



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:58 AM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

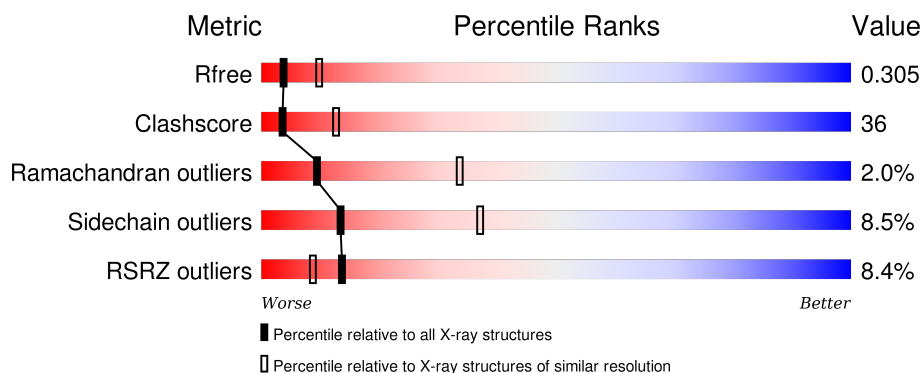
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



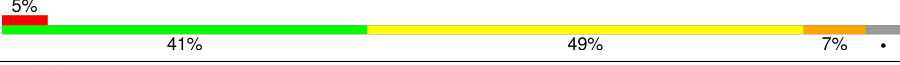
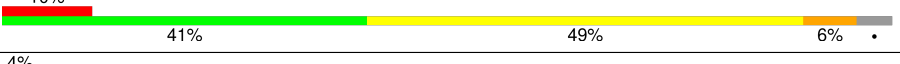

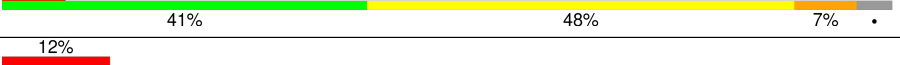
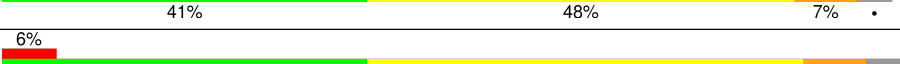
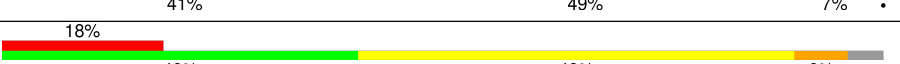
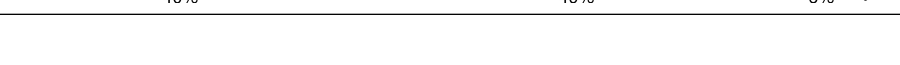
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	377	<div> <div>3%</div> <div>40% 50% 6% .</div> </div>
1	B	377	<div> <div>3%</div> <div>41% 49% 6% .</div> </div>
1	C	377	<div> <div>9%</div> <div>41% 49% 6% .</div> </div>
1	D	377	<div> <div>8%</div> <div>40% 49% 7% .</div> </div>
1	E	377	<div> <div>9%</div> <div>40% 50% 6% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	377	
1	G	377	
1	H	377	
1	I	377	
1	J	377	
1	K	377	
1	L	377	

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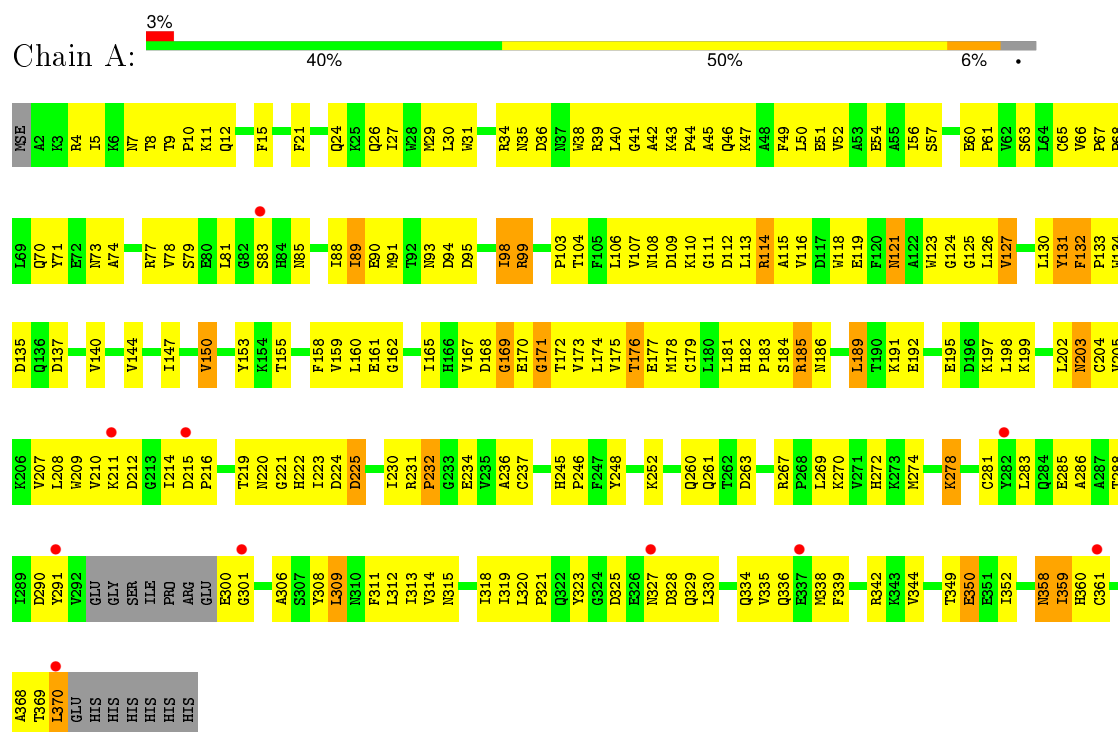
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	17	Total	O	0	0
			17	17		
2	L	13	Total	O	0	0
			13	13		

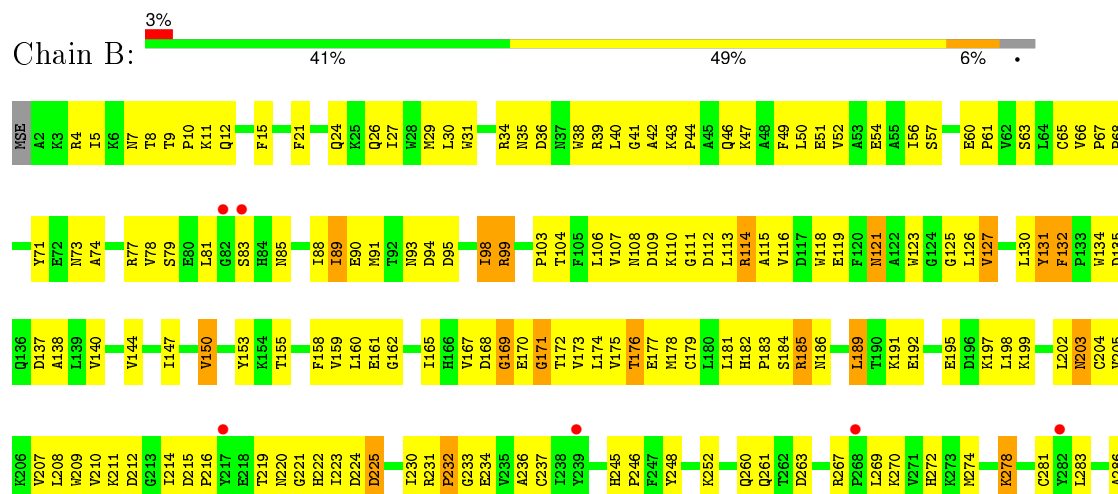
3 Residue-property plots

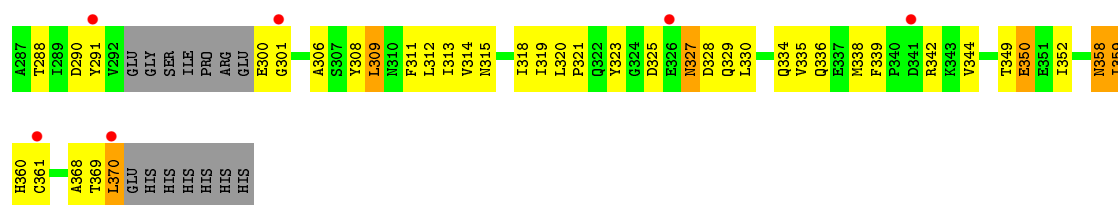
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: Putative agmatine deiminase

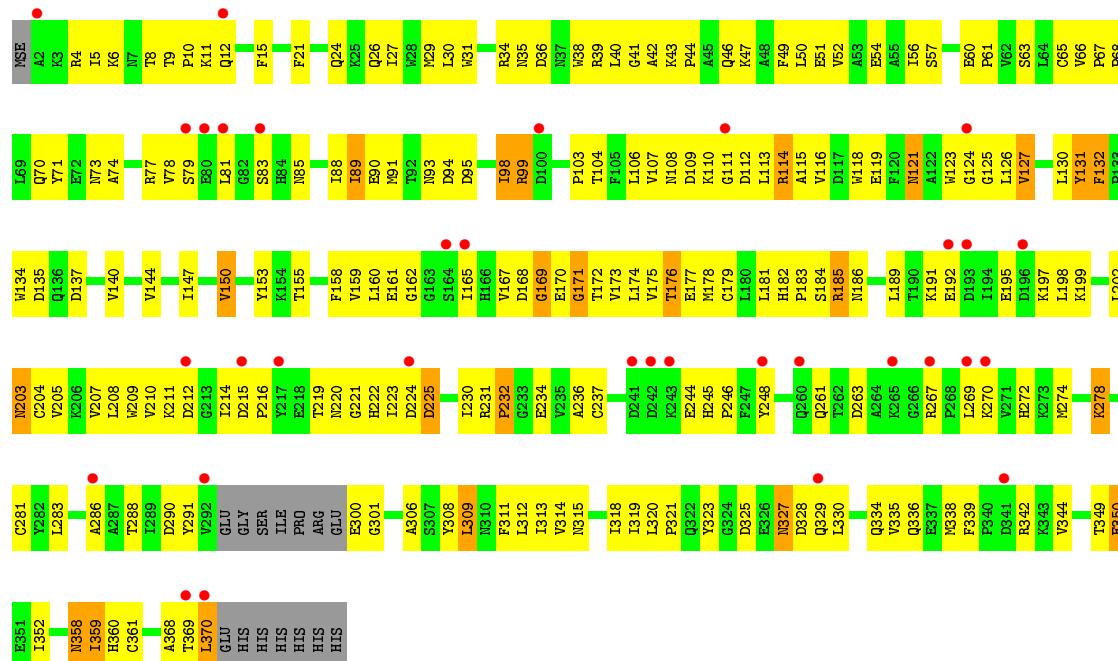


- Molecule 1: Putative agmatine deiminase

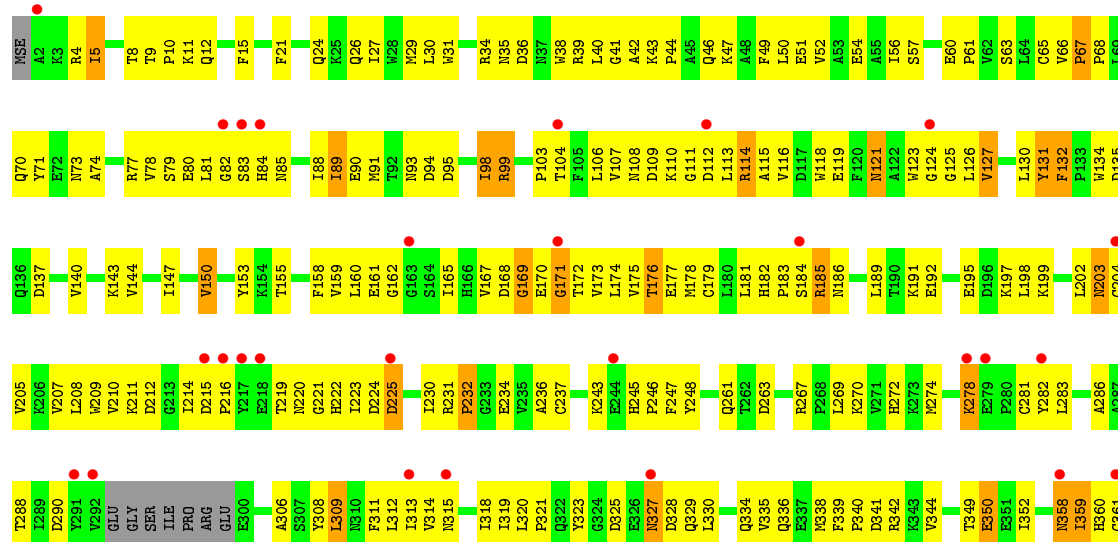
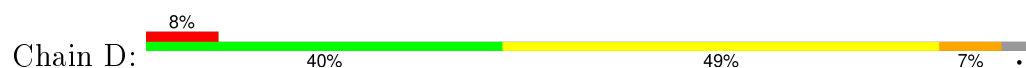


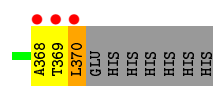


• Molecule 1: Putative agmatine deiminase

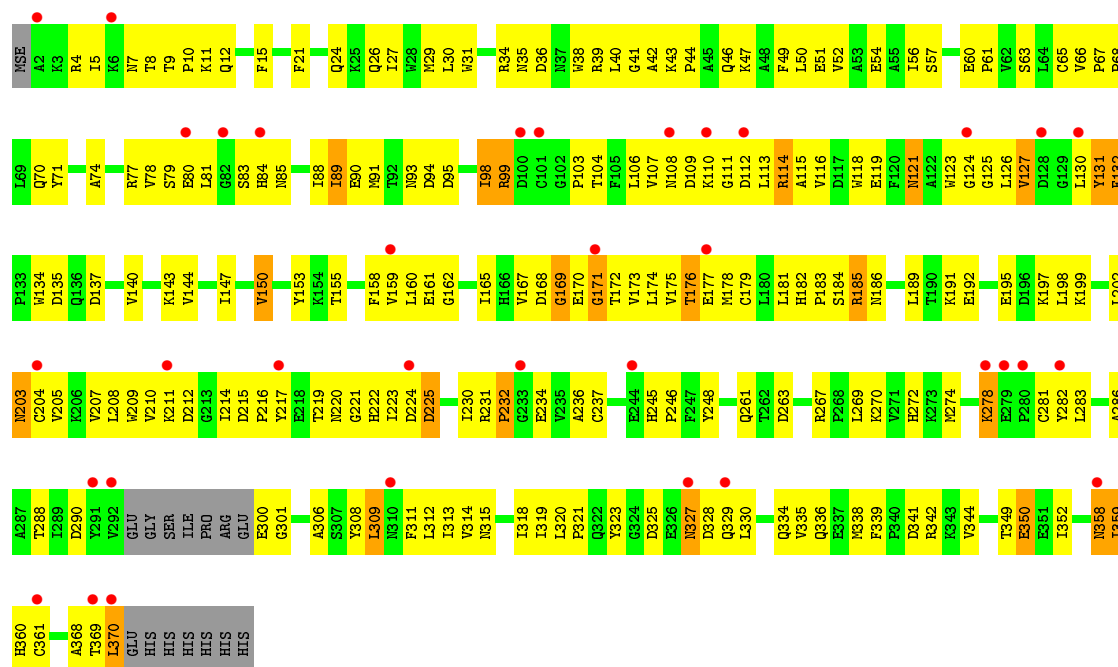
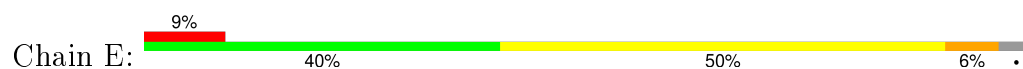


• Molecule 1: Putative agmatine deiminase

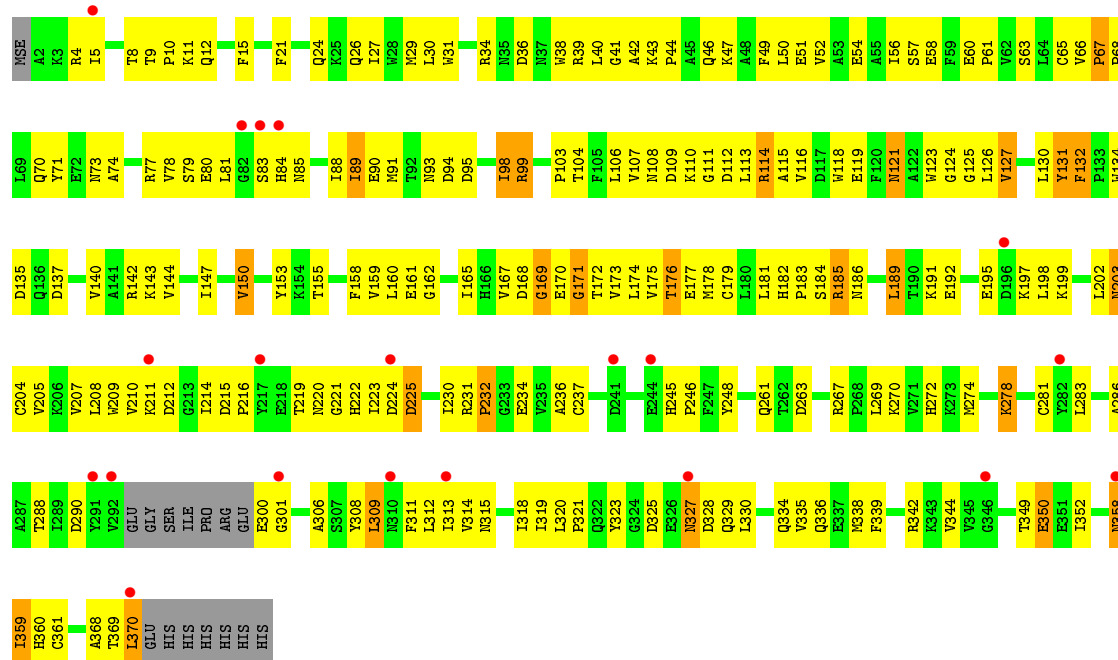
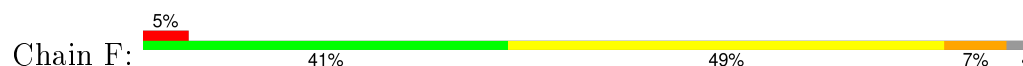




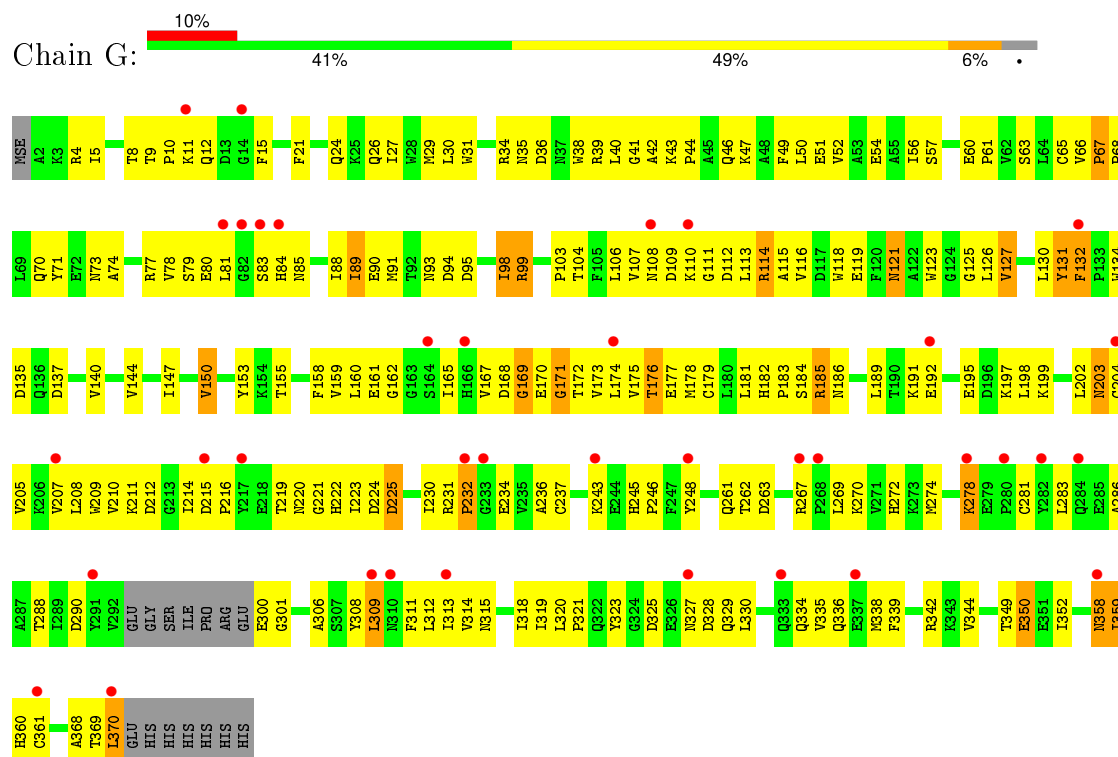
● Molecule 1: Putative agmatine deiminase



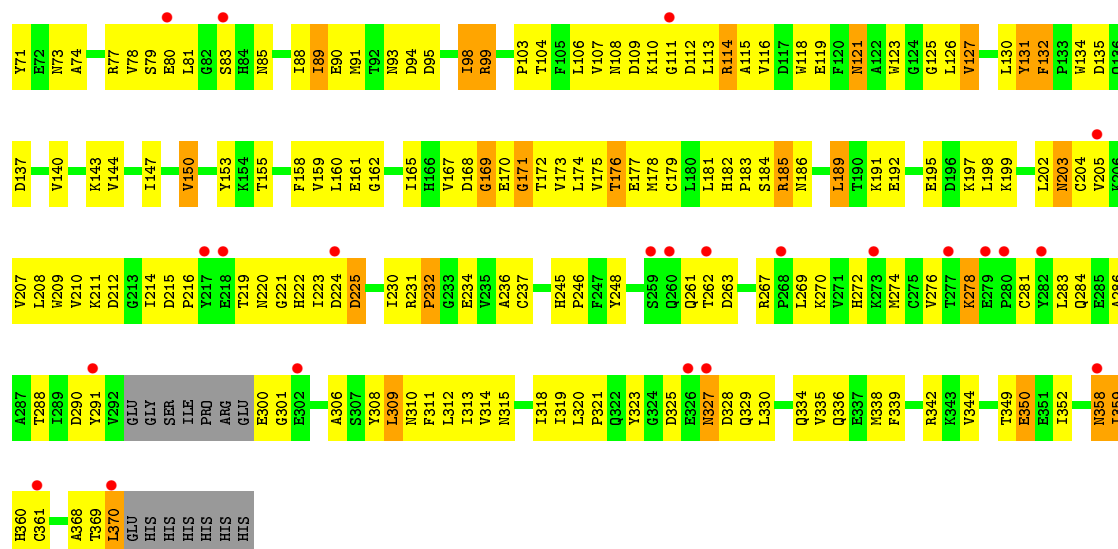
● Molecule 1: Putative agmatine deiminase



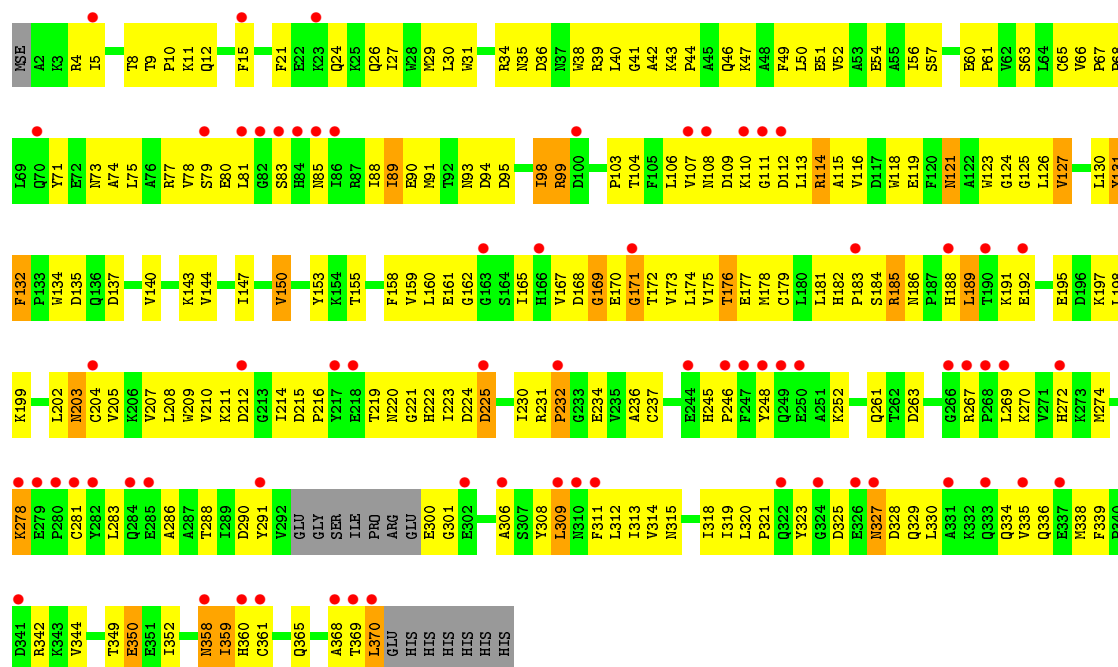
• Molecule 1: Putative agmatine deiminase







● Molecule 1: Putative agmatine deiminase



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 29.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	83.8 (19.99-2.90) 98.5 (29.95-2.90)	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 0.282 , 0.305	Depositor DCC
R_{free} test set	5222 reflections (4.93%)	DCC
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 , 20.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 218714 reflections	Xtriage
F_o, F_c correlation	0.83	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, 0.375 respectively for untwinned datasets, and 0.333, 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:HG2	1:G:211:LYS:O	1.41	1.16
1:J:211:LYS:HG2	1:J:211:LYS:O	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:I:211:LYS:O	1:I:211:LYS:HG2	1.41	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:LYS:O	1:D:211:LYS:HG2	1.41	1.10
1:E:211:LYS:HG2	1:E: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:O	1:C:211:LYS:HG2	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:C:369:THR:HG23	1:C:370:LEU:N	1.71	1.06
1:A:211:LYS:O	1:A:211:LYS:HG2	1.41	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:HB2	1:J:185:ARG:HH11	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:J:167:VAL:HB	2:J:387:HOH:O	1.55	1.03
1:I:185:ARG:HH11	1:I:185:ARG:HB2	1.22	1.03
1:E:185:ARG:HB2	1:E:185:ARG:HH11	1.22	1.03
1:D:369:THR:HG23	1:D:370:LEU:N	1.71	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:HH11	1:F:185:ARG:HB2	1.22	1.02
1:L:185:ARG:HB2	1:L:185:ARG:HH11	1.22	1.02
1:G:185:ARG:HB2	1:G:185:ARG:HH11	1.22	1.02
1:F:369:THR:HG23	1:F:370:LEU:N	1.71	1.02
1:K:185:ARG:HH11	1:K:185:ARG:HB2	1.22	1.02
1:B:185:ARG:HH11	1:B:185:ARG:HB2	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:D:341:ASP:OD2	1:F:58:GLU:CA	2.09	1.00
1:C:185:ARG:HB2	1:C:185:ARG:HH11	1.22	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:K:369:THR:O	1:K:370:LEU:HB2	1.64	0.95
1:B:369:THR:O	1:B: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:G:369:THR:HG23	1:G:370:LEU:H	1.26	0.94
1:D:89:ILE:HG22	1:I:147:ILE:HG22	1.49	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:K:369:THR:CG2	1:K:370:LEU:H	1.81	0.94
1:B:369:THR:CG2	1:B: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:J:369:THR:O	1:J:370:LEU:HB2	1.64	0.93
1:G:79:SER:HA	1:G:83:SER:HB2	1.51	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:J:369:THR:CG2	1:J:370:LEU:H	1.80	0.93
1:G:369:THR:CG2	1:G:370:LEU:H	1.81	0.93
1:D:147:ILE:HG22	1:I:89:ILE:HG22	1.50	0.92
1:D:79:SER:HA	1:D:83:SER:HB2	1.51	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:K:369:THR:HG23	1:K:370:LEU:H	1.26	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: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:H	1:L:89:ILE:HD13	1.38	0.88
1:K:99:ARG:HD2	1:K:360:HIS:O	1.72	0.88
1:F:99:ARG:HD2	1:F:360:HIS:O	1.72	0.88
1:D:99:ARG:HD2	1:D:360:HIS:O	1.72	0.88
1:A:89:ILE:H	1:A:89:ILE:HD13	1.38	0.88
1:A:89:ILE:HG22	1:F:147:ILE:HG22	1.56	0.88
1:I:89:ILE:H	1:I:89:ILE:HD13	1.38	0.88
1:C:369:THR:CG2	1:C:370:LEU:N	2.37	0.88
1:J:89:ILE:H	1:J:89:ILE:HD13	1.39	0.88
1:J:99:ARG:HD2	1:J:360:HIS:O	1.72	0.88
1:G:99:ARG:HD2	1:G:360:HIS:O	1.72	0.88
1:D:341:ASP:CB	1:F:58:GLU:HA	2.03	0.87
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: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:I:211:LYS:O	1:I:211:LYS:CG	2.22	0.87
1:B:89:ILE:HD13	1:B:89:ILE:H	1.38	0.87
1:E:89:ILE:H	1:E:89:ILE:HD13	1.38	0.87
1:G:89:ILE:H	1:G:89:ILE:HD13	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:ILE:H	1:D:89:ILE:HD13	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:369:THR:CG2	1:K:370:LEU:N	2.37	0.86
1:K:165:ILE:HG22	1:K:175:VAL:HG12	1.58	0.86
1:E:165:ILE:HG22	1:E:175:VAL:HG12	1.58	0.86
1:D:247:PHE:HE2	2:D:390:HOH:O	1.59	0.86
1:D:341:ASP:CA	1:F:84:HIS:NE2	2.38	0.86
1:J:193:ASP:HA	2:J:381:HOH:O	1.75	0.86
1:D:165:ILE:HG22	1:D:175:VAL:HG12	1.58	0.86
1:A:165:ILE:HG22	1:A:175:VAL:HG12	1.58	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:HD13	1:K:89:ILE:H	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: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:C:165:ILE:HG22	1:C:175:VAL:HG12	1.58	0.85
1:J:165:ILE:HG22	1:J:175:VAL:HG12	1.58	0.85
1:F:369:THR:CG2	1:F:370:LEU:N	2.37	0.85
1:F:89:ILE:H	1:F:89:ILE:HD13	1.38	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:CG	1:L:211:LYS:O	2.22	0.84
1:D:341:ASP:C	1:F:84:HIS:CD2	2.49	0.84
1:L:165:ILE:HG22	1:L:175:VAL:HG12	1.58	0.84
1:D:5:ILE:HD12	2:D:384:HOH:O	1.76	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:E:111:GLY:O	1:E:369:THR:OG1	1.96	0.83
1:A:147:ILE:HG22	1:F:89:ILE:HG22	1.61	0.83
1:B:185:ARG:NH1	1:B:185:ARG:HB2	1.94	0.82
1:K:185:ARG:NH1	1:K:185:ARG:HB2	1.94	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:H:43:LYS:HB2	1:H:44:PRO:HD3	1.61	0.82
1:F:185:ARG:NH1	1:F:185:ARG:HB2	1.94	0.82
1:H:147:ILE:HG22	1:L:89:ILE:HG22	1.58	0.82
1:I:111:GLY:O	1:I:369:THR:OG1	1.96	0.82
1:D:111:GLY:O	1:D: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:K:111:GLY:O	1:K:369:THR:OG1	1.96	0.82
1:F:111:GLY:O	1:F:369:THR:OG1	1.96	0.82
1:D:185:ARG:NH1	1:D:185:ARG:HB2	1.94	0.81
1:I:185:ARG:NH1	1:I:185:ARG:HB2	1.94	0.81
1:L:111:GLY:O	1:L:369:THR:OG1	1.96	0.81
1:J:185:ARG:HB2	1:J:185:ARG:NH1	1.94	0.81
1:C:185:ARG:HB2	1:C:185:ARG:NH1	1.94	0.81
1:J:211:LYS:CG	1:J:211:LYS:O	2.22	0.81
1:H:42:ALA:O	1:H:46:GLN:HG3	1.79	0.81
1:L:185:ARG:HB2	1:L:185:ARG:NH1	1.94	0.81
1:G:185:ARG:HB2	1:G:185:ARG:NH1	1.94	0.81
1:A:185:ARG:HB2	1:A:185:ARG:NH1	1.94	0.81
1:A:111:GLY:O	1:A:369:THR:OG1	1.96	0.81
1:G:111:GLY:O	1:G:369:THR:OG1	1.96	0.80
1:G:211:LYS:CG	1:G:211:LYS:O	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:CG	1:E:211:LYS:O	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:D:171:GLY:HA2	1:D:204:CYS:HA	1.67	0.77
1:C:171:GLY:HA2	1:C: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:HH11	1:H:185:ARG:HB2	1.47	0.77
1:J:171:GLY:HA2	1:J:204:CYS:HA	1.67	0.77
1:I:171:GLY:HA2	1:I: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:A:171:GLY:HA2	1:A: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:H:24:GLN:H	1:H:315:ASN:ND2	1.84	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: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:J:107:VAL:HG22	1:J:109:ASP:H	1.49	0.76
1:I:274:MSE:HE1	1:I:335:VAL:HG12	1.68	0.76
1:G:274:MSE:HE1	1:G:335:VAL:HG12	1.68	0.76
1:J:274:MSE:HE1	1:J:335:VAL:HG12	1.68	0.76
1:E:274:MSE:HE1	1:E:335:VAL:HG12	1.68	0.76
1:I:26:GLN:HB3	1:I:61:PRO:HG2	1.68	0.76
1:A:274:MSE:HE1	1:A: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:L:171:GLY:HA2	1:L:204:CYS:HA	1.67	0.75
1:F:107:VAL:HG22	1:F:109:ASP:H	1.49	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:G:171:GLY:HA2	1:G:204:CYS:HA	1.67	0.75
1:B:171:GLY:HA2	1:B:204:CYS:HA	1.67	0.75
1:C:107:VAL:HG22	1:C:109:ASP:H	1.49	0.75
1:I:107:VAL:HG22	1:I:109:ASP:H	1.49	0.75
1:D:107:VAL:HG22	1:D:109:ASP:H	1.49	0.75
1:B:41:GLY:HA3	1:F:41:GLY:HA3	1.69	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: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: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:A:26:GLN:HB3	1:A:61:PRO:HG2	1.68	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:F:121:ASN:H	1:F:121:ASN:HD22	1.34	0.74
1:C:274:MSE:HE1	1:C:335:VAL:HG12	1.68	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:HD22	1:C:121:ASN:H	1.34	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:I:234:GLU:HG2	1:I:270:LYS:HB3	1.70	0.73
1:B:211:LYS:CG	1:B:211:LYS:O	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: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:A:168:ASP:OD1	1:A:172:THR:HB	1.89	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:J:121:ASN:H	1:J:121:ASN:HD22	1.34	0.73
1:G:234:GLU:HG2	1:G:270:LYS:HB3	1.70	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:A:121:ASN:HD22	1:A: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:B:121:ASN:H	1:B:121:ASN:HD22	1.34	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: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:C:234:GLU:HG2	1:C:270:LYS:HB3	1.70	0.72
1:C:168:ASP:OD1	1:C:172:THR:HB	1.89	0.72
1:B:234:GLU:HG2	1:B:270:LYS:HB3	1.70	0.72
1:E:126:LEU:HD12	1:L:126:LEU:HD12	1.71	0.72
1:B:290:ASP:HB3	1:F:73:ASN:ND2	2.05	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:I:121:ASN:H	1:I:121:ASN:HD22	1.34	0.72
1:K:73:ASN:ND2	1:L:290:ASP:HB3	2.03	0.72
1:B:168:ASP:OD1	1:B:172:THR:HB	1.89	0.72
1:L:234:GLU:HG2	1:L:270:LYS:HB3	1.70	0.72
1:G:168:ASP:OD1	1:G:172:THR:HB	1.89	0.72
1:F:234:GLU:HG2	1:F:270:LYS:HB3	1.70	0.72
1:J:168:ASP:OD1	1:J:172:THR:HB	1.89	0.71
1:H:318:ILE:HD13	1:H:342:ARG:HD3	1.72	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:L:349:THR:HG21	1:L:359:ILE:HG12	1.73	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: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:K:24:GLN:H	1:K:315:ASN:HD22	1.39	0.71
1:J:234:GLU:HG2	1:J:270:LYS:HB3	1.70	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:HD22	1:H:121:ASN:H	1.38	0.70
1:C:24:GLN:H	1:C:315:ASN:HD22	1.39	0.70
1:B:349:THR:HG21	1:B:359:ILE:HG12	1.73	0.70
1:K:349:THR:HG21	1:K:359:ILE:HG12	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLN:H	1:A:315:ASN:HD22	1.39	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:H:43:LYS:NZ	1:H:46:GLN:HE22	1.89	0.69
1:A:135:ASP:HB3	1:B:132:PHE:CE2	2.27	0.69
1:F:159:VAL:H	1:F:186:ASN:HD21	1.40	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: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:I:159:VAL:H	1:I:186:ASN:HD21	1.40	0.69
1:L:159:VAL:H	1:L:186:ASN:HD21	1.40	0.69
1:K:159:VAL:H	1:K:186:ASN:HD21	1.40	0.69
1:D:283:LEU:HD12	1:D:286:ALA:HB2	1.75	0.69
1:C:283:LEU:HD12	1:C:286:ALA:HB2	1.75	0.69
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:C:135:ASP:HB3	1:I:132:PHE:CE2	2.28	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:A:283:LEU:HD12	1:A:286:ALA:HB2	1.75	0.68
1:J:159:VAL:H	1:J:186:ASN:HD21	1.40	0.68
1:I:24:GLN:HG3	1:I:60:GLU:OE1	1.94	0.68
1:E:24:GLN:HG3	1:E:60:GLU:OE1	1.94	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:I:27:ILE:HD12	1:I:56:ILE:HG21	1.76	0.68
1:G:24:GLN:H	1:G:315:ASN:HD22	1.39	0.68
1:D:24:GLN:HG3	1:D:60:GLU:OE1	1.94	0.68
1:H:123:TRP:HB2	1:H:130:LEU:HD13	1.73	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:B:27:ILE:HD12	1:B:56:ILE:HG21	1.76	0.68
1:A:24:GLN:HG3	1:A:60:GLU:OE1	1.94	0.68
1:A:159:VAL:H	1:A:186:ASN:HD21	1.40	0.68
1:F:24:GLN:HG3	1:F:60:GLU:OE1	1.94	0.68
1:E:283:LEU:HD12	1:E:286:ALA:HB2	1.75	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:E:27:ILE:HD12	1:E:56:ILE:HG21	1.75	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:G:261:GLN:NE2	2:G:392:HOH:O	2.26	0.68
1:B:283:LEU:HD12	1:B:286:ALA:HB2	1.74	0.68
1:H:43:LYS:HZ1	1:H:46:GLN:HE22	1.41	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:E:159:VAL:H	1:E:186:ASN:HD21	1.40	0.67
1:B:24:GLN:HG3	1:B:60:GLU:OE1	1.94	0.67
1:I:24:GLN:H	1:I:315:ASN:HD22	1.39	0.67
1:K:24:GLN:HG3	1:K:60:GLU:OE1	1.94	0.67
1:D:24:GLN:HA	1:D:368:ALA:H	1.59	0.67
1:J:283:LEU:HD12	1:J:286:ALA:HB2	1.75	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:D:27:ILE:HD12	1:D:56:ILE:HG21	1.76	0.67
1:L:24:GLN:HG3	1:L:60:GLU:OE1	1.94	0.67
1:A:24:GLN:HA	1:A:368:ALA:H	1.59	0.67
1:J:27:ILE:HD12	1:J:56:ILE:HG21	1.75	0.67
1:F:27:ILE:HD12	1:F:56:ILE:HG21	1.76	0.67
1:G:159:VAL:H	1:G:186:ASN:HD21	1.40	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:A:290:ASP:HB3	1:G:73:ASN:ND2	2.09	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:C:27:ILE:HD12	1:C:56:ILE:HG21	1.76	0.66
1:B:24:GLN:HA	1:B:368:ALA:H	1.60	0.66
1:I:73:ASN:ND2	1:J:290:ASP:HB3	2.10	0.66
1:J:24:GLN:HA	1:J:368:ALA:H	1.59	0.66
1:A:132:PHE:CE2	1:B:135:ASP:HB3	2.29	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:L:24:GLN:HA	1:L:368:ALA:H	1.59	0.65
1:H:177:GLU:HB3	1:H:209:TRP:HE3	1.62	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:H:198:LEU:HD22	1:H:202:LEU:HD22	1.78	0.65
1:A:315:ASN:HB3	2:A:379:HOH:O	1.97	0.65
1:A:121:ASN:ND2	2:A:392:HOH:O	2.30	0.64
1:C:290:ASP:HB3	1:D:73:ASN:ND2	2.11	0.64
1:A:133:PRO:HG2	2:A:390:HOH:O	1.96	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:G:262:THR:HG22	2:G:392:HOH:O	1.95	0.64
1:E:29:MSE:HA	1:E:98:ILE:HG21	1.80	0.64
1:A:135:ASP:HB3	1:B:132:PHE:CD2	2.33	0.64
1:F:29:MSE:HA	1:F:98:ILE:HG21	1.80	0.64
1:B:29:MSE:HA	1:B: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:L:27:ILE:HD11	1:L:314:VAL:HG12	1.81	0.63
1:K:29:MSE:HA	1:K:98:ILE:HG21	1.80	0.63
1:I:191:LYS:O	1:I:195:GLU:HG3	1.99	0.63
1:F:27:ILE:HD11	1:F:314:VAL:HG12	1.81	0.63
1:A:132:PHE:CD2	1:B:135:ASP:HB3	2.34	0.63
1:G:215:ASP:CG	2:G:401:HOH:O	2.37	0.63
1:F:185:ARG:HH22	1:F:220:ASN:HD22	1.47	0.63
1:E:27:ILE:HD11	1:E:314:VAL:HG12	1.81	0.63
1:K:191:LYS:O	1:K:195:GLU:HG3	1.99	0.63
1:K:185:ARG:HH22	1:K:220:ASN:HD22	1.47	0.63
1:J:29:MSE:HA	1:J:98:ILE:HG21	1.80	0.63
1:A:73:ASN:ND2	1:G:290:ASP:HB3	2.14	0.63
1:J:103:PRO:HD3	1:J:144:VAL:HG11	1.81	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:27:ILE:HD11	1:J:314:VAL:HG12	1.80	0.63
1:C:29:MSE:HA	1:C:98:ILE:HG21	1.80	0.63
1:I:103:PRO:HD3	1:I:144:VAL:HG11	1.81	0.63
1:H:312:LEU:HD22	1:H:313:ILE:N	2.13	0.63
1:A:29:MSE:HA	1:A:98:ILE:HG21	1.80	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:L:103:PRO:HD3	1:L:144:VAL:HG11	1.81	0.62
1:G:191:LYS:O	1:G:195:GLU:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:ARG:HH22	1:E:220:ASN:HD22	1.47	0.62
1:A:103:PRO:HD3	1:A:144:VAL:HG11	1.81	0.62
1:F:191:LYS:O	1:F:195:GLU:HG3	1.99	0.62
1:D:27:ILE:HD11	1:D:314:VAL:HG12	1.81	0.62
1:H:100:ASP:HB3	1:H:161:GLU:HB2	1.80	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: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: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:K:103:PRO:HD3	1:K:144:VAL:HG11	1.81	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:C:15:PHE:CE2	1:C:114:ARG:HD3	2.35	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:D:159:VAL:HG22	1:D:185:ARG:HD2	1.82	0.62
1:C:27:ILE:HD11	1:C:314:VAL:HG12	1.81	0.62
1:I:15:PHE:CE2	1:I:114:ARG:HD3	2.35	0.62
1:G:159:VAL:HG22	1:G:185:ARG:HD2	1.82	0.62
1:E:103:PRO:HD3	1:E:144:VAL:HG11	1.81	0.62
1:A:15:PHE:CE2	1:A:114:ARG:HD3	2.35	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: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:J:191:LYS:O	1:J:195:GLU:HG3	1.99	0.61
1:A:191:LYS:O	1:A:195:GLU:HG3	1.99	0.61
1:A:27:ILE:HD11	1:A:314:VAL:HG12	1.81	0.61
1:L:191:LYS:O	1:L:195:GLU:HG3	1.99	0.61
1:H:139:LEU:HB3	1:H:143:LYS:HE3	1.82	0.61
1:E:159:VAL:HG22	1:E:185:ARG:HD2	1.82	0.61
1:I:159:VAL:HG22	1:I:185:ARG:HD2	1.82	0.61
1:G:185:ARG:HH22	1:G:220:ASN:HD22	1.47	0.61
1:K:159:VAL:HG22	1:K:185:ARG:HD2	1.82	0.61
1:C:185:ARG:HH22	1:C:220:ASN:HD22	1.47	0.61
1:B:103:PRO:HD3	1:B:144:VAL:HG11	1.81	0.61
1:B:27:ILE:HD11	1:B:314:VAL:HG12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:PHE:CE2	1:B:114:ARG:HD3	2.35	0.61
1:J:278:LYS:HA	1:J:278:LYS:HE2	1.83	0.61
1:I:185:ARG:HH22	1:I:220:ASN:HD22	1.47	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:K:27:ILE:HD11	1:K:314:VAL:HG12	1.81	0.61
1:J:185:ARG:HH22	1:J:220:ASN:HD22	1.47	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:B:159:VAL:HG22	1:B:185:ARG:HD2	1.82	0.61
1:D:103:PRO:HD3	1:D:144:VAL:HG11	1.81	0.61
1:D:15:PHE:CE2	1:D:114:ARG:HD3	2.35	0.61
1:K:15:PHE:CE2	1:K:114:ARG:HD3	2.35	0.61
1:B:278:LYS:HA	1:B:278:LYS:HE2	1.83	0.61
1:C:278:LYS:HE2	1:C:278:LYS:HA	1.83	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:HE2	1:G:278:LYS:HA	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:H:358:ASN:HD22	1:H:359:ILE:N	1.93	0.60
1:G:214:ILE:HG13	2:G:401:HOH:O	2.00	0.60
1:K:278:LYS:HA	1:K:278:LYS:HE2	1.83	0.60
1:F:15:PHE:CE2	1:F:114:ARG:HB2	2.37	0.60
1:L:159:VAL:HG22	1:L:185:ARG:HD2	1.82	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:A:278:LYS:HA	1:A:278:LYS:HE2	1.83	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:A:15:PHE:CE2	1:A:114:ARG:HB2	2.37	0.60
1:H:4:ARG:HH22	1:H:154:LYS:HD3	1.66	0.60
1:I:278:LYS:HA	1:I:278:LYS:HE2	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: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:E:198:LEU:O	1:E:202:LEU:HB2	2.02	0.60
1:F:198:LEU:O	1:F:202:LEU:HB2	2.02	0.60
1:E:278:LYS:HE2	1:E:278:LYS:HA	1.83	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:179:CYS:HB2	1:C:220:ASN:O	2.01	0.59
1:K:89:ILE:N	1:K:89:ILE:HD13	2.14	0.59
1:C:15:PHE:CE2	1:C:114:ARG:HB2	2.37	0.59
1:J:198:LEU:O	1:J:202:LEU:HB2	2.02	0.59
1:I:179:CYS:HB2	1:I:220:ASN:O	2.02	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: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:J:89:ILE:N	1:J:89:ILE:HD13	2.15	0.59
1:L:15:PHE:CE2	1:L:114:ARG:HB2	2.37	0.59
1:K:15:PHE:CE2	1:K:114:ARG:HB2	2.37	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:G:104:THR:HB	1:G:116:VAL:HG13	1.84	0.59
1:F:132:PHE:CE2	1:G:135:ASP:HB3	2.36	0.59
1:E:369:THR:CG2	1:E:370:LEU:N	2.37	0.59
1:B:15:PHE:CE2	1:B:114:ARG:HB2	2.37	0.59
1:D:15:PHE:CE2	1:D:114:ARG:HB2	2.37	0.59
1:E:15:PHE:CE2	1:E:114:ARG:HB2	2.37	0.59
1:D:104:THR:HB	1:D:116:VAL:HG13	1.84	0.59
1:C:132:PHE:CE2	1:I:135:ASP:HB3	2.38	0.59
1:A:198:LEU:O	1:A:202:LEU:HB2	2.02	0.59
1:D:278:LYS:HE2	1:D:278:LYS:HA	1.83	0.59
1:K:179:CYS:HB2	1:K:220:ASN:O	2.02	0.59
1:D:198:LEU:O	1:D:202:LEU:HB2	2.02	0.59
1:L:9:THR:HG22	1:L:12:GLN:CD	2.23	0.59
1:L:179:CYS:HB2	1:L:220:ASN:O	2.01	0.59
1:D:9:THR:HG22	1:D:12:GLN:CD	2.23	0.59
1:K:9:THR:HG22	1:K:12:GLN:CD	2.23	0.59
1:F:278:LYS:HA	1:F:278:LYS:HE2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:9:THR:HG22	1:I:12:GLN:CD	2.23	0.59
1:J:15:PHE:CE2	1:J:114:ARG:HB2	2.37	0.59
1:J:179:CYS:HB2	1:J:220:ASN:O	2.01	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:H:318:ILE:CD1	1:H:342:ARG:HD3	2.32	0.59
1:H:142:ARG:CZ	1:L:75:LEU:HD21	2.33	0.59
1:F:104:THR:HB	1:F:116:VAL:HG13	1.84	0.59
1:B:9:THR:HG22	1:B:12:GLN:CD	2.23	0.59
1:L:278:LYS:HE2	1:L:278:LYS:HA	1.83	0.59
1:J:199:LYS:HG2	1:J:204:CYS:O	2.03	0.58
1:F:9:THR:HG22	1:F:12:GLN:CD	2.23	0.58
1:B:89:ILE:N	1:B:89:ILE:HD13	2.14	0.58
1:D:199:LYS:HG2	1:D:204:CYS:O	2.03	0.58
1:I:263:ASP:OD2	1:I:267:ARG:NH1	2.37	0.58
1:G:198:LEU:O	1:G:202:LEU:HB2	2.02	0.58
1:J:263:ASP:OD2	1:J:267:ARG:NH1	2.36	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:L:121:ASN:N	1:L:121:ASN:HD22	1.96	0.58
1:C:171:GLY:HA3	1:C:205:VAL:HG22	1.85	0.58
1:I:104:THR:HB	1:I:116:VAL:HG13	1.84	0.58
1:C:263:ASP:OD2	1:C:267:ARG:NH1	2.37	0.58
1:B:198:LEU:O	1:B:202:LEU:HB2	2.02	0.58
1:E:89:ILE:N	1:E:89:ILE:HD13	2.14	0.58
1:F:199:LYS:HG2	1:F:204:CYS:O	2.03	0.58
1:J:171:GLY:HA3	1:J:205:VAL:HG22	1.85	0.58
1:I:171:GLY:HA3	1:I:205:VAL:HG22	1.86	0.58
1:A:199:LYS:HG2	1:A:204:CYS:O	2.03	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:A:263:ASP:OD2	1:A:267:ARG:NH1	2.36	0.58
1:K:198:LEU:O	1:K:202:LEU:HB2	2.02	0.58
1:B:263:ASP:OD2	1:B:267:ARG:NH1	2.37	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:A:104:THR:HB	1:A:116:VAL:HG13	1.84	0.58
1:D:121:ASN:N	1:D:121:ASN:HD22	1.96	0.58
1:F:171:GLY:HA3	1:F:205:VAL:HG22	1.85	0.58
1:I:199:LYS:HG2	1:I:204:CYS:O	2.03	0.58
1:E:199:LYS:HG2	1:E:204:CYS:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:GLY:HA3	1:G:205:VAL:HG22	1.86	0.58
1:K:171:GLY:HA3	1:K:205:VAL:HG22	1.85	0.58
1:G:114:ARG:HG2	1:G:153:TYR:CE1	2.39	0.58
1:G:114:ARG:HG2	1:G:153:TYR:HE1	1.69	0.58
1:L:104:THR:HB	1:L:116:VAL:HG13	1.84	0.58
1:D:263:ASP:OD2	1:D:267:ARG:NH1	2.37	0.58
1:G:199:LYS:HG2	1:G:204:CYS:O	2.03	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:I:114:ARG:HG2	1:I:153:TYR:CE1	2.39	0.58
1:A:114:ARG:HG2	1:A:153:TYR:CE1	2.39	0.58
1:L:114:ARG:HG2	1:L:153:TYR:HE1	1.69	0.58
1:D:114:ARG:HG2	1:D:153:TYR:HE1	1.69	0.58
1:J:69:LEU:HG	2:J:380:HOH:O	2.02	0.58
1:E:159:VAL:HG12	1:E:186:ASN:ND2	2.19	0.58
1:D:147:ILE:CG2	1:I:89:ILE:HG22	2.30	0.58
1:C:199:LYS:HG2	1:C:204:CYS:O	2.03	0.58
1:E:263:ASP:OD2	1:E:267:ARG:NH1	2.37	0.58
1:B:104:THR:HB	1:B:116:VAL:HG13	1.84	0.58
1:H:108:ASN:ND2	1:H:110:LYS:HB2	2.18	0.58
1:H:105:PHE:O	1:H:106:LEU:HD23	2.03	0.58
1:K:27:ILE:HD12	1:K:56:ILE:CG2	2.34	0.58
1:D:27:ILE:HD12	1:D:56:ILE:CG2	2.34	0.58
1:F:27:ILE:HD12	1:F:56:ILE:CG2	2.34	0.58
1:J:114:ARG:HG2	1:J:153:TYR:HE1	1.69	0.58
1:A:114:ARG:HG2	1:A:153:TYR:HE1	1.69	0.58
1:E:114:ARG:HG2	1:E:153:TYR:HE1	1.69	0.58
1:H:231:ARG:HD2	1:H:234:GLU:OE2	2.04	0.58
1:G:177:GLU:HB3	1:G:209:TRP:CE3	2.39	0.58
1:D:31:TRP:HB2	1:D:66:VAL:HG12	1.86	0.58
1:K:31:TRP:HB2	1:K:66:VAL:HG12	1.86	0.58
1:I:159:VAL:HG12	1:I:186:ASN:ND2	2.19	0.58
1:K:159:VAL:HG12	1:K:186:ASN:ND2	2.19	0.58
1:H:321:PRO:HB3	1:H:358:ASN:ND2	2.19	0.58
1:G:89:ILE:HD13	1:G:89:ILE:N	2.14	0.58
1:A:312:LEU:HD13	1:A:313:ILE:N	2.19	0.58
1:I:170:GLU:O	1:I:172:THR:N	2.37	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:J:31:TRP:HB2	1:J:66:VAL:HG12	1.86	0.58
1:C:114:ARG:HG2	1:C:153:TYR:HE1	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:114:ARG:HG2	1:K:153:TYR:CE1	2.39	0.58
1:K:34:ARG:HD2	1:K:94:ASP:O	2.04	0.58
1:C:89:ILE:N	1:C:89:ILE:HD13	2.14	0.58
1:C:312:LEU:HD13	1:C:313:ILE:N	2.19	0.58
1:K:312:LEU:HD13	1:K:313:ILE:N	2.19	0.58
1:D:312:LEU:HD13	1:D:313:ILE:N	2.19	0.58
1:D:114:ARG:HG2	1:D:153:TYR:CE1	2.39	0.58
1:K:114:ARG:HG2	1:K:153:TYR:HE1	1.69	0.58
1:E:114:ARG:HG2	1:E:153:TYR:CE1	2.39	0.58
1:H:142:ARG:NH1	1:H:146:GLU:HG2	2.19	0.58
1:D:177:GLU:HB3	1:D:209:TRP:CE3	2.39	0.58
1:H:88:ILE:HD12	1:H:88:ILE:N	2.19	0.58
1:D:170:GLU:O	1:D:172:THR:N	2.37	0.57
1:J:170:GLU:O	1:J:172:THR:N	2.37	0.57
1:D:89:ILE:N	1:D:89:ILE:HD13	2.14	0.57
1:C:34:ARG:HD2	1:C:94:ASP:O	2.04	0.57
1:L:89:ILE:N	1:L:89:ILE:HD13	2.14	0.57
1:B:312:LEU:HD13	1:B:313:ILE:N	2.19	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: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:F:170:GLU:O	1:F:172:THR:N	2.37	0.57
1:C:167:VAL:HG22	1:C:173:VAL:HG23	1.86	0.57
1:E:177:GLU:HB3	1:E:209:TRP:CE3	2.39	0.57
1:B:177:GLU:HB3	1:B:209:TRP:CE3	2.39	0.57
1:A:31:TRP:HB2	1:A:66:VAL:HG12	1.86	0.57
1:D:121:ASN:ND2	1:D:159:VAL:HG21	2.19	0.57
1:G:159:VAL:HG12	1:G:186:ASN:ND2	2.19	0.57
1:L:34:ARG:HD2	1:L:94:ASP:O	2.04	0.57
1:C:170:GLU:O	1:C:172:THR:N	2.37	0.57
1:K:170:GLU:O	1:K:172:THR:N	2.37	0.57
1:F:114:ARG:HG2	1:F:153:TYR:HE1	1.69	0.57
1:K:104:THR:HB	1:K:116:VAL:HG13	1.84	0.57
1:H:167:VAL:HG13	1:H:172:THR:O	2.02	0.57
1:E:104:THR:HB	1:E:116:VAL:HG13	1.84	0.57
1:L:177:GLU:HB3	1:L:209:TRP:CE3	2.39	0.57
1:L:159:VAL:HG12	1:L:186:ASN:ND2	2.19	0.57
1:I:89:ILE:N	1:I:89:ILE:HD13	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:224:ASP:HB2	1:H:360:HIS:CD2	2.40	0.57
1:F:263:ASP:OD2	1:F:267:ARG:NH1	2.37	0.57
1:A:159:VAL:HG12	1:A:186:ASN:ND2	2.19	0.57
1:D:159:VAL:HG12	1:D:186:ASN:ND2	2.19	0.57
1:F:159:VAL:HG12	1:F:186:ASN:ND2	2.19	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:E:312:LEU:HD13	1:E:313:ILE:N	2.19	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:F:312:LEU:HD13	1:F:313:ILE:N	2.19	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:C:31:TRP:HB2	1:C:66:VAL:HG12	1.86	0.57
1:H:90:GLU:OE2	1:L:90:GLU:OE2	2.22	0.57
1:B:34:ARG:HD2	1:B:94:ASP:O	2.04	0.57
1:F:167:VAL:HG22	1:F:173:VAL:HG23	1.86	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:E:121:ASN:N	1:E:121:ASN:HD22	1.96	0.57
1:H:319:ILE:HG22	1:H:359:ILE:HD13	1.85	0.57
1:H:61:PRO:CA	1:H:85:ASN:HD22	2.13	0.57
1:E:171:GLY:HA3	1:E:205:VAL:HG22	1.86	0.57
1:C:27:ILE:HD12	1:C:56:ILE:CG2	2.34	0.57
1:G:27:ILE:HD12	1:G:56:ILE:CG2	2.34	0.57
1:E:27:ILE:HD12	1:E:56:ILE:CG2	2.34	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:K:167:VAL:HG22	1:K:173:VAL:HG23	1.86	0.57
1:J:114:ARG:HG2	1:J:153:TYR:CE1	2.39	0.57
1:G:263:ASP:OD2	1:G:267:ARG:NH1	2.37	0.57
1:A:177:GLU:HB3	1:A:209:TRP:CE3	2.39	0.57
1:J:159:VAL:HG12	1:J:186:ASN:ND2	2.19	0.57
1:I:121:ASN:ND2	1:I:159:VAL:HG21	2.20	0.57
1:G:34:ARG:HD2	1:G:94:ASP:O	2.04	0.57
1:B:170:GLU:O	1:B:172:THR:N	2.37	0.57
1:D:171:GLY:HA3	1:D:205:VAL:HG22	1.85	0.57
1:C:135:ASP:HB3	1:I:132:PHE:CD2	2.40	0.57
1:C:114:ARG:HG2	1:C:153:TYR:CE1	2.39	0.57
1:I:177:GLU:HB3	1:I:209:TRP:CE3	2.39	0.57
1:A:121:ASN:ND2	1:A:159:VAL:HG21	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:ASN:ND2	1:G:159:VAL:HG21	2.19	0.57
1:K:121:ASN:ND2	1:K:159:VAL:HG21	2.20	0.57
1:A:34:ARG:HD2	1:A:94:ASP:O	2.04	0.57
1:A:171:GLY:HA3	1:A:205:VAL:HG22	1.86	0.57
1:L:171:GLY:HA3	1:L:205:VAL:HG22	1.85	0.57
1:J:177:GLU:HB3	1:J:209:TRP:CE3	2.39	0.57
1:E:31:TRP:HB2	1:E:66:VAL:HG12	1.86	0.57
1:G:312:LEU:HD13	1:G:313:ILE:N	2.19	0.57
1:F:114:ARG:HG2	1:F:153:TYR:CE1	2.39	0.57
1:E:290:ASP:HB3	1:H:73:ASN:ND2	2.20	0.57
1:B:77:ARG:O	1:B:81:LEU:HG	2.05	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:J:121:ASN:ND2	1:J:159:VAL:HG21	2.20	0.56
1:D:167:VAL:HG22	1:D:173:VAL:HG23	1.86	0.56
1:L:121:ASN:ND2	1:L:159:VAL:HG21	2.19	0.56
1:I:34:ARG:HD2	1:I:94:ASP:O	2.04	0.56
1:E:167:VAL:HG22	1:E:173:VAL:HG23	1.86	0.56
1:B:114:ARG:HG2	1:B:153:TYR:CE1	2.39	0.56
1:F:177:GLU:HB3	1:F:209:TRP:CE3	2.39	0.56
1:D:342:ARG:N	1:F:84:HIS:CE1	2.72	0.56
1:F:121:ASN:ND2	1:F:159:VAL:HG21	2.19	0.56
1:F:34:ARG:HD2	1:F:94:ASP:O	2.04	0.56
1:B:27:ILE:HD12	1:B:56:ILE:CG2	2.34	0.56
1:K:77:ARG:O	1:K:81:LEU:HG	2.05	0.56
1:E:170:GLU:O	1:E:172:THR:N	2.37	0.56
1:C:6:LYS:HB2	2:C:393:HOH:O	2.05	0.56
1:H:330:LEU:O	1:H:334:GLN:HG3	2.05	0.56
1:F:31:TRP:HB2	1:F:66:VAL:HG12	1.86	0.56
1:H:87:ARG:HG3	1:H:87:ARG:O	2.04	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:B:159:VAL:HG12	1:B:186:ASN:ND2	2.19	0.56
1:J:34:ARG:HD2	1:J:94:ASP:O	2.04	0.56
1:A:167:VAL:HG22	1:A:173:VAL:HG23	1.86	0.56
1:L:167:VAL:HG22	1:L:173:VAL:HG23	1.86	0.56
1:A:77:ARG:O	1:A:81:LEU:HG	2.05	0.56
1:B:31:TRP:HB2	1:B:66:VAL:HG12	1.86	0.56
1:K:106:LEU:O	1:K:113:LEU:HD12	2.06	0.56
1:G:31:TRP:HB2	1:G:66:VAL:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:LEU:O	1:C:113:LEU:HD12	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:B:9:THR:HG22	1:B:12:GLN:OE1	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:E:9:THR:HG22	1:E:12:GLN:OE1	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:A:106:LEU:O	1:A:113:LEU:HD12	2.06	0.56
1:D:106:LEU:O	1:D:113:LEU:HD12	2.06	0.56
1:K:174:LEU:HB3	1:K:223:ILE:HD13	1.88	0.56
1:E:106:LEU:O	1:E:113:LEU:HD12	2.06	0.56
1:E:34:ARG:HD2	1:E:94:ASP:O	2.04	0.56
1:B:174:LEU:HB3	1:B:223:ILE:HD13	1.88	0.56
1:L:174:LEU:HB3	1:L:223:ILE:HD13	1.88	0.56
1:F:135:ASP:HB3	1:G:132:PHE:CE2	2.40	0.56
1:A:9:THR:HG22	1:A:12:GLN:OE1	2.06	0.56
1:I:167:VAL:HG22	1:I:173:VAL:HG23	1.86	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:K:177:GLU:HB3	1:K:209:TRP:CE3	2.39	0.56
1:B:106:LEU:O	1:B:113:LEU:HD12	2.06	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:B:127:VAL:HG13	1:B:184:SER:HB2	1.88	0.56
1:K:127:VAL:HG13	1:K:184:SER:HB2	1.88	0.56
1:C:77:ARG:O	1:C:81:LEU:HG	2.05	0.56
1:I:65:CYS:SG	1:I:89:ILE:HD11	2.46	0.56
1:L:65:CYS:SG	1:L:89:ILE:HD11	2.46	0.56
1:A:89:ILE:N	1:A:89:ILE:HD13	2.14	0.56
1:J:65:CYS:SG	1:J:89:ILE:HD11	2.46	0.56
1:F:174:LEU:HB3	1:F:223:ILE:HD13	1.88	0.56
1:J:106:LEU:O	1:J:113:LEU:HD12	2.06	0.56
1:F:43:LYS:NZ	1:F:46:GLN:HE22	2.04	0.56
1:H:337:GLU:O	1:H:340:PRO:HD3	2.06	0.56
1:C:43:LYS:NZ	1:C:46:GLN:HE22	2.04	0.56
1:A:127:VAL:HG13	1:A:184:SER:HB2	1.88	0.56
1:F:127:VAL:HG13	1:F:184:SER:HB2	1.88	0.56
1:J:174:LEU:HB3	1:J:223:ILE:HD13	1.88	0.56
1:D:340:PRO:HG2	1:F:58:GLU:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:165:ILE:HG22	1:H:175:VAL:CG1	2.36	0.56
1:D:195:GLU:O	1:D:199:LYS:HG3	2.06	0.56
1:C:349:THR:HG21	1:C:359:ILE:CG1	2.36	0.56
1:K:195:GLU:O	1:K:199:LYS:HG3	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:I:127:VAL:HG13	1:I:184:SER:HB2	1.88	0.56
1:L:43:LYS:NZ	1:L:46:GLN:HE22	2.04	0.56
1:J:127:VAL:HG13	1:J:184:SER:HB2	1.88	0.56
1:G:77:ARG:O	1:G:81:LEU:HG	2.05	0.56
1:A:65:CYS:SG	1:A:89:ILE:HD11	2.47	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:L:195:GLU:O	1:L:199:LYS:HG3	2.06	0.55
1:C:9:THR:HG22	1:C:12:GLN:OE1	2.06	0.55
1:K:43:LYS:NZ	1:K:46:GLN:HE22	2.04	0.55
1:B:65:CYS:SG	1:B:89:ILE:HD11	2.46	0.55
1:A:195:GLU:O	1:A:199:LYS:HG3	2.06	0.55
1:I:174:LEU:HB3	1:I:223:ILE:HD13	1.88	0.55
1:B:167:VAL:HG22	1:B:173:VAL:HG23	1.86	0.55
1:K:9:THR:HG22	1:K:12:GLN:OE1	2.06	0.55
1:G:106:LEU:O	1:G:113:LEU:HD12	2.06	0.55
1:D:127:VAL:HG13	1:D:184:SER:HB2	1.88	0.55
1:G:127:VAL:HG13	1:G:184:SER:HB2	1.88	0.55
1:I:252:LYS:HD3	2:I:387:HOH:O	2.06	0.55
1:A:43:LYS:NZ	1:A:46:GLN:HE22	2.04	0.55
1:L:127:VAL:HG13	1:L:184:SER:HB2	1.88	0.55
1:I:43:LYS:NZ	1:I:46:GLN:HE22	2.04	0.55
1:G:174:LEU:HB3	1:G:223:ILE:HD13	1.88	0.55
1:E:65:CYS:SG	1:E:89:ILE:HD11	2.46	0.55
1:G:65:CYS:SG	1:G:89:ILE:HD11	2.46	0.55
1:B:349:THR:HG21	1:B:359:ILE:CG1	2.36	0.55
1:K:349:THR:HG21	1:K:359:ILE:CG1	2.36	0.55
1:K:283:LEU:CD1	1:K:286:ALA:HB2	2.37	0.55
1:I:77:ARG:O	1:I:81:LEU:HG	2.05	0.55
1:C:174:LEU:HB3	1:C:223:ILE:HD13	1.88	0.55
1:G:43:LYS:NZ	1:G:46:GLN:HE22	2.04	0.55
1:F:77:ARG:O	1:F:81:LEU:HG	2.05	0.55
1:D:65:CYS:SG	1:D:89:ILE:HD11	2.46	0.55
1:H:65:CYS:HB3	1:H:91:MSE:HB3	1.88	0.55
1:A:318:ILE:HB	1:A:344:VAL:HG22	1.89	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:K:65:CYS:SG	1:K:89:ILE:HD11	2.46	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:A:349:THR:HG21	1:A:359:ILE:CG1	2.36	0.55
1:E:174:LEU:HB3	1:E:223:ILE:HD13	1.88	0.55
1:D:281:CYS:SG	1:D:306:ALA:HB2	2.47	0.55
1:D:43:LYS:NZ	1:D:46:GLN:HE22	2.04	0.55
1:E:40:LEU:HD12	1:H:40:LEU:HD12	1.89	0.55
1:C:127:VAL:HG13	1:C:184:SER:HB2	1.88	0.55
1:J:121:ASN:N	1:J:121:ASN:HD22	1.96	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:F:9:THR:HG22	1:F:12:GLN:OE1	2.06	0.55
1:K:281:CYS:SG	1:K:306:ALA:HB2	2.47	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:I:349:THR:HG21	1:I:359:ILE:CG1	2.36	0.55
1:B:283:LEU:CD1	1:B:286:ALA:HB2	2.36	0.55
1:L:9:THR:HG22	1:L:12:GLN:OE1	2.06	0.55
1:A:174:LEU:HB3	1:A:223:ILE:HD13	1.88	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:B:281:CYS:SG	1:B:306:ALA:HB2	2.47	0.55
1:E:195:GLU:O	1:E:199:LYS:HG3	2.06	0.55
1:L:349:THR:HG21	1:L:359:ILE:CG1	2.37	0.55
1:F:349:THR:HG21	1:F:359:ILE:CG1	2.36	0.55
1:A:12:GLN:CD	1:D:82:GLY:CA	2.75	0.55
2:C:392:HOH:O	1:J:147:ILE:C	2.44	0.55
1:F:65:CYS:SG	1:F:89:ILE:HD11	2.46	0.55
1:B:195:GLU:O	1:B:199:LYS:HG3	2.06	0.55
1:D:135:ASP:HB3	1:J:132:PHE:HE2	1.70	0.55
1:L:283:LEU:CD1	1:L:286:ALA:HB2	2.37	0.55
1:A:283:LEU:CD1	1:A:286:ALA:HB2	2.37	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:A:281:CYS:SG	1:A:306:ALA:HB2	2.47	0.55
1:B:73:ASN:ND2	1:F:290:ASP:HB3	2.22	0.55
1:D:174:LEU:HB3	1:D:223:ILE:HD13	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:9:THR:HG22	1:L:12:GLN:HG3	1.89	0.54
1:H:122:ALA:O	1:H:129:GLY:HA2	2.07	0.54
1:G:281:CYS:SG	1:G:306:ALA:HB2	2.47	0.54
1:A:74:ALA:O	1:A:78:VAL:HG23	2.07	0.54
1:H:252:LYS:HG2	1:H:256:ASP:OD2	2.07	0.54
1:B:43:LYS:NZ	1:B:46:GLN:HE22	2.04	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:C:283:LEU:CD1	1:C:286:ALA:HB2	2.37	0.54
1:B:74:ALA:O	1:B:78:VAL:HG23	2.08	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:J:321:PRO:HD3	1:J:359:ILE:HD12	1.90	0.54
1:E:309:LEU:O	1:E:309:LEU:HD13	2.08	0.54
1:J:9:THR:HG22	1:J:12:GLN:OE1	2.06	0.54
1:D:9:THR:HG22	1:D:12:GLN:HG3	1.89	0.54
1:J:43:LYS:NZ	1:J:46:GLN:HE22	2.04	0.54
1:L:318:ILE:HB	1:L:344:VAL:HG22	1.89	0.54
1:I:281:CYS:SG	1:I:306:ALA:HB2	2.47	0.54
1:E:43:LYS:NZ	1:E:46:GLN:HE22	2.04	0.54
1:J:74:ALA:O	1:J:78:VAL:HG23	2.07	0.54
1:F:74:ALA:O	1:F:78:VAL:HG23	2.08	0.54
1:I:74:ALA:O	1:I:78:VAL:HG23	2.07	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:L:74:ALA:O	1:L:78:VAL:HG23	2.07	0.54
1:E:127:VAL:HG13	1:E:184:SER:HB2	1.88	0.54
1:C:309:LEU:O	1:C:309:LEU:HD13	2.08	0.54
1:G:309:LEU:O	1:G:309:LEU:HD13	2.08	0.54
1:L:309:LEU:HD13	1:L:309:LEU:O	2.08	0.54
1:F:283:LEU:CD1	1:F:286:ALA:HB2	2.37	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: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:D:309:LEU:O	1:D:309:LEU:HD13	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: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: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:K:320:LEU:HD13	1:K:335:VAL:HG11	1.90	0.54
1:E:9:THR:HG22	1:E:12:GLN:HG3	1.90	0.54
1:D:9:THR:HG22	1:D:12:GLN:OE1	2.06	0.54
1:K:318:ILE:HB	1:K:344:VAL:HG22	1.89	0.54
1:G:321:PRO:HD3	1:G:359:ILE:HD12	1.90	0.54
1:J:309:LEU:HD13	1:J:309:LEU:O	2.08	0.54
1:K:321:PRO:HD3	1:K:359:ILE:HD12	1.90	0.54
1:F:318:ILE:HB	1:F:344:VAL:HG22	1.89	0.54
1:J:88:ILE:HD12	1:J:88:ILE:N	2.23	0.54
1:B:121:ASN:HD22	1:B:121:ASN:N	1.96	0.54
1:H:43:LYS:NZ	1:H:46:GLN:NE2	2.55	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:C:88:ILE:HD12	1:C:88:ILE:N	2.23	0.54
1:A:9:THR:HG22	1:A:12:GLN:HG3	1.90	0.54
1:A:121:ASN:N	1:A:121:ASN:HD22	1.96	0.54
1:C:89:ILE:HG22	1:J:147:ILE:CG2	2.32	0.54
1:B:321:PRO:HD3	1:B:359:ILE:HD12	1.90	0.54
1:G:320:LEU:HD13	1:G:335:VAL:HG11	1.90	0.54
1:F:309:LEU:O	1:F:309:LEU:HD13	2.08	0.54
1:C:15:PHE:CD2	1:C:114:ARG:HB2	2.43	0.54
1:K:9:THR:HG22	1:K:12:GLN:HG3	1.89	0.54
1:D:74:ALA:O	1:D:78:VAL:HG23	2.07	0.54
1:J:318:ILE:HB	1:J:344:VAL:HG22	1.89	0.54
1:B:88:ILE:N	1:B:88:ILE:HD12	2.23	0.54
1:B:369:THR:O	1:B:370:LEU:CB	2.47	0.53
1:F:121:ASN:N	1:F:121:ASN:HD22	1.96	0.53
1:H:27:ILE:HD12	1:H:56:ILE:HD12	1.90	0.53
1:E:320:LEU:HD13	1:E:335:VAL:HG11	1.90	0.53
1:L:321:PRO:HD3	1:L:359:ILE:HD12	1.90	0.53
1:H:176:THR:HG21	1:H:221:GLY:O	2.07	0.53
1:D:283:LEU:CD1	1:D:286:ALA:HB2	2.37	0.53
1:C:318:ILE:HB	1:C:344:VAL:HG22	1.89	0.53
1:G:88:ILE:N	1:G:88:ILE:HD12	2.23	0.53
1:D:88:ILE:HD12	1:D:88:ILE:N	2.23	0.53
1:F:88:ILE:N	1:F:88:ILE:HD12	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:15:PHE:CD2	1:J:114:ARG:HB2	2.43	0.53
1:G:9:THR:HG22	1:G:12:GLN:HG3	1.89	0.53
1:H:124:GLY:HA3	1:H:128:ASP:C	2.28	0.53
1:H:66:VAL:CG2	1:H:71:TYR:HA	2.38	0.53
1:B:320:LEU:HD13	1:B:335:VAL:HG11	1.90	0.53
1:G:349:THR:HG21	1:G:359:ILE:CG1	2.36	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:B:291:TYR:OH	1:F:80:GLU:HB2	2.08	0.53
1:A:309:LEU:HD13	1:A:309:LEU:O	2.08	0.53
1:G:15:PHE:CD2	1:G:114:ARG:HB2	2.44	0.53
1:D:15:PHE:CD2	1:D:114:ARG:HB2	2.43	0.53
1:K:15:PHE:CZ	1:K:114:ARG:HD3	2.44	0.53
1:B:9:THR:HG22	1:B:12:GLN:HG3	1.89	0.53
1:E:132:PHE:CE2	1:L:135:ASP:HB3	2.43	0.53
1:L:88:ILE:N	1:L:88:ILE:HD12	2.23	0.53
1:K:121:ASN:HD22	1:K:121:ASN:N	1.96	0.53
1:H:185:ARG:HH22	1:H:220:ASN:HD22	1.57	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:I:15:PHE:CZ	1:I:114:ARG:HD3	2.44	0.53
1:J:9:THR:HG22	1:J:12:GLN:HG3	1.89	0.53
1:I:43:LYS:NZ	1:J:35:ASN:HD22	2.06	0.53
1:A:7:ASN:HB2	1:D:84:HIS:NE2	2.22	0.53
1:I:312:LEU:HD12	1:I:314:VAL:CG1	2.39	0.53
1:D:312:LEU:HD12	1:D:314:VAL:CG1	2.39	0.53
1:I:283:LEU:CD1	1:I:286:ALA:HB2	2.37	0.53
1:I:15:PHE:CD2	1:I:114:ARG:HB2	2.44	0.53
1:L:15:PHE:CZ	1:L:114:ARG:HD3	2.44	0.53
1:K:15:PHE:CD2	1:K:114:ARG:HB2	2.43	0.53
1:C:121:ASN:N	1:C:121:ASN:HD22	1.96	0.53
1:C:320:LEU:HD13	1:C:335:VAL:HG11	1.90	0.53
1:A:312:LEU:HD12	1:A:314:VAL:CG1	2.39	0.53
1:A:15:PHE:CZ	1:A:114:ARG:HD3	2.44	0.53
1:F:15:PHE:CZ	1:F:114:ARG:HD3	2.44	0.53
1:L:15:PHE:CD2	1:L:114:ARG:HB2	2.43	0.53
1:K:74:ALA:O	1:K:78:VAL:HG23	2.07	0.53
1:E:74:ALA:O	1:E:78:VAL:HG23	2.08	0.53
1:K:312:LEU:HD12	1:K:314:VAL:CG1	2.39	0.53
1:F:312:LEU:HD12	1:F:314:VAL:CG1	2.39	0.53
1:E:135:ASP:HB3	1:L:132:PHE:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:PHE:CD2	1:F:114:ARG:HB2	2.43	0.53
1:G:210:VAL:HG12	1:G:211:LYS:N	2.24	0.53
1:D:243:LYS:HZ3	1:H:192:GLU:HG3	1.73	0.53
1:B:309:LEU:HD13	1:B:309:LEU:O	2.08	0.53
1:F:321:PRO:HD3	1:F:359:ILE:HD12	1.90	0.53
1:J:15:PHE:CZ	1:J:114:ARG:HD3	2.44	0.53
1:B:15:PHE:CD2	1:B:114:ARG:HB2	2.44	0.53
1:C:9:THR:HG22	1:C:12:GLN:HG3	1.89	0.53
1:H:174:LEU:HD22	1:H:223:ILE:HD11	1.91	0.53
1:G:121:ASN:HD22	1:G:121:ASN:N	1.96	0.53
1:L:312:LEU:HD12	1:L:314:VAL:CG1	2.39	0.53
1:F:320:LEU:HD13	1:F:335:VAL:HG11	1.90	0.53
1:C:15:PHE:CZ	1:C:114:ARG:HD3	2.44	0.53
1:G:15:PHE:CZ	1:G:114:ARG:HD3	2.44	0.53
1:A:15:PHE:CD2	1:A:114:ARG:HB2	2.44	0.53
1:H:124:GLY:O	1:H:128:ASP:N	2.39	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:K:88:ILE:HD12	1:K:88:ILE:N	2.23	0.53
1:I:121:ASN:ND2	1:I:121:ASN:H	2.06	0.52
1:I:309:LEU:HD13	1:I:309:LEU:O	2.08	0.52
1:J:320:LEU:HD13	1:J:335:VAL:HG11	1.90	0.52
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:J:11:LYS:HG3	1:J:203:ASN:HD21	1.74	0.52
1:E:312:LEU:HD12	1:E:314:VAL:CG1	2.39	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:N	1:E:88:ILE:HD12	2.23	0.52
1:A:312:LEU:HD12	1:A:314:VAL:HG12	1.92	0.52
1:B:290:ASP:CB	1:F:73:ASN:ND2	2.72	0.52
1:B:261:GLN:O	1:B:269:LEU:HD13	2.10	0.52
1:A:88:ILE:HD12	1:A:88:ILE:N	2.23	0.52
1:K:210:VAL:HG12	1:K:211:LYS:N	2.24	0.52
1:L:210:VAL:HG12	1:L:211:LYS:N	2.24	0.52
1:C:121:ASN:ND2	1:C:121:ASN:H	2.07	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:J:312:LEU:HD12	1:J:314:VAL:CG1	2.39	0.52
1:E:15:PHE:CD2	1:E:114:ARG:HB2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:26:GLN:HG2	1:H:366:GLN:HE21	1.75	0.52
1:L:123:TRP:HB2	1:L:130:LEU:HD13	1.92	0.52
1:I:121:ASN:N	1:I:121:ASN:HD22	1.96	0.52
1:B:121:ASN:H	1:B:121:ASN:ND2	2.07	0.52
1:E:89:ILE:HG22	1:K:147:ILE:CG2	2.31	0.52
1:E:15:PHE:CZ	1:E:114:ARG:HD3	2.44	0.52
1:L:11:LYS:HG3	1:L:203:ASN:HD21	1.74	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:K:261:GLN:O	1:K:269:LEU:HD13	2.10	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:D:214:ILE:C	1:D:216:PRO:HD3	2.30	0.52
1:D:123:TRP:HB2	1:D:130:LEU:HD13	1.92	0.52
1:I:88:ILE:HD12	1:I:88:ILE:N	2.23	0.52
1:F:210:VAL:HG12	1:F:211:LYS:N	2.24	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: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: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:D:15:PHE:CZ	1:D:114:ARG:HD3	2.44	0.52
1:A:11:LYS:HG3	1:A:203:ASN:HD21	1.74	0.52
1:J:312:LEU:HD12	1:J:314:VAL:HG12	1.92	0.52
1:D:311:PHE:HB3	1:D:320:LEU:HD12	1.92	0.52
1:D:135:ASP:HB3	1:J:132:PHE:CD2	2.44	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:C:214:ILE:C	1:C:216:PRO:HD3	2.30	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:311:PHE:HB3	1:G:320:LEU:HD12	1.92	0.52
1:K:312:LEU:HD12	1:K:314:VAL:HG12	1.92	0.52
1:G:261:GLN:O	1:G:269:LEU:HD13	2.10	0.52
1:K:281:CYS:HA	2:K:391:HOH:O	2.10	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:H:215:ASP:HB3	1:H:218:GLU:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:THR:OG1	1:C:10:PRO:HD2	2.11	0.51
1:L:43:LYS:HB2	1:L:44:PRO:HD3	1.93	0.51
1:A:43:LYS:HB2	1:A:44:PRO:HD3	1.93	0.51
1:A:214:ILE:C	1:A:216:PRO:HD3	2.30	0.51
1:K:123:TRP:HB2	1:K:130:LEU:HD13	1.92	0.51
1:L:214:ILE:C	1:L:216:PRO:HD3	2.30	0.51
1:J:210:VAL:HG12	1:J:211:LYS:N	2.24	0.51
1:A:210:VAL:HG12	1:A:211:LYS:N	2.24	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:B:9:THR:OG1	1:B:10:PRO:HD2	2.10	0.51
1:I:261:GLN:O	1:I: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:H:274:MSE:HE1	1:H:311:PHE:HE2	1.75	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:49:PHE:O	1:E:52:VAL:HG12	2.10	0.51
1:J:49:PHE:O	1:J:52:VAL:HG12	2.10	0.51
1:E:9:THR:OG1	1:E:10:PRO:HD2	2.11	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:E:261:GLN:O	1:E:269:LEU:HD13	2.10	0.51
1:J:261:GLN:O	1:J:269:LEU:HD13	2.10	0.51
1:J:159:VAL:HG12	1:J:186:ASN:HD21	1.76	0.51
1:L:137:ASP:HA	1:L:140:VAL:HG23	1.92	0.51
1:C:311:PHE:HB3	1:C:320:LEU:HD12	1.92	0.51
1:B:311:PHE:HB3	1:B:320:LEU:HD12	1.92	0.51
1:K:49:PHE:O	1:K:52:VAL:HG12	2.10	0.51
1:I:43:LYS:HB2	1:I:44:PRO:HD3	1.93	0.51
1:H:26:GLN:HG2	1:H:366:GLN:NE2	2.25	0.51
1:A:261:GLN:O	1:A:269:LEU:HD13	2.09	0.51
1:F:123:TRP:HB2	1:F:130:LEU:HD13	1.92	0.51
1:E:11:LYS:HG3	1:E:203:ASN:HD21	1.74	0.51
1:B:11:LYS:HG3	1:B:203:ASN:HD21	1.74	0.51
1:G:123:TRP:HB2	1:G:130:LEU:HD13	1.92	0.51
1:A:137:ASP:HA	1:A:140:VAL:HG23	1.92	0.51
1:B:49:PHE:O	1:B:52:VAL:HG12	2.10	0.51
1:C:49:PHE:O	1:C:52:VAL:HG12	2.10	0.51
1:L:9:THR:OG1	1:L:10:PRO:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:9:THR:OG1	1:I:10:PRO:HD2	2.11	0.51
1:F:9:THR:OG1	1:F:10:PRO:HD2	2.11	0.51
1:F:43:LYS:HB2	1:F:44:PRO:HD3	1.92	0.51
1:L:261:GLN:O	1:L:269:LEU:HD13	2.10	0.51
1:I:123:TRP:HB2	1:I:130:LEU:HD13	1.92	0.51
1:A:123:TRP:HB2	1:A: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: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:E:43:LYS:HB2	1:E:44:PRO:HD3	1.92	0.51
1:C:123:TRP:HB2	1:C:130:LEU:HD13	1.92	0.51
1:D:121:ASN:ND2	1:D:121:ASN:H	2.07	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:D:261:GLN:O	1:D:269:LEU:HD13	2.10	0.51
1:D:137:ASP:HA	1:D:140:VAL:HG23	1.92	0.51
1:I:68:PRO:HG3	1:I:90:GLU:OE2	2.11	0.51
1:C:68:PRO:HG3	1:C:90:GLU:OE2	2.11	0.51
1:H:317:GLY:O	1:H:318:ILE:HD12	2.11	0.51
1:A:49:PHE:O	1:A:52:VAL:HG12	2.10	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:K:174:LEU:O	1:K:223:ILE:HD13	2.11	0.51
1:J:43:LYS:HB2	1:J:44:PRO:HD3	1.93	0.51
1:A:9:THR:OG1	1:A:10:PRO:HD2	2.11	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:L:312:LEU:HD12	1:L:314:VAL:HG12	1.92	0.51
1:A:315:ASN:CA	2:A:379:HOH:O	2.58	0.51
1:F:49:PHE:O	1:F:52:VAL:HG12	2.10	0.51
1:K:177:GLU:HB3	1:K:209:TRP:HE3	1.76	0.51
1:B:214:ILE:C	1:B:216:PRO:HD3	2.30	0.51
1:K:214:ILE:C	1:K:216:PRO:HD3	2.30	0.51
1:A:159:VAL:HG12	1:A:186:ASN:HD21	1.76	0.51
1:D:68:PRO:HG3	1:D:90:GLU:OE2	2.11	0.51
1:I:49:PHE:O	1:I:52:VAL:HG12	2.10	0.51
1:L:68:PRO:HG3	1:L:90:GLU:OE2	2.11	0.51
1:J:174:LEU:O	1:J:223:ILE:HD13	2.11	0.51
1:D:43:LYS:HB2	1:D:44:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:PHE:O	1:E:134:TRP:CE3	2.64	0.51
1:B:210:VAL:HG12	1:B:211:LYS:N	2.24	0.50
1:E:210:VAL:HG12	1:E:211:LYS:N	2.24	0.50
1:C:290:ASP:OD1	1:D:77:ARG:NH2	2.36	0.50
1:D:140:VAL:O	1:D:144:VAL:HG12	2.12	0.50
1:I:137:ASP:HA	1:I:140:VAL:HG23	1.92	0.50
1:K:137:ASP:HA	1:K:140:VAL:HG23	1.92	0.50
1:E:140:VAL:O	1:E:144:VAL:HG12	2.12	0.50
1:C:137:ASP:HA	1:C:140:VAL:HG23	1.92	0.50
1:B:137:ASP:HA	1:B:140:VAL:HG23	1.92	0.50
1:D:9:THR:OG1	1:D:10:PRO:HD2	2.11	0.50
1:I:177:GLU:HB3	1:I:209:TRP:HE3	1.76	0.50
1:C:11:LYS:HG3	1:C:203:ASN:HD21	1.74	0.50
1:I:159:VAL:HG12	1:I:186:ASN:HD21	1.76	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:E:312:LEU:HD12	1:E:314:VAL:HG12	1.92	0.50
1:K:311:PHE:HB3	1:K:320:LEU:HD12	1.92	0.50
1:J:132:PHE:O	1:J:134:TRP:CE3	2.64	0.50
1:F:174:LEU:O	1:F:223:ILE:HD13	2.11	0.50
1:I:174:LEU:O	1:I:223:ILE:HD13	2.11	0.50
1:C:174:LEU:O	1:C:223:ILE:HD13	2.11	0.50
1:B:123:TRP:HB2	1:B:130:LEU:HD13	1.92	0.50
1:D:174:LEU:O	1:D:223:ILE:HD13	2.11	0.50
1:H:43:LYS:HZ1	1:H:46:GLN:NE2	2.08	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:K:43:LYS:HZ2	1:K:46:GLN:HE22	1.57	0.50
1:D:158:PHE:HE1	1:D:160:LEU:HB2	1.76	0.50
1:I:140:VAL:O	1:I:144:VAL:HG12	2.12	0.50
1:H:311:PHE:HE1	1:H:313:ILE:HD11	1.75	0.50
1:E:311:PHE:HB3	1:E:320:LEU:HD12	1.92	0.50
1:F:132:PHE:O	1:F:134:TRP:CE3	2.64	0.50
1:F:132:PHE:CD2	1:G:135:ASP:HB3	2.47	0.50
1:E:41:GLY:O	1:E:42:ALA:HB3	2.12	0.50
1:B:158:PHE:HE1	1:B:160:LEU:HB2	1.76	0.50
1:K:158:PHE:HE1	1:K:160:LEU:HB2	1.76	0.50
1:E:123:TRP:HB2	1:E:130:LEU:HD13	1.92	0.50
1:A:7:ASN:CG	1:D:84:HIS:ND1	2.53	0.50
1:J:68:PRO:HG3	1:J:90:GLU:OE2	2.11	0.50
1:H:27:ILE:CD1	1:H:312:LEU:HD11	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLY:O	1:A:42:ALA:HB3	2.12	0.50
1:B:41:GLY:O	1:B:42:ALA:HB3	2.12	0.50
1:L:132:PHE:O	1:L:134:TRP:CE3	2.64	0.50
1:C:41:GLY:O	1:C:42:ALA:HB3	2.12	0.50
1:K:9:THR:OG1	1:K:10:PRO:HD2	2.11	0.50
1:D:177:GLU:HB3	1:D:209:TRP:HE3	1.76	0.50
1:C:177:GLU:HB3	1:C:209:TRP:HE3	1.76	0.50
1:B:43:LYS:HB2	1:B:44:PRO:HD3	1.92	0.50
1:L:365:GLN:NE2	2:L:383:HOH:O	2.42	0.50
1:C:158:PHE:HE1	1:C:160:LEU:HB2	1.77	0.50
1:F:214:ILE:C	1:F:216:PRO:HD3	2.30	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:E:68:PRO:HG3	1:E:90:GLU:OE2	2.11	0.50
1:H:219:THR:O	1:H:220:ASN:HB2	2.10	0.50
1:H:52:VAL:O	1:H:56:ILE:HG12	2.12	0.50
1:I:311:PHE:HB3	1:I:320:LEU:HD12	1.93	0.50
1:F:311:PHE:HB3	1:F:320:LEU:HD12	1.92	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:D:132:PHE:O	1:D:134:TRP:CE3	2.64	0.50
1:I:121:ASN:N	1:I:121:ASN:ND2	2.60	0.50
1:B:121:ASN:ND2	2:B:387:HOH:O	2.44	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:I:132:PHE:O	1:I:134:TRP:CE3	2.64	0.50
1:D:41:GLY:O	1:D:42:ALA:HB3	2.12	0.50
1:A:132:PHE:O	1:A:134:TRP:CE3	2.64	0.50
1:G:158:PHE:HE1	1:G:160:LEU:HB2	1.76	0.50
1:J:121:ASN:N	1:J:121:ASN:ND2	2.60	0.50
1:L:159:VAL:HG12	1:L:186:ASN:HD21	1.76	0.50
1:A:68:PRO:HG3	1:A:90:GLU:OE2	2.11	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:B:358:ASN:O	1:B:361:CYS:N	2.45	0.50
1:I:358:ASN:O	1:I:361:CYS:N	2.45	0.50
1:D:358:ASN:O	1:D:361:CYS:N	2.45	0.50
1:J:9:THR:OG1	1:J:10:PRO:HD2	2.10	0.50
1:L:8:THR:HB	1:L:12:GLN:NE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:THR:HB	1:B:12:GLN:NE2	2.27	0.50
1:F:8:THR:HB	1:F:12:GLN:NE2	2.27	0.50
1:C:43:LYS:HB2	1:C:44:PRO:HD3	1.93	0.50
1:G:174:LEU:O	1:G:223:ILE:HD13	2.11	0.50
1:H:296:ILE:N	1:H:297:PRO:HD3	2.26	0.50
1:A:8:THR:HB	1:A:12:GLN:NE2	2.27	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:A:358:ASN:O	1:A:361:CYS:N	2.45	0.50
1:K:43:LYS:HB2	1:K:44:PRO:HD3	1.93	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:D:159:VAL:HG12	1:D:186:ASN:HD21	1.76	0.49
1:K:41:GLY:O	1:K:42:ALA:HB3	2.12	0.49
1:J:177:GLU:HB3	1:J:209:TRP:HE3	1.76	0.49
1:B:174:LEU:O	1:B:223:ILE:HD13	2.11	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:K:132:PHE:O	1:K:134:TRP:CE3	2.64	0.49
1:L:41:GLY:O	1:L:42:ALA:HB3	2.12	0.49
1:F:26:GLN:NE2	1:F:63:SER:OG	2.45	0.49
1:I:26:GLN:NE2	1:I:63:SER:OG	2.45	0.49
1:E:8:THR:HB	1:E:12:GLN:NE2	2.27	0.49
1:C:132:PHE:O	1:C:134:TRP:CE3	2.64	0.49
1:K:8:THR:HB	1:K:12:GLN:NE2	2.27	0.49
1:F:158:PHE:HE1	1:F:160:LEU:HB2	1.76	0.49
1:G:159:VAL:HG12	1:G:186:ASN:HD21	1.76	0.49
1:K:68:PRO:HG3	1:K:90:GLU:OE2	2.11	0.49
1:C:312:LEU:HD12	1:C:314:VAL:HG12	1.92	0.49
1:A:26:GLN:NE2	1:A:63:SER:OG	2.45	0.49
1:K:290:ASP:CB	1:L:73:ASN:ND2	2.76	0.49
1:J:8:THR:HB	1:J:12:GLN:NE2	2.27	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:K:43:LYS:NZ	1:L:35:ASN:HD22	2.10	0.49
1:L:108:ASN:ND2	1:L:110:LYS:HB2	2.28	0.49
1:A:121:ASN:N	1:A:121:ASN:ND2	2.60	0.49
1:B:26:GLN:NE2	1:B:63:SER:OG	2.45	0.49
1:E:26:GLN:NE2	1:E:63:SER:OG	2.45	0.49
1:B:132:PHE:O	1:B:134:TRP:CE3	2.64	0.49
1:D:8:THR:HB	1:D:12:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:113:LEU:O	1:J:150:VAL:HG23	2.13	0.49
1:A:174:LEU:O	1:A:223:ILE:HD13	2.11	0.49
1:F:113:LEU:O	1:F:150:VAL:HG23	2.13	0.49
1:H:296:ILE:O	1:H:296:ILE:HG12	2.12	0.49
1:K:262:THR:HG22	2:K:387:HOH:O	2.12	0.49
1:I:108:ASN:ND2	1:I:110:LYS:HB2	2.28	0.49
1:B:108:ASN:ND2	1:B:110:LYS:HB2	2.28	0.49
1:G:108:ASN:ND2	1:G:110:LYS:HB2	2.28	0.49
1:C:147:ILE:CG2	1:J:89:ILE:HG22	2.37	0.49
1:H:185:ARG:NH1	1:H:185:ARG:HB2	2.23	0.49
1:C:321:PRO:HB3	1:C:358:ASN:HD22	1.78	0.49
1:L:358:ASN:O	1:L:361:CYS:N	2.45	0.49
1:L:26:GLN:NE2	1:L:63:SER:OG	2.45	0.49
1:I:41:GLY:O	1:I:42:ALA:HB3	2.12	0.49
1:I:8:THR:HB	1:I:12:GLN:NE2	2.27	0.49
1:A:177:GLU:HB3	1:A:209:TRP:HE3	1.76	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:B:231:ARG:HG2	2:B:389:HOH:O	2.12	0.49
1:D:369:THR:O	1:D:370:LEU:CB	2.47	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:G:140:VAL:O	1:G:144:VAL:HG12	2.12	0.49
1:H:132:PHE:O	1:H:134:TRP:CE3	2.65	0.49
1:C:26:GLN:NE2	1:C:63:SER:OG	2.45	0.49
1:G:321:PRO:HB3	1:G:358:ASN:HD22	1.78	0.49
1:K:26:GLN:NE2	1:K:63:SER:OG	2.45	0.49
1:D:321:PRO:HB3	1:D:358:ASN:HD22	1.78	0.49
1:F:41:GLY:O	1:F:42:ALA:HB3	2.12	0.49
1:A:315:ASN:HA	2:A:379:HOH:O	2.11	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:E:230:ILE:HG22	1:E:339:PHE:CE1	2.48	0.49
1:L:230:ILE:HG22	1:L:339:PHE:CE1	2.48	0.49
1:B:230:ILE:HG22	1:B:339:PHE:CE1	2.48	0.49
1:C:108:ASN:ND2	1:C:110:LYS:HB2	2.28	0.49
1:A:158:PHE:HE1	1:A:160:LEU:HB2	1.76	0.49
1:H:182:HIS:CG	1:H:183:PRO:HD2	2.48	0.49
1:H:132:PHE:CD2	1:K:135:ASP:HB3	2.46	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:A:43:LYS:NZ	1:G:35:ASN:HD22	2.11	0.49
1:K:80:GLU:HB2	1:L:291:TYR:OH	2.13	0.49
1:C:140:VAL:O	1:C:144:VAL:HG12	2.12	0.49
1:H:15:PHE:CZ	1:H:114:ARG:HD3	2.48	0.49
1:B:321:PRO:HB3	1:B:358:ASN:HD22	1.78	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:A:230:ILE:HG22	1:A:339:PHE:CE1	2.48	0.49
1:I:230:ILE:HG22	1:I:339:PHE:CE1	2.48	0.49
1:C:230:ILE:HG22	1:C:339:PHE:CE1	2.48	0.49
1:I:231:ARG:HG3	1:I:232:PRO:HD2	1.95	0.49
1:B:140:VAL:O	1:B:144:VAL:HG12	2.11	0.49
1:F:358:ASN:O	1:F:361:CYS:N	2.45	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:E:113:LEU:O	1:E:150:VAL:HG23	2.13	0.49
1:I:158:PHE:HE1	1:I:160:LEU:HB2	1.76	0.49
1:D:231:ARG:HG3	1:D:232:PRO:HD2	1.95	0.49
1:J:158:PHE:HE1	1:J:160:LEU:HB2	1.76	0.49
1:D:121:ASN:N	1:D:121:ASN:ND2	2.60	0.49
1:H:28:TRP:CH2	1:H:144:VAL:HG23	2.48	0.49
1:J:140:VAL:O	1:J:144:VAL:HG12	2.12	0.49
1:H:27:ILE:HD11	1:H:314:VAL:HG12	1.93	0.49
1:J:26:GLN:NE2	1:J:63:SER:OG	2.45	0.49
1:E:321:PRO:HB3	1:E:358:ASN:HD22	1.78	0.49
1:D:26:GLN:NE2	1:D:63:SER:OG	2.45	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:G:177:GLU:HB3	1:G:209:TRP:HE3	1.76	0.49
1:H:50:LEU:HD11	1:H:78:VAL:HG22	1.95	0.49
1:J:108:ASN:ND2	1:J:110:LYS:HB2	2.27	0.49
1:D:108:ASN:ND2	1:D:110:LYS:HB2	2.28	0.49
1:C:320:LEU:HD12	1:C:321:PRO:HD2	1.95	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:G:8:THR:HB	1:G:12:GLN:NE2	2.27	0.48
1:A:113:LEU:O	1:A:150:VAL:HG23	2.13	0.48
1:L:113:LEU:O	1:L:150:VAL:HG23	2.13	0.48
1:F:230:ILE:HG22	1:F:339:PHE:CE1	2.48	0.48
1:A:108:ASN:ND2	1:A:110:LYS:HB2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:369:THR:O	1:I:370:LEU:CB	2.47	0.48
1:B:121:ASN:ND2	1:B:121:ASN:N	2.60	0.48
1:H:30:LEU:HB2	1:H:96:ALA:HB1	1.95	0.48
1:E:358:ASN:O	1:E:361:CYS:N	2.45	0.48
1:H:104:THR:HB	1:H:116:VAL:CG1	2.43	0.48
1:E:177:GLU:O	1:E:181:LEU:HB2	2.13	0.48
1:B:113:LEU:O	1:B:150:VAL:HG23	2.13	0.48
1:A:231:ARG:HG3	1:A:232:PRO:HD2	1.95	0.48
1:C:73:ASN:ND2	1:D:290:ASP:HB3	2.28	0.48
1:H:278:LYS:N	1:H:325:ASP:OD2	2.43	0.48
1:H:237:CYS:SG	1:H:238:ILE:N	2.87	0.48
1:L:158:PHE:HE1	1:L:160:LEU:HB2	1.76	0.48
1:K:140:VAL:O	1:K:144:VAL:HG12	2.12	0.48
1:I:321:PRO:HB3	1:I:358:ASN:HD22	1.78	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:C:272:HIS:ND1	1:C:338:MSE:HG2	2.29	0.48
1:F:108:ASN:ND2	1:F:110:LYS:HB2	2.28	0.48
1:J:272:HIS:ND1	1:J:338:MSE:HG2	2.29	0.48
1:A:291:TYR:OH	1:G:80:GLU:HB2	2.12	0.48
1:D:272:HIS:ND1	1:D:338:MSE:HG2	2.29	0.48
1:A:9:THR:HG22	1:A:12:GLN:CG	2.44	0.48
1:D:369:THR:CG2	1:D:370:LEU:N	2.37	0.48
1:H:30:LEU:HB2	1:H:96:ALA:CB	2.44	0.48
1:J:60:GLU:HB2	1:J:61:PRO:HD2	1.96	0.48
1:H:161:GLU:CD	1:H:161:GLU:H	2.16	0.48
1:L:177:GLU:HB3	1:L:209:TRP:HE3	1.76	0.48
1:C:177:GLU:O	1:C:181:LEU:HB2	2.13	0.48
1:I:177:GLU:O	1:I:181:LEU:HB2	2.13	0.48
1:K:108:ASN:ND2	1:K:110:LYS:HB2	2.28	0.48
1:B:272:HIS:ND1	1:B:338:MSE:HG2	2.29	0.48
1:H:169:GLY:HA3	2:H:393:HOH:O	2.13	0.48
1:F:231:ARG:HG3	1:F:232:PRO:HD2	1.95	0.48
1:J:231:ARG:HG3	1:J:232:PRO:HD2	1.95	0.48
1:E:231:ARG:HG3	1:E:232:PRO:HD2	1.95	0.48
1:D:230:ILE:HG22	1:D:339:PHE:CE1	2.48	0.48
1:J:121:ASN:H	1:J:121:ASN:ND2	2.07	0.48
1:J:56:ILE:HD13	1:J:319:ILE:HG13	1.96	0.48
1:K:177:GLU:O	1:K:181:LEU:HB2	2.13	0.48
1:J:230:ILE:HG22	1:J:339:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ARG:HG3	1:C:232:PRO:HD2	1.95	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: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:F:320:LEU:HD12	1:F:321:PRO:HD2	1.95	0.48
1:E:60:GLU:HB2	1:E:61:PRO:HD2	1.96	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:K:230:ILE:HG22	1:K:339:PHE:CE1	2.48	0.48
1:L:121:ASN:ND2	1:L:121:ASN:H	2.07	0.48
1:K:121:ASN:H	1:K:121:ASN:ND2	2.07	0.48
1:H:103:PRO:HD3	1:H:144:VAL:HG11	1.94	0.48
1:F:60:GLU:HB2	1:F:61:PRO:HD2	1.96	0.48
1:K:320:LEU:HD12	1:K:321:PRO:HD2	1.95	0.48
1:F:321:PRO:HB3	1:F:358:ASN:HD22	1.78	0.48
1:E:71:TYR:CZ	1:K:143:LYS:HG2	2.49	0.48
1:I:113:LEU:O	1:I:150:VAL:HG23	2.13	0.48
1:L:272:HIS:ND1	1:L:338:MSE:HG2	2.29	0.48
1:A:272:HIS:ND1	1:A:338:MSE:HG2	2.29	0.48
1:E:308:TYR:OH	1:E:325:ASP:HB3	2.14	0.48
1:H:9:THR:HG22	1:H:12:GLN:CD	2.33	0.48
1:D:341:ASP:HB3	1:F:57:SER:O	2.14	0.48
1:E:210:VAL:CG1	1:E:211:LYS:N	2.77	0.48
1:A:369:THR:O	1:A:370:LEU:CB	2.47	0.48
1:G:320:LEU:HD12	1:G:321:PRO:HD2	1.95	0.48
1:H:224:ASP:OD2	1:H:360:HIS:HD2	1.96	0.48
1:H:177:GLU:HG2	1:H:211:LYS:HA	1.96	0.48
1:K:9:THR:HG22	1:K:12:GLN:CG	2.44	0.48
1:E:177:GLU:HB3	1:E:209:TRP:HE3	1.76	0.48
1:B:177:GLU:O	1:B:181:LEU:HB2	2.13	0.48
1:F:210:VAL:CG1	1:F:211:LYS:N	2.77	0.48
1:C:56:ILE:HD13	1:C:319:ILE:HG13	1.96	0.48
1:C:9:THR:HG22	1:C:12:GLN:CG	2.44	0.48
1:E:143:LYS:HG2	1:K:71:TYR:CZ	2.49	0.48
1:D:177:GLU:O	1:D:181:LEU:HB2	2.13	0.48
1:A:177:GLU:O	1:A:181:LEU:HB2	2.13	0.48
1:L:308:TYR:OH	1:L:325:ASP:HB3	2.14	0.48
1:J:308:TYR:OH	1:J:325:ASP:HB3	2.14	0.48
1:G:272:HIS:ND1	1:G:338:MSE:HG2	2.29	0.48
1:D:340:PRO:CG	1:F:58:GLU:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:VAL:CG1	1:D:211:LYS:N	2.77	0.48
1:J:321:PRO:HB3	1:J:358:ASN:HD22	1.78	0.48
1:E:320:LEU:HD12	1:E:321:PRO:HD2	1.95	0.48
1:D:60:GLU:HB2	1:D:61:PRO:HD2	1.96	0.48
1:H:207:VAL:HG22	1:H:209:TRP:NE1	2.28	0.48
1:F:177:GLU:O	1:F:181:LEU:HB2	2.13	0.48
1:L:203:ASN:HD22	1:L:203:ASN:HA	1.50	0.48
1:B:231:ARG:HG3	1:B:232:PRO:HD2	1.95	0.48
1:F:47:LYS:O	1:F:51:GLU:HG3	2.14	0.48
1:I:272:HIS:ND1	1:I:338:MSE:HG2	2.29	0.48
1:G:210:VAL:CG1	1:G:211:LYS:N	2.77	0.47
1:I:210:VAL:CG1	1:I:211:LYS:N	2.77	0.47
1:A:210:VAL:CG1	1:A:211:LYS:N	2.77	0.47
1:C:121:ASN:ND2	1:C:121:ASN:N	2.60	0.47
1:L:47:LYS:HD3	2:L:388:HOH:O	2.13	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:C:61:PRO:HA	1:C:85:ASN:ND2	2.29	0.47
1:A:56:ILE:HD13	1:A:319:ILE:HG13	1.96	0.47
1:A:320:LEU:HD12	1:A:321:PRO:HD2	1.95	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:L:320:LEU:HD12	1:L:321:PRO:HD2	1.95	0.47
1:G:176:THR:HG21	1:G:221:GLY:O	2.14	0.47
1:B:9:THR:HG22	1:B:12:GLN:CG	2.44	0.47
1:F:231:ARG:CG	1:F:232:PRO:HD2	2.44	0.47
1:J:231:ARG:CG	1:J:232:PRO:HD2	2.44	0.47
1:G:308:TYR:OH	1:G:325:ASP:HB3	2.14	0.47
1:D:47:LYS:O	1:D:51:GLU:HG3	2.14	0.47
1:C:308:TYR:OH	1:C:325:ASP:HB3	2.14	0.47
1:F:308:TYR:OH	1:F:325:ASP:HB3	2.14	0.47
1:K:308:TYR:OH	1:K:325:ASP:HB3	2.14	0.47
1:E:272:HIS:ND1	1:E:338:MSE:HG2	2.29	0.47
1:J:210:VAL:CG1	1:J:211:LYS:N	2.77	0.47
1:D:341:ASP:CA	1:F:84:HIS:HD2	2.19	0.47
1:H:119:GLU:O	1:H:159:VAL:HG23	2.14	0.47
1:I:56:ILE:HD13	1:I:319:ILE:HG13	1.96	0.47
1:L:61:PRO:HA	1:L:85:ASN:ND2	2.29	0.47
1:E:61:PRO:HA	1:E:85:ASN:ND2	2.29	0.47
1:H:181:LEU:HD21	1:H:191:LYS:HG3	1.96	0.47
1:J:9:THR:HG22	1:J:12:GLN:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:9:THR:HG22	1:L:12:GLN:CG	2.44	0.47
1:I:9:THR:HG22	1:I:12:GLN:CG	2.44	0.47
1:H:267:ARG:C	1:H:268:PRO:O	2.50	0.47
1:A:176:THR:HG21	1:A:221:GLY:O	2.14	0.47
1:F:176:THR:HG21	1:F:221:GLY:O	2.14	0.47
1:D:21:PHE:CZ	1:D:232:PRO:HD3	2.50	0.47
1:F:272:HIS:ND1	1:F:338:MSE:HG2	2.29	0.47
1:K:272:HIS:ND1	1:K:338:MSE:HG2	2.29	0.47
1:J:47:LYS:O	1:J:51:GLU:HG3	2.14	0.47
1:K:231:ARG:HG3	1:K:232:PRO:HD2	1.95	0.47
1:A:7:ASN:HB2	1:D:84:HIS:CG	2.49	0.47
1:E:121:ASN:ND2	1:E:121:ASN:N	2.60	0.47
1:H:27:ILE:HD11	1:H:312:LEU:HD11	1.97	0.47
1:A:321:PRO:HB3	1:A:358:ASN:HD22	1.78	0.47
1:D:56:ILE:HD13	1:D:319:ILE:HG13	1.96	0.47
1:L:60:GLU:HB2	1:L:61:PRO:HD2	1.96	0.47
1:G:336:GLN:CG	2:G:404:HOH:O	2.54	0.47
1:C:176:THR:HG21	1:C:221:GLY:O	2.14	0.47
1:E:323:TYR:HA	1:E:350:GLU:HB3	1.97	0.47
1:D:39:ARG:HG3	1:D:40:LEU:HD23	1.97	0.47
1:L:21:PHE:CZ	1:L:232:PRO:HD3	2.50	0.47
1:G:39:ARG:HG3	1:G:40:LEU:HD23	1.97	0.47
1:C:47:LYS:O	1:C:51:GLU:HG3	2.14	0.47
1:L:47:LYS:O	1:L:51:GLU:HG3	2.14	0.47
1:D:171:GLY:CA	1:D:204:CYS:HA	2.43	0.47
1:J:61:PRO:HA	1:J:85:ASN:ND2	2.29	0.47
1:L:321:PRO:HB3	1:L:358:ASN:HD22	1.78	0.47
1:A:61:PRO:HA	1:A:85:ASN:ND2	2.29	0.47
1:G:339:PHE:HB3	2:G:391:HOH:O	2.15	0.47
1:B:21:PHE:CZ	1:B:232:PRO:HD3	2.50	0.47
1:D:231:ARG:CG	1:D:232:PRO:HD2	2.44	0.47
1:C:231:ARG:CG	1:C:232:PRO:HD2	2.44	0.47
1:A:308:TYR:OH	1:A:325:ASP:HB3	2.14	0.47
1:B:308:TYR:OH	1:B:325:ASP:HB3	2.14	0.47
1:I:47:LYS:O	1:I:51:GLU:HG3	2.14	0.47
1:H:68:PRO:HD2	2:H:386:HOH:O	2.14	0.47
1:B:60:GLU:HB2	1:B:61:PRO:HD2	1.96	0.47
1:L:56:ILE:HD13	1:L:319:ILE:HG13	1.96	0.47
1:F:56:ILE:HD13	1:F:319:ILE:HG13	1.96	0.47
1:I:66:VAL:CG2	1:I:71:TYR:HA	2.45	0.47
1:J:177:GLU:O	1:J:181:LEU:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:ARG:HG3	1:E:40:LEU:HD23	1.97	0.47
1:I:231:ARG:CG	1:I:232:PRO:HD2	2.44	0.47
1:A:21:PHE:CZ	1:A:232:PRO:HD3	2.50	0.47
1:E:21:PHE:CZ	1:E:232:PRO:HD3	2.50	0.47
1:K:176:THR:HG21	1:K:221:GLY:O	2.14	0.47
1:A:126:LEU:HD12	1:B:126:LEU:HD12	1.96	0.47
1:J:39:ARG:HG3	1:J:40:LEU:HD23	1.97	0.47
1:J:323:TYR:HA	1:J:350:GLU:HB3	1.97	0.47
1:L:210:VAL:CG1	1:L:211:LYS:N	2.77	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:K:61:PRO:HA	1:K:85:ASN:ND2	2.29	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:D:143:LYS:HG2	1:I:71:TYR:CZ	2.50	0.47
1:H:266:GLY:O	1:H:267:ARG:C	2.53	0.47
1:F:66:VAL:CG2	1:F:71:TYR:HA	2.45	0.47
1:E:176:THR:HG21	1:E:221:GLY:O	2.14	0.47
1:I:176:THR:HG21	1:I:221:GLY:O	2.14	0.47
1:J:176:THR:HG21	1:J:221:GLY:O	2.14	0.47
1:J:21:PHE:CZ	1:J:232:PRO:HD3	2.50	0.47
1:K:231:ARG:CG	1:K:232:PRO:HD2	2.44	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:D:308:TYR:OH	1:D:325:ASP:HB3	2.14	0.47
1:H:108:ASN:HD21	1:H:110:LYS:HB2	1.80	0.47
1:F:61:PRO:HA	1:F:85:ASN:ND2	2.29	0.47
1:D:320:LEU:HD12	1:D:321:PRO:HD2	1.95	0.47
1:D:61:PRO:HA	1:D:85:ASN:ND2	2.29	0.47
1:H:188:HIS:CE1	1:H:189:LEU:HD13	2.49	0.47
1:A:168:ASP:O	1:A:169:GLY:C	2.53	0.47
1:H:181:LEU:HD21	1:H:191:LYS:CG	2.45	0.47
1:E:9:THR:HG22	1:E:12:GLN:CG	2.44	0.47
1:D:9:THR:HG22	1:D:12:GLN:CG	2.44	0.47
1:F:9:THR:HG22	1:F:12:GLN:CG	2.44	0.47
1:A:66:VAL:CG2	1:A:71:TYR:HA	2.45	0.47
1:B:177:GLU:HB3	1:B:209:TRP:HE3	1.76	0.47
1:L:177:GLU:O	1:L:181:LEU:HB2	2.13	0.47
1:A:318:ILE:HD11	1:A:339:PHE:CD1	2.50	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:G:318:ILE:HD11	1:G:339:PHE:CD1	2.50	0.47
1:L:318:ILE:HD11	1:L:339:PHE:CD1	2.50	0.47
1:L:176:THR:HG21	1:L:221:GLY:O	2.14	0.47
1:B:231:ARG:CG	1:B:232:PRO:HD2	2.45	0.47
1:G:21:PHE:CZ	1:G:232:PRO:HD3	2.50	0.47
1:C:21:PHE:CZ	1:C:232:PRO:HD3	2.50	0.47
1:A:39:ARG:HG3	1:A:40:LEU:HD23	1.97	0.47
1:H:69:LEU:HG	2:H:386:HOH:O	2.15	0.47
1:L:54:GLU:O	1:L:57:SER:HB2	2.15	0.47
1:C:39:ARG:HG3	1:C:40:LEU:HD23	1.97	0.47
1:B:54:GLU:O	1:B:57:SER:HB2	2.15	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:C:323:TYR:HA	1:C:350:GLU:HB3	1.97	0.47
1:G:118:TRP:CZ3	1:G:155:THR:HG21	2.50	0.47
1:G:121:ASN:H	1:G:121:ASN:ND2	2.07	0.47
1:L:65:CYS:HB3	1:L:91:MSE:HB3	1.97	0.47
1:A:65:CYS:HB3	1:A:91:MSE:HB3	1.97	0.47
1:F:65:CYS:HB3	1:F:91:MSE:HB3	1.97	0.47
1:C:171:GLY:CA	1:C:204:CYS:HA	2.43	0.47
1:H:159:VAL:O	1:H:159:VAL:HG13	2.15	0.47
1:B:320:LEU:HD12	1:B:321:PRO:HD2	1.95	0.47
1:I:61:PRO:HA	1:I:85:ASN:ND2	2.29	0.47
1:L:168:ASP:O	1:L:169:GLY:C	2.53	0.47
1:C:168:ASP:O	1:C:169:GLY:C	2.53	0.47
1:L:66:VAL:CG2	1:L:71:TYR:HA	2.45	0.47
1:K:113:LEU:O	1:K:150:VAL:HG23	2.13	0.47
1:B:118:TRP:CZ3	1:B:155:THR:HG21	2.50	0.47
1:G:47:LYS:O	1:G:51:GLU:HG3	2.15	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:I:54:GLU:O	1:I:57:SER:HB2	2.15	0.47
1:K:323:TYR:HA	1:K:350:GLU:HB3	1.97	0.47
1:C:210:VAL:CG1	1:C:211:LYS:N	2.77	0.47
1:K:224:ASP:HB2	1:K:360:HIS:HD2	1.80	0.47
1:D:224:ASP:HB2	1:D:360:HIS:HD2	1.80	0.47
1:C:60:GLU:HB2	1:C:61:PRO:HD2	1.96	0.47
1:B:309:LEU:HD22	1:B:311:PHE:HE2	1.80	0.47
1:D:66:VAL:CG2	1:D:71:TYR:HA	2.45	0.47
1:K:66:VAL:CG2	1:K:71:TYR:HA	2.45	0.47
1:G:66:VAL:CG2	1:G:71:TYR:HA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:LYS:HZ2	1:C:46:GLN:HE22	1.63	0.47
1:C:174:LEU:O	1:C:223:ILE:HG21	2.15	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:H:124:GLY:O	1:H:127:VAL:HG13	2.15	0.47
1:C:54:GLU:O	1:C:57:SER:HB2	2.15	0.47
1:J:54:GLU:O	1:J:57:SER:HB2	2.15	0.47
1:E:47:LYS:O	1:E:51:GLU:HG3	2.14	0.47
1:D:318:ILE:HD11	1:D:339:PHE:CD1	2.50	0.47
1:J:168:ASP:O	1:J:169:GLY:C	2.53	0.47
1:E:224:ASP:HB2	1:E:360:HIS:HD2	1.80	0.47
1:J:65:CYS:HB3	1:J:91:MSE:HB3	1.97	0.47
1:C:68:PRO:HG3	1:C:90:GLU:CD	2.36	0.47
1:B:56:ILE:HD13	1:B:319:ILE:HG13	1.96	0.47
1:K:309:LEU:HD22	1:K:311:PHE:HE2	1.80	0.47
1:J:318:ILE:HD11	1:J:339:PHE:CD1	2.50	0.47
1:B:176:THR:HG21	1:B:221:GLY:O	2.14	0.47
1:G:231:ARG:CG	1:G:232:PRO:HD2	2.44	0.47
1:F:21:PHE:CZ	1:F:232:PRO:HD3	2.50	0.47
1:J:118:TRP:CZ3	1:J:155:THR:HG21	2.50	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:K:210:VAL:CG1	1:K:211:LYS:N	2.77	0.46
1:D:174:LEU:O	1:D:223:ILE:HG21	2.15	0.46
1:A:224:ASP:HB2	1:A:360:HIS:HD2	1.80	0.46
1:I:68:PRO:HG3	1:I:90:GLU:CD	2.36	0.46
1:F:68:PRO:HG3	1:F:90:GLU:CD	2.36	0.46
1:H:27:ILE:HD11	1:H:314:VAL:CG1	2.45	0.46
1:G:61:PRO:HA	1:G:85:ASN:ND2	2.29	0.46
1:J:320:LEU:HD12	1:J:321:PRO:HD2	1.95	0.46
1:E:309:LEU:HD22	1:E:311:PHE:HE2	1.80	0.46
1:E:56:ILE:HD13	1:E:319:ILE:HG13	1.96	0.46
1:G:168:ASP:O	1:G:169:GLY:C	2.53	0.46
1:E:168:ASP:O	1:E:169:GLY:C	2.53	0.46
1:C:29:MSE:HE1	1:C:52:VAL:HG13	1.97	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:L:174:LEU:O	1:L:223:ILE:HG21	2.15	0.46
1:I:318:ILE:HD11	1:I:339:PHE:CD1	2.50	0.46
1:B:318:ILE:HD11	1:B:339:PHE:CD1	2.50	0.46
1:I:21:PHE:CZ	1:I:232:PRO:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:CG	1:A:232:PRO:HD2	2.44	0.46
1:G:245:HIS:ND1	1:G:246:PRO:HD2	2.30	0.46
1:K:47:LYS:O	1:K:51:GLU:HG3	2.14	0.46
1:I:308:TYR:OH	1:I:325:ASP:HB3	2.14	0.46
1:I:245:HIS:ND1	1:I:246:PRO:HD2	2.30	0.46
1:I:118:TRP:CZ3	1:I:155:THR:HG21	2.50	0.46
1:F:369:THR:O	1:F:370:LEU:CB	2.47	0.46
1:I:224:ASP:HB2	1:I:360:HIS:HD2	1.80	0.46
1:F:224:ASP:HB2	1:F:360:HIS:HD2	1.80	0.46
1:L:224:ASP:HB2	1:L:360:HIS:HD2	1.80	0.46
1:J:68:PRO:HG3	1:J:90:GLU:CD	2.36	0.46
1:I:171:GLY:CA	1:I:204:CYS:HA	2.43	0.46
1:A:171:GLY:CA	1:A:204:CYS:HA	2.43	0.46
1:D:309:LEU:HD22	1:D:311:PHE:HE2	1.80	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:C:318:ILE:HD11	1:C:339:PHE:CD1	2.50	0.46
1:A:11:LYS:HG3	1:A:203:ASN:ND2	2.31	0.46
1:C:11:LYS:HG3	1:C:203:ASN:ND2	2.31	0.46
1:D:323:TYR:HA	1:D:350:GLU:HB3	1.97	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:L:245:HIS:ND1	1:L:246:PRO:HD2	2.30	0.46
1:E:121:ASN:H	1:E:121:ASN:ND2	2.07	0.46
1:I:65:CYS:HB3	1:I:91:MSE:HB3	1.97	0.46
1:E:65:CYS:HB3	1:E:91:MSE:HB3	1.97	0.46
1:B:224:ASP:HB2	1:B:360:HIS:HD2	1.80	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:29:MSE:HA	1:H:98:ILE:HG21	1.96	0.46
1:C:311:PHE:CE1	1:C:313:ILE:HD11	2.51	0.46
1:B:311:PHE:CE1	1:B:313:ILE:HD11	2.51	0.46
1:L:311:PHE:CE1	1:L:313:ILE:HD11	2.51	0.46
1:K:77:ARG:NH2	1:L:290:ASP:OD1	2.38	0.46
1:H:16:ARG:HH12	1:H:109:ASP:CG	2.19	0.46
1:L:68:PRO:HG3	1:L:90:GLU:CD	2.36	0.46
1:E:66:VAL:CG2	1:E:71:TYR:HA	2.45	0.46
1:K:318:ILE:HD11	1:K:339:PHE:CD1	2.50	0.46
1:A:118:TRP:CZ3	1:A:155:THR:HG21	2.50	0.46
1:J:39:ARG:HH11	1:J:40:LEU:HD23	1.81	0.46
1:F:245:HIS:ND1	1:F:246:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:ARG:HH11	1:F:40:LEU:HD23	1.81	0.46
1:B:336:GLN:HA	1:B:336:GLN:OE1	2.15	0.46
1:F:54:GLU:O	1:F:57:SER:HB2	2.15	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:A:89:ILE:HG22	1:F:147:ILE:CG2	2.36	0.46
1:K:68:PRO:HG3	1:K:90:GLU:CD	2.36	0.46
1:F:171:GLY:CA	1:F:204:CYS:HA	2.43	0.46
1:I:311:PHE:CE1	1:I:313:ILE:HD11	2.51	0.46
1:F:174:LEU:O	1:F:223:ILE:HG21	2.15	0.46
1:B:168:ASP:O	1:B:169:GLY:C	2.53	0.46
1:K:11:LYS:HG3	1:K:203:ASN:ND2	2.31	0.46
1:K:203:ASN:HD22	1:K:203:ASN:HA	1.50	0.46
1:J:215:ASP:HB2	1:J:221:GLY:HA2	1.98	0.46
1:K:21:PHE:CZ	1:K:232:PRO:HD3	2.50	0.46
1:K:245:HIS:ND1	1:K:246:PRO:HD2	2.31	0.46
1:D:168:ASP:O	1:D:169:GLY:C	2.53	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:L:309:LEU:HD22	1:L:311:PHE:HE2	1.80	0.46
1:I:168:ASP:O	1:I:169:GLY:C	2.53	0.46
1:K:174:LEU:O	1:K:223:ILE:HG21	2.15	0.46
1:C:35:ASN:HD22	1:D:43:LYS:NZ	2.14	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:D:118:TRP:CZ3	1:D:155:THR:HG21	2.50	0.46
1:J:158:PHE:CE1	1:J:160:LEU:HB2	2.51	0.46
1:D:39:ARG:HH11	1:D:40:LEU:HD23	1.81	0.46
1:K:65:CYS:HB3	1:K:91:MSE:HB3	1.97	0.46
1:B:68:PRO:HG3	1:B:90:GLU:CD	2.36	0.46
1:D:68:PRO:HG3	1:D:90:GLU:CD	2.36	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:E:311:PHE:CE1	1:E:313:ILE:HD11	2.51	0.46
1:K:311:PHE:CE1	1:K:313:ILE:HD11	2.51	0.46
1:F:168:ASP:O	1:F:169:GLY:C	2.53	0.46
1:D:29:MSE:HE1	1:D:52:VAL:HG13	1.97	0.46
1:L:29:MSE:HE1	1:L:52:VAL:HG13	1.98	0.46
1:C:66:VAL:CG2	1:C:71:TYR:HA	2.45	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:C:215:ASP:HB2	1:C:221:GLY:HA2	1.98	0.46
1:K:158:PHE:CE1	1:K:160:LEU:HB2	2.51	0.46
1:E:231:ARG:CG	1:E:232:PRO:HD2	2.44	0.46
1:G:39:ARG:HH11	1:G:40:LEU:HD23	1.80	0.46
1:B:323:TYR:HA	1:B:350:GLU:HB3	1.97	0.46
1:J:245:HIS:ND1	1:J:246:PRO:HD2	2.31	0.46
1:E:118:TRP:CZ3	1:E:155:THR:HG21	2.50	0.46
1:J:224:ASP:HB2	1:J:360:HIS:HD2	1.80	0.46
1:C:309:LEU:HD22	1:C:311:PHE:HE2	1.80	0.46
1:B:61:PRO:HA	1:B:85:ASN:ND2	2.29	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:F:29:MSE:HE1	1:F:52:VAL:HG13	1.98	0.46
1:A:71:TYR:CZ	1:F:143:LYS:HG2	2.50	0.46
1:F:135:ASP:HB3	1:G:132:PHE:CD2	2.51	0.46
1:E:11:LYS:HG3	1:E:203:ASN:ND2	2.31	0.46
1:B:215:ASP:HB2	1:B:221:GLY:HA2	1.98	0.46
1:F:158:PHE:CE1	1:F:160:LEU:HB2	2.51	0.46
1:C:39:ARG:HH11	1:C:40:LEU:HD23	1.81	0.46
1:H:243:LYS:HA	1:H:248:TYR:CG	2.50	0.46
1:D:245:HIS:ND1	1:D:246:PRO:HD2	2.31	0.46
1:C:336:GLN:OE1	1:C:336:GLN:HA	2.15	0.46
1:G:11:LYS:HG3	1:G:203:ASN:ND2	2.31	0.46
1:H:113:LEU:O	1:H:114:ARG:HG3	2.15	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:L:49:PHE:HA	1:L:52:VAL:HG12	1.98	0.46
1:G:215:ASP:HB2	1:G:221:GLY:HA2	1.98	0.46
1:J:29:MSE:HE1	1:J:52:VAL:HG13	1.97	0.46
1:A:29:MSE:HE1	1:A:52:VAL:HG13	1.98	0.46
1:J:336:GLN:HA	1:J:336:GLN:OE1	2.15	0.46
1:F:215:ASP:HB2	1:F:221:GLY:HA2	1.98	0.46
1:I:158:PHE:CE1	1:I:160:LEU:HB2	2.51	0.46
1:I:39:ARG:HG3	1:I:40:LEU:HD23	1.97	0.46
1:C:245:HIS:ND1	1:C:246:PRO:HD2	2.30	0.46
1:F:118:TRP:CZ3	1:F:155:THR:HG21	2.50	0.46
1:F:336:GLN:HA	1:F:336:GLN:OE1	2.15	0.46
1:F:121:ASN:CG	1:F:159:VAL:HG21	2.37	0.46
1:D:65:CYS:HB3	1:D:91:MSE:HB3	1.97	0.46
1:E:68:PRO:HG3	1:E:90:GLU:CD	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:132:PHE:CB	1:H:133:PRO:HD3	2.40	0.46
1:F:311:PHE:CE1	1:F:313:ILE:HD11	2.51	0.46
1:D:49:PHE:HA	1:D:52:VAL:HG12	1.98	0.46
1:E:49:PHE:HA	1:E:52:VAL:HG12	1.98	0.46
1:I:29:MSE:HE1	1:I:52:VAL:HG13	1.98	0.46
1:B:50:LEU:HG	1:B:81:LEU:HD11	1.98	0.46
1:J:174:LEU:O	1:J:223:ILE:HG21	2.15	0.46
1:G:50:LEU:HG	1:G:81:LEU:HD11	1.98	0.46
1:E:46:GLN:NE2	2:E:379:HOH:O	2.48	0.46
1:I:11:LYS:HG3	1:I:203:ASN:ND2	2.31	0.46
1:D:158:PHE:CE1	1:D:160:LEU:HB2	2.51	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:B:245:HIS:ND1	1:B:246:PRO:HD2	2.31	0.46
1:K:118:TRP:CZ3	1:K:155:THR:HG21	2.50	0.46
1:E:245:HIS:ND1	1:E:246:PRO:HD2	2.30	0.46
1:J:121:ASN:CG	1:J:159:VAL:HG21	2.37	0.46
1:J:94:ASP:HB2	1:J:137:ASP:OD2	2.16	0.46
1:J:171:GLY:CA	1:J:204:CYS:HA	2.43	0.46
1:J:49:PHE:HA	1:J:52:VAL:HG12	1.98	0.46
1:H:4:ARG:NH2	1:H:154:LYS:HD3	2.31	0.46
1:B:11:LYS:HG3	1:B:203:ASN:ND2	2.30	0.46
1:E:158:PHE:CE1	1:E:160:LEU:HB2	2.51	0.46
1:A:158:PHE:CE1	1:A:160:LEU:HB2	2.51	0.46
1:C:118:TRP:CZ3	1:C:155:THR:HG21	2.50	0.46
1:I:336:GLN:HA	1:I:336:GLN:OE1	2.15	0.46
1:L:94:ASP:HB2	1:L:137:ASP:OD2	2.16	0.45
1:C:224:ASP:HB2	1:C:360:HIS:HD2	1.80	0.45
1:H:159:VAL:HG12	1:H:186:ASN:ND2	2.31	0.45
1:A:49:PHE:HA	1:A:52:VAL:HG12	1.98	0.45
1:E:203:ASN:HD22	1:E:203:ASN:HA	1.50	0.45
1:C:158:PHE:CE1	1:C:160:LEU:HB2	2.51	0.45
1:B:39:ARG:HH11	1:B:40:LEU:HD23	1.81	0.45
1:F:39:ARG:HG3	1:F:40:LEU:HD23	1.97	0.45
1:K:291:TYR:OH	1:L:80:GLU:HB2	2.15	0.45
1:A:323:TYR:HA	1:A:350:GLU:HB3	1.97	0.45
1:A:38:TRP:HZ3	1:A:352:ILE:HA	1.81	0.45
1:G:54:GLU:O	1:G:57:SER:HB2	2.15	0.45
1:J:38:TRP:HZ3	1:J:352:ILE:HA	1.81	0.45
1:L:118:TRP:CZ3	1:L:155:THR:HG21	2.50	0.45
1:B:121:ASN:CG	1:B:159:VAL:HG21	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:224:ASP:HB2	1:G:360:HIS:HD2	1.80	0.45
1:B:65:CYS:HB3	1:B:91:MSE:HB3	1.97	0.45
1:E:29:MSE:HE1	1:E:52:VAL:HG13	1.97	0.45
1:I:49:PHE:HA	1:I:52:VAL:HG12	1.98	0.45
1:D:11:LYS:HG3	1:D:203:ASN:ND2	2.31	0.45
1:L:11:LYS:HG3	1:L:203:ASN:ND2	2.30	0.45
1:F:323:TYR:HA	1:F:350:GLU:HB3	1.97	0.45
1:F:38:TRP:HZ3	1:F:352:ILE:HA	1.81	0.45
1:A:161:GLU:HG3	1:A:222:HIS:CE1	2.52	0.45
1:H:351:GLU:HA	1:H:354:TYR:HD2	1.82	0.45
1:E:121:ASN:CG	1:E:159:VAL:HG21	2.37	0.45
1:L:121:ASN:CG	1:L:159:VAL:HG21	2.37	0.45
1:I:94:ASP:HB2	1:I:137:ASP:OD2	2.16	0.45
1:F:94:ASP:HB2	1:F:137:ASP:OD2	2.16	0.45
1:I:309:LEU:HD22	1:I:311:PHE:HE2	1.80	0.45
1:G:336:GLN:HA	1:G:336:GLN:OE1	2.15	0.45
1:I:174:LEU:O	1:I:223:ILE:HG21	2.15	0.45
1:I:50:LEU:HG	1:I: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:J:50:LEU:HG	1:J:81:LEU:HD11	1.98	0.45
1:L:158:PHE:CE1	1:L:160:LEU:HB2	2.51	0.45
1:I:39:ARG:HH11	1:I:40:LEU:HD23	1.81	0.45
1:E:38:TRP:HZ3	1:E:352:ILE:HA	1.81	0.45
1:D:54:GLU:O	1:D:57:SER:HB2	2.15	0.45
1:H:34:ARG:HD2	1:H:94:ASP:O	2.17	0.45
1:G:161:GLU:HG3	1:G:222:HIS:CE1	2.52	0.45
1:D:341:ASP:OD2	1:F:58:GLU:HB3	2.09	0.45
1:F:121:ASN:H	1:F:121:ASN:ND2	2.07	0.45
1:C:121:ASN:CG	1:C:159:VAL:HG21	2.37	0.45
1:E:94:ASP:HB2	1:E:137:ASP:OD2	2.16	0.45
1:G:309:LEU:HD22	1:G:311:PHE:HE2	1.80	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:A:174:LEU:O	1:A:223:ILE:HG21	2.15	0.45
1:L:38:TRP:HZ3	1:L:352:ILE:HA	1.82	0.45
1:J:161:GLU:HG3	1:J:222:HIS:CE1	2.52	0.45
1:I:161:GLU:HG3	1:I:222:HIS:CE1	2.52	0.45
1:A:7:ASN:HB3	1:D:84:HIS:CG	2.50	0.45
1:G:121:ASN:CG	1:G:159:VAL:HG21	2.37	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:J:99:ARG:O	1:J:162:GLY:HA3	2.17	0.45
1:G:65:CYS:HB3	1:G:91:MSE:HB3	1.97	0.45
1:K:168:ASP:O	1:K:169:GLY:C	2.53	0.45
1:A:50:LEU:HG	1:A:81:LEU:HD11	1.98	0.45
1:H:231:ARG:CB	1:H:231:ARG:NH1	2.79	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:L:215:ASP:HB2	1:L:221:GLY:HA2	1.98	0.45
1:D:161:GLU:HG3	1:D:222:HIS:CE1	2.52	0.45
1:L:336:GLN:OE1	1:L:336:GLN:HA	2.15	0.45
1:E:336:GLN:HA	1:E:336:GLN:OE1	2.15	0.45
1:D:38:TRP:HZ3	1:D:352:ILE:HA	1.81	0.45
1:G:99:ARG:O	1:G:162:GLY:HA3	2.17	0.45
1:C:99:ARG:O	1:C:162:GLY:HA3	2.17	0.45
1:A:309:LEU:HD22	1:A:311:PHE:HE2	1.80	0.45
1:D:234:GLU:OE1	1:D:270:LYS:HD3	2.17	0.45
1:F:234:GLU:OE1	1:F:270:LYS:HD3	2.17	0.45
1:B:49:PHE:HA	1:B:52:VAL:HG12	1.98	0.45
1:G:49:PHE:HA	1:G:52:VAL:HG12	1.98	0.45
1:E:339:PHE:HB3	1:E:342:ARG:HB2	1.99	0.45
1:C:339:PHE:HB3	1:C:342:ARG:HB2	1.99	0.45
1:E:215:ASP:HB2	1:E:221:GLY:HA2	1.98	0.45
1:I:203:ASN:HA	1:I:203:ASN:HD22	1.50	0.45
1:G:158:PHE:CE1	1:G:160:LEU:HB2	2.51	0.45
1:E:54:GLU:O	1:E:57:SER:HB2	2.15	0.45
1:C:38:TRP:HZ3	1:C:352:ILE:HA	1.81	0.45
1:H:5:ILE:HG23	1:H:5:ILE:O	2.15	0.45
1:A:336:GLN:OE1	1:A:336:GLN:HA	2.16	0.45
1:A:121:ASN:CG	1:A:159:VAL:HG21	2.37	0.45
1:D:121:ASN:CG	1:D:159:VAL:HG21	2.37	0.45
1:I:219:THR:O	1:I:220:ASN:HB2	2.17	0.45
1:I:99:ARG:O	1:I:162:GLY:HA3	2.17	0.45
1:K:234:GLU:OE1	1:K:270:LYS:HD3	2.17	0.45
1:A:234:GLU:OE1	1:A:270:LYS:HD3	2.17	0.45
1:F:49:PHE:HA	1:F:52:VAL:HG12	1.98	0.45
1:K:49:PHE:HA	1:K:52:VAL:HG12	1.98	0.45
1:E:39:ARG:HH11	1:E:40:LEU:HD23	1.81	0.45
1:A:174:LEU:HD23	1:A:208:LEU:HB2	1.99	0.45
1:H:223:ILE:C	1:H:225:ASP:H	2.19	0.45
1:K:80:GLU:HB2	1:L:291:TYR:HH	1.82	0.45
1:L:39:ARG:HH11	1:L:40:LEU:HD23	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:GLU:HG3	1:F:222:HIS:CE1	2.52	0.45
1:H:339:PHE:HB3	1:H:342:ARG:HG3	1.99	0.45
1:K:195:GLU:HG2	1:K:207:VAL:HG11	1.99	0.45
1:I:174:LEU:HD23	1:I:208:LEU:HB2	1.99	0.45
1:C:234:GLU:OE1	1:C:270:LYS:HD3	2.17	0.45
1:H:191:LYS:HD2	2:H:397:HOH:O	2.17	0.45
1:H:104:THR:O	1:H:104:THR:HG22	2.17	0.45
1:D:43:LYS:HZ2	1:D:46:GLN:HE22	1.63	0.45
1:K:215:ASP:HB2	1:K:221:GLY:HA2	1.98	0.45
1:A:245:HIS:ND1	1:A:246:PRO:HD2	2.30	0.45
1:J:219:THR:O	1:J:220:ASN:HB2	2.17	0.45
1:I:121:ASN:CG	1:I:159:VAL:HG21	2.37	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:J:67:PRO:HA	1:J:68:PRO:HD3	1.80	0.45
1:F:167:VAL:HG12	1:F:168:ASP:N	2.32	0.45
1:K:50:LEU:HG	1:K:81:LEU:HD11	1.98	0.45
1:L:234:GLU:OE1	1:L:270:LYS:HD3	2.17	0.45
1:H:142:ARG:HH12	1:H:146:GLU:HG2	1.81	0.45
1:H:231:ARG:HB2	1:H:231:ARG:CZ	2.47	0.45
1:L:223:ILE:C	1:L:225:ASP:H	2.21	0.45
1:C:50:LEU:HG	1:C:81:LEU:HD11	1.98	0.45
1:G:339:PHE:HB3	1:G:342:ARG:HB2	1.99	0.45
1:B:339:PHE:HB3	1:B:342:ARG:HB2	1.99	0.45
1:A:215:ASP:HB2	1:A:221:GLY:HA2	1.98	0.45
1:A:39:ARG:HH11	1:A:40:LEU:HD23	1.81	0.45
1:K:310:ASN:ND2	2:K:389:HOH:O	2.49	0.45
1:J:330:LEU:O	1:J:334:GLN:HG3	2.17	0.45
1:H:329:GLN:H	1:H:329:GLN:CD	2.21	0.45
1:K:38:TRP:HZ3	1:K:352:ILE:HA	1.82	0.45
1:D:339:PHE:HB3	1:D:342:ARG:HB2	1.99	0.45
1:A:219:THR:O	1:A:220:ASN:HB2	2.17	0.45
1:C:195:GLU:HG2	1:C:207:VAL:HG11	1.99	0.45
1:E:167:VAL:HG12	1:E:168:ASP:N	2.33	0.45
1:K:223:ILE:C	1:K:225:ASP:H	2.21	0.45
1:B:158:PHE:CE1	1:B:160:LEU:HB2	2.51	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:F:327:ASN:HA	1:F:327:ASN:HD22	1.63	0.45
1:D:327:ASN:HD22	1:D:327:ASN:HA	1.63	0.45
1:L:219:THR:O	1:L:220:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:219:THR:O	1:G:220:ASN:HB2	2.17	0.44
1:K:121:ASN:CG	1:K:159:VAL:HG21	2.37	0.44
1:E:369:THR:O	1:E:370:LEU:CB	2.47	0.44
1:C:94:ASP:HB2	1:C:137:ASP:OD2	2.17	0.44
1:L:99:ARG:O	1:L:162:GLY:HA3	2.17	0.44
1:L:195:GLU:HG2	1:L:207:VAL:HG11	1.99	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:C:174:LEU:HD23	1:C:208:LEU:HB2	1.99	0.44
1:G:43:LYS:HZ2	1:G:46:GLN:HE22	1.64	0.44
1:K:40:LEU:HD12	1:L:40:LEU:HB3	1.97	0.44
1:L:161:GLU:HG3	1:L:222:HIS:CE1	2.52	0.44
1:K:336:GLN:OE1	1:K:336:GLN:HA	2.15	0.44
1:D:50:LEU:HG	1:D:81:LEU:HD11	1.98	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: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:E:234:GLU:OE1	1:E:270:LYS:HD3	2.17	0.44
1:B:234:GLU:OE1	1:B:270:LYS:HD3	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:G:223:ILE:C	1:G:225:ASP:H	2.21	0.44
1:C:223:ILE:C	1:C:225:ASP:H	2.21	0.44
1:F:339:PHE:HB3	1:F:342:ARG:HB2	1.99	0.44
1:C:161:GLU:HG3	1:C:222:HIS:CE1	2.52	0.44
1:K:161:GLU:HG3	1:K:222:HIS:CE1	2.52	0.44
1:I:327:ASN:HD22	1:I:327:ASN:HA	1.63	0.44
1:D:336:GLN:OE1	1:D:336:GLN:HA	2.16	0.44
1:D:167:VAL:HG12	1:D:168:ASP:N	2.32	0.44
1:K:121:ASN:N	1:K:121:ASN:ND2	2.60	0.44
1:B:219:THR:O	1:B:220:ASN:HB2	2.17	0.44
1:D:91:MSE:SE	1:D:140:VAL:HG13	2.67	0.44
1:C:91:MSE:SE	1:C:140:VAL:HG13	2.68	0.44
1:A:94:ASP:HB2	1:A:137:ASP:OD2	2.17	0.44
1:B:94:ASP:HB2	1:B:137:ASP:OD2	2.17	0.44
1: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:F:67:PRO:HA	1:F:68:PRO:HD3	1.80	0.44
1:J:195:GLU:HG2	1:J:207:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:234:GLU:OE1	1:I:270:LYS:HD3	2.17	0.44
1:B:167:VAL:HG12	1:B:168:ASP:N	2.32	0.44
1:J:234:GLU:OE1	1:J:270:LYS:HD3	2.17	0.44
1:F:50:LEU:HG	1:F:81:LEU:HD11	1.98	0.44
1:A:223:ILE:C	1:A:225:ASP:H	2.21	0.44
1:L:339:PHE:HB3	1:L:342:ARG:HB2	1.99	0.44
1:B:330:LEU:O	1:B:334:GLN:HG3	2.17	0.44
1:I:330:LEU:O	1:I:334:GLN:HG3	2.17	0.44
1:D:330:LEU:O	1:D:334:GLN:HG3	2.17	0.44
1:G:119:GLU:HB2	1:G:159:VAL:HA	2.00	0.44
1:C:119:GLU:HB2	1:C:159:VAL:HA	2.00	0.44
1:D:94:ASP:HB2	1:D:137:ASP:OD2	2.17	0.44
1:E:99:ARG:O	1:E:162:GLY:HA3	2.17	0.44
1:A:99:ARG:O	1:A:162:GLY:HA3	2.17	0.44
1:D:99:ARG:O	1:D:162:GLY:HA3	2.17	0.44
1:G:91:MSE:SE	1:G:140:VAL:HG13	2.68	0.44
1:H:57:SER:HA	1:H:85:ASN:HD21	1.82	0.44
1:D:30:LEU:HD22	1:D:93:ASN:HD22	1.83	0.44
1:A:195:GLU:HG2	1:A:207:VAL:HG11	1.99	0.44
1:A:167:VAL:HG12	1:A:168:ASP:N	2.32	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: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:B:161:GLU:HG3	1:B:222:HIS:CE1	2.52	0.44
1:G:30:LEU:HD22	1:G:93:ASN:HD22	1.83	0.44
1:J:369:THR:O	1:J:370:LEU:CB	2.47	0.44
1:D:223:ILE:C	1:D:225:ASP:H	2.21	0.44
1:J:167:VAL:HG12	1:J:168:ASP:N	2.32	0.44
1:K:219:THR:O	1:K:220:ASN:HB2	2.17	0.44
1:B:91:MSE:SE	1:B:140:VAL:HG13	2.68	0.44
1:H:119:GLU:HB2	1:H:159:VAL:HA	2.00	0.44
1:I:161:GLU:HG3	1:I:222:HIS:NE2	2.33	0.44
1:I:30:LEU:HD22	1:I:93:ASN:HD22	1.83	0.44
1:A:12:GLN:HB3	1:D:81:LEU:C	2.38	0.44
1:I:185:ARG:CB	1:I:185:ARG:HH11	2.11	0.44
1:E:219:THR:O	1:E:220:ASN:HB2	2.17	0.44
1:K:119:GLU:HB2	1:K:159:VAL:HA	2.00	0.44
1:J:91:MSE:SE	1:J:140:VAL:HG13	2.67	0.44
1:I:223:ILE:C	1:I:225:ASP:H	2.21	0.44
1:H:215:ASP:HB2	1:H:221:GLY:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:43:LYS:HZ2	1:I:46:GLN:HE22	1.65	0.44
1:A:339:PHE:HB3	1:A:342:ARG:HB2	1.99	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:E:161:GLU:HG3	1:E:222:HIS:CE1	2.52	0.44
1:C:30:LEU:HD22	1:C:93:ASN:HD22	1.83	0.44
1:J:119:GLU:HB2	1:J:159:VAL:HA	2.00	0.44
1:A:119:GLU:HB2	1:A:159:VAL:HA	2.00	0.44
1:E:119:GLU:HB2	1:E:159:VAL:HA	2.00	0.44
1:L:119:GLU:HB2	1:L:159:VAL:HA	2.00	0.44
1:K:339:PHE:HB3	1:K:342:ARG:HB2	1.99	0.44
1:B:118:TRP:HA	1:B:155:THR:OG1	2.18	0.44
1:F:161:GLU:HG3	1:F:222:HIS:NE2	2.33	0.44
1:K:161:GLU:HG3	1:K:222:HIS:NE2	2.33	0.44
1:B:161:GLU:HG3	1:B:222:HIS:NE2	2.33	0.44
1:E:161:GLU:HG3	1:E:222:HIS:NE2	2.33	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:F:330:LEU:O	1:F:334:GLN:HG3	2.17	0.44
1:D:174:LEU:HD23	1:D:208:LEU:HB2	1.99	0.44
1:B:195:GLU:HG2	1:B:207:VAL:HG11	1.99	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:C:108:ASN:OD1	1:C:112:ASP:HB2	2.18	0.44
1:F:108:ASN:OD1	1:F:112:ASP:HB2	2.18	0.44
1:J:325:ASP:O	1:J:328:ASP:HB2	2.18	0.44
1:C:325:ASP:O	1:C:328:ASP:HB2	2.18	0.44
1:B:325:ASP:O	1:B:328:ASP:HB2	2.18	0.44
1:C:161:GLU:HG3	1:C:222:HIS:NE2	2.33	0.44
1:E:30:LEU:HD22	1:E:93:ASN:HD22	1.83	0.44
1:C:95:ASP:HB2	1:C:131:TYR:CE2	2.53	0.44
1:A:30:LEU:HD22	1:A:93:ASN:HD22	1.83	0.44
1:J:95:ASP:HB2	1:J:131:TYR:CE2	2.53	0.44
1:D:219:THR:O	1:D:220:ASN:HB2	2.17	0.44
1:G:234:GLU:OE1	1:G:270:LYS:HD3	2.17	0.44
1:F:223:ILE:C	1:F:225:ASP:H	2.21	0.44
1:B:114:ARG:NH1	2:B:380:HOH:O	2.31	0.44
1:I:215:ASP:HB2	1:I:221:GLY:HA2	1.98	0.44
1:I:108:ASN:OD1	1:I:112:ASP:HB2	2.18	0.44
1:D:325:ASP:O	1:D:328:ASP:HB2	2.18	0.44
1:I:325:ASP:O	1:I:328:ASP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:118:TRP:HA	1:K:155:THR:OG1	2.18	0.44
1:C:118:TRP:HA	1:C:155:THR:OG1	2.18	0.44
1:L:118:TRP:HA	1:L:155:THR:OG1	2.18	0.44
1:L:95:ASP:HB2	1:L:131:TYR:CE2	2.53	0.44
1:A:329:GLN:H	1:A:329:GLN:CD	2.22	0.44
1:B:119:GLU:HB2	1:B:159:VAL:HA	2.00	0.43
1:H:121:ASN:O	1:H:125:GLY:HA2	2.18	0.43
1:K:174:LEU:HD23	1:K:208:LEU:HB2	1.99	0.43
1:J:223:ILE:C	1:J:225:ASP:H	2.21	0.43
1:B:203:ASN:HD22	1:B:203:ASN:HA	1.50	0.43
1:F:118:TRP:HA	1:F:155:THR:OG1	2.18	0.43
1:G:161:GLU:HG3	1:G:222:HIS:NE2	2.33	0.43
1:B:38:TRP:HZ3	1:B:352:ILE:HA	1.82	0.43
1:F:142:ARG:N	2:F:388:HOH:O	2.46	0.43
1:E:330:LEU:O	1:E:334:GLN:HG3	2.17	0.43
1:K:91:MSE:SE	1:K:140:VAL:HG13	2.67	0.43
1:E:91:MSE:SE	1:E:140:VAL:HG13	2.68	0.43
1:A:91:MSE:SE	1:A:140:VAL:HG13	2.68	0.43
1:F:91:MSE:SE	1:F:140:VAL:HG13	2.68	0.43
1:G:195:GLU:HG2	1:G:207:VAL:HG11	1.99	0.43
1:G:167:VAL:HG12	1:G:168:ASP:N	2.32	0.43
1:L:174:LEU:HD23	1:L:208:LEU:HB2	1.99	0.43
1:E:174:LEU:HD23	1:E:208:LEU:HB2	1.99	0.43
1:D:118:TRP:HA	1:D:155:THR:OG1	2.18	0.43
1:B:108:ASN:OD1	1:B:112:ASP:HB2	2.18	0.43
1:E:325:ASP:O	1:E:328:ASP:HB2	2.18	0.43
1:L:325:ASP:O	1:L:328:ASP:HB2	2.18	0.43
1:K:330:LEU:O	1:K:334:GLN:HG3	2.17	0.43
1:B:329:GLN:H	1:B:329:GLN:CD	2.22	0.43
1:K:369:THR:O	1:K:370:LEU:CB	2.47	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:L:121:ASN:ND2	1:L:121:ASN:N	2.60	0.43
1:D:195:GLU:HG2	1:D:207:VAL:HG11	1.99	0.43
1:I:167:VAL:HG12	1:I:168:ASP:N	2.33	0.43
1:J:339:PHE:HB3	1:J:342:ARG:HB2	1.99	0.43
1:G:325:ASP:O	1:G:328:ASP:HB2	2.18	0.43
1:E:118:TRP:HA	1:E:155:THR:OG1	2.18	0.43
1:J:161:GLU:HG3	1:J:222:HIS:NE2	2.33	0.43
1:L:161:GLU:HG3	1:L:222:HIS:NE2	2.33	0.43
1:B:95:ASP:HB2	1:B:131:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:ASP:HB2	1:D:131:TYR:CE2	2.53	0.43
1:E:95:ASP:HB2	1:E:131:TYR:CE2	2.53	0.43
1:A:189:LEU:HA	1:A:189:LEU:HD12	1.84	0.43
1:K:329:GLN:CD	1:K:329:GLN:H	2.22	0.43
1:I:189:LEU:HD12	1:I:189:LEU:HA	1.84	0.43
1:L:91:MSE:SE	1:L:140:VAL:HG13	2.68	0.43
1:E:195:GLU:HG2	1:E:207:VAL:HG11	1.99	0.43
1:J:321:PRO:HB3	1:J:358:ASN:ND2	2.34	0.43
1:L:167:VAL:HG12	1:L:168:ASP:N	2.33	0.43
1:C:167:VAL:HG12	1:C:168:ASP:N	2.32	0.43
1:K:167:VAL:HG12	1:K:168:ASP:N	2.33	0.43
1:D:161:GLU:HG3	1:D:222:HIS:NE2	2.33	0.43
1:F:30:LEU:HD22	1:F:93:ASN:HD22	1.83	0.43
1:A:330:LEU:O	1:A:334:GLN:HG3	2.17	0.43
1:D:329:GLN:CD	1:D:329:GLN:H	2.22	0.43
1:L:330:LEU:O	1:L:334:GLN:HG3	2.17	0.43
1:E:185:ARG:CB	1:E:185:ARG:HH11	2.11	0.43
1:H:80:GLU:C	1:H:82:GLY:H	2.22	0.43
1:J:174:LEU:HD23	1:J:208:LEU:HB2	1.99	0.43
1:J:118:TRP:HA	1:J:155:THR:OG1	2.18	0.43
1:H:5:ILE:HD13	1:H:153:TYR:CE2	2.54	0.43
1:K:95:ASP:HB2	1:K:131:TYR:CE2	2.53	0.43
1:E:236:ALA:O	1:E:237:CYS:HB2	2.19	0.43
1:I:329:GLN:CD	1:I:329:GLN:H	2.22	0.43
1:J:327:ASN:HD22	1:J:327:ASN:HA	1.63	0.43
1:I:119:GLU:HB2	1:I:159:VAL:HA	2.00	0.43
1:B:321:PRO:HB3	1:B:358:ASN:ND2	2.34	0.43
1:K:66:VAL:HG21	1:K:71:TYR:HA	2.01	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:B:236:ALA:O	1:B:237:CYS:HB2	2.19	0.43
1:C:330:LEU:O	1:C:334:GLN:HG3	2.17	0.43
1:F:236:ALA:O	1:F:237:CYS:HB2	2.19	0.43
1:F:95:ASP:HB2	1:F:131:TYR:CE2	2.53	0.43
1:J:329:GLN:H	1:J:329:GLN:CD	2.22	0.43
1:E:329:GLN:CD	1:E:329:GLN:H	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:118:TRP:HA	1:I:155:THR:OG1	2.18	0.43
1:I:95:ASP:HB2	1:I:131:TYR:CE2	2.53	0.43
1:K:236:ALA:O	1:K:237:CYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:30:LEU:HD22	1:L:93:ASN:HD22	1.83	0.43
1:L:329:GLN:H	1:L:329:GLN:CD	2.22	0.43
1:F:329:GLN:H	1:F:329:GLN:CD	2.22	0.43
1:C:327:ASN:HD22	1:C:327:ASN:HA	1.63	0.43
1:G:89:ILE:H	1:G:89:ILE:CD1	2.22	0.43
1:H:224:ASP:HB2	1:H:360:HIS:HD2	1.81	0.43
1:C:132:PHE:CD2	1:I:135:ASP:HB3	2.53	0.43
1:I:66:VAL:HG21	1:I:71:TYR:HA	2.01	0.43
1:A:66:VAL:HG21	1:A:71:TYR:HA	2.01	0.43
1:E:223:ILE:C	1:E:225:ASP:H	2.21	0.43
1:K:108:ASN:OD1	1:K:112:ASP:HB2	2.18	0.43
1:G:236:ALA:O	1:G:237:CYS:HB2	2.19	0.43
1:C:329:GLN:H	1:C:329:GLN:CD	2.22	0.43
1:K:327:ASN:HD22	1:K:327:ASN:HA	1.63	0.43
1:I:195:GLU:HG2	1:I:207:VAL:HG11	1.99	0.43
1:E:321:PRO:HB3	1:E:358:ASN:ND2	2.34	0.43
1:E:135:ASP:HB3	1:L:132:PHE:HE2	1.78	0.43
1:E:66:VAL:HG21	1:E:71:TYR:HA	2.01	0.43
1:B:174:LEU:HD23	1:B:208:LEU:HB2	1.99	0.43
1:A:325:ASP:O	1:A:328:ASP:HB2	2.18	0.43
1:G:118:TRP:HA	1:G:155:THR:OG1	2.18	0.43
1:J:185:ARG:CB	1:J:185:ARG:HH11	2.11	0.43
1:A:121:ASN:H	1:A:121:ASN:ND2	2.07	0.43
1:H:15:PHE:CE2	1:H:108:ASN:HB3	2.54	0.43
1:F:195:GLU:HG2	1:F:207:VAL:HG11	1.99	0.43
1:C:321:PRO:HB3	1:C:358:ASN:ND2	2.34	0.43
1:B:171:GLY:CA	1:B:204:CYS:HA	2.43	0.43
1:F:98:ILE:HG22	2:F:379:HOH:O	2.18	0.43
1:C:66:VAL:HG21	1:C:71:TYR:HA	2.01	0.43
1:A:43:LYS:HZ2	1:A:46:GLN:HE22	1.66	0.43
1:E:40:LEU:HD22	1:E:288:THR:OG1	2.19	0.43
1:A:118:TRP:HA	1:A:155:THR:OG1	2.18	0.43
1:J:108:ASN:OD1	1:J:112:ASP:HB2	2.18	0.43
1:K:325:ASP:O	1:K:328:ASP:HB2	2.18	0.43
1:F:40:LEU:HD22	1:F:288:THR:OG1	2.19	0.43
1:G:95:ASP:HB2	1:G:131:TYR:CE2	2.53	0.43
1:L:236:ALA:O	1:L:237:CYS:HB2	2.19	0.43
1:C:185:ARG:HH11	1:C:185:ARG:CB	2.11	0.42
1:C:311:PHE:HE1	1:C:313:ILE:HD11	1.84	0.42
1:A:321:PRO:HB3	1:A:358:ASN:ND2	2.34	0.42
1:L:311:PHE:HE1	1:L:313:ILE:HD11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:GLU:OE1	1:H:360:HIS:HE1	2.02	0.42
1:G:66:VAL:HG21	1:G:71:TYR:HA	2.01	0.42
1:D:203:ASN:HA	1:D:203:ASN:HD22	1.50	0.42
1:J:203:ASN:HA	1:J:203:ASN:HD22	1.50	0.42
1:L:108:ASN:OD1	1:L:112:ASP:HB2	2.18	0.42
1:F:325:ASP:O	1:F:328:ASP:HB2	2.18	0.42
1:K:40:LEU:HD22	1:K:288:THR:OG1	2.19	0.42
1:B:138:ALA:HB1	2:B:384:HOH:O	2.19	0.42
1:I:236:ALA:O	1:I:237:CYS:HB2	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:B:40:LEU:HD22	1:B:288:THR:OG1	2.19	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: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:A:315:ASN:CB	2:A:379:HOH:O	2.63	0.42
1:I:339:PHE:HB3	1:I:342:ARG:HB2	1.99	0.42
1:I:40:LEU:HD22	1:I:288:THR:OG1	2.19	0.42
1:F:142:ARG:HB2	2:F:388:HOH:O	2.20	0.42
1:A:236:ALA:O	1:A:237:CYS:HB2	2.19	0.42
1:C:291:TYR:OH	1:D:80:GLU:HB2	2.19	0.42
1:F:321:PRO:HB3	1:F:358:ASN:ND2	2.34	0.42
1:B:66:VAL:HG21	1:B:71:TYR:HA	2.01	0.42
1:H:263:ASP:C	1:H:265:LYS:H	2.23	0.42
1:G:329:GLN:H	1:G:329:GLN:CD	2.22	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:G:321:PRO:HB3	1:G:358:ASN:ND2	2.34	0.42
1:H:178:MSE:SE	1:H:221:GLY:HA3	2.69	0.42
1:J:66:VAL:HG21	1:J:71:TYR:HA	2.01	0.42
1:D:66:VAL:HG21	1:D:71:TYR:HA	2.01	0.42
1:A:127:VAL:HG12	2:A:382:HOH:O	2.19	0.42
1:E:108:ASN:OD1	1:E:112:ASP:HB2	2.18	0.42
1:H:11:LYS:HG3	1:H:203:ASN:ND2	2.34	0.42
1:L:252:LYS:HE2	1:L:252:LYS:HB3	1.92	0.42
1:H:310:ASN:OD1	1:H:358:ASN:HB3	2.19	0.42
1:E:171:GLY:CA	1:E:204:CYS:HA	2.43	0.42
1:B:311:PHE:HE1	1:B:313:ILE:HD11	1.84	0.42
1:L:321:PRO:HB3	1:L:358:ASN:ND2	2.34	0.42
1:D:108:ASN:OD1	1:D:112:ASP:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD22	1:A:288:THR:OG1	2.19	0.42
1:J:40:LEU:HD22	1:J:288:THR:OG1	2.19	0.42
1:H:5:ILE:HD11	1:H:8:THR:OG1	2.19	0.42
1:D:236:ALA:O	1:D:237:CYS:HB2	2.19	0.42
1:A:35:ASN:N	1:A:35:ASN:OD1	2.53	0.42
1:A:7:ASN:HB2	1:D:84:HIS:CD2	2.54	0.42
1:F:185:ARG:CB	1:F:185:ARG:HH11	2.11	0.42
1:K:121:ASN:O	1:K:125:GLY:HA2	2.20	0.42
1:H:313:ILE:HD12	1:H:318:ILE:HD11	2.00	0.42
1:K:311:PHE:HE1	1:K:313:ILE:HD11	1.84	0.42
1:I:174:LEU:HB3	1:I:223:ILE:CD1	2.50	0.42
1:C:71:TYR:CZ	1:J:143:LYS:HG2	2.54	0.42
1:C:35:ASN:OD1	1:C:35:ASN:N	2.53	0.42
1:C:40:LEU:HD22	1:C:288:THR:OG1	2.19	0.42
1:C:236:ALA:O	1:C:237:CYS:HB2	2.19	0.42
1:H:230:ILE:O	1:H:231:ARG:HB2	2.20	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:325:ASP:N	1:H:328:ASP:OD1	2.50	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:C:224:ASP:HB2	1:C:360:HIS:CD2	2.55	0.42
1:K:321:PRO:HB3	1:K:358:ASN:ND2	2.34	0.42
1:A:203:ASN:HD22	1:A:203:ASN:HA	1.50	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:I:121:ASN:O	1:I:125:GLY:HA2	2.20	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:B:121:ASN:O	1:B:125:GLY:HA2	2.20	0.42
1:L:35:ASN:OD1	1:L:35:ASN:N	2.53	0.42
1:G:40:LEU:HD22	1:G:288:THR:OG1	2.19	0.42
1:F:182:HIS:ND1	1:F:183:PRO:HD2	2.35	0.42
1:G:182:HIS:ND1	1:G:183:PRO:HD2	2.35	0.42
1:B:182:HIS:ND1	1:B:183:PRO:HD2	2.35	0.42
1:J:121:ASN:O	1:J:125:GLY:HA2	2.20	0.41
1:F:121:ASN:N	1:F:121:ASN:ND2	2.60	0.41
1:G:185:ARG:CB	1:G:185:ARG:HH11	2.11	0.41
1:L:224:ASP:HB2	1:L:360:HIS:CD2	2.55	0.41
1:I:309:LEU:HD22	1:I:309:LEU:HA	1.92	0.41
1:J:311:PHE:HE1	1:J:313:ILE:HD11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:171:GLY:CA	1:L:204:CYS:HA	2.43	0.41
1:F:311:PHE:HE1	1:F:313:ILE:HD11	1.84	0.41
1:L:115:ALA:O	1:L:153:TYR:HD1	2.03	0.41
1:H:231:ARG:HB3	1:H:231:ARG:HH11	1.85	0.41
1:D:40:LEU:HD22	1:D:288:THR:OG1	2.19	0.41
1:K:189:LEU:HA	1:K:189:LEU:HD12	1.84	0.41
1:L:121:ASN:O	1:L:125:GLY:HA2	2.20	0.41
1:G:215:ASP:N	1:G:216:PRO:HD3	2.36	0.41
1:I:215:ASP:N	1:I:216:PRO:HD3	2.36	0.41
1:H:94:ASP:OD2	1:H:136:GLN:HB2	2.20	0.41
1:A:182:HIS:ND1	1:A:183:PRO:HD2	2.35	0.41
1:B:189:LEU:HD12	1:B:189:LEU:HA	1.84	0.41
1:B:35:ASN:N	1:B:35:ASN:OD1	2.53	0.41
1:J:224:ASP:HB2	1:J:360:HIS:CD2	2.55	0.41
1:I:311:PHE:HE1	1:I:313:ILE:HD11	1.84	0.41
1:H:171:GLY:HA2	1:H:204:CYS:HA	2.01	0.41
1:K:35:ASN:N	1:K:35:ASN:OD1	2.53	0.41
1:F:189:LEU:HA	1:F:189:LEU:HD12	1.84	0.41
1:D:121:ASN:O	1:D:125:GLY:HA2	2.20	0.41
1:B:56:ILE:HG12	1:B:56:ILE:H	1.67	0.41
1:J:56:ILE:HG12	1:J:56:ILE:H	1.67	0.41
1:F:174:LEU:HB3	1:F:223:ILE:CD1	2.50	0.41
1:D:215:ASP:N	1:D:216:PRO:HD3	2.36	0.41
1:B:215:ASP:N	1:B:216:PRO:HD3	2.36	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:J:189:LEU:HD12	1:J:189:LEU:HA	1.84	0.41
1:D:35:ASN:N	1:D:35:ASN:OD1	2.53	0.41
1:K:103:PRO:CD	1:K:144:VAL:HG11	2.50	0.41
1:K:67:PRO:HA	1:K:68:PRO:HD3	1.80	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:L:43:LYS:HZ2	1:L:46:GLN:HE22	1.67	0.41
1:G:35:ASN:OD1	1:G:35:ASN:N	2.53	0.41
1:J:35:ASN:N	1:J:35:ASN:OD1	2.53	0.41
1:E:215:ASP:N	1:E:216:PRO:HD3	2.36	0.41
1:A:40:LEU:HD12	1:G:40:LEU:HB3	2.02	0.41
1:I:182:HIS:ND1	1:I:183:PRO:HD2	2.35	0.41
1:H:198:LEU:CD2	1:H:202:LEU:HD22	2.48	0.41
1:H:105:PHE:CB	1:H:367:PRO:HD2	2.51	0.41
1:H:100:ASP:CB	1:H:161:GLU:HB2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ALA:O	1:C:153:TYR:HD1	2.03	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:H:8:THR:HB	1:H:13:ASP:OD1	2.20	0.41
1:E:327:ASN:HD22	1:E:327:ASN:HA	1.63	0.41
1:D:182:HIS:ND1	1:D:183:PRO:HD2	2.36	0.41
1:B:224:ASP:HB2	1:B:360:HIS:CD2	2.55	0.41
1:G:171:GLY:CA	1:G:204:CYS:HA	2.43	0.41
1:D:115:ALA:O	1:D:153:TYR:HD1	2.03	0.41
1:L:66:VAL:HG21	1:L:71:TYR:HA	2.01	0.41
1:G:161:GLU:HG3	1:G:222:HIS:HE2	1.86	0.41
1:A:121:ASN:O	1:A:125:GLY:HA2	2.20	0.41
1:C:103:PRO:CD	1:C:144:VAL:HG11	2.50	0.41
1:G:224:ASP:HB2	1:G:360:HIS:CD2	2.55	0.41
1:G:103:PRO:CD	1:G:144:VAL:HG11	2.50	0.41
1:D:67:PRO:HA	1:D:68:PRO:HD3	1.80	0.41
1:J:24:GLN:HA	1:J:368:ALA:N	2.33	0.41
1:A:311:PHE:HE1	1:A:313:ILE:HD11	1.84	0.41
1:H:121:ASN:O	1:H:125:GLY:N	2.51	0.41
1:F:115:ALA:O	1:F:153:TYR:HD1	2.03	0.41
1:H:172:THR:HG22	1:H:173:VAL:H	1.86	0.41
1:G:300:GLU:HG2	1:G:301:GLY:N	2.36	0.41
1:F:300:GLU:HG2	1:F:301:GLY:N	2.36	0.41
1:B:252:LYS:HB3	1:B:252:LYS:HE2	1.92	0.41
1:A:12:GLN:NE2	1:D:82:GLY:HA2	2.19	0.41
1:B:185:ARG:HH11	1:B:185:ARG:CB	2.11	0.41
1:I:103:PRO:CD	1:I:144:VAL:HG11	2.50	0.41
1:B:103:PRO:CD	1:B:144:VAL:HG11	2.50	0.41
1:H:133:PRO:HG3	1:K:135:ASP:CG	2.41	0.41
1:H:24:GLN:NE2	1:H:314:VAL:HG12	2.36	0.41
1:E:311:PHE:HE1	1:E:313:ILE:HD11	1.84	0.41
1:A:24:GLN:HA	1:A:368:ALA:N	2.33	0.41
1:I:115:ALA:O	1:I:153:TYR:HD1	2.03	0.41
1:H:173:VAL:HG12	1:H:206:LYS:O	2.20	0.41
1:F:66:VAL:HG21	1:F:71:TYR:HA	2.01	0.41
1:A:124:GLY:O	1:A:127:VAL:HG13	2.21	0.41
1:B:43:LYS:HZ2	1:B:46:GLN:HE22	1.68	0.41
1:A:215:ASP:N	1:A:216:PRO:HD3	2.36	0.41
1:C:203:ASN:HA	1:C:203:ASN:HD22	1.50	0.41
1:B:300:GLU:HG2	1:B:301:GLY:N	2.36	0.41
1:I:300:GLU:HG2	1:I:301:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:HE2	1:A:252:LYS:HB3	1.92	0.41
1:I:80:GLU:HB2	1:J:291:TYR:OH	2.21	0.41
1:A:300:GLU:HG2	1:A:301:GLY:N	2.36	0.41
1:L:300:GLU:HG2	1:L:301:GLY:N	2.36	0.41
1:J:182:HIS:ND1	1:J:183:PRO:HD2	2.36	0.41
1:E:35:ASN:N	1:E:35:ASN:OD1	2.53	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:F:99:ARG:HD3	1:F:360:HIS:CD2	2.56	0.41
1:B:27:ILE:HG13	1:B:60:GLU:OE2	2.21	0.41
1:G:311:PHE:HE1	1:G:313:ILE:HD11	1.84	0.41
1:A:174:LEU:HB3	1:A:223:ILE:CD1	2.50	0.41
1:C:215:ASP:N	1:C:216:PRO:HD3	2.36	0.41
1:B:233:GLY:N	2:B:397:HOH:O	2.54	0.41
1:C:182:HIS:ND1	1:C:183:PRO:HD2	2.35	0.41
1:B:327:ASN:HA	1:B:327:ASN:HD22	1.63	0.41
1:E:224:ASP:HB2	1:E:360:HIS:CD2	2.55	0.40
1:J:27:ILE:HG13	1:J:60:GLU:OE2	2.21	0.40
1:K:171:GLY:CA	1:K:204:CYS:HA	2.43	0.40
1:H:4:ARG:NH1	1:H:142:ARG:HD3	2.35	0.40
1:H:231:ARG:HB2	1:H:231:ARG:NH1	2.36	0.40
1:F:124:GLY:O	1:F:127:VAL:HG13	2.21	0.40
1:L:124:GLY:O	1:L:127:VAL:HG13	2.21	0.40
1:C:124:GLY:O	1:C:127:VAL:HG13	2.21	0.40
1:J:215:ASP:N	1:J:216:PRO:HD3	2.36	0.40
1:F:215:ASP:N	1:F:216:PRO:HD3	2.36	0.40
1:H:296:ILE:O	1:H:296:ILE:HG23	2.20	0.40
1:L:327:ASN:HD22	1:L:327:ASN:HA	1.63	0.40
1:D:173:VAL:HG22	1:D:174:LEU:N	2.37	0.40
1:A:224:ASP:HB2	1:A:360:HIS:CD2	2.55	0.40
1:D:243:LYS:NZ	1:H:192:GLU:CG	2.73	0.40
1:H:113:LEU:O	1:H:150:VAL:HG23	2.20	0.40
1:G:27:ILE:HG13	1:G:60:GLU:OE2	2.21	0.40
1:F:173:VAL:HG22	1:F:174:LEU:N	2.37	0.40
1:I:173:VAL:HG22	1:I:174:LEU:N	2.36	0.40
1:H:100:ASP:OD1	1:H:100:ASP:N	2.54	0.40
1:B:115:ALA:O	1:B:153:TYR:HD1	2.03	0.40
1:D:124:GLY:O	1:D:127:VAL:HG13	2.21	0.40
1:A:155:THR:HB	1:A:158:PHE:HB3	2.04	0.40
1:E:182:HIS:ND1	1:E:183:PRO:HD2	2.35	0.40
1:C:300:GLU:HG2	1:C:301:GLY: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:I:99:ARG:HD3	1:I:360:HIS:CD2	2.56	0.40
1:E:99:ARG:HD3	1:E:360:HIS:CD2	2.56	0.40
1:G:99:ARG:HD3	1:G:360:HIS:CD2	2.56	0.40
1:E:124:GLY:O	1:E:127:VAL:HG13	2.21	0.40
1:H:17:MSE:HB2	1:H:106:LEU:CD2	2.51	0.40
1:C:27:ILE:HG13	1:C:60:GLU:OE2	2.21	0.40
1:G:115:ALA:O	1:G:153:TYR:HD1	2.04	0.40
1:K:115:ALA:O	1:K:153:TYR:HD1	2.03	0.40
1:I:30:LEU:HD22	1:I:93:ASN:ND2	2.37	0.40
1:J:300:GLU:HG2	1:J:301:GLY:N	2.36	0.40
1:E:300:GLU:HG2	1:E:301:GLY:N	2.36	0.40
1:L:189:LEU:HA	1:L:189:LEU:HD12	1.84	0.40
1:C:121:ASN:O	1:C:125:GLY:HA2	2.20	0.40
1:E:103:PRO:CD	1:E:144:VAL:HG11	2.50	0.40
1:B:99:ARG:HD3	1:B:360:HIS:CD2	2.56	0.40
1:L:99:ARG:HD3	1:L:360:HIS:CD2	2.56	0.40
1:D:68:PRO:HG3	1:D:90:GLU:CG	2.52	0.40
1:K:68:PRO:HG3	1:K:90:GLU:CG	2.52	0.40
1:E:174:LEU:HB3	1:E:223:ILE:CD1	2.50	0.40
1:D:155:THR:HB	1:D:158:PHE:HB3	2.04	0.40
1:F:30:LEU:HD22	1:F:93:ASN:ND2	2.37	0.40
1:K:27:ILE:HG13	1:K:60:GLU:OE2	2.21	0.40
1:L:27:ILE:HG13	1:L:60:GLU:OE2	2.21	0.40
1:H:226:VAL:HG23	1:H:227:ALA:N	2.37	0.40
1:K:182:HIS:ND1	1:K:183:PRO:HD2	2.35	0.40
1:I:35:ASN:N	1:I:35:ASN:OD1	2.53	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: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:A:329:GLN:CG	1:E:282:TYR:OH[2_646]	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: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
1:A:330:LEU:N	1:E:282:TYR:CE2[2_646]	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%)	<div>9</div> <div>33</div>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	9	33
1	C	358/377 (95%)	291 (81%)	60 (17%)	7 (2%)	9	33
1	D	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	9	33
1	E	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	9	33
1	F	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	9	33
1	G	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	9	33
1	H	367/377 (97%)	303 (83%)	54 (15%)	10 (3%)	6	25
1	I	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	9	33
1	J	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	9	33
1	K	358/377 (95%)	293 (82%)	58 (16%)	7 (2%)	9	33
1	L	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	9	33
All	All	4305/4524 (95%)	3515 (82%)	703 (16%)	87 (2%)	9	33

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%)	14	37
1	B	310/316 (98%)	284 (92%)	26 (8%)	14	37
1	C	310/316 (98%)	284 (92%)	26 (8%)	14	37
1	D	310/316 (98%)	284 (92%)	26 (8%)	14	37
1	E	310/316 (98%)	284 (92%)	26 (8%)	14	37
1	F	310/316 (98%)	284 (92%)	26 (8%)	14	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	310/316 (98%)	284 (92%)	26 (8%)	14	37
1	H	316/316 (100%)	286 (90%)	30 (10%)	11	31
1	I	310/316 (98%)	284 (92%)	26 (8%)	14	37
1	J	310/316 (98%)	284 (92%)	26 (8%)	14	37
1	K	310/316 (98%)	285 (92%)	25 (8%)	15	39
1	L	310/316 (98%)	284 (92%)	26 (8%)	14	37
All	All	3726/3792 (98%)	3411 (92%)	315 (8%)	13	37

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

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	355/377 (94%)	0.36	10 (2%) 56 50	10, 17, 47, 60	1 (0%)
1	B	355/377 (94%)	0.31	12 (3%) 49 41	10, 20, 54, 60	1 (0%)
1	C	355/377 (94%)	0.66	33 (9%) 11 7	10, 40, 60, 60	1 (0%)
1	D	355/377 (94%)	0.59	30 (8%) 13 8	10, 34, 60, 60	1 (0%)
1	E	355/377 (94%)	0.63	35 (9%) 9 5	10, 35, 60, 60	1 (0%)
1	F	355/377 (94%)	0.58	20 (5%) 28 21	10, 36, 60, 60	1 (0%)
1	G	355/377 (94%)	0.70	37 (10%) 8 5	10, 37, 60, 60	1 (0%)
1	H	362/377 (96%)	0.19	14 (3%) 43 36	10, 33, 59, 60	1 (0%)
1	I	355/377 (94%)	0.56	28 (7%) 15 10	10, 38, 60, 60	1 (0%)
1	J	355/377 (94%)	0.80	45 (12%) 5 3	11, 49, 60, 60	1 (0%)
1	K	355/377 (94%)	0.56	24 (6%) 20 14	10, 45, 60, 60	1 (0%)
1	L	355/377 (94%)	1.10	69 (19%) 1 1	15, 56, 60, 60	1 (0%)
All	All	4267/4524 (94%)	0.59	357 (8%) 14 9	10, 37, 60, 60	12 (0%)

All (357) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	294	GLY	6.9
1	B	370	LEU	6.4
1	C	370	LEU	6.3
1	E	217	TYR	6.3
1	J	83	SER	6.1
1	E	282	TYR	5.6
1	F	83	SER	5.6
1	D	370	LEU	5.5
1	J	282	TYR	5.3
1	C	83	SER	5.0
1	G	370	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	282	TYR	4.8
1	A	370	LEU	4.7
1	L	370	LEU	4.6
1	J	281	CYS	4.6
1	L	267	ARG	4.5
1	J	217	TYR	4.5
1	K	83	SER	4.5
1	K	280	PRO	4.5
1	E	279	GLU	4.4
1	K	370	LEU	4.4
1	L	217	TYR	4.3
1	I	279	GLU	4.2
1	L	282	TYR	4.2
1	J	218	GLU	4.2
1	I	282	TYR	4.1
1	E	291	TYR	4.0
1	L	246	PRO	4.0
1	F	370	LEU	4.0
1	H	295	SER	3.9
1	L	108	ASN	3.9
1	D	279	GLU	3.9
1	H	6	LYS	3.8
1	L	79	SER	3.8
1	L	310	ASN	3.8
1	L	333	GLN	3.8
1	G	217	TYR	3.8
1	L	192	GLU	3.8
1	E	369	THR	3.8
1	L	327	ASN	3.8
1	C	265	LYS	3.7
1	E	370	LEU	3.7
1	L	369	THR	3.7
1	F	358	ASN	3.7
1	B	291	TYR	3.7
1	F	291	TYR	3.6
1	B	361	CYS	3.6
1	L	204	CYS	3.6
1	G	310	ASN	3.6
1	D	2	ALA	3.6
1	I	128	ASP	3.6
1	I	84	HIS	3.6
1	F	310	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	L	358	ASN	3.6
1	D	184	SER	3.6
1	K	326	GLU	3.5
1	H	370	LEU	3.5
1	J	270	LYS	3.5
1	B	217	TYR	3.5
1	K	327	ASN	3.5
1	L	218	GLU	3.5
1	F	301	GLY	3.5
1	I	327	ASN	3.5
1	A	83	SER	3.4
1	G	280	PRO	3.4
1	E	112	ASP	3.4
1	I	281	CYS	3.4
1	I	283	LEU	3.4
1	D	244	GLU	3.3
1	K	218	GLU	3.3
1	D	217	TYR	3.3
1	K	217	TYR	3.3
1	L	244	GLU	3.3
1	I	370	LEU	3.3
1	J	6	LYS	3.3
1	C	212	ASP	3.3
1	C	269	LEU	3.3
1	L	285	GLU	3.3
1	E	2	ALA	3.3
1	C	341	ASP	3.3
1	I	83	SER	3.3
1	L	225	ASP	3.2
1	J	225	ASP	3.2
1	L	212	ASP	3.2
1	B	282	TYR	3.2
1	L	110	LYS	3.2
1	J	326	GLU	3.1
1	G	361	CYS	3.1
1	F	292	VAL	3.1
1	J	192	GLU	3.1
1	C	79	SER	3.1
1	L	360	HIS	3.1
1	A	282	TYR	3.1
1	F	346	GLY	3.1
1	L	335	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	262	THR	3.0
1	E	211	LYS	3.0
1	H	296	ILE	3.0
1	D	82	GLY	3.0
1	K	205	VAL	3.0
1	C	124	GLY	3.0
1	J	241	ASP	3.0
1	L	112	ASP	3.0
1	D	291	TYR	3.0
1	J	164	SER	3.0
1	I	292	VAL	3.0
1	E	233	GLY	3.0
1	L	291	TYR	3.0
1	C	217	TYR	3.0
1	I	361	CYS	3.0
1	J	310	ASN	2.9
1	K	282	TYR	2.9
1	D	368	ALA	2.9
1	L	107	VAL	2.9
1	L	250	GLU	2.9
1	L	331	ALA	2.9
1	G	108	ASN	2.9
1	A	337	GLU	2.9
1	L	247	PHE	2.9
1	L	248	TYR	2.9
1	E	292	VAL	2.9
1	E	310	ASN	2.9
1	D	171	GLY	2.9
1	I	310	ASN	2.9
1	L	84	HIS	2.9
1	E	100	ASP	2.9
1	J	128	ASP	2.9
1	J	279	GLU	2.9
1	L	324	GLY	2.9
1	C	241	ASP	2.8
1	G	291	TYR	2.8
1	J	333	GLN	2.8
1	K	273	LYS	2.8
1	K	358	ASN	2.8
1	D	204	CYS	2.8
1	F	196	ASP	2.8
1	G	248	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	260	GLN	2.8
1	G	82	GLY	2.8
1	J	283	LEU	2.8
1	D	216	PRO	2.8
1	J	84	HIS	2.8
1	G	358	ASN	2.8
1	L	81	LEU	2.8
1	G	337	GLU	2.8
1	L	280	PRO	2.8
1	L	266	GLY	2.7
1	H	128	ASP	2.7
1	L	269	LEU	2.7
1	E	177	GLU	2.7
1	L	23	LYS	2.7
1	E	171	GLY	2.7
1	J	7	ASN	2.7
1	A	291	TYR	2.7
1	H	291	TYR	2.7
1	J	215	ASP	2.7
1	B	82	GLY	2.7
1	I	217	TYR	2.7
1	J	169	GLY	2.7
1	K	111	GLY	2.7
1	J	280	PRO	2.7
1	C	80	GLU	2.7
1	K	58	GLU	2.7
1	L	306	ALA	2.6
1	L	83	SER	2.6
1	J	300	GLU	2.6
1	D	225	ASP	2.6
1	H	84	HIS	2.6
1	A	327	ASN	2.6
1	L	86	ILE	2.6
1	C	196	ASP	2.6
1	G	232	PRO	2.6
1	L	163	GLY	2.6
1	L	284	GLN	2.6
1	D	327	ASN	2.6
1	F	217	TYR	2.6
1	G	215	ASP	2.6
1	K	80	GLU	2.6
1	D	278	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	337	GLU	2.6
1	L	337	GLU	2.6
1	E	278	LYS	2.6
1	J	370	LEU	2.5
1	J	301	GLY	2.5
1	E	110	LYS	2.5
1	E	82	GLY	2.5
1	E	358	ASN	2.5
1	E	124	GLY	2.5
1	C	224	ASP	2.5
1	B	268	PRO	2.5
1	I	268	PRO	2.5
1	L	232	PRO	2.5
1	J	111	GLY	2.5
1	G	282	TYR	2.5
1	F	5	ILE	2.5
1	D	358	ASN	2.5
1	E	108	ASN	2.5
1	J	286	ALA	2.5
1	D	215	ASP	2.5
1	J	292	VAL	2.5
1	K	268	PRO	2.5
1	G	267	ARG	2.5
1	C	369	THR	2.4
1	J	369	THR	2.4
1	E	128	ASP	2.4
1	G	83	SER	2.4
1	G	268	PRO	2.4
1	F	84	HIS	2.4
1	G	166	HIS	2.4
1	J	284	GLN	2.4
1	D	313	ILE	2.4
1	K	291	TYR	2.4
1	L	166	HIS	2.4
1	I	80	GLU	2.4
1	J	170	GLU	2.4
1	L	322	GLN	2.4
1	I	280	PRO	2.4
1	G	174	LEU	2.4
1	D	315	ASN	2.4
1	E	224	ASP	2.4
1	F	241	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	6	LYS	2.4
1	B	301	GLY	2.4
1	J	163	GLY	2.4
1	L	279	GLU	2.4
1	C	248	TYR	2.4
1	B	341	ASP	2.4
1	B	326	GLU	2.4
1	C	267	ARG	2.4
1	F	82	GLY	2.4
1	J	244	GLU	2.4
1	E	329	GLN	2.3
1	J	162	GLY	2.3
1	L	111	GLY	2.3
1	L	15	PHE	2.3
1	F	313	ILE	2.3
1	L	311	PHE	2.3
1	J	268	PRO	2.3
1	H	292	VAL	2.3
1	F	211	LYS	2.3
1	K	361	CYS	2.3
1	H	249	GLN	2.3
1	L	368	ALA	2.3
1	G	11	LYS	2.3
1	L	278	LYS	2.3
1	L	326	GLU	2.3
1	C	242	ASP	2.3
1	D	163	GLY	2.3
1	L	5	ILE	2.3
1	G	110	LYS	2.3
1	I	240	THR	2.3
1	D	292	VAL	2.3
1	G	207	VAL	2.3
1	L	268	PRO	2.3
1	C	286	ALA	2.3
1	L	85	ASN	2.3
1	G	233	GLY	2.3
1	E	361	CYS	2.3
1	J	224	ASP	2.2
1	D	83	SER	2.2
1	G	84	HIS	2.2
1	G	192	GLU	2.2
1	H	83	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	249	GLN	2.2
1	J	256	ASP	2.2
1	C	12	GLN	2.2
1	L	70	GLN	2.2
1	G	204	CYS	2.2
1	L	272	HIS	2.2
1	A	301	GLY	2.2
1	L	171	GLY	2.2
1	G	309	LEU	2.2
1	J	364	GLN	2.2
1	L	361	CYS	2.2
1	K	302	GLU	2.2
1	A	215	ASP	2.2
1	C	215	ASP	2.2
1	J	112	ASP	2.2
1	L	183	PRO	2.2
1	B	83	SER	2.2
1	E	80	GLU	2.2
1	G	278	LYS	2.2
1	H	297	PRO	2.2
1	D	84	HIS	2.2
1	K	279	GLU	2.2
1	F	327	ASN	2.2
1	K	259	SER	2.2
1	E	280	PRO	2.2
1	G	313	ILE	2.2
1	I	110	LYS	2.2
1	L	190	THR	2.2
1	C	292	VAL	2.2
1	F	282	TYR	2.2
1	C	2	ALA	2.2
1	K	224	ASP	2.2
1	I	209	TRP	2.2
1	L	188	HIS	2.2
1	G	327	ASN	2.2
1	L	100	ASP	2.1
1	C	111	GLY	2.1
1	J	202	LEU	2.1
1	B	239	TYR	2.1
1	G	243	LYS	2.1
1	I	341	ASP	2.1
1	H	299	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	81	LEU	2.1
1	J	275	CYS	2.1
1	D	112	ASP	2.1
1	F	244	GLU	2.1
1	I	256	ASP	2.1
1	J	216	PRO	2.1
1	C	193	ASP	2.1
1	D	361	CYS	2.1
1	I	204	CYS	2.1
1	L	341	ASP	2.1
1	E	244	GLU	2.1
1	J	227	ALA	2.1
1	C	100	ASP	2.1
1	C	243	LYS	2.1
1	C	270	LYS	2.1
1	G	164	SER	2.1
1	C	329	GLN	2.1
1	K	260	GLN	2.1
1	C	165	ILE	2.1
1	L	309	LEU	2.1
1	J	165	ILE	2.1
1	E	204	CYS	2.1
1	D	104	THR	2.1
1	I	277	THR	2.1
1	C	81	LEU	2.1
1	L	82	GLY	2.0
1	A	211	LYS	2.0
1	F	224	ASP	2.0
1	I	223	ILE	2.0
1	L	281	CYS	2.0
1	C	192	GLU	2.0
1	D	218	GLU	2.0
1	I	225	ASP	2.0
1	G	284	GLN	2.0
1	G	333	GLN	2.0
1	A	361	CYS	2.0
1	E	101	CYS	2.0
1	E	327	ASN	2.0
1	K	277	THR	2.0
1	D	124	GLY	2.0
1	H	82	GLY	2.0
1	J	222	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	260	GLN	2.0
1	D	369	THR	2.0
1	E	130	LEU	2.0
1	E	159	VAL	2.0
1	C	164	SER	2.0
1	G	132	PHE	2.0
1	L	302	GLU	2.0
1	E	84	HIS	2.0
1	I	278	LYS	2.0
1	G	14	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.