



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2016 – 03:33 PM EDT

PDB ID : 5G2E
Title : Structure of the Nap1 H2A H2B complex
Authors : AguilarGurrieri, C.; Larabi, A.; Vinayachandran, V.; Patel, N.A.; Yen, K.;
Reja, R.; Ebong, I.O.; Schoehn, G.; Robinson, C.V.; Pugh, B.F.; Panne, D.
Deposited on : 2016-04-07
Resolution : 6.70 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

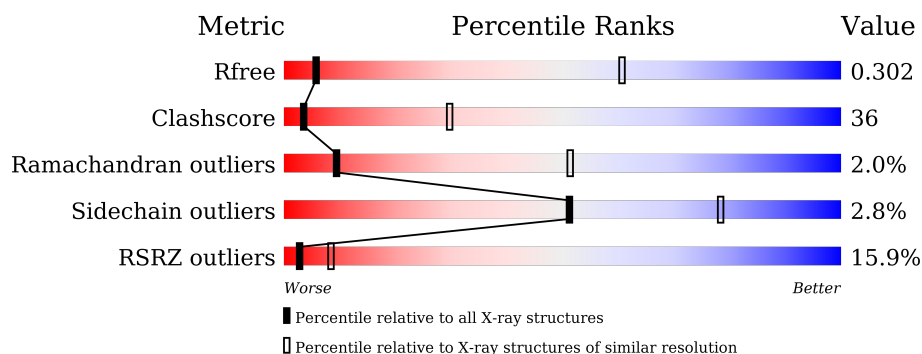
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.70 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	1014 (9.50-3.66)
Clashscore	102246	1062 (9.50-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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	310	<div> <div>10%</div> <div> <div>35%</div> <div>43%</div> <div>•</div> <div>19%</div> </div> </div>
1	B	310	<div> <div>9%</div> <div> <div>33%</div> <div>45%</div> <div>•</div> <div>21%</div> </div> </div>
1	E	310	<div> <div>13%</div> <div> <div>35%</div> <div>43%</div> <div>•</div> <div>19%</div> </div> </div>
1	F	310	<div> <div>16%</div> <div> <div>34%</div> <div>43%</div> <div>•</div> <div>21%</div> </div> </div>
1	I	310	<div> <div>11%</div> <div> <div>35%</div> <div>43%</div> <div>•</div> <div>19%</div> </div> </div>
1	J	310	<div> <div>18%</div> <div> <div>35%</div> <div>42%</div> <div>•</div> <div>21%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	M	310	
1	N	310	
1	Q	310	
1	R	310	
1	U	310	
1	V	310	
2	C	107	
2	G	107	
2	K	107	
2	O	107	
2	S	107	
2	W	107	
3	D	100	
3	H	100	
3	L	100	
3	P	100	
3	T	100	
3	X	100	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32814 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 NUCLEOSOME ASSEMBLY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2067	1328	323	412	4			
1	B	245	Total	C	N	O	S	0	0	0
			2009	1297	315	393	4			
1	E	252	Total	C	N	O	S	0	0	0
			2067	1328	323	412	4			
1	F	245	Total	C	N	O	S	0	0	0
			2009	1297	315	393	4			
1	I	252	Total	C	N	O	S	0	0	0
			2067	1328	323	412	4			
1	J	245	Total	C	N	O	S	0	0	0
			2009	1297	315	393	4			
1	M	252	Total	C	N	O	S	0	0	0
			2067	1328	323	412	4			
1	N	245	Total	C	N	O	S	0	0	0
			2009	1297	315	393	4			
1	Q	252	Total	C	N	O	S	0	0	0
			2067	1328	323	412	4			
1	R	245	Total	C	N	O	S	0	0	0
			2009	1297	315	393	4			
1	U	252	Total	C	N	O	S	0	0	0
			2067	1328	323	412	4			
1	V	245	Total	C	N	O	S	0	0	0
			2009	1297	315	393	4			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	SER	-	EXPRESSION TAG	UNP P25293
A	64	GLN	-	EXPRESSION TAG	UNP P25293
A	65	ASP	-	EXPRESSION TAG	UNP P25293
A	66	PRO	-	EXPRESSION TAG	UNP P25293
A	67	GLU	-	EXPRESSION TAG	UNP P25293

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Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ASN	-	EXPRESSION TAG	UNP P25293
A	69	LEU	-	EXPRESSION TAG	UNP P25293
A	70	TYR	-	EXPRESSION TAG	UNP P25293
A	71	PHE	-	EXPRESSION TAG	UNP P25293
A	72	GLN	-	EXPRESSION TAG	UNP P25293
A	73	GLY	-	EXPRESSION TAG	UNP P25293
B	63	SER	-	EXPRESSION TAG	UNP P25293
B	64	GLN	-	EXPRESSION TAG	UNP P25293
B	65	ASP	-	EXPRESSION TAG	UNP P25293
B	66	PRO	-	EXPRESSION TAG	UNP P25293
B	67	GLU	-	EXPRESSION TAG	UNP P25293
B	68	ASN	-	EXPRESSION TAG	UNP P25293
B	69	LEU	-	EXPRESSION TAG	UNP P25293
B	70	TYR	-	EXPRESSION TAG	UNP P25293
B	71	PHE	-	EXPRESSION TAG	UNP P25293
B	72	GLN	-	EXPRESSION TAG	UNP P25293
B	73	GLY	-	EXPRESSION TAG	UNP P25293
E	63	SER	-	EXPRESSION TAG	UNP P25293
E	64	GLN	-	EXPRESSION TAG	UNP P25293
E	65	ASP	-	EXPRESSION TAG	UNP P25293
E	66	PRO	-	EXPRESSION TAG	UNP P25293
E	67	GLU	-	EXPRESSION TAG	UNP P25293
E	68	ASN	-	EXPRESSION TAG	UNP P25293
E	69	LEU	-	EXPRESSION TAG	UNP P25293
E	70	TYR	-	EXPRESSION TAG	UNP P25293
E	71	PHE	-	EXPRESSION TAG	UNP P25293
E	72	GLN	-	EXPRESSION TAG	UNP P25293
E	73	GLY	-	EXPRESSION TAG	UNP P25293
F	63	SER	-	EXPRESSION TAG	UNP P25293
F	64	GLN	-	EXPRESSION TAG	UNP P25293
F	65	ASP	-	EXPRESSION TAG	UNP P25293
F	66	PRO	-	EXPRESSION TAG	UNP P25293
F	67	GLU	-	EXPRESSION TAG	UNP P25293
F	68	ASN	-	EXPRESSION TAG	UNP P25293
F	69	LEU	-	EXPRESSION TAG	UNP P25293
F	70	TYR	-	EXPRESSION TAG	UNP P25293
F	71	PHE	-	EXPRESSION TAG	UNP P25293
F	72	GLN	-	EXPRESSION TAG	UNP P25293
F	73	GLY	-	EXPRESSION TAG	UNP P25293
I	63	SER	-	EXPRESSION TAG	UNP P25293
I	64	GLN	-	EXPRESSION TAG	UNP P25293
I	65	ASP	-	EXPRESSION TAG	UNP P25293

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Chain	Residue	Modelled	Actual	Comment	Reference
I	66	PRO	-	EXPRESSION TAG	UNP P25293
I	67	GLU	-	EXPRESSION TAG	UNP P25293
I	68	ASN	-	EXPRESSION TAG	UNP P25293
I	69	LEU	-	EXPRESSION TAG	UNP P25293
I	70	TYR	-	EXPRESSION TAG	UNP P25293
I	71	PHE	-	EXPRESSION TAG	UNP P25293
I	72	GLN	-	EXPRESSION TAG	UNP P25293
I	73	GLY	-	EXPRESSION TAG	UNP P25293
J	63	SER	-	EXPRESSION TAG	UNP P25293
J	64	GLN	-	EXPRESSION TAG	UNP P25293
J	65	ASP	-	EXPRESSION TAG	UNP P25293
J	66	PRO	-	EXPRESSION TAG	UNP P25293
J	67	GLU	-	EXPRESSION TAG	UNP P25293
J	68	ASN	-	EXPRESSION TAG	UNP P25293
J	69	LEU	-	EXPRESSION TAG	UNP P25293
J	70	TYR	-	EXPRESSION TAG	UNP P25293
J	71	PHE	-	EXPRESSION TAG	UNP P25293
J	72	GLN	-	EXPRESSION TAG	UNP P25293
J	73	GLY	-	EXPRESSION TAG	UNP P25293
M	63	SER	-	EXPRESSION TAG	UNP P25293
M	64	GLN	-	EXPRESSION TAG	UNP P25293
M	65	ASP	-	EXPRESSION TAG	UNP P25293
M	66	PRO	-	EXPRESSION TAG	UNP P25293
M	67	GLU	-	EXPRESSION TAG	UNP P25293
M	68	ASN	-	EXPRESSION TAG	UNP P25293
M	69	LEU	-	EXPRESSION TAG	UNP P25293
M	70	TYR	-	EXPRESSION TAG	UNP P25293
M	71	PHE	-	EXPRESSION TAG	UNP P25293
M	72	GLN	-	EXPRESSION TAG	UNP P25293
M	73	GLY	-	EXPRESSION TAG	UNP P25293
N	63	SER	-	EXPRESSION TAG	UNP P25293
N	64	GLN	-	EXPRESSION TAG	UNP P25293
N	65	ASP	-	EXPRESSION TAG	UNP P25293
N	66	PRO	-	EXPRESSION TAG	UNP P25293
N	67	GLU	-	EXPRESSION TAG	UNP P25293
N	68	ASN	-	EXPRESSION TAG	UNP P25293
N	69	LEU	-	EXPRESSION TAG	UNP P25293
N	70	TYR	-	EXPRESSION TAG	UNP P25293
N	71	PHE	-	EXPRESSION TAG	UNP P25293
N	72	GLN	-	EXPRESSION TAG	UNP P25293
N	73	GLY	-	EXPRESSION TAG	UNP P25293
Q	63	SER	-	EXPRESSION TAG	UNP P25293

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	64	GLN	-	EXPRESSION TAG	UNP P25293
Q	65	ASP	-	EXPRESSION TAG	UNP P25293
Q	66	PRO	-	EXPRESSION TAG	UNP P25293
Q	67	GLU	-	EXPRESSION TAG	UNP P25293
Q	68	ASN	-	EXPRESSION TAG	UNP P25293
Q	69	LEU	-	EXPRESSION TAG	UNP P25293
Q	70	TYR	-	EXPRESSION TAG	UNP P25293
Q	71	PHE	-	EXPRESSION TAG	UNP P25293
Q	72	GLN	-	EXPRESSION TAG	UNP P25293
Q	73	GLY	-	EXPRESSION TAG	UNP P25293
R	63	SER	-	EXPRESSION TAG	UNP P25293
R	64	GLN	-	EXPRESSION TAG	UNP P25293
R	65	ASP	-	EXPRESSION TAG	UNP P25293
R	66	PRO	-	EXPRESSION TAG	UNP P25293
R	67	GLU	-	EXPRESSION TAG	UNP P25293
R	68	ASN	-	EXPRESSION TAG	UNP P25293
R	69	LEU	-	EXPRESSION TAG	UNP P25293
R	70	TYR	-	EXPRESSION TAG	UNP P25293
R	71	PHE	-	EXPRESSION TAG	UNP P25293
R	72	GLN	-	EXPRESSION TAG	UNP P25293
R	73	GLY	-	EXPRESSION TAG	UNP P25293
U	63	SER	-	EXPRESSION TAG	UNP P25293
U	64	GLN	-	EXPRESSION TAG	UNP P25293
U	65	ASP	-	EXPRESSION TAG	UNP P25293
U	66	PRO	-	EXPRESSION TAG	UNP P25293
U	67	GLU	-	EXPRESSION TAG	UNP P25293
U	68	ASN	-	EXPRESSION TAG	UNP P25293
U	69	LEU	-	EXPRESSION TAG	UNP P25293
U	70	TYR	-	EXPRESSION TAG	UNP P25293
U	71	PHE	-	EXPRESSION TAG	UNP P25293
U	72	GLN	-	EXPRESSION TAG	UNP P25293
U	73	GLY	-	EXPRESSION TAG	UNP P25293
V	63	SER	-	EXPRESSION TAG	UNP P25293
V	64	GLN	-	EXPRESSION TAG	UNP P25293
V	65	ASP	-	EXPRESSION TAG	UNP P25293
V	66	PRO	-	EXPRESSION TAG	UNP P25293
V	67	GLU	-	EXPRESSION TAG	UNP P25293
V	68	ASN	-	EXPRESSION TAG	UNP P25293
V	69	LEU	-	EXPRESSION TAG	UNP P25293
V	70	TYR	-	EXPRESSION TAG	UNP P25293
V	71	PHE	-	EXPRESSION TAG	UNP P25293
V	72	GLN	-	EXPRESSION TAG	UNP P25293

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Chain	Residue	Modelled	Actual	Comment	Reference
V	73	GLY	-	EXPRESSION TAG	UNP P25293

- Molecule 2 is a protein called HISTONE H2A TYPE 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	90	Total	C	N	O	0	0	0
			699	437	139	123			
2	G	90	Total	C	N	O	0	0	0
			699	437	139	123			
2	K	90	Total	C	N	O	0	0	0
			699	437	139	123			
2	O	90	Total	C	N	O	0	0	0
			699	437	139	123			
2	S	90	Total	C	N	O	0	0	0
			699	437	139	123			
2	W	90	Total	C	N	O	0	0	0
			699	437	139	123			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	12	MET	-	EXPRESSION TAG	UNP P06897
C	99	ARG	GLY	CONFLICT	UNP P06897
G	12	MET	-	EXPRESSION TAG	UNP P06897
G	99	ARG	GLY	CONFLICT	UNP P06897
K	12	MET	-	EXPRESSION TAG	UNP P06897
K	99	ARG	GLY	CONFLICT	UNP P06897
O	12	MET	-	EXPRESSION TAG	UNP P06897
O	99	ARG	GLY	CONFLICT	UNP P06897
S	12	MET	-	EXPRESSION TAG	UNP P06897
S	99	ARG	GLY	CONFLICT	UNP P06897
W	12	MET	-	EXPRESSION TAG	UNP P06897
W	99	ARG	GLY	CONFLICT	UNP P06897

- Molecule 3 is a protein called HISTONE H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	89	Total	C	N	O	S	0	0	0
			694	439	123	130	2			
3	H	89	Total	C	N	O	S	0	0	0
			694	439	123	130	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	89	Total 694	C 439	N 123	O 130	S 2	0	0	0
3	P	89	Total 694	C 439	N 123	O 130	S 2	0	0	0
3	T	89	Total 694	C 439	N 123	O 130	S 2	0	0	0
3	X	89	Total 694	C 439	N 123	O 130	S 2	0	0	0

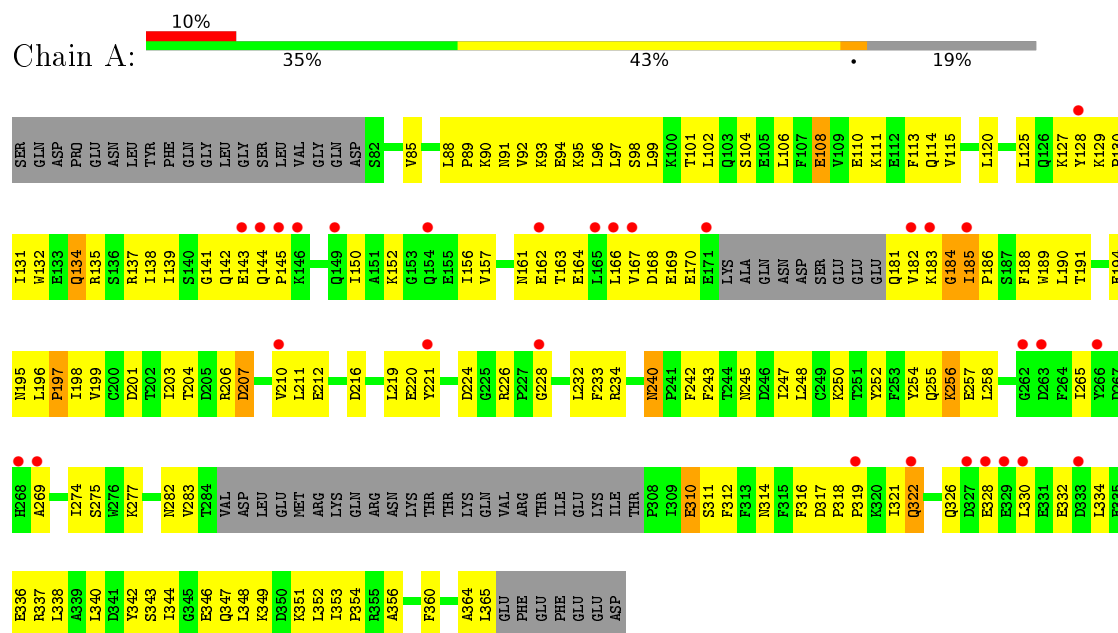
There are 12 discrepancies between the modelled and reference sequences:

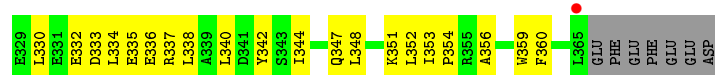
Chain	Residue	Modelled	Actual	Comment	Reference
D	23	MET	-	EXPRESSION TAG	UNP P02281
D	29	THR	SER	CONFLICT	UNP P02281
H	23	MET	-	EXPRESSION TAG	UNP P02281
H	29	THR	SER	CONFLICT	UNP P02281
L	23	MET	-	EXPRESSION TAG	UNP P02281
L	29	THR	SER	CONFLICT	UNP P02281
P	23	MET	-	EXPRESSION TAG	UNP P02281
P	29	THR	SER	CONFLICT	UNP P02281
T	23	MET	-	EXPRESSION TAG	UNP P02281
T	29	THR	SER	CONFLICT	UNP P02281
X	23	MET	-	EXPRESSION TAG	UNP P02281
X	29	THR	SER	CONFLICT	UNP P02281

3 Residue-property plots

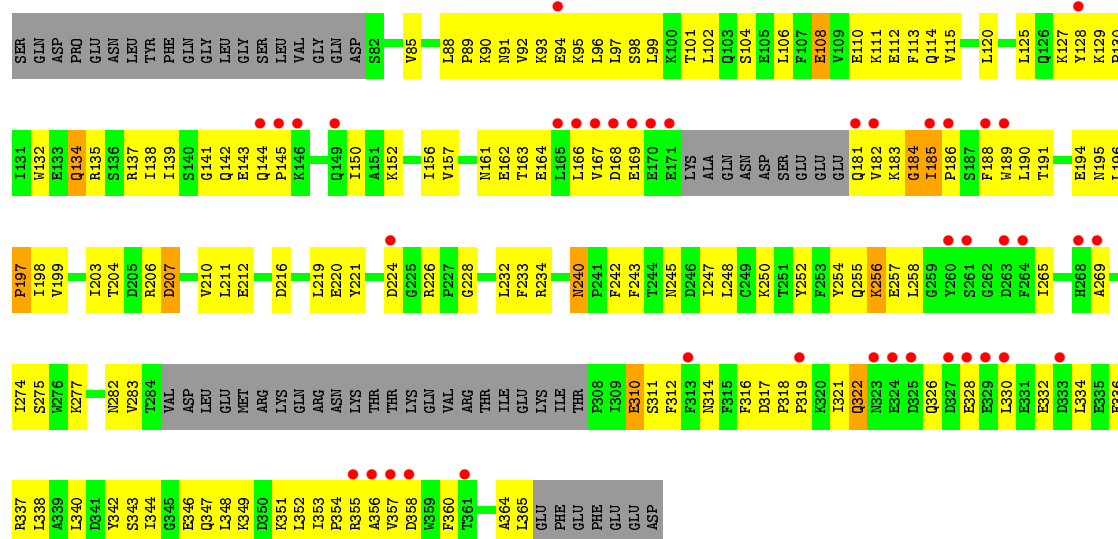
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: NUCLEOSOME ASSEMBLY PROTEIN

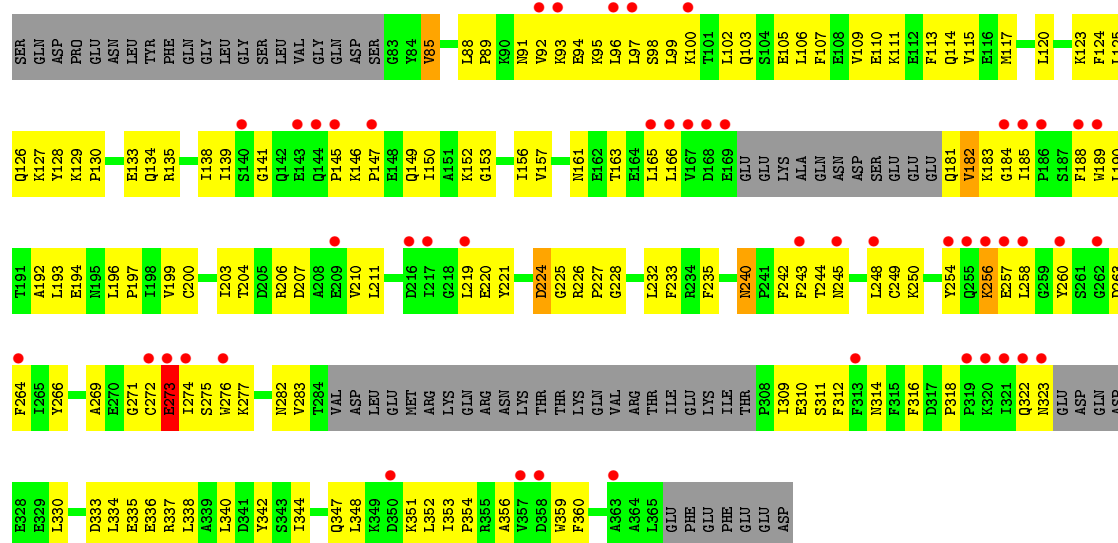




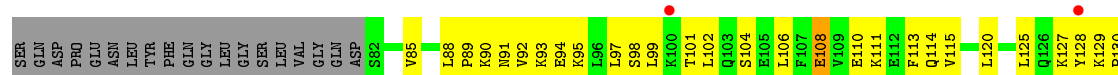
• Molecule 1: NUCLEOSOME ASSEMBLY PROTEIN

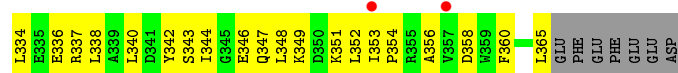


• Molecule 1: NUCLEOSOME ASSEMBLY PROTEIN

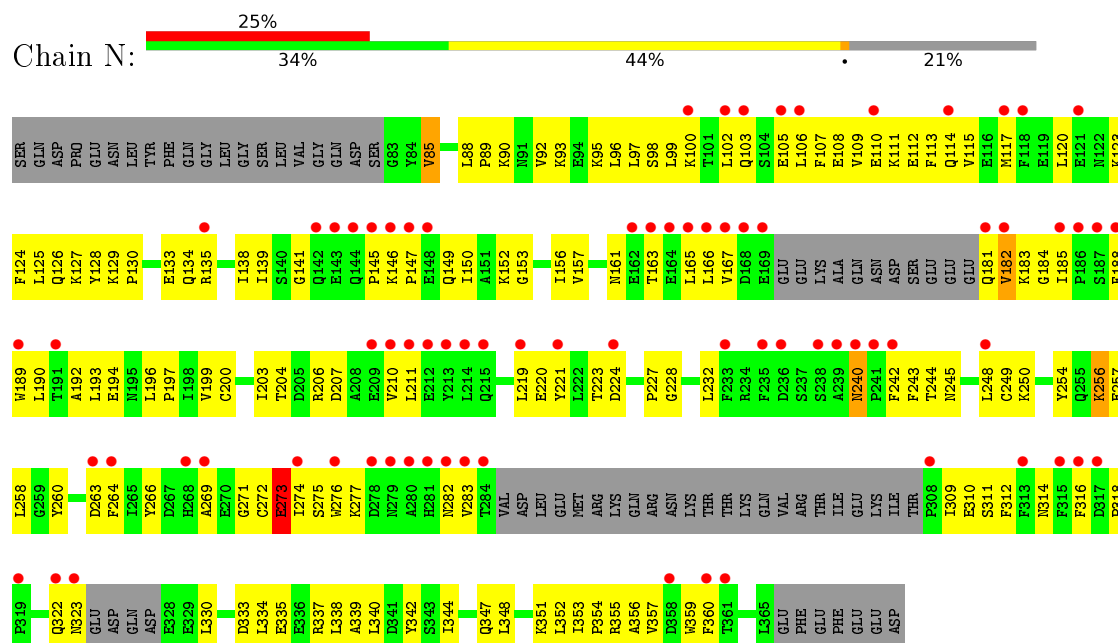


• Molecule 1: NUCLEOSOME ASSEMBLY PROTEIN

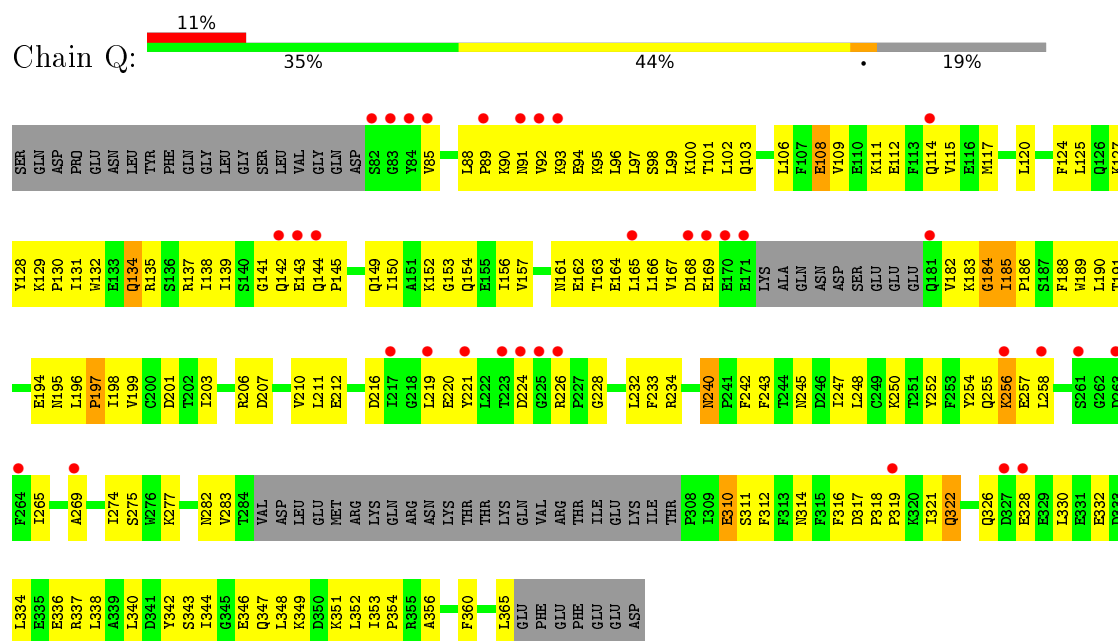




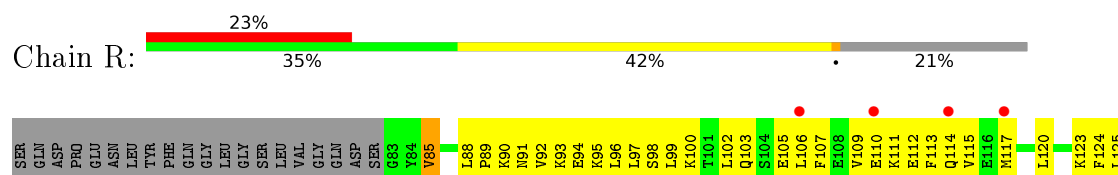
• Molecule 1: NUCLEOSOME ASSEMBLY PROTEIN

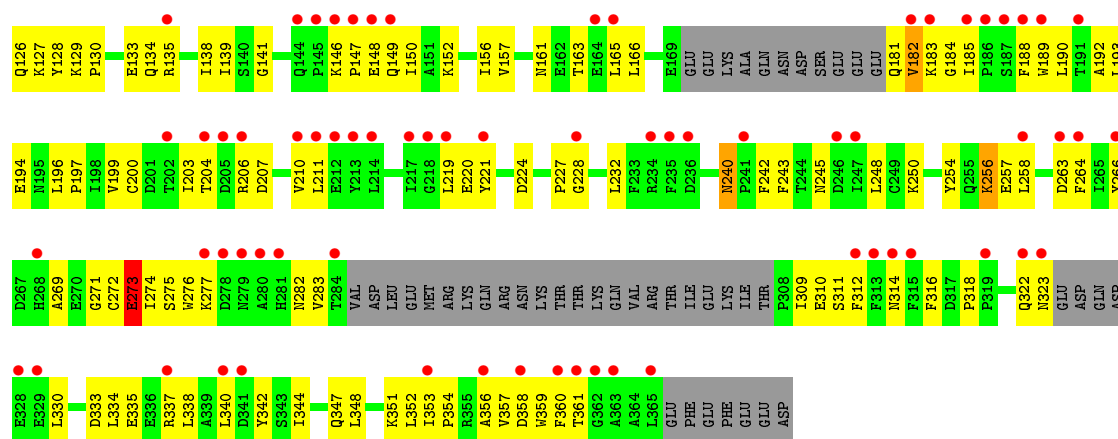


• Molecule 1: NUCLEOSOME ASSEMBLY PROTEIN

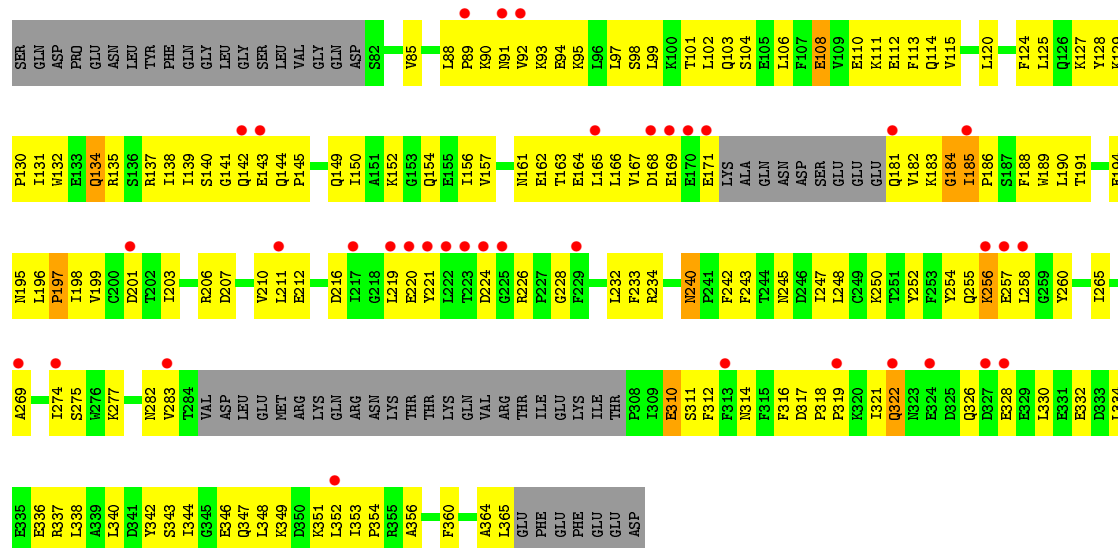


• Molecule 1: NUCLEOSOME ASSEMBLY PROTEIN

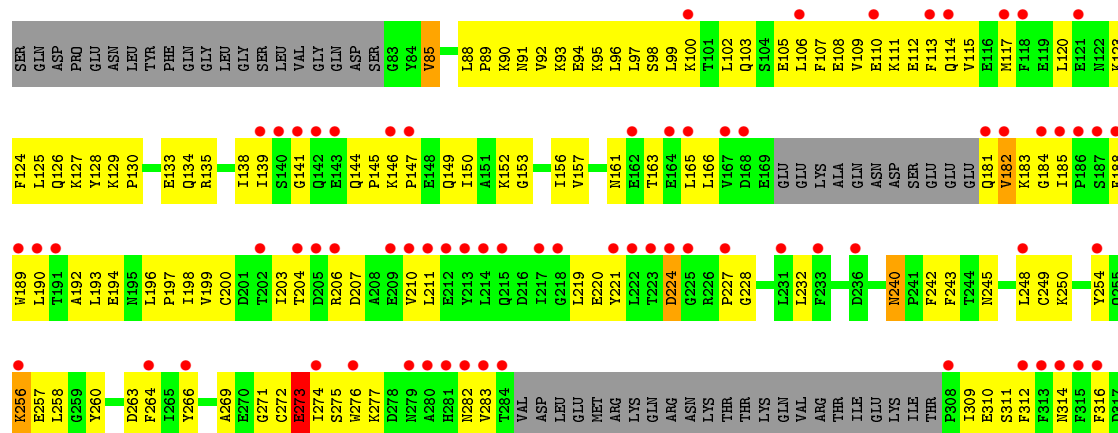


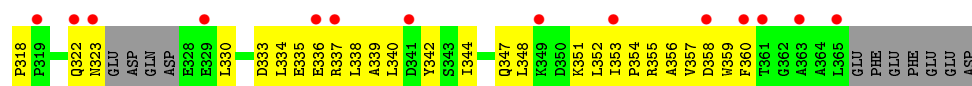


• Molecule 1: NUCLEOSOME ASSEMBLY PROTEIN

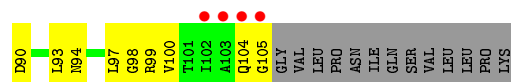
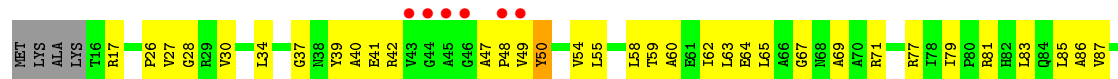


• Molecule 1: NUCLEOSOME ASSEMBLY PROTEIN

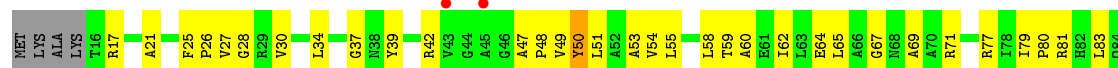




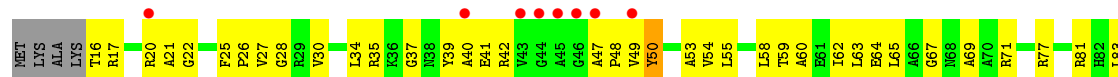
• Molecule 2: HISTONE H2A TYPE 1



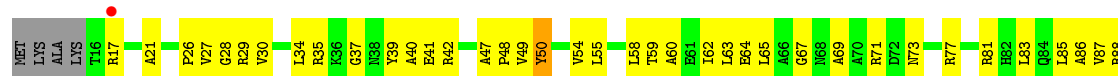
• Molecule 2: HISTONE H2A TYPE 1



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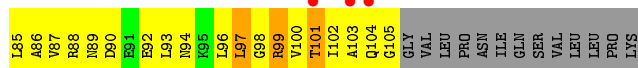
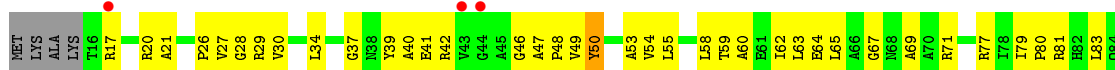


• Molecule 2: HISTONE H2A TYPE 1





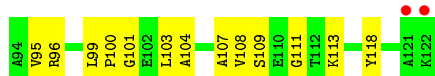
• Molecule 2: HISTONE H2A TYPE 1



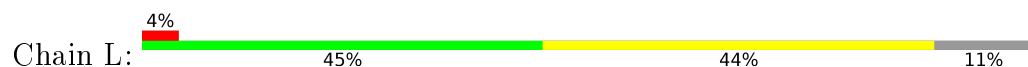
• Molecule 3: HISTONE H2B 1.1



• Molecule 3: HISTONE H2B 1.1

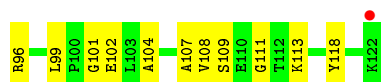


• Molecule 3: HISTONE H2B 1.1

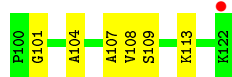


• Molecule 3: HISTONE H2B 1.1

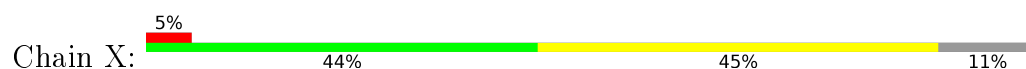




- Molecule 3: HISTONE H2B 1.1



- Molecule 3: HISTONE H2B 1.1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.47Å 211.13Å 126.57Å 90.00° 99.72° 90.00°	Depositor
Resolution (Å)	50.00 – 6.70 56.52 – 6.72	Depositor EDS
% Data completeness (in resolution range)	97.0 (50.00-6.70) 98.1 (56.52-6.72)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 6.69Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.263 , 0.310 0.267 , 0.302	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	276.9	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 344.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	32814	wwPDB-VP
Average B, all atoms (Å ²)	363.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/2112	0.45	0/2853
1	B	0.26	0/2053	0.46	0/2772
1	E	0.26	0/2112	0.45	0/2853
1	F	0.26	0/2053	0.46	0/2772
1	I	0.26	0/2112	0.45	0/2853
1	J	0.26	0/2053	0.46	0/2772
1	M	0.26	0/2112	0.45	0/2853
1	N	0.26	0/2053	0.46	0/2772
1	Q	0.26	0/2112	0.45	0/2853
1	R	0.26	0/2053	0.46	0/2772
1	U	0.26	0/2112	0.45	0/2853
1	V	0.26	0/2053	0.46	0/2772
2	C	0.22	0/707	0.41	0/953
2	G	0.38	0/707	0.57	0/953
2	K	0.22	0/707	0.62	2/953 (0.2%)
2	O	0.30	0/707	1.09	3/953 (0.3%)
2	S	62.54	2/707 (0.3%)	1.51	3/953 (0.3%)
2	W	0.21	0/707	0.40	0/953
3	D	0.24	0/705	0.42	0/949
3	H	0.24	0/705	0.42	0/949
3	L	0.24	0/705	0.42	0/949
3	P	0.24	0/705	0.42	0/949
3	T	0.24	0/705	0.42	0/949
3	X	0.24	0/705	0.42	0/949
All	All	9.09	2/33462 (0.0%)	0.52	8/45162 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	S	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	105	GLY	C-O	1662.54	27.83	1.23
2	S	94	ASN	C-N	-28.57	0.68	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	105	GLY	CA-C-O	-43.57	42.17	120.60
2	O	95	LYS	O-C-N	-22.19	87.19	122.70
2	O	95	LYS	CA-C-N	15.51	151.33	117.20
2	O	95	LYS	C-N-CA	14.63	158.27	121.70
2	K	94	ASN	O-C-N	-13.31	101.40	122.70
2	S	94	ASN	CA-C-N	-9.40	96.52	117.20
2	S	94	ASN	C-N-CA	-5.39	108.21	121.70
2	K	94	ASN	C-N-CA	5.02	134.24	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	94	ASN	Mainchain
2	S	94	ASN	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2067	0	1986	156	0
1	B	2009	0	1946	150	0
1	E	2067	0	1986	176	0
1	F	2009	0	1946	169	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2067	0	1986	172	0
1	J	2009	0	1946	141	0
1	M	2067	0	1986	192	0
1	N	2009	0	1946	172	0
1	Q	2067	0	1986	197	0
1	R	2009	0	1946	164	0
1	U	2067	0	1986	183	0
1	V	2009	0	1946	155	0
2	C	699	0	735	59	0
2	G	699	0	732	81	0
2	K	699	0	733	115	0
2	O	699	0	735	108	0
2	S	699	0	734	65	0
2	W	699	0	733	98	0
3	D	694	0	716	41	0
3	H	694	0	716	53	0
3	L	694	0	715	63	0
3	P	694	0	714	47	0
3	T	694	0	714	52	0
3	X	694	0	713	55	0
All	All	32814	0	32282	2358	0

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 (2358) 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)
2:S:94:ASN:C	2:S:95:LYS:CA	1.79	1.48
2:S:94:ASN:CA	2:S:95:LYS:N	1.74	1.48
2:W:99:ARG:NH2	2:W:102:ILE:CG1	1.71	1.48
2:W:99:ARG:NH2	2:W:102:ILE:HG12	1.20	1.48
2:K:103:ALA:CA	2:O:81:ARG:NH1	1.88	1.36
2:S:100:VAL:CG2	3:T:65:ASP:OD2	1.70	1.36
2:K:105:GLY:C	2:O:73:ASN:OD1	1.65	1.34
2:K:96:LEU:HD13	3:L:99:LEU:CD2	1.59	1.31
2:G:87:VAL:HG22	2:G:93:LEU:CD1	1.60	1.29
2:W:99:ARG:O	2:W:102:ILE:HG13	1.28	1.29
2:K:103:ALA:HA	2:O:81:ARG:NH1	0.96	1.27
2:K:96:LEU:CD1	3:L:99:LEU:HD23	1.69	1.23
2:S:94:ASN:O	2:S:95:LYS:N	1.72	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:100:VAL:HG22	3:T:65:ASP:OD2	1.04	1.20
2:W:99:ARG:NH2	2:W:102:ILE:CD1	2.02	1.19
2:G:87:VAL:CG2	2:G:93:LEU:HD13	1.73	1.19
1:N:88:LEU:HB3	1:N:89:PRO:HD2	1.26	1.17
2:K:100:VAL:HG22	3:L:69:ARG:HD2	1.26	1.17
1:Q:99:LEU:HD22	1:R:135:ARG:HG3	1.24	1.16
1:J:88:LEU:HB3	1:J:89:PRO:HD2	1.26	1.15
1:R:88:LEU:HB3	1:R:89:PRO:HD2	1.26	1.14
1:V:88:LEU:HB3	1:V:89:PRO:HD2	1.26	1.14
2:G:97:LEU:O	3:H:69:ARG:NH2	1.82	1.10
2:O:87:VAL:HG11	2:O:97:LEU:CD1	1.80	1.10
2:O:87:VAL:CG1	2:O:97:LEU:HD12	1.80	1.10
2:G:62:ILE:HD12	2:G:93:LEU:HD11	1.26	1.10
1:F:88:LEU:HB3	1:F:89:PRO:HD2	1.26	1.09
2:S:100:VAL:HG13	3:T:65:ASP:CG	1.73	1.09
1:B:88:LEU:HB3	1:B:89:PRO:HD2	1.26	1.09
2:G:87:VAL:HG13	2:G:93:LEU:HB3	1.10	1.08
2:S:102:ILE:CG2	2:S:103:ALA:H	1.65	1.07
2:S:97:LEU:O	2:S:101:THR:HG23	1.53	1.07
2:S:102:ILE:HG22	2:S:103:ALA:N	1.65	1.07
2:W:42:ARG:HB2	3:X:85:THR:HG22	1.32	1.06
2:S:102:ILE:HG22	2:S:103:ALA:H	0.92	1.06
2:S:87:VAL:HG11	2:S:97:LEU:HD12	1.10	1.05
2:K:96:LEU:CD1	3:L:99:LEU:CD2	2.30	1.05
2:K:103:ALA:HB2	2:O:85:LEU:HD21	1.38	1.05
2:K:96:LEU:HD13	3:L:99:LEU:HD23	1.05	1.04
2:K:97:LEU:CD1	2:O:104:GLN:HG3	1.88	1.03
2:O:42:ARG:HB2	3:P:85:THR:HG22	1.37	1.02
1:B:328:GLU:OE1	2:W:105:GLY:O	1.79	1.00
2:W:99:ARG:NH2	2:W:102:ILE:HD11	1.75	0.99
2:G:62:ILE:CD1	2:G:93:LEU:HD11	1.93	0.99
2:G:97:LEU:HD11	3:H:62:PHE:CD1	1.98	0.98
1:J:245:ASN:HD21	1:J:275:SER:H	1.11	0.98
2:O:87:VAL:HG11	2:O:97:LEU:HD12	1.01	0.98
1:M:245:ASN:HD21	1:M:275:SER:H	1.08	0.98
2:K:97:LEU:HD11	2:O:104:GLN:HE21	1.28	0.98
2:C:81:ARG:HB3	2:W:104:GLN:CD	1.84	0.98
2:C:99:ARG:HH12	2:W:85:LEU:HA	1.29	0.97
1:B:245:ASN:HD21	1:B:275:SER:H	1.11	0.97
1:F:245:ASN:HD21	1:F:275:SER:H	1.11	0.97
2:G:96:LEU:HG	3:H:100:PRO:HD3	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:94:ASN:O	2:S:95:LYS:CA	2.10	0.97
2:K:100:VAL:HG22	3:L:69:ARG:CD	1.85	0.96
2:S:92:GLU:O	2:S:95:LYS:HB3	1.65	0.96
1:J:183:LYS:HG3	1:J:184:GLY:H	1.31	0.96
2:K:42:ARG:HB2	3:L:85:THR:HG22	1.44	0.96
1:V:183:LYS:HG3	1:V:184:GLY:H	1.31	0.96
1:F:183:LYS:HG3	1:F:184:GLY:H	1.31	0.96
1:R:183:LYS:HG3	1:R:184:GLY:H	1.31	0.95
2:C:99:ARG:NH1	2:W:85:LEU:HA	1.82	0.95
2:S:87:VAL:HG11	2:S:97:LEU:CD1	1.96	0.95
1:N:183:LYS:HG3	1:N:184:GLY:H	1.31	0.95
1:Q:245:ASN:HD21	1:Q:275:SER:H	1.08	0.95
1:Q:95:LYS:NZ	1:R:184:GLY:HA2	1.82	0.95
2:K:103:ALA:HA	2:O:81:ARG:CZ	1.97	0.94
2:K:94:ASN:ND2	2:O:94:ASN:HD21	1.64	0.94
1:B:183:LYS:HG3	1:B:184:GLY:H	1.31	0.94
1:I:245:ASN:HD21	1:I:275:SER:H	1.08	0.94
1:E:245:ASN:HD21	1:E:275:SER:H	1.08	0.94
2:G:87:VAL:CG1	2:G:93:LEU:HB3	1.98	0.94
2:C:105:GLY:O	2:W:104:GLN:HB3	1.68	0.94
1:Q:137:ARG:HD2	1:U:142:GLN:HE21	1.32	0.94
2:K:84:GLN:HE21	2:O:102:ILE:C	1.70	0.93
2:W:99:ARG:O	2:W:102:ILE:CG1	2.15	0.93
2:S:87:VAL:CG1	2:S:97:LEU:HD12	1.98	0.93
2:K:97:LEU:HD11	2:O:104:GLN:NE2	1.81	0.93
2:K:103:ALA:CB	2:O:85:LEU:HD21	1.99	0.93
1:V:245:ASN:HD21	1:V:275:SER:H	1.11	0.93
1:A:170:GLU:HG3	1:I:169:GLU:OE2	1.67	0.92
2:O:88:ARG:CZ	2:O:97:LEU:HD13	2.00	0.92
1:A:245:ASN:HD21	1:A:275:SER:H	1.08	0.92
1:U:245:ASN:HD21	1:U:275:SER:H	1.08	0.92
2:K:99:ARG:CD	3:L:98:LEU:O	2.19	0.91
2:C:94:ASN:HD21	2:W:94:ASN:HD21	1.14	0.91
1:N:245:ASN:HD21	1:N:275:SER:H	1.11	0.91
1:E:95:LYS:HD2	1:F:145:PRO:HG2	1.51	0.91
1:F:245:ASN:ND2	1:F:275:SER:H	1.70	0.90
1:R:245:ASN:HD21	1:R:275:SER:H	1.11	0.90
1:J:245:ASN:ND2	1:J:275:SER:H	1.70	0.89
2:W:99:ARG:HA	2:W:99:ARG:CZ	2.01	0.89
2:S:100:VAL:CG2	3:T:69:ARG:CZ	2.48	0.89
1:R:245:ASN:ND2	1:R:275:SER:H	1.70	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:97:LEU:HD11	2:O:104:GLN:HG3	1.54	0.89
1:Q:142:GLN:HE21	1:U:142:GLN:HG2	1.38	0.89
2:G:87:VAL:HG22	2:G:93:LEU:HD13	0.89	0.88
2:K:94:ASN:HD21	2:O:94:ASN:HD21	0.93	0.88
2:S:100:VAL:CB	3:T:65:ASP:OD2	2.20	0.88
1:B:245:ASN:ND2	1:B:275:SER:H	1.70	0.88
2:S:100:VAL:CG1	3:T:65:ASP:OD2	2.21	0.88
2:G:92:GLU:OE1	3:H:103:LEU:CB	2.21	0.88
2:S:94:ASN:N	2:S:95:LYS:N	2.22	0.88
1:N:245:ASN:ND2	1:N:275:SER:H	1.70	0.88
1:E:364:ALA:HA	1:F:260:TYR:HE2	1.35	0.88
1:V:245:ASN:ND2	1:V:275:SER:H	1.70	0.87
2:K:94:ASN:HD21	2:O:94:ASN:ND2	1.72	0.87
1:Q:95:LYS:HZ1	1:R:184:GLY:HA2	1.39	0.87
2:C:42:ARG:HB2	3:D:85:THR:HG22	1.56	0.86
2:G:87:VAL:HG13	2:G:93:LEU:CB	2.01	0.86
2:K:97:LEU:HD11	2:O:104:GLN:CG	2.06	0.85
2:K:97:LEU:CD1	2:O:104:GLN:CG	2.53	0.85
1:M:145:PRO:HB3	1:N:98:SER:HB3	1.56	0.85
2:S:100:VAL:HG13	3:T:65:ASP:OD2	1.77	0.85
2:C:105:GLY:O	2:W:104:GLN:CB	2.24	0.84
1:M:201:ASP:OD1	2:O:29:ARG:HB2	1.78	0.84
1:A:95:LYS:HD2	1:B:145:PRO:HG2	1.59	0.83
1:E:185:ILE:HD12	1:F:96:LEU:HD11	1.60	0.83
1:F:336:GLU:HA	2:G:77:ARG:NH2	1.93	0.83
2:K:100:VAL:CG2	3:L:69:ARG:HD2	2.07	0.83
2:S:99:ARG:HB2	3:T:69:ARG:NH1	1.94	0.83
1:B:226:ARG:NE	1:F:225:GLY:HA2	1.93	0.83
1:Q:198:ILE:HD13	3:T:36:ILE:HD13	1.60	0.82
2:K:103:ALA:HA	2:O:81:ARG:HH12	1.40	0.82
2:K:105:GLY:CA	2:O:73:ASN:OD1	2.27	0.82
1:E:185:ILE:HD12	1:F:96:LEU:CD1	2.08	0.82
1:I:142:GLN:O	1:V:224:ASP:OD2	1.98	0.82
1:V:88:LEU:HB3	1:V:89:PRO:CD	2.09	0.82
1:B:270:GLU:OE2	1:F:224:ASP:HB3	1.80	0.82
1:J:88:LEU:HB3	1:J:89:PRO:CD	2.09	0.81
2:S:94:ASN:C	2:S:95:LYS:HA	1.99	0.81
2:S:94:ASN:O	2:S:95:LYS:HA	1.78	0.81
2:G:92:GLU:O	2:G:96:LEU:HB3	1.79	0.81
2:K:97:LEU:CD1	2:O:104:GLN:HE21	1.93	0.80
2:G:92:GLU:OE1	3:H:103:LEU:HB3	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:88:LEU:HB3	1:R:89:PRO:CD	2.09	0.80
2:S:42:ARG:HB2	3:T:85:THR:HG22	1.62	0.80
2:K:100:VAL:CG2	3:L:69:ARG:CD	2.54	0.80
1:Q:142:GLN:HG2	1:U:142:GLN:CG	2.11	0.80
2:C:99:ARG:HH22	2:W:89:ASN:HD21	1.26	0.80
2:K:84:GLN:NE2	2:O:102:ILE:O	2.14	0.80
2:K:103:ALA:CA	2:O:81:ARG:HH11	1.65	0.80
2:K:97:LEU:HD21	2:O:104:GLN:HE21	1.46	0.80
1:I:245:ASN:ND2	1:I:275:SER:H	1.80	0.79
2:K:97:LEU:HD21	2:O:104:GLN:NE2	1.97	0.79
1:U:245:ASN:ND2	1:U:275:SER:H	1.80	0.79
1:A:245:ASN:ND2	1:A:275:SER:H	1.80	0.79
1:I:95:LYS:HD2	1:J:145:PRO:HG2	1.64	0.79
1:E:364:ALA:HA	1:F:260:TYR:CE2	2.17	0.79
1:Q:245:ASN:ND2	1:Q:275:SER:H	1.80	0.79
1:M:245:ASN:ND2	1:M:275:SER:H	1.80	0.79
2:K:105:GLY:C	2:O:73:ASN:CG	2.42	0.78
1:E:245:ASN:ND2	1:E:275:SER:H	1.80	0.78
1:I:185:ILE:HD12	1:J:96:LEU:HD11	1.65	0.78
1:Q:245:ASN:HD21	1:Q:275:SER:N	1.82	0.78
2:K:98:GLY:HA2	2:K:101:THR:OG1	1.83	0.78
2:S:17:ARG:HH21	2:S:28:GLY:HA2	1.48	0.78
1:Q:163:THR:HG23	1:Q:166:LEU:HD12	1.66	0.78
1:M:112:GLU:HG3	1:N:124:PHE:CZ	2.17	0.78
2:G:17:ARG:HH21	2:G:28:GLY:HA2	1.49	0.78
2:O:17:ARG:HH21	2:O:28:GLY:HA2	1.49	0.78
1:I:245:ASN:HD21	1:I:275:SER:N	1.82	0.77
2:K:17:ARG:HH21	2:K:28:GLY:HA2	1.49	0.77
1:M:163:THR:HG23	1:M:166:LEU:HD12	1.66	0.77
1:E:245:ASN:HD21	1:E:275:SER:N	1.82	0.77
1:R:243:PHE:HD2	1:R:245:ASN:HB2	1.50	0.77
1:B:88:LEU:HB3	1:B:89:PRO:CD	2.09	0.77
1:I:163:THR:HG23	1:I:166:LEU:HD12	1.66	0.77
1:M:201:ASP:CG	2:O:29:ARG:HB2	2.04	0.77
1:V:146:LYS:HB2	1:V:149:GLN:HG3	1.67	0.77
1:E:163:THR:HG23	1:E:166:LEU:HD12	1.66	0.77
2:K:96:LEU:HD13	3:L:99:LEU:HD22	1.63	0.77
2:C:17:ARG:HH21	2:C:28:GLY:HA2	1.49	0.77
1:M:112:GLU:HG3	1:N:124:PHE:HZ	1.48	0.77
2:W:17:ARG:HH21	2:W:28:GLY:HA2	1.48	0.77
3:D:93:THR:HG22	3:D:96:ARG:HH12	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:LEU:HB3	1:F:89:PRO:CD	2.09	0.76
3:H:93:THR:HG22	3:H:96:ARG:HH12	1.50	0.76
3:T:93:THR:HG22	3:T:96:ARG:HH12	1.51	0.76
1:B:243:PHE:HD2	1:B:245:ASN:HB2	1.50	0.76
1:J:243:PHE:HD2	1:J:245:ASN:HB2	1.50	0.76
1:M:245:ASN:HD21	1:M:275:SER:N	1.82	0.76
1:U:163:THR:HG23	1:U:166:LEU:HD12	1.66	0.76
1:V:243:PHE:HD2	1:V:245:ASN:HB2	1.50	0.76
2:C:79:ILE:CD1	2:C:81:ARG:NH2	2.49	0.76
1:F:243:PHE:HD2	1:F:245:ASN:HB2	1.50	0.76
2:G:96:LEU:O	2:G:96:LEU:HD22	1.86	0.76
1:A:163:THR:HG23	1:A:166:LEU:HD12	1.66	0.76
3:P:93:THR:HG22	3:P:96:ARG:HH12	1.51	0.75
2:K:92:GLU:O	2:K:95:LYS:HB3	1.87	0.75
1:F:146:LYS:HB2	1:F:149:GLN:HG3	1.67	0.75
1:N:88:LEU:HB3	1:N:89:PRO:CD	2.09	0.75
1:R:245:ASN:HD21	1:R:275:SER:N	1.84	0.75
1:U:245:ASN:HD21	1:U:275:SER:N	1.82	0.75
2:C:105:GLY:C	2:W:104:GLN:HB3	2.06	0.75
2:W:41:GLU:HB3	3:X:84:SER:HB3	1.68	0.75
1:B:146:LYS:HB2	1:B:149:GLN:HG3	1.67	0.75
1:J:146:LYS:HB2	1:J:149:GLN:HG3	1.67	0.75
1:N:245:ASN:HD21	1:N:275:SER:N	1.84	0.75
2:G:97:LEU:HD11	3:H:62:PHE:HD1	1.46	0.75
2:K:103:ALA:HB2	2:O:85:LEU:CD2	2.17	0.75
1:R:146:LYS:HB2	1:R:149:GLN:HG3	1.67	0.75
1:A:245:ASN:HD21	1:A:275:SER:N	1.82	0.75
1:U:145:PRO:HB3	1:V:98:SER:HB3	1.67	0.74
1:N:243:PHE:HD2	1:N:245:ASN:HB2	1.50	0.74
1:B:245:ASN:HD21	1:B:275:SER:N	1.84	0.74
1:I:353:ILE:HB	1:I:354:PRO:HD3	1.70	0.74
1:M:131:ILE:HD12	1:N:106:LEU:HD23	1.69	0.74
2:G:93:LEU:O	2:G:97:LEU:HB2	1.86	0.74
2:G:99:ARG:HG3	2:G:100:VAL:H	1.52	0.74
1:Q:112:GLU:HG3	1:R:124:PHE:CZ	2.22	0.74
2:W:99:ARG:NH2	2:W:102:ILE:HG13	1.96	0.74
2:G:42:ARG:HB2	3:H:85:THR:HG22	1.68	0.74
1:I:364:ALA:HA	1:J:260:TYR:HE2	1.52	0.74
1:Q:112:GLU:HG3	1:R:124:PHE:HZ	1.50	0.74
1:M:353:ILE:HB	1:M:354:PRO:HD3	1.70	0.74
1:M:124:PHE:CE1	1:N:112:GLU:HG3	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:353:ILE:HB	1:Q:354:PRO:HD3	1.70	0.74
3:L:93:THR:HG22	3:L:96:ARG:HH12	1.50	0.74
2:C:79:ILE:HD12	2:C:81:ARG:CZ	2.17	0.74
1:Q:168:ASP:OD1	1:R:90:LYS:HE2	1.86	0.74
1:E:353:ILE:HB	1:E:354:PRO:HD3	1.70	0.74
1:R:207:ASP:HB3	1:R:283:VAL:HG11	1.70	0.74
1:V:207:ASP:HB3	1:V:283:VAL:HG11	1.70	0.74
3:X:93:THR:HG22	3:X:96:ARG:HH12	1.50	0.74
1:A:353:ILE:HB	1:A:354:PRO:HD3	1.70	0.73
1:F:207:ASP:HB3	1:F:283:VAL:HG11	1.70	0.73
1:M:205:ASP:OD2	2:O:35:ARG:NH1	2.21	0.73
1:Q:142:GLN:HG2	1:U:142:GLN:HG3	1.69	0.73
1:I:311:SER:H	1:I:314:ASN:ND2	1.86	0.73
1:B:207:ASP:HB3	1:B:283:VAL:HG11	1.70	0.73
1:E:181:GLN:HG3	1:F:91:ASN:ND2	2.04	0.73
1:E:311:SER:H	1:E:314:ASN:ND2	1.86	0.73
1:J:336:GLU:HA	2:K:77:ARG:NH2	2.03	0.73
1:U:311:SER:H	1:U:314:ASN:ND2	1.86	0.73
1:B:135:ARG:NH1	1:B:356:ALA:HB3	2.04	0.73
1:J:245:ASN:HD21	1:J:275:SER:N	1.84	0.73
1:J:207:ASP:HB3	1:J:283:VAL:HG11	1.70	0.73
2:S:94:ASN:C	2:S:95:LYS:N	0.68	0.73
1:U:353:ILE:HB	1:U:354:PRO:HD3	1.70	0.73
1:N:146:LYS:HB2	1:N:149:GLN:HG3	1.68	0.73
1:F:245:ASN:HD21	1:F:275:SER:N	1.84	0.73
1:V:135:ARG:NH1	1:V:356:ALA:HB3	2.04	0.73
1:R:135:ARG:NH1	1:R:356:ALA:HB3	2.03	0.73
1:V:245:ASN:HD21	1:V:275:SER:N	1.84	0.73
1:F:135:ARG:NH1	1:F:356:ALA:HB3	2.04	0.72
1:M:113:PHE:HA	1:N:124:PHE:CE2	2.23	0.72
1:A:219:LEU:HD11	1:A:349:LYS:HG3	1.71	0.72
1:M:165:LEU:HD22	1:N:96:LEU:HD23	1.70	0.72
1:M:311:SER:H	1:M:314:ASN:ND2	1.86	0.72
1:N:207:ASP:HB3	1:N:283:VAL:HG11	1.70	0.72
2:O:97:LEU:CD2	2:O:102:ILE:HG13	2.19	0.72
1:Q:311:SER:H	1:Q:314:ASN:ND2	1.86	0.72
2:W:98:GLY:O	2:W:101:THR:OG1	2.07	0.72
1:U:219:LEU:HD11	1:U:349:LYS:HG3	1.72	0.72
1:A:114:GLN:HG3	1:A:258:LEU:HD11	1.72	0.72
2:G:92:GLU:OE1	3:H:103:LEU:HB2	1.88	0.72
1:M:190:LEU:HD23	1:M:211:LEU:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:114:GLN:HG3	1:U:258:LEU:HD11	1.72	0.72
1:Q:137:ARG:CD	1:U:142:GLN:HE21	2.02	0.72
1:A:311:SER:H	1:A:314:ASN:ND2	1.86	0.72
1:J:135:ARG:NH1	1:J:356:ALA:HB3	2.04	0.72
2:K:97:LEU:HD13	2:O:104:GLN:HG3	1.71	0.72
1:I:114:GLN:HG3	1:I:258:LEU:HD11	1.72	0.72
1:M:114:GLN:HG3	1:M:258:LEU:HD11	1.71	0.72
1:N:135:ARG:NH1	1:N:356:ALA:HB3	2.03	0.72
2:C:79:ILE:CD1	2:C:81:ARG:CZ	2.68	0.72
2:K:99:ARG:HD2	3:L:98:LEU:O	1.89	0.72
2:C:26:PRO:HD3	3:D:37:TYR:CD1	2.25	0.71
1:I:219:LEU:HD11	1:I:349:LYS:HG3	1.72	0.71
1:M:219:LEU:HD11	1:M:349:LYS:HG3	1.71	0.71
1:Q:190:LEU:HD23	1:Q:211:LEU:HB2	1.72	0.71
2:S:99:ARG:HB2	3:T:69:ARG:HH12	1.54	0.71
2:W:100:VAL:C	2:W:102:ILE:H	1.94	0.71
1:B:336:GLU:HG2	2:C:77:ARG:HH21	1.54	0.71
1:A:190:LEU:HD23	1:A:211:LEU:HB2	1.72	0.71
2:K:96:LEU:O	3:L:69:ARG:NH1	2.23	0.71
1:R:188:PHE:HA	1:R:360:PHE:CE2	2.26	0.71
1:I:145:PRO:HB3	1:J:98:SER:HB3	1.71	0.71
2:S:100:VAL:HG22	3:T:69:ARG:CZ	2.20	0.71
2:S:100:VAL:HG23	3:T:69:ARG:CZ	2.20	0.71
1:U:190:LEU:HD23	1:U:211:LEU:HB2	1.72	0.71
1:B:225:GLY:HA2	1:F:226:ARG:NE	2.05	0.71
1:I:190:LEU:HD23	1:I:211:LEU:HB2	1.72	0.71
1:Q:114:GLN:HG3	1:Q:258:LEU:HD11	1.72	0.71
1:Q:219:LEU:HD11	1:Q:349:LYS:HG3	1.72	0.71
1:V:188:PHE:HA	1:V:360:PHE:CE2	2.26	0.71
2:S:71:ARG:HH21	3:T:46:HIS:CD2	2.08	0.71
2:K:84:GLN:HG2	2:O:102:ILE:O	1.90	0.70
1:E:190:LEU:HD23	1:E:211:LEU:HB2	1.72	0.70
2:C:105:GLY:O	2:W:104:GLN:HA	1.90	0.70
1:R:353:ILE:HB	1:R:354:PRO:HD3	1.73	0.70
1:I:135:ARG:HB2	1:J:99:LEU:HD22	1.72	0.70
1:N:188:PHE:HA	1:N:360:PHE:CE2	2.26	0.70
1:E:114:GLN:HG3	1:E:258:LEU:HD11	1.72	0.70
2:K:97:LEU:HD13	2:O:104:GLN:CG	2.21	0.70
1:M:99:LEU:HD22	1:N:135:ARG:HG3	1.73	0.70
1:B:188:PHE:HA	1:B:360:PHE:CE2	2.26	0.70
1:M:125:LEU:HD22	1:M:221:TYR:CD1	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:95:LYS:HB2	1:R:185:ILE:HG12	1.73	0.70
1:B:353:ILE:HB	1:B:354:PRO:HD3	1.73	0.70
1:I:185:ILE:HD12	1:J:96:LEU:CD1	2.21	0.70
1:Q:91:ASN:O	1:Q:95:LYS:HG2	1.92	0.70
2:S:102:ILE:CG2	2:S:103:ALA:N	2.35	0.70
1:A:120:LEU:HD13	1:B:120:LEU:HD12	1.73	0.70
1:F:129:LYS:HB2	1:F:130:PRO:HD3	1.74	0.70
1:V:353:ILE:HB	1:V:354:PRO:HD3	1.74	0.70
1:A:125:LEU:HD22	1:A:221:TYR:CD1	2.27	0.69
1:A:145:PRO:HB3	1:B:98:SER:HB3	1.73	0.69
1:E:219:LEU:HD11	1:E:349:LYS:HG3	1.72	0.69
2:C:105:GLY:C	2:W:104:GLN:HA	2.12	0.69
1:F:353:ILE:HB	1:F:354:PRO:HD3	1.73	0.69
1:N:129:LYS:HB2	1:N:130:PRO:HD3	1.74	0.69
1:F:188:PHE:HA	1:F:360:PHE:CE2	2.27	0.69
1:E:135:ARG:HB2	1:F:99:LEU:HD22	1.75	0.69
1:J:188:PHE:HA	1:J:360:PHE:CE2	2.27	0.69
1:Q:154:GLN:N	1:R:97:LEU:HD12	2.08	0.69
1:A:364:ALA:HA	1:B:260:TYR:HE2	1.58	0.69
1:N:353:ILE:HB	1:N:354:PRO:HD3	1.74	0.69
1:U:120:LEU:HD13	1:V:120:LEU:HD12	1.73	0.69
1:A:91:ASN:O	1:A:95:LYS:HG2	1.93	0.69
2:K:97:LEU:CD2	2:O:104:GLN:HE21	2.06	0.69
2:W:93:LEU:HA	2:W:96:LEU:CD2	2.23	0.69
1:E:125:LEU:HD22	1:E:221:TYR:CD1	2.27	0.69
1:J:353:ILE:HB	1:J:354:PRO:HD3	1.74	0.68
1:E:91:ASN:O	1:E:95:LYS:HG2	1.93	0.68
1:V:339:ALA:HB3	2:W:77:ARG:HH22	1.58	0.68
1:V:129:LYS:HB2	1:V:130:PRO:HD3	1.74	0.68
2:C:81:ARG:HB3	2:W:104:GLN:NE2	2.08	0.68
1:F:163:THR:HG23	1:F:166:LEU:HD12	1.75	0.68
1:I:125:LEU:HD22	1:I:221:TYR:CD1	2.27	0.68
1:Q:125:LEU:HD22	1:Q:221:TYR:CD1	2.28	0.68
1:U:91:ASN:O	1:U:95:LYS:HG2	1.93	0.68
2:C:71:ARG:HH21	3:D:46:HIS:CD2	2.11	0.68
1:J:163:THR:HG23	1:J:166:LEU:HD12	1.75	0.68
1:N:163:THR:HG23	1:N:166:LEU:HD12	1.75	0.68
2:W:99:ARG:NH1	2:W:99:ARG:HA	2.08	0.68
1:I:198:ILE:HB	1:I:347:GLN:HG3	1.75	0.68
1:R:163:THR:HG23	1:R:166:LEU:HD12	1.75	0.68
1:U:99:LEU:HD22	1:V:135:ARG:HG3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:81:ARG:HG2	2:W:104:GLN:HB2	1.76	0.68
1:U:131:ILE:HD12	1:V:106:LEU:HD23	1.76	0.68
1:A:181:GLN:HG3	1:B:91:ASN:ND2	2.09	0.68
1:R:129:LYS:HB2	1:R:130:PRO:HD3	1.74	0.68
1:B:129:LYS:HB2	1:B:130:PRO:HD3	1.74	0.68
1:M:141:GLY:HA3	1:M:183:LYS:HD3	1.76	0.68
2:O:41:GLU:HB3	3:P:84:SER:HB3	1.75	0.68
1:A:198:ILE:HB	1:A:347:GLN:HG3	1.76	0.68
1:E:360:PHE:HE1	1:F:96:LEU:HD21	1.58	0.68
1:J:129:LYS:HB2	1:J:130:PRO:HD3	1.74	0.68
1:M:149:GLN:HB3	1:N:98:SER:HA	1.76	0.68
1:Q:198:ILE:HB	1:Q:347:GLN:HG3	1.76	0.68
1:U:198:ILE:HB	1:U:347:GLN:HG3	1.76	0.68
1:U:125:LEU:HD22	1:U:221:TYR:CD1	2.27	0.68
1:M:91:ASN:O	1:M:95:LYS:HG2	1.93	0.67
1:V:250:LYS:HE3	1:V:318:PRO:HG3	1.76	0.67
1:U:98:SER:HB3	1:V:145:PRO:HB3	1.76	0.67
1:F:111:LYS:NZ	1:F:258:LEU:HD13	2.10	0.67
2:G:96:LEU:HD13	2:G:97:LEU:N	2.09	0.67
1:I:91:ASN:O	1:I:95:LYS:HG2	1.93	0.67
1:U:120:LEU:CD1	1:V:120:LEU:HD12	2.25	0.67
1:B:111:LYS:NZ	1:B:258:LEU:HD13	2.10	0.67
1:N:111:LYS:NZ	1:N:258:LEU:HD13	2.09	0.67
1:B:163:THR:HG23	1:B:166:LEU:HD12	1.75	0.67
1:E:181:GLN:N	1:F:91:ASN:ND2	2.42	0.67
1:R:111:LYS:NZ	1:R:258:LEU:HD13	2.09	0.67
1:R:250:LYS:HE3	1:R:318:PRO:HG3	1.76	0.67
2:G:26:PRO:HD3	3:H:37:TYR:CD1	2.29	0.67
1:B:336:GLU:HA	2:C:77:ARG:NH2	2.10	0.67
1:V:111:LYS:NZ	1:V:258:LEU:HD13	2.09	0.67
2:C:94:ASN:ND2	2:W:94:ASN:HD21	1.89	0.67
1:Q:153:GLY:C	1:R:97:LEU:HD12	2.15	0.67
1:J:250:LYS:HE3	1:J:318:PRO:HG3	1.77	0.66
1:Q:142:GLN:HG2	1:U:142:GLN:HG2	1.76	0.66
1:E:141:GLY:HA3	1:E:183:LYS:HD3	1.78	0.66
1:J:111:LYS:NZ	1:J:258:LEU:HD13	2.10	0.66
1:M:198:ILE:HB	1:M:347:GLN:HG3	1.76	0.66
2:O:88:ARG:NH2	2:O:97:LEU:HD13	2.10	0.66
2:O:97:LEU:HD22	2:O:102:ILE:HG13	1.76	0.66
1:V:163:THR:HG23	1:V:166:LEU:HD12	1.75	0.66
1:I:144:GLN:OE1	1:J:95:LYS:HE3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLN:HG3	1:B:91:ASN:HD22	1.59	0.66
1:Q:141:GLY:HA3	1:Q:183:LYS:HD3	1.77	0.66
2:W:92:GLU:OE2	3:X:102:GLU:HB3	1.95	0.66
1:U:199:VAL:HG22	1:U:344:ILE:HG23	1.78	0.66
1:A:120:LEU:CD1	1:B:120:LEU:HD12	2.26	0.66
1:I:141:GLY:HA3	1:I:183:LYS:HD3	1.78	0.66
2:O:97:LEU:CD2	2:O:102:ILE:CD1	2.72	0.66
1:N:250:LYS:HE3	1:N:318:PRO:HG3	1.77	0.66
2:C:81:ARG:CB	2:W:104:GLN:CD	2.56	0.66
1:E:125:LEU:HA	1:E:128:TYR:HD2	1.61	0.66
1:E:198:ILE:HB	1:E:347:GLN:HG3	1.76	0.66
1:F:127:LYS:HE3	1:U:169:GLU:OE1	1.95	0.66
1:A:199:VAL:HG22	1:A:344:ILE:HG23	1.78	0.65
1:I:199:VAL:HG22	1:I:344:ILE:HG23	1.77	0.65
1:Q:95:LYS:NZ	1:R:184:GLY:CA	2.56	0.65
1:B:250:LYS:HE3	1:B:318:PRO:HG3	1.77	0.65
1:Q:199:VAL:HG22	1:Q:344:ILE:HG23	1.77	0.65
1:U:125:LEU:HA	1:U:128:TYR:HD2	1.61	0.65
1:M:199:VAL:HG22	1:M:344:ILE:HG23	1.78	0.65
1:Q:131:ILE:HD12	1:R:106:LEU:HD23	1.77	0.65
1:F:183:LYS:HG3	1:F:184:GLY:N	2.10	0.65
1:I:125:LEU:HA	1:I:128:TYR:HD2	1.61	0.65
2:K:81:ARG:HH22	2:O:101:THR:HA	1.62	0.65
2:S:100:VAL:CG1	3:T:65:ASP:CG	2.56	0.65
2:W:100:VAL:O	2:W:102:ILE:N	2.30	0.65
2:G:93:LEU:O	2:G:97:LEU:CB	2.44	0.65
2:G:87:VAL:HA	2:G:93:LEU:HD12	1.79	0.65
1:Q:100:LYS:HA	1:R:357:VAL:HG11	1.78	0.65
1:Q:149:GLN:HB3	1:R:98:SER:HA	1.79	0.65
2:W:99:ARG:NE	2:W:99:ARG:HA	2.08	0.65
1:A:125:LEU:HA	1:A:128:TYR:HD2	1.61	0.65
2:G:87:VAL:CG2	2:G:93:LEU:CD1	2.52	0.65
1:A:141:GLY:HA3	1:A:183:LYS:HD3	1.78	0.65
1:M:125:LEU:HA	1:M:128:TYR:HD2	1.61	0.65
1:F:250:LYS:HE3	1:F:318:PRO:HG3	1.78	0.64
2:G:100:VAL:O	2:G:101:THR:HG23	1.98	0.64
2:C:99:ARG:HH22	2:W:89:ASN:ND2	1.94	0.64
1:B:311:SER:H	1:B:314:ASN:ND2	1.96	0.64
1:F:311:SER:H	1:F:314:ASN:ND2	1.96	0.64
1:Q:125:LEU:HA	1:Q:128:TYR:HD2	1.61	0.64
1:Q:137:ARG:HD2	1:U:142:GLN:NE2	2.08	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:196:LEU:HD21	1:I:347:GLN:HB3	1.80	0.64
1:M:95:LYS:HD2	1:N:145:PRO:HG2	1.79	0.64
1:N:311:SER:H	1:N:314:ASN:ND2	1.96	0.64
1:U:141:GLY:HA3	1:U:183:LYS:HD3	1.77	0.64
2:W:77:ARG:HG3	3:X:51:ILE:N	2.11	0.64
1:R:311:SER:H	1:R:314:ASN:ND2	1.96	0.64
1:U:99:LEU:HD21	1:V:138:ILE:HB	1.80	0.64
1:E:199:VAL:HG22	1:E:344:ILE:HG23	1.78	0.64
1:U:256:LYS:HD2	1:U:257:GLU:H	1.63	0.64
1:J:219:LEU:HD23	1:J:220:GLU:N	2.13	0.64
1:B:206:ARG:HH21	1:B:283:VAL:HA	1.63	0.64
1:N:206:ARG:HH21	1:N:283:VAL:HA	1.63	0.64
3:T:91:ILE:O	3:T:95:VAL:HG23	1.98	0.64
1:E:196:LEU:HD21	1:E:347:GLN:HB3	1.80	0.63
1:F:336:GLU:HA	2:G:77:ARG:HH22	1.58	0.63
1:M:256:LYS:HD2	1:M:257:GLU:H	1.63	0.63
1:N:85:VAL:HA	1:N:88:LEU:HD12	1.80	0.63
1:V:206:ARG:HH21	1:V:283:VAL:HA	1.63	0.63
2:C:105:GLY:O	2:W:104:GLN:CA	2.46	0.63
1:B:219:LEU:HD23	1:B:220:GLU:N	2.13	0.63
1:V:219:LEU:HD23	1:V:220:GLU:N	2.13	0.63
1:A:190:LEU:O	1:A:194:GLU:HG2	1.99	0.63
3:L:91:ILE:O	3:L:95:VAL:HG23	1.98	0.63
1:Q:95:LYS:HZ1	1:R:184:GLY:CA	2.10	0.63
1:U:190:LEU:O	1:U:194:GLU:HG2	1.99	0.63
1:A:256:LYS:HD2	1:A:257:GLU:H	1.63	0.63
1:I:190:LEU:O	1:I:194:GLU:HG2	1.99	0.63
1:Q:203:ILE:HD12	1:Q:203:ILE:O	1.99	0.63
1:Q:256:LYS:HD2	1:Q:257:GLU:H	1.63	0.63
1:U:196:LEU:HD21	1:U:347:GLN:HB3	1.80	0.63
1:M:203:ILE:HD12	1:M:203:ILE:O	1.99	0.63
1:E:203:ILE:O	1:E:203:ILE:HD12	1.99	0.63
1:E:256:LYS:HD2	1:E:257:GLU:H	1.63	0.63
2:G:97:LEU:HD11	3:H:62:PHE:CE1	2.34	0.63
2:K:26:PRO:HD3	3:L:37:TYR:CD1	2.34	0.63
1:M:196:LEU:HD21	1:M:347:GLN:HB3	1.80	0.63
1:M:93:LYS:HD2	1:N:167:VAL:HG22	1.80	0.63
1:Q:196:LEU:HD21	1:Q:347:GLN:HB3	1.80	0.63
1:R:219:LEU:HD23	1:R:220:GLU:N	2.13	0.63
2:S:99:ARG:CB	3:T:69:ARG:NH1	2.61	0.63
2:G:100:VAL:HG12	2:G:101:THR:OG1	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:125:LEU:HD22	1:I:221:TYR:HD1	1.64	0.63
1:J:134:GLN:O	1:J:138:ILE:HG12	1.99	0.63
1:J:183:LYS:HG3	1:J:184:GLY:N	2.10	0.63
1:J:206:ARG:HH21	1:J:283:VAL:HA	1.63	0.63
1:M:190:LEU:O	1:M:194:GLU:HG2	1.99	0.63
2:K:84:GLN:NE2	2:O:102:ILE:C	2.48	0.63
1:U:206:ARG:NH2	1:U:283:VAL:HA	2.14	0.63
1:V:311:SER:H	1:V:314:ASN:ND2	1.95	0.63
1:E:360:PHE:CE1	1:F:96:LEU:HD21	2.33	0.63
1:I:256:LYS:HD2	1:I:257:GLU:H	1.63	0.63
1:M:154:GLN:N	1:N:97:LEU:HD12	2.13	0.63
1:U:203:ILE:O	1:U:203:ILE:HD12	1.99	0.63
1:U:243:PHE:HD2	1:U:245:ASN:HB2	1.64	0.63
1:V:85:VAL:HA	1:V:88:LEU:HD12	1.80	0.63
1:A:196:LEU:HD21	1:A:347:GLN:HB3	1.80	0.63
1:A:243:PHE:HD2	1:A:245:ASN:HB2	1.64	0.63
1:F:219:LEU:HD23	1:F:220:GLU:N	2.13	0.63
1:J:311:SER:H	1:J:314:ASN:ND2	1.96	0.63
1:N:219:LEU:HD23	1:N:220:GLU:N	2.13	0.63
1:B:85:VAL:HA	1:B:88:LEU:HD12	1.80	0.62
1:E:125:LEU:HD22	1:E:221:TYR:HD1	1.64	0.62
1:E:185:ILE:HG13	1:F:92:VAL:HG13	1.80	0.62
1:E:97:LEU:HD13	1:F:157:VAL:HG21	1.80	0.62
3:H:91:ILE:O	3:H:95:VAL:HG23	1.98	0.62
1:N:190:LEU:HD23	1:N:211:LEU:HB2	1.81	0.62
1:V:190:LEU:HD23	1:V:211:LEU:HB2	1.81	0.62
1:A:195:ASN:HB3	1:A:365:LEU:HD21	1.81	0.62
1:B:190:LEU:HD23	1:B:211:LEU:HB2	1.81	0.62
1:I:195:ASN:HB3	1:I:365:LEU:HD21	1.81	0.62
1:I:203:ILE:O	1:I:203:ILE:HD12	1.99	0.62
1:J:85:VAL:HA	1:J:88:LEU:HD12	1.80	0.62
1:M:206:ARG:NH2	1:M:283:VAL:HA	2.14	0.62
3:X:91:ILE:O	3:X:95:VAL:HG23	1.98	0.62
1:A:203:ILE:HD12	1:A:203:ILE:O	1.99	0.62
1:E:190:LEU:O	1:E:194:GLU:HG2	1.99	0.62
1:E:243:PHE:HD2	1:E:245:ASN:HB2	1.64	0.62
1:M:116:GLU:C	1:N:120:LEU:HD11	2.20	0.62
1:R:206:ARG:HH21	1:R:283:VAL:HA	1.63	0.62
1:F:206:ARG:HH21	1:F:283:VAL:HA	1.63	0.62
1:N:134:GLN:O	1:N:138:ILE:HG12	1.99	0.62
3:P:91:ILE:O	3:P:95:VAL:HG23	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:GLN:O	1:B:138:ILE:HG12	1.99	0.62
1:Q:190:LEU:O	1:Q:194:GLU:HG2	1.99	0.62
1:Q:243:PHE:HD2	1:Q:245:ASN:HB2	1.64	0.62
1:Q:99:LEU:CD2	1:R:135:ARG:HG3	2.14	0.62
1:U:195:ASN:HB3	1:U:365:LEU:HD21	1.82	0.62
1:F:85:VAL:HA	1:F:88:LEU:HD12	1.80	0.62
2:O:37:GLY:HA3	2:O:39:TYR:CE2	2.35	0.62
1:U:103:GLN:OE1	1:V:357:VAL:HB	2.00	0.62
1:A:206:ARG:NH2	1:A:283:VAL:HA	2.14	0.62
1:F:134:GLN:O	1:F:138:ILE:HG12	1.99	0.62
1:I:181:GLN:N	1:J:91:ASN:ND2	2.48	0.62
1:M:195:ASN:HB3	1:M:365:LEU:HD21	1.81	0.62
1:U:125:LEU:HD22	1:U:221:TYR:HD1	1.64	0.62
1:N:183:LYS:HG3	1:N:184:GLY:N	2.10	0.62
3:D:91:ILE:O	3:D:95:VAL:HG23	1.98	0.61
1:E:186:PRO:CD	1:F:92:VAL:HG22	2.30	0.61
1:I:206:ARG:NH2	1:I:283:VAL:HA	2.14	0.61
3:D:93:THR:HG22	3:D:96:ARG:NH1	2.15	0.61
1:E:357:VAL:HG11	1:F:100:LYS:HA	1.82	0.61
2:G:37:GLY:HA3	2:G:39:TYR:CE2	2.35	0.61
1:I:243:PHE:HD2	1:I:245:ASN:HB2	1.64	0.61
1:J:190:LEU:HD23	1:J:211:LEU:HB2	1.81	0.61
2:S:37:GLY:HA3	2:S:39:TYR:CE2	2.35	0.61
2:C:37:GLY:HA3	2:C:39:TYR:CE2	2.35	0.61
1:A:169:GLU:O	1:I:169:GLU:OE1	2.19	0.61
1:J:200:CYS:O	1:J:203:ILE:HG13	2.01	0.61
2:K:37:GLY:HA3	2:K:39:TYR:CE2	2.35	0.61
2:K:96:LEU:HD11	3:L:99:LEU:CD2	2.28	0.61
1:Q:206:ARG:NH2	1:Q:283:VAL:HA	2.14	0.61
1:R:243:PHE:CD2	1:R:245:ASN:HB2	2.35	0.61
1:V:134:GLN:O	1:V:138:ILE:HG12	1.99	0.61
1:Q:195:ASN:HB3	1:Q:365:LEU:HD21	1.82	0.61
1:R:183:LYS:HG3	1:R:184:GLY:N	2.09	0.61
1:A:125:LEU:HD22	1:A:221:TYR:HD1	1.64	0.61
1:M:124:PHE:CZ	1:N:112:GLU:HG3	2.35	0.61
1:M:260:TYR:O	1:N:355:ARG:NH2	2.34	0.61
1:R:141:GLY:HA3	1:R:183:LYS:HE2	1.83	0.61
1:B:200:CYS:O	1:B:203:ILE:HG13	2.01	0.61
1:F:190:LEU:HD23	1:F:211:LEU:HB2	1.81	0.61
2:G:97:LEU:HG	3:H:62:PHE:HE1	1.64	0.61
1:M:124:PHE:HE1	1:N:112:GLU:HG3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:141:GLY:HA3	1:N:183:LYS:HE2	1.82	0.61
1:R:190:LEU:HD23	1:R:211:LEU:HB2	1.81	0.61
2:S:26:PRO:HD3	3:T:37:TYR:CD1	2.35	0.61
1:E:206:ARG:NH2	1:E:283:VAL:HA	2.14	0.61
1:V:183:LYS:HG3	1:V:184:GLY:N	2.10	0.61
2:W:37:GLY:HA3	2:W:39:TYR:CE2	2.35	0.61
1:F:200:CYS:O	1:F:203:ILE:HG13	2.01	0.61
2:G:97:LEU:CD1	3:H:62:PHE:CE1	2.84	0.61
1:M:98:SER:HB3	1:N:145:PRO:HB3	1.81	0.61
1:N:200:CYS:O	1:N:203:ILE:HG13	2.01	0.61
1:V:141:GLY:HA3	1:V:183:LYS:HE2	1.83	0.61
2:K:97:LEU:HD11	2:O:104:GLN:CD	2.20	0.61
1:N:242:PHE:O	1:N:277:LYS:HG2	2.01	0.61
1:Q:125:LEU:HD22	1:Q:221:TYR:HD1	1.64	0.61
1:R:200:CYS:O	1:R:203:ILE:HG13	2.01	0.61
2:S:100:VAL:HG23	3:T:69:ARG:NH1	2.15	0.61
1:V:200:CYS:O	1:V:203:ILE:HG13	2.01	0.61
2:O:77:ARG:HG3	3:P:51:ILE:N	2.15	0.60
1:R:85:VAL:HA	1:R:88:LEU:HD12	1.80	0.60
3:T:93:THR:HG22	3:T:96:ARG:NH1	2.16	0.60
1:V:242:PHE:O	1:V:277:LYS:HG2	2.01	0.60
1:M:125:LEU:HD22	1:M:221:TYR:HD1	1.64	0.60
1:R:134:GLN:O	1:R:138:ILE:HG12	1.99	0.60
1:Q:145:PRO:HG2	1:R:95:LYS:HD3	1.83	0.60
2:C:105:GLY:C	2:W:104:GLN:CA	2.70	0.60
1:E:129:LYS:NZ	1:E:220:GLU:HG2	2.17	0.60
3:X:93:THR:HG22	3:X:96:ARG:NH1	2.16	0.60
3:D:46:HIS:HB3	3:D:49:THR:HB	1.84	0.60
1:F:243:PHE:CD2	1:F:245:ASN:HB2	2.35	0.60
1:M:243:PHE:HD2	1:M:245:ASN:HB2	1.64	0.60
3:P:93:THR:HG22	3:P:96:ARG:NH1	2.16	0.60
1:Q:96:LEU:HD21	1:R:360:PHE:HE1	1.67	0.60
1:Q:135:ARG:HB2	1:R:99:LEU:HD22	1.83	0.60
3:X:46:HIS:HB3	3:X:49:THR:HB	1.84	0.60
1:F:242:PHE:O	1:F:277:LYS:HG2	2.01	0.60
1:M:129:LYS:NZ	1:M:220:GLU:HG2	2.16	0.60
1:N:243:PHE:CD2	1:N:245:ASN:HB2	2.35	0.60
2:S:101:THR:O	2:S:102:ILE:O	2.20	0.60
1:B:242:PHE:O	1:B:277:LYS:HG2	2.01	0.60
1:J:141:GLY:HA3	1:J:183:LYS:HE2	1.83	0.60
2:K:103:ALA:HB1	2:O:81:ARG:HD3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:339:ALA:HB3	2:O:77:ARG:HH22	1.67	0.60
2:O:99:ARG:CG	2:O:99:ARG:HH11	2.14	0.60
1:Q:124:PHE:CD2	1:R:113:PHE:HD1	2.20	0.60
1:R:242:PHE:O	1:R:277:LYS:HG2	2.01	0.60
1:E:195:ASN:HB3	1:E:365:LEU:HD21	1.81	0.60
2:G:96:LEU:HD13	2:G:96:LEU:C	2.22	0.60
1:R:114:GLN:HE21	1:R:263:ASP:HA	1.67	0.60
1:U:95:LYS:HD2	1:V:145:PRO:HG2	1.84	0.60
1:B:243:PHE:CD2	1:B:245:ASN:HB2	2.35	0.60
1:Q:129:LYS:NZ	1:Q:220:GLU:HG2	2.17	0.60
3:T:46:HIS:HB3	3:T:49:THR:HB	1.84	0.60
1:U:260:TYR:O	1:V:355:ARG:NH2	2.34	0.60
1:U:198:ILE:HD13	3:X:36:ILE:HD13	1.84	0.60
2:O:63:LEU:HD13	3:P:42:LEU:HB2	1.83	0.59
1:V:114:GLN:HE21	1:V:263:ASP:HA	1.67	0.59
1:A:196:LEU:HD12	1:A:197:PRO:HD2	1.84	0.59
1:A:201:ASP:OD2	3:D:37:TYR:OH	2.21	0.59
3:H:93:THR:HG22	3:H:96:ARG:NH1	2.15	0.59
1:J:242:PHE:O	1:J:277:LYS:HG2	2.01	0.59
1:E:250:LYS:HE2	1:E:318:PRO:CG	2.33	0.59
2:G:87:VAL:O	2:G:90:ASP:O	2.20	0.59
1:F:141:GLY:HA3	1:F:183:LYS:HE2	1.83	0.59
1:I:129:LYS:NZ	1:I:220:GLU:HG2	2.17	0.59
2:O:99:ARG:NH1	2:O:99:ARG:HG2	2.16	0.59
1:B:141:GLY:HA3	1:B:183:LYS:HE2	1.83	0.59
3:P:46:HIS:HB3	3:P:49:THR:HB	1.84	0.59
1:J:114:GLN:HE21	1:J:263:ASP:HA	1.68	0.59
1:Q:250:LYS:HE2	1:Q:318:PRO:CG	2.32	0.59
2:C:81:ARG:O	2:C:85:LEU:HG	2.03	0.59
2:G:62:ILE:HD11	2:G:93:LEU:HD21	1.83	0.59
2:G:81:ARG:O	2:G:85:LEU:HG	2.03	0.59
1:M:128:TYR:CE1	1:N:110:GLU:HG2	2.37	0.59
2:O:81:ARG:O	2:O:85:LEU:HG	2.03	0.59
2:O:88:ARG:NH1	2:O:97:LEU:HD13	2.17	0.59
1:V:243:PHE:CD2	1:V:245:ASN:HB2	2.35	0.59
1:A:129:LYS:NZ	1:A:220:GLU:HG2	2.17	0.59
3:H:46:HIS:HB3	3:H:49:THR:HB	1.84	0.59
3:L:93:THR:HG22	3:L:96:ARG:NH1	2.16	0.59
1:N:114:GLN:HE21	1:N:263:ASP:HA	1.67	0.59
1:B:114:GLN:HE21	1:B:263:ASP:HA	1.68	0.58
2:K:81:ARG:O	2:K:85:LEU:HG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:124:PHE:CD1	1:V:127:LYS:HD2	2.38	0.58
2:W:81:ARG:O	2:W:85:LEU:HG	2.03	0.58
1:A:250:LYS:HE2	1:A:318:PRO:CG	2.33	0.58
1:A:337:ARG:NH1	1:A:337:ARG:HB2	2.19	0.58
1:F:124:PHE:CD1	1:F:127:LYS:HD2	2.38	0.58
1:I:250:LYS:HE2	1:I:318:PRO:CG	2.33	0.58
1:J:124:PHE:CD1	1:J:127:LYS:HD2	2.38	0.58
3:L:46:HIS:HB3	3:L:49:THR:HB	1.84	0.58
1:Q:196:LEU:HD12	1:Q:197:PRO:HD2	1.84	0.58
2:W:96:LEU:HG	2:W:97:LEU:N	2.19	0.58
1:E:120:LEU:HD13	1:F:120:LEU:HD12	1.86	0.58
1:I:131:ILE:HD12	1:J:106:LEU:HD23	1.85	0.58
1:I:138:ILE:HB	1:J:99:LEU:HD21	1.84	0.58
2:O:26:PRO:HD3	3:P:37:TYR:CD1	2.39	0.58
1:U:129:LYS:NZ	1:U:220:GLU:HG2	2.17	0.58
1:B:105:GLU:O	1:B:109:VAL:HG23	2.04	0.58
1:I:196:LEU:HD12	1:I:197:PRO:HD2	1.84	0.58
1:J:105:GLU:O	1:J:109:VAL:HG23	2.04	0.58
1:I:310:GLU:HG2	2:K:16:THR:CA	2.33	0.58
1:N:105:GLU:O	1:N:109:VAL:HG23	2.04	0.58
1:N:124:PHE:CD1	1:N:127:LYS:HD2	2.38	0.58
1:B:124:PHE:CD1	1:B:127:LYS:HD2	2.38	0.58
1:M:196:LEU:HD12	1:M:197:PRO:HD2	1.84	0.58
1:M:250:LYS:HE2	1:M:318:PRO:CG	2.33	0.58
1:R:124:PHE:CD1	1:R:127:LYS:HD2	2.38	0.58
1:U:337:ARG:NH1	1:U:337:ARG:HB2	2.19	0.58
1:V:105:GLU:O	1:V:109:VAL:HG23	2.04	0.58
1:E:196:LEU:HD12	1:E:197:PRO:HD2	1.84	0.58
1:F:114:GLN:HE21	1:F:263:ASP:HA	1.68	0.58
1:I:99:LEU:HD22	1:J:135:ARG:HG3	1.85	0.58
1:Q:337:ARG:NH1	1:Q:337:ARG:HB2	2.19	0.58
2:S:81:ARG:O	2:S:85:LEU:HG	2.03	0.58
1:U:250:LYS:HE2	1:U:318:PRO:CG	2.33	0.58
2:W:96:LEU:HB3	3:X:100:PRO:HD3	1.84	0.58
1:M:337:ARG:HB2	1:M:337:ARG:NH1	2.19	0.58
1:A:182:VAL:HG21	1:A:186:PRO:HD3	1.86	0.58
1:E:182:VAL:HG21	1:E:186:PRO:HD3	1.86	0.58
2:G:97:LEU:HA	3:H:69:ARG:HH12	1.68	0.58
2:K:103:ALA:HA	2:O:81:ARG:HH11	0.75	0.58
2:W:39:TYR:HB3	3:X:75:SER:HB2	1.86	0.58
1:I:337:ARG:HB2	1:I:337:ARG:NH1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:182:VAL:HG21	1:M:186:PRO:HD3	1.86	0.57
1:E:337:ARG:HB2	1:E:337:ARG:NH1	2.19	0.57
1:F:111:LYS:O	1:F:115:VAL:HG23	2.04	0.57
1:F:125:LEU:HD21	1:F:219:LEU:O	2.05	0.57
1:I:181:GLN:HG3	1:J:91:ASN:ND2	2.20	0.57
1:E:85:VAL:HG23	1:E:88:LEU:HD12	1.87	0.57
2:G:97:LEU:O	3:H:69:ARG:CZ	2.51	0.57
1:I:182:VAL:HG21	1:I:186:PRO:HD3	1.86	0.57
1:J:125:LEU:HD21	1:J:219:LEU:O	2.04	0.57
1:Q:182:VAL:HG21	1:Q:186:PRO:HD3	1.86	0.57
1:Q:85:VAL:HG23	1:Q:88:LEU:HD12	1.86	0.57
1:Q:95:LYS:HB3	1:R:185:ILE:HG13	1.85	0.57
1:V:125:LEU:HD21	1:V:219:LEU:O	2.04	0.57
1:N:111:LYS:O	1:N:115:VAL:HG23	2.04	0.57
1:R:105:GLU:O	1:R:109:VAL:HG23	2.04	0.57
1:E:184:GLY:HA2	1:F:95:LYS:HE2	1.85	0.57
1:I:85:VAL:HG23	1:I:88:LEU:HD12	1.87	0.57
2:K:99:ARG:NE	3:L:98:LEU:O	2.37	0.57
1:M:85:VAL:HG23	1:M:88:LEU:HD12	1.86	0.57
1:F:129:LYS:O	1:F:133:GLU:HG3	2.04	0.57
1:F:227:PRO:HB2	1:F:254:TYR:HB2	1.87	0.57
1:N:125:LEU:HD21	1:N:219:LEU:O	2.04	0.57
1:U:196:LEU:HD12	1:U:197:PRO:HD2	1.84	0.57
1:B:183:LYS:HG3	1:B:184:GLY:N	2.10	0.57
1:Q:95:LYS:HB2	1:R:185:ILE:CG1	2.35	0.57
1:R:129:LYS:O	1:R:133:GLU:HG3	2.04	0.57
2:W:40:ALA:CB	3:X:86:ILE:HG13	2.34	0.57
1:E:181:GLN:HG3	1:F:91:ASN:HD22	1.69	0.57
1:F:105:GLU:O	1:F:109:VAL:HG23	2.04	0.57
3:H:95:VAL:HG13	3:H:99:LEU:HD12	1.87	0.57
1:R:125:LEU:HD21	1:R:219:LEU:O	2.04	0.57
1:B:111:LYS:O	1:B:115:VAL:HG23	2.04	0.57
1:J:111:LYS:O	1:J:115:VAL:HG23	2.04	0.57
1:R:210:VAL:HG22	1:R:242:PHE:CE2	2.40	0.57
1:V:129:LYS:O	1:V:133:GLU:HG3	2.04	0.57
1:E:322:GLN:NE2	1:E:334:LEU:HD22	2.20	0.57
3:H:92:GLN:HE21	3:H:108:VAL:HG13	1.69	0.57
1:M:117:MET:HA	1:N:120:LEU:CD1	2.35	0.57
3:P:92:GLN:HE21	3:P:108:VAL:HG13	1.70	0.57
1:R:227:PRO:HB2	1:R:254:TYR:HB2	1.87	0.57
1:U:182:VAL:HG21	1:U:186:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:54:VAL:HG13	3:X:107:ALA:HB1	1.87	0.57
1:A:102:LEU:HD11	1:B:149:GLN:NE2	2.20	0.56
1:F:210:VAL:HG22	1:F:242:PHE:CE2	2.40	0.56
1:J:129:LYS:O	1:J:133:GLU:HG3	2.04	0.56
1:I:310:GLU:HG2	2:K:16:THR:HA	1.87	0.56
3:L:92:GLN:HE21	3:L:108:VAL:HG13	1.70	0.56
1:M:124:PHE:CD2	1:N:113:PHE:HD1	2.23	0.56
1:N:129:LYS:O	1:N:133:GLU:HG3	2.04	0.56
1:Q:95:LYS:HZ3	1:R:184:GLY:HA2	1.66	0.56
2:W:103:ALA:C	2:W:104:GLN:HG3	2.25	0.56
1:M:322:GLN:NE2	1:M:334:LEU:HD22	2.20	0.56
2:O:64:GLU:OE1	3:P:45:VAL:HB	2.05	0.56
3:D:92:GLN:HE21	3:D:108:VAL:HG13	1.70	0.56
1:I:120:LEU:HD13	1:J:120:LEU:HD12	1.88	0.56
1:J:227:PRO:HB2	1:J:254:TYR:HB2	1.87	0.56
1:M:252:TYR:HE2	1:M:342:TYR:HA	1.70	0.56
3:P:34:TYR:O	3:P:38:VAL:HG23	2.06	0.56
1:Q:322:GLN:NE2	1:Q:334:LEU:HD22	2.20	0.56
1:R:111:LYS:O	1:R:115:VAL:HG23	2.04	0.56
3:X:92:GLN:HE21	3:X:108:VAL:HG13	1.69	0.56
1:A:85:VAL:HG23	1:A:88:LEU:HD12	1.87	0.56
1:B:270:GLU:OE2	1:F:224:ASP:CB	2.52	0.56
1:E:181:GLN:CG	1:F:91:ASN:HD22	2.18	0.56
1:V:210:VAL:HG22	1:V:242:PHE:CE2	2.40	0.56
3:H:34:TYR:O	3:H:38:VAL:HG23	2.06	0.56
1:J:210:VAL:HG22	1:J:242:PHE:CE2	2.40	0.56
1:M:168:ASP:OD1	1:N:90:LYS:HE2	2.04	0.56
1:Q:198:ILE:CD1	3:T:36:ILE:HD13	2.32	0.56
1:U:322:GLN:NE2	1:U:334:LEU:HD22	2.20	0.56
1:A:252:TYR:HE2	1:A:342:TYR:HA	1.70	0.56
1:B:125:LEU:HD21	1:B:219:LEU:O	2.05	0.56
1:E:185:ILE:CD1	1:F:96:LEU:HD11	2.33	0.56
2:G:87:VAL:CG1	2:G:94:ASN:N	2.69	0.56
1:J:243:PHE:CD2	1:J:245:ASN:HB2	2.35	0.56
2:K:41:GLU:HB3	3:L:84:SER:HB3	1.87	0.56
1:V:111:LYS:O	1:V:115:VAL:HG23	2.04	0.56
3:L:34:TYR:O	3:L:38:VAL:HG23	2.06	0.56
1:B:129:LYS:O	1:B:133:GLU:HG3	2.04	0.56
1:U:85:VAL:HG23	1:U:88:LEU:HD12	1.86	0.56
2:C:81:ARG:HG2	2:W:104:GLN:CB	2.35	0.56
2:W:30:VAL:O	2:W:34:LEU:HG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:34:TYR:O	3:X:38:VAL:HG23	2.06	0.56
1:I:120:LEU:CD1	1:J:120:LEU:HD12	2.36	0.56
2:O:40:ALA:CB	3:P:86:ILE:HG13	2.36	0.56
3:T:34:TYR:O	3:T:38:VAL:HG23	2.06	0.56
1:I:252:TYR:HE2	1:I:342:TYR:HA	1.71	0.56
1:Q:252:TYR:HE2	1:Q:342:TYR:HA	1.71	0.56
1:B:210:VAL:HG22	1:B:242:PHE:CE2	2.40	0.56
2:K:71:ARG:HH21	3:L:46:HIS:CD2	2.24	0.56
2:K:77:ARG:HG3	3:L:51:ILE:N	2.21	0.56
1:N:210:VAL:HG22	1:N:242:PHE:CE2	2.40	0.56
3:T:92:GLN:HE21	3:T:108:VAL:HG13	1.69	0.56
2:W:64:GLU:OE1	3:X:45:VAL:HB	2.06	0.56
1:U:135:ARG:NH1	1:U:356:ALA:HB3	2.21	0.55
1:V:227:PRO:HB2	1:V:254:TYR:HB2	1.87	0.55
1:A:185:ILE:HD11	1:A:360:PHE:CZ	2.41	0.55
2:O:97:LEU:HD21	2:O:102:ILE:CD1	2.35	0.55
3:T:95:VAL:HG13	3:T:99:LEU:HD12	1.87	0.55
2:G:30:VAL:O	2:G:34:LEU:HG	2.06	0.55
1:I:322:GLN:NE2	1:I:334:LEU:HD22	2.20	0.55
3:L:95:VAL:HG13	3:L:99:LEU:HD12	1.87	0.55
1:Q:135:ARG:NH1	1:Q:356:ALA:HB3	2.22	0.55
2:K:105:GLY:C	2:O:73:ASN:CB	2.75	0.55
2:K:30:VAL:O	2:K:34:LEU:HG	2.06	0.55
1:Q:99:LEU:HD22	1:R:135:ARG:CG	2.17	0.55
1:U:149:GLN:NE2	1:V:102:LEU:HD11	2.21	0.55
1:U:250:LYS:HE2	1:U:318:PRO:HG3	1.89	0.55
2:C:30:VAL:O	2:C:34:LEU:HG	2.06	0.55
1:E:330:LEU:O	1:E:334:LEU:HD13	2.07	0.55
1:E:357:VAL:HG22	1:F:99:LEU:HB3	1.88	0.55
1:J:336:GLU:HA	2:K:77:ARG:HH21	1.72	0.55
3:P:95:VAL:HG13	3:P:99:LEU:HD12	1.87	0.55
3:T:36:ILE:HG13	3:T:37:TYR:N	2.22	0.55
1:A:322:GLN:NE2	1:A:334:LEU:HD22	2.20	0.55
3:D:34:TYR:O	3:D:38:VAL:HG23	2.06	0.55
3:D:95:VAL:HG13	3:D:99:LEU:HD12	1.87	0.55
1:M:99:LEU:HD11	1:N:185:ILE:HD12	1.89	0.55
1:N:227:PRO:HB2	1:N:254:TYR:HB2	1.87	0.55
2:K:97:LEU:CG	2:O:104:GLN:HE21	2.20	0.55
1:Q:330:LEU:O	1:Q:334:LEU:HD13	2.07	0.55
2:S:30:VAL:O	2:S:34:LEU:HG	2.06	0.55
1:U:330:LEU:O	1:U:334:LEU:HD13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:185:ILE:HD11	1:U:360:PHE:CZ	2.42	0.55
2:W:100:VAL:C	2:W:102:ILE:N	2.60	0.55
3:X:95:VAL:HG13	3:X:99:LEU:HD12	1.87	0.55
1:E:135:ARG:NH1	1:E:356:ALA:HB3	2.22	0.55
2:G:87:VAL:CB	2:G:93:LEU:HD13	2.34	0.55
2:W:92:GLU:CD	3:X:102:GLU:HB3	2.27	0.55
1:A:250:LYS:HE2	1:A:318:PRO:HG3	1.89	0.55
1:E:252:TYR:HE2	1:E:342:TYR:HA	1.71	0.55
2:G:71:ARG:HH21	3:H:46:HIS:CD2	2.25	0.55
1:I:185:ILE:HD11	1:I:360:PHE:CZ	2.42	0.55
3:L:113:LYS:HB3	3:L:113:LYS:NZ	2.22	0.55
2:O:97:LEU:CD2	2:O:102:ILE:CG1	2.85	0.55
2:O:30:VAL:O	2:O:34:LEU:HG	2.06	0.55
3:P:113:LYS:HB3	3:P:113:LYS:NZ	2.22	0.55
3:P:36:ILE:HG13	3:P:37:TYR:N	2.22	0.55
2:S:98:GLY:O	2:S:101:THR:OG1	2.19	0.55
1:B:328:GLU:CD	2:W:105:GLY:O	2.45	0.55
2:G:96:LEU:HD22	2:G:96:LEU:C	2.27	0.55
1:A:135:ARG:NH1	1:A:356:ALA:HB3	2.22	0.55
1:B:227:PRO:HB2	1:B:254:TYR:HB2	1.87	0.55
1:I:135:ARG:NH1	1:I:356:ALA:HB3	2.22	0.55
2:K:65:LEU:HB2	2:K:86:ALA:HB1	1.89	0.55
1:M:135:ARG:NH1	1:M:356:ALA:HB3	2.21	0.55
1:Q:185:ILE:HD11	1:Q:360:PHE:CZ	2.42	0.55
3:D:36:ILE:HG13	3:D:37:TYR:N	2.23	0.54
1:I:330:LEU:O	1:I:334:LEU:HD13	2.07	0.54
3:L:36:ILE:HG13	3:L:37:TYR:N	2.22	0.54
1:M:124:PHE:CE2	1:N:113:PHE:HA	2.42	0.54
1:U:252:TYR:HE2	1:U:342:TYR:HA	1.71	0.54
1:U:113:PHE:HA	1:V:124:PHE:CE2	2.42	0.54
1:B:336:GLU:HA	2:C:77:ARG:HH22	1.72	0.54
1:E:129:LYS:HB2	1:E:130:PRO:HD3	1.90	0.54
2:G:65:LEU:HB2	2:G:86:ALA:HB1	1.89	0.54
1:M:330:LEU:O	1:M:334:LEU:HD13	2.07	0.54
1:M:134:GLN:OE1	1:N:102:LEU:HD21	2.07	0.54
1:V:211:LEU:HD21	1:V:312:PHE:HE2	1.72	0.54
2:W:96:LEU:O	2:W:100:VAL:HG23	2.07	0.54
1:A:104:SER:OG	1:B:156:ILE:HD13	2.07	0.54
3:H:36:ILE:HG13	3:H:37:TYR:N	2.22	0.54
1:J:125:LEU:HD22	1:J:221:TYR:CD1	2.43	0.54
1:M:185:ILE:HD11	1:M:360:PHE:CZ	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:103:ALA:N	2:O:81:ARG:NH1	2.53	0.54
1:Q:248:LEU:HD22	1:Q:274:ILE:HG12	1.90	0.54
3:T:113:LYS:NZ	3:T:113:LYS:HB3	2.22	0.54
2:G:50:TYR:OH	3:H:92:GLN:HG3	2.07	0.54
1:J:183:LYS:CG	1:J:184:GLY:H	2.13	0.54
1:M:250:LYS:HE2	1:M:318:PRO:HG3	1.89	0.54
1:M:248:LEU:HD22	1:M:274:ILE:HG12	1.90	0.54
1:U:129:LYS:HB2	1:U:130:PRO:HD3	1.90	0.54
1:V:250:LYS:HE2	1:V:269:ALA:HB1	1.90	0.54
1:A:330:LEU:O	1:A:334:LEU:HD13	2.07	0.54
1:B:125:LEU:HD22	1:B:221:TYR:CD1	2.43	0.54
2:K:47:ALA:N	2:K:48:PRO:HD2	2.23	0.54
2:S:47:ALA:N	2:S:48:PRO:HD2	2.23	0.54
1:V:206:ARG:NH2	1:V:283:VAL:HA	2.22	0.54
2:C:105:GLY:C	2:W:104:GLN:CB	2.75	0.54
2:W:65:LEU:HB2	2:W:86:ALA:HB1	1.89	0.54
1:A:364:ALA:HA	1:B:260:TYR:CE2	2.40	0.54
1:E:185:ILE:HD11	1:E:360:PHE:CZ	2.42	0.54
3:H:113:LYS:HB3	3:H:113:LYS:NZ	2.22	0.54
1:J:206:ARG:NH2	1:J:283:VAL:HA	2.22	0.54
1:V:125:LEU:HD22	1:V:221:TYR:CD1	2.43	0.54
3:X:36:ILE:HG13	3:X:37:TYR:N	2.22	0.54
1:B:125:LEU:HG	1:B:129:LYS:HE3	1.90	0.54
1:E:248:LEU:HD22	1:E:274:ILE:HG12	1.90	0.54
1:A:129:LYS:HB2	1:A:130:PRO:HD3	1.90	0.54
1:A:135:ARG:O	1:A:139:ILE:HG13	2.08	0.54
1:A:348:LEU:HA	1:A:352:LEU:HB3	1.90	0.54
2:C:65:LEU:HB2	2:C:86:ALA:HB1	1.89	0.54
2:C:40:ALA:HB2	3:D:86:ILE:HG13	1.90	0.54
1:I:348:LEU:HA	1:I:352:LEU:HB3	1.90	0.54
1:Q:124:PHE:CE2	1:R:113:PHE:HA	2.43	0.54
1:R:190:LEU:O	1:R:194:GLU:HG3	2.08	0.54
1:R:125:LEU:HD22	1:R:221:TYR:CD1	2.42	0.54
1:A:131:ILE:HD12	1:B:106:LEU:HD23	1.90	0.54
1:B:250:LYS:HE2	1:B:269:ALA:HB1	1.90	0.54
2:C:94:ASN:HD21	2:W:94:ASN:ND2	1.96	0.54
1:F:125:LEU:HD22	1:F:221:TYR:CD1	2.43	0.54
1:I:250:LYS:HE2	1:I:318:PRO:HG3	1.89	0.54
1:M:198:ILE:HD13	3:P:36:ILE:CD1	2.38	0.54
2:O:47:ALA:N	2:O:48:PRO:HD2	2.23	0.54
1:U:255:GLN:HG2	1:U:265:ILE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:113:PHE:HD1	1:V:124:PHE:CD2	2.25	0.54
1:V:272:CYS:O	1:V:273:GLU:HG3	2.08	0.54
1:E:135:ARG:O	1:E:139:ILE:HG13	2.08	0.54
1:E:250:LYS:HE2	1:E:318:PRO:HG3	1.89	0.54
1:I:129:LYS:HB2	1:I:130:PRO:HD3	1.90	0.54
1:J:190:LEU:O	1:J:194:GLU:HG3	2.08	0.54
1:M:255:GLN:HG2	1:M:265:ILE:O	2.08	0.54
1:N:125:LEU:HG	1:N:129:LYS:HE3	1.90	0.54
1:N:190:LEU:O	1:N:194:GLU:HG3	2.08	0.54
1:Q:135:ARG:O	1:Q:139:ILE:HG13	2.08	0.54
1:R:250:LYS:HE2	1:R:269:ALA:HB1	1.90	0.54
3:X:113:LYS:NZ	3:X:113:LYS:HB3	2.22	0.54
2:C:47:ALA:N	2:C:48:PRO:HD2	2.23	0.53
3:D:113:LYS:HB3	3:D:113:LYS:NZ	2.22	0.53
3:D:56:MET:HE3	3:D:59:MET:HB2	1.89	0.53
1:E:186:PRO:HD2	1:F:92:VAL:HG22	1.90	0.53
1:E:255:GLN:HG2	1:E:265:ILE:O	2.08	0.53
1:F:190:LEU:O	1:F:194:GLU:HG3	2.08	0.53
1:F:272:CYS:O	1:F:273:GLU:HG3	2.08	0.53
1:M:135:ARG:O	1:M:139:ILE:HG13	2.08	0.53
2:O:92:GLU:OE2	3:P:102:GLU:HB3	2.08	0.53
1:R:206:ARG:NH2	1:R:283:VAL:HA	2.22	0.53
2:W:97:LEU:O	2:W:101:THR:HG23	2.08	0.53
1:E:114:GLN:HG3	1:E:258:LEU:CD1	2.39	0.53
1:E:97:LEU:HD12	1:F:153:GLY:C	2.28	0.53
1:F:206:ARG:NH2	1:F:283:VAL:HA	2.22	0.53
1:I:210:VAL:HG22	1:I:242:PHE:CE2	2.43	0.53
1:Q:210:VAL:HG22	1:Q:242:PHE:CE2	2.43	0.53
1:A:255:GLN:HG2	1:A:265:ILE:O	2.08	0.53
1:I:135:ARG:O	1:I:139:ILE:HG13	2.08	0.53
1:I:364:ALA:HA	1:J:260:TYR:CE2	2.38	0.53
1:J:125:LEU:HG	1:J:129:LYS:HE3	1.90	0.53
1:N:206:ARG:NH2	1:N:283:VAL:HA	2.22	0.53
1:M:165:LEU:CD2	1:N:96:LEU:HD23	2.35	0.53
1:Q:129:LYS:HB2	1:Q:130:PRO:HD3	1.90	0.53
1:Q:250:LYS:HE2	1:Q:318:PRO:HG3	1.89	0.53
1:A:228:GLY:HA2	1:A:254:TYR:CD2	2.44	0.53
1:E:93:LYS:O	1:E:97:LEU:HD23	2.09	0.53
1:F:125:LEU:HG	1:F:129:LYS:HE3	1.90	0.53
1:F:250:LYS:HE2	1:F:269:ALA:HB1	1.89	0.53
1:M:311:SER:H	1:M:314:ASN:HD21	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:40:ALA:HB2	3:P:86:ILE:HG13	1.91	0.53
1:R:211:LEU:HD21	1:R:312:PHE:HE2	1.72	0.53
1:U:248:LEU:HD22	1:U:274:ILE:HG12	1.90	0.53
2:W:47:ALA:N	2:W:48:PRO:HD2	2.23	0.53
1:B:211:LEU:HD21	1:B:312:PHE:HE2	1.74	0.53
1:I:108:GLU:O	1:I:111:LYS:HB3	2.09	0.53
1:I:181:GLN:HG3	1:J:91:ASN:HD22	1.73	0.53
1:Q:128:TYR:CE1	1:R:110:GLU:HG2	2.44	0.53
1:R:250:LYS:HE3	1:R:318:PRO:CG	2.39	0.53
1:U:135:ARG:O	1:U:139:ILE:HG13	2.08	0.53
2:W:71:ARG:HH21	3:X:46:HIS:CD2	2.27	0.53
1:E:210:VAL:HG22	1:E:242:PHE:CE2	2.43	0.53
2:G:101:THR:O	2:G:102:ILE:HG12	2.08	0.53
2:G:47:ALA:N	2:G:48:PRO:HD2	2.23	0.53
2:O:88:ARG:HH22	2:O:97:LEU:HD22	1.74	0.53
1:Q:108:GLU:O	1:Q:111:LYS:HB3	2.09	0.53
1:Q:348:LEU:HA	1:Q:352:LEU:HB3	1.90	0.53
1:U:108:GLU:O	1:U:111:LYS:HB3	2.09	0.53
3:X:56:MET:HE3	3:X:59:MET:HB2	1.90	0.53
1:A:108:GLU:O	1:A:111:LYS:HB3	2.09	0.53
1:A:93:LYS:O	1:A:97:LEU:HD23	2.09	0.53
1:E:112:GLU:HB2	1:U:171:GLU:CG	2.39	0.53
1:F:211:LEU:HD21	1:F:312:PHE:HE2	1.74	0.53
1:I:311:SER:H	1:I:314:ASN:HD21	1.57	0.53
1:J:250:LYS:HE2	1:J:269:ALA:HB1	1.90	0.53
1:N:125:LEU:HD22	1:N:221:TYR:CD1	2.42	0.53
1:Q:228:GLY:HA2	1:Q:254:TYR:CD2	2.44	0.53
1:U:95:LYS:NZ	1:V:184:GLY:HA2	2.24	0.53
1:A:114:GLN:HG3	1:A:258:LEU:CD1	2.39	0.53
1:E:185:ILE:HD12	1:F:96:LEU:HD12	1.90	0.53
1:F:135:ARG:O	1:F:139:ILE:HG13	2.09	0.53
1:F:340:LEU:O	1:F:344:ILE:HG13	2.09	0.53
1:J:250:LYS:HE3	1:J:318:PRO:CG	2.39	0.53
1:M:129:LYS:HB2	1:M:130:PRO:HD3	1.90	0.53
1:M:93:LYS:O	1:M:97:LEU:HD23	2.09	0.53
1:N:340:LEU:O	1:N:344:ILE:HG13	2.09	0.53
1:R:135:ARG:O	1:R:139:ILE:HG13	2.09	0.53
1:U:348:LEU:HA	1:U:352:LEU:HB3	1.90	0.53
1:V:125:LEU:HG	1:V:129:LYS:HE3	1.90	0.53
1:V:250:LYS:HE3	1:V:318:PRO:CG	2.39	0.53
1:A:141:GLY:HA3	1:A:183:LYS:CD	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ARG:NH2	1:B:283:VAL:HA	2.22	0.53
2:C:50:TYR:CE1	3:D:111:GLY:HA3	2.44	0.53
1:I:248:LEU:HD22	1:I:274:ILE:HG12	1.90	0.53
1:I:93:LYS:O	1:I:97:LEU:HD23	2.09	0.53
3:L:56:MET:HE3	3:L:59:MET:HB2	1.91	0.53
1:M:210:VAL:HG22	1:M:242:PHE:CE2	2.44	0.53
1:N:211:LEU:HD21	1:N:312:PHE:HE2	1.73	0.53
1:Q:255:GLN:HG2	1:Q:265:ILE:O	2.08	0.53
1:B:135:ARG:O	1:B:139:ILE:HG13	2.09	0.53
1:E:145:PRO:HB3	1:F:98:SER:HB3	1.89	0.53
1:E:141:GLY:HA3	1:E:183:LYS:CD	2.39	0.53
1:J:272:CYS:O	1:J:273:GLU:HG3	2.08	0.53
1:M:124:PHE:CZ	1:N:113:PHE:HA	2.44	0.53
1:R:125:LEU:HG	1:R:129:LYS:HE3	1.90	0.53
1:Q:109:VAL:HG23	1:R:128:TYR:CE1	2.44	0.53
1:Q:145:PRO:CG	1:R:95:LYS:HD3	2.39	0.53
1:Q:142:GLN:NE2	1:U:142:GLN:HG2	2.17	0.53
1:V:340:LEU:O	1:V:344:ILE:HG13	2.09	0.53
1:B:190:LEU:O	1:B:194:GLU:HG3	2.08	0.52
2:C:41:GLU:HB3	3:D:84:SER:HB3	1.91	0.52
1:E:269:ALA:HB3	1:E:318:PRO:HB3	1.91	0.52
1:J:135:ARG:O	1:J:139:ILE:HG13	2.09	0.52
2:O:65:LEU:HB2	2:O:86:ALA:HB1	1.89	0.52
1:Q:109:VAL:HG23	1:R:128:TYR:HE1	1.74	0.52
1:U:141:GLY:HA3	1:U:183:LYS:CD	2.39	0.52
1:U:210:VAL:HG22	1:U:242:PHE:CE2	2.43	0.52
1:V:199:VAL:HG22	1:V:344:ILE:HG23	1.91	0.52
1:E:317:ASP:N	1:E:318:PRO:HD3	2.25	0.52
1:E:348:LEU:HA	1:E:352:LEU:HB3	1.90	0.52
2:O:99:ARG:HG2	2:O:99:ARG:HH11	1.72	0.52
1:Q:99:LEU:HB3	1:R:357:VAL:HG22	1.90	0.52
1:Q:95:LYS:CB	1:R:185:ILE:CG1	2.87	0.52
2:S:65:LEU:HB2	2:S:86:ALA:HB1	1.89	0.52
1:U:114:GLN:HG3	1:U:258:LEU:CD1	2.39	0.52
1:F:250:LYS:HE3	1:F:318:PRO:CG	2.39	0.52
1:M:108:GLU:O	1:M:111:LYS:HB3	2.09	0.52
1:M:141:GLY:HA3	1:M:183:LYS:CD	2.38	0.52
1:M:348:LEU:HA	1:M:352:LEU:HB3	1.90	0.52
1:U:317:ASP:N	1:U:318:PRO:HD3	2.25	0.52
1:V:190:LEU:O	1:V:194:GLU:HG3	2.08	0.52
1:F:330:LEU:O	1:F:334:LEU:HD13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:141:GLY:HA3	1:I:183:LYS:CD	2.40	0.52
1:M:228:GLY:HA2	1:M:254:TYR:CD2	2.44	0.52
1:M:328:GLU:C	1:M:330:LEU:H	2.13	0.52
1:N:135:ARG:O	1:N:139:ILE:HG13	2.09	0.52
1:Q:93:LYS:O	1:Q:97:LEU:HD23	2.09	0.52
1:R:330:LEU:O	1:R:334:LEU:HD13	2.10	0.52
1:A:185:ILE:HD12	1:B:96:LEU:HD11	1.91	0.52
1:A:210:VAL:HG22	1:A:242:PHE:CE2	2.43	0.52
1:A:248:LEU:HD22	1:A:274:ILE:HG12	1.90	0.52
1:B:340:LEU:O	1:B:344:ILE:HG13	2.09	0.52
1:E:340:LEU:O	1:E:344:ILE:HG13	2.10	0.52
1:F:203:ILE:HD12	1:F:203:ILE:O	2.10	0.52
1:I:255:GLN:HG2	1:I:265:ILE:O	2.08	0.52
1:J:330:LEU:O	1:J:334:LEU:HD13	2.10	0.52
1:J:340:LEU:O	1:J:344:ILE:HG13	2.09	0.52
1:U:111:LYS:O	1:U:115:VAL:HG23	2.10	0.52
1:U:328:GLU:C	1:U:330:LEU:H	2.13	0.52
1:U:340:LEU:O	1:U:344:ILE:HG13	2.10	0.52
1:B:272:CYS:O	1:B:273:GLU:HG3	2.08	0.52
1:B:330:LEU:O	1:B:334:LEU:HD13	2.10	0.52
1:I:111:LYS:O	1:I:115:VAL:HG23	2.10	0.52
1:M:152:LYS:O	1:M:156:ILE:HG13	2.10	0.52
1:M:269:ALA:HB3	1:M:318:PRO:HB3	1.92	0.52
1:N:203:ILE:HD12	1:N:203:ILE:O	2.10	0.52
2:O:100:VAL:HG21	3:P:65:ASP:OD2	2.09	0.52
1:R:272:CYS:O	1:R:273:GLU:HG3	2.09	0.52
1:U:93:LYS:O	1:U:97:LEU:HD23	2.09	0.52
1:A:152:LYS:O	1:A:156:ILE:HG13	2.10	0.52
1:A:328:GLU:C	1:A:330:LEU:H	2.13	0.52
1:E:111:LYS:O	1:E:115:VAL:HG23	2.10	0.52
1:M:317:ASP:N	1:M:318:PRO:HD3	2.24	0.52
1:N:250:LYS:HE2	1:N:269:ALA:HB1	1.90	0.52
1:N:272:CYS:O	1:N:273:GLU:HG3	2.08	0.52
1:Q:141:GLY:HA3	1:Q:183:LYS:CD	2.39	0.52
1:U:152:LYS:O	1:U:156:ILE:HG13	2.10	0.52
1:U:228:GLY:HA2	1:U:254:TYR:CD2	2.44	0.52
1:E:108:GLU:O	1:E:111:LYS:HB3	2.09	0.52
1:F:199:VAL:HG22	1:F:344:ILE:HG23	1.92	0.52
1:I:228:GLY:HA2	1:I:254:TYR:CD2	2.44	0.52
1:N:250:LYS:HE3	1:N:318:PRO:CG	2.39	0.52
1:Q:111:LYS:O	1:Q:115:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:269:ALA:HB3	1:Q:318:PRO:HB3	1.91	0.52
1:A:243:PHE:CD2	1:A:245:ASN:HB2	2.45	0.52
1:A:245:ASN:HD22	1:A:274:ILE:HG23	1.75	0.52
1:B:199:VAL:HG22	1:B:344:ILE:HG23	1.92	0.52
1:B:250:LYS:HE3	1:B:318:PRO:CG	2.39	0.52
1:N:199:VAL:HG22	1:N:344:ILE:HG23	1.92	0.52
2:O:71:ARG:HH21	3:P:46:HIS:CD2	2.27	0.52
1:A:111:LYS:O	1:A:115:VAL:HG23	2.10	0.52
1:A:340:LEU:O	1:A:344:ILE:HG13	2.10	0.52
1:E:228:GLY:HA2	1:E:254:TYR:CD2	2.44	0.52
1:I:269:ALA:HB3	1:I:318:PRO:HB3	1.92	0.52
1:I:328:GLU:C	1:I:330:LEU:H	2.13	0.52
2:O:67:GLY:HA3	3:P:46:HIS:CD2	2.45	0.52
1:B:203:ILE:O	1:B:203:ILE:HD12	2.10	0.51
1:B:271:GLY:HA3	1:B:316:PHE:O	2.10	0.51
1:E:152:LYS:O	1:E:156:ILE:HG13	2.10	0.51
1:E:328:GLU:C	1:E:330:LEU:H	2.13	0.51
1:I:152:LYS:O	1:I:156:ILE:HG13	2.10	0.51
1:M:340:LEU:O	1:M:344:ILE:HG13	2.10	0.51
1:Q:340:LEU:O	1:Q:344:ILE:HG13	2.10	0.51
1:U:269:ALA:HB3	1:U:318:PRO:HB3	1.91	0.51
1:V:203:ILE:HD12	1:V:203:ILE:O	2.10	0.51
2:C:98:GLY:O	2:W:88:ARG:HG3	2.09	0.51
3:H:56:MET:HE3	3:H:59:MET:HB2	1.92	0.51
1:J:211:LEU:HD21	1:J:312:PHE:HE2	1.74	0.51
1:J:271:GLY:HA3	1:J:316:PHE:O	2.10	0.51
1:M:165:LEU:HD22	1:N:96:LEU:CD2	2.40	0.51
1:N:330:LEU:O	1:N:334:LEU:HD13	2.10	0.51
1:N:338:LEU:HD23	1:N:338:LEU:O	2.11	0.51
1:Q:152:LYS:O	1:Q:156:ILE:HG13	2.10	0.51
3:T:56:MET:HE3	3:T:59:MET:HB2	1.92	0.51
1:V:135:ARG:O	1:V:139:ILE:HG13	2.09	0.51
1:E:125:LEU:HA	1:E:128:TYR:CD2	2.44	0.51
1:E:127:LYS:C	1:E:130:PRO:HD2	2.31	0.51
1:F:271:GLY:HA3	1:F:316:PHE:O	2.10	0.51
1:J:203:ILE:O	1:J:203:ILE:HD12	2.10	0.51
1:M:127:LYS:C	1:M:130:PRO:HD2	2.31	0.51
1:Q:243:PHE:CD2	1:Q:245:ASN:HB2	2.45	0.51
1:R:199:VAL:HG22	1:R:344:ILE:HG23	1.92	0.51
1:J:125:LEU:HA	1:J:128:TYR:HD2	1.76	0.51
3:L:73:GLU:HA	3:L:76:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:271:GLY:HA3	1:N:316:PHE:O	2.10	0.51
1:Q:127:LYS:C	1:Q:130:PRO:HD2	2.31	0.51
1:Q:245:ASN:HD22	1:Q:274:ILE:HG23	1.75	0.51
1:Q:317:ASP:N	1:Q:318:PRO:HD3	2.25	0.51
1:R:125:LEU:HD22	1:R:221:TYR:HD1	1.75	0.51
3:X:93:THR:HA	3:X:96:ARG:NH1	2.26	0.51
1:E:120:LEU:CD1	1:F:120:LEU:HD12	2.40	0.51
1:E:245:ASN:HD22	1:E:274:ILE:HG23	1.75	0.51
1:F:232:LEU:N	1:F:232:LEU:HD12	2.26	0.51
2:K:98:GLY:CA	2:K:101:THR:OG1	2.55	0.51
1:M:114:GLN:HG3	1:M:258:LEU:CD1	2.39	0.51
2:O:97:LEU:CD2	2:O:102:ILE:HD11	2.40	0.51
1:Q:233:PHE:O	1:Q:247:ILE:HA	2.11	0.51
1:R:340:LEU:O	1:R:344:ILE:HG13	2.09	0.51
1:Q:201:ASP:OD2	2:S:29:ARG:NE	2.44	0.51
3:T:93:THR:HA	3:T:96:ARG:NH1	2.25	0.51
1:V:232:LEU:N	1:V:232:LEU:HD12	2.26	0.51
1:A:269:ALA:HB3	1:A:318:PRO:HB3	1.91	0.51
1:E:181:GLN:CB	1:F:91:ASN:HD22	2.23	0.51
3:L:93:THR:HA	3:L:96:ARG:NH1	2.26	0.51
1:M:232:LEU:HD12	1:M:232:LEU:N	2.26	0.51
1:R:232:LEU:N	1:R:232:LEU:HD12	2.26	0.51
1:Q:142:GLN:CD	1:U:142:GLN:O	2.49	0.51
1:U:233:PHE:O	1:U:247:ILE:HA	2.11	0.51
1:U:243:PHE:CD2	1:U:245:ASN:HB2	2.45	0.51
3:X:73:GLU:HA	3:X:76:ARG:HH11	1.76	0.51
1:A:282:ASN:O	1:A:283:VAL:HB	2.11	0.51
1:B:139:ILE:HD13	1:B:188:PHE:CD2	2.46	0.51
2:C:58:LEU:O	2:C:62:ILE:HG12	2.11	0.51
1:E:232:LEU:HD12	1:E:232:LEU:N	2.26	0.51
1:I:232:LEU:N	1:I:232:LEU:HD12	2.26	0.51
1:I:317:ASP:N	1:I:318:PRO:HD3	2.25	0.51
1:M:111:LYS:O	1:M:115:VAL:HG23	2.10	0.51
2:K:97:LEU:HD22	2:O:105:GLY:O	2.11	0.51
1:Q:114:GLN:HG3	1:Q:258:LEU:CD1	2.39	0.51
1:Q:310:GLU:HG2	2:S:16:THR:HA	1.91	0.51
1:U:232:LEU:N	1:U:232:LEU:HD12	2.26	0.51
1:V:125:LEU:HD22	1:V:221:TYR:HD1	1.75	0.51
1:V:330:LEU:O	1:V:334:LEU:HD13	2.10	0.51
1:B:92:VAL:O	1:B:96:LEU:HD13	2.11	0.51
3:D:93:THR:HA	3:D:96:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:ASN:O	1:E:283:VAL:HB	2.11	0.51
1:I:340:LEU:O	1:I:344:ILE:HG13	2.10	0.51
2:K:58:LEU:O	2:K:62:ILE:HG12	2.11	0.51
1:M:233:PHE:O	1:M:247:ILE:HA	2.11	0.51
1:M:282:ASN:O	1:M:283:VAL:HB	2.11	0.51
2:O:58:LEU:O	2:O:62:ILE:HG12	2.11	0.51
3:P:56:MET:HE3	3:P:59:MET:HB2	1.92	0.51
1:Q:232:LEU:N	1:Q:232:LEU:HD12	2.26	0.51
1:Q:328:GLU:C	1:Q:330:LEU:H	2.13	0.51
1:R:139:ILE:HD13	1:R:188:PHE:CD2	2.45	0.51
1:U:245:ASN:HD22	1:U:274:ILE:HG23	1.75	0.51
1:V:139:ILE:HD13	1:V:188:PHE:CD2	2.46	0.51
2:W:67:GLY:HA3	3:X:46:HIS:CD2	2.44	0.51
1:E:186:PRO:HD3	1:F:92:VAL:HG22	1.91	0.51
1:J:232:LEU:HD12	1:J:232:LEU:N	2.26	0.51
3:L:113:LYS:HB3	3:L:113:LYS:HZ3	1.76	0.51
1:M:245:ASN:HD22	1:M:274:ILE:HG23	1.75	0.51
1:N:232:LEU:HD12	1:N:232:LEU:N	2.26	0.51
3:P:93:THR:HA	3:P:96:ARG:NH1	2.25	0.51
1:Q:282:ASN:O	1:Q:283:VAL:HB	2.11	0.51
1:R:203:ILE:HD12	1:R:203:ILE:O	2.10	0.51
1:U:91:ASN:ND2	1:V:181:GLN:O	2.44	0.51
1:A:317:ASP:N	1:A:318:PRO:HD3	2.25	0.51
1:B:348:LEU:HA	1:B:352:LEU:HB3	1.93	0.51
1:J:338:LEU:O	1:J:338:LEU:HD23	2.11	0.51
2:K:99:ARG:O	2:K:102:ILE:HG13	2.11	0.51
3:P:73:GLU:HA	3:P:76:ARG:HH11	1.76	0.51
1:R:114:GLN:HA	1:R:117:MET:HB3	1.93	0.51
1:R:125:LEU:HA	1:R:128:TYR:HD2	1.75	0.51
1:U:181:GLN:HG3	1:V:91:ASN:HD22	1.75	0.51
2:W:60:ALA:O	2:W:64:GLU:HB2	2.11	0.51
3:X:104:ALA:O	3:X:108:VAL:HG23	2.11	0.51
1:I:233:PHE:O	1:I:247:ILE:HA	2.11	0.50
1:I:245:ASN:HD22	1:I:274:ILE:HG23	1.75	0.50
1:I:282:ASN:O	1:I:283:VAL:HB	2.11	0.50
1:J:348:LEU:HA	1:J:352:LEU:HB3	1.93	0.50
1:M:149:GLN:NE2	1:N:102:LEU:HD11	2.25	0.50
1:N:125:LEU:HA	1:N:128:TYR:HD2	1.76	0.50
3:P:104:ALA:O	3:P:108:VAL:HG23	2.11	0.50
2:W:69:ALA:HB1	2:W:85:LEU:HD12	1.93	0.50
1:A:233:PHE:O	1:A:247:ILE:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:GLN:HA	1:F:117:MET:HB3	1.94	0.50
1:F:125:LEU:HA	1:F:128:TYR:HD2	1.76	0.50
1:F:338:LEU:O	1:F:338:LEU:HD23	2.11	0.50
2:G:58:LEU:O	2:G:62:ILE:HG12	2.11	0.50
3:H:93:THR:HA	3:H:96:ARG:NH1	2.26	0.50
1:I:243:PHE:CD2	1:I:245:ASN:HB2	2.45	0.50
2:K:105:GLY:HA3	2:O:73:ASN:CG	2.32	0.50
2:O:50:TYR:CE1	3:P:111:GLY:HA3	2.45	0.50
1:Q:95:LYS:NZ	1:R:183:LYS:O	2.44	0.50
1:R:188:PHE:HA	1:R:360:PHE:HE2	1.76	0.50
1:R:271:GLY:HA3	1:R:316:PHE:O	2.11	0.50
3:T:104:ALA:O	3:T:108:VAL:HG23	2.11	0.50
1:U:127:LYS:C	1:U:130:PRO:HD2	2.31	0.50
1:V:348:LEU:HA	1:V:352:LEU:HB3	1.93	0.50
1:A:127:LYS:C	1:A:130:PRO:HD2	2.31	0.50
1:B:125:LEU:HD22	1:B:221:TYR:HD1	1.75	0.50
2:C:60:ALA:O	2:C:64:GLU:HB2	2.11	0.50
1:E:120:LEU:HD23	1:E:120:LEU:C	2.32	0.50
1:F:183:LYS:CG	1:F:184:GLY:H	2.13	0.50
2:G:69:ALA:HB1	2:G:85:LEU:HD12	1.94	0.50
1:I:127:LYS:C	1:I:130:PRO:HD2	2.31	0.50
1:J:127:LYS:HG2	1:R:148:GLU:OE2	2.12	0.50
1:N:125:LEU:HD22	1:N:221:TYR:HD1	1.75	0.50
1:M:97:LEU:HB3	1:N:150:ILE:HA	1.93	0.50
1:Q:211:LEU:HD21	1:Q:312:PHE:CE2	2.47	0.50
1:R:348:LEU:HA	1:R:352:LEU:HB3	1.93	0.50
2:S:60:ALA:O	2:S:64:GLU:HB2	2.11	0.50
1:V:92:VAL:O	1:V:96:LEU:HD13	2.11	0.50
1:B:338:LEU:HD23	1:B:338:LEU:O	2.11	0.50
1:E:243:PHE:CD2	1:E:245:ASN:HB2	2.45	0.50
1:E:233:PHE:O	1:E:247:ILE:HA	2.11	0.50
1:I:114:GLN:HG3	1:I:258:LEU:CD1	2.39	0.50
1:J:92:VAL:O	1:J:96:LEU:HD13	2.11	0.50
1:N:248:LEU:HD22	1:N:274:ILE:HG12	1.94	0.50
1:N:92:VAL:O	1:N:96:LEU:HD13	2.11	0.50
1:F:139:ILE:HD13	1:F:188:PHE:CD2	2.46	0.50
2:G:60:ALA:O	2:G:64:GLU:HB2	2.11	0.50
3:L:104:ALA:O	3:L:108:VAL:HG23	2.11	0.50
3:L:73:GLU:O	3:L:77:LEU:HD23	2.12	0.50
1:N:139:ILE:HD13	1:N:188:PHE:CD2	2.46	0.50
2:O:60:ALA:O	2:O:64:GLU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:131:ILE:HG23	1:R:102:LEU:HB3	1.93	0.50
3:T:73:GLU:HA	3:T:76:ARG:HH11	1.76	0.50
1:U:145:PRO:HB3	1:V:98:SER:CB	2.40	0.50
1:U:99:LEU:HD11	1:V:185:ILE:HD12	1.94	0.50
1:A:132:TRP:HA	1:A:135:ARG:HG2	1.94	0.50
1:B:248:LEU:HD22	1:B:274:ILE:HG12	1.94	0.50
3:D:73:GLU:O	3:D:77:LEU:HD23	2.12	0.50
1:F:125:LEU:HD22	1:F:221:TYR:HD1	1.76	0.50
1:E:95:LYS:CD	1:F:145:PRO:HG2	2.34	0.50
2:K:40:ALA:CB	3:L:86:ILE:HG13	2.42	0.50
1:M:144:GLN:OE1	1:N:95:LYS:HE3	2.12	0.50
1:M:243:PHE:CD2	1:M:245:ASN:HB2	2.45	0.50
1:R:92:VAL:O	1:R:96:LEU:HD13	2.11	0.50
1:U:240:ASN:ND2	1:U:242:PHE:H	2.10	0.50
1:A:120:LEU:C	1:A:120:LEU:HD23	2.32	0.50
1:A:240:ASN:ND2	1:A:242:PHE:H	2.10	0.50
3:D:73:GLU:HA	3:D:76:ARG:HH11	1.76	0.50
1:I:211:LEU:HD21	1:I:312:PHE:CE2	2.46	0.50
1:J:114:GLN:HA	1:J:117:MET:HB3	1.93	0.50
1:J:248:LEU:HD22	1:J:274:ILE:HG12	1.94	0.50
2:K:60:ALA:O	2:K:64:GLU:HB2	2.11	0.50
2:K:63:LEU:HD13	3:L:42:LEU:HB2	1.93	0.50
1:M:138:ILE:HB	1:N:99:LEU:HD21	1.94	0.50
1:N:146:LYS:HB2	1:N:149:GLN:CG	2.41	0.50
1:M:145:PRO:HG2	1:N:95:LYS:HA	1.94	0.50
2:O:49:VAL:HG21	3:P:118:TYR:CD2	2.47	0.50
2:S:58:LEU:O	2:S:62:ILE:HG12	2.11	0.50
1:U:120:LEU:HD23	1:U:120:LEU:C	2.32	0.50
1:U:132:TRP:HA	1:U:135:ARG:HG2	1.94	0.50
1:V:338:LEU:HD23	1:V:338:LEU:O	2.11	0.50
2:W:93:LEU:HA	2:W:96:LEU:HD21	1.92	0.50
1:A:211:LEU:HD21	1:A:312:PHE:CE2	2.47	0.50
1:E:219:LEU:HD23	1:E:220:GLU:N	2.27	0.50
1:F:248:LEU:HD22	1:F:274:ILE:HG12	1.94	0.50
1:J:199:VAL:HG22	1:J:344:ILE:HG23	1.92	0.50
1:M:211:LEU:HD21	1:M:312:PHE:CE2	2.47	0.50
3:P:73:GLU:O	3:P:77:LEU:HD23	2.12	0.50
1:Q:99:LEU:HD11	1:R:185:ILE:HD12	1.94	0.50
1:R:338:LEU:O	1:R:338:LEU:HD23	2.11	0.50
2:W:58:LEU:O	2:W:62:ILE:HG12	2.11	0.50
1:A:232:LEU:HD12	1:A:232:LEU:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LEU:N	1:B:232:LEU:HD12	2.26	0.50
1:F:348:LEU:HA	1:F:352:LEU:HB3	1.93	0.50
1:I:120:LEU:HD23	1:I:120:LEU:C	2.32	0.50
1:I:125:LEU:HA	1:I:128:TYR:CD2	2.44	0.50
1:J:125:LEU:HD22	1:J:221:TYR:HD1	1.75	0.50
2:K:69:ALA:HB1	2:K:85:LEU:HD12	1.93	0.50
1:M:240:ASN:ND2	1:M:242:PHE:H	2.10	0.50
1:R:147:PRO:HA	1:R:150:ILE:HD12	1.93	0.50
1:V:125:LEU:HA	1:V:128:TYR:HD2	1.76	0.50
1:V:248:LEU:HD22	1:V:274:ILE:HG12	1.94	0.50
2:W:21:ALA:HB2	3:X:118:TYR:HB2	1.93	0.50
1:F:188:PHE:HA	1:F:360:PHE:HE2	1.77	0.49
3:H:104:ALA:O	3:H:108:VAL:HG23	2.11	0.49
1:I:219:LEU:HD23	1:I:220:GLU:N	2.27	0.49
1:J:139:ILE:HD13	1:J:188:PHE:CD2	2.46	0.49
1:M:219:LEU:HD23	1:M:220:GLU:N	2.27	0.49
1:Q:132:TRP:HA	1:Q:135:ARG:HG2	1.94	0.49
2:S:93:LEU:C	2:S:95:LYS:N	2.64	0.49
1:B:147:PRO:HA	1:B:150:ILE:HD12	1.94	0.49
3:D:104:ALA:O	3:D:108:VAL:HG23	2.11	0.49
1:F:147:PRO:HA	1:F:150:ILE:HD12	1.93	0.49
3:H:43:LYS:O	3:H:47:PRO:HG3	2.13	0.49
1:M:120:LEU:C	1:M:120:LEU:HD23	2.32	0.49
1:Q:145:PRO:HB2	1:Q:150:ILE:HD11	1.95	0.49
1:Q:310:GLU:OE2	2:S:16:THR:N	2.45	0.49
1:A:206:ARG:HH22	1:A:283:VAL:H	1.60	0.49
2:C:69:ALA:HB1	2:C:85:LEU:HD12	1.93	0.49
1:I:145:PRO:HB2	1:I:150:ILE:HD11	1.95	0.49
1:M:125:LEU:HA	1:M:128:TYR:CD2	2.44	0.49
1:Q:120:LEU:C	1:Q:120:LEU:HD23	2.32	0.49
1:Q:240:ASN:ND2	1:Q:242:PHE:H	2.10	0.49
2:S:69:ALA:HB1	2:S:85:LEU:HD12	1.93	0.49
1:U:282:ASN:O	1:U:283:VAL:HB	2.11	0.49
1:V:147:PRO:HA	1:V:150:ILE:HD12	1.94	0.49
3:X:73:GLU:O	3:X:77:LEU:HD23	2.12	0.49
1:A:170:GLU:HG3	1:I:169:GLU:CD	2.33	0.49
1:B:114:GLN:HA	1:B:117:MET:HB3	1.93	0.49
1:B:185:ILE:HG21	1:B:188:PHE:HD1	1.78	0.49
3:D:43:LYS:O	3:D:47:PRO:HG3	2.13	0.49
1:E:113:PHE:CE1	1:F:120:LEU:HD22	2.48	0.49
1:F:92:VAL:O	1:F:96:LEU:HD13	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:73:GLU:O	3:H:77:LEU:HD23	2.12	0.49
2:K:50:TYR:OH	3:L:92:GLN:HG3	2.12	0.49
1:M:113:PHE:HD1	1:N:124:PHE:CD2	2.31	0.49
1:N:348:LEU:HA	1:N:352:LEU:HB3	1.93	0.49
1:Q:311:SER:H	1:Q:314:ASN:HD21	1.57	0.49
1:Q:124:PHE:CZ	1:R:113:PHE:HA	2.48	0.49
1:R:185:ILE:HG21	1:R:188:PHE:HD1	1.78	0.49
1:R:93:LYS:O	1:R:97:LEU:HD23	2.13	0.49
3:T:73:GLU:O	3:T:77:LEU:HD23	2.12	0.49
1:U:211:LEU:HD21	1:U:312:PHE:CE2	2.47	0.49
1:V:185:ILE:HG21	1:V:188:PHE:HD1	1.78	0.49
1:E:311:SER:H	1:E:314:ASN:HD21	1.57	0.49
2:G:99:ARG:HG3	2:G:100:VAL:HG23	1.94	0.49
1:I:185:ILE:HD13	1:I:188:PHE:HD1	1.78	0.49
2:K:21:ALA:HB2	3:L:118:TYR:HB2	1.94	0.49
3:L:43:LYS:O	3:L:47:PRO:HG3	2.13	0.49
1:M:198:ILE:HD13	3:P:36:ILE:HD13	1.94	0.49
1:M:206:ARG:HH22	1:M:283:VAL:H	1.60	0.49
2:W:99:ARG:O	2:W:102:ILE:CD1	2.60	0.49
1:B:125:LEU:HA	1:B:128:TYR:HD2	1.76	0.49
1:E:132:TRP:HA	1:E:135:ARG:HG2	1.94	0.49
2:G:99:ARG:HB3	3:H:69:ARG:NH2	2.26	0.49
1:I:185:ILE:HG13	1:J:92:VAL:HG13	1.95	0.49
1:N:114:GLN:HA	1:N:117:MET:HB3	1.94	0.49
1:M:117:MET:HA	1:N:120:LEU:HD13	1.93	0.49
1:R:248:LEU:HD22	1:R:274:ILE:HG12	1.94	0.49
1:E:211:LEU:HD21	1:E:312:PHE:CE2	2.47	0.49
1:F:93:LYS:O	1:F:97:LEU:HD23	2.13	0.49
1:N:196:LEU:HD23	1:N:199:VAL:HG21	1.95	0.49
1:M:103:GLN:OE1	1:N:357:VAL:HB	2.13	0.49
1:N:93:LYS:O	1:N:97:LEU:HD23	2.13	0.49
1:U:145:PRO:HB2	1:U:150:ILE:HD11	1.95	0.49
1:U:219:LEU:HD23	1:U:220:GLU:N	2.27	0.49
2:W:42:ARG:O	3:X:85:THR:HA	2.12	0.49
1:E:185:ILE:HD13	1:E:188:PHE:HD1	1.77	0.49
1:F:185:ILE:HG21	1:F:188:PHE:HD1	1.78	0.49
3:H:73:GLU:HA	3:H:76:ARG:HH11	1.76	0.49
1:I:132:TRP:HA	1:I:135:ARG:HG2	1.93	0.49
1:I:205:ASP:OD2	2:K:35:ARG:HD2	2.12	0.49
3:T:43:LYS:O	3:T:47:PRO:HG3	2.13	0.49
1:U:206:ARG:HH22	1:U:283:VAL:H	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:HD23	1:A:220:GLU:N	2.27	0.49
1:A:96:LEU:HB3	1:B:165:LEU:HD21	1.94	0.49
1:U:185:ILE:HD13	1:U:188:PHE:HD1	1.78	0.49
1:U:319:PRO:HB2	1:U:338:LEU:CD2	2.43	0.49
1:E:206:ARG:HH22	1:E:283:VAL:H	1.60	0.49
1:J:147:PRO:HA	1:J:150:ILE:HD12	1.93	0.49
1:J:93:LYS:O	1:J:97:LEU:HD23	2.13	0.49
1:Q:219:LEU:HD23	1:Q:220:GLU:N	2.27	0.49
1:Q:316:PHE:C	1:Q:318:PRO:HD3	2.34	0.49
1:R:146:LYS:HB2	1:R:149:GLN:CG	2.41	0.49
1:U:316:PHE:C	1:U:318:PRO:HD3	2.34	0.49
1:V:114:GLN:HA	1:V:117:MET:HB3	1.94	0.49
1:V:196:LEU:HD23	1:V:199:VAL:HG21	1.95	0.49
1:A:181:GLN:CG	1:B:91:ASN:HD22	2.25	0.48
1:E:145:PRO:HB2	1:E:150:ILE:HD11	1.95	0.48
1:I:206:ARG:HH22	1:I:283:VAL:H	1.61	0.48
1:I:319:PRO:HB2	1:I:338:LEU:CD2	2.43	0.48
1:M:131:ILE:HG21	1:N:106:LEU:HG	1.94	0.48
1:M:157:VAL:HG13	1:M:162:GLU:HB2	1.95	0.48
2:O:69:ALA:HB1	2:O:85:LEU:HD12	1.93	0.48
1:Q:99:LEU:O	1:R:357:VAL:HG21	2.13	0.48
1:R:196:LEU:HD23	1:R:199:VAL:HG21	1.95	0.48
1:V:211:LEU:HD21	1:V:312:PHE:CE2	2.47	0.48
1:V:271:GLY:HA3	1:V:316:PHE:O	2.12	0.48
3:X:43:LYS:O	3:X:47:PRO:HG3	2.13	0.48
1:A:234:ARG:HG2	1:A:247:ILE:HG12	1.95	0.48
1:A:319:PRO:HB2	1:A:338:LEU:CD2	2.43	0.48
1:E:240:ASN:ND2	1:E:242:PHE:H	2.10	0.48
1:E:319:PRO:HB2	1:E:338:LEU:CD2	2.43	0.48
1:I:240:ASN:ND2	1:I:242:PHE:H	2.10	0.48
1:J:185:ILE:HG21	1:J:188:PHE:HD1	1.78	0.48
1:Q:274:ILE:HG22	1:Q:275:SER:N	2.29	0.48
1:U:132:TRP:O	1:U:135:ARG:HG2	2.13	0.48
1:U:274:ILE:HG22	1:U:275:SER:N	2.28	0.48
1:A:132:TRP:O	1:A:135:ARG:HG2	2.13	0.48
1:A:274:ILE:HG22	1:A:275:SER:N	2.28	0.48
1:E:132:TRP:O	1:E:135:ARG:HG2	2.13	0.48
1:M:132:TRP:O	1:M:135:ARG:HG2	2.13	0.48
1:Q:256:LYS:HE3	1:Q:256:LYS:H	1.79	0.48
1:R:211:LEU:HD21	1:R:312:PHE:CE2	2.48	0.48
1:A:145:PRO:HB2	1:A:150:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LEU:HD12	1:B:153:GLY:C	2.33	0.48
1:E:316:PHE:C	1:E:318:PRO:HD3	2.34	0.48
1:M:316:PHE:C	1:M:318:PRO:HD3	2.34	0.48
1:N:147:PRO:HA	1:N:150:ILE:HD12	1.93	0.48
1:N:185:ILE:HG21	1:N:188:PHE:HD1	1.78	0.48
2:K:84:GLN:NE2	2:O:102:ILE:HB	2.28	0.48
1:Q:125:LEU:HA	1:Q:128:TYR:CD2	2.43	0.48
1:Q:137:ARG:HB3	1:Q:142:GLN:HB3	1.96	0.48
1:V:93:LYS:O	1:V:97:LEU:HD23	2.13	0.48
1:A:316:PHE:C	1:A:318:PRO:HD3	2.34	0.48
1:I:157:VAL:HG13	1:I:162:GLU:HB2	1.95	0.48
3:L:46:HIS:HB3	3:L:49:THR:CB	2.44	0.48
3:L:76:ARG:HB3	3:L:80:TYR:CZ	2.49	0.48
2:K:40:ALA:HB2	3:L:86:ILE:HG13	1.95	0.48
1:M:274:ILE:HG22	1:M:275:SER:N	2.28	0.48
1:M:99:LEU:HD21	1:N:138:ILE:HB	1.95	0.48
1:Q:167:VAL:HG12	1:Q:168:ASP:N	2.29	0.48
1:U:167:VAL:HG12	1:U:168:ASP:N	2.29	0.48
1:U:234:ARG:HG2	1:U:247:ILE:HG12	1.96	0.48
1:B:196:LEU:HD23	1:B:199:VAL:HG21	1.95	0.48
2:C:50:TYR:O	2:C:54:VAL:HG23	2.14	0.48
3:H:62:PHE:O	3:H:66:VAL:HG23	2.14	0.48
1:I:106:LEU:HD13	1:I:106:LEU:O	2.14	0.48
1:M:132:TRP:HA	1:M:135:ARG:HG2	1.94	0.48
1:M:256:LYS:HE3	1:M:256:LYS:H	1.78	0.48
2:O:50:TYR:O	2:O:54:VAL:HG23	2.14	0.48
1:Q:117:MET:SD	1:R:117:MET:CE	3.02	0.48
1:Q:319:PRO:HB2	1:Q:338:LEU:CD2	2.43	0.48
1:A:125:LEU:HA	1:A:128:TYR:CD2	2.44	0.48
1:A:157:VAL:HG13	1:A:162:GLU:HB2	1.95	0.48
1:A:185:ILE:HD13	1:A:188:PHE:HD1	1.78	0.48
1:A:135:ARG:HB2	1:B:99:LEU:HD22	1.96	0.48
2:C:40:ALA:CB	3:D:86:ILE:HG13	2.43	0.48
3:D:34:TYR:HA	3:D:37:TYR:HD2	1.79	0.48
2:G:50:TYR:O	2:G:54:VAL:HG23	2.14	0.48
2:G:87:VAL:HG12	2:G:94:ASN:HB2	1.95	0.48
3:H:46:HIS:HB3	3:H:49:THR:CB	2.44	0.48
3:H:76:ARG:HB3	3:H:80:TYR:CZ	2.49	0.48
1:I:316:PHE:C	1:I:318:PRO:HD3	2.34	0.48
1:J:196:LEU:HD23	1:J:199:VAL:HG21	1.95	0.48
1:M:125:LEU:HD22	1:M:221:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:319:PRO:HB2	1:M:338:LEU:CD2	2.43	0.48
1:N:106:LEU:O	1:N:110:GLU:HG3	2.14	0.48
3:P:43:LYS:O	3:P:47:PRO:HG3	2.13	0.48
1:Q:132:TRP:O	1:Q:135:ARG:HG2	2.13	0.48
3:T:46:HIS:HB3	3:T:49:THR:CB	2.44	0.48
3:D:62:PHE:O	3:D:66:VAL:HG23	2.14	0.48
1:E:125:LEU:HD22	1:E:221:TYR:CE1	2.49	0.48
1:I:132:TRP:O	1:I:135:ARG:HG2	2.13	0.48
1:J:211:LEU:HD21	1:J:312:PHE:CE2	2.49	0.48
2:K:50:TYR:O	2:K:54:VAL:HG23	2.14	0.48
1:M:106:LEU:O	1:M:106:LEU:HD13	2.14	0.48
1:M:137:ARG:HB3	1:M:142:GLN:HB3	1.96	0.48
1:M:167:VAL:HG12	1:M:168:ASP:N	2.29	0.48
3:P:76:ARG:HB3	3:P:80:TYR:CZ	2.49	0.48
1:Q:106:LEU:O	1:Q:106:LEU:HD13	2.14	0.48
1:Q:125:LEU:HD22	1:Q:221:TYR:CE1	2.49	0.48
2:S:50:TYR:O	2:S:54:VAL:HG23	2.14	0.48
1:U:137:ARG:HB3	1:U:142:GLN:HB3	1.95	0.48
1:U:157:VAL:HG13	1:U:162:GLU:HB2	1.95	0.48
1:B:93:LYS:O	1:B:97:LEU:HD23	2.13	0.48
3:D:65:ASP:O	3:D:69:ARG:HG3	2.13	0.48
2:K:103:ALA:CA	2:O:81:ARG:CZ	2.75	0.48
3:L:65:ASP:O	3:L:69:ARG:HG3	2.13	0.48
2:K:84:GLN:CG	2:O:102:ILE:O	2.59	0.48
3:P:65:ASP:O	3:P:69:ARG:HG3	2.13	0.48
1:U:102:LEU:HD11	1:V:149:GLN:NE2	2.28	0.48
1:U:106:LEU:HD13	1:U:106:LEU:O	2.14	0.48
2:W:99:ARG:NE	2:W:99:ARG:CA	2.73	0.48
1:A:311:SER:H	1:A:314:ASN:HD21	1.57	0.48
1:E:167:VAL:HG12	1:E:168:ASP:N	2.29	0.48
1:E:256:LYS:H	1:E:256:LYS:HE3	1.79	0.48
1:E:355:ARG:NH2	1:F:110:GLU:OE1	2.46	0.48
1:F:196:LEU:HD23	1:F:199:VAL:HG21	1.95	0.48
3:P:46:HIS:HB3	3:P:49:THR:CB	2.44	0.48
1:Q:352:LEU:HD13	1:Q:352:LEU:C	2.35	0.48
3:T:76:ARG:HB3	3:T:80:TYR:CZ	2.49	0.48
1:U:154:GLN:N	1:V:97:LEU:HD12	2.29	0.48
1:U:99:LEU:CD1	1:V:185:ILE:HD12	2.44	0.48
1:A:256:LYS:HE3	1:A:256:LYS:H	1.78	0.47
1:B:211:LEU:HD21	1:B:312:PHE:CE2	2.49	0.47
3:D:46:HIS:HB3	3:D:49:THR:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:VAL:HG13	1:E:162:GLU:HB2	1.95	0.47
1:E:358:ASP:OD1	1:F:100:LYS:HE2	2.14	0.47
1:E:102:LEU:HD11	1:F:149:GLN:NE2	2.29	0.47
1:I:125:LEU:HD22	1:I:221:TYR:CE1	2.49	0.47
1:I:167:VAL:HG12	1:I:168:ASP:N	2.29	0.47
1:I:352:LEU:C	1:I:352:LEU:HD13	2.35	0.47
1:M:150:ILE:HA	1:N:97:LEU:HB3	1.95	0.47
1:R:352:LEU:C	1:R:352:LEU:HD13	2.35	0.47
3:X:76:ARG:HB3	3:X:80:TYR:CZ	2.49	0.47
1:M:91:ASN:ND2	1:N:181:GLN:O	2.47	0.47
1:N:211:LEU:HD21	1:N:312:PHE:CE2	2.48	0.47
1:N:352:LEU:HD13	1:N:352:LEU:C	2.35	0.47
1:Q:201:ASP:CG	2:S:29:ARG:HB2	2.35	0.47
1:Q:206:ARG:HH22	1:Q:283:VAL:H	1.61	0.47
1:U:165:LEU:HD22	1:V:96:LEU:HD23	1.95	0.47
2:W:90:ASP:OD2	2:W:93:LEU:HG	2.14	0.47
1:B:225:GLY:HA2	1:F:226:ARG:HE	1.75	0.47
1:A:144:GLN:OE1	1:B:95:LYS:HE3	2.13	0.47
1:F:106:LEU:O	1:F:110:GLU:HG3	2.15	0.47
1:I:190:LEU:C	1:I:190:LEU:HD13	2.35	0.47
1:M:145:PRO:HB2	1:M:150:ILE:HD11	1.95	0.47
1:M:190:LEU:C	1:M:190:LEU:HD13	2.35	0.47
1:M:234:ARG:HG2	1:M:247:ILE:HG12	1.96	0.47
1:Q:157:VAL:HG13	1:Q:162:GLU:HB2	1.95	0.47
3:T:65:ASP:O	3:T:69:ARG:HG3	2.13	0.47
1:B:188:PHE:HA	1:B:360:PHE:HE2	1.77	0.47
1:I:274:ILE:HG22	1:I:275:SER:N	2.28	0.47
1:J:190:LEU:HD13	1:J:190:LEU:C	2.35	0.47
3:L:62:PHE:O	3:L:66:VAL:HG23	2.14	0.47
1:M:185:ILE:HD13	1:M:188:PHE:HD1	1.78	0.47
1:M:352:LEU:HD13	1:M:352:LEU:C	2.35	0.47
3:P:62:PHE:O	3:P:66:VAL:HG23	2.14	0.47
1:U:311:SER:H	1:U:314:ASN:HD21	1.57	0.47
3:X:34:TYR:HA	3:X:37:TYR:HD2	1.79	0.47
2:W:40:ALA:HB2	3:X:86:ILE:HG13	1.96	0.47
1:A:167:VAL:HG12	1:A:168:ASP:N	2.29	0.47
3:D:76:ARG:HB3	3:D:80:TYR:CZ	2.49	0.47
1:F:211:LEU:HD21	1:F:312:PHE:CE2	2.49	0.47
3:H:34:TYR:HA	3:H:37:TYR:HD2	1.79	0.47
3:H:65:ASP:O	3:H:69:ARG:HG3	2.13	0.47
1:I:332:GLU:O	1:I:336:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:106:LEU:O	1:J:110:GLU:HG3	2.14	0.47
2:K:105:GLY:CA	2:O:73:ASN:CG	2.81	0.47
1:R:106:LEU:O	1:R:110:GLU:HG3	2.14	0.47
1:V:190:LEU:C	1:V:190:LEU:HD13	2.35	0.47
1:V:352:LEU:C	1:V:352:LEU:HD13	2.35	0.47
1:A:137:ARG:HB3	1:A:142:GLN:HB3	1.96	0.47
1:E:352:LEU:C	1:E:352:LEU:HD13	2.35	0.47
1:I:137:ARG:HB3	1:I:142:GLN:HB3	1.96	0.47
1:I:256:LYS:HE3	1:I:256:LYS:H	1.79	0.47
1:Q:91:ASN:ND2	1:R:181:GLN:O	2.48	0.47
3:T:62:PHE:O	3:T:66:VAL:HG23	2.14	0.47
1:U:125:LEU:HA	1:U:128:TYR:CD2	2.44	0.47
1:V:183:LYS:CG	1:V:184:GLY:H	2.13	0.47
2:W:50:TYR:O	2:W:54:VAL:HG23	2.14	0.47
3:X:62:PHE:O	3:X:66:VAL:HG23	2.14	0.47
3:X:65:ASP:O	3:X:69:ARG:HG3	2.13	0.47
1:A:125:LEU:HD22	1:A:221:TYR:CE1	2.49	0.47
1:E:106:LEU:HD13	1:E:106:LEU:O	2.14	0.47
1:E:190:LEU:HD13	1:E:190:LEU:C	2.35	0.47
3:H:37:TYR:O	3:H:41:VAL:HG23	2.15	0.47
1:I:310:GLU:CG	2:K:16:THR:HA	2.44	0.47
1:Q:185:ILE:HD13	1:Q:188:PHE:HD1	1.78	0.47
1:R:190:LEU:HD13	1:R:190:LEU:C	2.35	0.47
2:S:95:LYS:HB2	2:S:95:LYS:HE3	1.76	0.47
1:U:190:LEU:HD13	1:U:190:LEU:C	2.35	0.47
1:U:203:ILE:C	1:U:203:ILE:HD12	2.35	0.47
3:X:37:TYR:O	3:X:41:VAL:HG23	2.15	0.47
3:X:46:HIS:HB3	3:X:49:THR:CB	2.44	0.47
1:A:106:LEU:O	1:A:106:LEU:HD13	2.13	0.47
1:A:203:ILE:C	1:A:203:ILE:HD12	2.35	0.47
1:B:106:LEU:O	1:B:110:GLU:HG3	2.14	0.47
1:A:185:ILE:HD12	1:B:96:LEU:CD1	2.44	0.47
1:E:274:ILE:HG22	1:E:275:SER:N	2.28	0.47
2:O:90:ASP:OD2	2:O:93:LEU:HG	2.14	0.47
2:S:41:GLU:HB3	3:T:84:SER:HB3	1.96	0.47
1:A:134:GLN:NE2	1:A:143:GLU:OE1	2.48	0.47
1:B:352:LEU:HD13	1:B:352:LEU:C	2.35	0.47
1:B:98:SER:O	1:B:102:LEU:HD13	2.15	0.47
1:E:137:ARG:HB3	1:E:142:GLN:HB3	1.96	0.47
1:E:234:ARG:HG2	1:E:247:ILE:HG12	1.96	0.47
1:F:336:GLU:HA	2:G:77:ARG:HH21	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:352:LEU:HD13	1:F:352:LEU:C	2.35	0.47
1:F:98:SER:O	1:F:102:LEU:HD13	2.15	0.47
1:J:98:SER:O	1:J:102:LEU:HD13	2.15	0.47
1:J:352:LEU:C	1:J:352:LEU:HD13	2.35	0.47
2:K:90:ASP:OD2	2:K:93:LEU:HG	2.14	0.47
1:M:191:THR:O	1:M:194:GLU:HB2	2.15	0.47
3:P:34:TYR:HA	3:P:37:TYR:HD2	1.79	0.47
1:Q:124:PHE:CZ	1:R:112:GLU:HG3	2.50	0.47
1:U:125:LEU:HD22	1:U:221:TYR:CE1	2.49	0.47
2:W:63:LEU:HD13	3:X:42:LEU:HB2	1.96	0.47
1:E:319:PRO:HB2	1:E:338:LEU:HD21	1.97	0.47
1:I:234:ARG:HG2	1:I:247:ILE:HG12	1.96	0.47
1:J:204:THR:H	1:J:207:ASP:CG	2.18	0.47
2:K:105:GLY:HA3	2:O:73:ASN:OD1	2.11	0.47
1:Q:234:ARG:HG2	1:Q:247:ILE:HG12	1.95	0.47
1:Q:95:LYS:HZ3	1:R:184:GLY:CA	2.25	0.47
1:R:344:ILE:O	1:R:348:LEU:HD23	2.15	0.47
1:V:336:GLU:OE2	2:W:79:ILE:HD13	2.15	0.47
3:D:37:TYR:O	3:D:41:VAL:HG23	2.15	0.47
1:M:120:LEU:CD1	1:N:120:LEU:HD12	2.44	0.47
1:Q:332:GLU:O	1:Q:336:GLU:HG3	2.15	0.47
3:T:34:TYR:HA	3:T:37:TYR:HD2	1.79	0.47
3:T:37:TYR:O	3:T:41:VAL:HG23	2.15	0.47
1:U:344:ILE:O	1:U:348:LEU:HD23	2.15	0.47
2:C:90:ASP:OD2	2:C:93:LEU:HG	2.14	0.46
1:F:146:LYS:HB2	1:F:149:GLN:CG	2.41	0.46
1:I:185:ILE:HD13	1:I:188:PHE:CD1	2.50	0.46
3:L:34:TYR:HA	3:L:37:TYR:HD2	1.79	0.46
1:M:145:PRO:HB3	1:N:98:SER:CB	2.37	0.46
1:N:98:SER:O	1:N:102:LEU:HD13	2.15	0.46
1:Q:190:LEU:C	1:Q:190:LEU:HD13	2.35	0.46
1:Q:344:ILE:O	1:Q:348:LEU:HD23	2.15	0.46
2:S:90:ASP:OD2	2:S:93:LEU:HG	2.14	0.46
1:V:106:LEU:O	1:V:110:GLU:HG3	2.14	0.46
2:W:99:ARG:CZ	2:W:102:ILE:HD11	2.44	0.46
1:A:248:LEU:HB3	1:A:316:PHE:CE2	2.51	0.46
1:A:319:PRO:HB2	1:A:338:LEU:HD21	1.97	0.46
1:B:146:LYS:HB2	1:B:149:GLN:CG	2.41	0.46
1:B:256:LYS:HD2	1:B:257:GLU:H	1.81	0.46
2:C:97:LEU:HD22	2:C:100:VAL:HG21	1.97	0.46
1:E:191:THR:O	1:E:194:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:LYS:HE2	1:E:318:PRO:HG2	1.98	0.46
1:E:310:GLU:HG2	2:G:17:ARG:N	2.30	0.46
1:I:203:ILE:C	1:I:203:ILE:HD12	2.35	0.46
1:I:97:LEU:HD13	1:J:157:VAL:HG21	1.97	0.46
1:M:113:PHE:HA	1:N:124:PHE:CD2	2.50	0.46
1:M:344:ILE:O	1:M:348:LEU:HD23	2.15	0.46
2:O:102:ILE:HG22	2:O:103:ALA:N	2.30	0.46
2:K:103:ALA:CB	2:O:81:ARG:CZ	2.93	0.46
1:U:352:LEU:HD13	1:U:352:LEU:C	2.35	0.46
1:A:344:ILE:O	1:A:348:LEU:HD23	2.15	0.46
1:A:352:LEU:HD13	1:A:352:LEU:C	2.35	0.46
1:E:332:GLU:O	1:E:336:GLU:HG3	2.15	0.46
1:F:190:LEU:C	1:F:190:LEU:HD13	2.35	0.46
2:K:97:LEU:HD13	2:O:104:GLN:HG2	1.95	0.46
1:M:332:GLU:O	1:M:336:GLU:HG3	2.15	0.46
1:M:98:SER:O	1:M:102:LEU:HD13	2.16	0.46
2:O:97:LEU:HD23	2:O:102:ILE:HD11	1.97	0.46
1:R:204:THR:H	1:R:207:ASP:CG	2.18	0.46
2:S:98:GLY:HA2	2:S:101:THR:OG1	2.16	0.46
1:V:98:SER:O	1:V:102:LEU:HD13	2.15	0.46
2:W:26:PRO:O	2:W:30:VAL:HG23	2.16	0.46
1:E:185:ILE:HD13	1:E:188:PHE:CD1	2.50	0.46
3:H:83:ARG:NH1	3:H:83:ARG:HB3	2.31	0.46
1:I:344:ILE:O	1:I:348:LEU:HD23	2.15	0.46
1:J:146:LYS:HB2	1:J:149:GLN:CG	2.41	0.46
2:K:54:VAL:HG13	3:L:107:ALA:HB1	1.96	0.46
3:L:37:TYR:O	3:L:41:VAL:HG23	2.15	0.46
3:L:83:ARG:HB3	3:L:83:ARG:NH1	2.31	0.46
1:R:188:PHE:HA	1:R:360:PHE:CD2	2.50	0.46
1:R:219:LEU:HD12	1:R:353:ILE:HD12	1.98	0.46
1:U:191:THR:O	1:U:194:GLU:HB2	2.15	0.46
1:U:256:LYS:H	1:U:256:LYS:HE3	1.79	0.46
1:U:319:PRO:HB2	1:U:338:LEU:HD21	1.97	0.46
1:A:190:LEU:HD13	1:A:190:LEU:C	2.35	0.46
1:B:204:THR:H	1:B:207:ASP:CG	2.18	0.46
1:E:185:ILE:H	1:F:95:LYS:HG3	1.80	0.46
1:B:226:ARG:CD	1:F:225:GLY:HA2	2.45	0.46
1:F:240:ASN:ND2	1:F:242:PHE:H	2.14	0.46
1:I:98:SER:O	1:I:102:LEU:HD13	2.16	0.46
1:I:250:LYS:HE2	1:I:318:PRO:HG2	1.97	0.46
2:K:26:PRO:O	2:K:30:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:190:LEU:C	1:N:190:LEU:HD13	2.35	0.46
1:N:204:THR:H	1:N:207:ASP:CG	2.18	0.46
1:Q:319:PRO:HB2	1:Q:338:LEU:HD21	1.97	0.46
1:R:98:SER:O	1:R:102:LEU:HD13	2.15	0.46
2:S:26:PRO:O	2:S:30:VAL:HG23	2.16	0.46
1:V:120:LEU:O	1:V:123:LYS:HB3	2.16	0.46
1:A:250:LYS:HE2	1:A:318:PRO:HG2	1.98	0.46
1:I:162:GLU:C	1:I:164:GLU:H	2.19	0.46
1:I:319:PRO:HB2	1:I:338:LEU:HD21	1.97	0.46
1:M:182:VAL:HG21	1:M:186:PRO:CD	2.46	0.46
1:M:203:ILE:HD12	1:M:203:ILE:C	2.35	0.46
3:P:37:TYR:O	3:P:41:VAL:HG23	2.15	0.46
1:Q:144:GLN:OE1	1:R:95:LYS:HE3	2.15	0.46
1:U:112:GLU:HG3	1:V:124:PHE:CZ	2.51	0.46
1:V:152:LYS:O	1:V:156:ILE:HG13	2.16	0.46
1:I:248:LEU:HB3	1:I:316:PHE:CE2	2.51	0.46
1:M:319:PRO:HB2	1:M:338:LEU:HD21	1.97	0.46
1:Q:162:GLU:C	1:Q:164:GLU:H	2.19	0.46
1:Q:182:VAL:HG21	1:Q:186:PRO:CD	2.46	0.46
2:S:50:TYR:OH	3:T:92:GLN:HG3	2.15	0.46
1:U:127:LYS:O	1:U:130:PRO:HD2	2.16	0.46
1:B:120:LEU:O	1:B:123:LYS:HB3	2.16	0.46
1:B:344:ILE:O	1:B:348:LEU:HD23	2.15	0.46
1:F:256:LYS:HD2	1:F:257:GLU:H	1.81	0.46
2:G:77:ARG:HG3	3:H:51:ILE:N	2.31	0.46
2:G:87:VAL:HA	2:G:93:LEU:CD1	2.45	0.46
2:K:87:VAL:HG11	2:K:97:LEU:HD12	1.98	0.46
1:M:127:LYS:O	1:M:130:PRO:HD2	2.16	0.46
1:M:248:LEU:HB3	1:M:316:PHE:CE2	2.50	0.46
1:N:120:LEU:O	1:N:123:LYS:HB3	2.16	0.46
1:Q:191:THR:O	1:Q:194:GLU:HB2	2.15	0.46
1:Q:248:LEU:HB3	1:Q:316:PHE:CE2	2.51	0.46
1:R:120:LEU:O	1:R:123:LYS:HB3	2.16	0.46
1:U:248:LEU:HB3	1:U:316:PHE:CE2	2.51	0.46
1:U:332:GLU:O	1:U:336:GLU:HG3	2.15	0.46
1:V:204:THR:H	1:V:207:ASP:CG	2.18	0.46
1:V:344:ILE:O	1:V:348:LEU:HD23	2.15	0.46
2:W:20:ARG:O	3:X:118:TYR:HA	2.16	0.46
1:A:127:LYS:O	1:A:130:PRO:HD2	2.16	0.46
1:A:185:ILE:HD13	1:A:188:PHE:CD1	2.51	0.46
1:A:191:THR:O	1:A:194:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:LEU:C	1:E:219:LEU:HD23	2.37	0.46
1:F:219:LEU:HD12	1:F:353:ILE:HD12	1.98	0.46
2:G:26:PRO:O	2:G:30:VAL:HG23	2.16	0.46
2:K:20:ARG:HB3	3:L:121:ALA:HB3	1.98	0.46
1:M:219:LEU:C	1:M:219:LEU:HD23	2.37	0.46
1:N:240:ASN:ND2	1:N:242:PHE:H	2.13	0.46
1:Q:134:GLN:NE2	1:Q:143:GLU:OE1	2.48	0.46
1:Q:203:ILE:HD12	1:Q:203:ILE:C	2.35	0.46
1:Q:98:SER:O	1:Q:102:LEU:HD13	2.16	0.46
1:U:219:LEU:C	1:U:219:LEU:HD23	2.37	0.46
2:W:53:ALA:HB3	3:X:111:GLY:HA2	1.98	0.46
2:C:27:VAL:HG11	2:C:49:VAL:HG22	1.98	0.46
2:C:83:LEU:O	2:C:87:VAL:HG23	2.16	0.46
1:E:134:GLN:HA	1:E:137:ARG:NH2	2.32	0.46
1:E:344:ILE:O	1:E:348:LEU:HD23	2.15	0.46
1:F:152:LYS:O	1:F:156:ILE:HG13	2.16	0.46
2:G:83:LEU:O	2:G:87:VAL:HG23	2.16	0.46
1:J:256:LYS:HD2	1:J:257:GLU:H	1.81	0.46
1:M:120:LEU:HD13	1:N:120:LEU:HD12	1.98	0.46
1:R:256:LYS:HD2	1:R:256:LYS:N	2.31	0.46
1:R:256:LYS:HD2	1:R:257:GLU:H	1.81	0.46
1:V:256:LYS:HD2	1:V:257:GLU:H	1.81	0.46
1:E:182:VAL:HG21	1:E:186:PRO:CD	2.46	0.45
1:E:203:ILE:C	1:E:203:ILE:HD12	2.35	0.45
1:F:344:ILE:O	1:F:348:LEU:HD23	2.15	0.45
2:G:99:ARG:CG	2:G:100:VAL:N	2.79	0.45
1:I:191:THR:O	1:I:194:GLU:HB2	2.15	0.45
1:J:120:LEU:O	1:J:123:LYS:HB3	2.16	0.45
1:J:256:LYS:N	1:J:256:LYS:HD2	2.31	0.45
1:J:344:ILE:O	1:J:348:LEU:HD23	2.15	0.45
1:N:256:LYS:HD2	1:N:257:GLU:H	1.81	0.45
1:N:188:PHE:HA	1:N:360:PHE:CD2	2.51	0.45
2:O:54:VAL:HG13	3:P:107:ALA:HB1	1.99	0.45
3:T:83:ARG:HB3	3:T:83:ARG:NH1	2.31	0.45
1:V:146:LYS:HB2	1:V:149:GLN:CG	2.40	0.45
1:V:188:PHE:HA	1:V:360:PHE:CD2	2.50	0.45
3:D:83:ARG:HB3	3:D:83:ARG:NH1	2.31	0.45
1:I:219:LEU:C	1:I:219:LEU:HD23	2.37	0.45
1:N:219:LEU:HD12	1:N:353:ILE:HD12	1.98	0.45
1:R:152:LYS:O	1:R:156:ILE:HG13	2.16	0.45
1:U:250:LYS:HE2	1:U:318:PRO:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:27:VAL:HG11	2:W:49:VAL:HG22	1.98	0.45
1:A:162:GLU:C	1:A:164:GLU:H	2.19	0.45
1:A:332:GLU:O	1:A:336:GLU:HG3	2.15	0.45
1:B:190:LEU:HD13	1:B:190:LEU:C	2.35	0.45
1:I:127:LYS:O	1:I:130:PRO:HD2	2.16	0.45
1:I:134:GLN:HA	1:I:137:ARG:NH2	2.32	0.45
1:J:188:PHE:HA	1:J:360:PHE:CD2	2.51	0.45
1:N:256:LYS:N	1:N:256:LYS:HD2	2.31	0.45
1:N:344:ILE:O	1:N:348:LEU:HD23	2.15	0.45
3:P:83:ARG:HB3	3:P:83:ARG:NH1	2.31	0.45
1:Q:185:ILE:HD13	1:Q:188:PHE:CD1	2.51	0.45
2:S:88:ARG:NH2	2:S:97:LEU:HD13	2.31	0.45
3:X:83:ARG:NH1	3:X:83:ARG:HB3	2.31	0.45
1:E:98:SER:O	1:E:102:LEU:HD13	2.16	0.45
1:F:348:LEU:O	1:F:353:ILE:HG13	2.17	0.45
1:I:89:PRO:HD2	1:I:92:VAL:HG21	1.99	0.45
1:N:219:LEU:HB2	1:N:353:ILE:HD13	1.99	0.45
1:Q:250:LYS:HE2	1:Q:318:PRO:HG2	1.97	0.45
1:U:185:ILE:HD13	1:U:188:PHE:CD1	2.51	0.45
1:U:318:PRO:HA	1:U:319:PRO:HD3	1.87	0.45
1:V:240:ASN:ND2	1:V:242:PHE:H	2.13	0.45
2:W:83:LEU:O	2:W:87:VAL:HG23	2.17	0.45
1:B:256:LYS:HD2	1:B:256:LYS:N	2.31	0.45
2:C:26:PRO:O	2:C:30:VAL:HG23	2.16	0.45
3:D:113:LYS:HB3	3:D:113:LYS:HZ3	1.80	0.45
1:J:152:LYS:O	1:J:156:ILE:HG13	2.16	0.45
1:M:185:ILE:HD13	1:M:188:PHE:CD1	2.51	0.45
1:N:152:LYS:O	1:N:156:ILE:HG13	2.16	0.45
1:N:348:LEU:O	1:N:353:ILE:HG13	2.17	0.45
1:Q:219:LEU:HD23	1:Q:219:LEU:C	2.37	0.45
1:R:240:ASN:ND2	1:R:242:PHE:H	2.13	0.45
1:U:98:SER:O	1:U:102:LEU:HD13	2.16	0.45
2:W:92:GLU:OE1	3:X:102:GLU:HB3	2.17	0.45
1:A:310:GLU:HG2	2:C:17:ARG:N	2.32	0.45
1:B:240:ASN:ND2	1:B:242:PHE:H	2.14	0.45
2:C:79:ILE:HD13	2:C:81:ARG:NH2	2.28	0.45
1:E:248:LEU:HB3	1:E:316:PHE:CE2	2.51	0.45
1:F:120:LEU:O	1:F:123:LYS:HB3	2.16	0.45
1:F:204:THR:H	1:F:207:ASP:CG	2.18	0.45
1:E:186:PRO:HD2	1:F:92:VAL:CG2	2.46	0.45
1:J:113:PHE:CZ	1:J:117:MET:HE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:240:ASN:ND2	1:J:242:PHE:H	2.13	0.45
2:K:83:LEU:O	2:K:87:VAL:HG23	2.17	0.45
1:M:134:GLN:HA	1:M:137:ARG:NH2	2.32	0.45
1:R:219:LEU:HB2	1:R:353:ILE:HD13	1.99	0.45
1:R:348:LEU:O	1:R:353:ILE:HG13	2.17	0.45
1:U:134:GLN:NE2	1:U:143:GLU:OE1	2.48	0.45
1:V:256:LYS:HD2	1:V:256:LYS:N	2.31	0.45
1:A:89:PRO:HD2	1:A:92:VAL:HG21	1.99	0.45
1:I:182:VAL:HG21	1:I:186:PRO:CD	2.46	0.45
1:J:188:PHE:HA	1:J:360:PHE:HE2	1.77	0.45
2:K:49:VAL:HG21	3:L:118:TYR:CD2	2.51	0.45
3:T:59:MET:O	3:T:63:VAL:HG23	2.17	0.45
1:A:182:VAL:HG21	1:A:186:PRO:CD	2.46	0.45
1:B:152:LYS:O	1:B:156:ILE:HG13	2.16	0.45
1:B:309:ILE:HG22	1:B:310:GLU:N	2.32	0.45
1:E:245:ASN:ND2	1:E:274:ILE:HG23	2.32	0.45
1:E:95:LYS:HE3	1:F:145:PRO:HD3	1.98	0.45
2:G:54:VAL:HG13	3:H:107:ALA:HB1	1.98	0.45
3:H:59:MET:O	3:H:63:VAL:HG23	2.17	0.45
1:I:245:ASN:ND2	1:I:274:ILE:HG23	2.32	0.45
1:M:112:GLU:HG3	1:N:124:PHE:CE1	2.52	0.45
2:O:26:PRO:O	2:O:30:VAL:HG23	2.16	0.45
2:O:83:LEU:O	2:O:87:VAL:HG23	2.16	0.45
3:P:59:MET:O	3:P:63:VAL:HG23	2.17	0.45
2:W:93:LEU:O	2:W:96:LEU:HD23	2.17	0.45
1:A:318:PRO:HA	1:A:319:PRO:HD3	1.87	0.45
1:E:127:LYS:O	1:E:130:PRO:HD2	2.16	0.45
1:F:135:ARG:HG2	1:F:139:ILE:HD11	1.99	0.45
1:F:256:LYS:N	1:F:256:LYS:HD2	2.31	0.45
1:E:144:GLN:OE1	1:F:95:LYS:HE3	2.16	0.45
1:E:138:ILE:HG21	1:F:98:SER:OG	2.17	0.45
1:J:322:GLN:O	1:J:323:ASN:HB2	2.17	0.45
1:M:250:LYS:HE2	1:M:318:PRO:HG2	1.98	0.45
1:N:322:GLN:O	1:N:323:ASN:HB2	2.17	0.45
3:P:36:ILE:HD11	3:P:37:TYR:CZ	2.52	0.45
1:U:134:GLN:HA	1:U:137:ARG:NH2	2.32	0.45
1:U:124:PHE:CE1	1:V:112:GLU:HG3	2.52	0.45
2:C:54:VAL:HG13	3:D:107:ALA:HB1	1.99	0.45
3:H:113:LYS:HZ3	3:H:113:LYS:HB3	1.81	0.45
1:J:348:LEU:O	1:J:353:ILE:HG13	2.17	0.45
1:M:201:ASP:OD2	2:O:26:PRO:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:128:TYR:HE1	1:N:110:GLU:HG2	1.79	0.45
1:N:125:LEU:O	1:N:129:LYS:HG3	2.17	0.45
1:Q:90:LYS:O	1:Q:94:GLU:HG3	2.17	0.45
1:R:322:GLN:O	1:R:323:ASN:HB2	2.17	0.45
1:V:135:ARG:HG2	1:V:139:ILE:HD11	1.99	0.45
1:A:98:SER:O	1:A:102:LEU:HD13	2.16	0.44
1:B:125:LEU:O	1:B:129:LYS:HG3	2.17	0.44
1:E:162:GLU:C	1:E:164:GLU:H	2.19	0.44
2:G:91:GLU:O	2:G:95:LYS:HB3	2.16	0.44
1:M:139:ILE:HD13	1:M:188:PHE:CD2	2.53	0.44
1:U:112:GLU:HG3	1:V:124:PHE:HZ	1.83	0.44
1:U:260:TYR:CE1	1:V:355:ARG:HG3	2.52	0.44
1:U:90:LYS:O	1:U:94:GLU:HG3	2.17	0.44
1:V:322:GLN:O	1:V:323:ASN:HB2	2.17	0.44
1:E:243:PHE:HA	1:E:277:LYS:HG3	1.99	0.44
2:K:27:VAL:HG11	2:K:49:VAL:HG22	1.98	0.44
2:K:53:ALA:HB3	3:L:111:GLY:HA2	1.99	0.44
1:I:201:ASP:OD2	3:L:37:TYR:OH	2.36	0.44
1:M:89:PRO:HD2	1:M:92:VAL:HG21	1.99	0.44
1:Q:91:ASN:CG	1:R:182:VAL:HB	2.38	0.44
1:U:101:THR:OG1	1:V:149:GLN:O	2.34	0.44
1:V:348:LEU:O	1:V:353:ILE:HG13	2.17	0.44
1:A:219:LEU:C	1:A:219:LEU:HD23	2.37	0.44
1:B:135:ARG:HG2	1:B:139:ILE:HD11	1.99	0.44
1:B:188:PHE:HA	1:B:360:PHE:CD2	2.51	0.44
1:B:348:LEU:O	1:B:353:ILE:HG13	2.17	0.44
1:B:219:LEU:HD12	1:B:353:ILE:HD12	1.98	0.44
1:E:89:PRO:HD2	1:E:92:VAL:HG21	1.99	0.44
1:F:219:LEU:HB2	1:F:353:ILE:HD13	1.99	0.44
1:F:188:PHE:HA	1:F:360:PHE:CD2	2.51	0.44
2:G:27:VAL:HG11	2:G:49:VAL:HG22	1.98	0.44
1:I:128:TYR:CE1	1:J:110:GLU:HG2	2.52	0.44
1:J:125:LEU:O	1:J:129:LYS:HG3	2.17	0.44
1:I:138:ILE:HG21	1:J:98:SER:OG	2.17	0.44
1:M:90:LYS:O	1:M:94:GLU:HG3	2.17	0.44
1:M:95:LYS:NZ	1:N:184:GLY:HA2	2.32	0.44
2:O:27:VAL:HG11	2:O:49:VAL:HG22	1.98	0.44
1:Q:127:LYS:O	1:Q:130:PRO:HD2	2.16	0.44
1:Q:134:GLN:HA	1:Q:137:ARG:NH2	2.32	0.44
1:R:125:LEU:O	1:R:129:LYS:HG3	2.17	0.44
1:R:309:ILE:HG22	1:R:310:GLU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:27:VAL:HG11	2:S:49:VAL:HG22	1.98	0.44
1:V:309:ILE:HG22	1:V:310:GLU:N	2.32	0.44
1:U:144:GLN:OE1	1:V:95:LYS:HE3	2.17	0.44
3:D:59:MET:O	3:D:63:VAL:HG23	2.17	0.44
1:I:90:LYS:O	1:I:94:GLU:HG3	2.17	0.44
2:K:103:ALA:CA	2:O:81:ARG:HH12	2.09	0.44
1:M:245:ASN:ND2	1:M:274:ILE:HG23	2.32	0.44
1:R:135:ARG:HG2	1:R:139:ILE:HD11	2.00	0.44
1:V:125:LEU:O	1:V:129:LYS:HG3	2.17	0.44
1:U:138:ILE:HB	1:V:99:LEU:HD21	1.99	0.44
1:A:138:ILE:HB	1:B:99:LEU:HD21	1.98	0.44
1:A:334:LEU:N	1:A:334:LEU:HD12	2.33	0.44
1:E:318:PRO:HA	1:E:319:PRO:HD3	1.87	0.44
1:F:125:LEU:O	1:F:129:LYS:HG3	2.17	0.44
2:G:99:ARG:CG	2:G:100:VAL:H	2.18	0.44
1:I:104:SER:OG	1:J:156:ILE:HD13	2.17	0.44
3:L:59:MET:O	3:L:63:VAL:HG23	2.17	0.44
1:M:134:GLN:NE2	1:M:143:GLU:OE1	2.48	0.44
1:M:129:LYS:HZ1	1:M:220:GLU:HG2	1.83	0.44
2:O:21:ALA:HB2	3:P:118:TYR:HB2	1.98	0.44
1:Q:139:ILE:HD13	1:Q:188:PHE:CD2	2.52	0.44
1:Q:334:LEU:HD12	1:Q:334:LEU:N	2.33	0.44
1:R:189:TRP:O	1:R:193:LEU:HG	2.18	0.44
1:U:89:PRO:HD2	1:U:92:VAL:HG21	1.99	0.44
2:W:26:PRO:HD3	3:X:37:TYR:CD1	2.52	0.44
2:W:42:ARG:N	3:X:84:SER:O	2.50	0.44
2:W:49:VAL:HG21	3:X:118:TYR:CD2	2.53	0.44
1:F:113:PHE:CZ	1:F:117:MET:HE2	2.52	0.44
2:G:99:ARG:HG3	2:G:100:VAL:N	2.27	0.44
3:H:93:THR:HA	3:H:96:ARG:HH11	1.83	0.44
1:M:243:PHE:HA	1:M:277:LYS:HG3	1.99	0.44
2:K:103:ALA:CB	2:O:81:ARG:NH1	2.74	0.44
2:S:83:LEU:O	2:S:87:VAL:HG23	2.16	0.44
3:X:36:ILE:HD11	3:X:37:TYR:CZ	2.53	0.44
3:X:59:MET:O	3:X:63:VAL:HG23	2.17	0.44
1:A:245:ASN:ND2	1:A:274:ILE:HG23	2.32	0.44
1:A:90:LYS:O	1:A:94:GLU:HG3	2.17	0.44
2:C:63:LEU:HD13	3:D:42:LEU:HB2	1.99	0.44
1:E:139:ILE:HD13	1:E:188:PHE:CD2	2.53	0.44
1:B:225:GLY:CA	1:F:226:ARG:NE	2.79	0.44
2:K:99:ARG:O	2:K:102:ILE:CG1	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:126:GLN:HE22	1:N:129:LYS:NZ	2.16	0.44
1:Q:245:ASN:ND2	1:Q:274:ILE:HG23	2.32	0.44
1:Q:95:LYS:O	1:Q:99:LEU:HG	2.18	0.44
2:S:54:VAL:HG13	3:T:107:ALA:HB1	1.99	0.44
1:V:219:LEU:HD12	1:V:353:ILE:HD12	1.99	0.44
1:A:134:GLN:HA	1:A:137:ARG:NH2	2.32	0.44
1:A:243:PHE:HA	1:A:277:LYS:HG3	1.99	0.44
1:B:187:SER:HG	1:B:212:GLU:CD	2.21	0.44
1:F:309:ILE:HG22	1:F:310:GLU:N	2.32	0.44
1:I:129:LYS:HZ3	1:I:220:GLU:HG2	1.82	0.44
1:I:243:PHE:HA	1:I:277:LYS:HG3	1.99	0.44
1:I:334:LEU:HD12	1:I:334:LEU:N	2.33	0.44
1:J:120:LEU:HD23	1:J:120:LEU:O	2.18	0.44
1:J:219:LEU:HD12	1:J:353:ILE:HD12	1.98	0.44
1:Q:142:GLN:NE2	1:U:142:GLN:O	2.50	0.44
3:T:36:ILE:HD11	3:T:37:TYR:CZ	2.53	0.44
1:U:334:LEU:HD12	1:U:334:LEU:N	2.33	0.44
2:W:42:ARG:CB	3:X:85:THR:HG22	2.22	0.44
1:E:334:LEU:N	1:E:334:LEU:HD12	2.33	0.44
1:F:322:GLN:O	1:F:323:ASN:HB2	2.17	0.44
1:I:201:ASP:OD2	2:K:26:PRO:HG3	2.18	0.44
1:J:309:ILE:HG22	1:J:310:GLU:N	2.32	0.44
3:L:109:SER:O	3:L:113:LYS:HG3	2.18	0.44
1:M:162:GLU:C	1:M:164:GLU:H	2.19	0.44
1:N:120:LEU:O	1:N:120:LEU:HD23	2.18	0.44
2:O:97:LEU:HD21	2:O:102:ILE:HD12	1.99	0.44
1:U:162:GLU:C	1:U:164:GLU:H	2.19	0.44
1:B:189:TRP:O	1:B:193:LEU:HG	2.18	0.43
2:C:50:TYR:CD1	3:D:111:GLY:HA3	2.53	0.43
1:F:120:LEU:O	1:F:120:LEU:HD23	2.18	0.43
1:E:96:LEU:HB3	1:F:165:LEU:HD21	2.00	0.43
1:M:194:GLU:C	1:M:195:ASN:HD22	2.22	0.43
1:N:309:ILE:HG22	1:N:310:GLU:N	2.32	0.43
3:X:109:SER:O	3:X:113:LYS:HG3	2.18	0.43
1:B:100:LYS:O	1:B:103:GLN:HB3	2.18	0.43
1:B:120:LEU:HD23	1:B:120:LEU:O	2.18	0.43
1:B:322:GLN:O	1:B:323:ASN:HB2	2.17	0.43
1:E:134:GLN:NE2	1:E:143:GLU:OE1	2.48	0.43
1:E:95:LYS:O	1:E:99:LEU:HG	2.18	0.43
3:H:109:SER:O	3:H:113:LYS:HG3	2.18	0.43
1:I:139:ILE:HD13	1:I:188:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:126:GLN:HE22	1:J:129:LYS:NZ	2.16	0.43
3:P:93:THR:HA	3:P:96:ARG:HH11	1.83	0.43
1:Q:98:SER:O	1:Q:101:THR:HB	2.19	0.43
1:Q:194:GLU:C	1:Q:195:ASN:HD22	2.22	0.43
1:Q:334:LEU:HA	1:Q:337:ARG:NH1	2.34	0.43
3:T:93:THR:HA	3:T:96:ARG:HH11	1.83	0.43
1:V:126:GLN:HE22	1:V:129:LYS:NZ	2.16	0.43
1:A:194:GLU:C	1:A:195:ASN:HD22	2.22	0.43
1:B:126:GLN:HE22	1:B:129:LYS:NZ	2.16	0.43
1:E:90:LYS:O	1:E:94:GLU:HG3	2.17	0.43
1:F:189:TRP:O	1:F:193:LEU:HG	2.18	0.43
1:I:310:GLU:CG	2:K:16:THR:CA	2.96	0.43
1:Q:130:PRO:O	1:Q:134:GLN:HB2	2.19	0.43
1:Q:243:PHE:HA	1:Q:277:LYS:HG3	1.99	0.43
3:T:75:SER:HA	3:T:86:ILE:HD11	2.01	0.43
1:U:130:PRO:O	1:U:134:GLN:HB2	2.19	0.43
1:U:139:ILE:HD13	1:U:188:PHE:CD2	2.52	0.43
1:U:245:ASN:ND2	1:U:274:ILE:HG23	2.32	0.43
1:U:243:PHE:HA	1:U:277:LYS:HG3	1.99	0.43
1:A:139:ILE:HD13	1:A:188:PHE:CD2	2.53	0.43
3:D:95:VAL:CG1	3:D:99:LEU:HD12	2.49	0.43
1:F:100:LYS:O	1:F:103:GLN:HB3	2.18	0.43
3:H:36:ILE:HD11	3:H:37:TYR:CZ	2.53	0.43
3:H:95:VAL:CG1	3:H:99:LEU:HD12	2.49	0.43
1:I:194:GLU:C	1:I:195:ASN:HD22	2.22	0.43
1:I:334:LEU:HA	1:I:337:ARG:NH1	2.33	0.43
1:R:125:LEU:HA	1:R:128:TYR:CD2	2.54	0.43
1:R:266:TYR:HB3	1:R:342:TYR:CZ	2.54	0.43
1:U:182:VAL:HG21	1:U:186:PRO:CD	2.46	0.43
1:V:120:LEU:O	1:V:120:LEU:HD23	2.18	0.43
1:V:189:TRP:O	1:V:193:LEU:HG	2.18	0.43
1:A:88:LEU:O	1:A:93:LYS:HE3	2.19	0.43
1:B:219:LEU:HB2	1:B:353:ILE:HD13	1.99	0.43
2:G:88:ARG:HD3	2:G:94:ASN:CB	2.48	0.43
1:M:130:PRO:O	1:M:134:GLN:HB2	2.19	0.43
1:M:93:LYS:CD	1:N:167:VAL:HG22	2.47	0.43
1:N:339:ALA:CB	2:O:77:ARG:HH22	2.31	0.43
1:V:100:LYS:O	1:V:103:GLN:HB3	2.18	0.43
1:V:347:GLN:O	1:V:351:LYS:HB2	2.19	0.43
2:W:50:TYR:CE1	3:X:111:GLY:HA3	2.53	0.43
3:X:95:VAL:CG1	3:X:99:LEU:HD12	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LYS:CG	1:B:184:GLY:H	2.13	0.43
1:I:95:LYS:O	1:I:99:LEU:HG	2.18	0.43
1:J:100:LYS:O	1:J:103:GLN:HB3	2.18	0.43
2:K:55:LEU:O	2:K:59:THR:HG23	2.19	0.43
2:K:95:LYS:HB2	2:K:95:LYS:HE3	1.76	0.43
1:M:201:ASP:OD2	2:O:26:PRO:CB	2.66	0.43
1:M:334:LEU:HA	1:M:337:ARG:NH1	2.34	0.43
1:M:95:LYS:O	1:M:99:LEU:HG	2.19	0.43
1:N:113:PHE:CZ	1:N:117:MET:HE2	2.54	0.43
3:P:109:SER:O	3:P:113:LYS:HG3	2.18	0.43
3:P:75:SER:HA	3:P:86:ILE:HD11	2.01	0.43
1:U:321:ILE:O	1:U:322:GLN:O	2.37	0.43
1:U:88:LEU:O	1:U:93:LYS:HE3	2.19	0.43
2:W:102:ILE:O	2:W:104:GLN:HG3	2.18	0.43
1:A:98:SER:O	1:A:101:THR:HB	2.19	0.43
1:E:104:SER:OG	1:F:156:ILE:HD13	2.19	0.43
1:F:266:TYR:HB3	1:F:342:TYR:CZ	2.54	0.43
1:F:311:SER:H	1:F:314:ASN:HD21	1.65	0.43
2:G:55:LEU:O	2:G:59:THR:HG23	2.19	0.43
1:I:130:PRO:O	1:I:134:GLN:HB2	2.19	0.43
1:I:88:LEU:O	1:I:93:LYS:HE3	2.19	0.43
1:J:189:TRP:O	1:J:193:LEU:HG	2.18	0.43
2:K:99:ARG:HD3	3:L:98:LEU:O	2.10	0.43
1:Q:96:LEU:HD21	1:R:360:PHE:CE1	2.51	0.43
1:R:311:SER:H	1:R:314:ASN:HD21	1.65	0.43
1:R:347:GLN:O	1:R:351:LYS:HB2	2.19	0.43
3:T:95:VAL:CG1	3:T:99:LEU:HD12	2.49	0.43
1:U:95:LYS:O	1:U:99:LEU:HG	2.19	0.43
1:U:102:LEU:HD21	1:V:134:GLN:HB3	2.01	0.43
3:D:36:ILE:HD11	3:D:37:TYR:CZ	2.53	0.43
3:D:93:THR:HA	3:D:96:ARG:HH11	1.83	0.43
1:E:194:GLU:C	1:E:195:ASN:HD22	2.22	0.43
1:E:322:GLN:HE21	1:E:334:LEU:HD22	1.84	0.43
1:I:169:GLU:O	1:I:169:GLU:HG3	2.19	0.43
1:J:135:ARG:HG2	1:J:139:ILE:HD11	1.99	0.43
1:M:98:SER:HA	1:N:149:GLN:HB3	2.01	0.43
1:N:189:TRP:O	1:N:193:LEU:HG	2.18	0.43
1:N:228:GLY:HA2	1:N:254:TYR:CE2	2.54	0.43
1:R:126:GLN:HE22	1:R:129:LYS:NZ	2.16	0.43
3:T:109:SER:O	3:T:113:LYS:HG3	2.18	0.43
1:U:98:SER:O	1:U:101:THR:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:144:GLN:HA	1:V:145:PRO:HD3	1.93	0.43
1:V:219:LEU:HB2	1:V:353:ILE:HD13	2.00	0.43
1:A:334:LEU:HA	1:A:337:ARG:NH1	2.34	0.43
1:A:95:LYS:O	1:A:99:LEU:HG	2.18	0.43
1:E:130:PRO:O	1:E:134:GLN:HB2	2.19	0.43
1:E:334:LEU:HA	1:E:337:ARG:NH1	2.34	0.43
1:E:351:LYS:O	1:E:354:PRO:HD2	2.19	0.43
1:E:88:LEU:O	1:E:93:LYS:HE3	2.19	0.43
1:I:163:THR:HA	1:I:166:LEU:HG	2.01	0.43
1:J:266:TYR:HB3	1:J:342:TYR:CZ	2.54	0.43
1:I:310:GLU:HG2	2:K:16:THR:C	2.38	0.43
3:L:36:ILE:HD11	3:L:37:TYR:CZ	2.53	0.43
3:L:95:VAL:CG1	3:L:99:LEU:HD12	2.49	0.43
1:M:321:ILE:O	1:M:322:GLN:O	2.37	0.43
1:N:125:LEU:HA	1:N:128:TYR:CD2	2.54	0.43
2:O:55:LEU:O	2:O:59:THR:HG23	2.19	0.43
1:Q:85:VAL:HA	1:Q:88:LEU:HG	2.01	0.43
1:Q:89:PRO:HD2	1:Q:92:VAL:HG21	1.99	0.43
1:U:334:LEU:HA	1:U:337:ARG:NH1	2.34	0.43
1:V:188:PHE:HA	1:V:360:PHE:HE2	1.77	0.43
3:X:93:THR:HA	3:X:96:ARG:HH11	1.83	0.43
1:A:130:PRO:O	1:A:134:GLN:HB2	2.19	0.43
1:A:189:TRP:CE2	1:A:216:ASP:HA	2.54	0.43
1:I:144:GLN:HA	1:I:145:PRO:HD3	1.88	0.43
1:J:219:LEU:HB2	1:J:353:ILE:HD13	1.99	0.43
1:Q:351:LYS:O	1:Q:354:PRO:HD2	2.19	0.43
1:R:100:LYS:O	1:R:103:GLN:HB3	2.18	0.43
1:U:194:GLU:C	1:U:195:ASN:HD22	2.22	0.43
1:V:192:ALA:HA	1:V:359:TRP:O	2.19	0.43
1:V:266:TYR:HB3	1:V:342:TYR:CZ	2.54	0.43
1:A:163:THR:HA	1:A:166:LEU:HG	2.01	0.42
2:C:55:LEU:O	2:C:59:THR:HG23	2.19	0.42
3:D:109:SER:O	3:D:113:LYS:HG3	2.18	0.42
1:E:163:THR:HA	1:E:166:LEU:HG	2.01	0.42
1:E:210:VAL:HG22	1:E:242:PHE:CD2	2.54	0.42
1:E:321:ILE:O	1:E:322:GLN:O	2.37	0.42
1:F:347:GLN:O	1:F:351:LYS:HB2	2.19	0.42
3:H:75:SER:HA	3:H:86:ILE:HD11	2.01	0.42
1:I:189:TRP:CE2	1:I:216:ASP:HA	2.54	0.42
1:I:310:GLU:HG2	2:K:17:ARG:N	2.34	0.42
1:I:351:LYS:O	1:I:354:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:85:VAL:HA	1:M:88:LEU:HG	2.01	0.42
1:M:88:LEU:O	1:M:93:LYS:HE3	2.19	0.42
1:N:135:ARG:HG2	1:N:139:ILE:HD11	1.99	0.42
1:M:102:LEU:HD11	1:N:149:GLN:NE2	2.34	0.42
1:Q:210:VAL:HG22	1:Q:242:PHE:CD2	2.54	0.42
1:U:189:TRP:CE2	1:U:216:ASP:HA	2.54	0.42
1:V:125:LEU:HA	1:V:128:TYR:CD2	2.54	0.42
1:U:201:ASP:OD2	2:W:29:ARG:NE	2.52	0.42
1:A:351:LYS:O	1:A:354:PRO:HD2	2.19	0.42
1:B:196:LEU:HD23	1:B:199:VAL:CG2	2.49	0.42
1:E:129:LYS:HZ3	1:E:220:GLU:HG2	1.83	0.42
1:F:126:GLN:HE22	1:F:129:LYS:NZ	2.16	0.42
1:F:337:ARG:HH11	1:F:337:ARG:HB3	1.84	0.42
1:I:210:VAL:HG22	1:I:242:PHE:CD2	2.55	0.42
3:L:93:THR:HA	3:L:96:ARG:HH11	1.83	0.42
2:O:50:TYR:CD1	3:P:111:GLY:HA3	2.54	0.42
1:R:120:LEU:O	1:R:120:LEU:HD23	2.18	0.42
1:Q:95:LYS:CB	1:R:185:ILE:HG13	2.49	0.42
1:B:203:ILE:HD12	1:B:203:ILE:C	2.40	0.42
1:F:203:ILE:HD12	1:F:203:ILE:C	2.40	0.42
1:F:228:GLY:HA2	1:F:254:TYR:CE2	2.54	0.42
1:E:181:GLN:HB2	1:F:91:ASN:HD22	1.84	0.42
1:J:228:GLY:HA2	1:J:254:TYR:CE2	2.54	0.42
2:K:96:LEU:HD11	3:L:99:LEU:HD21	2.02	0.42
1:M:189:TRP:CE2	1:M:216:ASP:HA	2.54	0.42
1:M:343:SER:O	1:M:346:GLU:HB2	2.20	0.42
1:N:266:TYR:HB3	1:N:342:TYR:CZ	2.54	0.42
1:Q:95:LYS:C	1:R:185:ILE:HD11	2.40	0.42
1:Q:165:LEU:HD22	1:R:96:LEU:HD23	2.00	0.42
2:S:55:LEU:O	2:S:59:THR:HG23	2.19	0.42
1:V:333:ASP:C	1:V:335:GLU:H	2.23	0.42
2:W:55:LEU:O	2:W:59:THR:HG23	2.19	0.42
1:B:125:LEU:HA	1:B:128:TYR:CD2	2.54	0.42
1:E:98:SER:O	1:E:101:THR:HB	2.19	0.42
1:F:125:LEU:HA	1:F:128:TYR:CD2	2.54	0.42
1:F:181:GLN:O	1:F:182:VAL:HB	2.20	0.42
1:I:185:ILE:CD1	1:J:96:LEU:HD11	2.44	0.42
1:M:334:LEU:HD12	1:M:334:LEU:N	2.33	0.42
1:N:100:LYS:O	1:N:103:GLN:HB3	2.18	0.42
1:R:192:ALA:HA	1:R:359:TRP:O	2.19	0.42
1:R:196:LEU:HD23	1:R:199:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:333:ASP:C	1:R:335:GLU:H	2.23	0.42
1:U:169:GLU:O	1:U:169:GLU:HG3	2.19	0.42
1:A:111:LYS:HA	1:A:258:LEU:HD22	2.02	0.42
1:A:343:SER:O	1:A:346:GLU:HB2	2.20	0.42
1:E:189:TRP:CE2	1:E:216:ASP:HA	2.54	0.42
1:E:85:VAL:HA	1:E:88:LEU:HG	2.01	0.42
3:L:75:SER:HA	3:L:86:ILE:HD11	2.01	0.42
1:M:98:SER:O	1:M:101:THR:HB	2.19	0.42
1:N:333:ASP:C	1:N:335:GLU:H	2.23	0.42
1:Q:163:THR:HA	1:Q:166:LEU:HG	2.01	0.42
1:Q:189:TRP:CE2	1:Q:216:ASP:HA	2.54	0.42
1:Q:321:ILE:O	1:Q:322:GLN:O	2.37	0.42
1:Q:88:LEU:O	1:Q:93:LYS:HE3	2.19	0.42
1:U:111:LYS:HA	1:U:258:LEU:HD22	2.02	0.42
1:U:260:TYR:HE2	1:V:358:ASP:OD2	2.02	0.42
3:X:75:SER:HA	3:X:86:ILE:HD11	2.00	0.42
1:A:169:GLU:HG3	1:A:169:GLU:O	2.19	0.42
1:B:181:GLN:O	1:B:182:VAL:HB	2.20	0.42
2:G:88:ARG:CD	2:G:94:ASN:CB	2.98	0.42
1:J:181:GLN:O	1:J:182:VAL:HB	2.19	0.42
1:J:203:ILE:C	1:J:203:ILE:HD12	2.40	0.42
1:J:351:LYS:C	1:J:354:PRO:HD2	2.40	0.42
1:N:311:SER:H	1:N:314:ASN:HD21	1.65	0.42
1:Q:88:LEU:HA	1:Q:89:PRO:HD3	1.94	0.42
1:U:163:THR:HA	1:U:166:LEU:HG	2.01	0.42
1:V:181:GLN:O	1:V:182:VAL:HB	2.20	0.42
1:A:210:VAL:HG22	1:A:242:PHE:CD2	2.55	0.42
1:B:228:GLY:HA2	1:B:254:TYR:CE2	2.54	0.42
1:B:333:ASP:C	1:B:335:GLU:H	2.23	0.42
1:B:266:TYR:HB3	1:B:342:TYR:CZ	2.54	0.42
1:B:347:GLN:O	1:B:351:LYS:HB2	2.19	0.42
1:B:351:LYS:C	1:B:354:PRO:HD2	2.40	0.42
3:D:75:SER:HA	3:D:86:ILE:HD11	2.01	0.42
1:E:113:PHE:HE1	1:F:120:LEU:HD22	1.85	0.42
1:I:134:GLN:NE2	1:I:143:GLU:OE1	2.48	0.42
1:M:358:ASP:OD2	1:N:260:TYR:OH	2.22	0.42
1:N:347:GLN:O	1:N:351:LYS:HB2	2.19	0.42
1:Q:129:LYS:HZ1	1:Q:220:GLU:HG2	1.85	0.42
1:R:113:PHE:CZ	1:R:117:MET:HE2	2.54	0.42
1:R:228:GLY:HA2	1:R:254:TYR:CE2	2.54	0.42
1:V:351:LYS:C	1:V:354:PRO:HD2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:VAL:HG21	1:A:186:PRO:CG	2.50	0.42
1:J:337:ARG:HH11	1:J:337:ARG:HB3	1.84	0.42
1:M:310:GLU:OE1	1:M:310:GLU:HA	2.20	0.42
1:Q:184:GLY:O	1:Q:185:ILE:C	2.58	0.42
1:R:203:ILE:HD12	1:R:203:ILE:C	2.40	0.42
2:S:100:VAL:HG13	3:T:65:ASP:OD1	2.11	0.42
1:U:95:LYS:HA	1:V:145:PRO:HG2	2.01	0.42
1:B:192:ALA:HA	1:B:359:TRP:O	2.20	0.42
2:G:21:ALA:HB2	3:H:118:TYR:HB2	2.01	0.42
1:I:195:ASN:N	1:I:195:ASN:HD22	2.18	0.42
1:I:343:SER:O	1:I:346:GLU:HB2	2.20	0.42
1:M:111:LYS:HA	1:M:258:LEU:HD22	2.01	0.42
1:N:188:PHE:HA	1:N:360:PHE:HE2	1.76	0.42
1:N:203:ILE:C	1:N:203:ILE:HD12	2.40	0.42
1:R:181:GLN:O	1:R:182:VAL:HB	2.20	0.42
1:V:203:ILE:HD12	1:V:203:ILE:C	2.40	0.42
1:I:98:SER:O	1:I:101:THR:HB	2.19	0.42
1:I:321:ILE:O	1:I:322:GLN:O	2.37	0.42
1:J:192:ALA:HA	1:J:359:TRP:O	2.20	0.42
1:J:347:GLN:O	1:J:351:LYS:HB2	2.19	0.42
2:K:25:PHE:HE1	3:L:41:VAL:HG21	1.85	0.42
1:M:102:LEU:HD21	1:N:134:GLN:HB3	2.02	0.42
1:N:192:ALA:HA	1:N:359:TRP:O	2.20	0.42
1:N:196:LEU:HD23	1:N:199:VAL:CG2	2.50	0.42
1:N:249:CYS:H	1:N:272:CYS:HB2	1.85	0.42
1:Q:169:GLU:HG3	1:Q:169:GLU:O	2.19	0.42
1:R:219:LEU:HD23	1:R:219:LEU:C	2.40	0.42
1:Q:100:LYS:CA	1:R:357:VAL:HG11	2.46	0.42
1:U:104:SER:OG	1:V:156:ILE:HD13	2.20	0.42
1:V:196:LEU:HD23	1:V:199:VAL:CG2	2.49	0.42
2:W:103:ALA:C	2:W:104:GLN:CG	2.87	0.42
1:A:310:GLU:HA	1:A:310:GLU:OE1	2.20	0.41
1:B:276:TRP:CE3	1:B:282:ASN:HA	2.55	0.41
2:C:49:VAL:HG21	3:D:118:TYR:CD2	2.55	0.41
1:E:169:GLU:HG3	1:E:169:GLU:O	2.19	0.41
1:E:182:VAL:HG21	1:E:186:PRO:CG	2.50	0.41
1:E:343:SER:O	1:E:346:GLU:HB2	2.20	0.41
2:G:99:ARG:HD2	2:G:99:ARG:HA	1.71	0.41
1:I:182:VAL:HG21	1:I:186:PRO:CG	2.50	0.41
1:I:85:VAL:HA	1:I:88:LEU:HG	2.01	0.41
1:J:219:LEU:C	1:J:219:LEU:HD23	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:117:MET:N	1:N:120:LEU:HD11	2.34	0.41
1:R:337:ARG:HB3	1:R:337:ARG:HH11	1.84	0.41
1:U:85:VAL:HA	1:U:88:LEU:HG	2.01	0.41
1:V:228:GLY:HA2	1:V:254:TYR:CE2	2.54	0.41
1:A:321:ILE:O	1:A:322:GLN:O	2.37	0.41
1:A:181:GLN:N	1:B:91:ASN:ND2	2.68	0.41
1:E:99:LEU:HD22	1:F:135:ARG:HG3	2.01	0.41
1:F:333:ASP:C	1:F:335:GLU:H	2.23	0.41
1:F:351:LYS:C	1:F:354:PRO:HD2	2.40	0.41
2:G:97:LEU:O	3:H:69:ARG:NH1	2.52	0.41
1:J:187:SER:HG	1:J:212:GLU:CD	2.23	0.41
1:M:322:GLN:HE21	1:M:334:LEU:HD22	1.84	0.41
1:M:351:LYS:O	1:M:354:PRO:HD2	2.19	0.41
1:N:337:ARG:HB3	1:N:337:ARG:HH11	1.84	0.41
1:R:351:LYS:C	1:R:354:PRO:HD2	2.40	0.41
1:U:139:ILE:HD13	1:U:188:PHE:CE2	2.55	0.41
1:U:210:VAL:HG22	1:U:242:PHE:CD2	2.55	0.41
1:U:351:LYS:O	1:U:354:PRO:HD2	2.19	0.41
1:A:144:GLN:HA	1:A:145:PRO:HD3	1.88	0.41
1:A:85:VAL:HA	1:A:88:LEU:HG	2.01	0.41
1:F:249:CYS:H	1:F:272:CYS:HB2	1.85	0.41
2:G:67:GLY:O	2:G:71:ARG:HG3	2.21	0.41
2:K:103:ALA:N	2:O:81:ARG:HH12	2.18	0.41
1:M:182:VAL:HG21	1:M:186:PRO:CG	2.50	0.41
1:M:210:VAL:HG22	1:M:242:PHE:CD2	2.55	0.41
1:N:181:GLN:O	1:N:182:VAL:HB	2.20	0.41
1:N:351:LYS:C	1:N:354:PRO:HD2	2.40	0.41
3:P:95:VAL:CG1	3:P:99:LEU:HD12	2.49	0.41
1:Q:137:ARG:HG2	1:Q:142:GLN:NE2	2.35	0.41
1:Q:139:ILE:HD13	1:Q:188:PHE:CE2	2.56	0.41
1:U:343:SER:O	1:U:346:GLU:HB2	2.20	0.41
1:U:124:PHE:CD2	1:V:113:PHE:HD1	2.39	0.41
2:W:99:ARG:CA	2:W:99:ARG:CZ	2.86	0.41
2:W:46:GLY:O	3:X:88:SER:HB3	2.21	0.41
1:F:196:LEU:HD23	1:F:199:VAL:CG2	2.49	0.41
1:F:219:LEU:HD23	1:F:219:LEU:C	2.41	0.41
1:I:111:LYS:HA	1:I:258:LEU:HD22	2.02	0.41
1:I:102:LEU:HD11	1:J:149:GLN:NE2	2.35	0.41
1:J:276:TRP:CE3	1:J:282:ASN:HA	2.55	0.41
1:M:99:LEU:CD1	1:N:185:ILE:HD12	2.49	0.41
1:N:219:LEU:HD23	1:N:219:LEU:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:96:LEU:HD21	3:T:62:PHE:CE1	2.55	0.41
1:U:311:SER:H	1:U:314:ASN:HD22	1.67	0.41
1:B:219:LEU:HD23	1:B:219:LEU:C	2.40	0.41
1:B:337:ARG:HB3	1:B:337:ARG:HH11	1.84	0.41
2:G:25:PHE:HE1	3:H:41:VAL:HG21	1.84	0.41
2:G:51:LEU:HD21	3:H:67:PHE:CD1	2.55	0.41
1:J:311:SER:H	1:J:314:ASN:HD21	1.65	0.41
1:I:186:PRO:CD	1:J:92:VAL:HG22	2.51	0.41
1:M:169:GLU:O	1:M:169:GLU:HG3	2.19	0.41
1:M:139:ILE:HD13	1:M:188:PHE:CE2	2.56	0.41
1:R:276:TRP:CE3	1:R:282:ASN:HA	2.55	0.41
1:U:120:LEU:HD12	1:V:120:LEU:HD12	2.02	0.41
1:A:322:GLN:HE21	1:A:334:LEU:HD22	1.84	0.41
1:B:311:SER:H	1:B:314:ASN:HD21	1.65	0.41
1:E:184:GLY:O	1:E:185:ILE:C	2.58	0.41
1:E:256:LYS:N	1:E:256:LYS:HD2	2.36	0.41
1:E:319:PRO:HG2	1:E:337:ARG:HG2	2.03	0.41
1:F:276:TRP:CE3	1:F:282:ASN:HA	2.55	0.41
1:J:139:ILE:O	1:J:184:GLY:HA3	2.21	0.41
2:K:22:GLY:HA3	3:L:117:LYS:NZ	2.36	0.41
1:M:124:PHE:HE1	1:N:112:GLU:CG	2.31	0.41
1:N:96:LEU:N	1:N:96:LEU:HD12	2.36	0.41
1:Q:111:LYS:HA	1:Q:258:LEU:HD22	2.02	0.41
1:U:184:GLY:O	1:U:185:ILE:C	2.58	0.41
1:U:182:VAL:HG21	1:U:186:PRO:CG	2.50	0.41
1:A:184:GLY:O	1:A:185:ILE:C	2.58	0.41
1:A:348:LEU:HD22	1:A:348:LEU:N	2.36	0.41
1:I:322:GLN:HE21	1:I:334:LEU:HD22	1.84	0.41
1:J:107:PHE:O	1:J:111:LYS:HB2	2.21	0.41
1:M:348:LEU:N	1:M:348:LEU:HD22	2.36	0.41
1:R:183:LYS:CG	1:R:184:GLY:H	2.12	0.41
1:V:311:SER:H	1:V:314:ASN:HD21	1.65	0.41
2:W:67:GLY:O	2:W:71:ARG:HG3	2.21	0.41
1:B:332:GLU:OE1	2:C:81:ARG:NH1	2.53	0.41
1:F:336:GLU:HG2	2:G:77:ARG:HH21	1.85	0.41
1:F:96:LEU:N	1:F:96:LEU:HD12	2.35	0.41
1:I:139:ILE:HD13	1:I:188:PHE:CE2	2.56	0.41
1:I:256:LYS:N	1:I:256:LYS:HD2	2.36	0.41
1:I:319:PRO:HG2	1:I:337:ARG:HG2	2.03	0.41
1:J:125:LEU:HA	1:J:128:TYR:CD2	2.54	0.41
1:I:181:GLN:CG	1:J:91:ASN:HD22	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:195:ASN:HD22	1:M:195:ASN:N	2.18	0.41
1:V:139:ILE:O	1:V:184:GLY:HA3	2.21	0.41
1:V:337:ARG:HH11	1:V:337:ARG:HB3	1.84	0.41
1:A:139:ILE:HD13	1:A:188:PHE:CE2	2.56	0.41
1:B:249:CYS:H	1:B:272:CYS:HB2	1.85	0.41
1:E:139:ILE:HD13	1:E:188:PHE:CE2	2.56	0.41
1:F:139:ILE:O	1:F:184:GLY:HA3	2.21	0.41
1:F:192:ALA:HA	1:F:359:TRP:O	2.20	0.41
2:G:53:ALA:HB3	3:H:111:GLY:HA2	2.03	0.41
1:M:163:THR:HA	1:M:166:LEU:HG	2.01	0.41
1:N:107:PHE:O	1:N:111:LYS:HB2	2.21	0.41
1:Q:182:VAL:HG21	1:Q:186:PRO:CG	2.50	0.41
1:Q:195:ASN:HD22	1:Q:195:ASN:N	2.18	0.41
1:Q:343:SER:O	1:Q:346:GLU:HB2	2.20	0.41
1:R:107:PHE:O	1:R:111:LYS:HB2	2.21	0.41
1:U:140:SER:C	1:U:142:GLN:H	2.24	0.41
1:V:249:CYS:H	1:V:272:CYS:HB2	1.85	0.41
2:W:100:VAL:HG11	3:X:65:ASP:OD2	2.21	0.41
1:B:254:TYR:HB3	1:B:264:PHE:HB3	2.03	0.41
1:E:111:LYS:HA	1:E:258:LEU:HD22	2.02	0.41
1:F:254:TYR:HB3	1:F:264:PHE:HB3	2.03	0.41
1:F:244:THR:HG23	1:F:277:LYS:HE2	2.03	0.41
1:J:196:LEU:HD23	1:J:199:VAL:CG2	2.49	0.41
1:J:233:PHE:HB3	1:J:235:PHE:HE1	1.86	0.41
1:M:140:SER:C	1:M:142:GLN:H	2.24	0.41
1:N:244:THR:HG23	1:N:277:LYS:HE2	2.03	0.41
1:M:170:GLU:HB3	1:N:90:LYS:HZ3	1.86	0.41
1:Q:145:PRO:HB3	1:R:98:SER:HB3	2.02	0.41
1:Q:348:LEU:HD22	1:Q:348:LEU:N	2.36	0.41
1:R:157:VAL:HG11	1:R:165:LEU:O	2.21	0.41
1:R:139:ILE:O	1:R:184:GLY:HA3	2.20	0.41
1:R:111:LYS:HZ2	1:R:258:LEU:HD13	1.84	0.41
1:Q:96:LEU:HD23	1:R:361:THR:HG22	2.02	0.41
2:S:67:GLY:O	2:S:71:ARG:HG3	2.21	0.41
1:V:108:GLU:O	1:V:111:LYS:HB3	2.21	0.41
1:V:153:GLY:O	1:V:157:VAL:HG23	2.21	0.41
1:A:204:THR:H	1:A:207:ASP:HB2	1.86	0.41
1:B:233:PHE:HB3	1:B:235:PHE:HE1	1.86	0.41
1:B:96:LEU:N	1:B:96:LEU:HD12	2.36	0.41
2:C:67:GLY:O	2:C:71:ARG:HG3	2.21	0.41
1:E:138:ILE:HB	1:F:99:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:THR:H	1:E:207:ASP:HB2	1.86	0.41
1:F:107:PHE:O	1:F:111:LYS:HB2	2.21	0.41
1:F:91:ASN:HA	1:F:94:GLU:OE2	2.21	0.41
2:G:87:VAL:CG1	2:G:93:LEU:HD13	2.51	0.41
1:J:157:VAL:HG11	1:J:165:LEU:O	2.21	0.41
1:J:333:ASP:C	1:J:335:GLU:H	2.23	0.41
1:J:96:LEU:N	1:J:96:LEU:HD12	2.36	0.41
2:K:67:GLY:HA3	3:L:46:HIS:CD2	2.56	0.41
1:N:153:GLY:O	1:N:157:VAL:HG23	2.21	0.41
1:U:256:LYS:N	1:U:256:LYS:HD2	2.36	0.41
1:U:310:GLU:HA	1:U:310:GLU:OE1	2.20	0.41
1:V:107:PHE:O	1:V:111:LYS:HB2	2.21	0.41
1:A:256:LYS:HD2	1:A:256:LYS:N	2.36	0.40
1:I:110:GLU:O	1:I:113:PHE:HB3	2.22	0.40
1:I:137:ARG:HG2	1:I:142:GLN:NE2	2.36	0.40
1:N:254:TYR:HB3	1:N:264:PHE:HB3	2.03	0.40
1:Q:310:GLU:HA	1:Q:310:GLU:OE1	2.20	0.40
1:Q:318:PRO:HA	1:Q:319:PRO:HD3	1.87	0.40
1:Q:103:GLN:HE22	1:R:358:ASP:CG	2.25	0.40
1:R:91:ASN:HA	1:R:94:GLU:OE2	2.21	0.40
1:U:144:GLN:HA	1:U:145:PRO:HD3	1.88	0.40
1:U:129:LYS:HZ1	1:U:220:GLU:HG2	1.83	0.40
1:V:254:TYR:HB3	1:V:264:PHE:HB3	2.03	0.40
1:A:110:GLU:O	1:A:113:PHE:HB3	2.22	0.40
1:A:120:LEU:HD12	1:B:120:LEU:HD12	2.03	0.40
1:B:328:GLU:HG2	2:C:104:GLN:OE1	2.21	0.40
1:E:310:GLU:HA	1:E:310:GLU:OE1	2.20	0.40
1:I:184:GLY:O	1:I:185:ILE:C	2.58	0.40
1:N:108:GLU:O	1:N:111:LYS:HB3	2.21	0.40
1:N:139:ILE:O	1:N:184:GLY:HA3	2.21	0.40
1:N:223:THR:HG22	1:N:223:THR:O	2.22	0.40
1:N:135:ARG:CZ	1:N:356:ALA:HB3	2.51	0.40
2:O:67:GLY:O	2:O:71:ARG:HG3	2.21	0.40
1:Q:144:GLN:HA	1:Q:145:PRO:HD3	1.88	0.40
1:Q:256:LYS:HD2	1:Q:256:LYS:N	2.36	0.40
1:Q:337:ARG:NH1	1:Q:337:ARG:CB	2.84	0.40
1:R:110:GLU:O	1:R:113:PHE:HB3	2.22	0.40
1:R:256:LYS:HG2	1:R:257:GLU:N	2.36	0.40
1:U:337:ARG:NH1	1:U:337:ARG:CB	2.84	0.40
1:U:348:LEU:HD22	1:U:348:LEU:N	2.36	0.40
1:V:157:VAL:HG11	1:V:165:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:276:TRP:CE3	1:V:282:ASN:HA	2.55	0.40
2:W:93:LEU:O	2:W:97:LEU:HB2	2.21	0.40
1:A:137:ARG:HG2	1:A:142:GLN:NE2	2.36	0.40
1:B:110:GLU:O	1:B:113:PHE:HB3	2.22	0.40
1:B:144:GLN:HA	1:B:145:PRO:HD3	1.93	0.40
1:B:157:VAL:HG11	1:B:165:LEU:O	2.21	0.40
1:E:110:GLU:O	1:E:113:PHE:HB3	2.22	0.40
1:F:233:PHE:HB3	1:F:235:PHE:HE1	1.86	0.40
1:I:357:VAL:HG11	1:J:100:LYS:HA	2.03	0.40
1:I:134:GLN:OE1	1:J:102:LEU:HD21	2.21	0.40
1:M:110:GLU:O	1:M:113:PHE:HB3	2.21	0.40
1:N:276:TRP:CE3	1:N:282:ASN:HA	2.55	0.40
1:Q:322:GLN:HE21	1:Q:334:LEU:HD22	1.84	0.40
1:R:254:TYR:HB3	1:R:264:PHE:HB3	2.03	0.40
1:R:111:LYS:CE	1:R:258:LEU:HD13	2.52	0.40
1:U:110:GLU:O	1:U:113:PHE:HB3	2.22	0.40
1:U:195:ASN:HD22	1:U:195:ASN:N	2.18	0.40
2:W:79:ILE:HB	2:W:80:PRO:HD2	2.04	0.40
2:W:96:LEU:CG	2:W:97:LEU:N	2.83	0.40
1:A:156:ILE:HD13	1:B:104:SER:OG	2.22	0.40
1:B:125:LEU:HD21	1:B:220:GLU:HA	2.04	0.40
1:E:134:GLN:O	1:E:138:ILE:HG12	2.22	0.40
1:E:137:ARG:HG2	1:E:142:GLN:NE2	2.36	0.40
1:E:348:LEU:HD22	1:E:348:LEU:N	2.36	0.40
1:F:256:LYS:HG2	1:F:257:GLU:N	2.36	0.40
1:F:348:LEU:N	1:F:348:LEU:HD22	2.37	0.40
2:G:79:ILE:HB	2:G:80:PRO:HD2	2.04	0.40
1:I:204:THR:H	1:I:207:ASP:HB2	1.86	0.40
2:K:67:GLY:O	2:K:71:ARG:HG3	2.21	0.40
1:M:137:ARG:HG2	1:M:142:GLN:NE2	2.36	0.40
1:M:85:VAL:HG23	1:M:88:LEU:CD1	2.52	0.40
1:N:157:VAL:HG11	1:N:165:LEU:O	2.21	0.40
1:U:168:ASP:OD1	1:V:90:LYS:HE2	2.22	0.40
1:U:364:ALA:HA	1:V:260:TYR:HE2	1.85	0.40
1:V:91:ASN:HA	1:V:94:GLU:OE2	2.21	0.40
1:V:96:LEU:HD12	1:V:96:LEU:N	2.36	0.40
1:B:118:PHE:CE1	1:B:221:TYR:HD2	2.40	0.40
1:B:348:LEU:HD22	1:B:348:LEU:N	2.37	0.40
1:I:134:GLN:O	1:I:138:ILE:HG12	2.22	0.40
1:I:310:GLU:OE1	1:I:310:GLU:HA	2.20	0.40
1:I:88:LEU:HA	1:I:89:PRO:HD3	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:91:ASN:HA	1:J:94:GLU:OE2	2.21	0.40
1:M:128:TYR:HE1	1:N:110:GLU:CG	2.34	0.40
1:M:204:THR:H	1:M:207:ASP:HB2	1.86	0.40
1:Q:134:GLN:O	1:Q:138:ILE:HG12	2.22	0.40
1:R:96:LEU:N	1:R:96:LEU:HD12	2.36	0.40
1:U:149:GLN:HB3	1:V:98:SER:HA	2.02	0.40
1:V:256:LYS:HG2	1:V:257:GLU:N	2.36	0.40
1:V:198:ILE:HB	1:V:347:GLN:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/310 (79%)	208 (85%)	31 (13%)	7 (3%)	6	44
1	B	237/310 (76%)	202 (85%)	31 (13%)	4 (2%)	11	55
1	E	246/310 (79%)	209 (85%)	30 (12%)	7 (3%)	6	44
1	F	237/310 (76%)	202 (85%)	31 (13%)	4 (2%)	11	55
1	I	246/310 (79%)	209 (85%)	30 (12%)	7 (3%)	6	44
1	J	237/310 (76%)	202 (85%)	31 (13%)	4 (2%)	11	55
1	M	246/310 (79%)	209 (85%)	30 (12%)	7 (3%)	6	44
1	N	237/310 (76%)	201 (85%)	32 (14%)	4 (2%)	11	55
1	Q	246/310 (79%)	208 (85%)	31 (13%)	7 (3%)	6	44
1	R	237/310 (76%)	202 (85%)	31 (13%)	4 (2%)	11	55
1	U	246/310 (79%)	208 (85%)	31 (13%)	7 (3%)	6	44
1	V	237/310 (76%)	201 (85%)	32 (14%)	4 (2%)	11	55
2	C	88/107 (82%)	87 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	88/107 (82%)	84 (96%)	3 (3%)	1 (1%)	17	63
2	K	88/107 (82%)	84 (96%)	2 (2%)	2 (2%)	8	48
2	O	88/107 (82%)	87 (99%)	1 (1%)	0	100	100
2	S	88/107 (82%)	85 (97%)	2 (2%)	1 (1%)	17	63
2	W	88/107 (82%)	86 (98%)	1 (1%)	1 (1%)	17	63
3	D	87/100 (87%)	84 (97%)	2 (2%)	1 (1%)	17	63
3	H	87/100 (87%)	84 (97%)	2 (2%)	1 (1%)	17	63
3	L	87/100 (87%)	84 (97%)	2 (2%)	1 (1%)	17	63
3	P	87/100 (87%)	84 (97%)	2 (2%)	1 (1%)	17	63
3	T	87/100 (87%)	84 (97%)	2 (2%)	1 (1%)	17	63
3	X	87/100 (87%)	84 (97%)	2 (2%)	1 (1%)	17	63
All	All	3948/4962 (80%)	3478 (88%)	393 (10%)	77 (2%)	9	51

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ILE
1	A	322	GLN
1	B	273	GLU
1	E	185	ILE
1	E	322	GLN
1	F	273	GLU
1	I	185	ILE
1	I	322	GLN
1	J	273	GLU
1	M	185	ILE
1	M	322	GLN
1	N	273	GLU
1	Q	185	ILE
1	Q	322	GLN
1	R	273	GLU
2	S	102	ILE
1	U	185	ILE
1	U	322	GLN
1	V	273	GLU
2	W	101	THR
1	A	184	GLY
1	A	224	ASP

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Mol	Chain	Res	Type
1	B	182	VAL
3	D	101	GLY
1	E	184	GLY
1	E	224	ASP
1	F	182	VAL
3	H	101	GLY
1	I	184	GLY
1	I	224	ASP
1	J	182	VAL
3	L	101	GLY
1	M	184	GLY
1	M	224	ASP
1	N	182	VAL
3	P	101	GLY
1	Q	184	GLY
1	Q	224	ASP
1	R	182	VAL
3	T	101	GLY
1	U	184	GLY
1	U	224	ASP
1	V	182	VAL
3	X	101	GLY
2	G	101	THR
1	A	326	GLN
1	B	197	PRO
1	E	326	GLN
1	F	197	PRO
1	I	326	GLN
1	J	197	PRO
1	M	326	GLN
1	N	197	PRO
1	Q	326	GLN
1	R	197	PRO
1	U	326	GLN
1	V	197	PRO
1	A	226	ARG
1	E	226	ARG
1	I	226	ARG
2	K	102	ILE
1	M	226	ARG
1	Q	226	ARG
1	U	226	ARG

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Mol	Chain	Res	Type
1	A	197	PRO
1	E	197	PRO
1	I	197	PRO
2	K	94	ASN
1	M	197	PRO
1	Q	197	PRO
1	U	197	PRO
1	B	85	VAL
1	F	85	VAL
1	J	85	VAL
1	N	85	VAL
1	R	85	VAL
1	V	85	VAL

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	228/282 (81%)	220 (96%)	8 (4%)	43	74
1	B	221/282 (78%)	216 (98%)	5 (2%)	58	82
1	E	228/282 (81%)	220 (96%)	8 (4%)	43	74
1	F	221/282 (78%)	216 (98%)	5 (2%)	58	82
1	I	228/282 (81%)	220 (96%)	8 (4%)	43	74
1	J	221/282 (78%)	216 (98%)	5 (2%)	58	82
1	M	228/282 (81%)	220 (96%)	8 (4%)	43	74
1	N	221/282 (78%)	216 (98%)	5 (2%)	58	82
1	Q	228/282 (81%)	220 (96%)	8 (4%)	43	74
1	R	221/282 (78%)	216 (98%)	5 (2%)	58	82
1	U	228/282 (81%)	220 (96%)	8 (4%)	43	74
1	V	221/282 (78%)	216 (98%)	5 (2%)	58	82
2	C	70/85 (82%)	69 (99%)	1 (1%)	74	89
2	G	70/85 (82%)	62 (89%)	8 (11%)	7	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	70/85 (82%)	66 (94%)	4 (6%)	25	62
2	O	70/85 (82%)	65 (93%)	5 (7%)	18	55
2	S	70/85 (82%)	68 (97%)	2 (3%)	50	78
2	W	70/85 (82%)	67 (96%)	3 (4%)	35	70
3	D	75/86 (87%)	75 (100%)	0	100	100
3	H	75/86 (87%)	75 (100%)	0	100	100
3	L	75/86 (87%)	75 (100%)	0	100	100
3	P	75/86 (87%)	75 (100%)	0	100	100
3	T	75/86 (87%)	75 (100%)	0	100	100
3	X	75/86 (87%)	75 (100%)	0	100	100
All	All	3564/4410 (81%)	3463 (97%)	101 (3%)	51	78

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	GLU
1	A	134	GLN
1	A	161	ASN
1	A	207	ASP
1	A	212	GLU
1	A	240	ASN
1	A	256	LYS
1	A	310	GLU
1	B	161	ASN
1	B	224	ASP
1	B	240	ASN
1	B	256	LYS
1	B	273	GLU
2	C	50	TYR
1	E	108	GLU
1	E	134	GLN
1	E	161	ASN
1	E	207	ASP
1	E	212	GLU
1	E	240	ASN
1	E	256	LYS
1	E	310	GLU
1	F	161	ASN

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Mol	Chain	Res	Type
1	F	224	ASP
1	F	240	ASN
1	F	256	LYS
1	F	273	GLU
2	G	50	TYR
2	G	92	GLU
2	G	93	LEU
2	G	94	ASN
2	G	95	LYS
2	G	96	LEU
2	G	97	LEU
2	G	101	THR
1	I	108	GLU
1	I	134	GLN
1	I	161	ASN
1	I	207	ASP
1	I	212	GLU
1	I	240	ASN
1	I	256	LYS
1	I	310	GLU
1	J	161	ASN
1	J	224	ASP
1	J	240	ASN
1	J	256	LYS
1	J	273	GLU
2	K	50	TYR
2	K	97	LEU
2	K	101	THR
2	K	104	GLN
1	M	108	GLU
1	M	134	GLN
1	M	161	ASN
1	M	207	ASP
1	M	212	GLU
1	M	240	ASN
1	M	256	LYS
1	M	310	GLU
1	N	161	ASN
1	N	224	ASP
1	N	240	ASN
1	N	256	LYS
1	N	273	GLU

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Mol	Chain	Res	Type
2	O	50	TYR
2	O	97	LEU
2	O	99	ARG
2	O	101	THR
2	O	104	GLN
1	Q	108	GLU
1	Q	134	GLN
1	Q	161	ASN
1	Q	207	ASP
1	Q	212	GLU
1	Q	240	ASN
1	Q	256	LYS
1	Q	310	GLU
1	R	161	ASN
1	R	224	ASP
1	R	240	ASN
1	R	256	LYS
1	R	273	GLU
2	S	50	TYR
2	S	97	LEU
1	U	108	GLU
1	U	134	GLN
1	U	161	ASN
1	U	207	ASP
1	U	212	GLU
1	U	240	ASN
1	U	256	LYS
1	U	310	GLU
1	V	161	ASN
1	V	224	ASP
1	V	240	ASN
1	V	256	LYS
1	V	273	GLU
2	W	50	TYR
2	W	97	LEU
2	W	99	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	161	ASN

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Mol	Chain	Res	Type
1	A	195	ASN
1	A	240	ASN
1	A	245	ASN
1	A	314	ASN
1	A	322	GLN
1	B	91	ASN
1	B	114	GLN
1	B	126	GLN
1	B	142	GLN
1	B	161	ASN
1	B	195	ASN
1	B	240	ASN
1	B	245	ASN
2	C	68	ASN
2	C	73	ASN
2	C	94	ASN
3	D	46	HIS
3	D	64	ASN
3	D	92	GLN
1	E	142	GLN
1	E	161	ASN
1	E	195	ASN
1	E	240	ASN
1	E	245	ASN
1	E	314	ASN
1	E	322	GLN
1	F	91	ASN
1	F	126	GLN
1	F	142	GLN
1	F	161	ASN
1	F	195	ASN
1	F	240	ASN
1	F	245	ASN
2	G	68	ASN
2	G	73	ASN
3	H	64	ASN
3	H	92	GLN
1	I	142	GLN
1	I	161	ASN
1	I	195	ASN
1	I	240	ASN
1	I	245	ASN

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Mol	Chain	Res	Type
1	I	314	ASN
1	I	322	GLN
1	J	91	ASN
1	J	126	GLN
1	J	142	GLN
1	J	161	ASN
1	J	195	ASN
1	J	240	ASN
1	J	245	ASN
2	K	68	ASN
2	K	73	ASN
2	K	94	ASN
3	L	92	GLN
1	M	142	GLN
1	M	161	ASN
1	M	195	ASN
1	M	240	ASN
1	M	245	ASN
1	M	314	ASN
1	M	322	GLN
1	N	91	ASN
1	N	126	GLN
1	N	142	GLN
1	N	161	ASN
1	N	195	ASN
1	N	240	ASN
1	N	245	ASN
2	O	68	ASN
2	O	104	GLN
3	P	46	HIS
3	P	64	ASN
3	P	92	GLN
1	Q	142	GLN
1	Q	161	ASN
1	Q	195	ASN
1	Q	240	ASN
1	Q	245	ASN
1	Q	314	ASN
1	Q	322	GLN
1	R	126	GLN
1	R	142	GLN
1	R	161	ASN

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Mol	Chain	Res	Type
1	R	195	ASN
1	R	240	ASN
1	R	245	ASN
2	S	68	ASN
2	S	73	ASN
3	T	64	ASN
3	T	92	GLN
1	U	142	GLN
1	U	161	ASN
1	U	195	ASN
1	U	240	ASN
1	U	245	ASN
1	U	314	ASN
1	U	322	GLN
1	V	91	ASN
1	V	126	GLN
1	V	142	GLN
1	V	161	ASN
1	V	195	ASN
1	V	240	ASN
1	V	245	ASN
2	W	68	ASN
2	W	73	ASN
2	W	89	ASN
3	X	64	ASN
3	X	92	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	252/310 (81%)	0.87	30 (11%) 6 11	232, 361, 461, 501	0
1	B	245/310 (79%)	0.93	29 (11%) 6 12	281, 404, 471, 558	0
1	E	252/310 (81%)	0.99	41 (16%) 2 8	233, 361, 461, 502	0
1	F	245/310 (79%)	1.16	49 (20%) 1 7	281, 404, 470, 559	0
1	I	252/310 (81%)	1.01	34 (13%) 4 10	234, 362, 461, 502	0
1	J	245/310 (79%)	1.22	56 (22%) 1 6	281, 404, 471, 559	0
1	M	252/310 (81%)	0.88	43 (17%) 2 8	237, 362, 462, 502	0
1	N	245/310 (79%)	1.42	77 (31%) 1 5	280, 405, 470, 559	0
1	Q	252/310 (81%)	0.81	34 (13%) 4 10	235, 361, 461, 502	0
1	R	245/310 (79%)	1.44	72 (29%) 1 5	278, 406, 471, 559	0
1	U	252/310 (81%)	0.88	36 (14%) 4 9	235, 362, 462, 502	0
1	V	245/310 (79%)	1.55	85 (34%) 0 4	280, 405, 471, 559	0
2	C	90/107 (84%)	0.85	10 (11%) 7 12	159, 291, 414, 456	0
2	G	90/107 (84%)	0.48	2 (2%) 65 61	162, 288, 414, 457	0
2	K	90/107 (84%)	0.65	10 (11%) 7 12	164, 278, 362, 388	0
2	O	90/107 (84%)	0.37	1 (1%) 82 78	164, 278, 363, 388	0
2	S	90/107 (84%)	0.44	1 (1%) 82 78	164, 278, 363, 388	0
2	W	90/107 (84%)	0.65	6 (6%) 21 23	166, 290, 427, 456	0
3	D	89/100 (89%)	0.55	3 (3%) 49 46	196, 300, 396, 464	0
3	H	89/100 (89%)	0.64	6 (6%) 21 23	200, 302, 393, 464	0
3	L	89/100 (89%)	0.47	4 (4%) 37 36	199, 302, 393, 464	0
3	P	89/100 (89%)	0.60	6 (6%) 21 23	196, 302, 393, 462	0
3	T	89/100 (89%)	0.40	4 (4%) 37 36	197, 302, 392, 464	0
3	X	89/100 (89%)	0.56	5 (5%) 28 28	200, 302, 394, 462	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4056/4962 (81%)	0.95	644 (15%) 3 8	159, 363, 464, 559	0

All (644) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	145	PRO	9.1
1	I	328	GLU	8.5
1	J	274	ILE	8.2
1	V	186	PRO	8.0
1	M	181	GLN	7.6
1	V	187	SER	7.4
1	R	361	THR	7.3
1	I	329	GLU	7.1
1	U	142	GLN	7.0
1	M	171	GLU	6.8
1	I	144	GLN	6.6
1	J	184	GLY	6.6
1	M	170	GLU	6.5
1	Q	143	GLU	6.2
3	L	121	ALA	6.1
3	P	81	ASN	5.9
1	V	147	PRO	5.8
2	C	105	GLY	5.7
1	R	186	PRO	5.7
1	M	182	VAL	5.7
1	F	319	PRO	5.6
1	A	144	GLN	5.5
2	C	45	ALA	5.4
1	V	224	ASP	5.4
1	E	165	LEU	5.4
1	U	221	TYR	5.4
1	N	186	PRO	5.4
1	V	284	THR	5.3
1	U	257	GLU	5.3
1	Q	142	GLN	5.1
1	Q	82	SER	5.1
1	V	353	ILE	5.1
1	J	363	ALA	5.0
1	A	145	PRO	5.0
1	A	165	LEU	4.9
1	E	269	ALA	4.9
1	R	213	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
1	R	187	SER	4.9
1	E	171	GLU	4.9
1	A	329	GLU	4.8
1	M	143	GLU	4.8
1	A	166	LEU	4.8
3	T	81	ASN	4.8
1	V	188	PHE	4.8
1	I	168	ASP	4.7
1	N	313	PHE	4.7
3	X	81	ASN	4.7
1	R	164	GLU	4.7
1	E	167	VAL	4.7
1	J	169	GLU	4.7
1	J	141	GLY	4.7
1	E	329	GLU	4.7
1	F	167	VAL	4.6
1	J	143	GLU	4.6
1	J	323	ASN	4.6
1	R	323	ASN	4.6
1	A	269	ALA	4.6
1	V	185	ILE	4.5
1	U	327	ASP	4.5
1	J	183	LYS	4.5
1	B	142	GLN	4.5
3	D	122	LYS	4.5
3	H	122	LYS	4.5
1	I	327	ASP	4.5
1	E	328	GLU	4.5
1	I	319	PRO	4.5
1	N	110	GLU	4.4
1	F	144	GLN	4.4
1	V	117	MET	4.4
1	R	148	GLU	4.4
3	D	121	ALA	4.4
1	J	185	ILE	4.4
1	N	361	THR	4.4
1	F	257	GLU	4.4
1	J	273	GLU	4.4
1	B	140	SER	4.4
1	N	214	LEU	4.3
1	N	213	TYR	4.3
1	B	143	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	J	114	GLN	4.3
1	U	319	PRO	4.3
1	N	224	ASP	4.3
1	E	166	LEU	4.3
1	V	315	PHE	4.3
1	N	187	SER	4.3
1	N	148	GLU	4.3
1	E	327	ASP	4.2
1	M	221	TYR	4.2
1	R	353	ILE	4.2
3	L	122	LYS	4.2
1	V	146	LYS	4.2
1	J	167	VAL	4.2
1	R	284	THR	4.2
3	X	82	LYS	4.1
1	A	167	VAL	4.1
1	U	224	ASP	4.1
1	N	280	ALA	4.1
1	R	362	GLY	4.1
1	J	319	PRO	4.1
1	N	147	PRO	4.1
1	J	313	PHE	4.1
1	M	169	GLU	4.0
1	E	145	PRO	4.0
1	J	138	ILE	4.0
1	J	186	PRO	4.0
1	V	189	TRP	4.0
1	R	214	LEU	4.0
1	R	212	GLU	3.9
1	F	323	ASN	3.9
1	I	170	GLU	3.9
1	B	185	ILE	3.9
1	N	279	ASN	3.9
1	V	181	GLN	3.9
1	R	146	LYS	3.9
1	I	269	ALA	3.9
1	J	168	ASP	3.9
1	V	279	ASN	3.8
1	N	146	LYS	3.8
1	M	257	GLU	3.8
1	R	264	PHE	3.8
3	H	121	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	V	361	THR	3.8
1	I	165	LEU	3.8
1	F	169	GLU	3.8
1	R	217	ILE	3.8
1	E	182	VAL	3.8
1	N	168	ASP	3.8
1	V	206	ARG	3.8
1	R	363	ALA	3.7
1	M	223	THR	3.7
1	F	92	VAL	3.7
1	F	258	LEU	3.7
1	V	209	GLU	3.7
2	K	45	ALA	3.7
2	C	44	GLY	3.7
1	J	144	GLN	3.7
1	R	279	ASN	3.7
1	U	169	GLU	3.7
1	M	225	GLY	3.7
1	U	170	GLU	3.7
1	V	313	PHE	3.7
1	V	191	THR	3.6
3	P	122	LYS	3.6
1	N	323	ASN	3.6
1	V	167	VAL	3.6
1	N	114	GLN	3.6
1	R	315	PHE	3.6
1	V	280	ALA	3.6
1	Q	169	GLU	3.6
1	N	143	GLU	3.6
1	F	256	LYS	3.6
1	Q	170	GLU	3.6
1	Q	181	GLN	3.6
3	X	49	THR	3.6
3	L	49	THR	3.5
1	M	329	GLU	3.5
1	R	165	LEU	3.5
1	R	149	GLN	3.5
1	R	205	ASP	3.5
1	R	191	THR	3.5
1	I	221	TYR	3.5
1	N	164	GLU	3.5
1	N	165	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	R	202	THR	3.5
1	U	328	GLU	3.5
3	T	49	THR	3.5
1	V	225	GLY	3.5
1	N	278	ASP	3.5
1	N	319	PRO	3.5
1	J	316	PHE	3.5
1	U	165	LEU	3.5
1	J	320	LYS	3.4
1	V	221	TYR	3.4
1	N	106	LEU	3.4
1	M	90	LYS	3.4
1	I	146	LYS	3.4
1	B	183	LYS	3.4
2	C	104	GLN	3.4
1	Q	224	ASP	3.4
1	R	218	GLY	3.4
1	J	110	GLU	3.4
1	R	185	ILE	3.4
1	A	333	ASP	3.4
1	A	328	GLU	3.4
1	Q	85	VAL	3.4
1	V	142	GLN	3.4
1	Q	92	VAL	3.3
1	B	184	GLY	3.3
1	E	330	LEU	3.3
1	F	320	LYS	3.3
1	N	239	ALA	3.3
1	F	322	GLN	3.3
1	N	210	VAL	3.3
1	B	240	ASN	3.3
1	N	269	ALA	3.3
2	G	45	ALA	3.3
1	V	213	TYR	3.3
1	F	260	TYR	3.3
1	M	228	GLY	3.3
1	J	140	SER	3.2
1	J	106	LEU	3.2
1	N	185	ILE	3.2
1	V	121	GLU	3.2
1	A	330	LEU	3.2
1	E	170	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	V	282	ASN	3.2
1	R	360	PHE	3.2
2	K	46	GLY	3.2
2	K	43	VAL	3.2
1	I	143	GLU	3.2
1	Q	223	THR	3.2
1	F	255	GLN	3.2
1	R	188	PHE	3.2
1	I	330	LEU	3.2
1	N	241	PRO	3.2
1	V	308	PRO	3.2
1	E	319	PRO	3.2
1	V	114	GLN	3.2
1	M	144	GLN	3.1
1	A	171	GLU	3.1
1	J	258	LEU	3.1
1	J	361	THR	3.1
1	E	261	SER	3.1
1	J	322	GLN	3.1
1	M	165	LEU	3.1
1	I	167	VAL	3.1
1	F	262	GLY	3.1
1	J	281	HIS	3.1
1	E	263	ASP	3.1
1	U	256	LYS	3.1
1	N	235	PHE	3.1
1	M	258	LEU	3.1
1	J	264	PHE	3.1
1	U	223	THR	3.1
1	U	219	LEU	3.1
1	M	210	VAL	3.1
1	U	143	GLU	3.0
1	F	274	ILE	3.0
1	V	217	ILE	3.0
1	V	110	GLU	3.0
1	A	185	ILE	3.0
1	F	357	VAL	3.0
1	R	280	ALA	3.0
1	Q	258	LEU	3.0
1	F	189	TRP	3.0
1	N	162	GLU	3.0
1	R	189	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	185	ILE	3.0
1	F	145	PRO	3.0
2	W	103	ALA	3.0
1	I	268	HIS	3.0
1	N	322	GLN	3.0
1	N	238	SER	3.0
1	F	168	ASP	3.0
1	A	128	TYR	3.0
1	B	274	ILE	3.0
3	X	122	LYS	3.0
1	V	214	LEU	3.0
1	N	221	TYR	3.0
1	B	260	TYR	2.9
1	F	143	GLU	2.9
1	N	189	TRP	2.9
1	R	247	ILE	2.9
1	R	328	GLU	2.9
1	R	329	GLU	2.9
1	A	322	GLN	2.9
1	R	319	PRO	2.9
2	S	43	VAL	2.9
1	B	141	GLY	2.9
1	N	236	ASP	2.9
1	N	315	PHE	2.9
2	W	44	GLY	2.9
1	F	185	ILE	2.9
1	V	184	GLY	2.9
1	N	188	PHE	2.9
1	N	281	HIS	2.9
1	Q	165	LEU	2.9
1	B	110	GLU	2.9
1	B	242	PHE	2.9
1	I	229	PHE	2.9
1	R	313	PHE	2.9
1	V	337	ARG	2.9
1	V	210	VAL	2.9
1	Q	83	GLY	2.9
2	C	46	GLY	2.9
1	Q	91	ASN	2.9
1	N	169	GLU	2.9
1	V	162	GLU	2.9
1	F	219	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	N	167	VAL	2.8
1	B	114	GLN	2.8
1	R	211	LEU	2.8
1	V	312	PHE	2.8
1	B	210	VAL	2.8
1	E	323	ASN	2.8
1	B	139	ILE	2.8
1	U	313	PHE	2.8
1	N	282	ASN	2.8
1	R	235	PHE	2.8
1	Q	327	ASP	2.8
1	E	186	PRO	2.8
1	E	168	ASP	2.8
1	R	206	ARG	2.8
1	E	268	HIS	2.8
1	I	100	LYS	2.8
1	A	268	HIS	2.8
1	B	257	GLU	2.8
1	R	144	GLN	2.8
1	J	211	LEU	2.8
1	N	316	PHE	2.8
1	N	242	PHE	2.8
1	V	316	PHE	2.8
1	N	284	THR	2.8
1	R	277	LYS	2.8
1	R	341	ASP	2.8
1	Q	264	PHE	2.8
1	V	349	LYS	2.8
1	A	183	LYS	2.7
1	N	268	HIS	2.7
1	Q	84	TYR	2.7
1	N	240	ASN	2.7
2	K	44	GLY	2.7
1	E	188	PHE	2.7
1	J	257	GLU	2.7
1	V	212	GLU	2.7
2	K	105	GLY	2.7
1	M	328	GLU	2.7
3	X	83	ARG	2.7
1	N	145	PRO	2.7
1	E	169	GLU	2.7
1	F	276	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
2	K	104	GLN	2.7
1	J	266	TYR	2.7
1	Q	93	LYS	2.7
1	M	168	ASP	2.7
1	M	224	ASP	2.7
1	V	164	GLU	2.7
2	W	101	THR	2.7
1	R	210	VAL	2.7
1	M	94	GLU	2.7
1	V	205	ASP	2.7
3	L	86	ILE	2.7
1	B	243	PHE	2.7
1	M	319	PRO	2.7
1	J	321	ILE	2.7
1	V	314	ASN	2.7
1	N	360	PHE	2.7
1	E	355	ARG	2.7
1	U	91	ASN	2.7
1	N	274	ILE	2.7
1	R	236	ASP	2.6
1	J	100	LYS	2.6
1	V	256	LYS	2.6
1	N	103	GLN	2.6
1	R	246	ASP	2.6
1	R	258	LEU	2.6
1	V	165	LEU	2.6
1	N	121	GLU	2.6
1	V	329	GLU	2.6
1	Q	319	PRO	2.6
1	A	319	PRO	2.6
1	M	142	GLN	2.6
1	A	262	GLY	2.6
1	R	241	PRO	2.6
2	W	43	VAL	2.6
1	V	182	VAL	2.6
1	A	266	TYR	2.6
1	B	273	GLU	2.6
1	Q	263	ASP	2.6
1	J	139	ILE	2.6
1	F	96	LEU	2.6
1	U	201	ASP	2.6
1	J	280	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	252	TYR	2.6
1	J	235	PHE	2.6
1	V	360	PHE	2.6
2	C	49	VAL	2.6
1	J	279	ASN	2.6
1	R	147	PRO	2.6
1	N	215	GLN	2.6
1	Q	221	TYR	2.6
1	M	357	VAL	2.6
1	U	222	LEU	2.6
2	W	104	GLN	2.6
1	A	327	ASP	2.5
1	U	217	ILE	2.5
1	N	209	GLU	2.5
1	Q	225	GLY	2.5
1	U	220	GLU	2.5
1	V	363	ALA	2.5
1	F	272	CYS	2.5
1	R	312	PHE	2.5
3	D	34	TYR	2.5
1	J	241	PRO	2.5
1	I	219	LEU	2.5
1	J	219	LEU	2.5
1	F	184	GLY	2.5
1	A	162	GLU	2.5
1	R	182	VAL	2.5
1	U	269	ALA	2.5
1	U	283	VAL	2.5
1	E	324	GLU	2.5
2	C	103	ALA	2.5
1	N	163	THR	2.5
1	E	333	ASP	2.5
1	J	276	TRP	2.5
1	N	100	LYS	2.5
1	F	140	SER	2.5
1	F	254	TYR	2.5
1	I	225	GLY	2.5
1	J	165	LEU	2.5
1	J	248	LEU	2.5
1	U	171	GLU	2.5
1	Q	226	ARG	2.5
1	E	144	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	V	218	GLY	2.5
1	B	181	GLN	2.5
1	R	145	PRO	2.5
1	V	211	LEU	2.5
1	B	227	PRO	2.5
1	V	113	PHE	2.5
1	B	319	PRO	2.5
1	U	324	GLU	2.5
1	N	118	PHE	2.5
3	P	49	THR	2.5
1	B	323	ASN	2.5
3	H	86	ILE	2.4
1	Q	269	ALA	2.4
1	V	233	PHE	2.4
1	V	204	THR	2.4
1	V	141	GLY	2.4
1	N	358	ASP	2.4
1	V	143	GLU	2.4
1	N	276	TRP	2.4
1	J	142	GLN	2.4
1	R	278	ASP	2.4
1	F	350	ASP	2.4
1	N	181	GLN	2.4
1	J	149	GLN	2.4
1	J	275	SER	2.4
3	T	122	LYS	2.4
1	U	168	ASP	2.4
1	V	358	ASP	2.4
1	E	264	PHE	2.4
1	I	128	TYR	2.4
1	M	121	GLU	2.4
1	U	92	VAL	2.4
1	R	281	HIS	2.4
1	A	182	VAL	2.4
3	H	81	ASN	2.4
1	V	281	HIS	2.4
1	F	358	ASP	2.4
1	N	144	GLN	2.4
1	J	272	CYS	2.4
1	V	236	ASP	2.4
1	E	128	TYR	2.4
1	E	357	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	358	ASP	2.4
1	U	89	PRO	2.3
1	F	100	LYS	2.3
1	M	229	PHE	2.3
1	U	352	LEU	2.3
1	A	210	VAL	2.3
1	I	162	GLU	2.3
1	Q	168	ASP	2.3
1	V	336	GLU	2.3
1	U	181	GLN	2.3
1	V	264	PHE	2.3
1	N	248	LEU	2.3
1	M	114	GLN	2.3
1	E	189	TRP	2.3
1	F	97	LEU	2.3
1	M	128	TYR	2.3
1	J	83	GLY	2.3
1	B	219	LEU	2.3
1	M	116	GLU	2.3
2	C	102	ILE	2.3
1	F	264	PHE	2.3
1	J	284	THR	2.3
1	M	353	ILE	2.3
1	R	117	MET	2.3
1	E	325	ASP	2.3
1	F	165	LEU	2.3
1	R	234	ARG	2.3
1	N	102	LEU	2.3
1	F	321	ILE	2.3
1	N	191	THR	2.3
1	E	224	ASP	2.3
1	V	266	TYR	2.3
1	B	365	LEU	2.3
1	V	106	LEU	2.3
1	A	143	GLU	2.3
1	N	105	GLU	2.3
1	A	228	GLY	2.3
1	N	182	VAL	2.3
1	N	117	MET	2.3
1	V	248	LEU	2.3
1	F	147	PRO	2.3
1	N	308	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	149	GLN	2.3
1	V	202	THR	2.3
1	M	189	TRP	2.3
1	N	212	GLU	2.3
1	Q	219	LEU	2.3
1	R	110	GLU	2.3
1	E	146	LYS	2.3
1	I	353	ILE	2.3
1	M	254	TYR	2.3
1	N	283	VAL	2.3
1	R	266	TYR	2.3
1	R	322	GLN	2.3
1	A	154	GLN	2.3
1	A	221	TYR	2.2
1	E	361	THR	2.2
1	Q	171	GLU	2.2
1	J	98	SER	2.2
1	E	181	GLN	2.2
1	R	263	ASP	2.2
1	R	314	ASN	2.2
1	V	283	VAL	2.2
1	F	248	LEU	2.2
1	U	258	LEU	2.2
2	K	49	VAL	2.2
1	A	263	ASP	2.2
1	I	224	ASP	2.2
1	V	341	ASP	2.2
3	P	48	ASP	2.2
1	N	211	LEU	2.2
1	R	219	LEU	2.2
1	E	260	TYR	2.2
1	R	358	ASP	2.2
1	V	323	ASN	2.2
1	I	217	ILE	2.2
1	Q	89	PRO	2.2
1	E	313	PHE	2.2
1	F	313	PHE	2.2
1	B	100	LYS	2.2
1	N	264	PHE	2.2
1	R	221	TYR	2.2
1	R	228	GLY	2.2
1	V	319	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	117	MET	2.2
1	A	149	GLN	2.2
1	Q	328	GLU	2.2
1	F	273	GLU	2.2
1	V	100	LYS	2.2
1	V	140	SER	2.2
2	C	43	VAL	2.2
1	J	364	ALA	2.2
1	F	166	LEU	2.2
1	F	363	ALA	2.2
1	R	337	ARG	2.2
2	G	43	VAL	2.2
2	K	20	ARG	2.2
3	T	83	ARG	2.2
1	V	274	ILE	2.2
1	F	186	PRO	2.2
2	W	17	ARG	2.2
1	R	106	LEU	2.2
2	C	48	PRO	2.2
2	O	17	ARG	2.1
1	V	223	THR	2.1
1	N	135	ARG	2.1
2	K	40	ALA	2.1
1	R	365	LEU	2.1
1	E	94	GLU	2.1
2	K	47	ALA	2.1
1	J	278	ASP	2.1
1	J	283	VAL	2.1
1	V	227	PRO	2.1
1	J	312	PHE	2.1
3	H	45	VAL	2.1
1	I	169	GLU	2.1
1	N	219	LEU	2.1
1	I	228	GLY	2.1
1	Q	144	GLN	2.1
1	V	254	TYR	2.1
1	V	365	LEU	2.1
1	I	331	GLU	2.1
1	R	268	HIS	2.1
1	V	215	GLN	2.1
1	V	168	ASP	2.1
1	B	226	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	284	THR	2.1
1	R	204	THR	2.1
3	P	80	TYR	2.1
1	M	135	ARG	2.1
1	M	281	HIS	2.1
1	N	142	GLN	2.1
1	N	233	PHE	2.1
1	F	245	ASN	2.1
1	F	217	ILE	2.1
1	V	190	LEU	2.1
1	V	118	PHE	2.1
1	I	226	ARG	2.1
1	V	322	GLN	2.1
1	M	113	PHE	2.1
1	M	117	MET	2.1
1	M	188	PHE	2.1
1	M	259	GLY	2.1
1	N	317	ASP	2.1
1	U	211	LEU	2.1
1	V	222	LEU	2.1
1	U	185	ILE	2.1
1	Q	256	LYS	2.1
1	E	356	ALA	2.1
1	V	139	ILE	2.1
3	P	86	ILE	2.1
1	J	268	HIS	2.1
1	B	238	SER	2.1
1	E	149	GLN	2.1
1	F	93	LYS	2.1
1	R	183	LYS	2.1
1	J	85	VAL	2.1
1	M	145	PRO	2.1
1	R	356	ALA	2.1
1	V	231	LEU	2.0
1	M	151	ALA	2.0
1	Q	261	SER	2.0
1	V	276	TRP	2.0
1	M	91	ASN	2.0
1	B	281	HIS	2.0
1	Q	217	ILE	2.0
1	N	166	LEU	2.0
1	R	114	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	U	225	GLY	2.0
1	U	322	GLN	2.0
1	F	188	PHE	2.0
1	F	243	PHE	2.0
1	M	243	PHE	2.0
1	F	209	GLU	2.0
1	I	171	GLU	2.0
1	R	135	ARG	2.0
1	U	229	PHE	2.0
3	H	90	GLU	2.0
1	F	216	ASP	2.0
1	I	333	ASP	2.0
1	U	274	ILE	2.0
1	R	340	LEU	2.0
1	I	252	TYR	2.0
1	N	263	ASP	2.0
1	Q	114	GLN	2.0
1	A	146	LYS	2.0
1	M	256	LYS	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.