



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:06 PM UTC

PDB ID : 2EWO / pdb_00002ewo
Title : X-ray structure of putative agmatine deiminase Q8DW17, Northeast Structural Genomics target SmR6.
Authors : Kuzin, A.P.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2005-11-04
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

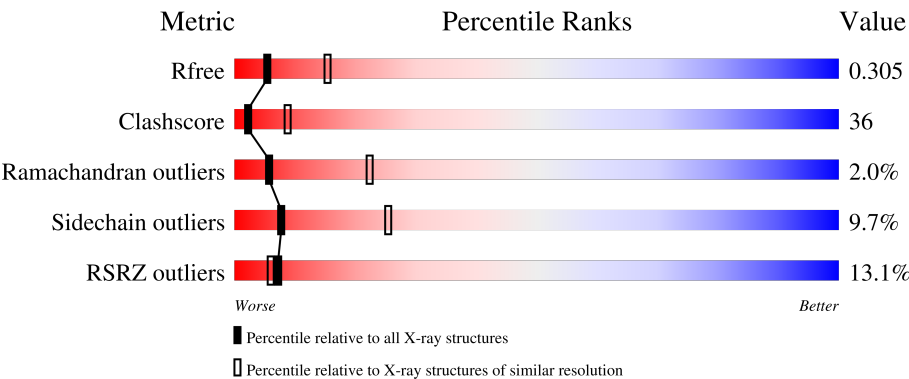
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	377	12% 40% 47% 9% .
1	B	377	13% 40% 46% 9% .
1	C	377	14% 41% 46% 9% .
1	D	377	16% 40% 47% 8% . .
1	E	377	18% 40% 47% 9% .

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Mol	Chain	Length	Quality of chain
1	F	377	16% 40% 47% 8%
1	G	377	14% 41% 46% 8%
1	H	377	2% 42% 46% 10%
1	I	377	12% 41% 46% 9%
1	J	377	15% 41% 46% 9%
1	K	377	3% 40% 47% 8%
1	L	377	14% 40% 46% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34934 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 Putative agmatine deiminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	B	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	C	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	D	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	E	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	F	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	G	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	H	369	Total	C	N	O	S	Se	0	0	0
			2942	1868	496	561	10	7			
1	I	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	J	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	K	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	L	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q8DW17
A	17	MSE	MET	modified residue	UNP Q8DW17
A	29	MSE	MET	modified residue	UNP Q8DW17
A	91	MSE	MET	modified residue	UNP Q8DW17
A	178	MSE	MET	modified residue	UNP Q8DW17

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Chain	Residue	Modelled	Actual	Comment	Reference
A	274	MSE	MET	modified residue	UNP Q8DW17
A	303	MSE	MET	modified residue	UNP Q8DW17
A	338	MSE	MET	modified residue	UNP Q8DW17
A	370	LEU	-	cloning artifact	UNP Q8DW17
A	371	GLU	-	cloning artifact	UNP Q8DW17
A	372	HIS	-	expression tag	UNP Q8DW17
A	373	HIS	-	expression tag	UNP Q8DW17
A	374	HIS	-	expression tag	UNP Q8DW17
A	375	HIS	-	expression tag	UNP Q8DW17
A	376	HIS	-	expression tag	UNP Q8DW17
A	377	HIS	-	expression tag	UNP Q8DW17
B	1	MSE	MET	modified residue	UNP Q8DW17
B	17	MSE	MET	modified residue	UNP Q8DW17
B	29	MSE	MET	modified residue	UNP Q8DW17
B	91	MSE	MET	modified residue	UNP Q8DW17
B	178	MSE	MET	modified residue	UNP Q8DW17
B	274	MSE	MET	modified residue	UNP Q8DW17
B	303	MSE	MET	modified residue	UNP Q8DW17
B	338	MSE	MET	modified residue	UNP Q8DW17
B	370	LEU	-	cloning artifact	UNP Q8DW17
B	371	GLU	-	cloning artifact	UNP Q8DW17
B	372	HIS	-	expression tag	UNP Q8DW17
B	373	HIS	-	expression tag	UNP Q8DW17
B	374	HIS	-	expression tag	UNP Q8DW17
B	375	HIS	-	expression tag	UNP Q8DW17
B	376	HIS	-	expression tag	UNP Q8DW17
B	377	HIS	-	expression tag	UNP Q8DW17
C	1	MSE	MET	modified residue	UNP Q8DW17
C	17	MSE	MET	modified residue	UNP Q8DW17
C	29	MSE	MET	modified residue	UNP Q8DW17
C	91	MSE	MET	modified residue	UNP Q8DW17
C	178	MSE	MET	modified residue	UNP Q8DW17
C	274	MSE	MET	modified residue	UNP Q8DW17
C	303	MSE	MET	modified residue	UNP Q8DW17
C	338	MSE	MET	modified residue	UNP Q8DW17
C	370	LEU	-	cloning artifact	UNP Q8DW17
C	371	GLU	-	cloning artifact	UNP Q8DW17
C	372	HIS	-	expression tag	UNP Q8DW17
C	373	HIS	-	expression tag	UNP Q8DW17
C	374	HIS	-	expression tag	UNP Q8DW17
C	375	HIS	-	expression tag	UNP Q8DW17
C	376	HIS	-	expression tag	UNP Q8DW17

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Chain	Residue	Modelled	Actual	Comment	Reference
C	377	HIS	-	expression tag	UNP Q8DW17
D	1	MSE	MET	modified residue	UNP Q8DW17
D	17	MSE	MET	modified residue	UNP Q8DW17
D	29	MSE	MET	modified residue	UNP Q8DW17
D	91	MSE	MET	modified residue	UNP Q8DW17
D	178	MSE	MET	modified residue	UNP Q8DW17
D	274	MSE	MET	modified residue	UNP Q8DW17
D	303	MSE	MET	modified residue	UNP Q8DW17
D	338	MSE	MET	modified residue	UNP Q8DW17
D	370	LEU	-	cloning artifact	UNP Q8DW17
D	371	GLU	-	cloning artifact	UNP Q8DW17
D	372	HIS	-	expression tag	UNP Q8DW17
D	373	HIS	-	expression tag	UNP Q8DW17
D	374	HIS	-	expression tag	UNP Q8DW17
D	375	HIS	-	expression tag	UNP Q8DW17
D	376	HIS	-	expression tag	UNP Q8DW17
D	377	HIS	-	expression tag	UNP Q8DW17
E	1	MSE	MET	modified residue	UNP Q8DW17
E	17	MSE	MET	modified residue	UNP Q8DW17
E	29	MSE	MET	modified residue	UNP Q8DW17
E	91	MSE	MET	modified residue	UNP Q8DW17
E	178	MSE	MET	modified residue	UNP Q8DW17
E	274	MSE	MET	modified residue	UNP Q8DW17
E	303	MSE	MET	modified residue	UNP Q8DW17
E	338	MSE	MET	modified residue	UNP Q8DW17
E	370	LEU	-	cloning artifact	UNP Q8DW17
E	371	GLU	-	cloning artifact	UNP Q8DW17
E	372	HIS	-	expression tag	UNP Q8DW17
E	373	HIS	-	expression tag	UNP Q8DW17
E	374	HIS	-	expression tag	UNP Q8DW17
E	375	HIS	-	expression tag	UNP Q8DW17
E	376	HIS	-	expression tag	UNP Q8DW17
E	377	HIS	-	expression tag	UNP Q8DW17
F	1	MSE	MET	modified residue	UNP Q8DW17
F	17	MSE	MET	modified residue	UNP Q8DW17
F	29	MSE	MET	modified residue	UNP Q8DW17
F	91	MSE	MET	modified residue	UNP Q8DW17
F	178	MSE	MET	modified residue	UNP Q8DW17
F	274	MSE	MET	modified residue	UNP Q8DW17
F	303	MSE	MET	modified residue	UNP Q8DW17
F	338	MSE	MET	modified residue	UNP Q8DW17
F	370	LEU	-	cloning artifact	UNP Q8DW17

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Chain	Residue	Modelled	Actual	Comment	Reference
F	371	GLU	-	cloning artifact	UNP Q8DW17
F	372	HIS	-	expression tag	UNP Q8DW17
F	373	HIS	-	expression tag	UNP Q8DW17
F	374	HIS	-	expression tag	UNP Q8DW17
F	375	HIS	-	expression tag	UNP Q8DW17
F	376	HIS	-	expression tag	UNP Q8DW17
F	377	HIS	-	expression tag	UNP Q8DW17
G	1	MSE	MET	modified residue	UNP Q8DW17
G	17	MSE	MET	modified residue	UNP Q8DW17
G	29	MSE	MET	modified residue	UNP Q8DW17
G	91	MSE	MET	modified residue	UNP Q8DW17
G	178	MSE	MET	modified residue	UNP Q8DW17
G	274	MSE	MET	modified residue	UNP Q8DW17
G	303	MSE	MET	modified residue	UNP Q8DW17
G	338	MSE	MET	modified residue	UNP Q8DW17
G	370	LEU	-	cloning artifact	UNP Q8DW17
G	371	GLU	-	cloning artifact	UNP Q8DW17
G	372	HIS	-	expression tag	UNP Q8DW17
G	373	HIS	-	expression tag	UNP Q8DW17
G	374	HIS	-	expression tag	UNP Q8DW17
G	375	HIS	-	expression tag	UNP Q8DW17
G	376	HIS	-	expression tag	UNP Q8DW17
G	377	HIS	-	expression tag	UNP Q8DW17
H	1	MSE	MET	modified residue	UNP Q8DW17
H	17	MSE	MET	modified residue	UNP Q8DW17
H	29	MSE	MET	modified residue	UNP Q8DW17
H	91	MSE	MET	modified residue	UNP Q8DW17
H	178	MSE	MET	modified residue	UNP Q8DW17
H	274	MSE	MET	modified residue	UNP Q8DW17
H	303	MSE	MET	modified residue	UNP Q8DW17
H	338	MSE	MET	modified residue	UNP Q8DW17
H	370	LEU	-	cloning artifact	UNP Q8DW17
H	371	GLU	-	cloning artifact	UNP Q8DW17
H	372	HIS	-	expression tag	UNP Q8DW17
H	373	HIS	-	expression tag	UNP Q8DW17
H	374	HIS	-	expression tag	UNP Q8DW17
H	375	HIS	-	expression tag	UNP Q8DW17
H	376	HIS	-	expression tag	UNP Q8DW17
H	377	HIS	-	expression tag	UNP Q8DW17
I	1	MSE	MET	modified residue	UNP Q8DW17
I	17	MSE	MET	modified residue	UNP Q8DW17
I	29	MSE	MET	modified residue	UNP Q8DW17

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Chain	Residue	Modelled	Actual	Comment	Reference
I	91	MSE	MET	modified residue	UNP Q8DW17
I	178	MSE	MET	modified residue	UNP Q8DW17
I	274	MSE	MET	modified residue	UNP Q8DW17
I	303	MSE	MET	modified residue	UNP Q8DW17
I	338	MSE	MET	modified residue	UNP Q8DW17
I	370	LEU	-	cloning artifact	UNP Q8DW17
I	371	GLU	-	cloning artifact	UNP Q8DW17
I	372	HIS	-	expression tag	UNP Q8DW17
I	373	HIS	-	expression tag	UNP Q8DW17
I	374	HIS	-	expression tag	UNP Q8DW17
I	375	HIS	-	expression tag	UNP Q8DW17
I	376	HIS	-	expression tag	UNP Q8DW17
I	377	HIS	-	expression tag	UNP Q8DW17
J	1	MSE	MET	modified residue	UNP Q8DW17
J	17	MSE	MET	modified residue	UNP Q8DW17
J	29	MSE	MET	modified residue	UNP Q8DW17
J	91	MSE	MET	modified residue	UNP Q8DW17
J	178	MSE	MET	modified residue	UNP Q8DW17
J	274	MSE	MET	modified residue	UNP Q8DW17
J	303	MSE	MET	modified residue	UNP Q8DW17
J	338	MSE	MET	modified residue	UNP Q8DW17
J	370	LEU	-	cloning artifact	UNP Q8DW17
J	371	GLU	-	cloning artifact	UNP Q8DW17
J	372	HIS	-	expression tag	UNP Q8DW17
J	373	HIS	-	expression tag	UNP Q8DW17
J	374	HIS	-	expression tag	UNP Q8DW17
J	375	HIS	-	expression tag	UNP Q8DW17
J	376	HIS	-	expression tag	UNP Q8DW17
J	377	HIS	-	expression tag	UNP Q8DW17
K	1	MSE	MET	modified residue	UNP Q8DW17
K	17	MSE	MET	modified residue	UNP Q8DW17
K	29	MSE	MET	modified residue	UNP Q8DW17
K	91	MSE	MET	modified residue	UNP Q8DW17
K	178	MSE	MET	modified residue	UNP Q8DW17
K	274	MSE	MET	modified residue	UNP Q8DW17
K	303	MSE	MET	modified residue	UNP Q8DW17
K	338	MSE	MET	modified residue	UNP Q8DW17
K	370	LEU	-	cloning artifact	UNP Q8DW17
K	371	GLU	-	cloning artifact	UNP Q8DW17
K	372	HIS	-	expression tag	UNP Q8DW17
K	373	HIS	-	expression tag	UNP Q8DW17
K	374	HIS	-	expression tag	UNP Q8DW17

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Chain	Residue	Modelled	Actual	Comment	Reference
K	375	HIS	-	expression tag	UNP Q8DW17
K	376	HIS	-	expression tag	UNP Q8DW17
K	377	HIS	-	expression tag	UNP Q8DW17
L	1	MSE	MET	modified residue	UNP Q8DW17
L	17	MSE	MET	modified residue	UNP Q8DW17
L	29	MSE	MET	modified residue	UNP Q8DW17
L	91	MSE	MET	modified residue	UNP Q8DW17
L	178	MSE	MET	modified residue	UNP Q8DW17
L	274	MSE	MET	modified residue	UNP Q8DW17
L	303	MSE	MET	modified residue	UNP Q8DW17
L	338	MSE	MET	modified residue	UNP Q8DW17
L	370	LEU	-	cloning artifact	UNP Q8DW17
L	371	GLU	-	cloning artifact	UNP Q8DW17
L	372	HIS	-	expression tag	UNP Q8DW17
L	373	HIS	-	expression tag	UNP Q8DW17
L	374	HIS	-	expression tag	UNP Q8DW17
L	375	HIS	-	expression tag	UNP Q8DW17
L	376	HIS	-	expression tag	UNP Q8DW17
L	377	HIS	-	expression tag	UNP Q8DW17

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	26	Total O 26 26	0	0
2	B	22	Total O 22 22	0	0
2	C	18	Total O 18 18	0	0
2	D	20	Total O 20 20	0	0
2	E	15	Total O 15 15	0	0
2	F	19	Total O 19 19	0	0
2	G	27	Total O 27 27	0	0
2	H	23	Total O 23 23	0	0
2	I	13	Total O 13 13	0	0
2	J	11	Total O 11 11	0	0

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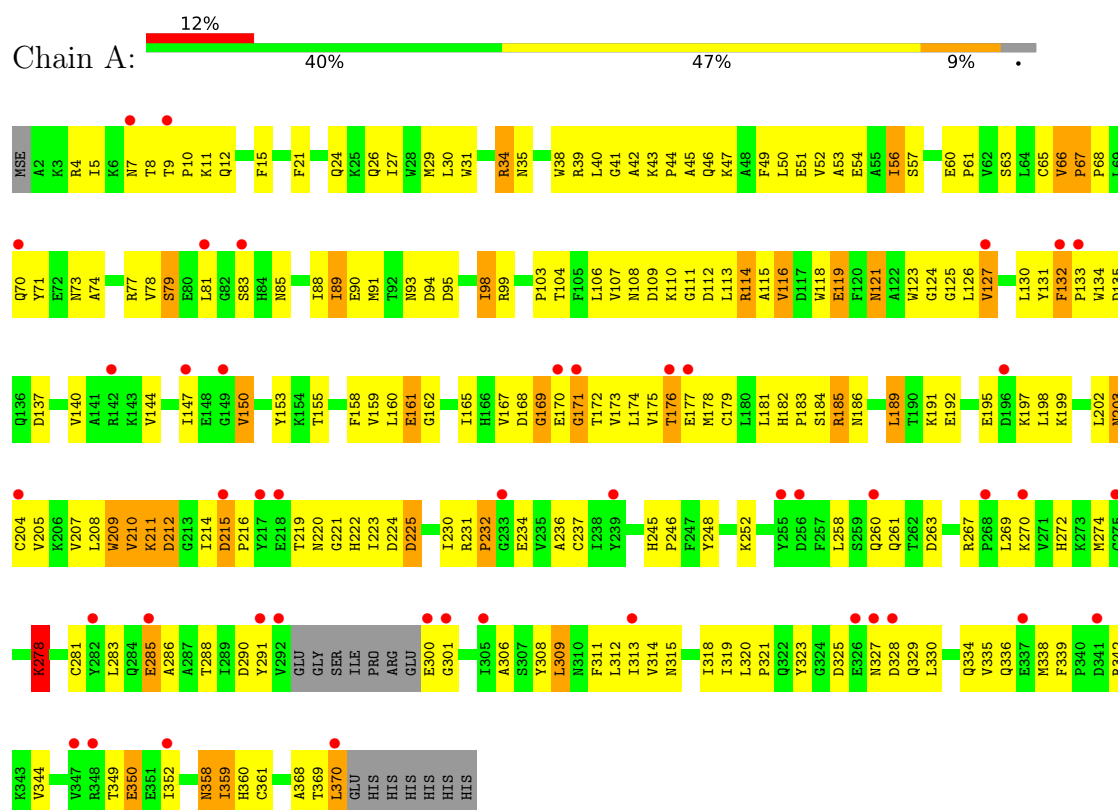
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	17	Total	O	0	0
			17	17		
2	L	13	Total	O	0	0
			13	13		

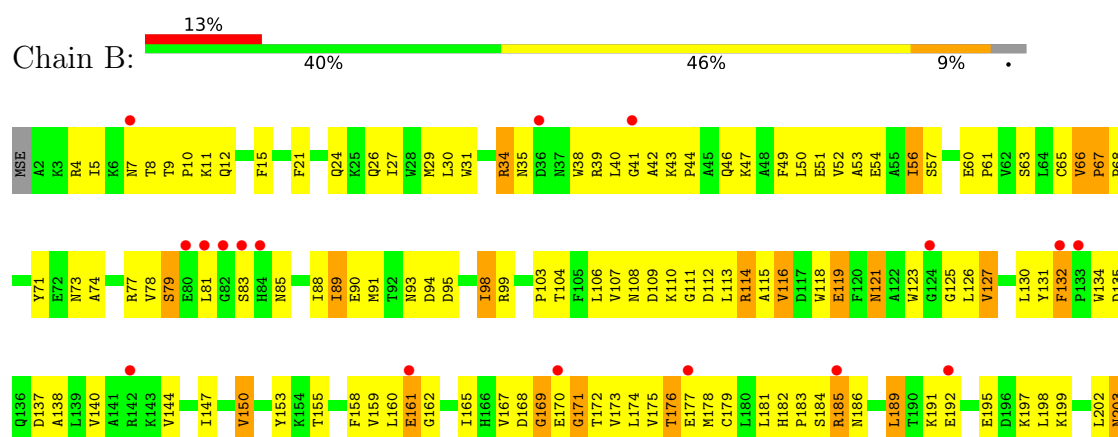
3 Residue-property plots

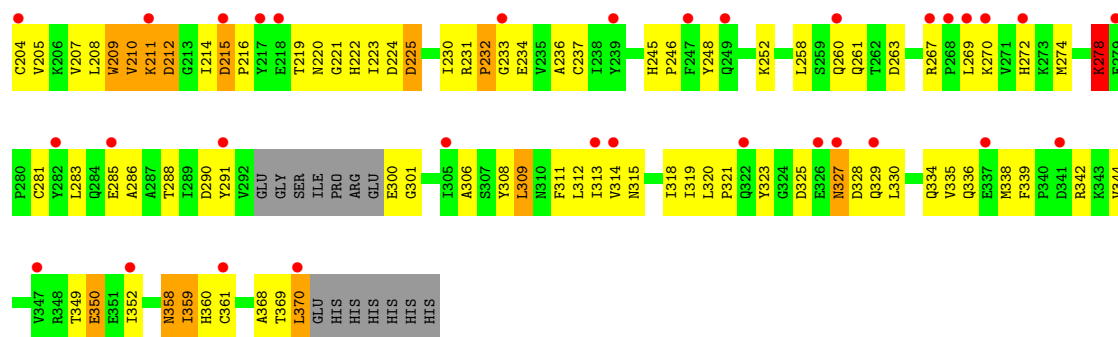
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Putative agmatine deiminase

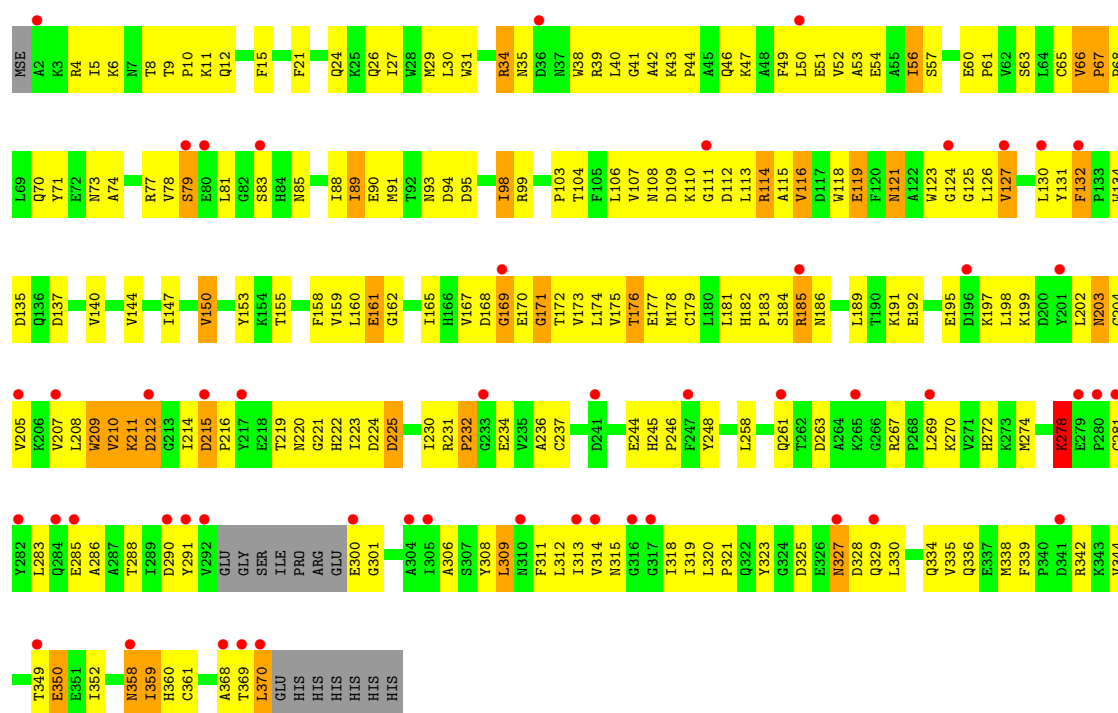
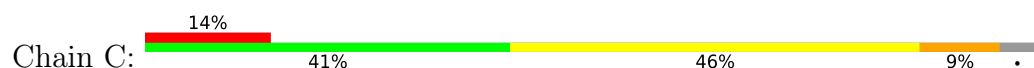


• Molecule 1: Putative agmatine deiminase

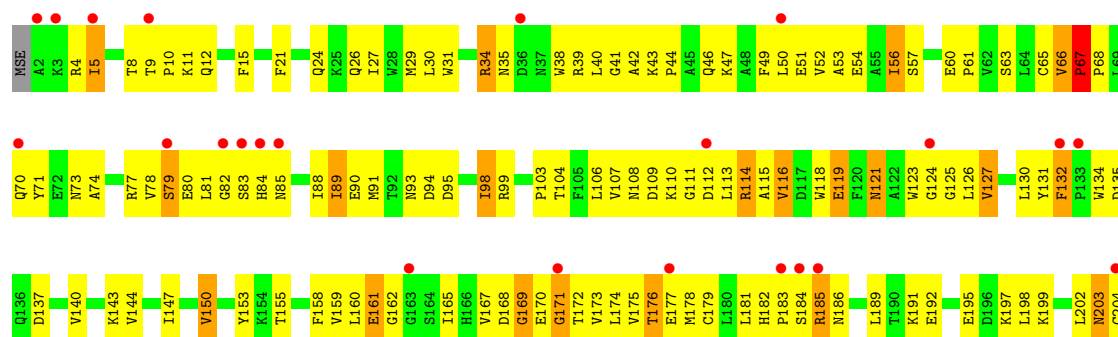


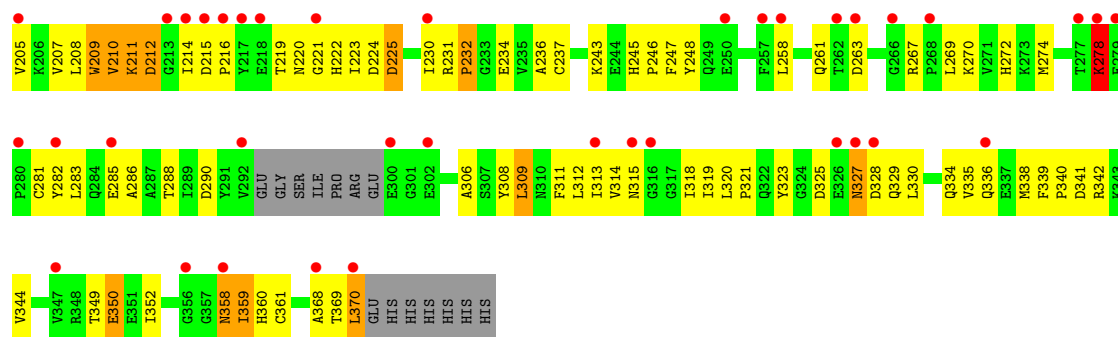


● Molecule 1: Putative agmatine deiminase

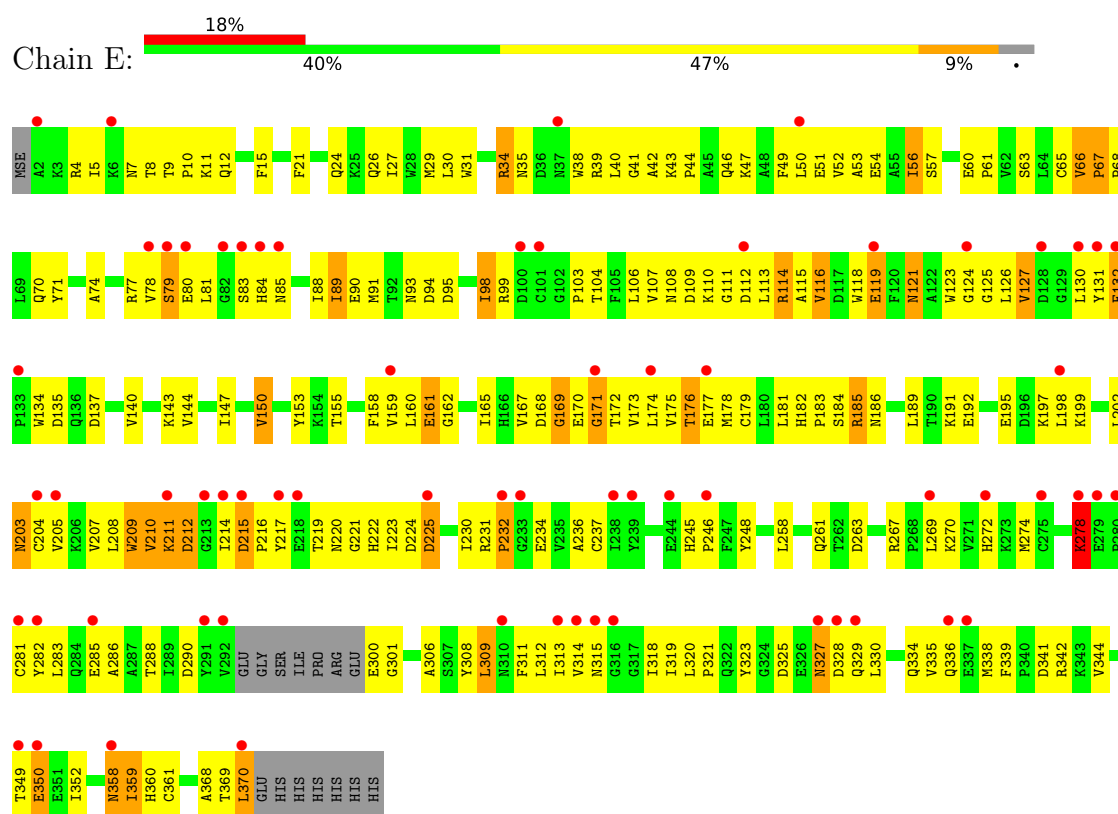


● Molecule 1: Putative agmatine deiminase

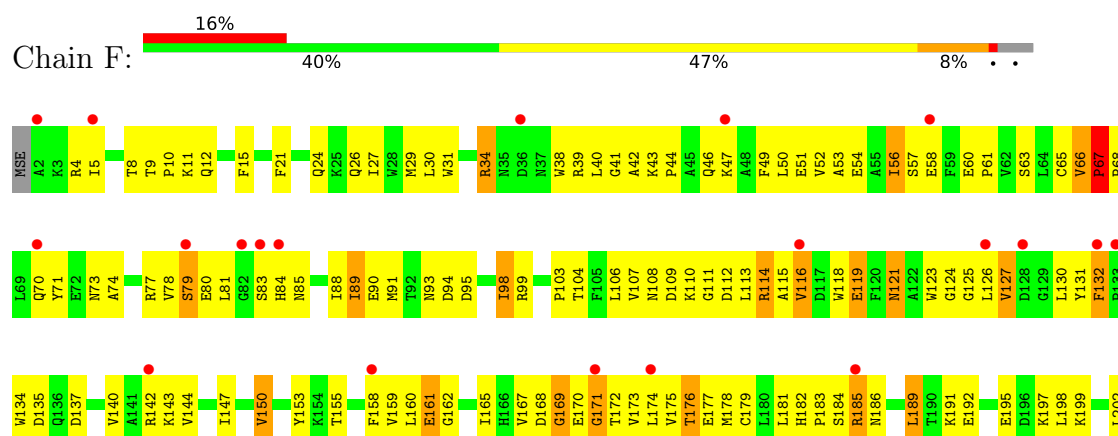


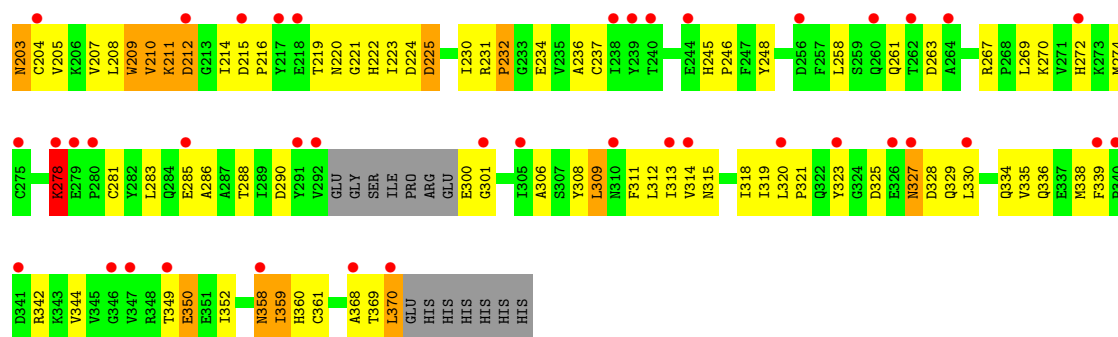


• Molecule 1: Putative agmatine deiminase

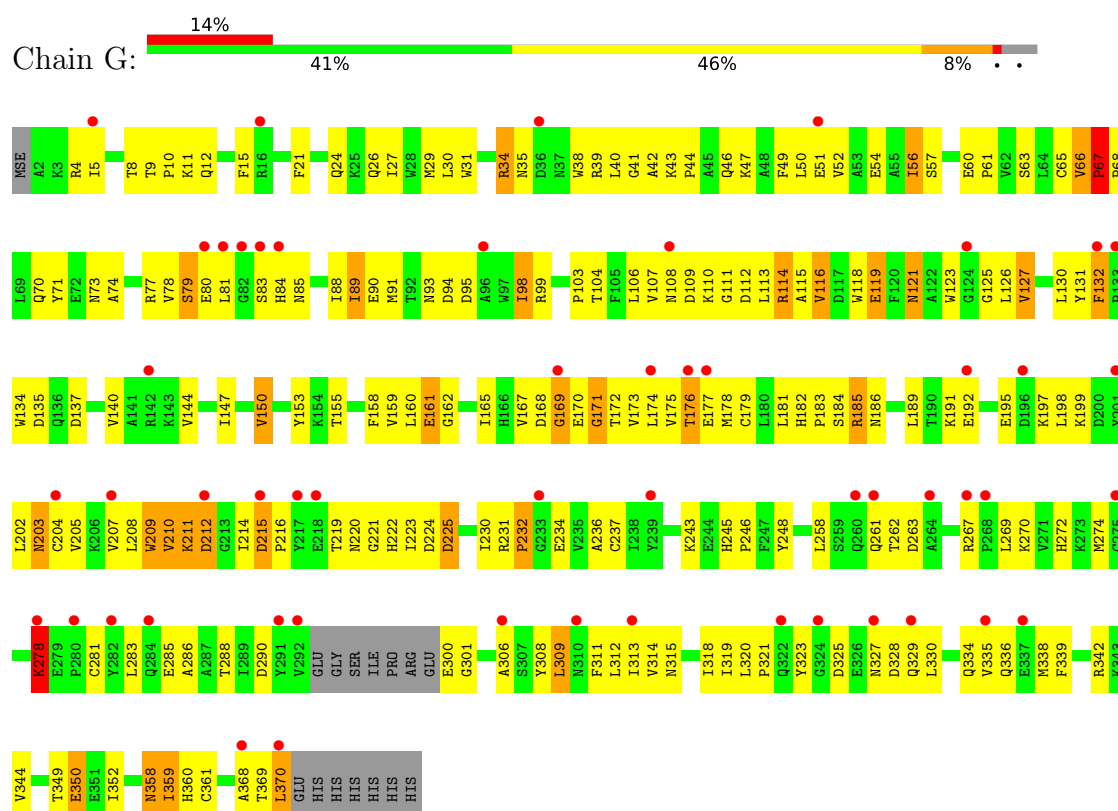


• Molecule 1: Putative agmatine deiminase

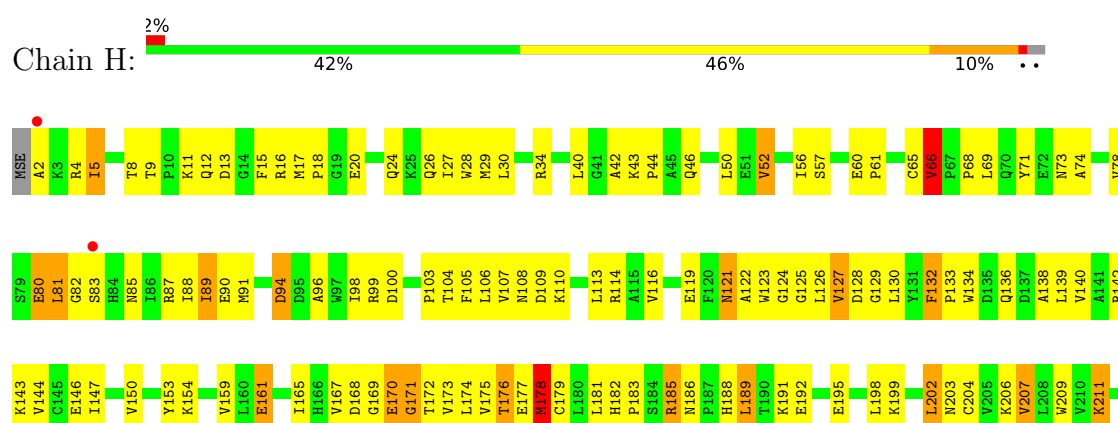


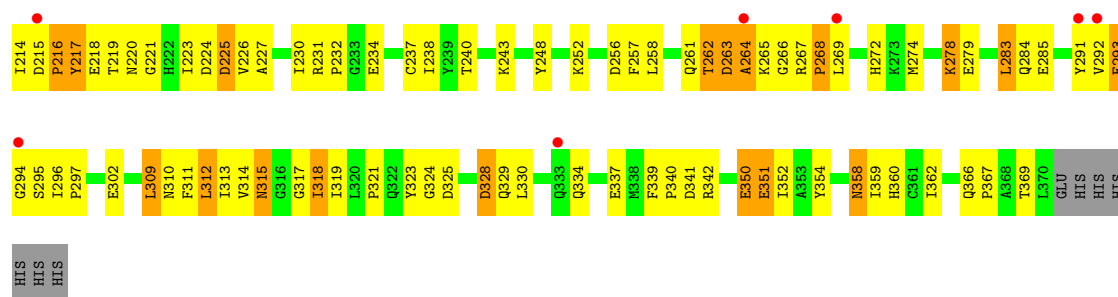


• Molecule 1: Putative agmatine deiminase

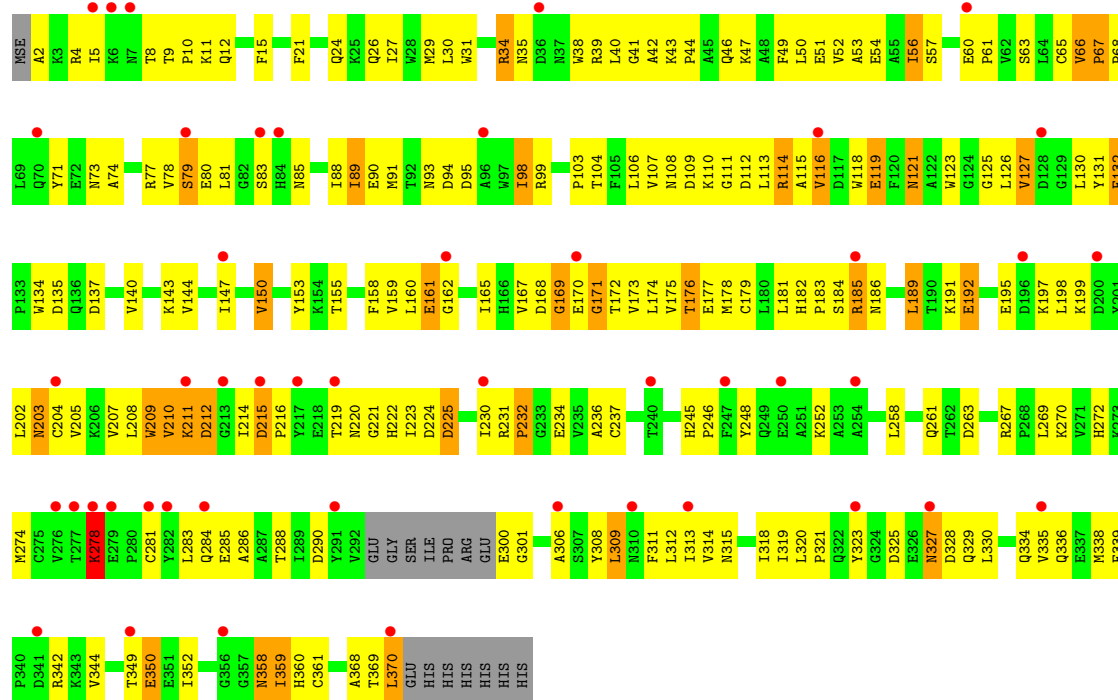
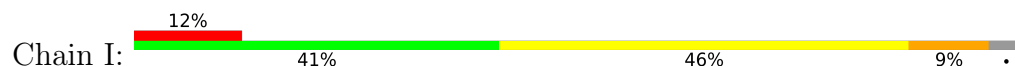


• Molecule 1: Putative agmatine deiminase

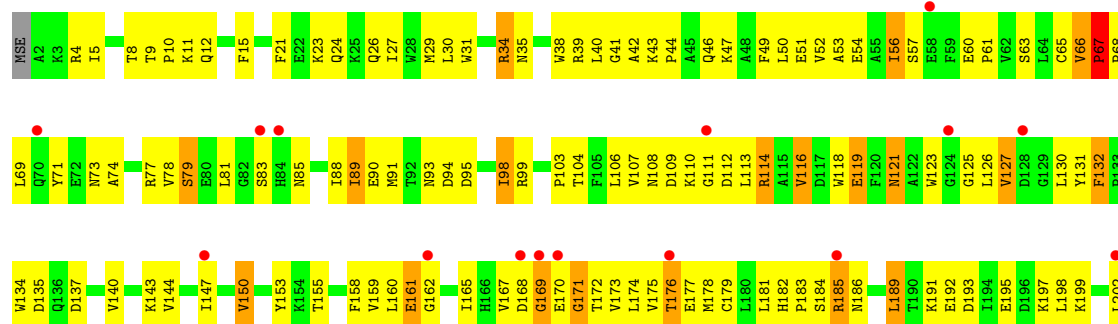


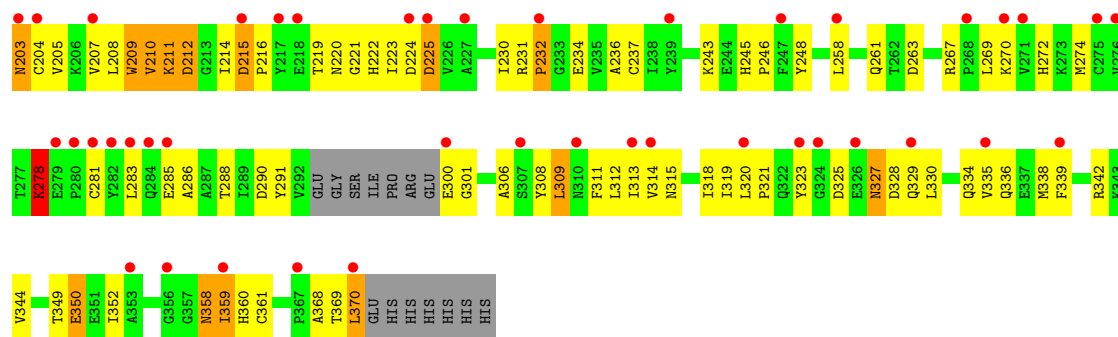


• Molecule 1: Putative agmatine deiminase

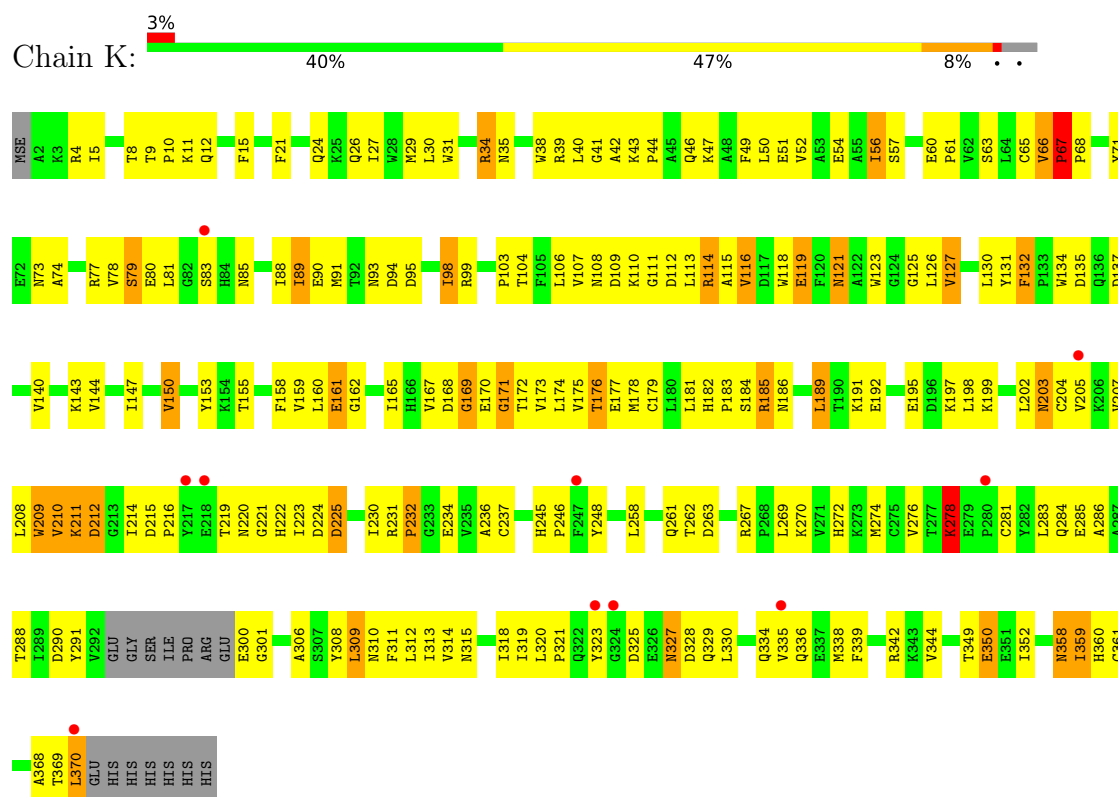


• Molecule 1: Putative agmatine deiminase

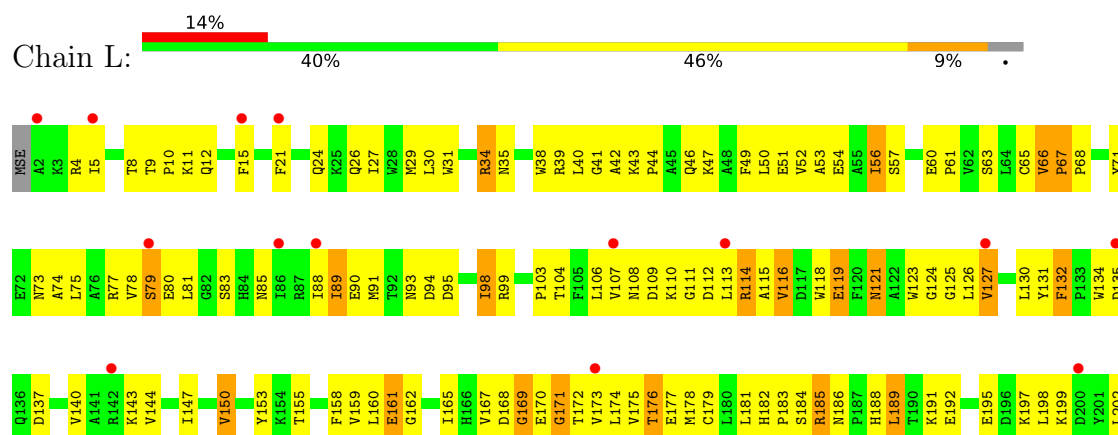


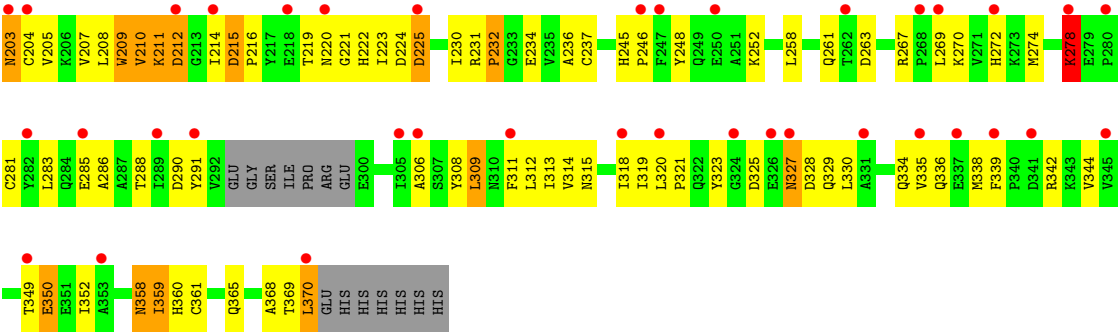


• Molecule 1: Putative agmatine deiminase



• Molecule 1: Putative agmatine deiminase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.52Å 203.69Å 139.54Å 90.00° 104.72° 90.00°	Depositor
Resolution (Å)	19.99 – 2.90 19.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	83.8 (19.99-2.90) 95.7 (19.99-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.269 0.280 , 0.305	Depositor DCC
R_{free} test set	10723 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 19.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	34934	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.58	4/2950 (0.1%)	0.99	12/3992 (0.3%)
1	B	0.58	4/2950 (0.1%)	0.99	12/3992 (0.3%)
1	C	0.58	4/2950 (0.1%)	0.99	12/3992 (0.3%)
1	D	0.58	4/2950 (0.1%)	0.99	10/3992 (0.3%)
1	E	0.58	4/2950 (0.1%)	0.99	12/3992 (0.3%)
1	F	0.58	4/2950 (0.1%)	0.99	10/3992 (0.3%)
1	G	0.58	4/2950 (0.1%)	0.99	12/3992 (0.3%)
1	H	0.59	0/3006	1.01	9/4069 (0.2%)
1	I	0.58	4/2950 (0.1%)	0.99	12/3992 (0.3%)
1	J	0.58	4/2950 (0.1%)	0.99	12/3992 (0.3%)
1	K	0.58	4/2950 (0.1%)	0.99	10/3992 (0.3%)
1	L	0.58	3/2950 (0.1%)	0.99	12/3992 (0.3%)
All	All	0.58	43/35456 (0.1%)	1.00	135/47981 (0.3%)

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	211	LYS	C-N	-5.92	1.26	1.33
1	J	211	LYS	C-N	-5.91	1.26	1.33
1	I	211	LYS	C-N	-5.91	1.26	1.33
1	L	211	LYS	C-N	-5.90	1.26	1.33
1	C	211	LYS	C-N	-5.89	1.26	1.33
1	G	211	LYS	C-N	-5.89	1.26	1.33
1	F	211	LYS	C-N	-5.88	1.26	1.33
1	K	211	LYS	C-N	-5.86	1.26	1.33
1	D	211	LYS	C-N	-5.85	1.26	1.33
1	E	211	LYS	C-N	-5.85	1.26	1.33
1	A	211	LYS	C-N	-5.83	1.26	1.33
1	F	209	TRP	NE1-CE2	-5.39	1.31	1.37
1	C	209	TRP	NE1-CE2	-5.38	1.31	1.37
1	E	209	TRP	NE1-CE2	-5.37	1.31	1.37
1	D	209	TRP	NE1-CE2	-5.33	1.31	1.37
1	A	209	TRP	NE1-CE2	-5.33	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	209	TRP	NE1-CE2	-5.31	1.31	1.37
1	B	209	TRP	NE1-CE2	-5.29	1.31	1.37
1	K	209	TRP	NE1-CE2	-5.29	1.31	1.37
1	G	209	TRP	NE1-CE2	-5.28	1.31	1.37
1	L	209	TRP	NE1-CE2	-5.28	1.31	1.37
1	I	209	TRP	NE1-CE2	-5.25	1.31	1.37
1	F	211	LYS	CG-CD	5.17	1.68	1.52
1	J	211	LYS	CG-CD	5.16	1.68	1.52
1	L	211	LYS	CG-CD	5.16	1.68	1.52
1	E	211	LYS	CG-CD	5.16	1.68	1.52
1	I	211	LYS	CG-CD	5.16	1.68	1.52
1	C	211	LYS	CG-CD	5.15	1.67	1.52
1	G	211	LYS	CG-CD	5.15	1.68	1.52
1	D	211	LYS	CG-CD	5.15	1.67	1.52
1	K	211	LYS	CG-CD	5.14	1.67	1.52
1	B	211	LYS	CG-CD	5.14	1.67	1.52
1	A	211	LYS	CG-CD	5.13	1.67	1.52
1	J	210	VAL	CA-C	-5.08	1.47	1.53
1	G	210	VAL	CA-C	-5.08	1.47	1.53
1	C	210	VAL	CA-C	-5.04	1.47	1.53
1	E	210	VAL	CA-C	-5.04	1.47	1.53
1	K	210	VAL	CA-C	-5.03	1.47	1.53
1	I	210	VAL	CA-C	-5.02	1.47	1.53
1	F	210	VAL	CA-C	-5.02	1.47	1.53
1	A	210	VAL	CA-C	-5.01	1.47	1.53
1	B	210	VAL	CA-C	-5.01	1.47	1.53
1	D	210	VAL	CA-C	-5.01	1.47	1.53

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	67	PRO	CA-C-N	7.49	128.15	119.47
1	F	67	PRO	C-N-CA	7.49	128.15	119.47
1	G	67	PRO	CA-C-N	7.45	128.12	119.47
1	G	67	PRO	C-N-CA	7.45	128.12	119.47
1	D	67	PRO	CA-C-N	7.45	128.11	119.47
1	D	67	PRO	C-N-CA	7.45	128.11	119.47
1	A	67	PRO	CA-C-N	7.45	128.11	119.47
1	A	67	PRO	C-N-CA	7.45	128.11	119.47
1	J	67	PRO	CA-C-N	7.45	128.11	119.47
1	J	67	PRO	C-N-CA	7.45	128.11	119.47
1	C	67	PRO	CA-C-N	7.44	128.09	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	67	PRO	C-N-CA	7.44	128.09	119.47
1	I	67	PRO	CA-C-N	7.43	128.09	119.47
1	I	67	PRO	C-N-CA	7.43	128.09	119.47
1	K	67	PRO	CA-C-N	7.43	128.09	119.47
1	K	67	PRO	C-N-CA	7.43	128.09	119.47
1	B	67	PRO	CA-C-N	7.40	128.06	119.47
1	B	67	PRO	C-N-CA	7.40	128.06	119.47
1	L	67	PRO	CA-C-N	7.39	128.04	119.47
1	L	67	PRO	C-N-CA	7.39	128.04	119.47
1	E	67	PRO	CA-C-N	7.38	128.03	119.47
1	E	67	PRO	C-N-CA	7.38	128.03	119.47
1	B	211	LYS	N-CA-C	7.21	122.10	112.30
1	E	211	LYS	N-CA-C	7.20	122.09	112.30
1	K	211	LYS	N-CA-C	7.17	122.05	112.30
1	J	211	LYS	N-CA-C	7.16	122.04	112.30
1	L	211	LYS	N-CA-C	7.16	122.03	112.30
1	I	211	LYS	N-CA-C	7.15	122.03	112.30
1	D	211	LYS	N-CA-C	7.15	122.03	112.30
1	G	211	LYS	N-CA-C	7.15	122.03	112.30
1	C	211	LYS	N-CA-C	7.15	122.02	112.30
1	A	211	LYS	N-CA-C	7.14	122.01	112.30
1	F	211	LYS	N-CA-C	7.11	121.97	112.30
1	H	268	PRO	N-CA-C	-6.83	101.56	111.33
1	H	66	VAL	CA-C-N	6.66	124.52	119.66
1	H	66	VAL	C-N-CA	6.66	124.52	119.66
1	H	178	MSE	N-CA-C	-6.06	105.85	113.18
1	H	350	GLU	N-CA-C	-5.90	104.77	111.14
1	L	210	VAL	CA-C-N	-5.86	112.36	122.14
1	L	210	VAL	C-N-CA	-5.86	112.36	122.14
1	F	210	VAL	CA-C-N	-5.83	112.41	122.14
1	F	210	VAL	C-N-CA	-5.83	112.41	122.14
1	B	210	VAL	CA-C-N	-5.83	112.41	122.14
1	B	210	VAL	C-N-CA	-5.83	112.41	122.14
1	C	210	VAL	CA-C-N	-5.83	112.41	122.14
1	C	210	VAL	C-N-CA	-5.83	112.41	122.14
1	A	210	VAL	CA-C-N	-5.82	112.42	122.14
1	A	210	VAL	C-N-CA	-5.82	112.42	122.14
1	G	210	VAL	CA-C-N	-5.81	112.43	122.14
1	G	210	VAL	C-N-CA	-5.81	112.43	122.14
1	K	210	VAL	CA-C-N	-5.81	112.44	122.14
1	K	210	VAL	C-N-CA	-5.81	112.44	122.14
1	J	210	VAL	CA-C-N	-5.80	112.45	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	210	VAL	C-N-CA	-5.80	112.45	122.14
1	D	210	VAL	CA-C-N	-5.79	112.47	122.14
1	D	210	VAL	C-N-CA	-5.79	112.47	122.14
1	E	210	VAL	CA-C-N	-5.79	112.47	122.14
1	E	210	VAL	C-N-CA	-5.79	112.47	122.14
1	I	210	VAL	CA-C-N	-5.76	112.52	122.14
1	I	210	VAL	C-N-CA	-5.76	112.52	122.14
1	C	278	LYS	N-CA-C	-5.67	106.35	113.72
1	K	278	LYS	N-CA-C	-5.67	106.35	113.72
1	H	324	GLY	N-CA-C	-5.66	105.13	114.76
1	F	278	LYS	N-CA-C	-5.66	106.36	113.72
1	J	278	LYS	N-CA-C	-5.66	106.36	113.72
1	I	212	ASP	N-CA-C	-5.66	99.71	108.42
1	A	278	LYS	N-CA-C	-5.66	106.37	113.72
1	C	212	ASP	N-CA-C	-5.66	99.71	108.42
1	L	212	ASP	N-CA-C	-5.65	99.72	108.42
1	A	212	ASP	N-CA-C	-5.65	99.72	108.42
1	K	212	ASP	N-CA-C	-5.65	99.72	108.42
1	I	278	LYS	N-CA-C	-5.64	106.38	113.72
1	B	278	LYS	N-CA-C	-5.64	106.39	113.72
1	D	278	LYS	N-CA-C	-5.64	106.39	113.72
1	G	212	ASP	N-CA-C	-5.64	99.73	108.42
1	E	212	ASP	N-CA-C	-5.64	99.73	108.42
1	G	278	LYS	N-CA-C	-5.64	106.39	113.72
1	B	212	ASP	N-CA-C	-5.64	99.74	108.42
1	E	278	LYS	N-CA-C	-5.63	106.39	113.72
1	F	212	ASP	N-CA-C	-5.63	99.74	108.42
1	L	278	LYS	N-CA-C	-5.63	106.39	113.72
1	D	212	ASP	N-CA-C	-5.63	99.75	108.42
1	J	212	ASP	N-CA-C	-5.60	99.79	108.42
1	K	211	LYS	CB-CA-C	-5.57	101.72	110.85
1	H	94	ASP	N-CA-C	-5.56	106.63	113.41
1	A	211	LYS	CB-CA-C	-5.56	101.74	110.85
1	E	211	LYS	CB-CA-C	-5.55	101.75	110.85
1	C	211	LYS	CB-CA-C	-5.55	101.75	110.85
1	D	211	LYS	CB-CA-C	-5.55	101.75	110.85
1	B	211	LYS	CB-CA-C	-5.54	101.76	110.85
1	F	211	LYS	CB-CA-C	-5.54	101.77	110.85
1	L	211	LYS	CB-CA-C	-5.54	101.77	110.85
1	H	170	GLU	N-CA-C	5.53	119.27	107.70
1	J	211	LYS	CB-CA-C	-5.53	101.79	110.85
1	G	211	LYS	CB-CA-C	-5.52	101.79	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	211	LYS	CB-CA-C	-5.50	101.83	110.85
1	G	79	SER	N-CA-C	-5.35	105.90	112.90
1	F	79	SER	N-CA-C	-5.35	105.90	112.90
1	K	79	SER	N-CA-C	-5.34	105.90	112.90
1	L	79	SER	N-CA-C	-5.34	105.90	112.90
1	J	79	SER	N-CA-C	-5.34	105.90	112.90
1	A	79	SER	N-CA-C	-5.34	105.91	112.90
1	E	79	SER	N-CA-C	-5.34	105.91	112.90
1	C	79	SER	N-CA-C	-5.31	105.94	112.90
1	I	79	SER	N-CA-C	-5.31	105.94	112.90
1	B	34	ARG	N-CA-C	5.31	118.01	110.10
1	D	79	SER	N-CA-C	-5.30	105.95	112.90
1	L	34	ARG	N-CA-C	5.30	118.00	110.10
1	B	79	SER	N-CA-C	-5.29	105.97	112.90
1	G	34	ARG	N-CA-C	5.29	117.97	110.10
1	H	268	PRO	O-C-N	-5.28	116.37	122.71
1	C	34	ARG	N-CA-C	5.26	117.94	110.10
1	E	34	ARG	N-CA-C	5.26	117.94	110.10
1	D	34	ARG	N-CA-C	5.26	117.94	110.10
1	I	34	ARG	N-CA-C	5.26	117.94	110.10
1	F	34	ARG	N-CA-C	5.26	117.93	110.10
1	A	34	ARG	N-CA-C	5.25	117.93	110.10
1	J	34	ARG	N-CA-C	5.25	117.93	110.10
1	K	34	ARG	N-CA-C	5.25	117.92	110.10
1	J	215	ASP	CA-C-N	5.03	126.13	119.84
1	J	215	ASP	C-N-CA	5.03	126.13	119.84
1	C	215	ASP	CA-C-N	5.02	126.12	119.84
1	C	215	ASP	C-N-CA	5.02	126.12	119.84
1	I	215	ASP	CA-C-N	5.02	126.11	119.84
1	I	215	ASP	C-N-CA	5.02	126.11	119.84
1	L	215	ASP	CA-C-N	5.02	126.11	119.84
1	L	215	ASP	C-N-CA	5.02	126.11	119.84
1	B	215	ASP	CA-C-N	5.01	126.10	119.84
1	B	215	ASP	C-N-CA	5.01	126.10	119.84
1	G	215	ASP	CA-C-N	5.01	126.10	119.84
1	G	215	ASP	C-N-CA	5.01	126.10	119.84
1	E	215	ASP	CA-C-N	5.00	126.09	119.84
1	E	215	ASP	C-N-CA	5.00	126.09	119.84
1	A	215	ASP	CA-C-N	5.00	126.09	119.84
1	A	215	ASP	C-N-CA	5.00	126.09	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2888	0	2800	239	8
1	B	2888	0	2800	209	11
1	C	2888	0	2800	207	2
1	D	2888	0	2800	260	6
1	E	2888	0	2800	209	19
1	F	2888	0	2800	230	2
1	G	2888	0	2800	214	5
1	H	2942	0	2852	220	2
1	I	2888	0	2800	214	3
1	J	2888	0	2800	212	8
1	K	2888	0	2800	211	3
1	L	2888	0	2800	209	1
2	A	26	0	0	10	0
2	B	22	0	0	5	0
2	C	18	0	0	5	0
2	D	20	0	0	9	0
2	E	15	0	0	5	0
2	F	19	0	0	6	0
2	G	27	0	0	13	0
2	H	23	0	0	6	0
2	I	13	0	0	3	0
2	J	11	0	0	5	0
2	K	17	0	0	4	0
2	L	13	0	0	4	0
All	All	34934	0	33652	2480	35

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 36.

All (2480) 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:A:7:ASN:ND2	1:D:84:HIS:CE1	1.86	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ASN:ND2	1:D:84:HIS:HE1	1.16	1.36
1:A:7:ASN:CG	1:D:84:HIS:CE1	2.06	1.33
1:A:7:ASN:CB	1:D:84:HIS:CE1	2.23	1.21
1:D:341:ASP:C	1:F:84:HIS:NE2	2.00	1.19
1:G:211:LYS:O	1:G:211:LYS:HG2	1.41	1.16
1:J:211:LYS:O	1:J:211:LYS:HG2	1.41	1.16
1:B:211:LYS:O	1:B:211:LYS:HG2	1.41	1.14
1:F:211:LYS:HG2	1:F:211:LYS:O	1.41	1.14
1:D:211:LYS:O	1:D:211:LYS:HG2	1.41	1.10
1:E:211:LYS:O	1:E:211:LYS:HG2	1.41	1.10
1:I:211:LYS:HG2	1:I:211:LYS:O	1.41	1.10
1:K:211:LYS:HG2	1:K:211:LYS:O	1.42	1.09
1:C:211:LYS:HG2	1:C:211:LYS:O	1.41	1.09
1:L:211:LYS:O	1:L:211:LYS:HG2	1.41	1.07
1:A:12:GLN:NE2	1:D:82:GLY:HA3	1.68	1.06
1:A:211:LYS:O	1:A:211:LYS:HG2	1.41	1.06
1:C:369:THR:HG23	1:C:370:LEU:N	1.71	1.06
1:A:7:ASN:CB	1:D:84:HIS:ND1	2.18	1.06
1:I:369:THR:HG23	1:I:370:LEU:N	1.71	1.06
1:J:369:THR:HG23	1:J:370:LEU:N	1.71	1.05
1:J:185:ARG:HH11	1:J:185:ARG:HB2	1.22	1.05
1:D:167:VAL:HB	2:D:391:HOH:O	1.56	1.05
1:A:185:ARG:HB2	1:A:185:ARG:HH11	1.22	1.05
1:A:369:THR:HG23	1:A:370:LEU:N	1.71	1.04
1:K:369:THR:HG23	1:K:370:LEU:N	1.71	1.04
1:D:185:ARG:HH11	1:D:185:ARG:HB2	1.22	1.03
1:I:185:ARG:HB2	1:I:185:ARG:HH11	1.22	1.03
1:J:167:VAL:HB	2:J:387:HOH:O	1.55	1.03
1:D:369:THR:HG23	1:D:370:LEU:N	1.71	1.03
1:E:185:ARG:HB2	1:E:185:ARG:HH11	1.22	1.03
1:B:369:THR:HG23	1:B:370:LEU:N	1.71	1.03
1:G:369:THR:HG23	1:G:370:LEU:N	1.71	1.03
1:F:185:ARG:HB2	1:F:185:ARG:HH11	1.22	1.02
1:L:185:ARG:HH11	1:L:185:ARG:HB2	1.22	1.02
1:G:185:ARG:HH11	1:G:185:ARG:HB2	1.22	1.02
1:B:185:ARG:HH11	1:B:185:ARG:HB2	1.22	1.02
1:K:185:ARG:HB2	1:K:185:ARG:HH11	1.22	1.02
1:L:369:THR:HG23	1:L:370:LEU:N	1.71	1.02
1:E:369:THR:HG23	1:E:370:LEU:N	1.71	1.01
1:F:369:THR:HG23	1:F:370:LEU:N	1.71	1.01
1:D:341:ASP:OD2	1:F:58:GLU:CB	2.08	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ARG:HB2	1:C:185:ARG:HH11	1.22	1.00
1:D:341:ASP:OD2	1:F:58:GLU:CA	2.09	1.00
1:A:7:ASN:HD22	1:D:84:HIS:CE1	1.71	1.00
1:D:342:ARG:N	1:F:84:HIS:NE2	2.08	1.00
1:I:2:ALA:HB2	2:I:384:HOH:O	1.61	1.00
1:A:7:ASN:HB3	1:D:84:HIS:ND1	1.77	1.00
1:D:341:ASP:HA	1:F:84:HIS:CD2	1.98	0.98
1:B:369:THR:HG23	1:B:370:LEU:H	1.26	0.98
1:C:70:GLN:HB3	2:C:382:HOH:O	1.62	0.98
1:G:11:LYS:HE3	2:G:389:HOH:O	1.61	0.98
1:H:358:ASN:HD22	1:H:359:ILE:H	1.12	0.98
1:A:7:ASN:HB2	1:D:84:HIS:CE1	1.95	0.97
1:E:369:THR:O	1:E:370:LEU:HB2	1.64	0.97
1:C:369:THR:HG23	1:C:370:LEU:H	1.26	0.97
1:D:369:THR:HG23	1:D:370:LEU:H	1.26	0.96
1:F:369:THR:HG23	1:F:370:LEU:H	1.26	0.96
1:D:341:ASP:HB3	1:F:58:GLU:HA	1.43	0.96
1:G:369:THR:O	1:G:370:LEU:HB2	1.64	0.96
1:I:369:THR:O	1:I:370:LEU:HB2	1.64	0.96
1:L:369:THR:HG23	1:L:370:LEU:H	1.26	0.96
1:A:369:THR:O	1:A:370:LEU:HB2	1.64	0.96
1:E:70:GLN:HB3	2:E:383:HOH:O	1.65	0.95
1:B:369:THR:O	1:B:370:LEU:HB2	1.64	0.95
1:K:369:THR:O	1:K:370:LEU:HB2	1.64	0.95
1:L:369:THR:O	1:L:370:LEU:HB2	1.64	0.95
1:F:369:THR:O	1:F:370:LEU:HB2	1.64	0.95
1:D:89:ILE:HG22	1:I:147:ILE:HG22	1.49	0.94
1:G:369:THR:HG23	1:G:370:LEU:H	1.26	0.94
1:D:341:ASP:OD2	1:F:58:GLU:HA	1.65	0.94
1:E:369:THR:CG2	1:E:370:LEU:H	1.81	0.94
1:B:369:THR:CG2	1:B:370:LEU:H	1.81	0.94
1:K:369:THR:CG2	1:K:370:LEU:H	1.81	0.94
1:A:369:THR:CG2	1:A:370:LEU:H	1.81	0.94
1:F:369:THR:CG2	1:F:370:LEU:H	1.81	0.93
1:L:369:THR:CG2	1:L:370:LEU:H	1.81	0.93
1:G:79:SER:HA	1:G:83:SER:HB2	1.51	0.93
1:J:369:THR:O	1:J:370:LEU:HB2	1.64	0.93
1:D:369:THR:O	1:D:370:LEU:HB2	1.64	0.93
1:C:369:THR:O	1:C:370:LEU:HB2	1.64	0.93
1:D:369:THR:CG2	1:D:370:LEU:H	1.81	0.93
1:I:369:THR:CG2	1:I:370:LEU:H	1.81	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:369:THR:CG2	1:G:370:LEU:H	1.81	0.93
1:J:369:THR:CG2	1:J:370:LEU:H	1.80	0.93
1:D:79:SER:HA	1:D:83:SER:HB2	1.51	0.92
1:D:147:ILE:HG22	1:I:89:ILE:HG22	1.50	0.92
1:B:79:SER:HA	1:B:83:SER:HB2	1.51	0.92
1:J:79:SER:HA	1:J:83:SER:HB2	1.51	0.92
1:K:79:SER:HA	1:K:83:SER:HB2	1.51	0.92
1:C:369:THR:CG2	1:C:370:LEU:H	1.81	0.92
1:J:369:THR:HG23	1:J:370:LEU:H	1.26	0.92
1:I:369:THR:HG23	1:I:370:LEU:H	1.26	0.92
1:E:147:ILE:HG22	1:K:89:ILE:HG22	1.50	0.91
1:A:369:THR:HG23	1:A:370:LEU:H	1.26	0.91
1:E:89:ILE:HG22	1:K:147:ILE:HG22	1.51	0.91
1:D:341:ASP:CA	1:F:84:HIS:CD2	2.52	0.91
1:L:79:SER:HA	1:L:83:SER:HB2	1.51	0.91
1:F:79:SER:HA	1:F:83:SER:HB2	1.51	0.90
1:L:47:LYS:HB3	2:L:388:HOH:O	1.70	0.90
1:C:79:SER:HA	1:C:83:SER:HB2	1.51	0.90
1:E:79:SER:HA	1:E:83:SER:HB2	1.51	0.90
1:K:369:THR:HG23	1:K:370:LEU:H	1.26	0.90
1:C:89:ILE:HG22	1:J:147:ILE:HG22	1.53	0.90
1:A:12:GLN:NE2	1:D:82:GLY:CA	2.34	0.90
1:E:369:THR:HG23	1:E:370:LEU:H	1.26	0.90
1:I:99:ARG:HD2	1:I:360:HIS:O	1.72	0.89
1:I:79:SER:HA	1:I:83:SER:HB2	1.51	0.89
1:E:99:ARG:HD2	1:E:360:HIS:O	1.72	0.89
1:B:99:ARG:HD2	1:B:360:HIS:O	1.72	0.89
1:A:99:ARG:HD2	1:A:360:HIS:O	1.72	0.89
1:A:79:SER:HA	1:A:83:SER:HB2	1.51	0.89
1:D:341:ASP:C	1:F:84:HIS:CD2	2.49	0.88
1:H:358:ASN:ND2	1:H:359:ILE:H	1.71	0.88
1:L:89:ILE:HD13	1:L:89:ILE:H	1.38	0.88
1:K:99:ARG:HD2	1:K:360:HIS:O	1.72	0.88
1:D:99:ARG:HD2	1:D:360:HIS:O	1.72	0.88
1:F:99:ARG:HD2	1:F:360:HIS:O	1.72	0.88
1:A:89:ILE:HD13	1:A:89:ILE:H	1.38	0.88
1:A:89:ILE:HG22	1:F:147:ILE:HG22	1.56	0.88
1:I:89:ILE:HD13	1:I:89:ILE:H	1.38	0.88
1:C:369:THR:CG2	1:C:370:LEU:N	2.37	0.88
1:G:99:ARG:HD2	1:G:360:HIS:O	1.72	0.88
1:J:89:ILE:HD13	1:J:89:ILE:H	1.39	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:99:ARG:HD2	1:J:360:HIS:O	1.72	0.88
1:A:211:LYS:O	1:A:211:LYS:CG	2.22	0.87
1:C:89:ILE:H	1:C:89:ILE:HD13	1.38	0.87
1:D:341:ASP:CB	1:F:58:GLU:HA	2.03	0.87
1:L:99:ARG:HD2	1:L:360:HIS:O	1.72	0.87
1:C:99:ARG:HD2	1:C:360:HIS:O	1.72	0.87
1:B:89:ILE:HD13	1:B:89:ILE:H	1.38	0.87
1:I:211:LYS:O	1:I:211:LYS:CG	2.22	0.87
1:E:89:ILE:HD13	1:E:89:ILE:H	1.38	0.87
1:G:89:ILE:HD13	1:G:89:ILE:H	1.38	0.87
1:D:89:ILE:HD13	1:D:89:ILE:H	1.38	0.86
1:D:243:LYS:NZ	1:H:192:GLU:HG3	1.90	0.86
1:H:61:PRO:HA	1:H:85:ASN:HD22	1.38	0.86
1:K:165:ILE:HG22	1:K:175:VAL:HG12	1.58	0.86
1:K:369:THR:CG2	1:K:370:LEU:N	2.37	0.86
1:D:247:PHE:HE2	2:D:390:HOH:O	1.59	0.86
1:E:165:ILE:HG22	1:E:175:VAL:HG12	1.58	0.86
1:D:341:ASP:CA	1:F:84:HIS:NE2	2.38	0.86
1:A:165:ILE:HG22	1:A:175:VAL:HG12	1.58	0.86
1:D:165:ILE:HG22	1:D:175:VAL:HG12	1.58	0.86
1:J:193:ASP:HA	2:J:381:HOH:O	1.75	0.86
1:B:90:GLU:OE2	1:G:90:GLU:OE2	1.94	0.85
1:C:211:LYS:O	1:C:211:LYS:CG	2.22	0.85
1:F:165:ILE:HG22	1:F:175:VAL:HG12	1.58	0.85
1:A:369:THR:CG2	1:A:370:LEU:N	2.37	0.85
1:K:89:ILE:H	1:K:89:ILE:HD13	1.39	0.85
1:I:165:ILE:HG22	1:I:175:VAL:HG12	1.58	0.85
1:G:165:ILE:HG22	1:G:175:VAL:HG12	1.58	0.85
1:B:165:ILE:HG22	1:B:175:VAL:HG12	1.58	0.85
1:C:165:ILE:HG22	1:C:175:VAL:HG12	1.58	0.85
1:D:211:LYS:O	1:D:211:LYS:CG	2.22	0.85
1:I:369:THR:CG2	1:I:370:LEU:N	2.37	0.85
1:J:165:ILE:HG22	1:J:175:VAL:HG12	1.58	0.85
1:F:89:ILE:H	1:F:89:ILE:HD13	1.38	0.85
1:F:369:THR:CG2	1:F:370:LEU:N	2.37	0.85
1:H:113:LEU:HB2	1:H:369:THR:HG21	1.57	0.85
1:K:41:GLY:HA3	1:L:41:GLY:HA3	1.59	0.84
1:L:211:LYS:O	1:L:211:LYS:CG	2.22	0.84
1:D:5:ILE:HD12	2:D:384:HOH:O	1.76	0.84
1:L:165:ILE:HG22	1:L:175:VAL:HG12	1.58	0.84
1:B:111:GLY:O	1:B:369:THR:OG1	1.96	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ILE:HG22	1:J:89:ILE:HG22	1.58	0.84
1:D:90:GLU:OE2	1:I:90:GLU:OE2	1.95	0.84
1:D:341:ASP:HA	1:F:84:HIS:NE2	1.92	0.83
1:C:111:GLY:O	1:C:369:THR:OG1	1.96	0.83
1:A:147:ILE:HG22	1:F:89:ILE:HG22	1.61	0.83
1:E:111:GLY:O	1:E:369:THR:OG1	1.96	0.83
1:B:185:ARG:HB2	1:B:185:ARG:NH1	1.94	0.82
1:H:43:LYS:HB2	1:H:44:PRO:HD3	1.61	0.82
1:H:65:CYS:SG	1:H:89:ILE:HD11	2.19	0.82
1:K:185:ARG:HB2	1:K:185:ARG:NH1	1.94	0.82
1:F:185:ARG:HB2	1:F:185:ARG:NH1	1.94	0.82
1:H:147:ILE:HG22	1:L:89:ILE:HG22	1.58	0.82
1:D:111:GLY:O	1:D:369:THR:OG1	1.96	0.82
1:I:111:GLY:O	1:I:369:THR:OG1	1.96	0.82
1:J:111:GLY:O	1:J:369:THR:OG1	1.96	0.82
1:E:185:ARG:HB2	1:E:185:ARG:NH1	1.94	0.82
1:F:111:GLY:O	1:F:369:THR:OG1	1.96	0.82
1:K:111:GLY:O	1:K:369:THR:OG1	1.96	0.82
1:D:185:ARG:HB2	1:D:185:ARG:NH1	1.94	0.81
1:I:185:ARG:HB2	1:I:185:ARG:NH1	1.94	0.81
1:L:111:GLY:O	1:L:369:THR:OG1	1.96	0.81
1:C:185:ARG:HB2	1:C:185:ARG:NH1	1.94	0.81
1:J:185:ARG:HB2	1:J:185:ARG:NH1	1.94	0.81
1:H:42:ALA:O	1:H:46:GLN:HG3	1.79	0.81
1:J:211:LYS:O	1:J:211:LYS:CG	2.22	0.81
1:G:185:ARG:HB2	1:G:185:ARG:NH1	1.94	0.81
1:L:185:ARG:HB2	1:L:185:ARG:NH1	1.94	0.81
1:A:111:GLY:O	1:A:369:THR:OG1	1.96	0.81
1:A:185:ARG:HB2	1:A:185:ARG:NH1	1.94	0.81
1:G:111:GLY:O	1:G:369:THR:OG1	1.96	0.80
1:A:7:ASN:CG	1:D:84:HIS:HE1	1.62	0.80
1:G:211:LYS:O	1:G:211:LYS:CG	2.22	0.80
1:E:90:GLU:OE2	1:K:90:GLU:OE2	1.99	0.80
1:E:127:VAL:HG11	2:E:386:HOH:O	1.80	0.80
1:C:90:GLU:OE2	1:J:90:GLU:OE2	2.00	0.79
1:D:341:ASP:CG	1:F:58:GLU:HA	2.07	0.79
1:H:165:ILE:HD13	1:H:202:LEU:HD21	1.64	0.79
1:A:90:GLU:OE2	1:F:90:GLU:OE2	2.00	0.79
1:D:126:LEU:HD12	1:J:126:LEU:HD12	1.64	0.79
1:D:341:ASP:OD2	1:F:58:GLU:HB2	1.83	0.79
1:E:211:LYS:O	1:E:211:LYS:CG	2.22	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:211:LYS:O	1:K:211:LYS:CG	2.22	0.79
1:G:70:GLN:HG3	2:G:383:HOH:O	1.83	0.78
1:B:107:VAL:HG22	1:B:109:ASP:H	1.49	0.78
1:L:107:VAL:HG22	1:L:109:ASP:H	1.49	0.78
1:D:67:PRO:HD3	2:D:385:HOH:O	1.83	0.77
1:D:70:GLN:HB3	2:D:387:HOH:O	1.84	0.77
1:C:171:GLY:HA2	1:C:204:CYS:HA	1.67	0.77
1:D:171:GLY:HA2	1:D:204:CYS:HA	1.67	0.77
1:E:107:VAL:HG22	1:E:109:ASP:H	1.49	0.77
1:F:171:GLY:HA2	1:F:204:CYS:HA	1.67	0.77
1:G:107:VAL:HG22	1:G:109:ASP:H	1.49	0.77
1:H:185:ARG:HB2	1:H:185:ARG:HH11	1.47	0.77
1:H:43:LYS:HZ1	1:H:46:GLN:HE22	1.32	0.77
1:J:171:GLY:HA2	1:J:204:CYS:HA	1.67	0.77
1:A:171:GLY:HA2	1:A:204:CYS:HA	1.67	0.77
1:E:171:GLY:HA2	1:E:204:CYS:HA	1.67	0.77
1:G:199:LYS:HD2	2:G:399:HOH:O	1.85	0.77
1:I:171:GLY:HA2	1:I:204:CYS:HA	1.67	0.77
1:K:107:VAL:HG22	1:K:109:ASP:H	1.49	0.77
1:H:132:PHE:HB3	1:H:133:PRO:HD3	1.64	0.76
1:A:41:GLY:HA3	1:G:41:GLY:HA3	1.67	0.76
1:C:315:ASN:HB3	2:C:390:HOH:O	1.85	0.76
1:H:24:GLN:H	1:H:315:ASN:ND2	1.84	0.76
1:F:26:GLN:HB3	1:F:61:PRO:HG2	1.68	0.76
1:A:107:VAL:HG22	1:A:109:ASP:H	1.49	0.76
1:B:274:MSE:HE1	1:B:335:VAL:HG12	1.68	0.76
1:I:274:MSE:HE1	1:I:335:VAL:HG12	1.68	0.76
1:J:107:VAL:HG22	1:J:109:ASP:H	1.49	0.76
1:A:274:MSE:HE1	1:A:335:VAL:HG12	1.68	0.76
1:E:274:MSE:HE1	1:E:335:VAL:HG12	1.68	0.76
1:G:274:MSE:HE1	1:G:335:VAL:HG12	1.68	0.76
1:I:26:GLN:HB3	1:I:61:PRO:HG2	1.68	0.76
1:J:274:MSE:HE1	1:J:335:VAL:HG12	1.68	0.76
1:G:121:ASN:HD22	1:G:121:ASN:H	1.34	0.76
1:K:274:MSE:HE1	1:K:335:VAL:HG12	1.68	0.76
1:F:107:VAL:HG22	1:F:109:ASP:H	1.49	0.75
1:L:171:GLY:HA2	1:L:204:CYS:HA	1.67	0.75
1:D:274:MSE:HE1	1:D:335:VAL:HG12	1.68	0.75
1:L:274:MSE:HE1	1:L:335:VAL:HG12	1.68	0.75
1:B:171:GLY:HA2	1:B:204:CYS:HA	1.67	0.75
1:G:171:GLY:HA2	1:G:204:CYS:HA	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:VAL:HG22	1:C:109:ASP:H	1.49	0.75
1:B:41:GLY:HA3	1:F:41:GLY:HA3	1.69	0.75
1:D:107:VAL:HG22	1:D:109:ASP:H	1.49	0.75
1:I:107:VAL:HG22	1:I:109:ASP:H	1.49	0.75
1:F:126:LEU:HD12	1:G:126:LEU:HD12	1.67	0.75
1:F:274:MSE:HE1	1:F:335:VAL:HG12	1.68	0.75
1:L:26:GLN:HB3	1:L:61:PRO:HG2	1.68	0.75
1:A:70:GLN:HB3	2:A:380:HOH:O	1.86	0.74
1:K:171:GLY:HA2	1:K:204:CYS:HA	1.67	0.74
1:A:12:GLN:HE21	1:D:82:GLY:HA3	1.52	0.74
1:A:26:GLN:HB3	1:A:61:PRO:HG2	1.68	0.74
1:B:26:GLN:HB3	1:B:61:PRO:HG2	1.68	0.74
1:E:26:GLN:HB3	1:E:61:PRO:HG2	1.68	0.74
1:E:121:ASN:H	1:E:121:ASN:HD22	1.34	0.74
1:E:127:VAL:CG1	2:E:386:HOH:O	2.33	0.74
1:C:26:GLN:HB3	1:C:61:PRO:HG2	1.68	0.74
1:G:26:GLN:HB3	1:G:61:PRO:HG2	1.68	0.74
1:B:369:THR:CG2	1:B:370:LEU:N	2.37	0.74
1:C:274:MSE:HE1	1:C:335:VAL:HG12	1.68	0.74
1:F:121:ASN:H	1:F:121:ASN:HD22	1.34	0.74
1:K:26:GLN:HB3	1:K:61:PRO:HG2	1.68	0.74
1:K:121:ASN:H	1:K:121:ASN:HD22	1.34	0.74
1:D:26:GLN:HB3	1:D:61:PRO:HG2	1.68	0.74
1:H:188:HIS:ND1	1:H:189:LEU:HD13	2.03	0.74
1:L:121:ASN:HD22	1:L:121:ASN:H	1.34	0.74
1:C:121:ASN:H	1:C:121:ASN:HD22	1.34	0.73
1:I:234:GLU:HG2	1:I:270:LYS:HB3	1.70	0.73
1:J:26:GLN:HB3	1:J:61:PRO:HG2	1.68	0.73
1:K:234:GLU:HG2	1:K:270:LYS:HB3	1.70	0.73
1:B:211:LYS:O	1:B:211:LYS:CG	2.22	0.73
1:D:135:ASP:HB3	1:J:132:PHE:CE2	2.23	0.73
1:A:234:GLU:HG2	1:A:270:LYS:HB3	1.70	0.73
1:G:336:GLN:HG2	2:G:404:HOH:O	1.87	0.73
1:B:89:ILE:HG22	1:G:147:ILE:HG22	1.69	0.73
1:D:234:GLU:HG2	1:D:270:LYS:HB3	1.70	0.73
1:A:168:ASP:OD1	1:A:172:THR:HB	1.89	0.73
1:F:211:LYS:O	1:F:211:LYS:CG	2.22	0.73
1:I:41:GLY:HA3	1:J:41:GLY:HA3	1.70	0.73
1:H:89:ILE:H	1:H:89:ILE:HD13	1.53	0.73
1:H:123:TRP:CE3	1:H:130:LEU:HD22	2.24	0.73
1:L:168:ASP:OD1	1:L:172:THR:HB	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:GLU:HG2	1:E:270:LYS:HB3	1.70	0.73
1:F:168:ASP:OD1	1:F:172:THR:HB	1.89	0.73
1:G:234:GLU:HG2	1:G:270:LYS:HB3	1.70	0.73
1:J:121:ASN:HD22	1:J:121:ASN:H	1.34	0.73
1:A:121:ASN:HD22	1:A:121:ASN:H	1.34	0.72
1:B:121:ASN:HD22	1:B:121:ASN:H	1.34	0.72
1:D:121:ASN:HD22	1:D:121:ASN:H	1.34	0.72
1:G:369:THR:CG2	1:G:370:LEU:N	2.37	0.72
1:I:168:ASP:OD1	1:I:172:THR:HB	1.89	0.72
1:C:234:GLU:HG2	1:C:270:LYS:HB3	1.70	0.72
1:H:89:ILE:HG22	1:L:147:ILE:HG22	1.70	0.72
1:H:165:ILE:HG22	1:H:175:VAL:HG12	1.69	0.72
1:B:234:GLU:HG2	1:B:270:LYS:HB3	1.70	0.72
1:B:290:ASP:HB3	1:F:73:ASN:ND2	2.05	0.72
1:C:168:ASP:OD1	1:C:172:THR:HB	1.89	0.72
1:E:126:LEU:HD12	1:L:126:LEU:HD12	1.71	0.72
1:D:168:ASP:OD1	1:D:172:THR:HB	1.89	0.72
1:D:243:LYS:HZ1	1:H:192:GLU:HG3	1.53	0.72
1:B:168:ASP:OD1	1:B:172:THR:HB	1.89	0.72
1:I:121:ASN:HD22	1:I:121:ASN:H	1.34	0.72
1:K:73:ASN:ND2	1:L:290:ASP:HB3	2.03	0.72
1:L:234:GLU:HG2	1:L:270:LYS:HB3	1.70	0.72
1:F:234:GLU:HG2	1:F:270:LYS:HB3	1.70	0.72
1:G:168:ASP:OD1	1:G:172:THR:HB	1.89	0.72
1:H:318:ILE:HD13	1:H:342:ARG:HD3	1.72	0.71
1:J:168:ASP:OD1	1:J:172:THR:HB	1.89	0.71
1:A:45:ALA:HB2	2:A:395:HOH:O	1.89	0.71
1:H:99:ARG:HD2	1:H:360:HIS:O	1.89	0.71
1:E:168:ASP:OD1	1:E:172:THR:HB	1.89	0.71
1:D:93:ASN:ND2	2:D:385:HOH:O	2.21	0.71
1:F:349:THR:HG21	1:F:359:ILE:HG12	1.73	0.71
1:K:168:ASP:OD1	1:K:172:THR:HB	1.89	0.71
1:L:349:THR:HG21	1:L:359:ILE:HG12	1.73	0.71
1:E:24:GLN:H	1:E:315:ASN:HD22	1.39	0.71
1:H:159:VAL:H	1:H:186:ASN:HD21	1.37	0.71
1:E:349:THR:HG21	1:E:359:ILE:HG12	1.73	0.71
1:G:349:THR:HG21	1:G:359:ILE:HG12	1.73	0.71
1:J:234:GLU:HG2	1:J:270:LYS:HB3	1.70	0.71
1:K:24:GLN:H	1:K:315:ASN:HD22	1.39	0.71
1:B:147:ILE:HG22	1:G:89:ILE:HG22	1.72	0.70
1:D:24:GLN:H	1:D:315:ASN:HD22	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:GLN:H	1:B:315:ASN:HD22	1.39	0.70
1:A:349:THR:HG21	1:A:359:ILE:HG12	1.73	0.70
1:H:274:MSE:HE3	1:H:309:LEU:HD22	1.72	0.70
1:H:24:GLN:H	1:H:315:ASN:HD22	1.38	0.70
1:A:12:GLN:CD	1:D:82:GLY:HA2	2.16	0.70
1:D:159:VAL:H	1:D:186:ASN:HD21	1.40	0.70
1:H:121:ASN:H	1:H:121:ASN:HD22	1.38	0.70
1:A:24:GLN:H	1:A:315:ASN:HD22	1.39	0.70
1:B:349:THR:HG21	1:B:359:ILE:HG12	1.73	0.70
1:C:24:GLN:H	1:C:315:ASN:HD22	1.39	0.70
1:K:349:THR:HG21	1:K:359:ILE:HG12	1.72	0.70
1:H:178:MSE:HG2	2:H:398:HOH:O	1.92	0.69
1:J:349:THR:HG21	1:J:359:ILE:HG12	1.73	0.69
1:I:349:THR:HG21	1:I:359:ILE:HG12	1.73	0.69
1:J:24:GLN:H	1:J:315:ASN:HD22	1.39	0.69
1:L:283:LEU:HD12	1:L:286:ALA:HB2	1.75	0.69
1:A:135:ASP:HB3	1:B:132:PHE:CE2	2.27	0.69
1:H:43:LYS:NZ	1:H:46:GLN:HE22	1.89	0.69
1:B:159:VAL:H	1:B:186:ASN:HD21	1.40	0.69
1:D:349:THR:HG21	1:D:359:ILE:HG12	1.73	0.69
1:F:159:VAL:H	1:F:186:ASN:HD21	1.40	0.69
1:L:24:GLN:H	1:L:315:ASN:HD22	1.39	0.69
1:C:349:THR:HG21	1:C:359:ILE:HG12	1.73	0.69
1:K:283:LEU:HD12	1:K:286:ALA:HB2	1.74	0.69
1:C:283:LEU:HD12	1:C:286:ALA:HB2	1.75	0.69
1:D:283:LEU:HD12	1:D:286:ALA:HB2	1.75	0.69
1:I:159:VAL:H	1:I:186:ASN:HD21	1.40	0.69
1:K:159:VAL:H	1:K:186:ASN:HD21	1.40	0.69
1:L:159:VAL:H	1:L:186:ASN:HD21	1.40	0.69
1:E:80:GLU:CD	1:H:291:TYR:OH	2.36	0.69
1:C:135:ASP:HB3	1:I:132:PHE:CE2	2.28	0.68
1:G:27:ILE:HD12	1:G:56:ILE:HG21	1.76	0.68
1:K:27:ILE:HD12	1:K:56:ILE:HG21	1.75	0.68
1:A:283:LEU:HD12	1:A:286:ALA:HB2	1.75	0.68
1:D:247:PHE:CE2	2:D:390:HOH:O	2.38	0.68
1:F:24:GLN:H	1:F:315:ASN:HD22	1.39	0.68
1:E:24:GLN:HG3	1:E:60:GLU:OE1	1.94	0.68
1:I:24:GLN:HG3	1:I:60:GLU:OE1	1.94	0.68
1:J:159:VAL:H	1:J:186:ASN:HD21	1.40	0.68
1:K:290:ASP:HB3	1:L:73:ASN:ND2	2.09	0.68
1:C:159:VAL:H	1:C:186:ASN:HD21	1.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:GLN:HG3	1:D:60:GLU:OE1	1.94	0.68
1:G:24:GLN:H	1:G:315:ASN:HD22	1.39	0.68
1:H:123:TRP:HB2	1:H:130:LEU:HD13	1.73	0.68
1:I:27:ILE:HD12	1:I:56:ILE:HG21	1.76	0.68
1:A:27:ILE:HD12	1:A:56:ILE:HG21	1.75	0.68
1:E:135:ASP:HB3	1:L:132:PHE:CE2	2.28	0.68
1:A:24:GLN:HG3	1:A:60:GLU:OE1	1.94	0.68
1:B:27:ILE:HD12	1:B:56:ILE:HG21	1.76	0.68
1:A:159:VAL:H	1:A:186:ASN:HD21	1.40	0.68
1:E:283:LEU:HD12	1:E:286:ALA:HB2	1.75	0.68
1:F:24:GLN:HG3	1:F:60:GLU:OE1	1.94	0.68
1:G:215:ASP:CG	2:G:401:HOH:O	2.37	0.68
1:G:283:LEU:HD12	1:G:286:ALA:HB2	1.75	0.68
1:B:283:LEU:HD12	1:B:286:ALA:HB2	1.74	0.68
1:E:27:ILE:HD12	1:E:56:ILE:HG21	1.75	0.68
1:G:261:GLN:NE2	2:G:392:HOH:O	2.26	0.68
1:I:24:GLN:HA	1:I:368:ALA:H	1.59	0.68
1:I:283:LEU:HD12	1:I:286:ALA:HB2	1.75	0.68
1:C:24:GLN:HG3	1:C:60:GLU:OE1	1.94	0.68
1:E:24:GLN:HA	1:E:368:ALA:H	1.59	0.68
1:F:283:LEU:HD12	1:F:286:ALA:HB2	1.75	0.68
1:B:24:GLN:HG3	1:B:60:GLU:OE1	1.94	0.67
1:E:159:VAL:H	1:E:186:ASN:HD21	1.40	0.67
1:D:24:GLN:HA	1:D:368:ALA:H	1.59	0.67
1:I:24:GLN:H	1:I:315:ASN:HD22	1.39	0.67
1:J:283:LEU:HD12	1:J:286:ALA:HB2	1.75	0.67
1:K:24:GLN:HG3	1:K:60:GLU:OE1	1.94	0.67
1:A:24:GLN:HA	1:A:368:ALA:H	1.59	0.67
1:D:27:ILE:HD12	1:D:56:ILE:HG21	1.76	0.67
1:F:24:GLN:HA	1:F:368:ALA:H	1.59	0.67
1:G:24:GLN:HA	1:G:368:ALA:H	1.59	0.67
1:J:24:GLN:HG3	1:J:60:GLU:OE1	1.94	0.67
1:L:24:GLN:HG3	1:L:60:GLU:OE1	1.94	0.67
1:F:27:ILE:HD12	1:F:56:ILE:HG21	1.76	0.67
1:J:27:ILE:HD12	1:J:56:ILE:HG21	1.75	0.67
1:A:290:ASP:HB3	1:G:73:ASN:ND2	2.09	0.67
1:C:24:GLN:HA	1:C:368:ALA:H	1.59	0.67
1:C:41:GLY:HA3	1:D:41:GLY:HA3	1.76	0.67
1:G:159:VAL:H	1:G:186:ASN:HD21	1.40	0.67
1:G:361:CYS:SG	2:G:393:HOH:O	2.53	0.67
1:K:24:GLN:HA	1:K:368:ALA:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:GLN:HG3	1:G:60:GLU:OE1	1.94	0.67
1:B:24:GLN:HA	1:B:368:ALA:H	1.60	0.66
1:C:27:ILE:HD12	1:C:56:ILE:HG21	1.76	0.66
1:I:73:ASN:ND2	1:J:290:ASP:HB3	2.10	0.66
1:A:132:PHE:CE2	1:B:135:ASP:HB3	2.29	0.66
1:J:24:GLN:HA	1:J:368:ALA:H	1.59	0.66
1:L:27:ILE:HD12	1:L:56:ILE:HG21	1.75	0.66
1:K:276:VAL:HG13	2:K:394:HOH:O	1.96	0.65
1:F:121:ASN:ND2	2:F:389:HOH:O	2.28	0.65
1:H:177:GLU:HB3	1:H:209:TRP:HE3	1.62	0.65
1:L:24:GLN:HA	1:L:368:ALA:H	1.59	0.65
1:A:315:ASN:HB3	2:A:379:HOH:O	1.97	0.65
1:H:198:LEU:HD22	1:H:202:LEU:HD22	1.78	0.65
1:C:9:THR:HG22	1:C:12:GLN:CD	2.23	0.64
1:A:121:ASN:ND2	2:A:392:HOH:O	2.30	0.64
1:A:133:PRO:HG2	2:A:390:HOH:O	1.96	0.64
1:C:290:ASP:HB3	1:D:73:ASN:ND2	2.11	0.64
1:A:9:THR:HG22	1:A:12:GLN:CD	2.23	0.64
1:D:29:MSE:HA	1:D:98:ILE:HG21	1.80	0.64
1:E:9:THR:HG22	1:E:12:GLN:CD	2.22	0.64
1:L:29:MSE:HA	1:L:98:ILE:HG21	1.80	0.64
1:E:29:MSE:HA	1:E:98:ILE:HG21	1.80	0.64
1:G:262:THR:HG22	2:G:392:HOH:O	1.95	0.64
1:L:9:THR:HG22	1:L:12:GLN:CD	2.23	0.64
1:A:135:ASP:HB3	1:B:132:PHE:CD2	2.33	0.64
1:B:29:MSE:HA	1:B:98:ILE:HG21	1.80	0.64
1:D:9:THR:HG22	1:D:12:GLN:CD	2.23	0.64
1:F:29:MSE:HA	1:F:98:ILE:HG21	1.80	0.64
1:I:9:THR:HG22	1:I:12:GLN:CD	2.23	0.64
1:K:9:THR:HG22	1:K:12:GLN:CD	2.23	0.64
1:J:71:TYR:N	2:J:386:HOH:O	2.31	0.63
1:D:191:LYS:O	1:D:195:GLU:HG3	1.99	0.63
1:I:27:ILE:HD11	1:I:314:VAL:HG12	1.81	0.63
1:J:9:THR:HG22	1:J:12:GLN:CD	2.23	0.63
1:K:29:MSE:HA	1:K:98:ILE:HG21	1.80	0.63
1:L:27:ILE:HD11	1:L:314:VAL:HG12	1.81	0.63
1:A:132:PHE:CD2	1:B:135:ASP:HB3	2.34	0.63
1:B:9:THR:HG22	1:B:12:GLN:CD	2.23	0.63
1:F:9:THR:HG22	1:F:12:GLN:CD	2.23	0.63
1:F:27:ILE:HD11	1:F:314:VAL:HG12	1.81	0.63
1:I:191:LYS:O	1:I:195:GLU:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:ILE:HD11	1:E:314:VAL:HG12	1.81	0.63
1:F:185:ARG:HH22	1:F:220:ASN:HD22	1.47	0.63
1:K:191:LYS:O	1:K:195:GLU:HG3	1.99	0.63
1:A:73:ASN:ND2	1:G:290:ASP:HB3	2.14	0.63
1:G:9:THR:HG22	1:G:12:GLN:CD	2.23	0.63
1:J:29:MSE:HA	1:J:98:ILE:HG21	1.80	0.63
1:K:185:ARG:HH22	1:K:220:ASN:HD22	1.47	0.63
1:B:191:LYS:O	1:B:195:GLU:HG3	1.99	0.63
1:I:29:MSE:HA	1:I:98:ILE:HG21	1.80	0.63
1:J:103:PRO:HD3	1:J:144:VAL:HG11	1.81	0.63
1:C:29:MSE:HA	1:C:98:ILE:HG21	1.80	0.63
1:J:27:ILE:HD11	1:J:314:VAL:HG12	1.80	0.63
1:A:29:MSE:HA	1:A:98:ILE:HG21	1.80	0.63
1:H:312:LEU:HD22	1:H:313:ILE:N	2.13	0.63
1:I:103:PRO:HD3	1:I:144:VAL:HG11	1.81	0.63
1:A:185:ARG:HH22	1:A:220:ASN:HD22	1.47	0.62
1:D:185:ARG:HG2	2:D:396:HOH:O	1.99	0.62
1:G:191:LYS:O	1:G:195:GLU:HG3	1.99	0.62
1:L:103:PRO:HD3	1:L:144:VAL:HG11	1.81	0.62
1:A:103:PRO:HD3	1:A:144:VAL:HG11	1.81	0.62
1:D:27:ILE:HD11	1:D:314:VAL:HG12	1.81	0.62
1:E:185:ARG:HH22	1:E:220:ASN:HD22	1.47	0.62
1:F:191:LYS:O	1:F:195:GLU:HG3	1.99	0.62
1:H:100:ASP:HB3	1:H:161:GLU:HB2	1.80	0.62
1:C:126:LEU:HD12	1:I:126:LEU:HD12	1.79	0.62
1:H:352:ILE:HD13	1:H:362:ILE:HD13	1.82	0.62
1:J:159:VAL:HG22	1:J:185:ARG:HD2	1.82	0.62
1:L:170:GLU:HA	2:L:389:HOH:O	1.99	0.62
1:F:159:VAL:HG22	1:F:185:ARG:HD2	1.82	0.62
1:G:103:PRO:HD3	1:G:144:VAL:HG11	1.81	0.62
1:C:15:PHE:CE2	1:C:114:ARG:HD3	2.35	0.62
1:C:191:LYS:O	1:C:195:GLU:HG3	1.99	0.62
1:K:103:PRO:HD3	1:K:144:VAL:HG11	1.81	0.62
1:G:15:PHE:CE2	1:G:114:ARG:HD3	2.35	0.62
1:J:15:PHE:CE2	1:J:114:ARG:HD3	2.35	0.62
1:A:159:VAL:HG22	1:A:185:ARG:HD2	1.82	0.62
1:C:27:ILE:HD11	1:C:314:VAL:HG12	1.81	0.62
1:D:159:VAL:HG22	1:D:185:ARG:HD2	1.82	0.62
1:I:15:PHE:CE2	1:I:114:ARG:HD3	2.35	0.62
1:A:15:PHE:CE2	1:A:114:ARG:HD3	2.35	0.62
1:E:103:PRO:HD3	1:E:144:VAL:HG11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:PHE:CE2	1:F:114:ARG:HD3	2.35	0.62
1:G:29:MSE:HA	1:G:98:ILE:HG21	1.80	0.62
1:G:159:VAL:HG22	1:G:185:ARG:HD2	1.82	0.62
1:I:290:ASP:HB3	1:J:73:ASN:ND2	2.15	0.62
1:L:15:PHE:CE2	1:L:114:ARG:HD3	2.35	0.62
1:E:191:LYS:O	1:E:195:GLU:HG3	1.99	0.61
1:A:27:ILE:HD11	1:A:314:VAL:HG12	1.81	0.61
1:A:191:LYS:O	1:A:195:GLU:HG3	1.99	0.61
1:H:139:LEU:HB3	1:H:143:LYS:HE3	1.82	0.61
1:J:191:LYS:O	1:J:195:GLU:HG3	1.99	0.61
1:L:191:LYS:O	1:L:195:GLU:HG3	1.99	0.61
1:E:159:VAL:HG22	1:E:185:ARG:HD2	1.82	0.61
1:G:185:ARG:HH22	1:G:220:ASN:HD22	1.47	0.61
1:I:159:VAL:HG22	1:I:185:ARG:HD2	1.82	0.61
1:K:159:VAL:HG22	1:K:185:ARG:HD2	1.82	0.61
1:B:15:PHE:CE2	1:B:114:ARG:HD3	2.35	0.61
1:B:27:ILE:HD11	1:B:314:VAL:HG12	1.81	0.61
1:B:103:PRO:HD3	1:B:144:VAL:HG11	1.81	0.61
1:C:185:ARG:HH22	1:C:220:ASN:HD22	1.47	0.61
1:J:278:LYS:HE2	1:J:278:LYS:HA	1.83	0.61
1:C:103:PRO:HD3	1:C:144:VAL:HG11	1.81	0.61
1:H:91:MSE:SE	1:H:140:VAL:HG13	2.49	0.61
1:I:185:ARG:HH22	1:I:220:ASN:HD22	1.47	0.61
1:K:27:ILE:HD11	1:K:314:VAL:HG12	1.81	0.61
1:D:185:ARG:HH22	1:D:220:ASN:HD22	1.47	0.61
1:H:18:PRO:HD3	1:H:107:VAL:HG12	1.83	0.61
1:J:185:ARG:HH22	1:J:220:ASN:HD22	1.47	0.61
1:B:159:VAL:HG22	1:B:185:ARG:HD2	1.82	0.61
1:B:278:LYS:HE2	1:B:278:LYS:HA	1.83	0.61
1:C:278:LYS:HE2	1:C:278:LYS:HA	1.83	0.61
1:D:15:PHE:CE2	1:D:114:ARG:HD3	2.35	0.61
1:D:103:PRO:HD3	1:D:144:VAL:HG11	1.81	0.61
1:K:15:PHE:CE2	1:K:114:ARG:HD3	2.35	0.61
1:B:185:ARG:HH22	1:B:220:ASN:HD22	1.47	0.61
1:E:15:PHE:CE2	1:E:114:ARG:HD3	2.35	0.61
1:G:278:LYS:HA	1:G:278:LYS:HE2	1.83	0.61
1:F:103:PRO:HD3	1:F:144:VAL:HG11	1.81	0.61
1:G:27:ILE:HD11	1:G:314:VAL:HG12	1.81	0.61
1:H:284:GLN:O	1:H:285:GLU:HB2	1.99	0.61
1:E:179:CYS:HB2	1:E:220:ASN:O	2.01	0.60
1:F:89:ILE:HD13	1:F:89:ILE:N	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:185:ARG:HH22	1:L:220:ASN:HD22	1.47	0.60
1:H:104:THR:HB	1:H:116:VAL:HG13	1.83	0.60
1:G:214:ILE:HG13	2:G:401:HOH:O	2.00	0.60
1:H:358:ASN:HD22	1:H:359:ILE:N	1.93	0.60
1:K:278:LYS:HE2	1:K:278:LYS:HA	1.83	0.60
1:F:15:PHE:CE2	1:F:114:ARG:HB2	2.37	0.60
1:A:278:LYS:HE2	1:A:278:LYS:HA	1.83	0.60
1:C:159:VAL:HG22	1:C:185:ARG:HD2	1.82	0.60
1:G:15:PHE:CE2	1:G:114:ARG:HB2	2.37	0.60
1:L:159:VAL:HG22	1:L:185:ARG:HD2	1.82	0.60
1:A:15:PHE:CE2	1:A:114:ARG:HB2	2.37	0.60
1:A:179:CYS:HB2	1:A:220:ASN:O	2.01	0.60
1:G:179:CYS:HB2	1:G:220:ASN:O	2.01	0.60
1:H:4:ARG:HH22	1:H:154:LYS:HD3	1.66	0.60
1:I:278:LYS:HE2	1:I:278:LYS:HA	1.83	0.60
1:C:198:LEU:O	1:C:202:LEU:HB2	2.02	0.60
1:I:198:LEU:O	1:I:202:LEU:HB2	2.02	0.60
1:L:198:LEU:O	1:L:202:LEU:HB2	2.02	0.60
1:E:198:LEU:O	1:E:202:LEU:HB2	2.02	0.60
1:E:278:LYS:HE2	1:E:278:LYS:HA	1.83	0.60
1:F:198:LEU:O	1:F:202:LEU:HB2	2.02	0.60
1:H:24:GLN:HA	1:H:367:PRO:HA	1.83	0.60
1:I:15:PHE:CE2	1:I:114:ARG:HB2	2.37	0.60
1:C:104:THR:HB	1:C:116:VAL:HG13	1.84	0.59
1:C:15:PHE:CE2	1:C:114:ARG:HB2	2.37	0.59
1:C:179:CYS:HB2	1:C:220:ASN:O	2.01	0.59
1:J:198:LEU:O	1:J:202:LEU:HB2	2.02	0.59
1:K:89:ILE:HD13	1:K:89:ILE:N	2.14	0.59
1:B:179:CYS:HB2	1:B:220:ASN:O	2.02	0.59
1:I:77:ARG:NH2	1:J:290:ASP:OD1	2.30	0.59
1:I:179:CYS:HB2	1:I:220:ASN:O	2.02	0.59
1:J:104:THR:HB	1:J:116:VAL:HG13	1.84	0.59
1:A:12:GLN:CD	1:D:82:GLY:CA	2.75	0.59
1:D:179:CYS:HB2	1:D:220:ASN:O	2.01	0.59
1:F:132:PHE:CE2	1:G:135:ASP:HB3	2.36	0.59
1:G:104:THR:HB	1:G:116:VAL:HG13	1.84	0.59
1:H:80:GLU:OE1	1:H:81:LEU:HD23	2.03	0.59
1:H:230:ILE:HD11	1:H:272:HIS:CD2	2.37	0.59
1:J:89:ILE:HD13	1:J:89:ILE:N	2.15	0.59
1:K:15:PHE:CE2	1:K:114:ARG:HB2	2.37	0.59
1:L:15:PHE:CE2	1:L:114:ARG:HB2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:O	1:A:202:LEU:HB2	2.02	0.59
1:B:15:PHE:CE2	1:B:114:ARG:HB2	2.37	0.59
1:C:132:PHE:CE2	1:I:135:ASP:HB3	2.38	0.59
1:D:15:PHE:CE2	1:D:114:ARG:HB2	2.37	0.59
1:D:104:THR:HB	1:D:116:VAL:HG13	1.84	0.59
1:D:278:LYS:HA	1:D:278:LYS:HE2	1.83	0.59
1:E:15:PHE:CE2	1:E:114:ARG:HB2	2.37	0.59
1:D:198:LEU:O	1:D:202:LEU:HB2	2.02	0.59
1:K:179:CYS:HB2	1:K:220:ASN:O	2.02	0.59
1:F:278:LYS:HE2	1:F:278:LYS:HA	1.83	0.59
1:L:179:CYS:HB2	1:L:220:ASN:O	2.01	0.59
2:C:392:HOH:O	1:J:147:ILE:C	2.44	0.59
1:J:15:PHE:CE2	1:J:114:ARG:HB2	2.37	0.59
1:D:89:ILE:HG22	1:I:147:ILE:CG2	2.29	0.59
1:E:147:ILE:CG2	1:K:89:ILE:HG22	2.29	0.59
1:F:104:THR:HB	1:F:116:VAL:HG13	1.84	0.59
1:H:142:ARG:CZ	1:L:75:LEU:HD21	2.33	0.59
1:H:318:ILE:CD1	1:H:342:ARG:HD3	2.32	0.59
1:J:179:CYS:HB2	1:J:220:ASN:O	2.01	0.59
1:H:43:LYS:HZ1	1:H:46:GLN:NE2	1.99	0.59
1:L:278:LYS:HA	1:L:278:LYS:HE2	1.83	0.59
1:J:199:LYS:HG2	1:J:204:CYS:O	2.03	0.58
1:B:89:ILE:HD13	1:B:89:ILE:N	2.14	0.58
1:D:199:LYS:HG2	1:D:204:CYS:O	2.03	0.58
1:G:198:LEU:O	1:G:202:LEU:HB2	2.02	0.58
1:I:263:ASP:OD2	1:I:267:ARG:NH1	2.37	0.58
1:J:263:ASP:OD2	1:J:267:ARG:NH1	2.36	0.58
1:B:198:LEU:O	1:B:202:LEU:HB2	2.02	0.58
1:C:171:GLY:HA3	1:C:205:VAL:HG22	1.85	0.58
1:C:263:ASP:OD2	1:C:267:ARG:NH1	2.37	0.58
1:D:185:ARG:CG	2:D:396:HOH:O	2.50	0.58
1:F:179:CYS:HB2	1:F:220:ASN:O	2.01	0.58
1:I:104:THR:HB	1:I:116:VAL:HG13	1.84	0.58
1:L:121:ASN:HD22	1:L:121:ASN:N	1.96	0.58
1:A:104:THR:HB	1:A:116:VAL:HG13	1.84	0.58
1:A:199:LYS:HG2	1:A:204:CYS:O	2.03	0.58
1:A:263:ASP:OD2	1:A:267:ARG:NH1	2.36	0.58
1:B:263:ASP:OD2	1:B:267:ARG:NH1	2.37	0.58
1:E:89:ILE:HD13	1:E:89:ILE:N	2.14	0.58
1:F:199:LYS:HG2	1:F:204:CYS:O	2.03	0.58
1:I:31:TRP:HB2	1:I:66:VAL:HG12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:171:GLY:HA3	1:I:205:VAL:HG22	1.86	0.58
1:J:171:GLY:HA3	1:J:205:VAL:HG22	1.85	0.58
1:K:198:LEU:O	1:K:202:LEU:HB2	2.02	0.58
1:K:263:ASP:OD2	1:K:267:ARG:NH1	2.37	0.58
1:L:263:ASP:OD2	1:L:267:ARG:NH1	2.37	0.58
1:D:121:ASN:HD22	1:D:121:ASN:N	1.96	0.58
1:D:263:ASP:OD2	1:D:267:ARG:NH1	2.37	0.58
1:E:199:LYS:HG2	1:E:204:CYS:O	2.03	0.58
1:F:171:GLY:HA3	1:F:205:VAL:HG22	1.85	0.58
1:G:114:ARG:HG2	1:G:153:TYR:HE1	1.69	0.58
1:G:114:ARG:HG2	1:G:153:TYR:CE1	2.39	0.58
1:G:171:GLY:HA3	1:G:205:VAL:HG22	1.86	0.58
1:I:199:LYS:HG2	1:I:204:CYS:O	2.03	0.58
1:K:171:GLY:HA3	1:K:205:VAL:HG22	1.85	0.58
1:L:104:THR:HB	1:L:116:VAL:HG13	1.84	0.58
1:A:114:ARG:HG2	1:A:153:TYR:CE1	2.39	0.58
1:B:171:GLY:HA3	1:B:205:VAL:HG22	1.85	0.58
1:B:199:LYS:HG2	1:B:204:CYS:O	2.03	0.58
1:D:114:ARG:HG2	1:D:153:TYR:HE1	1.69	0.58
1:G:199:LYS:HG2	1:G:204:CYS:O	2.03	0.58
1:I:114:ARG:HG2	1:I:153:TYR:CE1	2.39	0.58
1:J:69:LEU:HG	2:J:380:HOH:O	2.02	0.58
1:L:114:ARG:HG2	1:L:153:TYR:HE1	1.69	0.58
1:B:104:THR:HB	1:B:116:VAL:HG13	1.84	0.58
1:C:199:LYS:HG2	1:C:204:CYS:O	2.03	0.58
1:D:147:ILE:CG2	1:I:89:ILE:HG22	2.30	0.58
1:E:159:VAL:HG12	1:E:186:ASN:ND2	2.19	0.58
1:E:263:ASP:OD2	1:E:267:ARG:NH1	2.37	0.58
1:A:114:ARG:HG2	1:A:153:TYR:HE1	1.69	0.58
1:D:27:ILE:HD12	1:D:56:ILE:CG2	2.34	0.58
1:D:31:TRP:HB2	1:D:66:VAL:HG12	1.86	0.58
1:E:114:ARG:HG2	1:E:153:TYR:HE1	1.69	0.58
1:F:27:ILE:HD12	1:F:56:ILE:CG2	2.34	0.58
1:G:177:GLU:HB3	1:G:209:TRP:CE3	2.39	0.58
1:H:105:PHE:O	1:H:106:LEU:HD23	2.03	0.58
1:H:108:ASN:ND2	1:H:110:LYS:HB2	2.18	0.58
1:H:231:ARG:HD2	1:H:234:GLU:OE2	2.04	0.58
1:J:114:ARG:HG2	1:J:153:TYR:HE1	1.69	0.58
1:K:27:ILE:HD12	1:K:56:ILE:CG2	2.34	0.58
1:K:31:TRP:HB2	1:K:66:VAL:HG12	1.86	0.58
1:A:312:LEU:HD13	1:A:313:ILE:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ARG:HG2	1:C:153:TYR:HE1	1.69	0.58
1:G:89:ILE:HD13	1:G:89:ILE:N	2.14	0.58
1:G:167:VAL:HG22	1:G:173:VAL:HG23	1.86	0.58
1:G:170:GLU:O	1:G:172:THR:N	2.37	0.58
1:H:321:PRO:HB3	1:H:358:ASN:ND2	2.19	0.58
1:I:159:VAL:HG12	1:I:186:ASN:ND2	2.19	0.58
1:I:170:GLU:O	1:I:172:THR:N	2.37	0.58
1:J:31:TRP:HB2	1:J:66:VAL:HG12	1.86	0.58
1:K:114:ARG:HG2	1:K:153:TYR:CE1	2.39	0.58
1:K:159:VAL:HG12	1:K:186:ASN:ND2	2.19	0.58
1:C:89:ILE:HD13	1:C:89:ILE:N	2.14	0.58
1:C:312:LEU:HD13	1:C:313:ILE:N	2.19	0.58
1:D:114:ARG:HG2	1:D:153:TYR:CE1	2.39	0.58
1:D:177:GLU:HB3	1:D:209:TRP:CE3	2.39	0.58
1:D:312:LEU:HD13	1:D:313:ILE:N	2.19	0.58
1:E:114:ARG:HG2	1:E:153:TYR:CE1	2.39	0.58
1:H:88:ILE:HD12	1:H:88:ILE:N	2.19	0.58
1:H:142:ARG:NH1	1:H:146:GLU:HG2	2.19	0.58
1:K:34:ARG:HD2	1:K:94:ASP:O	2.04	0.58
1:K:114:ARG:HG2	1:K:153:TYR:HE1	1.69	0.58
1:K:312:LEU:HD13	1:K:313:ILE:N	2.19	0.58
1:A:31:TRP:HB2	1:A:66:VAL:HG12	1.86	0.57
1:B:177:GLU:HB3	1:B:209:TRP:CE3	2.39	0.57
1:B:312:LEU:HD13	1:B:313:ILE:N	2.19	0.57
1:C:34:ARG:HD2	1:C:94:ASP:O	2.04	0.57
1:C:167:VAL:HG22	1:C:173:VAL:HG23	1.86	0.57
1:D:89:ILE:HD13	1:D:89:ILE:N	2.14	0.57
1:D:170:GLU:O	1:D:172:THR:N	2.37	0.57
1:E:177:GLU:HB3	1:E:209:TRP:CE3	2.39	0.57
1:F:170:GLU:O	1:F:172:THR:N	2.37	0.57
1:H:124:GLY:HA3	1:H:128:ASP:C	2.28	0.57
1:I:27:ILE:HD12	1:I:56:ILE:CG2	2.34	0.57
1:I:312:LEU:HD13	1:I:313:ILE:N	2.19	0.57
1:J:170:GLU:O	1:J:172:THR:N	2.37	0.57
1:J:312:LEU:HD13	1:J:313:ILE:N	2.19	0.57
1:K:199:LYS:HG2	1:K:204:CYS:O	2.03	0.57
1:L:89:ILE:HD13	1:L:89:ILE:N	2.14	0.57
1:C:170:GLU:O	1:C:172:THR:N	2.37	0.57
1:D:121:ASN:ND2	1:D:159:VAL:HG21	2.19	0.57
1:E:104:THR:HB	1:E:116:VAL:HG13	1.84	0.57
1:F:114:ARG:HG2	1:F:153:TYR:HE1	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:VAL:HG12	1:G:186:ASN:ND2	2.19	0.57
1:H:167:VAL:HG13	1:H:172:THR:O	2.02	0.57
1:K:104:THR:HB	1:K:116:VAL:HG13	1.84	0.57
1:K:170:GLU:O	1:K:172:THR:N	2.37	0.57
1:L:34:ARG:HD2	1:L:94:ASP:O	2.04	0.57
1:L:177:GLU:HB3	1:L:209:TRP:CE3	2.39	0.57
1:A:27:ILE:HD12	1:A:56:ILE:CG2	2.34	0.57
1:A:170:GLU:O	1:A:172:THR:N	2.37	0.57
1:F:263:ASP:OD2	1:F:267:ARG:NH1	2.37	0.57
1:H:224:ASP:HB2	1:H:360:HIS:CD2	2.40	0.57
1:I:89:ILE:HD13	1:I:89:ILE:N	2.14	0.57
1:L:159:VAL:HG12	1:L:186:ASN:ND2	2.19	0.57
1:A:159:VAL:HG12	1:A:186:ASN:ND2	2.19	0.57
1:C:31:TRP:HB2	1:C:66:VAL:HG12	1.86	0.57
1:C:121:ASN:ND2	1:C:159:VAL:HG21	2.20	0.57
1:C:159:VAL:HG12	1:C:186:ASN:ND2	2.19	0.57
1:D:159:VAL:HG12	1:D:186:ASN:ND2	2.19	0.57
1:E:312:LEU:HD13	1:E:313:ILE:N	2.19	0.57
1:F:159:VAL:HG12	1:F:186:ASN:ND2	2.19	0.57
1:F:312:LEU:HD13	1:F:313:ILE:N	2.19	0.57
1:H:90:GLU:OE2	1:L:90:GLU:OE2	2.22	0.57
1:I:114:ARG:HG2	1:I:153:TYR:HE1	1.69	0.57
1:L:114:ARG:HG2	1:L:153:TYR:CE1	2.39	0.57
1:L:199:LYS:HG2	1:L:204:CYS:O	2.03	0.57
1:L:312:LEU:HD13	1:L:313:ILE:N	2.19	0.57
1:B:34:ARG:HD2	1:B:94:ASP:O	2.04	0.57
1:B:114:ARG:HG2	1:B:153:TYR:HE1	1.69	0.57
1:C:177:GLU:HB3	1:C:209:TRP:CE3	2.39	0.57
1:F:167:VAL:HG22	1:F:173:VAL:HG23	1.86	0.57
1:A:177:GLU:HB3	1:A:209:TRP:CE3	2.39	0.57
1:C:27:ILE:HD12	1:C:56:ILE:CG2	2.34	0.57
1:E:27:ILE:HD12	1:E:56:ILE:CG2	2.34	0.57
1:E:121:ASN:HD22	1:E:121:ASN:N	1.96	0.57
1:E:171:GLY:HA3	1:E:205:VAL:HG22	1.86	0.57
1:G:27:ILE:HD12	1:G:56:ILE:CG2	2.34	0.57
1:G:263:ASP:OD2	1:G:267:ARG:NH1	2.37	0.57
1:H:61:PRO:CA	1:H:85:ASN:HD22	2.13	0.57
1:H:319:ILE:HG22	1:H:359:ILE:HD13	1.85	0.57
1:J:114:ARG:HG2	1:J:153:TYR:CE1	2.39	0.57
1:K:167:VAL:HG22	1:K:173:VAL:HG23	1.86	0.57
1:L:27:ILE:HD12	1:L:56:ILE:CG2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:170:GLU:O	1:L:172:THR:N	2.37	0.57
1:B:170:GLU:O	1:B:172:THR:N	2.37	0.57
1:G:34:ARG:HD2	1:G:94:ASP:O	2.04	0.57
1:I:121:ASN:ND2	1:I:159:VAL:HG21	2.20	0.57
1:J:159:VAL:HG12	1:J:186:ASN:ND2	2.19	0.57
1:A:214:ILE:C	1:A:216:PRO:HD3	2.30	0.57
1:C:114:ARG:HG2	1:C:153:TYR:CE1	2.39	0.57
1:C:135:ASP:HB3	1:I:132:PHE:CD2	2.40	0.57
1:D:171:GLY:HA3	1:D:205:VAL:HG22	1.85	0.57
1:I:177:GLU:HB3	1:I:209:TRP:CE3	2.39	0.57
1:A:34:ARG:HD2	1:A:94:ASP:O	2.04	0.57
1:A:121:ASN:ND2	1:A:159:VAL:HG21	2.20	0.57
1:A:171:GLY:HA3	1:A:205:VAL:HG22	1.86	0.57
1:C:214:ILE:C	1:C:216:PRO:HD3	2.30	0.57
1:E:31:TRP:HB2	1:E:66:VAL:HG12	1.86	0.57
1:E:214:ILE:C	1:E:216:PRO:HD3	2.30	0.57
1:G:121:ASN:ND2	1:G:159:VAL:HG21	2.19	0.57
1:J:177:GLU:HB3	1:J:209:TRP:CE3	2.39	0.57
1:K:121:ASN:ND2	1:K:159:VAL:HG21	2.20	0.57
1:L:171:GLY:HA3	1:L:205:VAL:HG22	1.85	0.57
1:B:77:ARG:O	1:B:81:LEU:HG	2.05	0.57
1:D:214:ILE:C	1:D:216:PRO:HD3	2.30	0.57
1:E:290:ASP:HB3	1:H:73:ASN:ND2	2.20	0.57
1:F:114:ARG:HG2	1:F:153:TYR:CE1	2.39	0.57
1:G:312:LEU:HD13	1:G:313:ILE:N	2.19	0.57
1:J:77:ARG:O	1:J:81:LEU:HG	2.05	0.57
1:L:31:TRP:HB2	1:L:66:VAL:HG12	1.86	0.57
1:L:77:ARG:O	1:L:81:LEU:HG	2.05	0.57
1:B:114:ARG:HG2	1:B:153:TYR:CE1	2.39	0.56
1:D:167:VAL:HG22	1:D:173:VAL:HG23	1.86	0.56
1:E:167:VAL:HG22	1:E:173:VAL:HG23	1.86	0.56
1:F:177:GLU:HB3	1:F:209:TRP:CE3	2.39	0.56
1:I:34:ARG:HD2	1:I:94:ASP:O	2.04	0.56
1:J:121:ASN:ND2	1:J:159:VAL:HG21	2.20	0.56
1:L:121:ASN:ND2	1:L:159:VAL:HG21	2.19	0.56
1:B:27:ILE:HD12	1:B:56:ILE:CG2	2.34	0.56
1:C:6:LYS:HB2	2:C:393:HOH:O	2.05	0.56
1:D:342:ARG:N	1:F:84:HIS:CE1	2.72	0.56
1:E:170:GLU:O	1:E:172:THR:N	2.37	0.56
1:F:31:TRP:HB2	1:F:66:VAL:HG12	1.86	0.56
1:F:34:ARG:HD2	1:F:94:ASP:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:ASN:ND2	1:F:159:VAL:HG21	2.19	0.56
1:H:87:ARG:HG3	1:H:87:ARG:O	2.04	0.56
1:H:330:LEU:O	1:H:334:GLN:HG3	2.05	0.56
1:K:77:ARG:O	1:K:81:LEU:HG	2.05	0.56
1:A:77:ARG:O	1:A:81:LEU:HG	2.05	0.56
1:A:167:VAL:HG22	1:A:173:VAL:HG23	1.86	0.56
1:B:31:TRP:HB2	1:B:66:VAL:HG12	1.86	0.56
1:B:159:VAL:HG12	1:B:186:ASN:ND2	2.19	0.56
1:C:106:LEU:O	1:C:113:LEU:HD12	2.06	0.56
1:D:77:ARG:O	1:D:81:LEU:HG	2.05	0.56
1:E:121:ASN:ND2	1:E:159:VAL:HG21	2.19	0.56
1:F:214:ILE:C	1:F:216:PRO:HD3	2.30	0.56
1:G:31:TRP:HB2	1:G:66:VAL:HG12	1.86	0.56
1:I:214:ILE:C	1:I:216:PRO:HD3	2.30	0.56
1:J:34:ARG:HD2	1:J:94:ASP:O	2.04	0.56
1:J:214:ILE:C	1:J:216:PRO:HD3	2.30	0.56
1:K:106:LEU:O	1:K:113:LEU:HD12	2.06	0.56
1:L:167:VAL:HG22	1:L:173:VAL:HG23	1.86	0.56
1:B:9:THR:HG22	1:B:12:GLN:OE1	2.06	0.56
1:G:214:ILE:C	1:G:216:PRO:HD3	2.30	0.56
1:H:159:VAL:HG22	1:H:185:ARG:HD2	1.86	0.56
1:J:27:ILE:HD12	1:J:56:ILE:CG2	2.34	0.56
1:L:214:ILE:C	1:L:216:PRO:HD3	2.30	0.56
1:A:106:LEU:O	1:A:113:LEU:HD12	2.06	0.56
1:B:121:ASN:ND2	1:B:159:VAL:HG21	2.20	0.56
1:D:34:ARG:HD2	1:D:94:ASP:O	2.04	0.56
1:D:106:LEU:O	1:D:113:LEU:HD12	2.06	0.56
1:E:9:THR:HG22	1:E:12:GLN:OE1	2.06	0.56
1:E:106:LEU:O	1:E:113:LEU:HD12	2.06	0.56
1:H:283:LEU:HD12	1:H:302:GLU:HG2	1.87	0.56
1:I:106:LEU:O	1:I:113:LEU:HD12	2.06	0.56
1:K:174:LEU:HB3	1:K:223:ILE:HD13	1.88	0.56
1:B:174:LEU:HB3	1:B:223:ILE:HD13	1.88	0.56
1:E:34:ARG:HD2	1:E:94:ASP:O	2.04	0.56
1:F:135:ASP:HB3	1:G:132:PHE:CE2	2.40	0.56
1:L:174:LEU:HB3	1:L:223:ILE:HD13	1.88	0.56
1:A:9:THR:HG22	1:A:12:GLN:OE1	2.06	0.56
1:B:106:LEU:O	1:B:113:LEU:HD12	2.06	0.56
1:H:2:ALA:HB1	1:H:146:GLU:OE2	2.05	0.56
1:I:9:THR:HG22	1:I:12:GLN:OE1	2.06	0.56
1:I:167:VAL:HG22	1:I:173:VAL:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:177:GLU:HB3	1:K:209:TRP:CE3	2.39	0.56
1:B:127:VAL:HG13	1:B:184:SER:HB2	1.88	0.56
1:C:77:ARG:O	1:C:81:LEU:HG	2.05	0.56
1:J:167:VAL:HG22	1:J:173:VAL:HG23	1.86	0.56
1:J:195:GLU:O	1:J:199:LYS:HG3	2.06	0.56
1:K:127:VAL:HG13	1:K:184:SER:HB2	1.88	0.56
1:A:89:ILE:HD13	1:A:89:ILE:N	2.14	0.56
1:A:127:VAL:HG13	1:A:184:SER:HB2	1.88	0.56
1:C:43:LYS:NZ	1:C:46:GLN:HE22	2.04	0.56
1:F:43:LYS:NZ	1:F:46:GLN:HE22	2.04	0.56
1:F:127:VAL:HG13	1:F:184:SER:HB2	1.88	0.56
1:F:174:LEU:HB3	1:F:223:ILE:HD13	1.88	0.56
1:H:337:GLU:O	1:H:340:PRO:HD3	2.06	0.56
1:I:65:CYS:SG	1:I:89:ILE:HD11	2.46	0.56
1:J:65:CYS:SG	1:J:89:ILE:HD11	2.46	0.56
1:J:106:LEU:O	1:J:113:LEU:HD12	2.06	0.56
1:J:174:LEU:HB3	1:J:223:ILE:HD13	1.88	0.56
1:L:65:CYS:SG	1:L:89:ILE:HD11	2.46	0.56
1:C:349:THR:HG21	1:C:359:ILE:CG1	2.36	0.56
1:D:195:GLU:O	1:D:199:LYS:HG3	2.06	0.56
1:D:340:PRO:HG2	1:F:58:GLU:O	2.06	0.56
1:E:77:ARG:O	1:E:81:LEU:HG	2.05	0.56
1:G:9:THR:HG22	1:G:12:GLN:OE1	2.06	0.56
1:G:77:ARG:O	1:G:81:LEU:HG	2.05	0.56
1:H:165:ILE:HG22	1:H:175:VAL:CG1	2.36	0.56
1:I:127:VAL:HG13	1:I:184:SER:HB2	1.88	0.56
1:J:127:VAL:HG13	1:J:184:SER:HB2	1.88	0.56
1:K:195:GLU:O	1:K:199:LYS:HG3	2.06	0.56
1:K:214:ILE:C	1:K:216:PRO:HD3	2.30	0.56
1:L:43:LYS:NZ	1:L:46:GLN:HE22	2.04	0.56
1:A:65:CYS:SG	1:A:89:ILE:HD11	2.47	0.55
1:C:9:THR:HG22	1:C:12:GLN:OE1	2.06	0.55
1:C:195:GLU:O	1:C:199:LYS:HG3	2.06	0.55
1:I:195:GLU:O	1:I:199:LYS:HG3	2.06	0.55
1:K:43:LYS:NZ	1:K:46:GLN:HE22	2.04	0.55
1:L:195:GLU:O	1:L:199:LYS:HG3	2.06	0.55
1:A:195:GLU:O	1:A:199:LYS:HG3	2.06	0.55
1:B:65:CYS:SG	1:B:89:ILE:HD11	2.46	0.55
1:B:167:VAL:HG22	1:B:173:VAL:HG23	1.86	0.55
1:D:127:VAL:HG13	1:D:184:SER:HB2	1.88	0.55
1:G:106:LEU:O	1:G:113:LEU:HD12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:174:LEU:HB3	1:I:223:ILE:HD13	1.88	0.55
1:K:9:THR:HG22	1:K:12:GLN:OE1	2.06	0.55
1:A:7:ASN:HB3	1:D:84:HIS:HD1	1.67	0.55
1:A:43:LYS:NZ	1:A:46:GLN:HE22	2.04	0.55
1:G:127:VAL:HG13	1:G:184:SER:HB2	1.88	0.55
1:G:174:LEU:HB3	1:G:223:ILE:HD13	1.88	0.55
1:I:43:LYS:NZ	1:I:46:GLN:HE22	2.04	0.55
1:I:252:LYS:HD3	2:I:387:HOH:O	2.06	0.55
1:L:127:VAL:HG13	1:L:184:SER:HB2	1.88	0.55
1:B:214:ILE:C	1:B:216:PRO:HD3	2.30	0.55
1:B:349:THR:HG21	1:B:359:ILE:CG1	2.36	0.55
1:C:174:LEU:HB3	1:C:223:ILE:HD13	1.88	0.55
1:E:65:CYS:SG	1:E:89:ILE:HD11	2.46	0.55
1:F:77:ARG:O	1:F:81:LEU:HG	2.05	0.55
1:G:43:LYS:NZ	1:G:46:GLN:HE22	2.04	0.55
1:G:65:CYS:SG	1:G:89:ILE:HD11	2.46	0.55
1:I:77:ARG:O	1:I:81:LEU:HG	2.05	0.55
1:K:283:LEU:CD1	1:K:286:ALA:HB2	2.37	0.55
1:K:349:THR:HG21	1:K:359:ILE:CG1	2.36	0.55
1:A:318:ILE:HB	1:A:344:VAL:HG22	1.89	0.55
1:D:65:CYS:SG	1:D:89:ILE:HD11	2.46	0.55
1:H:65:CYS:HB3	1:H:91:MSE:HB3	1.88	0.55
1:I:318:ILE:HB	1:I:344:VAL:HG22	1.89	0.55
1:A:349:THR:HG21	1:A:359:ILE:CG1	2.36	0.55
1:C:127:VAL:HG13	1:C:184:SER:HB2	1.88	0.55
1:D:43:LYS:NZ	1:D:46:GLN:HE22	2.04	0.55
1:D:281:CYS:SG	1:D:306:ALA:HB2	2.47	0.55
1:E:40:LEU:HD12	1:H:40:LEU:HD12	1.89	0.55
1:E:174:LEU:HB3	1:E:223:ILE:HD13	1.88	0.55
1:G:195:GLU:O	1:G:199:LYS:HG3	2.06	0.55
1:J:349:THR:HG21	1:J:359:ILE:CG1	2.36	0.55
1:K:65:CYS:SG	1:K:89:ILE:HD11	2.46	0.55
1:E:281:CYS:SG	1:E:306:ALA:HB2	2.47	0.55
1:E:318:ILE:HB	1:E:344:VAL:HG22	1.89	0.55
1:F:9:THR:HG22	1:F:12:GLN:OE1	2.06	0.55
1:F:195:GLU:O	1:F:199:LYS:HG3	2.06	0.55
1:H:30:LEU:HG	1:H:98:ILE:HB	1.89	0.55
1:J:121:ASN:HD22	1:J:121:ASN:N	1.96	0.55
1:K:281:CYS:SG	1:K:306:ALA:HB2	2.47	0.55
1:A:174:LEU:HB3	1:A:223:ILE:HD13	1.88	0.55
1:B:281:CYS:SG	1:B:306:ALA:HB2	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:LEU:CD1	1:B:286:ALA:HB2	2.36	0.55
1:I:349:THR:HG21	1:I:359:ILE:CG1	2.36	0.55
1:L:9:THR:HG22	1:L:12:GLN:OE1	2.06	0.55
1:L:106:LEU:O	1:L:113:LEU:HD12	2.06	0.55
1:L:281:CYS:SG	1:L:306:ALA:HB2	2.47	0.55
1:E:195:GLU:O	1:E:199:LYS:HG3	2.06	0.55
1:F:349:THR:HG21	1:F:359:ILE:CG1	2.36	0.55
1:L:349:THR:HG21	1:L:359:ILE:CG1	2.37	0.55
1:A:281:CYS:SG	1:A:306:ALA:HB2	2.47	0.55
1:A:283:LEU:CD1	1:A:286:ALA:HB2	2.37	0.55
1:B:73:ASN:ND2	1:F:290:ASP:HB3	2.22	0.55
1:B:195:GLU:O	1:B:199:LYS:HG3	2.06	0.55
1:D:135:ASP:HB3	1:J:132:PHE:HE2	1.70	0.55
1:F:65:CYS:SG	1:F:89:ILE:HD11	2.46	0.55
1:F:106:LEU:O	1:F:113:LEU:HD12	2.06	0.55
1:J:281:CYS:SG	1:J:306:ALA:HB2	2.47	0.55
1:L:283:LEU:CD1	1:L:286:ALA:HB2	2.37	0.55
1:A:74:ALA:O	1:A:78:VAL:HG23	2.07	0.54
1:B:43:LYS:NZ	1:B:46:GLN:HE22	2.04	0.54
1:D:174:LEU:HB3	1:D:223:ILE:HD13	1.88	0.54
1:G:281:CYS:SG	1:G:306:ALA:HB2	2.47	0.54
1:H:122:ALA:O	1:H:129:GLY:HA2	2.07	0.54
1:H:252:LYS:HG2	1:H:256:ASP:OD2	2.07	0.54
1:I:321:PRO:HD3	1:I:359:ILE:HD12	1.89	0.54
1:J:283:LEU:CD1	1:J:286:ALA:HB2	2.37	0.54
1:L:9:THR:HG22	1:L:12:GLN:HG3	1.89	0.54
1:B:74:ALA:O	1:B:78:VAL:HG23	2.08	0.54
1:C:283:LEU:CD1	1:C:286:ALA:HB2	2.37	0.54
1:D:318:ILE:HB	1:D:344:VAL:HG22	1.89	0.54
1:E:349:THR:HG21	1:E:359:ILE:CG1	2.36	0.54
1:G:318:ILE:HB	1:G:344:VAL:HG22	1.89	0.54
1:C:65:CYS:SG	1:C:89:ILE:HD11	2.46	0.54
1:D:9:THR:HG22	1:D:12:GLN:HG3	1.89	0.54
1:E:43:LYS:NZ	1:E:46:GLN:HE22	2.04	0.54
1:E:309:LEU:O	1:E:309:LEU:HD13	2.08	0.54
1:F:74:ALA:O	1:F:78:VAL:HG23	2.08	0.54
1:I:281:CYS:SG	1:I:306:ALA:HB2	2.47	0.54
1:J:9:THR:HG22	1:J:12:GLN:OE1	2.06	0.54
1:J:43:LYS:NZ	1:J:46:GLN:HE22	2.04	0.54
1:J:74:ALA:O	1:J:78:VAL:HG23	2.07	0.54
1:J:321:PRO:HD3	1:J:359:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:318:ILE:HB	1:L:344:VAL:HG22	1.89	0.54
1:C:281:CYS:SG	1:C:306:ALA:HB2	2.47	0.54
1:H:262:THR:HG23	2:H:395:HOH:O	2.07	0.54
1:I:74:ALA:O	1:I:78:VAL:HG23	2.07	0.54
1:L:74:ALA:O	1:L:78:VAL:HG23	2.07	0.54
1:C:309:LEU:O	1:C:309:LEU:HD13	2.08	0.54
1:E:127:VAL:HG13	1:E:184:SER:HB2	1.88	0.54
1:F:283:LEU:CD1	1:F:286:ALA:HB2	2.37	0.54
1:G:309:LEU:O	1:G:309:LEU:HD13	2.08	0.54
1:H:107:VAL:HG22	1:H:109:ASP:H	1.73	0.54
1:I:9:THR:HG22	1:I:12:GLN:HG3	1.89	0.54
1:L:309:LEU:HD13	1:L:309:LEU:O	2.08	0.54
1:A:320:LEU:HD13	1:A:335:VAL:HG11	1.90	0.54
1:A:321:PRO:HD3	1:A:359:ILE:HD12	1.90	0.54
1:B:318:ILE:HB	1:B:344:VAL:HG22	1.89	0.54
1:C:74:ALA:O	1:C:78:VAL:HG23	2.07	0.54
1:D:309:LEU:HD13	1:D:309:LEU:O	2.08	0.54
1:G:283:LEU:CD1	1:G:286:ALA:HB2	2.37	0.54
1:H:170:GLU:HG3	1:H:267:ARG:HH22	1.72	0.54
1:H:257:PHE:O	1:H:261:GLN:HG2	2.08	0.54
1:A:7:ASN:CG	1:D:84:HIS:ND1	2.53	0.54
1:C:321:PRO:HD3	1:C:359:ILE:HD12	1.90	0.54
1:D:9:THR:HG22	1:D:12:GLN:OE1	2.06	0.54
1:E:9:THR:HG22	1:E:12:GLN:HG3	1.90	0.54
1:K:318:ILE:HB	1:K:344:VAL:HG22	1.89	0.54
1:K:320:LEU:HD13	1:K:335:VAL:HG11	1.90	0.54
1:F:318:ILE:HB	1:F:344:VAL:HG22	1.89	0.54
1:G:321:PRO:HD3	1:G:359:ILE:HD12	1.90	0.54
1:J:88:ILE:N	1:J:88:ILE:HD12	2.23	0.54
1:J:309:LEU:O	1:J:309:LEU:HD13	2.08	0.54
1:K:321:PRO:HD3	1:K:359:ILE:HD12	1.90	0.54
1:B:121:ASN:HD22	1:B:121:ASN:N	1.96	0.54
1:C:88:ILE:HD12	1:C:88:ILE:N	2.23	0.54
2:C:385:HOH:O	1:D:70:GLN:HG3	2.08	0.54
1:E:321:PRO:HD3	1:E:359:ILE:HD12	1.90	0.54
1:F:9:THR:HG22	1:F:12:GLN:HG3	1.89	0.54
1:F:281:CYS:SG	1:F:306:ALA:HB2	2.47	0.54
1:H:43:LYS:NZ	1:H:46:GLN:NE2	2.55	0.54
1:A:9:THR:HG22	1:A:12:GLN:HG3	1.90	0.54
1:A:121:ASN:HD22	1:A:121:ASN:N	1.96	0.54
1:B:88:ILE:N	1:B:88:ILE:HD12	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:PRO:HD3	1:B:359:ILE:HD12	1.90	0.54
1:C:15:PHE:CD2	1:C:114:ARG:HB2	2.43	0.54
1:C:89:ILE:HG22	1:J:147:ILE:CG2	2.32	0.54
1:D:74:ALA:O	1:D:78:VAL:HG23	2.07	0.54
1:F:309:LEU:O	1:F:309:LEU:HD13	2.08	0.54
1:G:320:LEU:HD13	1:G:335:VAL:HG11	1.90	0.54
1:J:318:ILE:HB	1:J:344:VAL:HG22	1.89	0.54
1:K:9:THR:HG22	1:K:12:GLN:HG3	1.89	0.54
1:B:369:THR:O	1:B:370:LEU:CB	2.47	0.53
1:C:318:ILE:HB	1:C:344:VAL:HG22	1.89	0.53
1:D:88:ILE:N	1:D:88:ILE:HD12	2.23	0.53
1:D:283:LEU:CD1	1:D:286:ALA:HB2	2.37	0.53
1:E:320:LEU:HD13	1:E:335:VAL:HG11	1.90	0.53
1:F:88:ILE:HD12	1:F:88:ILE:N	2.23	0.53
1:F:121:ASN:HD22	1:F:121:ASN:N	1.96	0.53
1:G:88:ILE:N	1:G:88:ILE:HD12	2.23	0.53
1:H:9:THR:HG22	1:H:12:GLN:CD	2.33	0.53
1:H:27:ILE:HD12	1:H:56:ILE:HD12	1.90	0.53
1:H:161:GLU:CD	1:H:161:GLU:H	2.16	0.53
1:H:176:THR:HG21	1:H:221:GLY:O	2.07	0.53
1:L:321:PRO:HD3	1:L:359:ILE:HD12	1.90	0.53
1:G:9:THR:HG22	1:G:12:GLN:HG3	1.89	0.53
1:H:66:VAL:CG2	1:H:71:TYR:HA	2.38	0.53
1:J:15:PHE:CD2	1:J:114:ARG:HB2	2.43	0.53
1:K:309:LEU:O	1:K:309:LEU:HD13	2.08	0.53
1:L:320:LEU:HD13	1:L:335:VAL:HG11	1.90	0.53
1:B:291:TYR:OH	1:F:80:GLU:HB2	2.08	0.53
1:B:320:LEU:HD13	1:B:335:VAL:HG11	1.90	0.53
1:D:349:THR:HG21	1:D:359:ILE:CG1	2.36	0.53
1:G:74:ALA:O	1:G:78:VAL:HG23	2.08	0.53
1:G:349:THR:HG21	1:G:359:ILE:CG1	2.36	0.53
1:A:309:LEU:HD13	1:A:309:LEU:O	2.08	0.53
1:B:9:THR:HG22	1:B:12:GLN:HG3	1.89	0.53
1:D:15:PHE:CD2	1:D:114:ARG:HB2	2.43	0.53
1:E:132:PHE:CE2	1:L:135:ASP:HB3	2.43	0.53
1:G:15:PHE:CD2	1:G:114:ARG:HB2	2.44	0.53
1:K:15:PHE:CZ	1:K:114:ARG:HD3	2.44	0.53
1:L:88:ILE:N	1:L:88:ILE:HD12	2.23	0.53
1:B:312:LEU:HD12	1:B:314:VAL:CG1	2.39	0.53
1:D:320:LEU:HD13	1:D:335:VAL:HG11	1.90	0.53
1:G:181:LEU:C	2:G:397:HOH:O	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:185:ARG:HH22	1:H:220:ASN:HD22	1.57	0.53
1:I:15:PHE:CZ	1:I:114:ARG:HD3	2.44	0.53
1:I:43:LYS:NZ	1:J:35:ASN:HD22	2.06	0.53
1:J:9:THR:HG22	1:J:12:GLN:HG3	1.89	0.53
1:K:121:ASN:HD22	1:K:121:ASN:N	1.96	0.53
1:A:7:ASN:HB2	1:D:84:HIS:NE2	2.22	0.53
1:D:312:LEU:HD12	1:D:314:VAL:CG1	2.39	0.53
1:I:15:PHE:CD2	1:I:114:ARG:HB2	2.44	0.53
1:I:283:LEU:CD1	1:I:286:ALA:HB2	2.37	0.53
1:I:312:LEU:HD12	1:I:314:VAL:CG1	2.39	0.53
1:K:15:PHE:CD2	1:K:114:ARG:HB2	2.43	0.53
1:L:15:PHE:CZ	1:L:114:ARG:HD3	2.44	0.53
1:A:15:PHE:CZ	1:A:114:ARG:HD3	2.44	0.53
1:A:312:LEU:HD12	1:A:314:VAL:CG1	2.39	0.53
1:C:121:ASN:HD22	1:C:121:ASN:N	1.96	0.53
1:C:320:LEU:HD13	1:C:335:VAL:HG11	1.90	0.53
1:E:74:ALA:O	1:E:78:VAL:HG23	2.08	0.53
1:F:15:PHE:CZ	1:F:114:ARG:HD3	2.44	0.53
1:K:74:ALA:O	1:K:78:VAL:HG23	2.07	0.53
1:L:15:PHE:CD2	1:L:114:ARG:HB2	2.43	0.53
1:E:135:ASP:HB3	1:L:132:PHE:CD2	2.44	0.53
1:F:15:PHE:CD2	1:F:114:ARG:HB2	2.43	0.53
1:F:312:LEU:HD12	1:F:314:VAL:CG1	2.39	0.53
1:H:293:GLU:C	1:H:295:SER:H	2.16	0.53
1:K:312:LEU:HD12	1:K:314:VAL:CG1	2.39	0.53
1:B:15:PHE:CD2	1:B:114:ARG:HB2	2.44	0.53
1:B:309:LEU:O	1:B:309:LEU:HD13	2.08	0.53
1:C:9:THR:HG22	1:C:12:GLN:HG3	1.89	0.53
1:D:243:LYS:HZ3	1:H:192:GLU:HG3	1.73	0.53
1:F:321:PRO:HD3	1:F:359:ILE:HD12	1.90	0.53
1:H:174:LEU:HD22	1:H:223:ILE:HD11	1.91	0.53
1:J:15:PHE:CZ	1:J:114:ARG:HD3	2.44	0.53
1:A:15:PHE:CD2	1:A:114:ARG:HB2	2.44	0.53
1:C:15:PHE:CZ	1:C:114:ARG:HD3	2.44	0.53
1:D:11:LYS:HG3	1:D:203:ASN:HD21	1.74	0.53
1:F:11:LYS:HG3	1:F:203:ASN:HD21	1.74	0.53
1:F:320:LEU:HD13	1:F:335:VAL:HG11	1.90	0.53
1:G:15:PHE:CZ	1:G:114:ARG:HD3	2.44	0.53
1:G:121:ASN:HD22	1:G:121:ASN:N	1.96	0.53
1:H:124:GLY:O	1:H:128:ASP:N	2.39	0.53
1:K:88:ILE:HD12	1:K:88:ILE:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:312:LEU:HD12	1:L:314:VAL:CG1	2.39	0.53
1:D:321:PRO:HD3	1:D:359:ILE:HD12	1.90	0.52
1:E:283:LEU:CD1	1:E:286:ALA:HB2	2.37	0.52
1:I:121:ASN:H	1:I:121:ASN:ND2	2.06	0.52
1:I:309:LEU:HD13	1:I:309:LEU:O	2.08	0.52
1:J:11:LYS:HG3	1:J:203:ASN:HD21	1.74	0.52
1:J:320:LEU:HD13	1:J:335:VAL:HG11	1.90	0.52
1:A:77:ARG:NH2	1:G:290:ASP:OD1	2.37	0.52
1:B:15:PHE:CZ	1:B:114:ARG:HD3	2.44	0.52
1:C:261:GLN:O	1:C:269:LEU:HD13	2.10	0.52
1:E:88:ILE:HD12	1:E:88:ILE:N	2.23	0.52
1:E:312:LEU:HD12	1:E:314:VAL:CG1	2.39	0.52
1:G:210:VAL:HG12	1:G:211:LYS:N	2.24	0.52
1:A:88:ILE:HD12	1:A:88:ILE:N	2.23	0.52
1:A:312:LEU:HD12	1:A:314:VAL:HG12	1.92	0.52
1:B:261:GLN:O	1:B:269:LEU:HD13	2.10	0.52
1:B:290:ASP:CB	1:F:73:ASN:ND2	2.72	0.52
1:C:121:ASN:H	1:C:121:ASN:ND2	2.07	0.52
1:E:15:PHE:CD2	1:E:114:ARG:HB2	2.43	0.52
1:G:11:LYS:CE	2:G:389:HOH:O	2.34	0.52
1:G:312:LEU:HD12	1:G:314:VAL:CG1	2.39	0.52
1:H:26:GLN:HG2	1:H:366:GLN:HE21	1.75	0.52
1:J:312:LEU:HD12	1:J:314:VAL:CG1	2.39	0.52
1:K:210:VAL:HG12	1:K:211:LYS:N	2.24	0.52
1:L:123:TRP:HB2	1:L:130:LEU:HD13	1.92	0.52
1:L:210:VAL:HG12	1:L:211:LYS:N	2.24	0.52
1:B:121:ASN:H	1:B:121:ASN:ND2	2.07	0.52
1:E:15:PHE:CZ	1:E:114:ARG:HD3	2.44	0.52
1:E:89:ILE:HG22	1:K:147:ILE:CG2	2.31	0.52
1:I:11:LYS:HG3	1:I:203:ASN:HD21	1.74	0.52
1:I:121:ASN:HD22	1:I:121:ASN:N	1.96	0.52
1:K:261:GLN:O	1:K:269:LEU:HD13	2.10	0.52
1:L:11:LYS:HG3	1:L:203:ASN:HD21	1.74	0.52
1:D:123:TRP:HB2	1:D:130:LEU:HD13	1.92	0.52
1:I:88:ILE:HD12	1:I:88:ILE:N	2.23	0.52
1:I:210:VAL:HG12	1:I:211:LYS:N	2.24	0.52
1:I:320:LEU:HD13	1:I:335:VAL:HG11	1.90	0.52
1:C:312:LEU:HD12	1:C:314:VAL:CG1	2.39	0.52
1:D:312:LEU:HD12	1:D:314:VAL:HG12	1.92	0.52
1:F:210:VAL:HG12	1:F:211:LYS:N	2.24	0.52
1:H:168:ASP:OD2	1:H:170:GLU:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:266:GLY:O	1:H:267:ARG:C	2.53	0.52
1:J:336:GLN:HG2	2:J:382:HOH:O	2.10	0.52
1:A:11:LYS:HG3	1:A:203:ASN:HD21	1.74	0.52
1:D:15:PHE:CZ	1:D:114:ARG:HD3	2.44	0.52
1:D:210:VAL:HG12	1:D:211:LYS:N	2.24	0.52
1:F:219:THR:HG21	2:F:396:HOH:O	2.09	0.52
1:I:312:LEU:HD12	1:I:314:VAL:HG12	1.92	0.52
1:A:168:ASP:O	1:A:169:GLY:C	2.53	0.52
1:D:135:ASP:HB3	1:J:132:PHE:CD2	2.44	0.52
1:D:311:PHE:HB3	1:D:320:LEU:HD12	1.92	0.52
1:J:312:LEU:HD12	1:J:314:VAL:HG12	1.92	0.52
1:K:11:LYS:HG3	1:K:203:ASN:HD21	1.74	0.52
1:F:137:ASP:HA	1:F:140:VAL:HG23	1.92	0.52
1:G:261:GLN:O	1:G:269:LEU:HD13	2.10	0.52
1:G:311:PHE:HB3	1:G:320:LEU:HD12	1.92	0.52
1:H:71:TYR:CZ	1:L:143:LYS:HG2	2.45	0.52
1:J:123:TRP:HB2	1:J:130:LEU:HD13	1.92	0.52
1:K:281:CYS:HA	2:K:391:HOH:O	2.10	0.52
1:K:312:LEU:HD12	1:K:314:VAL:HG12	1.92	0.52
1:A:43:LYS:HB2	1:A:44:PRO:HD3	1.93	0.51
1:C:9:THR:OG1	1:C:10:PRO:HD2	2.11	0.51
1:C:168:ASP:O	1:C:169:GLY:C	2.53	0.51
1:H:215:ASP:HB3	1:H:218:GLU:HB3	1.91	0.51
1:K:123:TRP:HB2	1:K:130:LEU:HD13	1.92	0.51
1:L:43:LYS:HB2	1:L:44:PRO:HD3	1.93	0.51
1:L:168:ASP:O	1:L:169:GLY:C	2.53	0.51
1:A:210:VAL:HG12	1:A:211:LYS:N	2.24	0.51
1:B:9:THR:OG1	1:B:10:PRO:HD2	2.10	0.51
1:C:159:VAL:HG12	1:C:186:ASN:HD21	1.76	0.51
1:F:312:LEU:HD12	1:F:314:VAL:HG12	1.92	0.51
1:G:49:PHE:O	1:G:52:VAL:HG12	2.10	0.51
1:I:261:GLN:O	1:I:269:LEU:HD13	2.10	0.51
1:J:210:VAL:HG12	1:J:211:LYS:N	2.24	0.51
1:A:311:PHE:HB3	1:A:320:LEU:HD12	1.92	0.51
1:D:49:PHE:O	1:D:52:VAL:HG12	2.10	0.51
1:E:9:THR:OG1	1:E:10:PRO:HD2	2.11	0.51
1:E:49:PHE:O	1:E:52:VAL:HG12	2.10	0.51
1:E:261:GLN:O	1:E:269:LEU:HD13	2.10	0.51
1:F:159:VAL:HG12	1:F:186:ASN:HD21	1.76	0.51
1:G:11:LYS:HG3	1:G:203:ASN:HD21	1.74	0.51
1:G:43:LYS:HB2	1:G:44:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:174:LEU:HD21	1:H:258:LEU:HD21	1.93	0.51
1:H:274:MSE:HE1	1:H:311:PHE:HE2	1.75	0.51
1:J:49:PHE:O	1:J:52:VAL:HG12	2.10	0.51
1:J:261:GLN:O	1:J:269:LEU:HD13	2.10	0.51
1:A:261:GLN:O	1:A:269:LEU:HD13	2.09	0.51
1:B:11:LYS:HG3	1:B:203:ASN:HD21	1.74	0.51
1:B:311:PHE:HB3	1:B:320:LEU:HD12	1.92	0.51
1:C:68:PRO:HG3	1:C:90:GLU:CD	2.36	0.51
1:C:311:PHE:HB3	1:C:320:LEU:HD12	1.92	0.51
1:E:11:LYS:HG3	1:E:203:ASN:HD21	1.74	0.51
1:E:168:ASP:O	1:E:169:GLY:C	2.53	0.51
1:F:68:PRO:HG3	1:F:90:GLU:CD	2.36	0.51
1:F:123:TRP:HB2	1:F:130:LEU:HD13	1.92	0.51
1:G:123:TRP:HB2	1:G:130:LEU:HD13	1.92	0.51
1:G:168:ASP:O	1:G:169:GLY:C	2.53	0.51
1:H:26:GLN:HG2	1:H:366:GLN:NE2	2.25	0.51
1:I:43:LYS:HB2	1:I:44:PRO:HD3	1.93	0.51
1:I:68:PRO:HG3	1:I:90:GLU:CD	2.36	0.51
1:J:159:VAL:HG12	1:J:186:ASN:HD21	1.76	0.51
1:K:49:PHE:O	1:K:52:VAL:HG12	2.10	0.51
1:L:137:ASP:HA	1:L:140:VAL:HG23	1.92	0.51
1:A:123:TRP:HB2	1:A:130:LEU:HD13	1.92	0.51
1:A:137:ASP:HA	1:A:140:VAL:HG23	1.92	0.51
1:B:49:PHE:O	1:B:52:VAL:HG12	2.10	0.51
1:C:49:PHE:O	1:C:52:VAL:HG12	2.10	0.51
1:F:9:THR:OG1	1:F:10:PRO:HD2	2.11	0.51
1:F:43:LYS:HB2	1:F:44:PRO:HD3	1.92	0.51
1:H:16:ARG:HH12	1:H:109:ASP:CG	2.19	0.51
1:I:9:THR:OG1	1:I:10:PRO:HD2	2.11	0.51
1:I:123:TRP:HB2	1:I:130:LEU:HD13	1.92	0.51
1:J:68:PRO:HG3	1:J:90:GLU:CD	2.36	0.51
1:L:9:THR:OG1	1:L:10:PRO:HD2	2.11	0.51
1:L:261:GLN:O	1:L:269:LEU:HD13	2.10	0.51
1:B:168:ASP:O	1:B:169:GLY:C	2.53	0.51
1:C:123:TRP:HB2	1:C:130:LEU:HD13	1.92	0.51
1:C:210:VAL:HG12	1:C:211:LYS:N	2.24	0.51
1:C:369:THR:O	1:C:370:LEU:CB	2.47	0.51
1:E:43:LYS:HB2	1:E:44:PRO:HD3	1.92	0.51
1:G:68:PRO:HG3	1:G:90:GLU:CD	2.36	0.51
1:H:321:PRO:HB3	1:H:358:ASN:HD21	1.73	0.51
1:J:137:ASP:HA	1:J:140:VAL:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:311:PHE:HB3	1:L:320:LEU:HD12	1.92	0.51
1:D:121:ASN:H	1:D:121:ASN:ND2	2.07	0.51
1:D:261:GLN:O	1:D:269:LEU:HD13	2.10	0.51
1:E:159:VAL:HG12	1:E:186:ASN:HD21	1.76	0.51
1:F:261:GLN:O	1:F:269:LEU:HD13	2.10	0.51
1:A:49:PHE:O	1:A:52:VAL:HG12	2.10	0.51
1:C:68:PRO:HG3	1:C:90:GLU:OE2	2.11	0.51
1:D:137:ASP:HA	1:D:140:VAL:HG23	1.92	0.51
1:D:168:ASP:O	1:D:169:GLY:C	2.53	0.51
1:G:9:THR:OG1	1:G:10:PRO:HD2	2.11	0.51
1:H:167:VAL:HG22	1:H:173:VAL:HG23	1.93	0.51
1:H:317:GLY:O	1:H:318:ILE:HD12	2.11	0.51
1:I:68:PRO:HG3	1:I:90:GLU:OE2	2.11	0.51
1:J:43:LYS:HB2	1:J:44:PRO:HD3	1.93	0.51
1:K:68:PRO:HG3	1:K:90:GLU:CD	2.36	0.51
1:K:174:LEU:O	1:K:223:ILE:HD13	2.11	0.51
1:A:9:THR:OG1	1:A:10:PRO:HD2	2.11	0.51
1:A:315:ASN:CA	2:A:379:HOH:O	2.58	0.51
1:F:49:PHE:O	1:F:52:VAL:HG12	2.10	0.51
1:G:137:ASP:HA	1:G:140:VAL:HG23	1.92	0.51
1:G:312:LEU:HD12	1:G:314:VAL:HG12	1.92	0.51
1:K:177:GLU:HB3	1:K:209:TRP:HE3	1.76	0.51
1:L:312:LEU:HD12	1:L:314:VAL:HG12	1.92	0.51
1:A:159:VAL:HG12	1:A:186:ASN:HD21	1.76	0.51
1:B:68:PRO:HG3	1:B:90:GLU:CD	2.36	0.51
1:D:43:LYS:HB2	1:D:44:PRO:HD3	1.93	0.51
1:D:68:PRO:HG3	1:D:90:GLU:CD	2.36	0.51
1:D:68:PRO:HG3	1:D:90:GLU:OE2	2.11	0.51
1:E:132:PHE:O	1:E:134:TRP:CE3	2.64	0.51
1:F:168:ASP:O	1:F:169:GLY:C	2.53	0.51
1:I:49:PHE:O	1:I:52:VAL:HG12	2.10	0.51
1:J:174:LEU:O	1:J:223:ILE:HD13	2.11	0.51
1:L:68:PRO:HG3	1:L:90:GLU:OE2	2.11	0.51
1:B:137:ASP:HA	1:B:140:VAL:HG23	1.92	0.50
1:B:210:VAL:HG12	1:B:211:LYS:N	2.24	0.50
1:C:11:LYS:HG3	1:C:203:ASN:HD21	1.74	0.50
1:C:137:ASP:HA	1:C:140:VAL:HG23	1.92	0.50
1:C:290:ASP:OD1	1:D:77:ARG:NH2	2.36	0.50
1:D:9:THR:OG1	1:D:10:PRO:HD2	2.11	0.50
1:D:140:VAL:O	1:D:144:VAL:HG12	2.12	0.50
1:E:140:VAL:O	1:E:144:VAL:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:VAL:HG12	1:E:211:LYS:N	2.24	0.50
1:I:137:ASP:HA	1:I:140:VAL:HG23	1.92	0.50
1:I:177:GLU:HB3	1:I:209:TRP:HE3	1.76	0.50
1:J:168:ASP:O	1:J:169:GLY:C	2.53	0.50
1:K:137:ASP:HA	1:K:140:VAL:HG23	1.92	0.50
1:A:68:PRO:HG3	1:A:90:GLU:CD	2.36	0.50
1:B:123:TRP:HB2	1:B:130:LEU:HD13	1.92	0.50
1:B:159:VAL:HG12	1:B:186:ASN:HD21	1.76	0.50
1:B:312:LEU:HD12	1:B:314:VAL:HG12	1.92	0.50
1:C:174:LEU:O	1:C:223:ILE:HD13	2.11	0.50
1:E:68:PRO:HG3	1:E:90:GLU:CD	2.36	0.50
1:E:312:LEU:HD12	1:E:314:VAL:HG12	1.92	0.50
1:F:121:ASN:CG	1:F:159:VAL:HG21	2.37	0.50
1:F:174:LEU:O	1:F:223:ILE:HD13	2.11	0.50
1:I:159:VAL:HG12	1:I:186:ASN:HD21	1.76	0.50
1:I:174:LEU:O	1:I:223:ILE:HD13	2.11	0.50
1:J:132:PHE:O	1:J:134:TRP:CE3	2.64	0.50
1:K:311:PHE:HB3	1:K:320:LEU:HD12	1.92	0.50
1:D:158:PHE:HE1	1:D:160:LEU:HB2	1.76	0.50
1:D:174:LEU:O	1:D:223:ILE:HD13	2.11	0.50
1:F:177:GLU:HB3	1:F:209:TRP:HE3	1.76	0.50
1:G:132:PHE:O	1:G:134:TRP:CE3	2.64	0.50
1:H:267:ARG:C	1:H:268:PRO:O	2.50	0.50
1:J:121:ASN:CG	1:J:159:VAL:HG21	2.37	0.50
1:B:158:PHE:HE1	1:B:160:LEU:HB2	1.76	0.50
1:E:41:GLY:O	1:E:42:ALA:HB3	2.12	0.50
1:E:123:TRP:HB2	1:E:130:LEU:HD13	1.92	0.50
1:E:311:PHE:HB3	1:E:320:LEU:HD12	1.92	0.50
1:F:132:PHE:CD2	1:G:135:ASP:HB3	2.47	0.50
1:F:132:PHE:O	1:F:134:TRP:CE3	2.64	0.50
1:H:311:PHE:HE1	1:H:313:ILE:HD11	1.75	0.50
1:I:140:VAL:O	1:I:144:VAL:HG12	2.12	0.50
1:K:158:PHE:HE1	1:K:160:LEU:HB2	1.76	0.50
1:L:68:PRO:HG3	1:L:90:GLU:CD	2.36	0.50
1:A:41:GLY:O	1:A:42:ALA:HB3	2.12	0.50
1:B:41:GLY:O	1:B:42:ALA:HB3	2.12	0.50
1:B:43:LYS:HB2	1:B:44:PRO:HD3	1.92	0.50
1:B:121:ASN:CG	1:B:159:VAL:HG21	2.37	0.50
1:C:41:GLY:O	1:C:42:ALA:HB3	2.12	0.50
1:C:158:PHE:HE1	1:C:160:LEU:HB2	1.77	0.50
1:C:177:GLU:HB3	1:C:209:TRP:HE3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:GLU:HB3	1:D:209:TRP:HE3	1.76	0.50
1:H:27:ILE:CD1	1:H:312:LEU:HD11	2.41	0.50
1:J:68:PRO:HG3	1:J:90:GLU:OE2	2.11	0.50
1:K:9:THR:OG1	1:K:10:PRO:HD2	2.11	0.50
1:L:132:PHE:O	1:L:134:TRP:CE3	2.64	0.50
1:L:365:GLN:NE2	2:L:383:HOH:O	2.42	0.50
1:A:7:ASN:CB	1:D:84:HIS:CG	2.92	0.50
1:A:140:VAL:O	1:A:144:VAL:HG12	2.12	0.50
1:B:68:PRO:HG3	1:B:90:GLU:OE2	2.11	0.50
1:D:132:PHE:O	1:D:134:TRP:CE3	2.64	0.50
1:E:68:PRO:HG3	1:E:90:GLU:OE2	2.11	0.50
1:E:121:ASN:CG	1:E:159:VAL:HG21	2.37	0.50
1:F:311:PHE:HB3	1:F:320:LEU:HD12	1.92	0.50
1:H:52:VAL:O	1:H:56:ILE:HG12	2.12	0.50
1:H:219:THR:O	1:H:220:ASN:HB2	2.10	0.50
1:I:311:PHE:HB3	1:I:320:LEU:HD12	1.93	0.50
1:L:49:PHE:O	1:L:52:VAL:HG12	2.10	0.50
1:L:121:ASN:CG	1:L:159:VAL:HG21	2.37	0.50
1:L:174:LEU:O	1:L:223:ILE:HD13	2.11	0.50
1:A:132:PHE:O	1:A:134:TRP:CE3	2.64	0.50
1:B:121:ASN:ND2	2:B:387:HOH:O	2.44	0.50
1:C:121:ASN:CG	1:C:159:VAL:HG21	2.37	0.50
1:D:41:GLY:O	1:D:42:ALA:HB3	2.12	0.50
1:E:137:ASP:HA	1:E:140:VAL:HG23	1.92	0.50
1:F:140:VAL:O	1:F:144:VAL:HG12	2.12	0.50
1:G:121:ASN:CG	1:G:159:VAL:HG21	2.37	0.50
1:G:158:PHE:HE1	1:G:160:LEU:HB2	1.76	0.50
1:I:121:ASN:ND2	1:I:121:ASN:N	2.60	0.50
1:I:132:PHE:O	1:I:134:TRP:CE3	2.64	0.50
1:A:68:PRO:HG3	1:A:90:GLU:OE2	2.11	0.50
1:B:8:THR:HB	1:B:12:GLN:NE2	2.27	0.50
1:B:358:ASN:O	1:B:361:CYS:N	2.45	0.50
1:C:43:LYS:HB2	1:C:44:PRO:HD3	1.93	0.50
1:D:358:ASN:O	1:D:361:CYS:N	2.45	0.50
1:F:8:THR:HB	1:F:12:GLN:NE2	2.27	0.50
1:F:68:PRO:HG3	1:F:90:GLU:OE2	2.11	0.50
1:G:41:GLY:O	1:G:42:ALA:HB3	2.12	0.50
1:G:174:LEU:O	1:G:223:ILE:HD13	2.11	0.50
1:H:296:ILE:N	1:H:297:PRO:HD3	2.26	0.50
1:I:358:ASN:O	1:I:361:CYS:N	2.45	0.50
1:J:9:THR:OG1	1:J:10:PRO:HD2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:121:ASN:ND2	1:J:121:ASN:N	2.60	0.50
1:K:168:ASP:O	1:K:169:GLY:C	2.53	0.50
1:L:8:THR:HB	1:L:12:GLN:NE2	2.27	0.50
1:L:159:VAL:HG12	1:L:186:ASN:HD21	1.76	0.50
1:A:8:THR:HB	1:A:12:GLN:NE2	2.27	0.50
1:A:358:ASN:O	1:A:361:CYS:N	2.45	0.50
1:E:158:PHE:HE1	1:E:160:LEU:HB2	1.76	0.50
1:F:70:GLN:HB3	2:F:387:HOH:O	2.11	0.50
1:G:68:PRO:HG3	1:G:90:GLU:OE2	2.11	0.50
1:H:223:ILE:C	1:H:225:ASP:H	2.19	0.50
1:J:311:PHE:HB3	1:J:320:LEU:HD12	1.92	0.50
1:K:43:LYS:HB2	1:K:44:PRO:HD3	1.93	0.50
1:A:121:ASN:CG	1:A:159:VAL:HG21	2.37	0.49
1:B:174:LEU:O	1:B:223:ILE:HD13	2.11	0.49
1:D:159:VAL:HG12	1:D:186:ASN:HD21	1.76	0.49
1:E:174:LEU:O	1:E:223:ILE:HD13	2.11	0.49
1:H:126:LEU:CD1	1:K:126:LEU:HD12	2.41	0.49
1:J:177:GLU:HB3	1:J:209:TRP:HE3	1.76	0.49
1:K:41:GLY:O	1:K:42:ALA:HB3	2.12	0.49
1:K:132:PHE:O	1:K:134:TRP:CE3	2.64	0.49
1:C:132:PHE:O	1:C:134:TRP:CE3	2.64	0.49
1:E:8:THR:HB	1:E:12:GLN:NE2	2.27	0.49
1:F:26:GLN:NE2	1:F:63:SER:OG	2.45	0.49
1:F:158:PHE:HE1	1:F:160:LEU:HB2	1.76	0.49
1:I:26:GLN:NE2	1:I:63:SER:OG	2.45	0.49
1:K:8:THR:HB	1:K:12:GLN:NE2	2.27	0.49
1:L:41:GLY:O	1:L:42:ALA:HB3	2.12	0.49
1:A:26:GLN:NE2	1:A:63:SER:OG	2.45	0.49
1:C:312:LEU:HD12	1:C:314:VAL:HG12	1.92	0.49
1:G:159:VAL:HG12	1:G:186:ASN:HD21	1.76	0.49
1:H:167:VAL:HG12	1:H:168:ASP:O	2.11	0.49
1:H:206:LYS:HB3	1:H:264:ALA:HB2	1.93	0.49
1:H:329:GLN:H	1:H:329:GLN:CD	2.21	0.49
1:I:121:ASN:CG	1:I:159:VAL:HG21	2.37	0.49
1:I:168:ASP:O	1:I:169:GLY:C	2.53	0.49
1:J:8:THR:HB	1:J:12:GLN:NE2	2.27	0.49
1:K:43:LYS:NZ	1:L:35:ASN:HD22	2.10	0.49
1:K:68:PRO:HG3	1:K:90:GLU:OE2	2.11	0.49
1:K:290:ASP:CB	1:L:73:ASN:ND2	2.76	0.49
1:L:108:ASN:ND2	1:L:110:LYS:HB2	2.28	0.49
1:A:174:LEU:O	1:A:223:ILE:HD13	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:GLN:NE2	1:B:63:SER:OG	2.45	0.49
1:B:108:ASN:ND2	1:B:110:LYS:HB2	2.28	0.49
1:B:132:PHE:O	1:B:134:TRP:CE3	2.64	0.49
1:D:8:THR:HB	1:D:12:GLN:NE2	2.27	0.49
1:E:26:GLN:NE2	1:E:63:SER:OG	2.45	0.49
1:F:113:LEU:O	1:F:150:VAL:HG23	2.13	0.49
1:G:108:ASN:ND2	1:G:110:LYS:HB2	2.28	0.49
1:I:108:ASN:ND2	1:I:110:LYS:HB2	2.28	0.49
1:J:113:LEU:O	1:J:150:VAL:HG23	2.13	0.49
1:K:223:ILE:C	1:K:225:ASP:H	2.21	0.49
1:K:262:THR:HG22	2:K:387:HOH:O	2.12	0.49
1:A:177:GLU:HB3	1:A:209:TRP:HE3	1.76	0.49
1:B:231:ARG:HG2	2:B:389:HOH:O	2.12	0.49
1:C:147:ILE:CG2	1:J:89:ILE:HG22	2.37	0.49
1:C:223:ILE:C	1:C:225:ASP:H	2.21	0.49
1:C:321:PRO:HB3	1:C:358:ASN:HD22	1.78	0.49
1:G:113:LEU:O	1:G:150:VAL:HG23	2.13	0.49
1:G:230:ILE:HG22	1:G:339:PHE:CE1	2.48	0.49
1:H:185:ARG:HB2	1:H:185:ARG:NH1	2.23	0.49
1:I:8:THR:HB	1:I:12:GLN:NE2	2.27	0.49
1:K:121:ASN:CG	1:K:159:VAL:HG21	2.37	0.49
1:L:26:GLN:NE2	1:L:63:SER:OG	2.45	0.49
1:L:358:ASN:O	1:L:361:CYS:N	2.45	0.49
1:A:158:PHE:HE1	1:A:160:LEU:HB2	1.76	0.49
1:A:315:ASN:HA	2:A:379:HOH:O	2.11	0.49
1:B:223:ILE:C	1:B:225:ASP:H	2.21	0.49
1:B:230:ILE:HG22	1:B:339:PHE:CE1	2.48	0.49
1:C:26:GLN:NE2	1:C:63:SER:OG	2.45	0.49
1:C:108:ASN:ND2	1:C:110:LYS:HB2	2.28	0.49
1:C:113:LEU:O	1:C:150:VAL:HG23	2.13	0.49
1:D:113:LEU:O	1:D:150:VAL:HG23	2.13	0.49
1:D:321:PRO:HB3	1:D:358:ASN:HD22	1.78	0.49
1:D:369:THR:O	1:D:370:LEU:CB	2.47	0.49
1:E:230:ILE:HG22	1:E:339:PHE:CE1	2.48	0.49
1:F:41:GLY:O	1:F:42:ALA:HB3	2.12	0.49
1:G:140:VAL:O	1:G:144:VAL:HG12	2.12	0.49
1:G:321:PRO:HB3	1:G:358:ASN:HD22	1.78	0.49
1:H:132:PHE:O	1:H:134:TRP:CE3	2.65	0.49
1:H:182:HIS:CG	1:H:183:PRO:HD2	2.48	0.49
1:K:26:GLN:NE2	1:K:63:SER:OG	2.45	0.49
1:K:159:VAL:HG12	1:K:186:ASN:HD21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:140:VAL:O	1:L:144:VAL:HG12	2.12	0.49
1:L:230:ILE:HG22	1:L:339:PHE:CE1	2.48	0.49
1:A:43:LYS:NZ	1:G:35:ASN:HD22	2.11	0.49
1:C:358:ASN:O	1:C:361:CYS:N	2.45	0.49
1:D:121:ASN:CG	1:D:159:VAL:HG21	2.37	0.49
1:F:43:LYS:HZ2	1:F:46:GLN:HE22	1.59	0.49
1:G:26:GLN:NE2	1:G:63:SER:OG	2.45	0.49
1:G:358:ASN:O	1:G:361:CYS:N	2.45	0.49
1:H:132:PHE:CD2	1:K:135:ASP:HB3	2.46	0.49
1:J:41:GLY:O	1:J:42:ALA:HB3	2.12	0.49
1:K:80:GLU:HB2	1:L:291:TYR:OH	2.13	0.49
1:A:223:ILE:C	1:A:225:ASP:H	2.21	0.49
1:A:230:ILE:HG22	1:A:339:PHE:CE1	2.48	0.49
1:B:321:PRO:HB3	1:B:358:ASN:HD22	1.78	0.49
1:C:140:VAL:O	1:C:144:VAL:HG12	2.12	0.49
1:C:230:ILE:HG22	1:C:339:PHE:CE1	2.48	0.49
1:H:15:PHE:CZ	1:H:114:ARG:HD3	2.48	0.49
1:I:230:ILE:HG22	1:I:339:PHE:CE1	2.48	0.49
1:I:231:ARG:HG3	1:I:232:PRO:HD2	1.95	0.49
1:J:358:ASN:O	1:J:361:CYS:N	2.45	0.49
1:K:358:ASN:O	1:K:361:CYS:N	2.45	0.49
1:B:140:VAL:O	1:B:144:VAL:HG12	2.11	0.49
1:C:8:THR:HB	1:C:12:GLN:NE2	2.27	0.49
1:D:71:TYR:CZ	1:I:143:LYS:HG2	2.48	0.49
1:D:223:ILE:C	1:D:225:ASP:H	2.21	0.49
1:D:231:ARG:HG3	1:D:232:PRO:HD2	1.95	0.49
1:E:113:LEU:O	1:E:150:VAL:HG23	2.13	0.49
1:F:358:ASN:O	1:F:361:CYS:N	2.45	0.49
1:G:223:ILE:C	1:G:225:ASP:H	2.21	0.49
1:I:41:GLY:O	1:I:42:ALA:HB3	2.12	0.49
1:I:158:PHE:HE1	1:I:160:LEU:HB2	1.76	0.49
1:J:158:PHE:HE1	1:J:160:LEU:HB2	1.76	0.49
1:A:12:GLN:HB3	1:D:81:LEU:C	2.38	0.49
1:D:26:GLN:NE2	1:D:63:SER:OG	2.45	0.49
1:D:108:ASN:ND2	1:D:110:LYS:HB2	2.28	0.49
1:E:321:PRO:HB3	1:E:358:ASN:HD22	1.78	0.49
1:G:177:GLU:HB3	1:G:209:TRP:HE3	1.76	0.49
1:H:27:ILE:HD11	1:H:314:VAL:HG12	1.93	0.49
1:H:28:TRP:CH2	1:H:144:VAL:HG23	2.48	0.49
1:H:50:LEU:HD11	1:H:78:VAL:HG22	1.95	0.49
1:H:176:THR:HG23	1:H:179:CYS:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:GLU:HG2	1:H:207:VAL:HG11	1.94	0.49
1:I:223:ILE:C	1:I:225:ASP:H	2.21	0.49
1:J:26:GLN:NE2	1:J:63:SER:OG	2.45	0.49
1:J:108:ASN:ND2	1:J:110:LYS:HB2	2.27	0.49
1:J:140:VAL:O	1:J:144:VAL:HG12	2.12	0.49
1:A:108:ASN:ND2	1:A:110:LYS:HB2	2.28	0.48
1:A:113:LEU:O	1:A:150:VAL:HG23	2.13	0.48
1:C:320:LEU:HD12	1:C:321:PRO:HD2	1.95	0.48
1:F:230:ILE:HG22	1:F:339:PHE:CE1	2.48	0.48
1:G:8:THR:HB	1:G:12:GLN:NE2	2.27	0.48
1:H:296:ILE:O	1:H:296:ILE:HG12	2.12	0.48
1:I:320:LEU:HD12	1:I:321:PRO:HD2	1.95	0.48
1:K:321:PRO:HB3	1:K:358:ASN:HD22	1.78	0.48
1:L:113:LEU:O	1:L:150:VAL:HG23	2.13	0.48
1:A:231:ARG:HG3	1:A:232:PRO:HD2	1.95	0.48
1:B:113:LEU:O	1:B:150:VAL:HG23	2.13	0.48
1:B:121:ASN:ND2	1:B:121:ASN:N	2.60	0.48
1:C:73:ASN:ND2	1:D:290:ASP:HB3	2.28	0.48
1:E:177:GLU:O	1:E:181:LEU:HB2	2.13	0.48
1:E:358:ASN:O	1:E:361:CYS:N	2.45	0.48
1:H:30:LEU:HB2	1:H:96:ALA:HB1	1.95	0.48
1:H:104:THR:HB	1:H:116:VAL:CG1	2.43	0.48
1:H:237:CYS:SG	1:H:238:ILE:N	2.87	0.48
1:H:278:LYS:N	1:H:325:ASP:OD2	2.43	0.48
1:I:369:THR:O	1:I:370:LEU:CB	2.47	0.48
1:L:158:PHE:HE1	1:L:160:LEU:HB2	1.76	0.48
1:A:291:TYR:OH	1:G:80:GLU:HB2	2.12	0.48
1:A:329:GLN:CD	1:A:329:GLN:H	2.22	0.48
1:C:272:HIS:ND1	1:C:338:MSE:HG2	2.29	0.48
1:D:272:HIS:ND1	1:D:338:MSE:HG2	2.29	0.48
1:F:108:ASN:ND2	1:F:110:LYS:HB2	2.28	0.48
1:G:177:GLU:O	1:G:181:LEU:HB2	2.13	0.48
1:G:231:ARG:HG3	1:G:232:PRO:HD2	1.95	0.48
1:I:321:PRO:HB3	1:I:358:ASN:HD22	1.78	0.48
1:J:272:HIS:ND1	1:J:338:MSE:HG2	2.29	0.48
1:K:140:VAL:O	1:K:144:VAL:HG12	2.12	0.48
1:A:9:THR:HG22	1:A:12:GLN:CG	2.44	0.48
1:B:272:HIS:ND1	1:B:338:MSE:HG2	2.29	0.48
1:C:177:GLU:O	1:C:181:LEU:HB2	2.13	0.48
1:E:80:GLU:CD	1:H:291:TYR:HH	2.21	0.48
1:E:231:ARG:HG3	1:E:232:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:223:ILE:C	1:F:225:ASP:H	2.21	0.48
1:F:231:ARG:HG3	1:F:232:PRO:HD2	1.95	0.48
1:H:30:LEU:HB2	1:H:96:ALA:CB	2.44	0.48
1:H:169:GLY:HA3	2:H:393:HOH:O	2.13	0.48
1:I:177:GLU:O	1:I:181:LEU:HB2	2.13	0.48
1:J:60:GLU:HB2	1:J:61:PRO:HD2	1.96	0.48
1:J:231:ARG:HG3	1:J:232:PRO:HD2	1.95	0.48
1:K:108:ASN:ND2	1:K:110:LYS:HB2	2.28	0.48
1:L:177:GLU:HB3	1:L:209:TRP:HE3	1.76	0.48
1:B:329:GLN:H	1:B:329:GLN:CD	2.22	0.48
1:C:231:ARG:HG3	1:C:232:PRO:HD2	1.95	0.48
1:D:230:ILE:HG22	1:D:339:PHE:CE1	2.48	0.48
1:E:108:ASN:ND2	1:E:110:LYS:HB2	2.28	0.48
1:J:56:ILE:HD13	1:J:319:ILE:HG13	1.96	0.48
1:J:121:ASN:H	1:J:121:ASN:ND2	2.07	0.48
1:J:230:ILE:HG22	1:J:339:PHE:CE1	2.48	0.48
1:K:177:GLU:O	1:K:181:LEU:HB2	2.13	0.48
1:A:60:GLU:HB2	1:A:61:PRO:HD2	1.96	0.48
1:A:290:ASP:CB	1:G:73:ASN:ND2	2.75	0.48
1:E:60:GLU:HB2	1:E:61:PRO:HD2	1.96	0.48
1:F:320:LEU:HD12	1:F:321:PRO:HD2	1.95	0.48
1:G:56:ILE:HD13	1:G:319:ILE:HG13	1.96	0.48
1:G:60:GLU:HB2	1:G:61:PRO:HD2	1.96	0.48
1:J:223:ILE:C	1:J:225:ASP:H	2.21	0.48
1:K:230:ILE:HG22	1:K:339:PHE:CE1	2.48	0.48
1:K:329:GLN:H	1:K:329:GLN:CD	2.22	0.48
1:A:272:HIS:ND1	1:A:338:MSE:HG2	2.29	0.48
1:E:71:TYR:CZ	1:K:143:LYS:HG2	2.49	0.48
1:E:308:TYR:OH	1:E:325:ASP:HB3	2.14	0.48
1:F:60:GLU:HB2	1:F:61:PRO:HD2	1.96	0.48
1:F:321:PRO:HB3	1:F:358:ASN:HD22	1.78	0.48
1:H:103:PRO:HD3	1:H:144:VAL:HG11	1.94	0.48
1:I:113:LEU:O	1:I:150:VAL:HG23	2.13	0.48
1:K:121:ASN:H	1:K:121:ASN:ND2	2.07	0.48
1:K:320:LEU:HD12	1:K:321:PRO:HD2	1.95	0.48
1:L:121:ASN:H	1:L:121:ASN:ND2	2.07	0.48
1:L:272:HIS:ND1	1:L:338:MSE:HG2	2.29	0.48
1:A:369:THR:O	1:A:370:LEU:CB	2.47	0.48
1:B:177:GLU:O	1:B:181:LEU:HB2	2.13	0.48
1:D:341:ASP:HB3	1:F:57:SER:O	2.14	0.48
1:E:177:GLU:HB3	1:E:209:TRP:HE3	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:VAL:CG1	1:E:211:LYS:N	2.77	0.48
1:G:320:LEU:HD12	1:G:321:PRO:HD2	1.95	0.48
1:H:80:GLU:C	1:H:82:GLY:H	2.22	0.48
1:H:177:GLU:HG2	1:H:211:LYS:HA	1.96	0.48
1:H:224:ASP:OD2	1:H:360:HIS:HD2	1.96	0.48
1:I:329:GLN:CD	1:I:329:GLN:H	2.22	0.48
1:K:9:THR:HG22	1:K:12:GLN:CG	2.44	0.48
1:A:177:GLU:O	1:A:181:LEU:HB2	2.13	0.48
1:C:9:THR:HG22	1:C:12:GLN:CG	2.44	0.48
1:C:56:ILE:HD13	1:C:319:ILE:HG13	1.96	0.48
1:D:177:GLU:O	1:D:181:LEU:HB2	2.13	0.48
1:E:143:LYS:HG2	1:K:71:TYR:CZ	2.49	0.48
1:E:329:GLN:H	1:E:329:GLN:CD	2.22	0.48
1:F:210:VAL:CG1	1:F:211:LYS:N	2.77	0.48
1:G:272:HIS:ND1	1:G:338:MSE:HG2	2.29	0.48
1:J:308:TYR:OH	1:J:325:ASP:HB3	2.14	0.48
1:J:329:GLN:H	1:J:329:GLN:CD	2.22	0.48
1:L:223:ILE:C	1:L:225:ASP:H	2.21	0.48
1:L:308:TYR:OH	1:L:325:ASP:HB3	2.14	0.48
1:L:329:GLN:CD	1:L:329:GLN:H	2.22	0.48
1:B:231:ARG:HG3	1:B:232:PRO:HD2	1.95	0.48
1:D:60:GLU:HB2	1:D:61:PRO:HD2	1.96	0.48
1:D:210:VAL:CG1	1:D:211:LYS:N	2.77	0.48
1:D:340:PRO:CG	1:F:58:GLU:O	2.61	0.48
1:E:320:LEU:HD12	1:E:321:PRO:HD2	1.95	0.48
1:F:47:LYS:O	1:F:51:GLU:HG3	2.14	0.48
1:F:177:GLU:O	1:F:181:LEU:HB2	2.13	0.48
1:F:329:GLN:H	1:F:329:GLN:CD	2.22	0.48
1:H:207:VAL:HG22	1:H:209:TRP:NE1	2.28	0.48
1:I:272:HIS:ND1	1:I:338:MSE:HG2	2.29	0.48
1:J:321:PRO:HB3	1:J:358:ASN:HD22	1.78	0.48
1:L:203:ASN:HD22	1:L:203:ASN:HA	1.50	0.48
1:A:56:ILE:HD13	1:A:319:ILE:HG13	1.96	0.47
1:A:210:VAL:CG1	1:A:211:LYS:N	2.77	0.47
1:A:320:LEU:HD12	1:A:321:PRO:HD2	1.95	0.47
1:B:9:THR:HG22	1:B:12:GLN:CG	2.44	0.47
1:C:61:PRO:HA	1:C:85:ASN:ND2	2.29	0.47
1:C:308:TYR:OH	1:C:325:ASP:HB3	2.14	0.47
1:C:329:GLN:H	1:C:329:GLN:CD	2.22	0.47
1:D:47:LYS:O	1:D:51:GLU:HG3	2.14	0.47
1:E:223:ILE:C	1:E:225:ASP:H	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:HIS:ND1	1:E:338:MSE:HG2	2.29	0.47
1:F:231:ARG:CG	1:F:232:PRO:HD2	2.44	0.47
1:F:308:TYR:OH	1:F:325:ASP:HB3	2.14	0.47
1:G:176:THR:HG21	1:G:221:GLY:O	2.14	0.47
1:G:210:VAL:CG1	1:G:211:LYS:N	2.77	0.47
1:G:308:TYR:OH	1:G:325:ASP:HB3	2.14	0.47
1:H:27:ILE:HG13	1:H:60:GLU:OE2	2.13	0.47
1:H:29:MSE:HE1	1:H:52:VAL:CG2	2.44	0.47
1:I:210:VAL:CG1	1:I:211:LYS:N	2.77	0.47
1:J:231:ARG:CG	1:J:232:PRO:HD2	2.44	0.47
1:K:56:ILE:HD13	1:K:319:ILE:HG13	1.96	0.47
1:K:60:GLU:HB2	1:K:61:PRO:HD2	1.96	0.47
1:K:308:TYR:OH	1:K:325:ASP:HB3	2.14	0.47
1:L:47:LYS:HD3	2:L:388:HOH:O	2.13	0.47
1:L:320:LEU:HD12	1:L:321:PRO:HD2	1.95	0.47
1:A:176:THR:HG21	1:A:221:GLY:O	2.14	0.47
1:D:21:PHE:CZ	1:D:232:PRO:HD3	2.50	0.47
1:D:341:ASP:CA	1:F:84:HIS:HD2	2.19	0.47
1:E:61:PRO:HA	1:E:85:ASN:ND2	2.29	0.47
1:F:176:THR:HG21	1:F:221:GLY:O	2.14	0.47
1:F:272:HIS:ND1	1:F:338:MSE:HG2	2.29	0.47
1:H:119:GLU:O	1:H:159:VAL:HG23	2.14	0.47
1:H:181:LEU:HD21	1:H:191:LYS:HG3	1.96	0.47
1:I:9:THR:HG22	1:I:12:GLN:CG	2.44	0.47
1:I:56:ILE:HD13	1:I:319:ILE:HG13	1.96	0.47
1:J:9:THR:HG22	1:J:12:GLN:CG	2.44	0.47
1:J:47:LYS:O	1:J:51:GLU:HG3	2.14	0.47
1:J:210:VAL:CG1	1:J:211:LYS:N	2.77	0.47
1:K:231:ARG:HG3	1:K:232:PRO:HD2	1.95	0.47
1:K:272:HIS:ND1	1:K:338:MSE:HG2	2.29	0.47
1:L:9:THR:HG22	1:L:12:GLN:CG	2.44	0.47
1:L:61:PRO:HA	1:L:85:ASN:ND2	2.29	0.47
1:A:7:ASN:HB2	1:D:84:HIS:CG	2.49	0.47
1:A:321:PRO:HB3	1:A:358:ASN:HD22	1.78	0.47
1:C:47:LYS:O	1:C:51:GLU:HG3	2.14	0.47
1:C:176:THR:HG21	1:C:221:GLY:O	2.14	0.47
1:D:39:ARG:HG3	1:D:40:LEU:HD23	1.97	0.47
1:D:56:ILE:HD13	1:D:319:ILE:HG13	1.96	0.47
1:E:121:ASN:N	1:E:121:ASN:ND2	2.60	0.47
1:E:323:TYR:HA	1:E:350:GLU:HB3	1.97	0.47
1:G:39:ARG:HG3	1:G:40:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:336:GLN:CG	2:G:404:HOH:O	2.54	0.47
1:H:27:ILE:HD11	1:H:312:LEU:HD11	1.97	0.47
1:L:21:PHE:CZ	1:L:232:PRO:HD3	2.50	0.47
1:L:60:GLU:HB2	1:L:61:PRO:HD2	1.96	0.47
1:A:61:PRO:HA	1:A:85:ASN:ND2	2.29	0.47
1:A:308:TYR:OH	1:A:325:ASP:HB3	2.14	0.47
1:B:21:PHE:CZ	1:B:232:PRO:HD3	2.50	0.47
1:B:308:TYR:OH	1:B:325:ASP:HB3	2.14	0.47
1:C:231:ARG:CG	1:C:232:PRO:HD2	2.44	0.47
1:D:171:GLY:CA	1:D:204:CYS:HA	2.43	0.47
1:D:231:ARG:CG	1:D:232:PRO:HD2	2.44	0.47
1:D:329:GLN:CD	1:D:329:GLN:H	2.22	0.47
1:G:339:PHE:HB3	2:G:391:HOH:O	2.15	0.47
1:H:68:PRO:HD2	2:H:386:HOH:O	2.14	0.47
1:I:47:LYS:O	1:I:51:GLU:HG3	2.14	0.47
1:J:61:PRO:HA	1:J:85:ASN:ND2	2.29	0.47
1:L:47:LYS:O	1:L:51:GLU:HG3	2.14	0.47
1:L:321:PRO:HB3	1:L:358:ASN:HD22	1.78	0.47
1:A:21:PHE:CZ	1:A:232:PRO:HD3	2.50	0.47
1:A:126:LEU:HD12	1:B:126:LEU:HD12	1.96	0.47
1:B:60:GLU:HB2	1:B:61:PRO:HD2	1.96	0.47
1:E:21:PHE:CZ	1:E:232:PRO:HD3	2.50	0.47
1:E:39:ARG:HG3	1:E:40:LEU:HD23	1.97	0.47
1:F:56:ILE:HD13	1:F:319:ILE:HG13	1.96	0.47
1:I:66:VAL:CG2	1:I:71:TYR:HA	2.45	0.47
1:I:231:ARG:CG	1:I:232:PRO:HD2	2.44	0.47
1:J:39:ARG:HG3	1:J:40:LEU:HD23	1.97	0.47
1:J:177:GLU:O	1:J:181:LEU:HB2	2.13	0.47
1:J:323:TYR:HA	1:J:350:GLU:HB3	1.97	0.47
1:K:176:THR:HG21	1:K:221:GLY:O	2.14	0.47
1:L:56:ILE:HD13	1:L:319:ILE:HG13	1.96	0.47
1:A:43:LYS:HZ2	1:A:46:GLN:HE22	1.61	0.47
1:D:143:LYS:HG2	1:I:71:TYR:CZ	2.50	0.47
1:D:308:TYR:OH	1:D:325:ASP:HB3	2.14	0.47
1:E:176:THR:HG21	1:E:221:GLY:O	2.14	0.47
1:F:66:VAL:CG2	1:F:71:TYR:HA	2.45	0.47
1:F:309:LEU:HD22	1:F:311:PHE:HE2	1.80	0.47
1:G:9:THR:HG22	1:G:12:GLN:CG	2.44	0.47
1:H:358:ASN:ND2	1:H:359:ILE:HG13	2.29	0.47
1:I:60:GLU:HB2	1:I:61:PRO:HD2	1.96	0.47
1:I:176:THR:HG21	1:I:221:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:21:PHE:CZ	1:J:232:PRO:HD3	2.50	0.47
1:J:176:THR:HG21	1:J:221:GLY:O	2.14	0.47
1:K:61:PRO:HA	1:K:85:ASN:ND2	2.29	0.47
1:K:231:ARG:CG	1:K:232:PRO:HD2	2.44	0.47
1:L:210:VAL:CG1	1:L:211:LYS:N	2.77	0.47
1:L:231:ARG:CG	1:L:232:PRO:HD2	2.44	0.47
1:L:231:ARG:HG3	1:L:232:PRO:HD2	1.95	0.47
1:L:323:TYR:HA	1:L:350:GLU:HB3	1.97	0.47
1:A:39:ARG:HG3	1:A:40:LEU:HD23	1.97	0.47
1:A:66:VAL:CG2	1:A:71:TYR:HA	2.45	0.47
1:A:318:ILE:HD11	1:A:339:PHE:CD1	2.50	0.47
1:B:54:GLU:O	1:B:57:SER:HB2	2.15	0.47
1:B:177:GLU:HB3	1:B:209:TRP:HE3	1.76	0.47
1:B:231:ARG:CG	1:B:232:PRO:HD2	2.45	0.47
1:C:21:PHE:CZ	1:C:232:PRO:HD3	2.50	0.47
1:C:39:ARG:HG3	1:C:40:LEU:HD23	1.97	0.47
1:C:323:TYR:HA	1:C:350:GLU:HB3	1.97	0.47
1:D:9:THR:HG22	1:D:12:GLN:CG	2.44	0.47
1:D:61:PRO:HA	1:D:85:ASN:ND2	2.29	0.47
1:D:320:LEU:HD12	1:D:321:PRO:HD2	1.95	0.47
1:E:9:THR:HG22	1:E:12:GLN:CG	2.44	0.47
1:E:318:ILE:HD11	1:E:339:PHE:CD1	2.50	0.47
1:F:9:THR:HG22	1:F:12:GLN:CG	2.44	0.47
1:F:61:PRO:HA	1:F:85:ASN:ND2	2.29	0.47
1:G:21:PHE:CZ	1:G:232:PRO:HD3	2.50	0.47
1:G:118:TRP:CZ3	1:G:155:THR:HG21	2.50	0.47
1:G:318:ILE:HD11	1:G:339:PHE:CD1	2.50	0.47
1:G:329:GLN:CD	1:G:329:GLN:H	2.22	0.47
1:H:69:LEU:HG	2:H:386:HOH:O	2.15	0.47
1:H:108:ASN:HD21	1:H:110:LYS:HB2	1.80	0.47
1:H:181:LEU:HD21	1:H:191:LYS:CG	2.45	0.47
1:H:188:HIS:CE1	1:H:189:LEU:HD13	2.49	0.47
1:H:263:ASP:C	1:H:265:LYS:H	2.23	0.47
1:J:43:LYS:HZ2	1:J:46:GLN:HE22	1.63	0.47
1:K:54:GLU:O	1:K:57:SER:HB2	2.15	0.47
1:L:39:ARG:HG3	1:L:40:LEU:HD23	1.97	0.47
1:L:54:GLU:O	1:L:57:SER:HB2	2.15	0.47
1:L:176:THR:HG21	1:L:221:GLY:O	2.14	0.47
1:L:177:GLU:O	1:L:181:LEU:HB2	2.13	0.47
1:L:318:ILE:HD11	1:L:339:PHE:CD1	2.50	0.47
1:A:65:CYS:HB3	1:A:91:MSE:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ARG:HG3	1:B:40:LEU:HD23	1.97	0.47
1:B:47:LYS:O	1:B:51:GLU:HG3	2.14	0.47
1:B:118:TRP:CZ3	1:B:155:THR:HG21	2.50	0.47
1:B:320:LEU:HD12	1:B:321:PRO:HD2	1.95	0.47
1:C:171:GLY:CA	1:C:204:CYS:HA	2.43	0.47
1:F:65:CYS:HB3	1:F:91:MSE:HB3	1.97	0.47
1:G:47:LYS:O	1:G:51:GLU:HG3	2.15	0.47
1:G:121:ASN:H	1:G:121:ASN:ND2	2.07	0.47
1:I:54:GLU:O	1:I:57:SER:HB2	2.15	0.47
1:I:61:PRO:HA	1:I:85:ASN:ND2	2.29	0.47
1:K:113:LEU:O	1:K:150:VAL:HG23	2.13	0.47
1:K:323:TYR:HA	1:K:350:GLU:HB3	1.97	0.47
1:L:65:CYS:HB3	1:L:91:MSE:HB3	1.97	0.47
1:L:66:VAL:CG2	1:L:71:TYR:HA	2.45	0.47
1:B:309:LEU:HD22	1:B:311:PHE:HE2	1.80	0.47
1:C:43:LYS:HZ2	1:C:46:GLN:HE22	1.63	0.47
1:C:54:GLU:O	1:C:57:SER:HB2	2.15	0.47
1:C:60:GLU:HB2	1:C:61:PRO:HD2	1.96	0.47
1:C:174:LEU:O	1:C:223:ILE:HG21	2.15	0.47
1:C:210:VAL:CG1	1:C:211:LYS:N	2.77	0.47
1:D:66:VAL:CG2	1:D:71:TYR:HA	2.45	0.47
1:D:224:ASP:HB2	1:D:360:HIS:HD2	1.80	0.47
1:E:47:LYS:O	1:E:51:GLU:HG3	2.14	0.47
1:E:174:LEU:O	1:E:223:ILE:HG21	2.15	0.47
1:F:318:ILE:HD11	1:F:339:PHE:CD1	2.50	0.47
1:G:66:VAL:CG2	1:G:71:TYR:HA	2.45	0.47
1:H:124:GLY:O	1:H:127:VAL:HG13	2.15	0.47
1:H:132:PHE:O	1:H:133:PRO:C	2.56	0.47
1:H:159:VAL:O	1:H:159:VAL:HG13	2.15	0.47
1:J:54:GLU:O	1:J:57:SER:HB2	2.15	0.47
1:K:43:LYS:HZ2	1:K:46:GLN:HE22	1.61	0.47
1:K:66:VAL:CG2	1:K:71:TYR:HA	2.45	0.47
1:K:224:ASP:HB2	1:K:360:HIS:HD2	1.80	0.47
1:B:56:ILE:HD13	1:B:319:ILE:HG13	1.96	0.47
1:B:176:THR:HG21	1:B:221:GLY:O	2.14	0.47
1:D:318:ILE:HD11	1:D:339:PHE:CD1	2.50	0.47
1:E:224:ASP:HB2	1:E:360:HIS:HD2	1.80	0.47
1:F:21:PHE:CZ	1:F:232:PRO:HD3	2.50	0.47
1:G:231:ARG:CG	1:G:232:PRO:HD2	2.44	0.47
1:G:323:TYR:HA	1:G:350:GLU:HB3	1.97	0.47
1:I:323:TYR:HA	1:I:350:GLU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:65:CYS:HB3	1:J:91:MSE:HB3	1.97	0.47
1:J:118:TRP:CZ3	1:J:155:THR:HG21	2.50	0.47
1:J:318:ILE:HD11	1:J:339:PHE:CD1	2.50	0.47
1:K:309:LEU:HD22	1:K:311:PHE:HE2	1.80	0.47
1:A:224:ASP:HB2	1:A:360:HIS:HD2	1.80	0.46
1:A:231:ARG:CG	1:A:232:PRO:HD2	2.44	0.46
1:B:66:VAL:CG2	1:B:71:TYR:HA	2.45	0.46
1:B:174:LEU:O	1:B:223:ILE:HG21	2.15	0.46
1:B:318:ILE:HD11	1:B:339:PHE:CD1	2.50	0.46
1:C:29:MSE:HE1	1:C:52:VAL:HG13	1.97	0.46
1:D:121:ASN:N	1:D:121:ASN:ND2	2.60	0.46
1:D:174:LEU:O	1:D:223:ILE:HG21	2.15	0.46
1:E:56:ILE:HD13	1:E:319:ILE:HG13	1.96	0.46
1:E:309:LEU:HD22	1:E:311:PHE:HE2	1.80	0.46
1:G:61:PRO:HA	1:G:85:ASN:ND2	2.29	0.46
1:G:245:HIS:ND1	1:G:246:PRO:HD2	2.30	0.46
1:H:27:ILE:HD11	1:H:314:VAL:CG1	2.45	0.46
1:H:339:PHE:C	1:H:341:ASP:H	2.21	0.46
1:I:21:PHE:CZ	1:I:232:PRO:HD3	2.50	0.46
1:I:118:TRP:CZ3	1:I:155:THR:HG21	2.50	0.46
1:I:245:HIS:ND1	1:I:246:PRO:HD2	2.30	0.46
1:I:308:TYR:OH	1:I:325:ASP:HB3	2.14	0.46
1:I:318:ILE:HD11	1:I:339:PHE:CD1	2.50	0.46
1:J:320:LEU:HD12	1:J:321:PRO:HD2	1.95	0.46
1:K:47:LYS:O	1:K:51:GLU:HG3	2.14	0.46
1:K:210:VAL:CG1	1:K:211:LYS:N	2.77	0.46
1:L:174:LEU:O	1:L:223:ILE:HG21	2.15	0.46
1:A:11:LYS:HG3	1:A:203:ASN:ND2	2.31	0.46
1:A:47:LYS:O	1:A:51:GLU:HG3	2.14	0.46
1:A:54:GLU:O	1:A:57:SER:HB2	2.15	0.46
1:A:171:GLY:CA	1:A:204:CYS:HA	2.43	0.46
1:C:11:LYS:HG3	1:C:203:ASN:ND2	2.31	0.46
1:C:318:ILE:HD11	1:C:339:PHE:CD1	2.50	0.46
1:D:309:LEU:HD22	1:D:311:PHE:HE2	1.80	0.46
1:D:323:TYR:HA	1:D:350:GLU:HB3	1.97	0.46
1:F:224:ASP:HB2	1:F:360:HIS:HD2	1.80	0.46
1:F:369:THR:O	1:F:370:LEU:CB	2.47	0.46
1:G:29:MSE:HE1	1:G:52:VAL:HG13	1.97	0.46
1:G:174:LEU:O	1:G:223:ILE:HG21	2.15	0.46
1:I:171:GLY:CA	1:I:204:CYS:HA	2.43	0.46
1:I:224:ASP:HB2	1:I:360:HIS:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:224:ASP:HB2	1:L:360:HIS:HD2	1.80	0.46
1:L:245:HIS:ND1	1:L:246:PRO:HD2	2.30	0.46
1:A:118:TRP:CZ3	1:A:155:THR:HG21	2.50	0.46
1:B:224:ASP:HB2	1:B:360:HIS:HD2	1.80	0.46
1:B:311:PHE:CE1	1:B:313:ILE:HD11	2.51	0.46
1:B:336:GLN:OE1	1:B:336:GLN:HA	2.15	0.46
1:C:311:PHE:CE1	1:C:313:ILE:HD11	2.51	0.46
1:E:65:CYS:HB3	1:E:91:MSE:HB3	1.97	0.46
1:E:66:VAL:CG2	1:E:71:TYR:HA	2.45	0.46
1:E:121:ASN:H	1:E:121:ASN:ND2	2.07	0.46
1:F:39:ARG:HH11	1:F:40:LEU:HD23	1.81	0.46
1:F:245:HIS:ND1	1:F:246:PRO:HD2	2.30	0.46
1:G:67:PRO:HA	1:G:68:PRO:HD3	1.80	0.46
1:H:29:MSE:HA	1:H:98:ILE:HG21	1.96	0.46
1:I:65:CYS:HB3	1:I:91:MSE:HB3	1.97	0.46
1:J:39:ARG:HH11	1:J:40:LEU:HD23	1.81	0.46
1:K:77:ARG:NH2	1:L:290:ASP:OD1	2.38	0.46
1:K:318:ILE:HD11	1:K:339:PHE:CD1	2.50	0.46
1:L:311:PHE:CE1	1:L:313:ILE:HD11	2.51	0.46
1:A:89:ILE:HG22	1:F:147:ILE:CG2	2.36	0.46
1:B:210:VAL:CG1	1:B:211:LYS:N	2.77	0.46
1:C:65:CYS:HB3	1:C:91:MSE:HB3	1.97	0.46
1:F:54:GLU:O	1:F:57:SER:HB2	2.15	0.46
1:F:171:GLY:CA	1:F:204:CYS:HA	2.43	0.46
1:F:174:LEU:O	1:F:223:ILE:HG21	2.15	0.46
1:I:311:PHE:CE1	1:I:313:ILE:HD11	2.51	0.46
1:J:215:ASP:HB2	1:J:221:GLY:HA2	1.98	0.46
1:K:11:LYS:HG3	1:K:203:ASN:ND2	2.31	0.46
1:K:21:PHE:CZ	1:K:232:PRO:HD3	2.50	0.46
1:K:203:ASN:HD22	1:K:203:ASN:HA	1.50	0.46
1:K:245:HIS:ND1	1:K:246:PRO:HD2	2.31	0.46
1:A:311:PHE:CE1	1:A:313:ILE:HD11	2.51	0.46
1:C:35:ASN:HD22	1:D:43:LYS:NZ	2.14	0.46
1:D:39:ARG:HH11	1:D:40:LEU:HD23	1.81	0.46
1:D:118:TRP:CZ3	1:D:155:THR:HG21	2.50	0.46
1:D:176:THR:HG21	1:D:221:GLY:O	2.14	0.46
1:D:215:ASP:HB2	1:D:221:GLY:HA2	1.98	0.46
1:J:158:PHE:CE1	1:J:160:LEU:HB2	2.51	0.46
1:K:174:LEU:O	1:K:223:ILE:HG21	2.15	0.46
1:L:309:LEU:HD22	1:L:311:PHE:HE2	1.80	0.46
1:B:323:TYR:HA	1:B:350:GLU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:VAL:CG2	1:C:71:TYR:HA	2.45	0.46
1:C:215:ASP:HB2	1:C:221:GLY:HA2	1.98	0.46
1:D:29:MSE:HE1	1:D:52:VAL:HG13	1.97	0.46
1:E:118:TRP:CZ3	1:E:155:THR:HG21	2.50	0.46
1:E:231:ARG:CG	1:E:232:PRO:HD2	2.44	0.46
1:E:311:PHE:CE1	1:E:313:ILE:HD11	2.51	0.46
1:G:39:ARG:HH11	1:G:40:LEU:HD23	1.80	0.46
1:H:330:LEU:O	1:H:330:LEU:HD12	2.16	0.46
1:J:11:LYS:HG3	1:J:203:ASN:ND2	2.31	0.46
1:J:245:HIS:ND1	1:J:246:PRO:HD2	2.31	0.46
1:J:309:LEU:HD22	1:J:311:PHE:HE2	1.80	0.46
1:J:311:PHE:CE1	1:J:313:ILE:HD11	2.51	0.46
1:K:65:CYS:HB3	1:K:91:MSE:HB3	1.97	0.46
1:K:158:PHE:CE1	1:K:160:LEU:HB2	2.51	0.46
1:K:311:PHE:CE1	1:K:313:ILE:HD11	2.51	0.46
1:L:29:MSE:HE1	1:L:52:VAL:HG13	1.98	0.46
1:A:71:TYR:CZ	1:F:143:LYS:HG2	2.50	0.46
1:B:61:PRO:HA	1:B:85:ASN:ND2	2.29	0.46
1:B:215:ASP:HB2	1:B:221:GLY:HA2	1.98	0.46
1:C:39:ARG:HH11	1:C:40:LEU:HD23	1.81	0.46
1:C:309:LEU:HD22	1:C:311:PHE:HE2	1.80	0.46
1:C:336:GLN:HA	1:C:336:GLN:OE1	2.15	0.46
1:D:245:HIS:ND1	1:D:246:PRO:HD2	2.31	0.46
1:E:11:LYS:HG3	1:E:203:ASN:ND2	2.31	0.46
1:F:29:MSE:HE1	1:F:52:VAL:HG13	1.98	0.46
1:F:135:ASP:HB3	1:G:132:PHE:CD2	2.51	0.46
1:F:158:PHE:CE1	1:F:160:LEU:HB2	2.51	0.46
1:G:311:PHE:CE1	1:G:313:ILE:HD11	2.51	0.46
1:H:195:GLU:O	1:H:199:LYS:HG3	2.16	0.46
1:H:243:LYS:HA	1:H:248:TYR:CG	2.50	0.46
1:J:224:ASP:HB2	1:J:360:HIS:HD2	1.80	0.46
1:A:29:MSE:HE1	1:A:52:VAL:HG13	1.98	0.46
1:C:245:HIS:ND1	1:C:246:PRO:HD2	2.30	0.46
1:D:311:PHE:CE1	1:D:313:ILE:HD11	2.51	0.46
1:E:50:LEU:HG	1:E:81:LEU:HD11	1.98	0.46
1:E:77:ARG:NH1	1:H:291:TYR:HE1	2.13	0.46
1:F:118:TRP:CZ3	1:F:155:THR:HG21	2.50	0.46
1:F:215:ASP:HB2	1:F:221:GLY:HA2	1.98	0.46
1:F:336:GLN:OE1	1:F:336:GLN:HA	2.15	0.46
1:G:11:LYS:HG3	1:G:203:ASN:ND2	2.31	0.46
1:G:215:ASP:HB2	1:G:221:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:113:LEU:O	1:H:114:ARG:HG3	2.15	0.46
1:I:39:ARG:HG3	1:I:40:LEU:HD23	1.97	0.46
1:I:158:PHE:CE1	1:I:160:LEU:HB2	2.51	0.46
1:J:29:MSE:HE1	1:J:52:VAL:HG13	1.97	0.46
1:J:336:GLN:OE1	1:J:336:GLN:HA	2.15	0.46
1:L:49:PHE:HA	1:L:52:VAL:HG12	1.98	0.46
1:B:50:LEU:HG	1:B:81:LEU:HD11	1.98	0.46
1:B:245:HIS:ND1	1:B:246:PRO:HD2	2.31	0.46
1:D:49:PHE:HA	1:D:52:VAL:HG12	1.98	0.46
1:D:65:CYS:HB3	1:D:91:MSE:HB3	1.97	0.46
1:D:158:PHE:CE1	1:D:160:LEU:HB2	2.51	0.46
1:E:46:GLN:NE2	2:E:379:HOH:O	2.48	0.46
1:E:49:PHE:HA	1:E:52:VAL:HG12	1.98	0.46
1:E:245:HIS:ND1	1:E:246:PRO:HD2	2.30	0.46
1:F:311:PHE:CE1	1:F:313:ILE:HD11	2.51	0.46
1:G:50:LEU:HG	1:G:81:LEU:HD11	1.98	0.46
1:H:132:PHE:CB	1:H:133:PRO:HD3	2.40	0.46
1:I:11:LYS:HG3	1:I:203:ASN:ND2	2.31	0.46
1:I:29:MSE:HE1	1:I:52:VAL:HG13	1.98	0.46
1:J:174:LEU:O	1:J:223:ILE:HG21	2.15	0.46
1:K:39:ARG:HG3	1:K:40:LEU:HD23	1.97	0.46
1:K:39:ARG:HH11	1:K:40:LEU:HD23	1.80	0.46
1:K:118:TRP:CZ3	1:K:155:THR:HG21	2.50	0.46
1:A:158:PHE:CE1	1:A:160:LEU:HB2	2.51	0.46
1:B:11:LYS:HG3	1:B:203:ASN:ND2	2.30	0.46
1:C:118:TRP:CZ3	1:C:155:THR:HG21	2.50	0.46
1:E:158:PHE:CE1	1:E:160:LEU:HB2	2.51	0.46
1:H:4:ARG:NH2	1:H:154:LYS:HD3	2.31	0.46
1:I:336:GLN:OE1	1:I:336:GLN:HA	2.15	0.46
1:J:49:PHE:HA	1:J:52:VAL:HG12	1.98	0.46
1:J:94:ASP:HB2	1:J:137:ASP:OD2	2.16	0.46
1:J:171:GLY:CA	1:J:204:CYS:HA	2.43	0.46
1:A:38:TRP:HZ3	1:A:352:ILE:HA	1.81	0.45
1:A:49:PHE:HA	1:A:52:VAL:HG12	1.98	0.45
1:A:323:TYR:HA	1:A:350:GLU:HB3	1.97	0.45
1:B:39:ARG:HH11	1:B:40:LEU:HD23	1.81	0.45
1:C:158:PHE:CE1	1:C:160:LEU:HB2	2.51	0.45
1:C:224:ASP:HB2	1:C:360:HIS:HD2	1.80	0.45
1:E:203:ASN:HD22	1:E:203:ASN:HA	1.50	0.45
1:F:39:ARG:HG3	1:F:40:LEU:HD23	1.97	0.45
1:G:54:GLU:O	1:G:57:SER:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:133:PRO:HG3	1:K:135:ASP:CG	2.41	0.45
1:H:159:VAL:HG12	1:H:186:ASN:ND2	2.31	0.45
1:J:38:TRP:HZ3	1:J:352:ILE:HA	1.81	0.45
1:K:291:TYR:OH	1:L:80:GLU:HB2	2.15	0.45
1:L:94:ASP:HB2	1:L:137:ASP:OD2	2.16	0.45
1:L:118:TRP:CZ3	1:L:155:THR:HG21	2.50	0.45
1:A:161:GLU:HG3	1:A:222:HIS:CE1	2.52	0.45
1:B:65:CYS:HB3	1:B:91:MSE:HB3	1.97	0.45
1:D:11:LYS:HG3	1:D:203:ASN:ND2	2.31	0.45
1:E:29:MSE:HE1	1:E:52:VAL:HG13	1.97	0.45
1:F:38:TRP:HZ3	1:F:352:ILE:HA	1.81	0.45
1:F:323:TYR:HA	1:F:350:GLU:HB3	1.97	0.45
1:G:224:ASP:HB2	1:G:360:HIS:HD2	1.80	0.45
1:H:351:GLU:HA	1:H:354:TYR:HD2	1.82	0.45
1:I:49:PHE:HA	1:I:52:VAL:HG12	1.98	0.45
1:L:11:LYS:HG3	1:L:203:ASN:ND2	2.30	0.45
1:D:54:GLU:O	1:D:57:SER:HB2	2.15	0.45
1:E:38:TRP:HZ3	1:E:352:ILE:HA	1.81	0.45
1:F:94:ASP:HB2	1:F:137:ASP:OD2	2.16	0.45
1:G:161:GLU:HG3	1:G:222:HIS:CE1	2.52	0.45
1:G:336:GLN:OE1	1:G:336:GLN:HA	2.15	0.45
1:H:34:ARG:HD2	1:H:94:ASP:O	2.17	0.45
1:I:39:ARG:HH11	1:I:40:LEU:HD23	1.81	0.45
1:I:43:LYS:HZ2	1:I:46:GLN:HE22	1.64	0.45
1:I:50:LEU:HG	1:I:81:LEU:HD11	1.98	0.45
1:I:94:ASP:HB2	1:I:137:ASP:OD2	2.16	0.45
1:I:174:LEU:O	1:I:223:ILE:HG21	2.15	0.45
1:I:309:LEU:HD22	1:I:311:PHE:HE2	1.80	0.45
1:J:50:LEU:HG	1:J:81:LEU:HD11	1.98	0.45
1:J:66:VAL:CG2	1:J:71:TYR:HA	2.45	0.45
1:K:29:MSE:HE1	1:K:52:VAL:HG13	1.98	0.45
1:L:158:PHE:CE1	1:L:160:LEU:HB2	2.51	0.45
1:A:174:LEU:O	1:A:223:ILE:HG21	2.15	0.45
1:B:29:MSE:HE1	1:B:52:VAL:HG13	1.98	0.45
1:C:49:PHE:HA	1:C:52:VAL:HG12	1.98	0.45
1:D:341:ASP:OD2	1:F:58:GLU:HB3	2.09	0.45
1:E:94:ASP:HB2	1:E:137:ASP:OD2	2.16	0.45
1:F:121:ASN:H	1:F:121:ASN:ND2	2.07	0.45
1:G:309:LEU:HD22	1:G:311:PHE:HE2	1.80	0.45
1:I:161:GLU:HG3	1:I:222:HIS:CE1	2.52	0.45
1:J:161:GLU:HG3	1:J:222:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:38:TRP:HZ3	1:L:352:ILE:HA	1.82	0.45
1:A:7:ASN:HB3	1:D:84:HIS:CG	2.50	0.45
1:A:50:LEU:HG	1:A:81:LEU:HD11	1.98	0.45
1:B:99:ARG:O	1:B:162:GLY:HA3	2.17	0.45
1:D:38:TRP:HZ3	1:D:352:ILE:HA	1.81	0.45
1:D:161:GLU:HG3	1:D:222:HIS:CE1	2.52	0.45
1:E:336:GLN:OE1	1:E:336:GLN:HA	2.15	0.45
1:E:339:PHE:HD2	2:E:391:HOH:O	1.99	0.45
1:F:11:LYS:HG3	1:F:203:ASN:ND2	2.31	0.45
1:G:65:CYS:HB3	1:G:91:MSE:HB3	1.97	0.45
1:H:231:ARG:CB	1:H:231:ARG:NH1	2.79	0.45
1:J:99:ARG:O	1:J:162:GLY:HA3	2.17	0.45
1:L:215:ASP:HB2	1:L:221:GLY:HA2	1.98	0.45
1:L:336:GLN:OE1	1:L:336:GLN:HA	2.15	0.45
1:A:309:LEU:HD22	1:A:311:PHE:HE2	1.80	0.45
1:B:49:PHE:HA	1:B:52:VAL:HG12	1.98	0.45
1:C:38:TRP:HZ3	1:C:352:ILE:HA	1.81	0.45
1:C:99:ARG:O	1:C:162:GLY:HA3	2.17	0.45
1:C:339:PHE:HB3	1:C:342:ARG:HB2	1.99	0.45
1:D:234:GLU:OE1	1:D:270:LYS:HD3	2.17	0.45
1:E:54:GLU:O	1:E:57:SER:HB2	2.15	0.45
1:E:215:ASP:HB2	1:E:221:GLY:HA2	1.98	0.45
1:E:339:PHE:HB3	1:E:342:ARG:HB2	1.99	0.45
1:F:234:GLU:OE1	1:F:270:LYS:HD3	2.17	0.45
1:G:49:PHE:HA	1:G:52:VAL:HG12	1.98	0.45
1:G:99:ARG:O	1:G:162:GLY:HA3	2.17	0.45
1:G:158:PHE:CE1	1:G:160:LEU:HB2	2.51	0.45
1:H:5:ILE:HG23	1:H:5:ILE:O	2.15	0.45
1:I:203:ASN:HD22	1:I:203:ASN:HA	1.50	0.45
1:A:174:LEU:HD23	1:A:208:LEU:HB2	1.99	0.45
1:A:234:GLU:OE1	1:A:270:LYS:HD3	2.17	0.45
1:A:336:GLN:OE1	1:A:336:GLN:HA	2.16	0.45
1:E:39:ARG:HH11	1:E:40:LEU:HD23	1.81	0.45
1:F:49:PHE:HA	1:F:52:VAL:HG12	1.98	0.45
1:F:161:GLU:HG3	1:F:222:HIS:CE1	2.52	0.45
1:I:99:ARG:O	1:I:162:GLY:HA3	2.17	0.45
1:I:219:THR:O	1:I:220:ASN:HB2	2.17	0.45
1:K:49:PHE:HA	1:K:52:VAL:HG12	1.98	0.45
1:K:234:GLU:OE1	1:K:270:LYS:HD3	2.17	0.45
1:L:39:ARG:HH11	1:L:40:LEU:HD23	1.81	0.45
1:A:245:HIS:ND1	1:A:246:PRO:HD2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:GLU:OE1	1:C:270:LYS:HD3	2.17	0.45
1:H:104:THR:O	1:H:104:THR:HG22	2.17	0.45
1:H:191:LYS:HD2	2:H:397:HOH:O	2.17	0.45
1:H:339:PHE:HB3	1:H:342:ARG:HG3	1.99	0.45
1:I:174:LEU:HD23	1:I:208:LEU:HB2	1.99	0.45
1:K:195:GLU:HG2	1:K:207:VAL:HG11	1.99	0.45
1:K:215:ASP:HB2	1:K:221:GLY:HA2	1.98	0.45
1:A:39:ARG:HH11	1:A:40:LEU:HD23	1.81	0.45
1:A:215:ASP:HB2	1:A:221:GLY:HA2	1.98	0.45
1:B:339:PHE:HB3	1:B:342:ARG:HB2	1.99	0.45
1:C:50:LEU:HG	1:C:81:LEU:HD11	1.98	0.45
1:F:99:ARG:O	1:F:162:GLY:HA3	2.17	0.45
1:F:167:VAL:HG12	1:F:168:ASP:N	2.32	0.45
1:G:339:PHE:HB3	1:G:342:ARG:HB2	1.99	0.45
1:H:142:ARG:HH12	1:H:146:GLU:HG2	1.81	0.45
1:H:231:ARG:CZ	1:H:231:ARG:HB2	2.47	0.45
1:J:67:PRO:HA	1:J:68:PRO:HD3	1.80	0.45
1:J:219:THR:O	1:J:220:ASN:HB2	2.17	0.45
1:J:330:LEU:O	1:J:334:GLN:HG3	2.17	0.45
1:K:38:TRP:HZ3	1:K:352:ILE:HA	1.82	0.45
1:K:50:LEU:HG	1:K:81:LEU:HD11	1.98	0.45
1:K:310:ASN:ND2	2:K:389:HOH:O	2.49	0.45
1:L:234:GLU:OE1	1:L:270:LYS:HD3	2.17	0.45
1:A:219:THR:O	1:A:220:ASN:HB2	2.17	0.45
1:B:158:PHE:CE1	1:B:160:LEU:HB2	2.51	0.45
1:C:195:GLU:HG2	1:C:207:VAL:HG11	1.99	0.45
1:D:327:ASN:HD22	1:D:327:ASN:HA	1.63	0.45
1:D:339:PHE:HB3	1:D:342:ARG:HB2	1.99	0.45
1:E:167:VAL:HG12	1:E:168:ASP:N	2.33	0.45
1:F:327:ASN:HD22	1:F:327:ASN:HA	1.63	0.45
1:G:38:TRP:HZ3	1:G:352:ILE:HA	1.82	0.45
1:I:38:TRP:HZ3	1:I:352:ILE:HA	1.82	0.45
1:C:94:ASP:HB2	1:C:137:ASP:OD2	2.17	0.44
1:C:174:LEU:HD23	1:C:208:LEU:HB2	1.99	0.44
1:E:369:THR:O	1:E:370:LEU:CB	2.47	0.44
1:G:43:LYS:HZ2	1:G:46:GLN:HE22	1.64	0.44
1:G:219:THR:O	1:G:220:ASN:HB2	2.17	0.44
1:H:177:GLU:HB3	1:H:209:TRP:CE3	2.46	0.44
1:H:181:LEU:HD13	1:H:209:TRP:HZ3	1.81	0.44
1:I:290:ASP:CB	1:J:73:ASN:ND2	2.80	0.44
1:K:40:LEU:HD12	1:L:40:LEU:HB3	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:336:GLN:OE1	1:K:336:GLN:HA	2.15	0.44
1:L:99:ARG:O	1:L:162:GLY:HA3	2.17	0.44
1:L:161:GLU:HG3	1:L:222:HIS:CE1	2.52	0.44
1:L:195:GLU:HG2	1:L:207:VAL:HG11	1.99	0.44
1:L:219:THR:O	1:L:220:ASN:HB2	2.17	0.44
1:A:98:ILE:HG22	2:A:393:HOH:O	2.16	0.44
1:B:234:GLU:OE1	1:B:270:LYS:HD3	2.17	0.44
1:C:161:GLU:HG3	1:C:222:HIS:CE1	2.52	0.44
1:D:50:LEU:HG	1:D:81:LEU:HD11	1.98	0.44
1:D:336:GLN:OE1	1:D:336:GLN:HA	2.16	0.44
1:E:234:GLU:OE1	1:E:270:LYS:HD3	2.17	0.44
1:F:339:PHE:HB3	1:F:342:ARG:HB2	1.99	0.44
1:H:24:GLN:HE21	1:H:60:GLU:CD	2.26	0.44
1:I:2:ALA:CB	2:I:384:HOH:O	2.40	0.44
1:I:91:MSE:SE	1:I:140:VAL:HG13	2.67	0.44
1:I:327:ASN:HD22	1:I:327:ASN:HA	1.63	0.44
1:K:94:ASP:HB2	1:K:137:ASP:OD2	2.17	0.44
1:K:99:ARG:O	1:K:162:GLY:HA3	2.17	0.44
1:K:161:GLU:HG3	1:K:222:HIS:CE1	2.52	0.44
1:A:94:ASP:HB2	1:A:137:ASP:OD2	2.17	0.44
1:B:94:ASP:HB2	1:B:137:ASP:OD2	2.17	0.44
1:B:167:VAL:HG12	1:B:168:ASP:N	2.32	0.44
1:B:219:THR:O	1:B:220:ASN:HB2	2.17	0.44
1:B:330:LEU:O	1:B:334:GLN:HG3	2.17	0.44
1:C:91:MSE:SE	1:C:140:VAL:HG13	2.68	0.44
1:D:91:MSE:SE	1:D:140:VAL:HG13	2.67	0.44
1:D:330:LEU:O	1:D:334:GLN:HG3	2.17	0.44
1:F:50:LEU:HG	1:F:81:LEU:HD11	1.98	0.44
1:F:67:PRO:HA	1:F:68:PRO:HD3	1.80	0.44
1:G:94:ASP:HB2	1:G:137:ASP:OD2	2.17	0.44
1:H:61:PRO:HA	1:H:85:ASN:ND2	2.18	0.44
1:I:234:GLU:OE1	1:I:270:LYS:HD3	2.17	0.44
1:I:330:LEU:O	1:I:334:GLN:HG3	2.17	0.44
1:J:195:GLU:HG2	1:J:207:VAL:HG11	1.99	0.44
1:J:234:GLU:OE1	1:J:270:LYS:HD3	2.17	0.44
1:K:121:ASN:ND2	1:K:121:ASN:N	2.60	0.44
1:L:339:PHE:HB3	1:L:342:ARG:HB2	1.99	0.44
1:A:99:ARG:O	1:A:162:GLY:HA3	2.17	0.44
1:A:167:VAL:HG12	1:A:168:ASP:N	2.32	0.44
1:A:195:GLU:HG2	1:A:207:VAL:HG11	1.99	0.44
1:B:161:GLU:HG3	1:B:222:HIS:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:GLU:HB2	1:C:159:VAL:HA	2.00	0.44
1:D:30:LEU:HD22	1:D:93:ASN:HD22	1.83	0.44
1:D:94:ASP:HB2	1:D:137:ASP:OD2	2.17	0.44
1:D:99:ARG:O	1:D:162:GLY:HA3	2.17	0.44
1:E:99:ARG:O	1:E:162:GLY:HA3	2.17	0.44
1:G:30:LEU:HD22	1:G:93:ASN:HD22	1.83	0.44
1:G:91:MSE:SE	1:G:140:VAL:HG13	2.68	0.44
1:G:119:GLU:HB2	1:G:159:VAL:HA	2.00	0.44
1:H:57:SER:HA	1:H:85:ASN:HD21	1.82	0.44
1:K:30:LEU:HD22	1:K:93:ASN:HD22	1.83	0.44
1:K:73:ASN:ND2	1:L:290:ASP:CB	2.76	0.44
1:L:50:LEU:HG	1:L:81:LEU:HD11	1.98	0.44
1:B:91:MSE:SE	1:B:140:VAL:HG13	2.68	0.44
1:H:119:GLU:HB2	1:H:159:VAL:HA	2.00	0.44
1:I:30:LEU:HD22	1:I:93:ASN:HD22	1.83	0.44
1:I:161:GLU:HG3	1:I:222:HIS:NE2	2.33	0.44
1:J:167:VAL:HG12	1:J:168:ASP:N	2.32	0.44
1:J:369:THR:O	1:J:370:LEU:CB	2.47	0.44
1:A:108:ASN:OD1	1:A:112:ASP:HB2	2.18	0.44
1:A:161:GLU:HG3	1:A:222:HIS:NE2	2.33	0.44
1:A:339:PHE:HB3	1:A:342:ARG:HB2	1.99	0.44
1:C:30:LEU:HD22	1:C:93:ASN:HD22	1.83	0.44
1:C:219:THR:O	1:C:220:ASN:HB2	2.17	0.44
1:E:161:GLU:HG3	1:E:222:HIS:CE1	2.52	0.44
1:E:219:THR:O	1:E:220:ASN:HB2	2.17	0.44
1:H:215:ASP:HB2	1:H:221:GLY:H	1.82	0.44
1:I:185:ARG:HH11	1:I:185:ARG:CB	2.11	0.44
1:J:91:MSE:SE	1:J:140:VAL:HG13	2.67	0.44
1:K:119:GLU:HB2	1:K:159:VAL:HA	2.00	0.44
1:A:119:GLU:HB2	1:A:159:VAL:HA	2.00	0.44
1:B:118:TRP:HA	1:B:155:THR:OG1	2.18	0.44
1:B:161:GLU:HG3	1:B:222:HIS:NE2	2.33	0.44
1:E:119:GLU:HB2	1:E:159:VAL:HA	2.00	0.44
1:E:161:GLU:HG3	1:E:222:HIS:NE2	2.33	0.44
1:F:161:GLU:HG3	1:F:222:HIS:NE2	2.33	0.44
1:F:330:LEU:O	1:F:334:GLN:HG3	2.17	0.44
1:G:330:LEU:O	1:G:334:GLN:HG3	2.17	0.44
1:J:30:LEU:HD22	1:J:93:ASN:HD22	1.83	0.44
1:J:119:GLU:HB2	1:J:159:VAL:HA	2.00	0.44
1:K:161:GLU:HG3	1:K:222:HIS:NE2	2.33	0.44
1:K:339:PHE:HB3	1:K:342:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:119:GLU:HB2	1:L:159:VAL:HA	2.00	0.44
1:A:30:LEU:HD22	1:A:93:ASN:HD22	1.83	0.44
1:B:195:GLU:HG2	1:B:207:VAL:HG11	1.99	0.44
1:B:325:ASP:O	1:B:328:ASP:HB2	2.18	0.44
1:C:95:ASP:HB2	1:C:131:TYR:CE2	2.53	0.44
1:C:108:ASN:OD1	1:C:112:ASP:HB2	2.18	0.44
1:C:161:GLU:HG3	1:C:222:HIS:NE2	2.33	0.44
1:C:325:ASP:O	1:C:328:ASP:HB2	2.18	0.44
1:D:174:LEU:HD23	1:D:208:LEU:HB2	1.99	0.44
1:E:30:LEU:HD22	1:E:93:ASN:HD22	1.83	0.44
1:E:43:LYS:HZ2	1:E:46:GLN:HE22	1.65	0.44
1:F:108:ASN:OD1	1:F:112:ASP:HB2	2.18	0.44
1:F:174:LEU:HD23	1:F:208:LEU:HB2	1.99	0.44
1:G:174:LEU:HD23	1:G:208:LEU:HB2	1.99	0.44
1:J:95:ASP:HB2	1:J:131:TYR:CE2	2.53	0.44
1:J:325:ASP:O	1:J:328:ASP:HB2	2.18	0.44
1:B:114:ARG:NH1	2:B:380:HOH:O	2.31	0.44
1:C:118:TRP:HA	1:C:155:THR:OG1	2.18	0.44
1:D:219:THR:O	1:D:220:ASN:HB2	2.17	0.44
1:D:325:ASP:O	1:D:328:ASP:HB2	2.18	0.44
1:G:234:GLU:OE1	1:G:270:LYS:HD3	2.17	0.44
1:I:108:ASN:OD1	1:I:112:ASP:HB2	2.18	0.44
1:I:215:ASP:HB2	1:I:221:GLY:HA2	1.98	0.44
1:I:325:ASP:O	1:I:328:ASP:HB2	2.18	0.44
1:K:118:TRP:HA	1:K:155:THR:OG1	2.18	0.44
1:L:95:ASP:HB2	1:L:131:TYR:CE2	2.53	0.44
1:L:118:TRP:HA	1:L:155:THR:OG1	2.18	0.44
1:B:38:TRP:HZ3	1:B:352:ILE:HA	1.82	0.43
1:B:119:GLU:HB2	1:B:159:VAL:HA	2.00	0.43
1:B:203:ASN:HD22	1:B:203:ASN:HA	1.50	0.43
1:D:43:LYS:HZ2	1:D:46:GLN:HE22	1.64	0.43
1:E:330:LEU:O	1:E:334:GLN:HG3	2.17	0.43
1:F:118:TRP:HA	1:F:155:THR:OG1	2.18	0.43
1:F:142:ARG:N	2:F:388:HOH:O	2.46	0.43
1:G:161:GLU:HG3	1:G:222:HIS:NE2	2.33	0.43
1:H:121:ASN:O	1:H:125:GLY:HA2	2.18	0.43
1:K:174:LEU:HD23	1:K:208:LEU:HB2	1.99	0.43
1:A:91:MSE:SE	1:A:140:VAL:HG13	2.68	0.43
1:B:108:ASN:OD1	1:B:112:ASP:HB2	2.18	0.43
1:D:118:TRP:HA	1:D:155:THR:OG1	2.18	0.43
1:E:91:MSE:SE	1:E:140:VAL:HG13	2.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:LEU:HD23	1:E:208:LEU:HB2	1.99	0.43
1:E:325:ASP:O	1:E:328:ASP:HB2	2.18	0.43
1:F:91:MSE:SE	1:F:140:VAL:HG13	2.68	0.43
1:G:167:VAL:HG12	1:G:168:ASP:N	2.32	0.43
1:G:195:GLU:HG2	1:G:207:VAL:HG11	1.99	0.43
1:K:91:MSE:SE	1:K:140:VAL:HG13	2.67	0.43
1:K:330:LEU:O	1:K:334:GLN:HG3	2.17	0.43
1:L:174:LEU:HD23	1:L:208:LEU:HB2	1.99	0.43
1:L:325:ASP:O	1:L:328:ASP:HB2	2.18	0.43
1:A:189:LEU:HD12	1:A:189:LEU:HA	1.84	0.43
1:B:95:ASP:HB2	1:B:131:TYR:CE2	2.53	0.43
1:D:95:ASP:HB2	1:D:131:TYR:CE2	2.53	0.43
1:D:195:GLU:HG2	1:D:207:VAL:HG11	1.99	0.43
1:E:95:ASP:HB2	1:E:131:TYR:CE2	2.53	0.43
1:E:118:TRP:HA	1:E:155:THR:OG1	2.18	0.43
1:F:119:GLU:HB2	1:F:159:VAL:HA	2.00	0.43
1:F:219:THR:O	1:F:220:ASN:HB2	2.17	0.43
1:G:325:ASP:O	1:G:328:ASP:HB2	2.18	0.43
1:I:167:VAL:HG12	1:I:168:ASP:N	2.33	0.43
1:I:189:LEU:HD12	1:I:189:LEU:HA	1.84	0.43
1:J:161:GLU:HG3	1:J:222:HIS:NE2	2.33	0.43
1:J:339:PHE:HB3	1:J:342:ARG:HB2	1.99	0.43
1:K:369:THR:O	1:K:370:LEU:CB	2.47	0.43
1:L:161:GLU:HG3	1:L:222:HIS:NE2	2.33	0.43
1:A:290:ASP:CG	1:G:73:ASN:CG	2.86	0.43
1:A:330:LEU:O	1:A:334:GLN:HG3	2.17	0.43
1:C:167:VAL:HG12	1:C:168:ASP:N	2.32	0.43
1:D:161:GLU:HG3	1:D:222:HIS:NE2	2.33	0.43
1:D:167:VAL:HG12	1:D:168:ASP:N	2.32	0.43
1:E:195:GLU:HG2	1:E:207:VAL:HG11	1.99	0.43
1:F:30:LEU:HD22	1:F:93:ASN:HD22	1.83	0.43
1:H:223:ILE:C	1:H:225:ASP:N	2.77	0.43
1:J:321:PRO:HB3	1:J:358:ASN:ND2	2.34	0.43
1:K:167:VAL:HG12	1:K:168:ASP:N	2.33	0.43
1:L:91:MSE:SE	1:L:140:VAL:HG13	2.68	0.43
1:L:167:VAL:HG12	1:L:168:ASP:N	2.33	0.43
1:L:330:LEU:O	1:L:334:GLN:HG3	2.17	0.43
1:E:185:ARG:HH11	1:E:185:ARG:CB	2.11	0.43
1:E:236:ALA:O	1:E:237:CYS:HB2	2.19	0.43
1:H:5:ILE:HD13	1:H:153:TYR:CE2	2.54	0.43
1:J:118:TRP:HA	1:J:155:THR:OG1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:174:LEU:HD23	1:J:208:LEU:HB2	1.99	0.43
1:J:327:ASN:HD22	1:J:327:ASN:HA	1.63	0.43
1:K:95:ASP:HB2	1:K:131:TYR:CE2	2.53	0.43
1:B:236:ALA:O	1:B:237:CYS:HB2	2.19	0.43
1:B:321:PRO:HB3	1:B:358:ASN:ND2	2.34	0.43
1:C:330:LEU:O	1:C:334:GLN:HG3	2.17	0.43
1:F:95:ASP:HB2	1:F:131:TYR:CE2	2.53	0.43
1:F:236:ALA:O	1:F:237:CYS:HB2	2.19	0.43
1:G:108:ASN:OD1	1:G:112:ASP:HB2	2.18	0.43
1:H:74:ALA:O	1:H:78:VAL:HG23	2.18	0.43
1:I:119:GLU:HB2	1:I:159:VAL:HA	2.00	0.43
1:K:66:VAL:HG21	1:K:71:TYR:HA	2.01	0.43
1:C:327:ASN:HD22	1:C:327:ASN:HA	1.63	0.43
1:H:132:PHE:HB3	1:H:133:PRO:CD	2.44	0.43
1:I:95:ASP:HB2	1:I:131:TYR:CE2	2.53	0.43
1:I:118:TRP:HA	1:I:155:THR:OG1	2.18	0.43
1:L:30:LEU:HD22	1:L:93:ASN:HD22	1.83	0.43
1:A:66:VAL:HG21	1:A:71:TYR:HA	2.01	0.43
1:C:132:PHE:CD2	1:I:135:ASP:HB3	2.53	0.43
1:G:89:ILE:H	1:G:89:ILE:CD1	2.22	0.43
1:G:236:ALA:O	1:G:237:CYS:HB2	2.19	0.43
1:H:203:ASN:C	1:H:203:ASN:HD22	2.25	0.43
1:H:224:ASP:HB2	1:H:360:HIS:HD2	1.81	0.43
1:I:66:VAL:HG21	1:I:71:TYR:HA	2.01	0.43
1:K:108:ASN:OD1	1:K:112:ASP:HB2	2.18	0.43
1:K:327:ASN:HD22	1:K:327:ASN:HA	1.63	0.43
1:A:325:ASP:O	1:A:328:ASP:HB2	2.18	0.43
1:B:174:LEU:HD23	1:B:208:LEU:HB2	1.99	0.43
1:E:66:VAL:HG21	1:E:71:TYR:HA	2.01	0.43
1:E:135:ASP:HB3	1:L:132:PHE:HE2	1.78	0.43
1:E:321:PRO:HB3	1:E:358:ASN:ND2	2.34	0.43
1:G:118:TRP:HA	1:G:155:THR:OG1	2.18	0.43
1:I:195:GLU:HG2	1:I:207:VAL:HG11	1.99	0.43
1:A:118:TRP:HA	1:A:155:THR:OG1	2.18	0.43
1:A:121:ASN:H	1:A:121:ASN:ND2	2.07	0.43
1:B:171:GLY:CA	1:B:204:CYS:HA	2.43	0.43
1:C:66:VAL:HG21	1:C:71:TYR:HA	2.01	0.43
1:C:321:PRO:HB3	1:C:358:ASN:ND2	2.34	0.43
1:E:40:LEU:HD22	1:E:288:THR:OG1	2.19	0.43
1:F:40:LEU:HD22	1:F:288:THR:OG1	2.19	0.43
1:F:98:ILE:HG22	2:F:379:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:GLU:HG2	1:F:207:VAL:HG11	1.99	0.43
1:G:95:ASP:HB2	1:G:131:TYR:CE2	2.53	0.43
1:H:15:PHE:CE2	1:H:108:ASN:HB3	2.54	0.43
1:H:312:LEU:HD22	1:H:312:LEU:C	2.44	0.43
1:J:108:ASN:OD1	1:J:112:ASP:HB2	2.18	0.43
1:J:185:ARG:HH11	1:J:185:ARG:CB	2.11	0.43
1:K:325:ASP:O	1:K:328:ASP:HB2	2.18	0.43
1:L:236:ALA:O	1:L:237:CYS:HB2	2.19	0.43
1:A:321:PRO:HB3	1:A:358:ASN:ND2	2.34	0.42
1:B:138:ALA:HB1	2:B:384:HOH:O	2.19	0.42
1:C:185:ARG:HH11	1:C:185:ARG:CB	2.11	0.42
1:C:311:PHE:HE1	1:C:313:ILE:HD11	1.84	0.42
1:D:203:ASN:HD22	1:D:203:ASN:HA	1.50	0.42
1:F:325:ASP:O	1:F:328:ASP:HB2	2.18	0.42
1:G:66:VAL:HG21	1:G:71:TYR:HA	2.01	0.42
1:H:20:GLU:OE1	1:H:360:HIS:HE1	2.02	0.42
1:I:236:ALA:O	1:I:237:CYS:HB2	2.19	0.42
1:J:203:ASN:HD22	1:J:203:ASN:HA	1.50	0.42
1:K:40:LEU:HD22	1:K:288:THR:OG1	2.19	0.42
1:L:108:ASN:OD1	1:L:112:ASP:HB2	2.18	0.42
1:L:311:PHE:HE1	1:L:313:ILE:HD11	1.84	0.42
1:A:95:ASP:HB2	1:A:131:TYR:CE2	2.53	0.42
1:B:30:LEU:HD22	1:B:93:ASN:HD22	1.83	0.42
1:B:40:LEU:HD22	1:B:288:THR:OG1	2.19	0.42
1:D:119:GLU:HB2	1:D:159:VAL:HA	2.00	0.42
1:H:223:ILE:HA	1:H:226:VAL:HG22	2.01	0.42
1:K:219:THR:O	1:K:220:ASN:HB2	2.17	0.42
1:A:236:ALA:O	1:A:237:CYS:HB2	2.19	0.42
1:A:315:ASN:CB	2:A:379:HOH:O	2.63	0.42
1:C:291:TYR:OH	1:D:80:GLU:HB2	2.19	0.42
1:D:311:PHE:HE1	1:D:313:ILE:HD11	1.84	0.42
1:D:321:PRO:HB3	1:D:358:ASN:ND2	2.34	0.42
1:F:142:ARG:HB2	2:F:388:HOH:O	2.20	0.42
1:I:40:LEU:HD22	1:I:288:THR:OG1	2.19	0.42
1:I:283:LEU:HD13	1:I:283:LEU:C	2.44	0.42
1:I:339:PHE:HB3	1:I:342:ARG:HB2	1.99	0.42
1:B:66:VAL:HG21	1:B:71:TYR:HA	2.01	0.42
1:F:321:PRO:HB3	1:F:358:ASN:ND2	2.34	0.42
1:J:51:GLU:C	1:J:53:ALA:N	2.77	0.42
1:K:236:ALA:O	1:K:237:CYS:HB2	2.19	0.42
1:A:127:VAL:HG12	2:A:382:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:C	1:A:283:LEU:HD13	2.44	0.42
1:D:66:VAL:HG21	1:D:71:TYR:HA	2.01	0.42
1:E:108:ASN:OD1	1:E:112:ASP:HB2	2.18	0.42
1:G:283:LEU:C	1:G:283:LEU:HD13	2.44	0.42
1:G:321:PRO:HB3	1:G:358:ASN:ND2	2.34	0.42
1:H:11:LYS:HG3	1:H:203:ASN:ND2	2.34	0.42
1:H:178:MSE:SE	1:H:221:GLY:HA3	2.69	0.42
1:I:321:PRO:HB3	1:I:358:ASN:ND2	2.34	0.42
1:J:66:VAL:HG21	1:J:71:TYR:HA	2.01	0.42
1:L:252:LYS:HB3	1:L:252:LYS:HE2	1.92	0.42
1:A:35:ASN:OD1	1:A:35:ASN:N	2.53	0.42
1:A:40:LEU:HD22	1:A:288:THR:OG1	2.19	0.42
1:B:311:PHE:HE1	1:B:313:ILE:HD11	1.84	0.42
1:D:108:ASN:OD1	1:D:112:ASP:HB2	2.18	0.42
1:D:236:ALA:O	1:D:237:CYS:HB2	2.19	0.42
1:E:171:GLY:CA	1:E:204:CYS:HA	2.43	0.42
1:H:5:ILE:HD11	1:H:8:THR:OG1	2.19	0.42
1:H:310:ASN:OD1	1:H:358:ASN:HB3	2.19	0.42
1:J:40:LEU:HD22	1:J:288:THR:OG1	2.19	0.42
1:L:321:PRO:HB3	1:L:358:ASN:ND2	2.34	0.42
1:A:7:ASN:HB2	1:D:84:HIS:CD2	2.54	0.42
1:C:35:ASN:OD1	1:C:35:ASN:N	2.53	0.42
1:C:40:LEU:HD22	1:C:288:THR:OG1	2.19	0.42
1:C:71:TYR:CZ	1:J:143:LYS:HG2	2.54	0.42
1:C:236:ALA:O	1:C:237:CYS:HB2	2.19	0.42
1:F:185:ARG:HH11	1:F:185:ARG:CB	2.11	0.42
1:H:313:ILE:HD12	1:H:318:ILE:HD11	2.00	0.42
1:I:174:LEU:HB3	1:I:223:ILE:CD1	2.50	0.42
1:K:121:ASN:O	1:K:125:GLY:HA2	2.20	0.42
1:K:311:PHE:HE1	1:K:313:ILE:HD11	1.84	0.42
1:L:283:LEU:C	1:L:283:LEU:HD13	2.45	0.42
1:B:290:ASP:CG	1:F:73:ASN:CG	2.88	0.42
1:C:121:ASN:ND2	1:C:121:ASN:N	2.60	0.42
1:D:132:PHE:CE2	1:J:135:ASP:HB3	2.54	0.42
1:H:230:ILE:O	1:H:231:ARG:HB2	2.20	0.42
1:H:325:ASP:N	1:H:328:ASP:OD1	2.50	0.42
1:J:283:LEU:C	1:J:283:LEU:HD13	2.44	0.42
1:A:203:ASN:HD22	1:A:203:ASN:HA	1.50	0.42
1:C:224:ASP:HB2	1:C:360:HIS:CD2	2.55	0.42
1:G:121:ASN:O	1:G:125:GLY:HA2	2.20	0.42
1:H:28:TRP:CZ3	1:H:144:VAL:HG23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:292:VAL:C	1:H:294:GLY:H	2.28	0.42
1:I:40:LEU:HD12	1:J:40:LEU:HB3	2.02	0.42
1:J:236:ALA:O	1:J:237:CYS:HB2	2.19	0.42
1:K:321:PRO:HB3	1:K:358:ASN:ND2	2.34	0.42
1:L:51:GLU:C	1:L:53:ALA:N	2.77	0.42
1:A:51:GLU:C	1:A:53:ALA:N	2.77	0.42
1:B:121:ASN:O	1:B:125:GLY:HA2	2.20	0.42
1:B:182:HIS:ND1	1:B:183:PRO:HD2	2.35	0.42
1:E:121:ASN:O	1:E:125:GLY:HA2	2.20	0.42
1:F:121:ASN:O	1:F:125:GLY:HA2	2.20	0.42
1:F:182:HIS:ND1	1:F:183:PRO:HD2	2.35	0.42
1:F:283:LEU:HD13	1:F:283:LEU:C	2.44	0.42
1:G:40:LEU:HD22	1:G:288:THR:OG1	2.19	0.42
1:G:182:HIS:ND1	1:G:183:PRO:HD2	2.35	0.42
1:I:121:ASN:O	1:I:125:GLY:HA2	2.20	0.42
1:L:35:ASN:OD1	1:L:35:ASN:N	2.53	0.42
1:B:283:LEU:C	1:B:283:LEU:HD13	2.45	0.41
1:C:283:LEU:HD13	1:C:283:LEU:C	2.45	0.41
1:D:40:LEU:HD22	1:D:288:THR:OG1	2.19	0.41
1:D:283:LEU:C	1:D:283:LEU:HD13	2.44	0.41
1:F:121:ASN:ND2	1:F:121:ASN:N	2.60	0.41
1:F:311:PHE:HE1	1:F:313:ILE:HD11	1.84	0.41
1:G:185:ARG:HH11	1:G:185:ARG:CB	2.11	0.41
1:H:231:ARG:HB3	1:H:231:ARG:HH11	1.85	0.41
1:I:309:LEU:HD22	1:I:309:LEU:HA	1.92	0.41
1:J:121:ASN:O	1:J:125:GLY:HA2	2.20	0.41
1:J:311:PHE:HE1	1:J:313:ILE:HD11	1.84	0.41
1:K:189:LEU:HD12	1:K:189:LEU:HA	1.84	0.41
1:L:115:ALA:O	1:L:153:TYR:HD1	2.03	0.41
1:L:171:GLY:CA	1:L:204:CYS:HA	2.43	0.41
1:L:224:ASP:HB2	1:L:360:HIS:CD2	2.55	0.41
1:A:182:HIS:ND1	1:A:183:PRO:HD2	2.35	0.41
1:B:35:ASN:N	1:B:35:ASN:OD1	2.53	0.41
1:B:51:GLU:C	1:B:53:ALA:N	2.77	0.41
1:B:189:LEU:HD12	1:B:189:LEU:HA	1.84	0.41
1:G:215:ASP:N	1:G:216:PRO:HD3	2.36	0.41
1:H:94:ASP:OD2	1:H:136:GLN:HB2	2.20	0.41
1:I:215:ASP:N	1:I:216:PRO:HD3	2.36	0.41
1:L:121:ASN:O	1:L:125:GLY:HA2	2.20	0.41
1:E:283:LEU:C	1:E:283:LEU:HD13	2.44	0.41
1:F:189:LEU:HD12	1:F:189:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:171:GLY:HA2	1:H:204:CYS:HA	2.01	0.41
1:I:311:PHE:HE1	1:I:313:ILE:HD11	1.84	0.41
1:J:224:ASP:HB2	1:J:360:HIS:CD2	2.55	0.41
1:K:35:ASN:N	1:K:35:ASN:OD1	2.53	0.41
1:B:56:ILE:H	1:B:56:ILE:HG12	1.67	0.41
1:B:215:ASP:N	1:B:216:PRO:HD3	2.36	0.41
1:C:51:GLU:C	1:C:53:ALA:N	2.77	0.41
1:D:35:ASN:OD1	1:D:35:ASN:N	2.53	0.41
1:D:121:ASN:O	1:D:125:GLY:HA2	2.20	0.41
1:D:215:ASP:N	1:D:216:PRO:HD3	2.36	0.41
1:F:174:LEU:HB3	1:F:223:ILE:CD1	2.50	0.41
1:H:214:ILE:C	1:H:216:PRO:HD3	2.45	0.41
1:J:56:ILE:H	1:J:56:ILE:HG12	1.67	0.41
1:J:189:LEU:HD12	1:J:189:LEU:HA	1.84	0.41
1:L:40:LEU:HD22	1:L:288:THR:OG1	2.19	0.41
1:L:182:HIS:ND1	1:L:183:PRO:HD2	2.35	0.41
1:A:40:LEU:HD12	1:G:40:LEU:HB3	2.02	0.41
1:A:115:ALA:O	1:A:153:TYR:HD1	2.03	0.41
1:E:115:ALA:O	1:E:153:TYR:HD1	2.03	0.41
1:E:215:ASP:N	1:E:216:PRO:HD3	2.36	0.41
1:G:35:ASN:OD1	1:G:35:ASN:N	2.53	0.41
1:H:203:ASN:C	1:H:203:ASN:ND2	2.78	0.41
1:I:182:HIS:ND1	1:I:183:PRO:HD2	2.35	0.41
1:J:35:ASN:OD1	1:J:35:ASN:N	2.53	0.41
1:K:67:PRO:HA	1:K:68:PRO:HD3	1.80	0.41
1:K:103:PRO:CD	1:K:144:VAL:HG11	2.50	0.41
1:C:115:ALA:O	1:C:153:TYR:HD1	2.03	0.41
1:D:182:HIS:ND1	1:D:183:PRO:HD2	2.36	0.41
1:E:327:ASN:HD22	1:E:327:ASN:HA	1.63	0.41
1:H:8:THR:HB	1:H:13:ASP:OD1	2.20	0.41
1:H:100:ASP:CB	1:H:161:GLU:HB2	2.49	0.41
1:H:105:PHE:CB	1:H:367:PRO:HD2	2.51	0.41
1:H:198:LEU:CD2	1:H:202:LEU:HD22	2.48	0.41
1:L:174:LEU:HB3	1:L:223:ILE:CD1	2.50	0.41
1:L:215:ASP:N	1:L:216:PRO:HD3	2.36	0.41
1:B:224:ASP:HB2	1:B:360:HIS:CD2	2.55	0.41
1:D:115:ALA:O	1:D:153:TYR:HD1	2.03	0.41
1:G:171:GLY:CA	1:G:204:CYS:HA	2.43	0.41
1:L:66:VAL:HG21	1:L:71:TYR:HA	2.01	0.41
1:A:121:ASN:O	1:A:125:GLY:HA2	2.20	0.41
1:A:311:PHE:HE1	1:A:313:ILE:HD11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LYS:HB3	1:B:252:LYS:HE2	1.92	0.41
1:C:103:PRO:CD	1:C:144:VAL:HG11	2.50	0.41
1:D:67:PRO:HA	1:D:68:PRO:HD3	1.80	0.41
1:F:115:ALA:O	1:F:153:TYR:HD1	2.03	0.41
1:F:300:GLU:HG2	1:F:301:GLY:N	2.36	0.41
1:G:103:PRO:CD	1:G:144:VAL:HG11	2.50	0.41
1:G:224:ASP:HB2	1:G:360:HIS:CD2	2.55	0.41
1:G:300:GLU:HG2	1:G:301:GLY:N	2.36	0.41
1:H:121:ASN:O	1:H:125:GLY:N	2.51	0.41
1:H:172:THR:HG22	1:H:173:VAL:H	1.86	0.41
1:H:231:ARG:O	1:H:232:PRO:C	2.64	0.41
1:J:24:GLN:HA	1:J:368:ALA:N	2.33	0.41
1:K:283:LEU:HD13	1:K:283:LEU:C	2.44	0.41
1:A:12:GLN:NE2	1:D:82:GLY:HA2	2.19	0.41
1:A:24:GLN:HA	1:A:368:ALA:N	2.33	0.41
1:A:124:GLY:O	1:A:127:VAL:HG13	2.21	0.41
1:A:215:ASP:N	1:A:216:PRO:HD3	2.36	0.41
1:A:252:LYS:HE2	1:A:252:LYS:HB3	1.92	0.41
1:A:300:GLU:HG2	1:A:301:GLY:N	2.36	0.41
1:B:43:LYS:HZ2	1:B:46:GLN:HE22	1.68	0.41
1:B:103:PRO:CD	1:B:144:VAL:HG11	2.50	0.41
1:B:185:ARG:HH11	1:B:185:ARG:CB	2.11	0.41
1:B:300:GLU:HG2	1:B:301:GLY:N	2.36	0.41
1:C:203:ASN:HD22	1:C:203:ASN:HA	1.50	0.41
1:D:51:GLU:C	1:D:53:ALA:N	2.77	0.41
1:E:35:ASN:N	1:E:35:ASN:OD1	2.53	0.41
1:E:311:PHE:HE1	1:E:313:ILE:HD11	1.84	0.41
1:F:51:GLU:C	1:F:53:ALA:N	2.77	0.41
1:F:66:VAL:HG21	1:F:71:TYR:HA	2.01	0.41
1:H:24:GLN:NE2	1:H:314:VAL:HG12	2.36	0.41
1:H:173:VAL:HG12	1:H:206:LYS:O	2.20	0.41
1:I:80:GLU:HB2	1:J:291:TYR:OH	2.21	0.41
1:I:103:PRO:CD	1:I:144:VAL:HG11	2.50	0.41
1:I:115:ALA:O	1:I:153:TYR:HD1	2.03	0.41
1:I:290:ASP:CG	1:J:73:ASN:CG	2.89	0.41
1:I:300:GLU:HG2	1:I:301:GLY:N	2.36	0.41
1:J:182:HIS:ND1	1:J:183:PRO:HD2	2.36	0.41
1:A:174:LEU:HB3	1:A:223:ILE:CD1	2.50	0.41
1:B:27:ILE:HG13	1:B:60:GLU:OE2	2.21	0.41
1:B:233:GLY:N	2:B:397:HOH:O	2.54	0.41
1:B:327:ASN:HD22	1:B:327:ASN:HA	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:HIS:ND1	1:C:183:PRO:HD2	2.35	0.41
1:C:215:ASP:N	1:C:216:PRO:HD3	2.36	0.41
1:F:99:ARG:HD3	1:F:360:HIS:CD2	2.56	0.41
1:G:311:PHE:HE1	1:G:313:ILE:HD11	1.84	0.41
1:H:28:TRP:CZ3	1:H:147:ILE:HD11	2.56	0.41
1:I:51:GLU:C	1:I:53:ALA:N	2.77	0.41
1:K:224:ASP:HB2	1:K:360:HIS:CD2	2.55	0.41
1:K:290:ASP:CG	1:L:73:ASN:CG	2.88	0.41
1:C:124:GLY:O	1:C:127:VAL:HG13	2.21	0.40
1:E:51:GLU:C	1:E:53:ALA:N	2.77	0.40
1:E:224:ASP:HB2	1:E:360:HIS:CD2	2.55	0.40
1:F:124:GLY:O	1:F:127:VAL:HG13	2.21	0.40
1:F:215:ASP:N	1:F:216:PRO:HD3	2.36	0.40
1:H:4:ARG:NH1	1:H:142:ARG:HD3	2.35	0.40
1:H:231:ARG:NH1	1:H:231:ARG:HB2	2.36	0.40
1:H:296:ILE:O	1:H:296:ILE:HG23	2.20	0.40
1:J:27:ILE:HG13	1:J:60:GLU:OE2	2.21	0.40
1:K:171:GLY:CA	1:K:204:CYS:HA	2.43	0.40
1:L:124:GLY:O	1:L:127:VAL:HG13	2.21	0.40
1:L:327:ASN:HD22	1:L:327:ASN:HA	1.63	0.40
1:A:155:THR:HB	1:A:158:PHE:HB3	2.04	0.40
1:A:224:ASP:HB2	1:A:360:HIS:CD2	2.55	0.40
1:B:115:ALA:O	1:B:153:TYR:HD1	2.03	0.40
1:C:300:GLU:HG2	1:C:301:GLY:N	2.36	0.40
1:D:124:GLY:O	1:D:127:VAL:HG13	2.21	0.40
1:D:173:VAL:HG22	1:D:174:LEU:N	2.37	0.40
1:D:243:LYS:NZ	1:H:192:GLU:CG	2.73	0.40
1:E:182:HIS:ND1	1:E:183:PRO:HD2	2.35	0.40
1:F:173:VAL:HG22	1:F:174:LEU:N	2.37	0.40
1:G:27:ILE:HG13	1:G:60:GLU:OE2	2.21	0.40
1:H:113:LEU:O	1:H:150:VAL:HG23	2.20	0.40
1:I:173:VAL:HG22	1:I:174:LEU:N	2.36	0.40
1:K:300:GLU:HG2	1:K:301:GLY:N	2.36	0.40
1:C:27:ILE:HG13	1:C:60:GLU:OE2	2.21	0.40
1:E:99:ARG:HD3	1:E:360:HIS:CD2	2.56	0.40
1:E:124:GLY:O	1:E:127:VAL:HG13	2.21	0.40
1:E:300:GLU:HG2	1:E:301:GLY:N	2.36	0.40
1:G:99:ARG:HD3	1:G:360:HIS:CD2	2.56	0.40
1:G:115:ALA:O	1:G:153:TYR:HD1	2.04	0.40
1:H:17:MSE:HB2	1:H:106:LEU:CD2	2.51	0.40
1:I:30:LEU:HD22	1:I:93:ASN:ND2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:99:ARG:HD3	1:I:360:HIS:CD2	2.56	0.40
1:J:300:GLU:HG2	1:J:301:GLY:N	2.36	0.40
1:K:115:ALA:O	1:K:153:TYR:HD1	2.03	0.40
1:L:189:LEU:HA	1:L:189:LEU:HD12	1.84	0.40
1:B:99:ARG:HD3	1:B:360:HIS:CD2	2.56	0.40
1:C:121:ASN:O	1:C:125:GLY:HA2	2.20	0.40
1:D:68:PRO:HG3	1:D:90:GLU:CG	2.52	0.40
1:D:155:THR:HB	1:D:158:PHE:HB3	2.04	0.40
1:E:103:PRO:CD	1:E:144:VAL:HG11	2.50	0.40
1:E:174:LEU:HB3	1:E:223:ILE:CD1	2.50	0.40
1:F:30:LEU:HD22	1:F:93:ASN:ND2	2.37	0.40
1:K:68:PRO:HG3	1:K:90:GLU:CG	2.52	0.40
1:L:99:ARG:HD3	1:L:360:HIS:CD2	2.56	0.40
1:H:226:VAL:HG23	1:H:227:ALA:N	2.37	0.40
1:H:263:ASP:CG	1:H:264:ALA:N	2.79	0.40
1:I:35:ASN:N	1:I:35:ASN:OD1	2.53	0.40
1:K:27:ILE:HG13	1:K:60:GLU:OE2	2.21	0.40
1:K:182:HIS:ND1	1:K:183:PRO:HD2	2.35	0.40
1:L:27:ILE:HG13	1:L:60:GLU:OE2	2.21	0.40

All (35) 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:G:243:LYS:NZ	1:K:284:GLN:NE2[1_556]	1.07	1.13
1:B:329:GLN:CB	1:D:282:TYR:OH[1_455]	1.18	1.02
1:A:329:GLN:CB	1:E:282:TYR:OH[2_646]	1.22	0.98
1:A:260:GLN:OE1	1:H:323:TYR:O[2_646]	1.34	0.86
1:E:217:TYR:OH	1:J:267:ARG:NE[2_655]	1.47	0.73
1:B:260:GLN:OE1	1:C:323:TYR:O[1_455]	1.56	0.64
1:E:217:TYR:OH	1:J:267:ARG:NH2[2_655]	1.70	0.50
1:E:217:TYR:OH	1:J:267:ARG:CZ[2_655]	1.71	0.49
1:J:23:LYS:NZ	1:L:188:HIS:O[2_645]	1.72	0.48
1:E:7:ASN:ND2	1:I:284:GLN:OE1[2_555]	1.78	0.42
1:A:285:GLU:OE2	1:J:243:LYS:NZ[1_556]	1.80	0.40
1:G:243:LYS:NZ	1:K:284:GLN:CD[1_556]	1.81	0.39
1:B:329:GLN:C	1:D:282:TYR:CE2[1_455]	1.86	0.34
1:C:244:GLU:OE2	1:H:217:TYR:OH[2_646]	1.86	0.34
1:A:329:GLN:C	1:E:282:TYR:CE2[2_646]	1.87	0.33
1:E:217:TYR:CZ	1:J:267:ARG:NE[2_655]	1.91	0.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ASN:ND2	1:E:84:HIS:CE1[2_546]	1.93	0.27
1:E:217:TYR:CE2	1:J:267:ARG:NE[2_655]	1.95	0.25
1:E:341:ASP:C	1:G:84:HIS:NE2[2_556]	1.98	0.22
1:E:217:TYR:CE2	1:J:267:ARG:CD[2_655]	2.00	0.20
1:B:7:ASN:CG	1:E:84:HIS:CE1[2_546]	2.01	0.19
1:A:329:GLN:CG	1:E:282:TYR:OH[2_646]	2.04	0.16
1:B:329:GLN:O	1:D:282:TYR:CE2[1_455]	2.04	0.16
1:F:211:LYS:CD	1:I:192:GLU:OE2[2_556]	2.04	0.16
1:B:7:ASN:CB	1:E:84:HIS:CE1[2_546]	2.08	0.12
1:A:329:GLN:O	1:E:282:TYR:CE2[2_646]	2.10	0.10
1:B:329:GLN:CG	1:D:282:TYR:OH[1_455]	2.11	0.09
1:B:7:ASN:CB	1:E:84:HIS:ND1[2_546]	2.12	0.08
1:A:329:GLN:CB	1:E:282:TYR:CZ[2_646]	2.14	0.06
1:B:330:LEU:N	1:D:282:TYR:CE2[1_455]	2.16	0.04
1:G:243:LYS:NZ	1:K:284:GLN:OE1[1_556]	2.17	0.03
1:F:211:LYS:NZ	1:I:192:GLU:OE1[2_556]	2.18	0.02
1:A:330:LEU:N	1:E:282:TYR:CE2[2_646]	2.19	0.01
1:B:329:GLN:CB	1:D:282:TYR:CZ[1_455]	2.19	0.01
1:E:342:ARG:N	1:G:84:HIS:NE2[2_556]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	6	22
1	B	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	6	22
1	C	358/377 (95%)	291 (81%)	60 (17%)	7 (2%)	6	22
1	D	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	6	22
1	E	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	6	22
1	F	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	6	22
1	G	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	6	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	367/377 (97%)	303 (83%)	54 (15%)	10 (3%)	4	16
1	I	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	6	22
1	J	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	6	22
1	K	358/377 (95%)	293 (82%)	58 (16%)	7 (2%)	6	22
1	L	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	6	22
All	All	4305/4524 (95%)	3515 (82%)	703 (16%)	87 (2%)	6	22

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	GLY
1	B	171	GLY
1	C	171	GLY
1	D	171	GLY
1	E	171	GLY
1	F	171	GLY
1	G	171	GLY
1	I	171	GLY
1	J	171	GLY
1	K	171	GLY
1	L	171	GLY
1	A	359	ILE
1	B	359	ILE
1	C	359	ILE
1	D	359	ILE
1	E	359	ILE
1	F	359	ILE
1	G	359	ILE
1	H	83	SER
1	I	359	ILE
1	J	359	ILE
1	K	359	ILE
1	L	359	ILE
1	A	248	TYR
1	B	248	TYR
1	C	248	TYR
1	D	248	TYR
1	E	248	TYR
1	F	248	TYR
1	G	248	TYR

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Mol	Chain	Res	Type
1	H	81	LEU
1	H	171	GLY
1	H	211	LYS
1	H	216	PRO
1	H	264	ALA
1	I	248	TYR
1	J	248	TYR
1	K	248	TYR
1	L	248	TYR
1	A	169	GLY
1	B	169	GLY
1	C	169	GLY
1	D	169	GLY
1	E	169	GLY
1	F	169	GLY
1	G	169	GLY
1	I	169	GLY
1	J	169	GLY
1	K	169	GLY
1	L	169	GLY
1	H	132	PHE
1	A	232	PRO
1	B	232	PRO
1	C	232	PRO
1	D	232	PRO
1	E	232	PRO
1	F	232	PRO
1	G	232	PRO
1	H	138	ALA
1	H	293	GLU
1	I	232	PRO
1	J	232	PRO
1	K	232	PRO
1	L	232	PRO
1	A	98	ILE
1	A	132	PHE
1	B	98	ILE
1	B	132	PHE
1	C	98	ILE
1	C	132	PHE
1	D	98	ILE
1	D	132	PHE

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Mol	Chain	Res	Type
1	E	98	ILE
1	E	132	PHE
1	F	98	ILE
1	F	132	PHE
1	G	98	ILE
1	G	132	PHE
1	I	98	ILE
1	I	132	PHE
1	J	98	ILE
1	J	132	PHE
1	K	98	ILE
1	K	132	PHE
1	L	98	ILE
1	L	132	PHE
1	H	5	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	310/316 (98%)	280 (90%)	30 (10%)	8	25
1	B	310/316 (98%)	280 (90%)	30 (10%)	8	25
1	C	310/316 (98%)	280 (90%)	30 (10%)	8	25
1	D	310/316 (98%)	280 (90%)	30 (10%)	8	25
1	E	310/316 (98%)	280 (90%)	30 (10%)	8	25
1	F	310/316 (98%)	280 (90%)	30 (10%)	8	25
1	G	310/316 (98%)	280 (90%)	30 (10%)	8	25
1	H	316/316 (100%)	286 (90%)	30 (10%)	8	26
1	I	310/316 (98%)	280 (90%)	30 (10%)	8	25
1	J	310/316 (98%)	280 (90%)	30 (10%)	8	25
1	K	310/316 (98%)	280 (90%)	30 (10%)	8	25
1	L	310/316 (98%)	280 (90%)	30 (10%)	8	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3726/3792 (98%)	3366 (90%)	360 (10%)	8 25

All (360) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	5	ILE
1	A	56	ILE
1	A	66	VAL
1	A	67	PRO
1	A	89	ILE
1	A	114	ARG
1	A	116	VAL
1	A	119	GLU
1	A	121	ASN
1	A	127	VAL
1	A	150	VAL
1	A	161	GLU
1	A	176	THR
1	A	178	MSE
1	A	185	ARG
1	A	189	LEU
1	A	192	GLU
1	A	197	LYS
1	A	203	ASN
1	A	212	ASP
1	A	225	ASP
1	A	258	LEU
1	A	278	LYS
1	A	285	GLU
1	A	309	LEU
1	A	327	ASN
1	A	350	GLU
1	A	358	ASN
1	A	370	LEU
1	B	4	ARG
1	B	5	ILE
1	B	56	ILE
1	B	66	VAL
1	B	67	PRO
1	B	89	ILE
1	B	114	ARG

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Mol	Chain	Res	Type
1	B	116	VAL
1	B	119	GLU
1	B	121	ASN
1	B	127	VAL
1	B	150	VAL
1	B	161	GLU
1	B	176	THR
1	B	178	MSE
1	B	185	ARG
1	B	189	LEU
1	B	192	GLU
1	B	197	LYS
1	B	203	ASN
1	B	212	ASP
1	B	225	ASP
1	B	258	LEU
1	B	278	LYS
1	B	285	GLU
1	B	309	LEU
1	B	327	ASN
1	B	350	GLU
1	B	358	ASN
1	B	370	LEU
1	C	4	ARG
1	C	5	ILE
1	C	56	ILE
1	C	66	VAL
1	C	67	PRO
1	C	89	ILE
1	C	114	ARG
1	C	116	VAL
1	C	119	GLU
1	C	121	ASN
1	C	127	VAL
1	C	150	VAL
1	C	161	GLU
1	C	176	THR
1	C	178	MSE
1	C	185	ARG
1	C	189	LEU
1	C	192	GLU
1	C	197	LYS

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Mol	Chain	Res	Type
1	C	203	ASN
1	C	212	ASP
1	C	225	ASP
1	C	258	LEU
1	C	278	LYS
1	C	285	GLU
1	C	309	LEU
1	C	327	ASN
1	C	350	GLU
1	C	358	ASN
1	C	370	LEU
1	D	4	ARG
1	D	5	ILE
1	D	56	ILE
1	D	66	VAL
1	D	67	PRO
1	D	89	ILE
1	D	114	ARG
1	D	116	VAL
1	D	119	GLU
1	D	121	ASN
1	D	127	VAL
1	D	150	VAL
1	D	161	GLU
1	D	176	THR
1	D	178	MSE
1	D	185	ARG
1	D	189	LEU
1	D	192	GLU
1	D	197	LYS
1	D	203	ASN
1	D	212	ASP
1	D	225	ASP
1	D	258	LEU
1	D	278	LYS
1	D	285	GLU
1	D	309	LEU
1	D	327	ASN
1	D	350	GLU
1	D	358	ASN
1	D	370	LEU
1	E	4	ARG

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Mol	Chain	Res	Type
1	E	5	ILE
1	E	56	ILE
1	E	66	VAL
1	E	67	PRO
1	E	89	ILE
1	E	114	ARG
1	E	116	VAL
1	E	119	GLU
1	E	121	ASN
1	E	127	VAL
1	E	150	VAL
1	E	161	GLU
1	E	176	THR
1	E	178	MSE
1	E	185	ARG
1	E	189	LEU
1	E	192	GLU
1	E	197	LYS
1	E	203	ASN
1	E	212	ASP
1	E	225	ASP
1	E	258	LEU
1	E	278	LYS
1	E	285	GLU
1	E	309	LEU
1	E	327	ASN
1	E	350	GLU
1	E	358	ASN
1	E	370	LEU
1	F	4	ARG
1	F	5	ILE
1	F	56	ILE
1	F	66	VAL
1	F	67	PRO
1	F	89	ILE
1	F	114	ARG
1	F	116	VAL
1	F	119	GLU
1	F	121	ASN
1	F	127	VAL
1	F	150	VAL
1	F	161	GLU

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Mol	Chain	Res	Type
1	F	176	THR
1	F	178	MSE
1	F	185	ARG
1	F	189	LEU
1	F	192	GLU
1	F	197	LYS
1	F	203	ASN
1	F	212	ASP
1	F	225	ASP
1	F	258	LEU
1	F	278	LYS
1	F	285	GLU
1	F	309	LEU
1	F	327	ASN
1	F	350	GLU
1	F	358	ASN
1	F	370	LEU
1	G	4	ARG
1	G	5	ILE
1	G	56	ILE
1	G	66	VAL
1	G	67	PRO
1	G	89	ILE
1	G	114	ARG
1	G	116	VAL
1	G	119	GLU
1	G	121	ASN
1	G	127	VAL
1	G	150	VAL
1	G	161	GLU
1	G	176	THR
1	G	178	MSE
1	G	185	ARG
1	G	189	LEU
1	G	192	GLU
1	G	197	LYS
1	G	203	ASN
1	G	212	ASP
1	G	225	ASP
1	G	258	LEU
1	G	278	LYS
1	G	285	GLU

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Mol	Chain	Res	Type
1	G	309	LEU
1	G	327	ASN
1	G	350	GLU
1	G	358	ASN
1	G	370	LEU
1	H	52	VAL
1	H	66	VAL
1	H	80	GLU
1	H	89	ILE
1	H	121	ASN
1	H	127	VAL
1	H	161	GLU
1	H	176	THR
1	H	178	MSE
1	H	185	ARG
1	H	189	LEU
1	H	202	LEU
1	H	207	VAL
1	H	217	TYR
1	H	225	ASP
1	H	240	THR
1	H	262	THR
1	H	263	ASP
1	H	269	LEU
1	H	278	LYS
1	H	279	GLU
1	H	283	LEU
1	H	309	LEU
1	H	312	LEU
1	H	315	ASN
1	H	318	ILE
1	H	328	ASP
1	H	350	GLU
1	H	351	GLU
1	H	358	ASN
1	I	4	ARG
1	I	5	ILE
1	I	56	ILE
1	I	66	VAL
1	I	67	PRO
1	I	89	ILE
1	I	114	ARG

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Mol	Chain	Res	Type
1	I	116	VAL
1	I	119	GLU
1	I	121	ASN
1	I	127	VAL
1	I	150	VAL
1	I	161	GLU
1	I	176	THR
1	I	178	MSE
1	I	185	ARG
1	I	189	LEU
1	I	192	GLU
1	I	197	LYS
1	I	203	ASN
1	I	212	ASP
1	I	225	ASP
1	I	258	LEU
1	I	278	LYS
1	I	285	GLU
1	I	309	LEU
1	I	327	ASN
1	I	350	GLU
1	I	358	ASN
1	I	370	LEU
1	J	4	ARG
1	J	5	ILE
1	J	56	ILE
1	J	66	VAL
1	J	67	PRO
1	J	89	ILE
1	J	114	ARG
1	J	116	VAL
1	J	119	GLU
1	J	121	ASN
1	J	127	VAL
1	J	150	VAL
1	J	161	GLU
1	J	176	THR
1	J	178	MSE
1	J	185	ARG
1	J	189	LEU
1	J	192	GLU
1	J	197	LYS

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Mol	Chain	Res	Type
1	J	203	ASN
1	J	212	ASP
1	J	225	ASP
1	J	258	LEU
1	J	278	LYS
1	J	285	GLU
1	J	309	LEU
1	J	327	ASN
1	J	350	GLU
1	J	358	ASN
1	J	370	LEU
1	K	4	ARG
1	K	5	ILE
1	K	56	ILE
1	K	66	VAL
1	K	67	PRO
1	K	89	ILE
1	K	114	ARG
1	K	116	VAL
1	K	119	GLU
1	K	121	ASN
1	K	127	VAL
1	K	150	VAL
1	K	161	GLU
1	K	176	THR
1	K	178	MSE
1	K	185	ARG
1	K	189	LEU
1	K	192	GLU
1	K	197	LYS
1	K	203	ASN
1	K	212	ASP
1	K	225	ASP
1	K	258	LEU
1	K	278	LYS
1	K	285	GLU
1	K	309	LEU
1	K	327	ASN
1	K	350	GLU
1	K	358	ASN
1	K	370	LEU
1	L	4	ARG

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Mol	Chain	Res	Type
1	L	5	ILE
1	L	56	ILE
1	L	66	VAL
1	L	67	PRO
1	L	89	ILE
1	L	114	ARG
1	L	116	VAL
1	L	119	GLU
1	L	121	ASN
1	L	127	VAL
1	L	150	VAL
1	L	161	GLU
1	L	176	THR
1	L	178	MSE
1	L	185	ARG
1	L	189	LEU
1	L	192	GLU
1	L	197	LYS
1	L	203	ASN
1	L	212	ASP
1	L	225	ASP
1	L	258	LEU
1	L	278	LYS
1	L	285	GLU
1	L	309	LEU
1	L	327	ASN
1	L	350	GLU
1	L	358	ASN
1	L	370	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (249) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	12	GLN
1	A	26	GLN
1	A	37	ASN
1	A	46	GLN
1	A	70	GLN
1	A	73	ASN
1	A	121	ASN
1	A	186	ASN

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Mol	Chain	Res	Type
1	A	203	ASN
1	A	220	ASN
1	A	249	GLN
1	A	261	GLN
1	A	284	GLN
1	A	310	ASN
1	A	315	ASN
1	A	327	ASN
1	A	333	GLN
1	A	358	ASN
1	A	360	HIS
1	A	366	GLN
1	B	12	GLN
1	B	26	GLN
1	B	46	GLN
1	B	70	GLN
1	B	73	ASN
1	B	121	ASN
1	B	186	ASN
1	B	203	ASN
1	B	220	ASN
1	B	249	GLN
1	B	261	GLN
1	B	284	GLN
1	B	310	ASN
1	B	315	ASN
1	B	327	ASN
1	B	333	GLN
1	B	358	ASN
1	B	360	HIS
1	B	366	GLN
1	C	12	GLN
1	C	26	GLN
1	C	35	ASN
1	C	37	ASN
1	C	46	GLN
1	C	70	GLN
1	C	73	ASN
1	C	121	ASN
1	C	186	ASN
1	C	203	ASN
1	C	220	ASN

Continued on next page...

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Mol	Chain	Res	Type
1	C	249	GLN
1	C	261	GLN
1	C	284	GLN
1	C	310	ASN
1	C	315	ASN
1	C	327	ASN
1	C	333	GLN
1	C	358	ASN
1	C	360	HIS
1	C	366	GLN
1	D	12	GLN
1	D	26	GLN
1	D	37	ASN
1	D	46	GLN
1	D	70	GLN
1	D	73	ASN
1	D	84	HIS
1	D	121	ASN
1	D	186	ASN
1	D	203	ASN
1	D	220	ASN
1	D	249	GLN
1	D	261	GLN
1	D	284	GLN
1	D	310	ASN
1	D	315	ASN
1	D	327	ASN
1	D	333	GLN
1	D	358	ASN
1	D	360	HIS
1	D	366	GLN
1	E	12	GLN
1	E	26	GLN
1	E	35	ASN
1	E	37	ASN
1	E	46	GLN
1	E	70	GLN
1	E	121	ASN
1	E	186	ASN
1	E	203	ASN
1	E	220	ASN
1	E	249	GLN

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Mol	Chain	Res	Type
1	E	261	GLN
1	E	284	GLN
1	E	310	ASN
1	E	315	ASN
1	E	327	ASN
1	E	333	GLN
1	E	358	ASN
1	E	360	HIS
1	E	366	GLN
1	F	12	GLN
1	F	26	GLN
1	F	35	ASN
1	F	37	ASN
1	F	46	GLN
1	F	70	GLN
1	F	73	ASN
1	F	121	ASN
1	F	186	ASN
1	F	203	ASN
1	F	220	ASN
1	F	249	GLN
1	F	261	GLN
1	F	284	GLN
1	F	310	ASN
1	F	315	ASN
1	F	327	ASN
1	F	333	GLN
1	F	358	ASN
1	F	360	HIS
1	F	366	GLN
1	G	12	GLN
1	G	26	GLN
1	G	35	ASN
1	G	37	ASN
1	G	46	GLN
1	G	70	GLN
1	G	73	ASN
1	G	121	ASN
1	G	186	ASN
1	G	203	ASN
1	G	220	ASN
1	G	249	GLN

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Mol	Chain	Res	Type
1	G	261	GLN
1	G	284	GLN
1	G	310	ASN
1	G	315	ASN
1	G	327	ASN
1	G	333	GLN
1	G	358	ASN
1	G	360	HIS
1	G	366	GLN
1	H	12	GLN
1	H	24	GLN
1	H	26	GLN
1	H	35	ASN
1	H	37	ASN
1	H	46	GLN
1	H	73	ASN
1	H	85	ASN
1	H	121	ASN
1	H	182	HIS
1	H	186	ASN
1	H	203	ASN
1	H	220	ASN
1	H	249	GLN
1	H	261	GLN
1	H	284	GLN
1	H	315	ASN
1	H	322	GLN
1	H	333	GLN
1	H	358	ASN
1	H	360	HIS
1	H	364	GLN
1	H	366	GLN
1	I	12	GLN
1	I	26	GLN
1	I	37	ASN
1	I	46	GLN
1	I	70	GLN
1	I	73	ASN
1	I	121	ASN
1	I	186	ASN
1	I	203	ASN
1	I	220	ASN

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Mol	Chain	Res	Type
1	I	249	GLN
1	I	261	GLN
1	I	284	GLN
1	I	310	ASN
1	I	315	ASN
1	I	327	ASN
1	I	333	GLN
1	I	358	ASN
1	I	360	HIS
1	I	366	GLN
1	J	12	GLN
1	J	26	GLN
1	J	35	ASN
1	J	37	ASN
1	J	46	GLN
1	J	70	GLN
1	J	73	ASN
1	J	121	ASN
1	J	186	ASN
1	J	203	ASN
1	J	220	ASN
1	J	249	GLN
1	J	261	GLN
1	J	284	GLN
1	J	310	ASN
1	J	315	ASN
1	J	327	ASN
1	J	333	GLN
1	J	358	ASN
1	J	360	HIS
1	J	366	GLN
1	K	12	GLN
1	K	26	GLN
1	K	37	ASN
1	K	46	GLN
1	K	70	GLN
1	K	73	ASN
1	K	121	ASN
1	K	186	ASN
1	K	203	ASN
1	K	220	ASN
1	K	249	GLN

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Mol	Chain	Res	Type
1	K	261	GLN
1	K	284	GLN
1	K	310	ASN
1	K	315	ASN
1	K	327	ASN
1	K	333	GLN
1	K	358	ASN
1	K	360	HIS
1	K	366	GLN
1	L	12	GLN
1	L	26	GLN
1	L	35	ASN
1	L	37	ASN
1	L	46	GLN
1	L	70	GLN
1	L	73	ASN
1	L	121	ASN
1	L	186	ASN
1	L	203	ASN
1	L	220	ASN
1	L	249	GLN
1	L	261	GLN
1	L	284	GLN
1	L	310	ASN
1	L	315	ASN
1	L	327	ASN
1	L	333	GLN
1	L	358	ASN
1	L	360	HIS
1	L	366	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	355/377 (94%)	0.89	45 (12%) 8 6	7, 17, 47, 60	1 (0%)
1	B	355/377 (94%)	0.87	49 (13%) 6 5	7, 20, 54, 60	1 (0%)
1	C	355/377 (94%)	1.04	51 (14%) 6 5	10, 40, 60, 60	1 (0%)
1	D	355/377 (94%)	1.09	60 (16%) 4 3	10, 34, 60, 60	1 (0%)
1	E	355/377 (94%)	1.16	66 (18%) 3 3	9, 35, 60, 60	1 (0%)
1	F	355/377 (94%)	1.04	60 (16%) 4 3	9, 36, 60, 60	1 (0%)
1	G	355/377 (94%)	1.11	53 (14%) 5 4	10, 37, 60, 60	1 (0%)
1	H	362/377 (96%)	0.41	9 (2%) 58 48	10, 33, 59, 60	1 (0%)
1	I	355/377 (94%)	0.92	47 (13%) 7 6	10, 38, 60, 60	1 (0%)
1	J	355/377 (94%)	1.13	57 (16%) 4 4	11, 49, 60, 60	1 (0%)
1	K	355/377 (94%)	0.61	10 (2%) 55 46	8, 45, 60, 60	1 (0%)
1	L	355/377 (94%)	1.15	51 (14%) 6 5	15, 56, 60, 60	1 (0%)
All	All	4267/4524 (94%)	0.95	558 (13%) 7 6	7, 37, 60, 60	12 (0%)

All (558) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	282	TYR	7.5
1	D	282	TYR	7.4
1	E	279	GLU	5.8
1	F	83	SER	5.7
1	D	82	GLY	5.3
1	G	124	GLY	5.3
1	B	260	GLN	5.2
1	E	124	GLY	5.2
1	J	218	GLU	5.1
1	E	82	GLY	4.9
1	D	171	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	327	ASN	4.7
1	D	279	GLU	4.7
1	B	217	TYR	4.7
1	E	280	PRO	4.6
1	A	83	SER	4.6
1	B	268	PRO	4.6
1	C	124	GLY	4.5
1	B	291	TYR	4.4
1	E	233	GLY	4.3
1	F	218	GLU	4.2
1	L	204	CYS	4.2
1	A	215	ASP	4.2
1	B	215	ASP	4.2
1	A	218	GLU	4.2
1	E	204	CYS	4.1
1	F	346	GLY	4.1
1	J	83	SER	4.1
1	C	341	ASP	4.1
1	E	217	TYR	4.1
1	D	2	ALA	4.0
1	G	82	GLY	4.0
1	L	335	VAL	4.0
1	D	370	LEU	4.0
1	F	82	GLY	3.9
1	G	207	VAL	3.9
1	F	264	ALA	3.9
1	A	370	LEU	3.9
1	C	2	ALA	3.9
1	C	217	TYR	3.9
1	B	124	GLY	3.9
1	A	9	THR	3.9
1	J	169	GLY	3.8
1	K	370	LEU	3.8
1	D	218	GLU	3.8
1	D	215	ASP	3.8
1	G	310	ASN	3.8
1	C	305	ILE	3.8
1	E	314	VAL	3.8
1	I	306	ALA	3.8
1	G	174	LEU	3.8
1	A	260	GLN	3.7
1	F	204	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	171	GLY	3.7
1	G	215	ASP	3.7
1	E	80	GLU	3.7
1	L	250	GLU	3.7
1	D	5	ILE	3.7
1	F	313	ILE	3.7
1	F	291	TYR	3.7
1	C	83	SER	3.6
1	G	84	HIS	3.6
1	D	368	ALA	3.6
1	A	337	GLU	3.6
1	I	370	LEU	3.6
1	E	2	ALA	3.6
1	B	282	TYR	3.6
1	C	281	CYS	3.6
1	F	370	LEU	3.6
1	F	310	ASN	3.6
1	E	292	VAL	3.5
1	C	279	GLU	3.5
1	C	79	SER	3.5
1	E	291	TYR	3.5
1	E	269	LEU	3.5
1	A	301	GLY	3.4
1	L	79	SER	3.4
1	G	327	ASN	3.4
1	B	185	ARG	3.4
1	C	291	TYR	3.4
1	J	124	GLY	3.4
1	A	326	GLU	3.4
1	D	177	GLU	3.4
1	A	268	PRO	3.4
1	A	291	TYR	3.4
1	D	263	ASP	3.4
1	E	100	ASP	3.4
1	E	329	GLN	3.3
1	K	218	GLU	3.3
1	I	291	TYR	3.3
1	A	327	ASN	3.3
1	D	315	ASN	3.3
1	D	327	ASN	3.3
1	E	315	ASN	3.3
1	D	313	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	370	LEU	3.3
1	A	292	VAL	3.3
1	D	83	SER	3.3
1	A	239	TYR	3.2
1	A	282	TYR	3.2
1	B	80	GLU	3.2
1	B	218	GLU	3.2
1	F	84	HIS	3.2
1	E	119	GLU	3.2
1	E	177	GLU	3.2
1	F	58	GLU	3.2
1	F	215	ASP	3.2
1	G	36	ASP	3.2
1	J	353	ALA	3.2
1	A	70	GLN	3.2
1	G	217	TYR	3.2
1	C	369	THR	3.2
1	D	204	CYS	3.2
1	B	239	TYR	3.2
1	C	215	ASP	3.2
1	C	269	LEU	3.2
1	E	159	VAL	3.2
1	K	280	PRO	3.2
1	D	280	PRO	3.1
1	J	217	TYR	3.1
1	E	83	SER	3.1
1	J	275	CYS	3.1
1	B	326	GLU	3.1
1	K	83	SER	3.1
1	D	216	PRO	3.1
1	F	2	ALA	3.1
1	C	247	PHE	3.1
1	I	341	ASP	3.1
1	A	313	ILE	3.1
1	E	238	ILE	3.1
1	F	5	ILE	3.1
1	C	80	GLU	3.1
1	F	285	GLU	3.1
1	L	370	LEU	3.1
1	J	335	VAL	3.0
1	L	345	VAL	3.0
1	L	262	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	85	ASN	3.0
1	D	278	LYS	3.0
1	B	370	LEU	3.0
1	C	370	LEU	3.0
1	F	244	GLU	3.0
1	J	313	ILE	3.0
1	A	204	CYS	3.0
1	I	279	GLU	3.0
1	G	313	ILE	3.0
1	E	370	LEU	3.0
1	I	356	GLY	3.0
1	C	241	ASP	3.0
1	J	281	CYS	3.0
1	C	292	VAL	2.9
1	L	142	ARG	2.9
1	J	202	LEU	2.9
1	L	331	ALA	2.9
1	E	133	PRO	2.9
1	E	358	ASN	2.9
1	A	275	CYS	2.9
1	G	233	GLY	2.9
1	K	324	GLY	2.9
1	I	250	GLU	2.9
1	A	7	ASN	2.9
1	F	358	ASN	2.9
1	L	203	ASN	2.9
1	I	276	VAL	2.9
1	L	247	PHE	2.9
1	G	169	GLY	2.8
1	I	215	ASP	2.8
1	D	214	ILE	2.8
1	A	233	GLY	2.8
1	J	232	PRO	2.8
1	D	285	GLU	2.8
1	J	170	GLU	2.8
1	B	327	ASN	2.8
1	C	212	ASP	2.8
1	F	171	GLY	2.8
1	G	96	ALA	2.8
1	I	310	ASN	2.8
1	C	233	GLY	2.8
1	G	268	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	337	GLU	2.8
1	A	348	ARG	2.8
1	D	292	VAL	2.8
1	A	132	PHE	2.8
1	I	282	TYR	2.8
1	I	5	ILE	2.8
1	A	149	GLY	2.8
1	E	336	GLN	2.7
1	G	142	ARG	2.7
1	L	285	GLU	2.7
1	G	204	CYS	2.7
1	D	205	VAL	2.7
1	A	217	TYR	2.7
1	E	174	LEU	2.7
1	G	81	LEU	2.7
1	E	278	LYS	2.7
1	L	135	ASP	2.7
1	B	83	SER	2.7
1	H	294	GLY	2.7
1	J	324	GLY	2.7
1	F	185	ARG	2.7
1	L	173	VAL	2.7
1	B	305	ILE	2.7
1	E	37	ASN	2.7
1	L	327	ASN	2.7
1	B	341	ASP	2.7
1	L	341	ASP	2.7
1	L	246	PRO	2.7
1	I	83	SER	2.7
1	J	314	VAL	2.7
1	D	258	LEU	2.7
1	C	280	PRO	2.7
1	D	36	ASP	2.7
1	E	128	ASP	2.7
1	D	70	GLN	2.7
1	D	84	HIS	2.7
1	D	217	TYR	2.7
1	I	204	CYS	2.7
1	A	328	ASP	2.7
1	G	192	GLU	2.7
1	I	70	GLN	2.7
1	B	313	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	79	SER	2.7
1	E	313	ILE	2.6
1	E	132	PHE	2.6
1	I	84	HIS	2.6
1	J	111	GLY	2.6
1	B	177	GLU	2.6
1	E	337	GLU	2.6
1	F	158	PHE	2.6
1	L	107	VAL	2.6
1	B	352	ILE	2.6
1	E	218	GLU	2.6
1	L	2	ALA	2.6
1	E	232	PRO	2.6
1	B	347	VAL	2.6
1	I	349	THR	2.6
1	L	320	LEU	2.6
1	F	339	PHE	2.6
1	J	225	ASP	2.6
1	D	184	SER	2.6
1	F	133	PRO	2.6
1	G	278	LYS	2.6
1	A	347	VAL	2.6
1	D	262	THR	2.6
1	E	101	CYS	2.6
1	D	185	ARG	2.5
1	J	84	HIS	2.5
1	B	133	PRO	2.5
1	D	266	GLY	2.5
1	G	133	PRO	2.5
1	C	282	TYR	2.5
1	G	282	TYR	2.5
1	J	147	ILE	2.5
1	L	349	THR	2.5
1	F	327	ASN	2.5
1	B	272	HIS	2.5
1	E	112	ASP	2.5
1	J	128	ASP	2.5
1	J	215	ASP	2.5
1	C	169	GLY	2.5
1	F	347	VAL	2.5
1	H	292	VAL	2.5
1	I	230	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	177	GLU	2.5
1	E	349	THR	2.5
1	G	176	THR	2.5
1	J	329	GLN	2.5
1	E	310	ASN	2.5
1	G	108	ASN	2.5
1	C	36	ASP	2.5
1	C	196	ASP	2.5
1	E	239	TYR	2.5
1	G	337	GLU	2.5
1	L	218	GLU	2.5
1	C	329	GLN	2.5
1	I	277	THR	2.5
1	E	84	HIS	2.5
1	J	320	LEU	2.5
1	A	133	PRO	2.5
1	A	171	GLY	2.5
1	D	124	GLY	2.5
1	E	213	GLY	2.5
1	H	83	SER	2.5
1	J	359	ILE	2.5
1	D	132	PHE	2.5
1	D	250	GLU	2.5
1	G	80	GLU	2.5
1	G	267	ARG	2.5
1	E	211	LYS	2.5
1	F	174	LEU	2.4
1	L	113	LEU	2.4
1	F	340	PRO	2.4
1	I	313	ILE	2.4
1	J	280	PRO	2.4
1	F	292	VAL	2.4
1	E	350	GLU	2.4
1	C	284	GLN	2.4
1	G	329	GLN	2.4
1	I	240	THR	2.4
1	D	358	ASN	2.4
1	F	275	CYS	2.4
1	E	78	VAL	2.4
1	F	314	VAL	2.4
1	J	162	GLY	2.4
1	E	244	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	131	TYR	2.4
1	G	260	GLN	2.4
1	E	275	CYS	2.4
1	E	215	ASP	2.4
1	C	132	PHE	2.4
1	F	240	THR	2.4
1	B	81	LEU	2.4
1	A	305	ILE	2.4
1	G	5	ILE	2.4
1	L	86	ILE	2.4
1	L	88	ILE	2.4
1	C	265	LYS	2.4
1	D	356	GLY	2.4
1	E	328	ASP	2.4
1	G	275	CYS	2.4
1	J	247	PHE	2.4
1	D	302	GLU	2.4
1	B	249	GLN	2.4
1	E	79	SER	2.4
1	E	130	LEU	2.4
1	C	327	ASN	2.3
1	G	335	VAL	2.3
1	J	310	ASN	2.3
1	B	82	GLY	2.3
1	C	316	GLY	2.3
1	I	213	GLY	2.3
1	H	215	ASP	2.3
1	B	192	GLU	2.3
1	B	279	GLU	2.3
1	C	285	GLU	2.3
1	G	218	GLU	2.3
1	I	254	ALA	2.3
1	A	176	THR	2.3
1	F	272	HIS	2.3
1	H	269	LEU	2.3
1	B	270	LYS	2.3
1	J	271	VAL	2.3
1	I	327	ASN	2.3
1	J	339	PHE	2.3
1	D	328	ASP	2.3
1	F	326	GLU	2.3
1	G	306	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	306	ALA	2.3
1	D	336	GLN	2.3
1	J	70	GLN	2.3
1	F	217	TYR	2.3
1	F	238	ILE	2.3
1	L	214	ILE	2.3
1	B	267	ARG	2.3
1	J	268	PRO	2.3
1	I	335	VAL	2.3
1	J	203	ASN	2.3
1	F	279	GLU	2.3
1	E	225	ASP	2.3
1	G	196	ASP	2.3
1	G	212	ASP	2.3
1	I	196	ASP	2.3
1	C	313	ILE	2.3
1	E	272	HIS	2.3
1	G	83	SER	2.3
1	I	211	LYS	2.3
1	L	318	ILE	2.3
1	G	16	ARG	2.3
1	I	217	TYR	2.3
1	K	323	TYR	2.3
1	C	205	VAL	2.3
1	D	213	GLY	2.3
1	D	316	GLY	2.3
1	G	264	ALA	2.3
1	B	329	GLN	2.3
1	C	50	LEU	2.3
1	F	126	LEU	2.3
1	F	256	ASP	2.3
1	F	320	LEU	2.3
1	L	289	ILE	2.3
1	I	79	SER	2.3
1	D	268	PRO	2.3
1	D	163	GLY	2.3
1	D	221	GLY	2.3
1	A	170	GLU	2.2
1	E	285	GLU	2.2
1	G	368	ALA	2.2
1	G	322	GLN	2.2
1	J	284	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	183	PRO	2.2
1	B	233	GLY	2.2
1	F	132	PHE	2.2
1	L	311	PHE	2.2
1	B	170	GLU	2.2
1	F	368	ALA	2.2
1	J	58	GLU	2.2
1	J	326	GLU	2.2
1	I	278	LYS	2.2
1	A	352	ILE	2.2
1	A	256	ASP	2.2
1	J	185	ARG	2.2
1	B	361	CYS	2.2
1	J	204	CYS	2.2
1	L	268	PRO	2.2
1	A	255	TYR	2.2
1	F	79	SER	2.2
1	J	307	SER	2.2
1	J	323	TYR	2.2
1	B	247	PHE	2.2
1	L	15	PHE	2.2
1	L	21	PHE	2.2
1	A	285	GLU	2.2
1	A	300	GLU	2.2
1	C	130	LEU	2.2
1	I	7	ASN	2.2
1	G	284	GLN	2.2
1	F	36	ASP	2.2
1	L	225	ASP	2.2
1	C	314	VAL	2.2
1	G	280	PRO	2.2
1	G	292	VAL	2.2
1	I	116	VAL	2.2
1	D	9	THR	2.2
1	D	277	THR	2.2
1	I	281	CYS	2.2
1	G	324	GLY	2.2
1	J	239	TYR	2.2
1	L	339	PHE	2.2
1	E	198	LEU	2.2
1	F	330	LEU	2.2
1	B	285	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	368	ALA	2.2
1	J	227	ALA	2.2
1	J	285	GLU	2.2
1	A	142	ARG	2.2
1	F	142	ARG	2.2
1	L	5	ILE	2.2
1	G	261	GLN	2.2
1	F	128	ASP	2.2
1	L	200	ASP	2.2
1	K	217	TYR	2.2
1	K	247	PHE	2.2
1	L	291	TYR	2.2
1	J	258	LEU	2.2
1	J	370	LEU	2.2
1	I	147	ILE	2.1
1	I	185	ARG	2.1
1	F	260	GLN	2.1
1	B	7	ASN	2.1
1	I	128	ASP	2.1
1	J	224	ASP	2.1
1	F	262	THR	2.1
1	I	219	THR	2.1
1	A	81	LEU	2.1
1	D	257	PHE	2.1
1	I	247	PHE	2.1
1	J	283	LEU	2.1
1	F	239	TYR	2.1
1	I	96	ALA	2.1
1	B	142	ARG	2.1
1	F	70	GLN	2.1
1	I	284	GLN	2.1
1	D	133	PRO	2.1
1	E	205	VAL	2.1
1	J	367	PRO	2.1
1	J	270	LYS	2.1
1	D	112	ASP	2.1
1	J	168	ASP	2.1
1	C	111	GLY	2.1
1	E	316	GLY	2.1
1	F	301	GLY	2.1
1	L	324	GLY	2.1
1	C	185	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	323	TYR	2.1
1	H	264	ALA	2.1
1	L	353	ALA	2.1
1	B	161	GLU	2.1
1	D	300	GLU	2.1
1	E	214	ILE	2.1
1	G	177	GLU	2.1
1	B	322	GLN	2.1
1	H	333	GLN	2.1
1	C	207	VAL	2.1
1	D	3	LYS	2.1
1	A	341	ASP	2.1
1	B	41	GLY	2.1
1	C	317	GLY	2.1
1	D	50	LEU	2.1
1	F	212	ASP	2.1
1	I	36	ASP	2.1
1	I	162	GLY	2.1
1	J	356	GLY	2.1
1	D	230	ILE	2.1
1	D	326	GLU	2.1
1	G	51	GLU	2.1
1	G	291	TYR	2.1
1	J	279	GLU	2.1
1	J	300	GLU	2.1
1	L	282	TYR	2.1
1	L	305	ILE	2.1
1	B	204	CYS	2.1
1	J	207	VAL	2.1
1	K	205	VAL	2.1
1	L	278	LYS	2.1
1	C	310	ASN	2.1
1	E	85	ASN	2.1
1	B	269	LEU	2.1
1	E	50	LEU	2.1
1	A	196	ASP	2.1
1	C	349	THR	2.1
1	F	341	ASP	2.1
1	F	349	THR	2.1
1	I	200	ASP	2.1
1	I	60	GLU	2.1
1	G	239	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	282	TYR	2.1
1	E	6	LYS	2.0
1	F	47	LYS	2.0
1	B	84	HIS	2.0
1	A	127	VAL	2.0
1	C	127	VAL	2.0
1	F	116	VAL	2.0
1	L	127	VAL	2.0
1	F	280	PRO	2.0
1	A	147	ILE	2.0
1	B	36	ASP	2.0
1	C	290	ASP	2.0
1	C	304	ALA	2.0
1	H	2	ALA	2.0
1	A	270	LYS	2.0
1	B	211	LYS	2.0
1	G	201	TYR	2.0
1	H	291	TYR	2.0
1	I	6	LYS	2.0
1	I	323	TYR	2.0
1	C	261	GLN	2.0
1	D	347	VAL	2.0
1	L	272	HIS	2.0
1	E	246	PRO	2.0
1	E	281	CYS	2.0
1	L	280	PRO	2.0
1	L	269	LEU	2.0
1	C	358	ASN	2.0
1	L	220	ASN	2.0
1	B	132	PHE	2.0
1	G	132	PHE	2.0
1	F	305	ILE	2.0
1	J	176	THR	2.0
1	C	300	GLU	2.0
1	F	278	LYS	2.0
1	I	170	GLU	2.0
1	L	212	ASP	2.0
1	L	326	GLU	2.0
1	L	337	GLU	2.0
1	C	201	TYR	2.0
1	B	314	VAL	2.0
1	J	276	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	K	335	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.