



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 04:25 PM EST

PDB ID : 2EWO
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

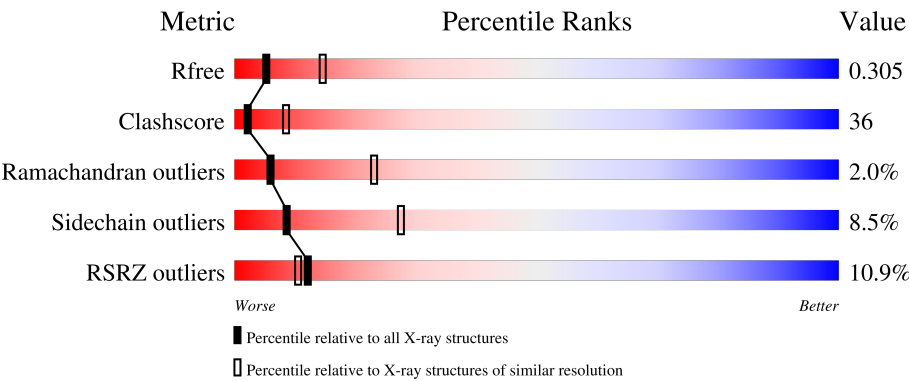
1 Overall quality at a glance i

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}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	377	<div><div>11%</div><div>40%</div><div>50%</div><div>6%</div><div>.</div></div>
1	B	377	<div><div>11%</div><div>41%</div><div>49%</div><div>6%</div><div>.</div></div>
1	C	377	<div><div>10%</div><div>41%</div><div>49%</div><div>6%</div><div>.</div></div>
1	D	377	<div><div>14%</div><div>40%</div><div>49%</div><div>7%</div><div>.</div></div>
1	E	377	<div><div>16%</div><div>40%</div><div>50%</div><div>6%</div><div>.</div></div>
1	F	377	<div><div>13%</div><div>41%</div><div>49%</div><div>7%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	G	377	<div><div></div><div>13%</div><div>41%</div><div>49%</div><div>6%</div><div></div></div>
1	H	377	<div><div></div><div>%</div><div>44%</div><div>45%</div><div>9%</div><div></div></div>
1	I	377	<div><div></div><div>10%</div><div>41%</div><div>48%</div><div>7%</div><div></div></div>
1	J	377	<div><div></div><div>13%</div><div>41%</div><div>48%</div><div>7%</div><div></div></div>
1	K	377	<div><div></div><div>2%</div><div>41%</div><div>49%</div><div>7%</div><div></div></div>
1	L	377	<div><div></div><div>10%</div><div>40%</div><div>49%</div><div>6%</div><div></div></div>



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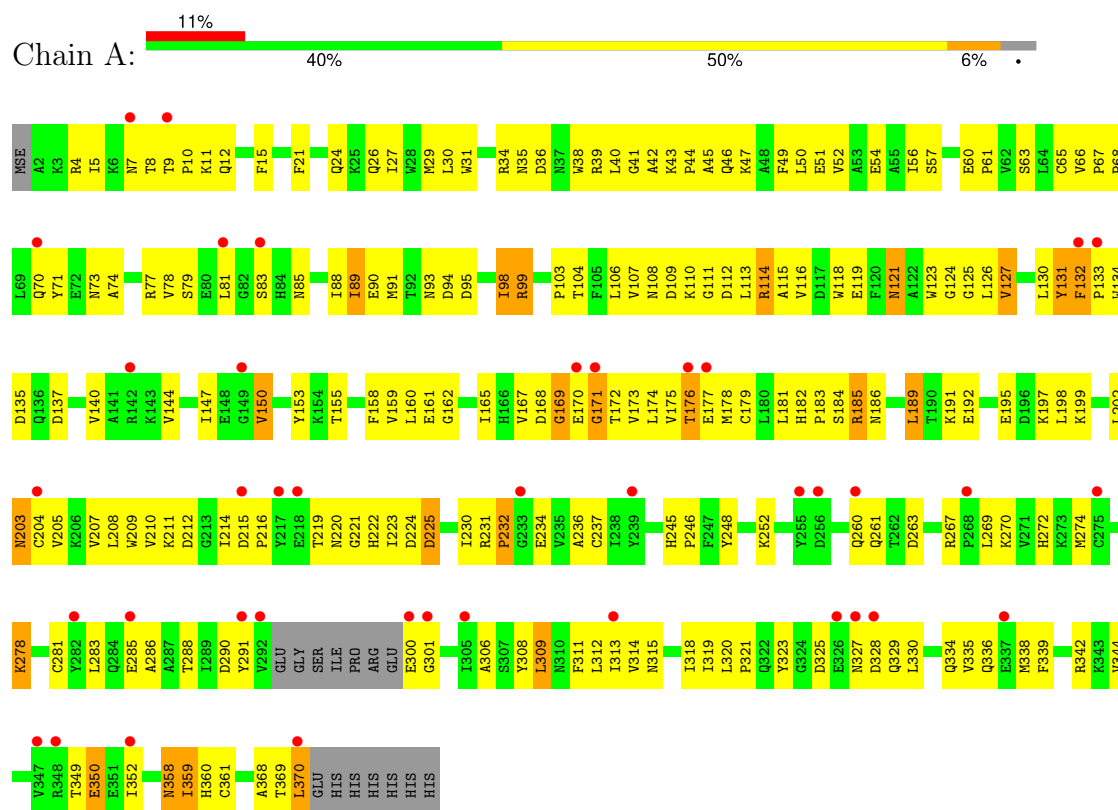
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	17	Total	O	0	0
			17	17		
2	L	13	Total	O	0	0
			13	13		

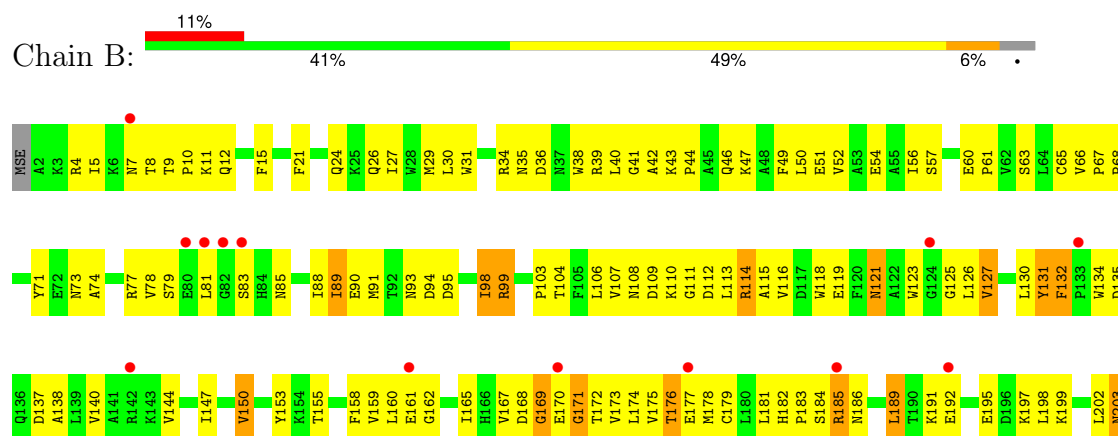
3 Residue-property plots

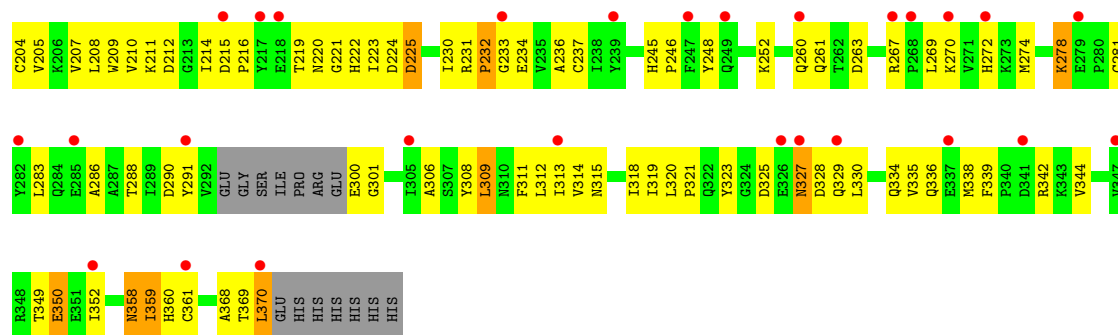
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

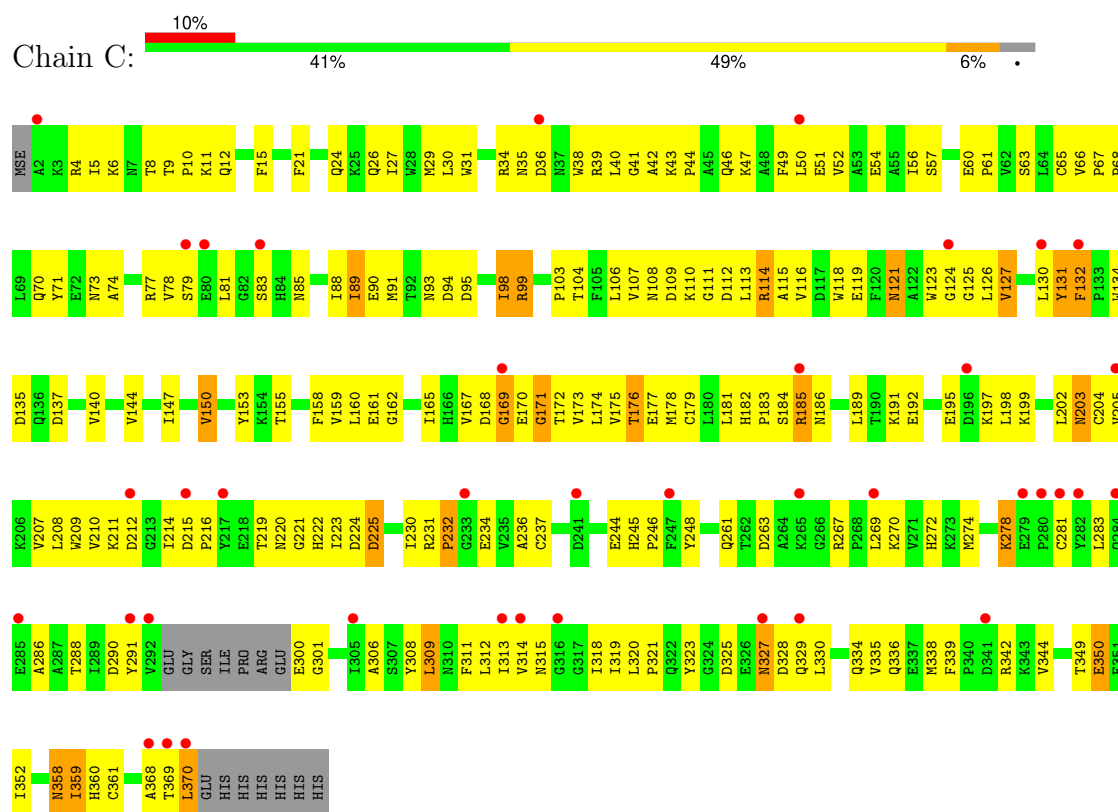


- Molecule 1: Putative agmatine deiminase

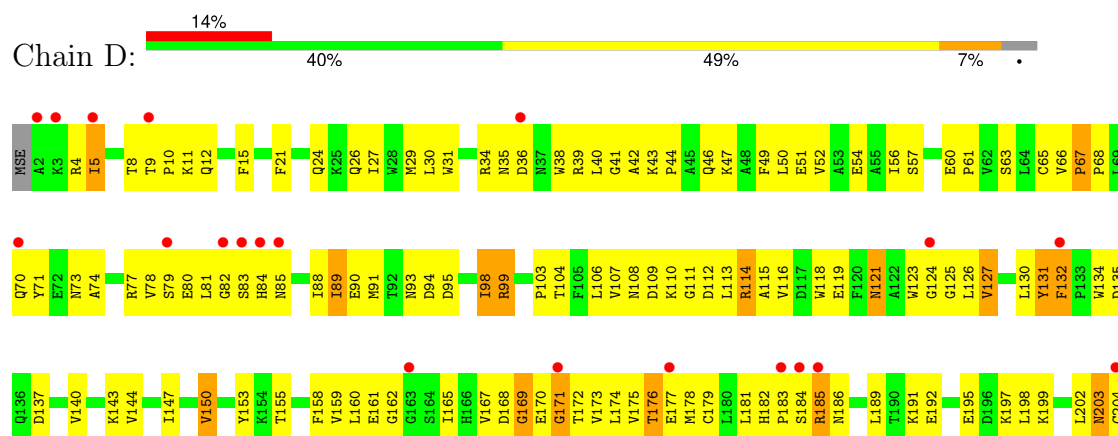


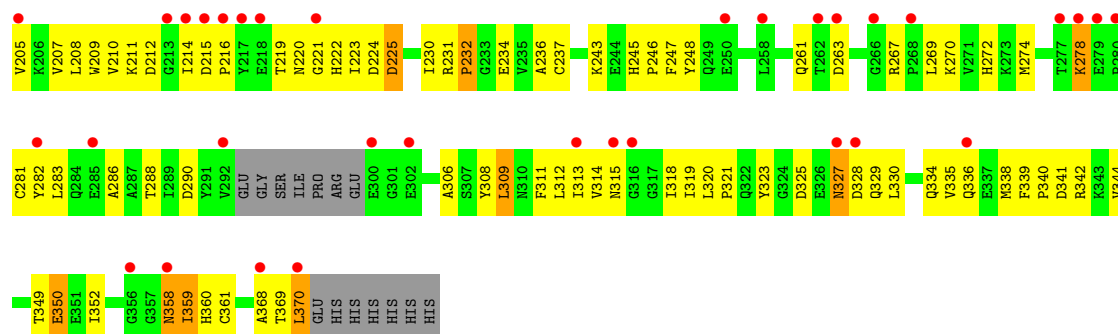


- Molecule 1: Putative agmatine deiminase



- Molecule 1: Putative agmatine deiminase

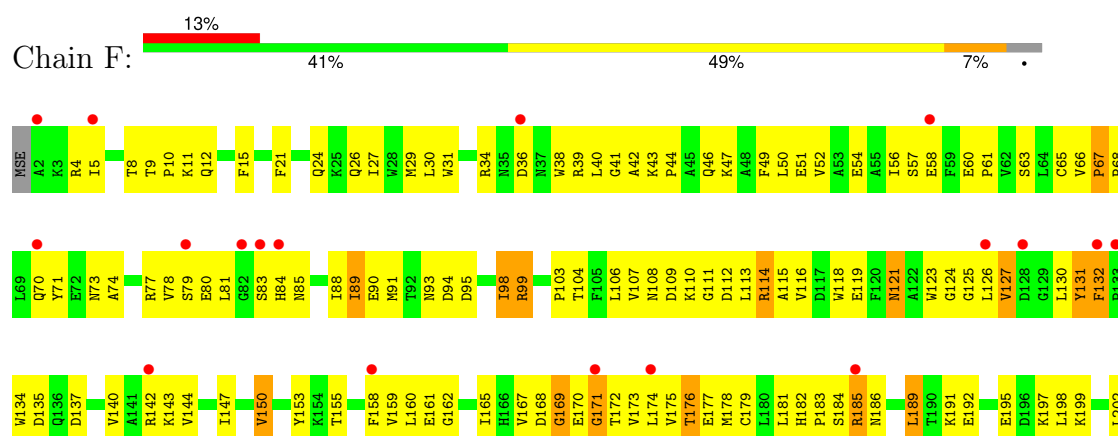


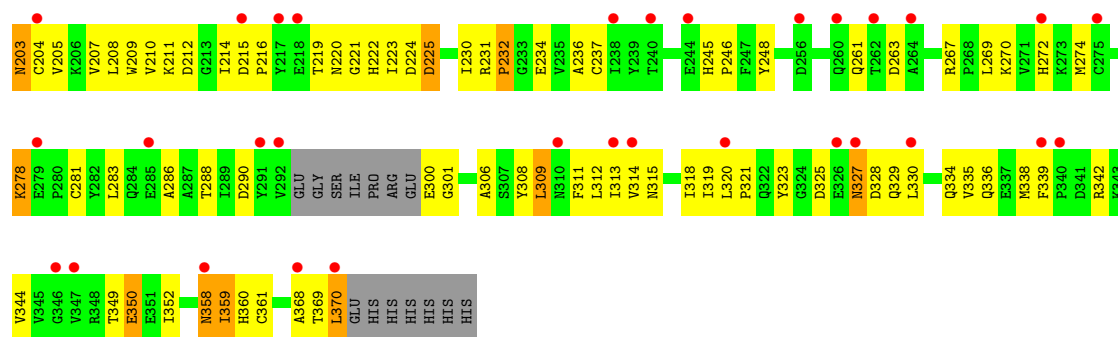


● Molecule 1: Putative agmatine deiminase

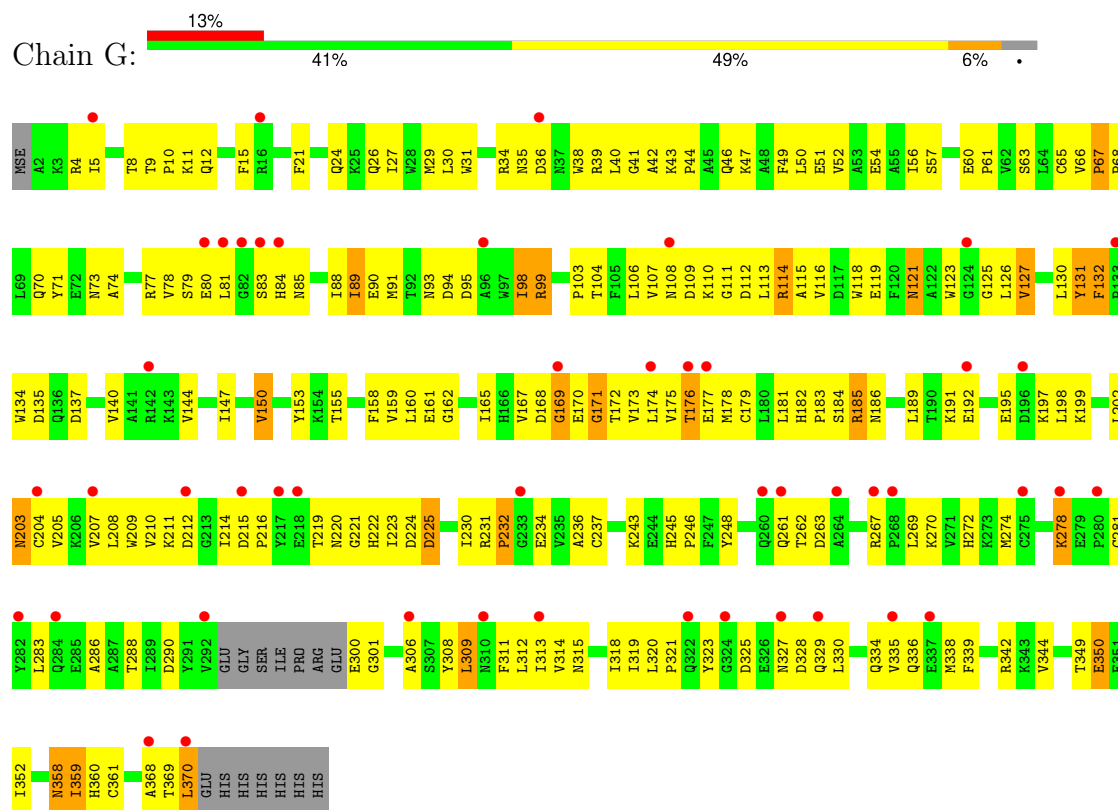


● Molecule 1: Putative agmatine deiminase

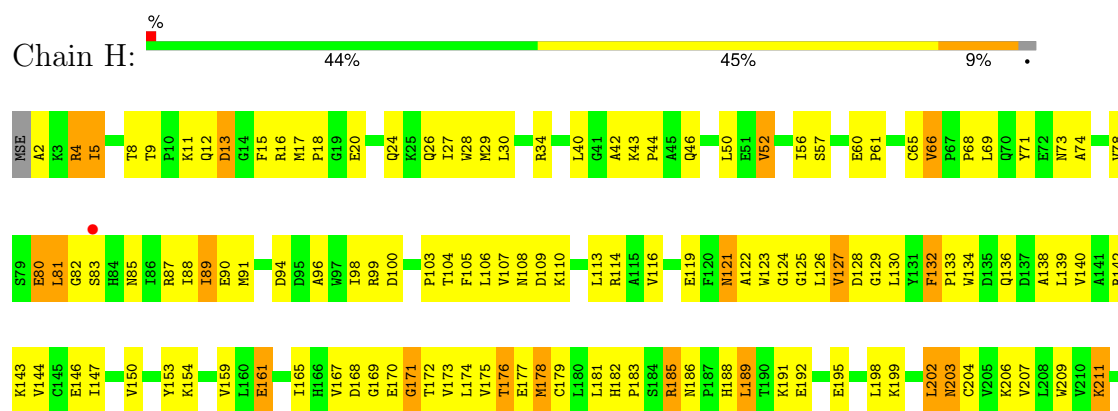


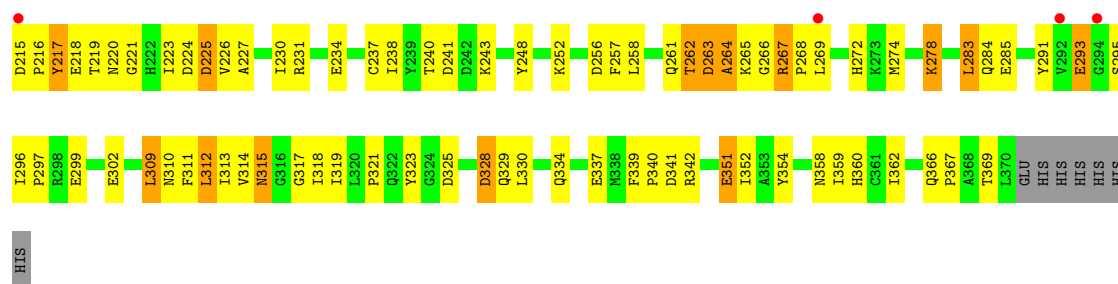


• Molecule 1: Putative agmatine deiminase

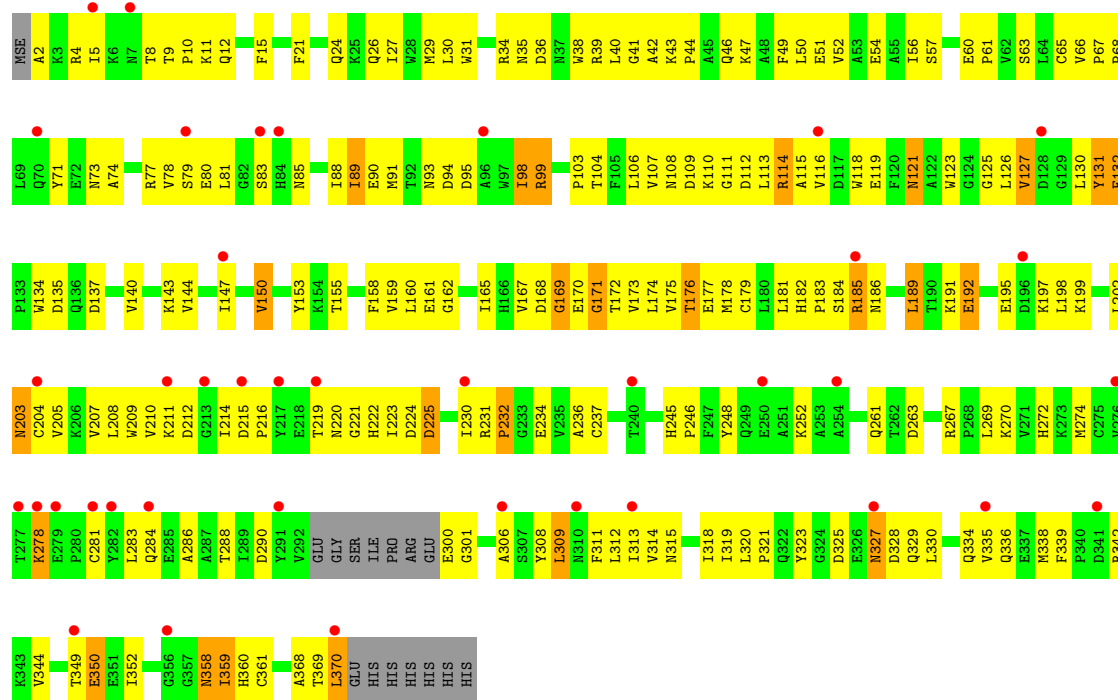
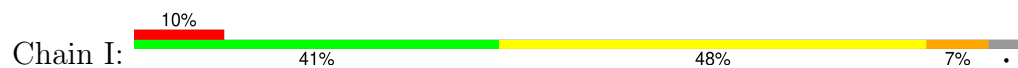


• Molecule 1: Putative agmatine deiminase

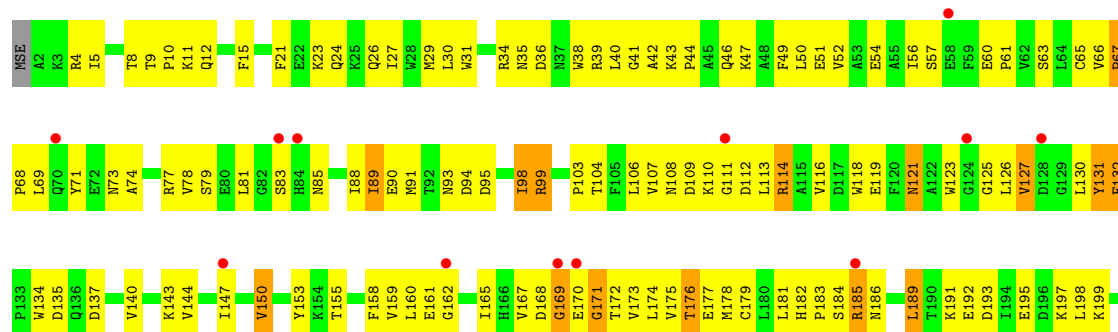


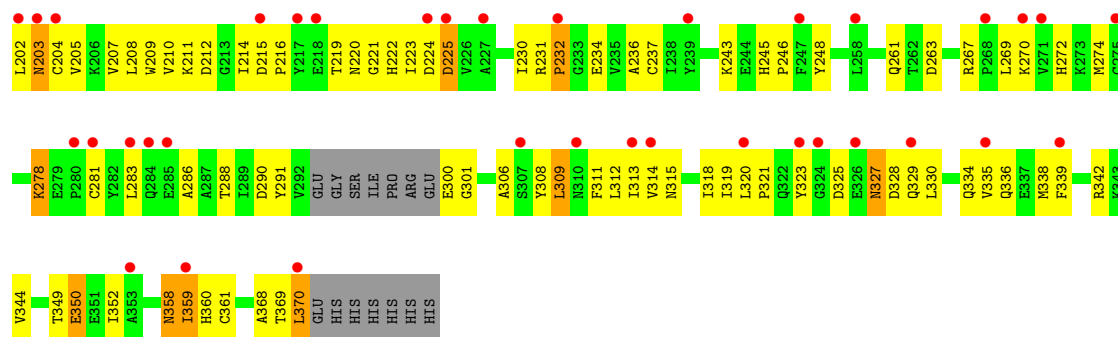


• Molecule 1: Putative agmatine deiminase

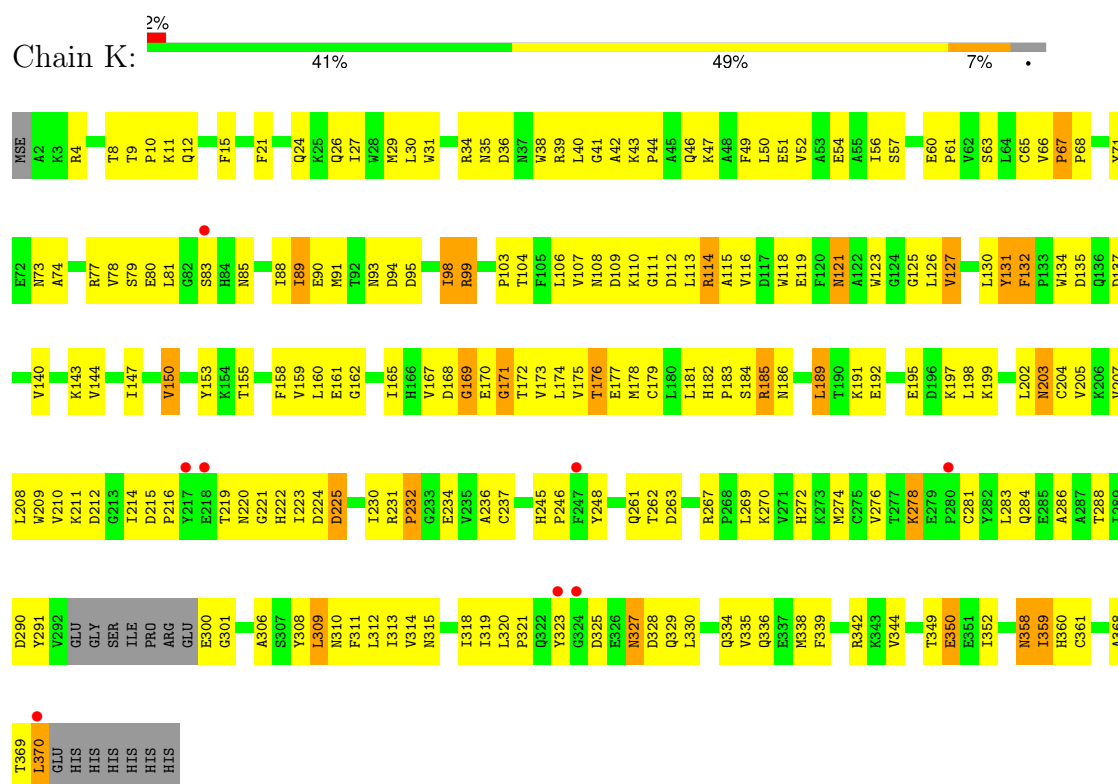


• Molecule 1: Putative agmatine deiminase

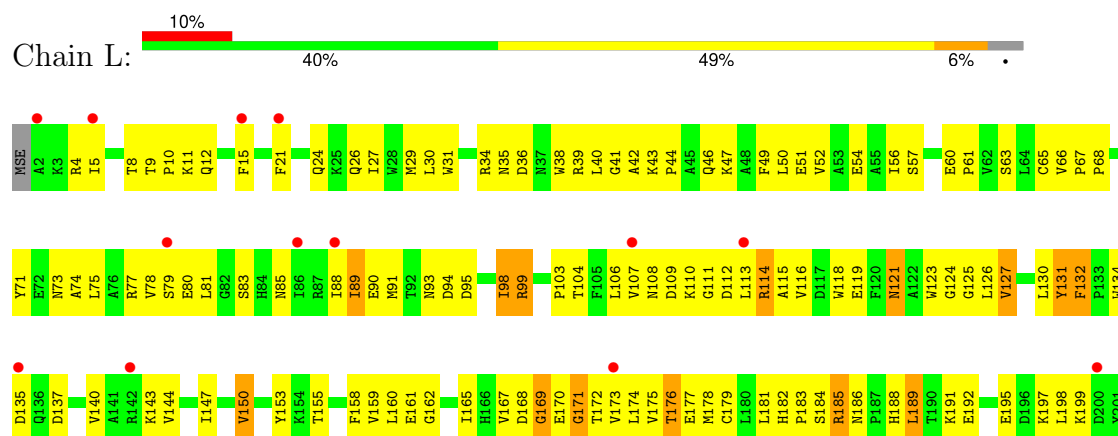


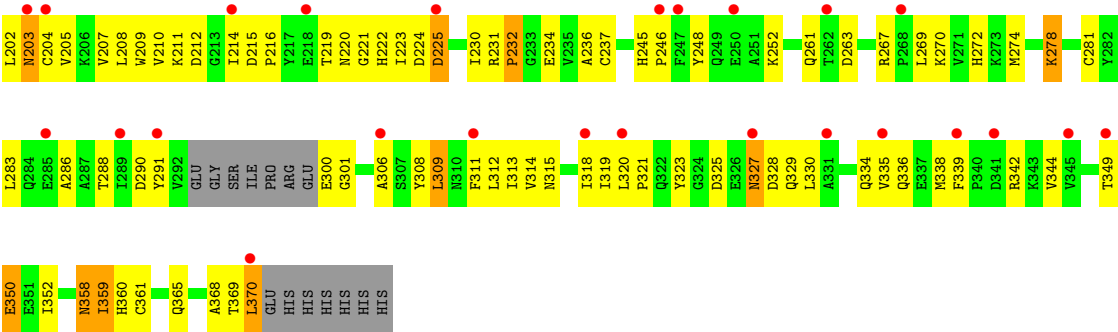


• Molecule 1: Putative agmatine deiminase



• 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	5404 reflections (4.93%)	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 [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.48	0/2950	0.65	0/3992
1	B	0.48	0/2950	0.65	0/3992
1	C	0.48	0/2950	0.65	0/3992
1	D	0.48	0/2950	0.65	0/3992
1	E	0.48	0/2950	0.65	0/3992
1	F	0.48	0/2950	0.65	0/3992
1	G	0.48	0/2950	0.65	0/3992
1	H	0.48	0/3006	0.68	1/4069 (0.0%)
1	I	0.48	0/2950	0.65	0/3992
1	J	0.48	0/2950	0.65	0/3992
1	K	0.48	0/2950	0.65	0/3992
1	L	0.48	0/2950	0.65	0/3992
All	All	0.48	0/35456	0.65	1/47981 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	267	ARG	NE-CZ-NH2	6.56	123.58	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2888	0	2800	236	8
1	B	2888	0	2800	207	11
1	C	2888	0	2800	205	2
1	D	2888	0	2800	258	6
1	E	2888	0	2800	207	19
1	F	2888	0	2800	227	2
1	G	2888	0	2800	213	5
1	H	2942	0	2852	212	2
1	I	2888	0	2800	211	3
1	J	2888	0	2800	211	8
1	K	2888	0	2800	210	3
1	L	2888	0	2800	210	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	2456	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 (2456) 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
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	1.28
1:A:7:ASN:CB	1:D:84:HIS:CE1	2.23	1.21
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:D:341:ASP:C	1:F:84:HIS:NE2	2.00	1.15
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:369:THR:HG23	1:F:370:LEU:N	1.71	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:D:341:ASP:OD2	1:F:58:GLU:CB	2.08	1.01
1:D:342:ARG:N	1:F:84:HIS:NE2	2.08	1.01
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:341:ASP:C	1:F:84:HIS:CD2	2.49	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:185:ARG:HB2	1:H:185:ARG:HH11	1.47	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:J:369:THR:CG2	1:J:370:LEU:N	2.37	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:A:7:ASN:CG	1:D:84:HIS:HE1	1.62	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
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:D:341:ASP:CG	1:F:58:GLU:HA	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:43:LYS:HZ1	1:H:46:GLN:HE22	1.41	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLN:CD	1:D:82:GLY:HA2	2.16	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: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:D:29:MSE:HA	1:D:98:ILE:HG21	1.80	0.64
1:E:80:GLU:CD	1:H:291:TYR:OH	2.36	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: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:F:29:MSE:HA	1:F:98:ILE:HG21	1.80	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: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:F:27:ILE:HD11	1:F:314:VAL:HG12	1.81	0.63
1:G:215:ASP:CG	2:G:401:HOH:O	2.37	0.63
1:I:191:LYS:O	1:I:195:GLU:HG3	1.99	0.63
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:80:GLU:CD	1:H:291:TYR:HH	2.03	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:9:THR:HG22	1:C:12:GLN:CD	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:9:THR:HG22	1:A:12:GLN:CD	2.23	0.59
1:C:104:THR:HB	1:C:116:VAL:HG13	1.84	0.59
1:E:9:THR:HG22	1:E:12:GLN:CD	2.22	0.59
1:J:9:THR:HG22	1:J:12:GLN:CD	2.23	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: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
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:E:369:THR:CG2	1:E:370:LEU:N	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:L:9:THR:HG22	1:L:12:GLN:CD	2.23	0.59
1:D:9:THR:HG22	1:D:12:GLN:CD	2.23	0.59
1:F:278:LYS:HE2	1:F:278:LYS:HA	1.83	0.59
1:I:9:THR:HG22	1:I:12:GLN:CD	2.23	0.59
1:K:9:THR:HG22	1:K:12:GLN:CD	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:179:CYS:HB2	1:L:220:ASN:O	2.01	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:B:9:THR:HG22	1:B:12:GLN:CD	2.23	0.59
1:L:278:LYS:HA	1:L:278:LYS:HE2	1.83	0.59
1:F:9:THR:HG22	1:F:12:GLN:CD	2.23	0.58
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:G:9:THR:HG22	1:G:12:GLN:CD	2.23	0.58
1:I:31:TRP:HB2	1:I:66:VAL:HG12	1.86	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:31:TRP:HB2	1:E:66:VAL:HG12	1.86	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: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
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:G:31:TRP:HB2	1:G:66:VAL:HG12	1.86	0.56
1:J:34:ARG:HD2	1:J:94:ASP:O	2.04	0.56
1:K:106:LEU:O	1:K:113:LEU:HD12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:12:GLN:CD	1:D:82:GLY:CA	2.75	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
2:C:392:HOH:O	1:J:147:ILE:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:27:ILE:HD12	1:H:56:ILE:HD12	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:GLY:HA3	1:H:128:ASP:C	2.28	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:210:VAL:HG12	1:G:211:LYS:N	2.24	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:214:ILE:C	1:E:216:PRO:HD3	2.30	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:D:214:ILE:C	1:D:216:PRO:HD3	2.30	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
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:C:214:ILE:C	1:C:216:PRO:HD3	2.30	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:G:214:ILE:C	1:G:216:PRO:HD3	2.30	0.52
1:I:214:ILE:C	1:I:216:PRO:HD3	2.30	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:J:214:ILE:C	1:J:216:PRO:HD3	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:C	1:A:216:PRO:HD3	2.30	0.51
1:C:9:THR:OG1	1:C:10:PRO:HD2	2.11	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:214:ILE:C	1:L:216:PRO:HD3	2.30	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
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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
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: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: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:B:214:ILE:C	1:B:216:PRO:HD3	2.30	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:K:214:ILE:C	1:K:216:PRO:HD3	2.30	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:D:43:LYS:HB2	1:D:44:PRO:HD3	1.93	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:K:137:ASP:HA	1:K:140:VAL:HG23	1.92	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:312:LEU:HD12	1:E:314:VAL:HG12	1.92	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:43:LYS:HZ1	1:H:46:GLN:NE2	2.08	0.50
1:K:43:LYS:HZ2	1:K:46:GLN:HE22	1.57	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:A:7:ASN:CG	1:D:84:HIS:ND1	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LYS:HB2	1:B:44:PRO:HD3	1.92	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
1:D:177:GLU:HB3	1:D:209:TRP:HE3	1.76	0.50
1:F:214:ILE:C	1:F:216:PRO:HD3	2.30	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: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:J:41:GLY:O	1:J:42:ALA:HB3	2.12	0.50
1:L:49:PHE:O	1:L:52:VAL:HG12	2.10	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:121:ASN:ND2	1:J:121:ASN:N	2.60	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: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: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: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:121:ASN:ND2	1:A:121:ASN:N	2.60	0.49
1:A:174:LEU:O	1:A:223:ILE:HD13	2.11	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:296:ILE:O	1:H:296:ILE:HG12	2.12	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: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: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:I:41:GLY:O	1:I:42:ALA:HB3	2.12	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: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
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:G:26:GLN:NE2	1:G:63:SER:OG	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:80:GLU:HB2	1:L:291:TYR:OH	2.13	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: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: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: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:D:121:ASN:N	1:D:121:ASN:ND2	2.60	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
1:H:195:GLU:HG2	1:H:207:VAL:HG11	1.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:181:LEU:C	2:G:397:HOH:O	2.51	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:D:369:THR:CG2	1:D:370:LEU:N	2.37	0.48
1:E:231:ARG:HG3	1:E:232:PRO:HD2	1.95	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:161:GLU:CD	1:H:161:GLU:H	2.16	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: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:H:293:GLU:C	1:H:295:SER:H	2.16	0.48
1:J:56:ILE:HD13	1:J:319:ILE:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:230:ILE:HG22	1:K:339:PHE:CE1	2.48	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:9:THR:HG22	1:H:12:GLN:CD	2.33	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
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: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: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: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:L:308:TYR:OH	1:L:325:ASP:HB3	2.14	0.48
1:B:231:ARG:HG3	1:B:232:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:121:ASN:ND2	1:C:121:ASN:N	2.60	0.47
1:C:308:TYR:OH	1:C:325:ASP:HB3	2.14	0.47
1:D:47:LYS:O	1:D:51:GLU:HG3	2.14	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:267:ARG:C	1:H:268:PRO:O	2.50	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:266:GLY:O	1:H:267:ARG:C	2.53	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
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:168:ASP:O	1:A:169:GLY:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:168:ASP:O	1:C:169:GLY:C	2.53	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:H:159:VAL:O	1:H:159:VAL:HG13	2.15	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:L:168:ASP:O	1:L:169:GLY:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:54:GLU:O	1:J:57:SER:HB2	2.15	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:C:68:PRO:HG3	1:C:90:GLU:CD	2.36	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
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:168:ASP:O	1:J:169:GLY:C	2.53	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: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:168:ASP:O	1:E:169:GLY:C	2.53	0.46
1:E:309:LEU:HD22	1:E:311:PHE:HE2	1.80	0.46
1:F:68:PRO:HG3	1:F:90:GLU:CD	2.36	0.46
1:G:61:PRO:HA	1:G:85:ASN:ND2	2.29	0.46
1:G:168:ASP:O	1:G:169:GLY:C	2.53	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:I:21:PHE:CZ	1:I:232:PRO:HD3	2.50	0.46
1:I:68:PRO:HG3	1:I:90:GLU:CD	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:68:PRO:HG3	1:J:90:GLU:CD	2.36	0.46
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:G:68:PRO:HG3	1:G:90:GLU:CD	2.36	0.46
1:H:16:ARG:HH12	1:H:109:ASP:CG	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:68:PRO:HG3	1:L:90:GLU:CD	2.36	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:168:ASP:O	1:B:169:GLY:C	2.53	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:68:PRO:HG3	1:K:90:GLU:CD	2.36	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:68:PRO:HG3	1:A:90:GLU:CD	2.36	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:168:ASP:O	1:D:169:GLY:C	2.53	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:I:168:ASP:O	1:I:169:GLY:C	2.53	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:68:PRO:HG3	1:B:90:GLU:CD	2.36	0.46
1:B:323:TYR:HA	1:B:350:GLU:HB3	1.97	0.46
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:D:68:PRO:HG3	1:D:90:GLU:CD	2.36	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:F:168:ASP:O	1:F:169:GLY:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:68:PRO:HG3	1:E:90:GLU:CD	2.36	0.46
1:E:245:HIS:ND1	1:E:246:PRO:HD2	2.30	0.46
1:F:121:ASN:CG	1:F:159:VAL:HG21	2.37	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:121:ASN:CG	1:J:159:VAL:HG21	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:CYS:HB3	1:B:91:MSE:HB3	1.97	0.45
1:B:121:ASN:CG	1:B:159:VAL:HG21	2.37	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:E:121:ASN:CG	1:E:159:VAL:HG21	2.37	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: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:121:ASN:CG	1:L:159:VAL:HG21	2.37	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:C:121:ASN:CG	1:C:159:VAL:HG21	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:121:ASN:CG	1:G:159:VAL:HG21	2.37	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:K:168:ASP:O	1:K:169:GLY:C	2.53	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:A:336:GLN:OE1	1:A:336:GLN:HA	2.16	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:121:ASN:CG	1:A:159:VAL:HG21	2.37	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:D:121:ASN:CG	1:D:159:VAL:HG21	2.37	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:H:223:ILE:C	1:H:225:ASP:H	2.19	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:80:GLU:HB2	1:L:291:TYR:HH	1.82	0.45
1:K:234:GLU:OE1	1:K:270:LYS:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:234:GLU:OE1	1:C:270:LYS:HD3	2.17	0.45
1:D:43:LYS:HZ2	1:D:46:GLN:HE22	1.63	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:C:219:THR:O	1:C:220:ASN:HB2	2.17	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:H:329:GLN:H	1:H:329:GLN:CD	2.21	0.45
1:I:121:ASN:CG	1:I:159:VAL:HG21	2.37	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:223:ILE:C	1:L:225:ASP:H	2.21	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:K:223:ILE:C	1:K:225:ASP:H	2.21	0.45
1:C:94:ASP:HB2	1:C:137:ASP:OD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:121:ASN:CG	1:K:159:VAL:HG21	2.37	0.44
1:K:336:GLN:HA	1:K:336:GLN:OE1	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:223:ILE:C	1:B:225:ASP:H	2.21	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:C:223:ILE:C	1:C:225:ASP:H	2.21	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:G:223:ILE:C	1:G:225:ASP:H	2.21	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:A:223:ILE:C	1:A:225:ASP:H	2.21	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:167:VAL:HG12	1:D:168:ASP:N	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:43:LYS:HZ2	1:J:46:GLN:HE22	1.66	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:D:223:ILE:C	1:D:225:ASP:H	2.21	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:K:219:THR:O	1:K:220:ASN:HB2	2.17	0.44
1:A:12:GLN:HB3	1:D:81:LEU:C	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:ASP:HB2	1:H:221:GLY:H	1.82	0.44
1:I:43:LYS:HZ2	1:I:46:GLN:HE22	1.65	0.44
1:I:185:ARG:HH11	1:I:185:ARG:CB	2.11	0.44
1:I:223:ILE:C	1:I:225:ASP:H	2.21	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
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: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:A:329:GLN:CD	1:A:329:GLN:H	2.22	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:F:223:ILE:C	1:F:225:ASP:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:J:223:ILE:C	1:J:225:ASP:H	2.21	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:B:329:GLN:H	1:B:329:GLN:CD	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:339:PHE:HB3	1:J:342:ARG:HB2	1.99	0.43
1:K:329:GLN:H	1:K:329:GLN:CD	2.22	0.43
1:K:369:THR:O	1:K:370:LEU:CB	2.47	0.43
1:L:121:ASN:N	1:L:121:ASN:ND2	2.60	0.43
1:L:161:GLU:HG3	1:L:222:HIS:NE2	2.33	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:329:GLN:CD	1:D:329:GLN:H	2.22	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: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:H:80:GLU:C	1:H:82:GLY:H	2.22	0.43
1:I:329:GLN:CD	1:I:329:GLN:H	2.22	0.43
1:J:118:TRP:HA	1:J:155:THR:OG1	2.18	0.43
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:E:329:GLN:H	1:E:329:GLN:CD	2.22	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:J:329:GLN:H	1:J:329:GLN:CD	2.22	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:F:329:GLN:H	1:F:329:GLN:CD	2.22	0.43
1:H:132:PHE:HB3	1:H:133:PRO:CD	2.44	0.43
1:H:132:PHE:O	1:H:133:PRO:C	2.56	0.43
1:I:95:ASP:HB2	1:I:131:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:118:TRP:HA	1:I:155:THR:OG1	2.18	0.43
1:K:236:ALA:O	1:K:237:CYS:HB2	2.19	0.43
1:L:30:LEU:HD22	1:L:93:ASN:HD22	1.83	0.43
1:L:329:GLN:CD	1:L:329:GLN:H	2.22	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:C:329:GLN:H	1:C:329:GLN:CD	2.22	0.43
1:E:223:ILE:C	1:E:225:ASP:H	2.21	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: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:43:LYS:HZ2	1:A:46:GLN:HE22	1.66	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:G:329:GLN:CD	1:G:329:GLN:H	2.22	0.42
1:H:263:ASP:C	1:H:265:LYS:H	2.23	0.42
1:A:127:VAL:HG12	2:A:382:HOH:O	2.19	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: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:H:339:PHE:C	1:H:341:ASP:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:C:35:ASN:OD1	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:B:291:TYR:HH	1:F:80:GLU:HB2	1.83	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: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
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: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: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:D:40:LEU:HD22	1:D:288:THR:OG1	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:189:LEU:HD12	1:F:189:LEU:HA	1.84	0.41
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: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: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: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:L:43:LYS:HZ2	1:L:46:GLN:HE22	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:161:GLU:HG3	1:G:222:HIS:HE2	1.86	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
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:J:24:GLN:HA	1:J:368:ALA:N	2.33	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: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: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:133:PRO:HG3	1:K:135:ASP:CG	2.41	0.41
1:H:173:VAL:HG12	1:H:206:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:L:300:GLU:HG2	1:L:301:GLY:N	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
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:K:224:ASP:HB2	1:K:360:HIS:CD2	2.55	0.41
1:C:124:GLY:O	1:C:127:VAL:HG13	2.21	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:J:215:ASP:N	1:J:216:PRO:HD3	2.36	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:100:ASP:N	1:H:100:ASP:OD1	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	6	23
1	C	358/377 (95%)	291 (81%)	60 (17%)	7 (2%)	6	23
1	D	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	6	23
1	E	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	6	23
1	F	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	6	23
1	G	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	6	23
1	H	367/377 (97%)	303 (83%)	54 (15%)	10 (3%)	4	17
1	I	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	6	23
1	J	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	6	23
1	K	358/377 (95%)	293 (82%)	58 (16%)	7 (2%)	6	23
1	L	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	6	23
All	All	4305/4524 (95%)	3515 (82%)	703 (16%)	87 (2%)	6	23

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	284 (92%)	26 (8%)	9	28
1	B	310/316 (98%)	284 (92%)	26 (8%)	9	28
1	C	310/316 (98%)	284 (92%)	26 (8%)	9	28
1	D	310/316 (98%)	284 (92%)	26 (8%)	9	28
1	E	310/316 (98%)	284 (92%)	26 (8%)	9	28
1	F	310/316 (98%)	284 (92%)	26 (8%)	9	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	310/316 (98%)	284 (92%)	26 (8%)	9	28
1	H	316/316 (100%)	286 (90%)	30 (10%)	7	22
1	I	310/316 (98%)	284 (92%)	26 (8%)	9	28
1	J	310/316 (98%)	284 (92%)	26 (8%)	9	28
1	K	310/316 (98%)	285 (92%)	25 (8%)	9	29
1	L	310/316 (98%)	284 (92%)	26 (8%)	9	28
All	All	3726/3792 (98%)	3411 (92%)	315 (8%)	8	27

All (315) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	5	ILE
1	A	36	ASP
1	A	67	PRO
1	A	89	ILE
1	A	99	ARG
1	A	114	ARG
1	A	121	ASN
1	A	127	VAL
1	A	131	TYR
1	A	150	VAL
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	278	LYS
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	36	ASP

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Mol	Chain	Res	Type
1	B	67	PRO
1	B	89	ILE
1	B	99	ARG
1	B	114	ARG
1	B	121	ASN
1	B	127	VAL
1	B	131	TYR
1	B	150	VAL
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	278	LYS
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	36	ASP
1	C	67	PRO
1	C	89	ILE
1	C	99	ARG
1	C	114	ARG
1	C	121	ASN
1	C	127	VAL
1	C	131	TYR
1	C	150	VAL
1	C	176	THR
1	C	178	MSE
1	C	185	ARG
1	C	189	LEU
1	C	192	GLU
1	C	197	LYS
1	C	203	ASN
1	C	212	ASP

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Mol	Chain	Res	Type
1	C	225	ASP
1	C	278	LYS
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	36	ASP
1	D	67	PRO
1	D	89	ILE
1	D	99	ARG
1	D	114	ARG
1	D	121	ASN
1	D	127	VAL
1	D	131	TYR
1	D	150	VAL
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	278	LYS
1	D	309	LEU
1	D	327	ASN
1	D	350	GLU
1	D	358	ASN
1	D	370	LEU
1	E	4	ARG
1	E	5	ILE
1	E	36	ASP
1	E	67	PRO
1	E	89	ILE
1	E	99	ARG
1	E	114	ARG
1	E	121	ASN
1	E	127	VAL

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Mol	Chain	Res	Type
1	E	131	TYR
1	E	150	VAL
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	278	LYS
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	36	ASP
1	F	67	PRO
1	F	89	ILE
1	F	99	ARG
1	F	114	ARG
1	F	121	ASN
1	F	127	VAL
1	F	131	TYR
1	F	150	VAL
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	278	LYS
1	F	309	LEU
1	F	327	ASN
1	F	350	GLU
1	F	358	ASN

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Mol	Chain	Res	Type
1	F	370	LEU
1	G	4	ARG
1	G	5	ILE
1	G	36	ASP
1	G	67	PRO
1	G	89	ILE
1	G	99	ARG
1	G	114	ARG
1	G	121	ASN
1	G	127	VAL
1	G	131	TYR
1	G	150	VAL
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	278	LYS
1	G	309	LEU
1	G	327	ASN
1	G	350	GLU
1	G	358	ASN
1	G	370	LEU
1	H	4	ARG
1	H	13	ASP
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	203	ASN

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Mol	Chain	Res	Type
1	H	217	TYR
1	H	225	ASP
1	H	240	THR
1	H	241	ASP
1	H	262	THR
1	H	263	ASP
1	H	269	LEU
1	H	278	LYS
1	H	283	LEU
1	H	299	GLU
1	H	309	LEU
1	H	312	LEU
1	H	315	ASN
1	H	328	ASP
1	H	351	GLU
1	I	4	ARG
1	I	5	ILE
1	I	36	ASP
1	I	67	PRO
1	I	89	ILE
1	I	99	ARG
1	I	114	ARG
1	I	121	ASN
1	I	127	VAL
1	I	131	TYR
1	I	150	VAL
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	278	LYS
1	I	309	LEU
1	I	327	ASN
1	I	350	GLU
1	I	358	ASN
1	I	370	LEU
1	J	4	ARG

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Mol	Chain	Res	Type
1	J	5	ILE
1	J	36	ASP
1	J	67	PRO
1	J	89	ILE
1	J	99	ARG
1	J	114	ARG
1	J	121	ASN
1	J	127	VAL
1	J	131	TYR
1	J	150	VAL
1	J	176	THR
1	J	178	MSE
1	J	185	ARG
1	J	189	LEU
1	J	192	GLU
1	J	197	LYS
1	J	203	ASN
1	J	212	ASP
1	J	225	ASP
1	J	278	LYS
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	36	ASP
1	K	67	PRO
1	K	89	ILE
1	K	99	ARG
1	K	114	ARG
1	K	121	ASN
1	K	127	VAL
1	K	131	TYR
1	K	150	VAL
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

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Mol	Chain	Res	Type
1	K	212	ASP
1	K	225	ASP
1	K	278	LYS
1	K	309	LEU
1	K	327	ASN
1	K	350	GLU
1	K	358	ASN
1	K	370	LEU
1	L	4	ARG
1	L	5	ILE
1	L	36	ASP
1	L	67	PRO
1	L	89	ILE
1	L	99	ARG
1	L	114	ARG
1	L	121	ASN
1	L	127	VAL
1	L	131	TYR
1	L	150	VAL
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	278	LYS
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 (255) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	12	GLN
1	A	26	GLN
1	A	35	ASN

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Mol	Chain	Res	Type
1	A	37	ASN
1	A	46	GLN
1	A	73	ASN
1	A	121	ASN
1	A	186	ASN
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	322	GLN
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	35	ASN
1	B	37	ASN
1	B	46	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	322	GLN
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

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Mol	Chain	Res	Type
1	C	37	ASN
1	C	46	GLN
1	C	73	ASN
1	C	121	ASN
1	C	186	ASN
1	C	203	ASN
1	C	220	ASN
1	C	249	GLN
1	C	261	GLN
1	C	284	GLN
1	C	310	ASN
1	C	315	ASN
1	C	322	GLN
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	35	ASN
1	D	37	ASN
1	D	46	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	322	GLN
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

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Mol	Chain	Res	Type
1	E	35	ASN
1	E	37	ASN
1	E	46	GLN
1	E	73	ASN
1	E	121	ASN
1	E	186	ASN
1	E	203	ASN
1	E	220	ASN
1	E	249	GLN
1	E	261	GLN
1	E	284	GLN
1	E	310	ASN
1	E	315	ASN
1	E	322	GLN
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	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	322	GLN
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

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Mol	Chain	Res	Type
1	G	35	ASN
1	G	37	ASN
1	G	46	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
1	G	261	GLN
1	G	284	GLN
1	G	310	ASN
1	G	315	ASN
1	G	322	GLN
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	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	329	GLN
1	H	333	GLN
1	H	358	ASN
1	H	360	HIS
1	H	366	GLN
1	I	12	GLN

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Mol	Chain	Res	Type
1	I	26	GLN
1	I	35	ASN
1	I	37	ASN
1	I	46	GLN
1	I	73	ASN
1	I	121	ASN
1	I	186	ASN
1	I	203	ASN
1	I	220	ASN
1	I	249	GLN
1	I	261	GLN
1	I	284	GLN
1	I	310	ASN
1	I	315	ASN
1	I	322	GLN
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	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	322	GLN
1	J	327	ASN
1	J	333	GLN
1	J	358	ASN
1	J	360	HIS
1	J	366	GLN
1	K	12	GLN

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Mol	Chain	Res	Type
1	K	26	GLN
1	K	35	ASN
1	K	37	ASN
1	K	46	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
1	K	261	GLN
1	K	284	GLN
1	K	310	ASN
1	K	315	ASN
1	K	322	GLN
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	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	322	GLN
1	L	327	ASN
1	L	333	GLN
1	L	358	ASN
1	L	360	HIS
1	L	366	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 ⓘ

Warning: The R factor obtained from EDS is 0.2878, which does not match the depositor's R factor of 0.235. Please interpret the results in this section carefully.

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%)	0.76	40 (11%)	11 10	7, 17, 47, 60	1 (0%)
1	B	355/377 (94%)	0.74	40 (11%)	11 10	7, 20, 54, 60	1 (0%)
1	C	355/377 (94%)	0.91	39 (10%)	12 10	10, 40, 60, 60	1 (0%)
1	D	355/377 (94%)	0.96	53 (14%)	7 6	10, 34, 60, 60	1 (0%)
1	E	355/377 (94%)	1.04	59 (16%)	5 5	9, 35, 60, 60	1 (0%)
1	F	355/377 (94%)	0.91	49 (13%)	8 7	9, 36, 60, 60	1 (0%)
1	G	355/377 (94%)	0.98	48 (13%)	8 7	10, 37, 60, 60	1 (0%)
1	H	362/377 (96%)	0.27	5 (1%)	73 68	10, 33, 59, 60	1 (0%)
1	I	355/377 (94%)	0.79	39 (10%)	12 10	10, 38, 60, 60	1 (0%)
1	J	355/377 (94%)	1.00	48 (13%)	8 7	11, 49, 60, 60	1 (0%)
1	K	355/377 (94%)	0.47	8 (2%)	61 54	8, 45, 60, 60	1 (0%)
1	L	355/377 (94%)	1.02	38 (10%)	12 11	15, 56, 60, 60	1 (0%)
All	All	4267/4524 (94%)	0.82	466 (10%)	12 10	7, 37, 60, 60	12 (0%)

All (466) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	282	TYR	7.4
1	D	282	TYR	7.3
1	E	279	GLU	5.9
1	F	83	SER	5.7
1	D	82	GLY	5.3
1	B	260	GLN	5.2
1	G	124	GLY	5.2
1	E	124	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	J	218	GLU	5.1
1	E	82	GLY	4.8
1	D	171	GLY	4.7
1	D	279	GLU	4.7
1	E	327	ASN	4.6
1	B	217	TYR	4.6
1	A	83	SER	4.6
1	E	280	PRO	4.5
1	B	268	PRO	4.5
1	C	124	GLY	4.4
1	B	291	TYR	4.3
1	F	218	GLU	4.2
1	E	233	GLY	4.2
1	A	218	GLU	4.2
1	A	215	ASP	4.1
1	B	215	ASP	4.1
1	L	204	CYS	4.1
1	J	83	SER	4.0
1	C	341	ASP	4.0
1	E	204	CYS	4.0
1	F	346	GLY	4.0
1	D	2	ALA	4.0
1	E	217	TYR	3.9
1	G	82	GLY	3.9
1	L	335	VAL	3.9
1	G	207	VAL	3.8
1	D	370	LEU	3.8
1	F	264	ALA	3.8
1	F	82	GLY	3.8
1	C	2	ALA	3.8
1	A	370	LEU	3.8
1	D	218	GLU	3.8
1	A	9	THR	3.8
1	B	124	GLY	3.8
1	C	217	TYR	3.8
1	G	310	ASN	3.7
1	D	215	ASP	3.7
1	J	169	GLY	3.7
1	K	370	LEU	3.7
1	C	305	ILE	3.7
1	A	260	GLN	3.7
1	E	314	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	306	ALA	3.7
1	E	80	GLU	3.7
1	L	250	GLU	3.7
1	G	174	LEU	3.6
1	G	215	ASP	3.6
1	E	171	GLY	3.6
1	D	5	ILE	3.6
1	F	313	ILE	3.6
1	A	337	GLU	3.6
1	F	204	CYS	3.6
1	C	83	SER	3.6
1	D	368	ALA	3.6
1	G	84	HIS	3.6
1	E	2	ALA	3.5
1	F	291	TYR	3.5
1	I	370	LEU	3.5
1	F	310	ASN	3.5
1	B	282	TYR	3.5
1	C	281	CYS	3.5
1	F	370	LEU	3.5
1	C	279	GLU	3.5
1	E	292	VAL	3.4
1	C	79	SER	3.4
1	B	185	ARG	3.4
1	L	79	SER	3.4
1	E	291	TYR	3.3
1	E	269	LEU	3.3
1	A	301	GLY	3.3
1	A	326	GLU	3.3
1	D	177	GLU	3.3
1	G	327	ASN	3.3
1	K	218	GLU	3.3
1	D	263	ASP	3.3
1	E	100	ASP	3.3
1	E	329	GLN	3.3
1	J	124	GLY	3.3
1	A	268	PRO	3.2
1	C	291	TYR	3.2
1	A	291	TYR	3.2
1	A	327	ASN	3.2
1	D	315	ASN	3.2
1	D	327	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	315	ASN	3.2
1	B	80	GLU	3.2
1	B	218	GLU	3.2
1	D	313	ILE	3.2
1	A	292	VAL	3.2
1	E	119	GLU	3.2
1	E	177	GLU	3.2
1	F	58	GLU	3.2
1	I	291	TYR	3.2
1	D	83	SER	3.2
1	G	370	LEU	3.2
1	F	84	HIS	3.1
1	A	70	GLN	3.1
1	F	215	ASP	3.1
1	G	36	ASP	3.1
1	J	353	ALA	3.1
1	A	239	TYR	3.1
1	A	282	TYR	3.1
1	C	369	THR	3.1
1	C	215	ASP	3.1
1	E	159	VAL	3.1
1	G	217	TYR	3.1
1	B	326	GLU	3.1
1	C	269	LEU	3.0
1	B	239	TYR	3.0
1	K	280	PRO	3.0
1	E	83	SER	3.0
1	D	204	CYS	3.0
1	D	280	PRO	3.0
1	C	80	GLU	3.0
1	F	285	GLU	3.0
1	K	83	SER	3.0
1	J	217	TYR	3.0
1	F	2	ALA	3.0
1	I	341	ASP	3.0
1	J	275	CYS	3.0
1	D	216	PRO	3.0
1	A	313	ILE	3.0
1	E	238	ILE	3.0
1	F	5	ILE	3.0
1	D	278	LYS	3.0
1	F	244	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	335	VAL	3.0
1	L	345	VAL	3.0
1	L	370	LEU	2.9
1	L	262	THR	2.9
1	D	85	ASN	2.9
1	I	279	GLU	2.9
1	C	247	PHE	2.9
1	B	370	LEU	2.9
1	C	370	LEU	2.9
1	J	313	ILE	2.9
1	L	142	ARG	2.9
1	C	241	ASP	2.9
1	G	313	ILE	2.9
1	E	370	LEU	2.8
1	I	356	GLY	2.8
1	A	204	CYS	2.8
1	C	292	VAL	2.8
1	L	331	ALA	2.8
1	J	281	CYS	2.8
1	I	250	GLU	2.8
1	E	358	ASN	2.8
1	J	202	LEU	2.8
1	A	7	ASN	2.8
1	F	358	ASN	2.8
1	L	203	ASN	2.8
1	E	133	PRO	2.8
1	I	276	VAL	2.8
1	D	285	GLU	2.8
1	J	170	GLU	2.8
1	G	233	GLY	2.8
1	K	324	GLY	2.8
1	I	215	ASP	2.7
1	A	275	CYS	2.7
1	D	214	ILE	2.7
1	G	169	GLY	2.7
1	B	327	ASN	2.7
1	A	348	ARG	2.7
1	C	212	ASP	2.7
1	B	337	GLU	2.7
1	L	247	PHE	2.7
1	A	233	GLY	2.7
1	J	232	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	142	ARG	2.7
1	I	310	ASN	2.7
1	G	96	ALA	2.7
1	L	285	GLU	2.7
1	F	171	GLY	2.7
1	F	185	ARG	2.7
1	D	292	VAL	2.7
1	E	278	LYS	2.7
1	E	336	GLN	2.7
1	I	5	ILE	2.7
1	C	233	GLY	2.7
1	G	268	PRO	2.7
1	D	205	VAL	2.6
1	B	83	SER	2.6
1	A	149	GLY	2.6
1	I	282	TYR	2.6
1	L	135	ASP	2.6
1	L	173	VAL	2.6
1	E	174	LEU	2.6
1	G	81	LEU	2.6
1	A	132	PHE	2.6
1	E	37	ASN	2.6
1	L	327	ASN	2.6
1	B	305	ILE	2.6
1	A	217	TYR	2.6
1	H	294	GLY	2.6
1	I	83	SER	2.6
1	J	324	GLY	2.6
1	B	341	ASP	2.6
1	L	341	ASP	2.6
1	J	314	VAL	2.6
1	G	204	CYS	2.6
1	D	70	GLN	2.6
1	G	192	GLU	2.6
1	L	246	PRO	2.6
1	D	36	ASP	2.6
1	E	128	ASP	2.6
1	D	258	LEU	2.6
1	I	70	GLN	2.6
1	B	177	GLU	2.6
1	C	280	PRO	2.6
1	D	84	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	337	GLU	2.6
1	D	79	SER	2.6
1	A	328	ASP	2.6
1	B	313	ILE	2.5
1	E	313	ILE	2.5
1	E	218	GLU	2.5
1	I	84	HIS	2.5
1	D	217	TYR	2.5
1	I	204	CYS	2.5
1	J	111	GLY	2.5
1	L	107	VAL	2.5
1	L	2	ALA	2.5
1	B	352	ILE	2.5
1	E	132	PHE	2.5
1	G	278	LYS	2.5
1	D	185	ARG	2.5
1	B	347	VAL	2.5
1	I	349	THR	2.5
1	F	158	PHE	2.5
1	D	184	SER	2.5
1	J	225	ASP	2.5
1	E	232	PRO	2.5
1	L	320	LEU	2.5
1	A	347	VAL	2.5
1	D	262	THR	2.5
1	F	133	PRO	2.4
1	J	84	HIS	2.4
1	A	177	GLU	2.4
1	F	327	ASN	2.4
1	J	147	ILE	2.4
1	F	339	PHE	2.4
1	L	349	THR	2.4
1	J	329	GLN	2.4
1	B	133	PRO	2.4
1	E	112	ASP	2.4
1	G	133	PRO	2.4
1	J	128	ASP	2.4
1	J	215	ASP	2.4
1	B	272	HIS	2.4
1	D	266	GLY	2.4
1	F	347	VAL	2.4
1	G	337	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	292	VAL	2.4
1	L	218	GLU	2.4
1	E	101	CYS	2.4
1	I	230	ILE	2.4
1	E	310	ASN	2.4
1	G	108	ASN	2.4
1	E	349	THR	2.4
1	G	176	THR	2.4
1	C	282	TYR	2.4
1	G	282	TYR	2.4
1	G	267	ARG	2.4
1	C	329	GLN	2.4
1	C	36	ASP	2.4
1	C	196	ASP	2.4
1	C	169	GLY	2.4
1	D	250	GLU	2.4
1	G	80	GLU	2.4
1	E	211	LYS	2.4
1	I	277	THR	2.4
1	E	84	HIS	2.4
1	H	83	SER	2.4
1	E	350	GLU	2.4
1	J	359	ILE	2.4
1	E	239	TYR	2.3
1	A	133	PRO	2.3
1	C	284	GLN	2.3
1	G	329	GLN	2.3
1	J	320	LEU	2.3
1	A	171	GLY	2.3
1	D	124	GLY	2.3
1	E	213	GLY	2.3
1	F	292	VAL	2.3
1	E	244	GLU	2.3
1	I	313	ILE	2.3
1	D	358	ASN	2.3
1	I	240	THR	2.3
1	F	174	LEU	2.3
1	F	340	PRO	2.3
1	J	280	PRO	2.3
1	L	113	LEU	2.3
1	G	260	GLN	2.3
1	E	78	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	314	VAL	2.3
1	D	132	PHE	2.3
1	C	265	LYS	2.3
1	J	162	GLY	2.3
1	D	302	GLU	2.3
1	E	215	ASP	2.3
1	F	240	THR	2.3
1	E	131	TYR	2.3
1	F	275	CYS	2.3
1	B	249	GLN	2.3
1	A	305	ILE	2.3
1	G	5	ILE	2.3
1	L	86	ILE	2.3
1	L	88	ILE	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	E	79	SER	2.3
1	E	328	ASP	2.3
1	B	81	LEU	2.3
1	B	270	LYS	2.3
1	C	327	ASN	2.2
1	J	310	ASN	2.2
1	D	356	GLY	2.2
1	E	275	CYS	2.2
1	G	335	VAL	2.2
1	C	132	PHE	2.2
1	B	267	ARG	2.2
1	F	326	GLU	2.2
1	I	254	ALA	2.2
1	E	130	LEU	2.2
1	H	215	ASP	2.2
1	A	176	THR	2.2
1	B	82	GLY	2.2
1	C	316	GLY	2.2
1	D	336	GLN	2.2
1	F	272	HIS	2.2
1	I	213	GLY	2.2
1	I	327	ASN	2.2
1	J	70	GLN	2.2
1	J	271	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	275	CYS	2.2
1	G	16	ARG	2.2
1	J	247	PHE	2.2
1	F	279	GLU	2.2
1	G	306	ALA	2.2
1	L	306	ALA	2.2
1	H	269	LEU	2.2
1	D	328	ASP	2.2
1	I	211	LYS	2.2
1	F	238	ILE	2.2
1	I	335	VAL	2.2
1	L	214	ILE	2.2
1	J	203	ASN	2.2
1	E	225	ASP	2.2
1	G	196	ASP	2.2
1	G	212	ASP	2.2
1	I	196	ASP	2.2
1	J	268	PRO	2.2
1	G	83	SER	2.2
1	C	205	VAL	2.2
1	C	313	ILE	2.2
1	L	318	ILE	2.2
1	B	329	GLN	2.2
1	E	272	HIS	2.2
1	F	217	TYR	2.2
1	J	339	PHE	2.2
1	G	264	ALA	2.2
1	A	170	GLU	2.2
1	E	285	GLU	2.2
1	F	256	ASP	2.2
1	I	79	SER	2.2
1	L	289	ILE	2.2
1	D	213	GLY	2.1
1	D	316	GLY	2.1
1	G	322	GLN	2.1
1	J	185	ARG	2.1
1	J	284	GLN	2.1
1	I	217	TYR	2.1
1	K	323	TYR	2.1
1	C	50	LEU	2.1
1	F	126	LEU	2.1
1	F	320	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	368	ALA	2.1
1	I	278	LYS	2.1
1	B	170	GLU	2.1
1	J	58	GLU	2.1
1	J	326	GLU	2.1
1	D	268	PRO	2.1
1	D	163	GLY	2.1
1	D	221	GLY	2.1
1	F	368	ALA	2.1
1	A	285	GLU	2.1
1	A	300	GLU	2.1
1	D	183	PRO	2.1
1	A	352	ILE	2.1
1	A	142	ARG	2.1
1	A	256	ASP	2.1
1	B	233	GLY	2.1
1	F	142	ARG	2.1
1	F	79	SER	2.1
1	J	307	SER	2.1
1	G	284	GLN	2.1
1	B	285	GLU	2.1
1	I	7	ASN	2.1
1	J	285	GLU	2.1
1	L	268	PRO	2.1
1	C	314	VAL	2.1
1	G	292	VAL	2.1
1	I	116	VAL	2.1
1	I	185	ARG	2.1
1	F	132	PHE	2.1
1	L	311	PHE	2.1
1	C	130	LEU	2.1
1	D	9	THR	2.1
1	D	277	THR	2.1
1	F	36	ASP	2.1
1	L	225	ASP	2.1
1	G	261	GLN	2.1
1	C	368	ALA	2.1
1	J	227	ALA	2.1
1	A	255	TYR	2.1
1	J	323	TYR	2.1
1	G	280	PRO	2.1
1	L	5	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	361	CYS	2.1
1	J	204	CYS	2.1
1	B	142	ARG	2.1
1	G	324	GLY	2.1
1	B	247	PHE	2.1
1	L	15	PHE	2.1
1	L	21	PHE	2.1
1	E	198	LEU	2.0
1	F	330	LEU	2.0
1	F	128	ASP	2.0
1	F	260	GLN	2.0
1	L	200	ASP	2.0
1	J	239	TYR	2.0
1	B	7	ASN	2.0
1	I	147	ILE	2.0
1	C	185	ARG	2.0
1	J	270	LYS	2.0
1	I	281	CYS	2.0
1	J	258	LEU	2.0
1	J	370	LEU	2.0
1	L	339	PHE	2.0
1	F	70	GLN	2.0
1	F	262	THR	2.0
1	I	219	THR	2.0
1	I	96	ALA	2.0
1	I	284	GLN	2.0
1	I	128	ASP	2.0
1	J	224	ASP	2.0
1	B	161	GLU	2.0
1	D	300	GLU	2.0
1	G	177	GLU	2.0
1	K	217	TYR	2.0
1	L	291	TYR	2.0
1	D	3	LYS	2.0
1	E	205	VAL	2.0
1	A	81	LEU	2.0
1	J	283	LEU	2.0
1	K	247	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.