU:CD1	2.30	0.40
1:J:306:ILE:HB	1:J:307:PRO:CD	2.44	0.40
1:K:218:GLN:O	1:K:222:LYS:HG3	2.22	0.40
1:K:281:LYS:HA	1:K:303:VAL:CG1	2.33	0.40
1:L:309:VAL:HG12	1:L:356:PHE:CZ	2.57	0.40
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.82	0.40
1:B:146:VAL:HG11	1:B:368:ILE:CG2	2.52	0.40
1:C:134:ASN:ND2	1:C:138:ARG:NH2	2.70	0.40
1:D:189:LYS:HB3	1:D:194:ILE:HG23	2.02	0.40
1:D:256:VAL:HG12	1:D:258:PHE:CD2	2.57	0.40
1:E:39:SER:HB3	1:E:57:VAL:HB	2.04	0.40
1:E:306:ILE:H	1:E:307:PRO:HD2	1.84	0.40
1:F:47:LYS:CG	1:F:48:VAL:N	2.81	0.40
1:F:106:LYS:HG3	1:F:113:ILE:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:LEU:HD23	1:G:127:LEU:HA	1.81	0.40
1:H:274:LEU:HD21	1:H:299:ILE:HD12	2.02	0.40
1:J:119:LEU:HD22	1:J:124:ILE:CD1	2.51	0.40
1:J:189:LYS:HB3	1:J:194:ILE:HG23	2.03	0.40
1:J:255:ARG:HH21	1:J:255:ARG:HD2	1.78	0.40
1:K:122:THR:CA	1:K:126:VAL:HG12	2.52	0.40
1:L:128:GLY:HA2	1:L:137:ILE:HD12	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLU:CA	1:K:167:ASP:OD2[1_455]	2.08	0.12

## 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	350/394 (89%)	323 (92%)	24 (7%)	3 (1%)	17	52
1	B	350/394 (89%)	322 (92%)	26 (7%)	2 (1%)	25	59
1	C	350/394 (89%)	323 (92%)	25 (7%)	2 (1%)	25	59
1	D	350/394 (89%)	322 (92%)	25 (7%)	3 (1%)	17	52
1	E	350/394 (89%)	323 (92%)	24 (7%)	3 (1%)	17	52
1	F	350/394 (89%)	322 (92%)	26 (7%)	2 (1%)	25	59
1	G	350/394 (89%)	322 (92%)	26 (7%)	2 (1%)	25	59
1	H	350/394 (89%)	322 (92%)	26 (7%)	2 (1%)	25	59
1	I	350/394 (89%)	322 (92%)	25 (7%)	3 (1%)	17	52
1	J	350/394 (89%)	322 (92%)	26 (7%)	2 (1%)	25	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	350/394 (89%)	322 (92%)	26 (7%)	2 (1%)	25	59
1	L	350/394 (89%)	323 (92%)	25 (7%)	2 (1%)	25	59
All	All	4200/4728 (89%)	3868 (92%)	304 (7%)	28 (1%)	22	57

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	ALA
1	A	304	GLY
1	B	293	ALA
1	B	304	GLY
1	C	293	ALA
1	C	304	GLY
1	D	293	ALA
1	D	304	GLY
1	E	293	ALA
1	E	304	GLY
1	F	293	ALA
1	F	304	GLY
1	G	293	ALA
1	G	304	GLY
1	H	293	ALA
1	H	304	GLY
1	I	293	ALA
1	I	304	GLY
1	J	293	ALA
1	J	304	GLY
1	K	293	ALA
1	K	304	GLY
1	L	293	ALA
1	L	304	GLY
1	A	98	HIS
1	D	98	HIS
1	E	98	HIS
1	I	98	HIS

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/346 (90%)	287 (92%)	25 (8%)	12	40
1	B	312/346 (90%)	287 (92%)	25 (8%)	12	40
1	C	312/346 (90%)	287 (92%)	25 (8%)	12	40
1	D	312/346 (90%)	287 (92%)	25 (8%)	12	40
1	E	312/346 (90%)	287 (92%)	25 (8%)	12	40
1	F	312/346 (90%)	287 (92%)	25 (8%)	12	40
1	G	312/346 (90%)	287 (92%)	25 (8%)	12	40
1	H	312/346 (90%)	287 (92%)	25 (8%)	12	40
1	I	312/346 (90%)	287 (92%)	25 (8%)	12	40
1	J	312/346 (90%)	286 (92%)	26 (8%)	11	38
1	K	312/346 (90%)	287 (92%)	25 (8%)	12	40
1	L	312/346 (90%)	287 (92%)	25 (8%)	12	40
All	All	3744/4152 (90%)	3443 (92%)	301 (8%)	12	40

All (301) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLU
1	A	59	VAL
1	A	65	PHE
1	A	86	ASN
1	A	92	VAL
1	A	113	ILE
1	A	122	THR
1	A	156	ASN
1	A	178	ARG
1	A	181	PHE
1	A	182	LYS
1	A	183	ARG
1	A	190	LYS
1	A	202	ILE
1	A	223	ILE
1	A	255	ARG
1	A	263	ASP
1	A	275	MET
1	A	278	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	279	SER
1	A	284	PHE
1	A	286	LEU
1	A	336	LYS
1	A	349	ARG
1	A	358	SER
1	B	56	GLU
1	B	59	VAL
1	B	65	PHE
1	B	86	ASN
1	B	92	VAL
1	B	113	ILE
1	B	122	THR
1	B	156	ASN
1	B	178	ARG
1	B	181	PHE
1	B	182	LYS
1	B	183	ARG
1	B	190	LYS
1	B	202	ILE
1	B	223	ILE
1	B	255	ARG
1	B	263	ASP
1	B	275	MET
1	B	278	LEU
1	B	279	SER
1	B	284	PHE
1	B	286	LEU
1	B	336	LYS
1	B	349	ARG
1	B	358	SER
1	C	56	GLU
1	C	59	VAL
1	C	65	PHE
1	C	86	ASN
1	C	92	VAL
1	C	113	ILE
1	C	122	THR
1	C	156	ASN
1	C	178	ARG
1	C	181	PHE
1	C	182	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	183	ARG
1	C	190	LYS
1	C	202	ILE
1	C	223	ILE
1	C	255	ARG
1	C	263	ASP
1	C	275	MET
1	C	278	LEU
1	C	279	SER
1	C	284	PHE
1	C	286	LEU
1	C	336	LYS
1	C	349	ARG
1	C	358	SER
1	D	56	GLU
1	D	59	VAL
1	D	65	PHE
1	D	86	ASN
1	D	92	VAL
1	D	113	ILE
1	D	122	THR
1	D	156	ASN
1	D	178	ARG
1	D	181	PHE
1	D	182	LYS
1	D	183	ARG
1	D	190	LYS
1	D	202	ILE
1	D	223	ILE
1	D	255	ARG
1	D	263	ASP
1	D	275	MET
1	D	278	LEU
1	D	279	SER
1	D	284	PHE
1	D	286	LEU
1	D	336	LYS
1	D	349	ARG
1	D	358	SER
1	E	56	GLU
1	E	59	VAL
1	E	65	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	86	ASN
1	E	92	VAL
1	E	113	ILE
1	E	122	THR
1	E	156	ASN
1	E	178	ARG
1	E	181	PHE
1	E	182	LYS
1	E	183	ARG
1	E	190	LYS
1	E	202	ILE
1	E	223	ILE
1	E	255	ARG
1	E	263	ASP
1	E	275	MET
1	E	278	LEU
1	E	279	SER
1	E	284	PHE
1	E	286	LEU
1	E	336	LYS
1	E	349	ARG
1	E	358	SER
1	F	56	GLU
1	F	59	VAL
1	F	65	PHE
1	F	86	ASN
1	F	92	VAL
1	F	113	ILE
1	F	122	THR
1	F	156	ASN
1	F	178	ARG
1	F	181	PHE
1	F	182	LYS
1	F	183	ARG
1	F	190	LYS
1	F	202	ILE
1	F	223	ILE
1	F	255	ARG
1	F	263	ASP
1	F	275	MET
1	F	278	LEU
1	F	279	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	284	PHE
1	F	286	LEU
1	F	336	LYS
1	F	349	ARG
1	F	358	SER
1	G	56	GLU
1	G	59	VAL
1	G	65	PHE
1	G	86	ASN
1	G	92	VAL
1	G	113	ILE
1	G	122	THR
1	G	156	ASN
1	G	178	ARG
1	G	181	PHE
1	G	182	LYS
1	G	183	ARG
1	G	190	LYS
1	G	202	ILE
1	G	223	ILE
1	G	255	ARG
1	G	263	ASP
1	G	275	MET
1	G	278	LEU
1	G	279	SER
1	G	284	PHE
1	G	286	LEU
1	G	336	LYS
1	G	349	ARG
1	G	358	SER
1	H	56	GLU
1	H	59	VAL
1	H	65	PHE
1	H	86	ASN
1	H	92	VAL
1	H	113	ILE
1	H	122	THR
1	H	156	ASN
1	H	178	ARG
1	H	181	PHE
1	H	182	LYS
1	H	183	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	190	LYS
1	H	202	ILE
1	H	223	ILE
1	H	255	ARG
1	H	263	ASP
1	H	275	MET
1	H	278	LEU
1	H	279	SER
1	H	284	PHE
1	H	286	LEU
1	H	336	LYS
1	H	349	ARG
1	H	358	SER
1	I	56	GLU
1	I	59	VAL
1	I	65	PHE
1	I	86	ASN
1	I	92	VAL
1	I	113	ILE
1	I	122	THR
1	I	156	ASN
1	I	178	ARG
1	I	181	PHE
1	I	182	LYS
1	I	183	ARG
1	I	190	LYS
1	I	202	ILE
1	I	223	ILE
1	I	255	ARG
1	I	263	ASP
1	I	275	MET
1	I	278	LEU
1	I	279	SER
1	I	284	PHE
1	I	286	LEU
1	I	336	LYS
1	I	349	ARG
1	I	358	SER
1	J	56	GLU
1	J	59	VAL
1	J	65	PHE
1	J	86	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	J	92	VAL
1	J	113	ILE
1	J	122	THR
1	J	156	ASN
1	J	178	ARG
1	J	181	PHE
1	J	182	LYS
1	J	183	ARG
1	J	190	LYS
1	J	195	SER
1	J	202	ILE
1	J	223	ILE
1	J	255	ARG
1	J	263	ASP
1	J	275	MET
1	J	278	LEU
1	J	279	SER
1	J	284	PHE
1	J	286	LEU
1	J	336	LYS
1	J	349	ARG
1	J	358	SER
1	K	56	GLU
1	K	59	VAL
1	K	65	PHE
1	K	86	ASN
1	K	92	VAL
1	K	113	ILE
1	K	122	THR
1	K	156	ASN
1	K	178	ARG
1	K	181	PHE
1	K	182	LYS
1	K	183	ARG
1	K	190	LYS
1	K	202	ILE
1	K	223	ILE
1	K	255	ARG
1	K	263	ASP
1	K	275	MET
1	K	278	LEU
1	K	279	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	K	284	PHE
1	K	286	LEU
1	K	336	LYS
1	K	349	ARG
1	K	358	SER
1	L	56	GLU
1	L	59	VAL
1	L	65	PHE
1	L	86	ASN
1	L	92	VAL
1	L	113	ILE
1	L	122	THR
1	L	156	ASN
1	L	178	ARG
1	L	181	PHE
1	L	182	LYS
1	L	183	ARG
1	L	190	LYS
1	L	202	ILE
1	L	223	ILE
1	L	255	ARG
1	L	263	ASP
1	L	275	MET
1	L	278	LEU
1	L	279	SER
1	L	284	PHE
1	L	286	LEU
1	L	336	LYS
1	L	349	ARG
1	L	358	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	98	HIS
1	A	134	ASN
1	A	165	ASN
1	A	173	ASN
1	A	214	GLN
1	A	312	HIS
1	A	330	GLN
1	A	333	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	364	GLN
1	B	98	HIS
1	B	134	ASN
1	B	165	ASN
1	B	173	ASN
1	B	214	GLN
1	B	312	HIS
1	B	330	GLN
1	B	333	GLN
1	B	364	GLN
1	C	98	HIS
1	C	134	ASN
1	C	159	HIS
1	C	165	ASN
1	C	173	ASN
1	C	214	GLN
1	C	312	HIS
1	C	330	GLN
1	C	333	GLN
1	C	364	GLN
1	D	98	HIS
1	D	134	ASN
1	D	165	ASN
1	D	173	ASN
1	D	214	GLN
1	D	312	HIS
1	D	330	GLN
1	D	333	GLN
1	D	364	GLN
1	E	98	HIS
1	E	134	ASN
1	E	165	ASN
1	E	173	ASN
1	E	214	GLN
1	E	312	HIS
1	E	330	GLN
1	E	333	GLN
1	E	364	GLN
1	F	98	HIS
1	F	134	ASN
1	F	135	ASN
1	F	165	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	173	ASN
1	F	214	GLN
1	F	312	HIS
1	F	330	GLN
1	F	333	GLN
1	F	364	GLN
1	G	98	HIS
1	G	134	ASN
1	G	165	ASN
1	G	173	ASN
1	G	214	GLN
1	G	312	HIS
1	G	330	GLN
1	G	333	GLN
1	G	364	GLN
1	H	98	HIS
1	H	134	ASN
1	H	165	ASN
1	H	173	ASN
1	H	214	GLN
1	H	312	HIS
1	H	330	GLN
1	H	333	GLN
1	H	364	GLN
1	I	98	HIS
1	I	134	ASN
1	I	165	ASN
1	I	173	ASN
1	I	214	GLN
1	I	312	HIS
1	I	330	GLN
1	I	333	GLN
1	I	364	GLN
1	J	98	HIS
1	J	134	ASN
1	J	165	ASN
1	J	173	ASN
1	J	214	GLN
1	J	312	HIS
1	J	330	GLN
1	J	333	GLN
1	J	364	GLN

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Mol	Chain	Res	Type
1	K	98	HIS
1	K	134	ASN
1	K	165	ASN
1	K	173	ASN
1	K	214	GLN
1	K	312	HIS
1	K	330	GLN
1	K	333	GLN
1	K	364	GLN
1	L	98	HIS
1	L	134	ASN
1	L	156	ASN
1	L	165	ASN
1	L	173	ASN
1	L	214	GLN
1	L	312	HIS
1	L	330	GLN
1	L	333	GLN
1	L	364	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	360/394 (91%)	0.02	3 (0%) 86 72	62, 92, 116, 125	0
1	B	360/394 (91%)	0.22	17 (4%) 31 15	63, 94, 116, 126	0
1	C	360/394 (91%)	0.18	8 (2%) 62 41	57, 93, 116, 125	0
1	D	360/394 (91%)	0.03	2 (0%) 89 78	58, 93, 115, 126	0
1	E	360/394 (91%)	0.12	6 (1%) 70 49	56, 92, 116, 125	0
1	F	360/394 (91%)	0.14	9 (2%) 57 34	57, 93, 116, 125	0
1	G	360/394 (91%)	0.05	4 (1%) 80 64	62, 93, 116, 125	0
1	H	360/394 (91%)	0.66	53 (14%) 2 1	63, 95, 117, 126	0
1	I	360/394 (91%)	0.22	9 (2%) 57 34	57, 92, 116, 125	0
1	J	360/394 (91%)	0.12	2 (0%) 89 78	38, 87, 116, 124	0
1	K	360/394 (91%)	0.16	8 (2%) 62 41	55, 90, 116, 124	0
1	L	360/394 (91%)	0.08	4 (1%) 80 64	61, 92, 115, 124	0
All	All	4320/4728 (91%)	0.17	125 (2%) 51 28	38, 92, 116, 126	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	177	GLU	5.2
1	H	190	LYS	4.4
1	H	257	LEU	4.3
1	H	263	ASP	4.1
1	H	272	SER	4.1
1	H	295	GLY	4.0
1	H	327	VAL	4.0
1	H	343	ASN	3.9
1	H	310	ILE	3.9
1	H	340	LEU	3.9
1	I	332	ILE	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	I	182	LYS	3.7
1	E	178	ARG	3.7
1	H	184	ASP	3.7
1	H	271	MET	3.6
1	H	339	GLU	3.6
1	H	200	ILE	3.5
1	B	188	LEU	3.4
1	D	182	LYS	3.3
1	I	313	GLY	3.1
1	E	332	ILE	3.1
1	B	314	ASP	3.0
1	H	264	ASN	3.0
1	E	336	LYS	3.0
1	B	187	GLN	3.0
1	H	185	MET	2.9
1	H	202	ILE	2.9
1	H	302	ARG	2.9
1	H	266	ALA	2.8
1	K	346	GLU	2.8
1	H	296	VAL	2.8
1	C	333	GLN	2.8
1	H	192	TYR	2.8
1	B	347	ARG	2.8
1	B	315	THR	2.7
1	C	223	ILE	2.7
1	H	244	LEU	2.7
1	H	162	VAL	2.7
1	B	309	VAL	2.7
1	H	188	LEU	2.7
1	H	229	ALA	2.7
1	G	187	GLN	2.7
1	C	184	ASP	2.6
1	H	341	HIS	2.6
1	H	350	GLU	2.6
1	F	335	LEU	2.6
1	H	223	ILE	2.6
1	L	182	LYS	2.6
1	K	271	MET	2.6
1	B	284	PHE	2.6
1	H	187	GLN	2.6
1	B	342	ARG	2.6
1	K	188	LEU	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	223	ILE	2.6
1	C	200	ILE	2.6
1	H	270	ALA	2.5
1	H	213	VAL	2.5
1	I	194	ILE	2.5
1	H	357	ARG	2.5
1	B	185	MET	2.5
1	F	314	ASP	2.5
1	E	182	LYS	2.5
1	H	182	LYS	2.5
1	I	328	ALA	2.5
1	I	229	ALA	2.4
1	B	200	ILE	2.4
1	I	186	THR	2.4
1	D	223	ILE	2.4
1	H	194	ILE	2.4
1	F	342	ARG	2.4
1	L	60	ASN	2.4
1	A	177	GLU	2.4
1	K	178	ARG	2.4
1	I	221	ALA	2.4
1	H	277	LEU	2.3
1	H	306	ILE	2.3
1	A	186	THR	2.3
1	K	187	GLN	2.3
1	C	186	THR	2.3
1	A	343	ASN	2.3
1	L	186	THR	2.3
1	E	334	LEU	2.3
1	H	349	ARG	2.3
1	F	185	MET	2.2
1	I	190	LYS	2.2
1	K	191	GLU	2.2
1	J	223	ILE	2.2
1	B	263	ASP	2.2
1	H	247	VAL	2.2
1	B	339	GLU	2.2
1	F	317	TYR	2.2
1	B	299	ILE	2.2
1	H	347	ARG	2.2
1	H	234	VAL	2.2
1	B	132	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	311	GLN	2.2
1	H	51	ASN	2.2
1	J	60	ASN	2.2
1	C	67	TYR	2.2
1	G	190	LYS	2.2
1	F	187	GLN	2.1
1	H	319	CYS	2.1
1	H	186	THR	2.1
1	H	191	GLU	2.1
1	H	314	ASP	2.1
1	B	345	GLY	2.1
1	H	300	GLY	2.1
1	K	349	ARG	2.1
1	C	269	LEU	2.1
1	G	314	ASP	2.1
1	H	273	ASP	2.1
1	F	223	ILE	2.0
1	B	183	ARG	2.0
1	F	227	VAL	2.0
1	H	216	VAL	2.0
1	K	167	ASP	2.0
1	G	188	LEU	2.0
1	F	334	LEU	2.0
1	C	185	MET	2.0
1	H	338	GLU	2.0
1	H	354	GLU	2.0
1	L	190	LYS	2.0
1	B	310	ILE	2.0
1	H	335	LEU	2.0
1	H	267	GLU	2.0

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

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

## 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.