



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:05 AM GMT

PDB ID : 1JYZ
Title : E. COLI (lacZ) BETA-GALACTOSIDASE IN COMPLEX WITH 2-F-LACTOSE. Chains I-P, see REMARK 400.
Authors : Juers, D.H.; McCarter, J.D.; Withers, S.G.; Matthews, B.W.
Deposited on : 2001-09-13
Resolution : 2.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

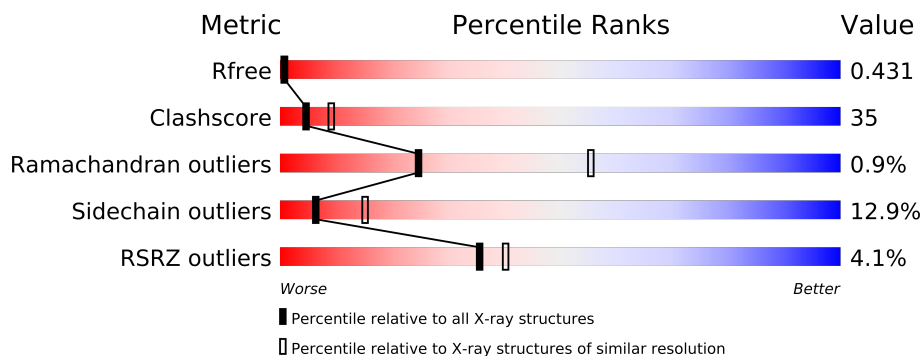
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	I	1023	
1	J	1023	
1	K	1023	
1	L	1023	
1	M	1023	
1	N	1023	
1	O	1023	
1	P	1023	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	2FL	J	2001	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	2FL	K	2001	-	X
2	2FL	L	2001	-	X
2	2FL	M	2001	-	X
2	2FL	N	2001	-	X
2	2FL	O	2001	-	X
2	2FL	P	2001	-	X
3	MG	N	3001	-	X
3	MG	O	3001	-	X
4	NA	J	3102	-	X
4	NA	K	3102	-	X
4	NA	N	3101	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 67264 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Beta-Galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	J	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	K	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	L	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	M	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	N	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	O	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	P	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			

There are 24 discrepancies between the modelled and reference sequences:

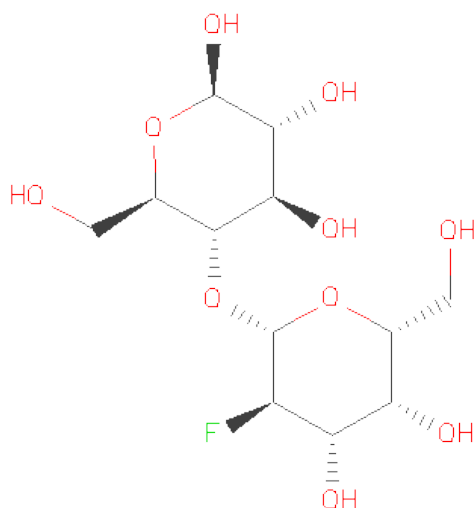
Chain	Residue	Modelled	Actual	Comment	Reference
I	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
I	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
I	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
J	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
J	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
J	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
K	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
K	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
K	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
L	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
L	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
L	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
M	748	CME	CYS	MODIFIED RESIDUE	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
M	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
M	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
N	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
N	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
N	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
O	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
O	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
O	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722
P	748	CME	CYS	MODIFIED RESIDUE	UNP P00722
P	914	CME	CYS	MODIFIED RESIDUE	UNP P00722
P	1021	CME	CYS	MODIFIED RESIDUE	UNP P00722

- Molecule 2 is 2-FLUORO-2-DEOXY-LACTOSE (three-letter code: 2FL) (formula: $C_{12}H_{21}FO_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total	C	F	O	0	0
			23	12	1	10		
2	J	1	Total	C	F	O	0	0
			23	12	1	10		
2	K	1	Total	C	F	O	0	0
			23	12	1	10		
2	L	1	Total	C	F	O	0	0
			23	12	1	10		
2	M	1	Total	C	F	O	0	0
			23	12	1	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	N	1	Total	C	F	O	0	0
			23	12	1	10		
2	O	1	Total	C	F	O	0	0
			23	12	1	10		
2	P	1	Total	C	F	O	0	0
			23	12	1	10		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	2	Total	Mg	0	0
			2	2		
3	J	2	Total	Mg	0	0
			2	2		
3	K	2	Total	Mg	0	0
			2	2		
3	I	2	Total	Mg	0	0
			2	2		
3	N	2	Total	Mg	0	0
			2	2		
3	O	2	Total	Mg	0	0
			2	2		
3	L	2	Total	Mg	0	0
			2	2		
3	M	2	Total	Mg	0	0
			2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	2	Total	Na	0	0
			2	2		
4	J	2	Total	Na	0	0
			2	2		
4	K	2	Total	Na	0	0
			2	2		
4	I	2	Total	Na	0	0
			2	2		
4	N	2	Total	Na	0	0
			2	2		
4	O	2	Total	Na	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	2	Total 2	Na 2	0	0
4	M	2	Total 2	Na 2	0	0

- Molecule 5 is water.

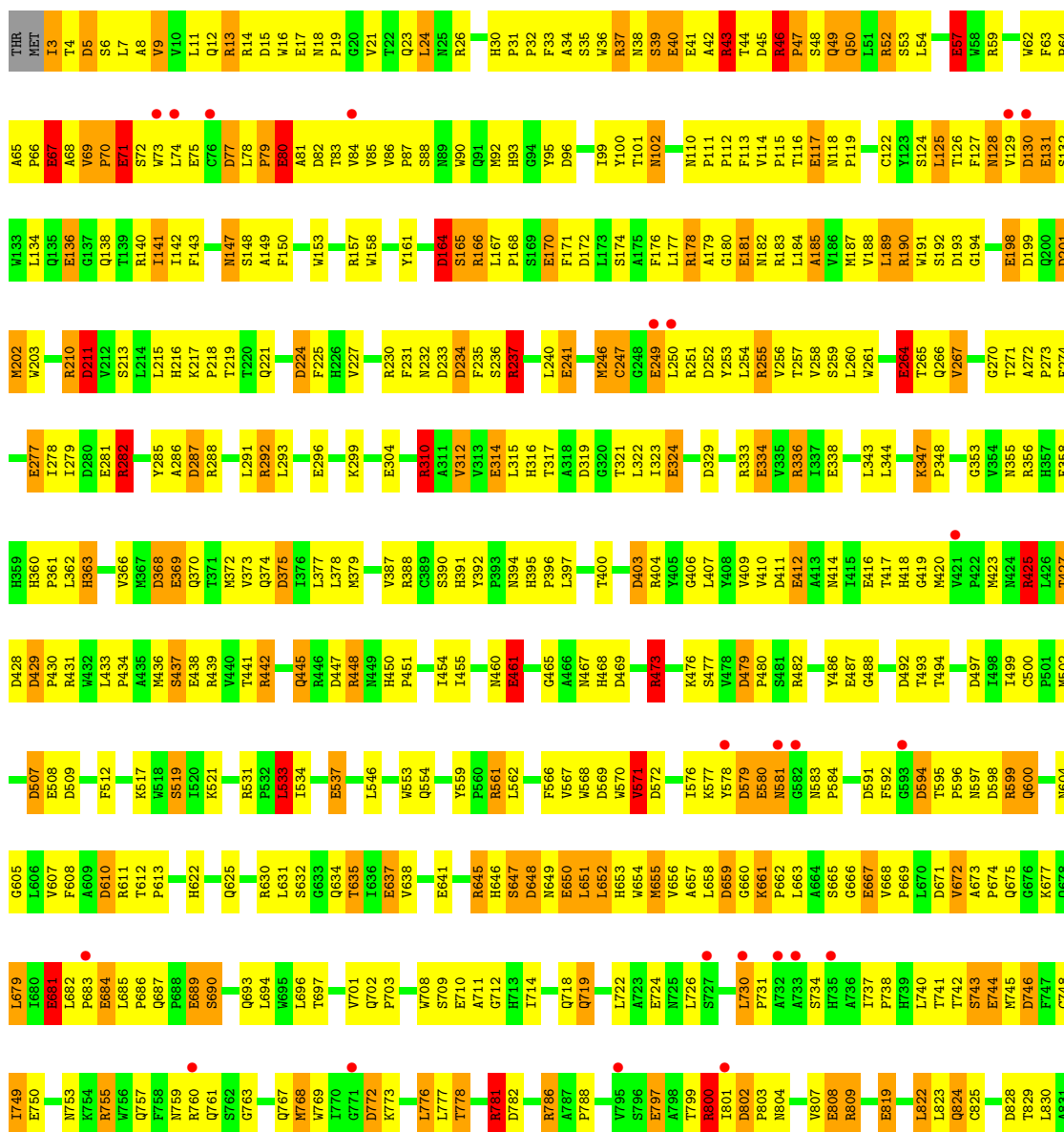
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	162	Total 162	O 162	0	0
5	J	162	Total 162	O 162	0	0
5	K	162	Total 162	O 162	0	0
5	L	162	Total 162	O 162	0	0
5	M	161	Total 161	O 161	0	0
5	N	163	Total 163	O 163	0	0
5	O	161	Total 161	O 161	0	0
5	P	163	Total 163	O 163	0	0

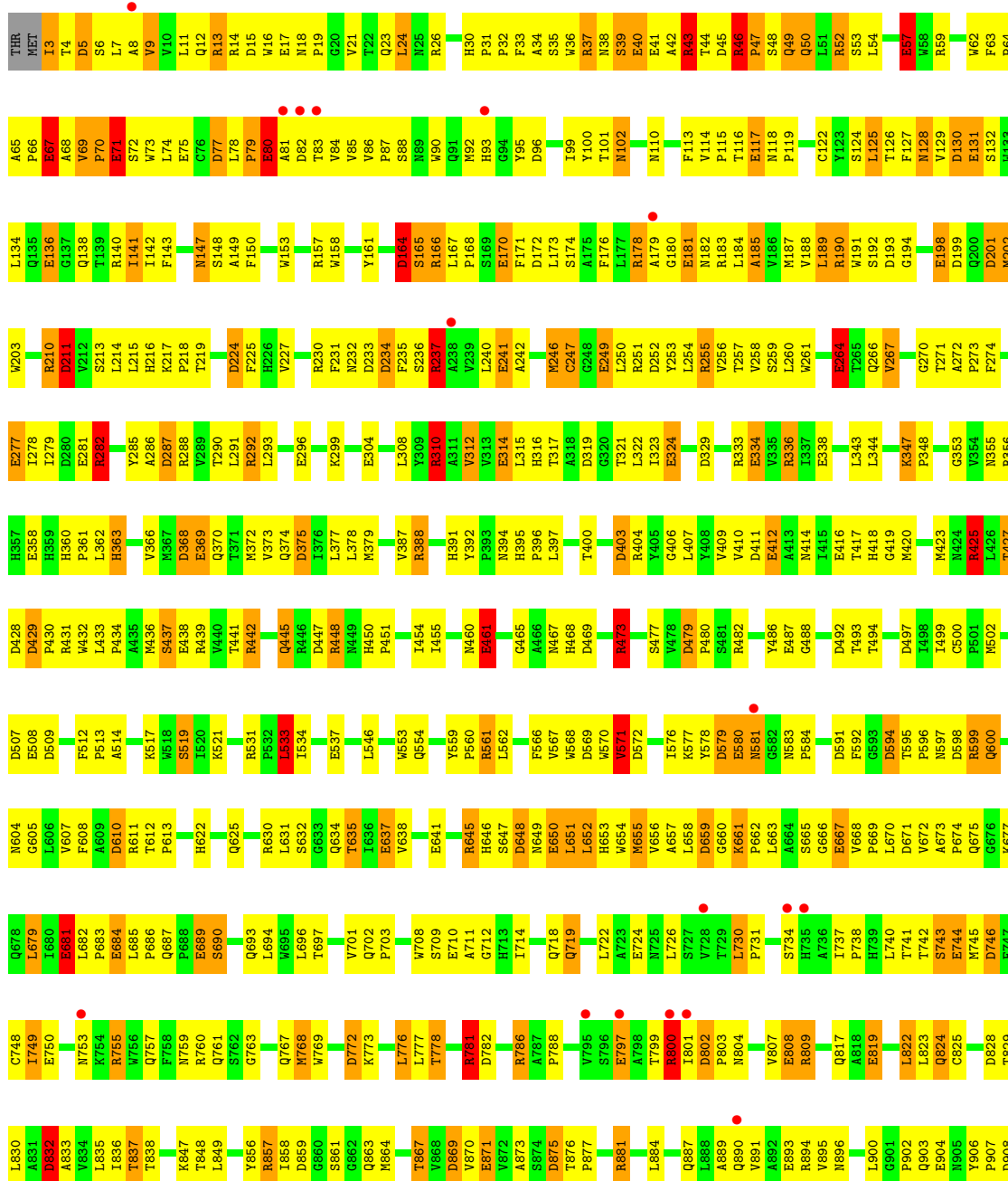
3 Residue-property plots

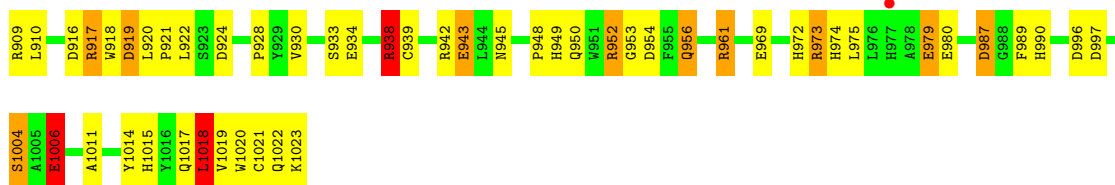
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Chain I: 

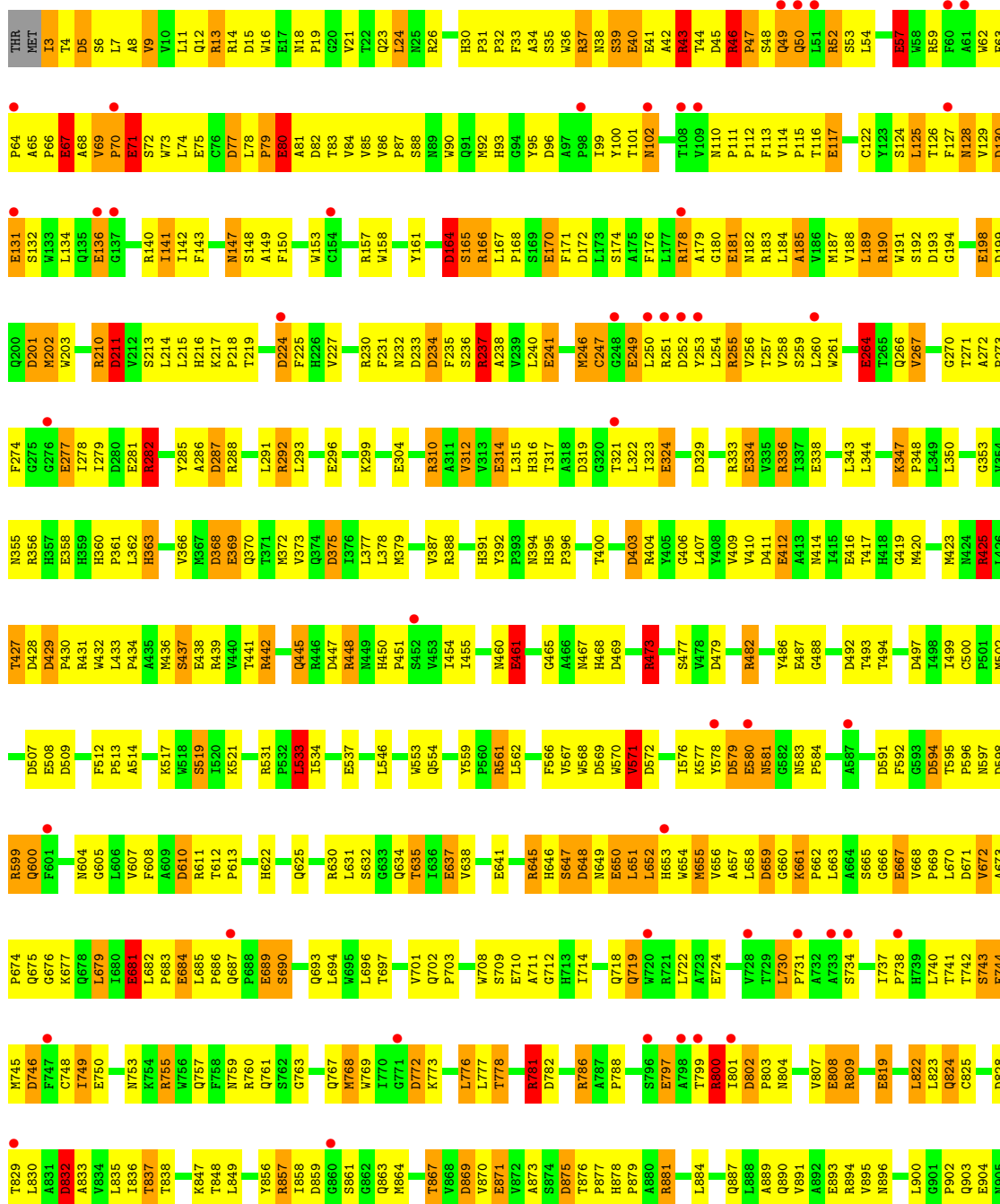






• Molecule 1: Beta-Galactosidase

Chain K:

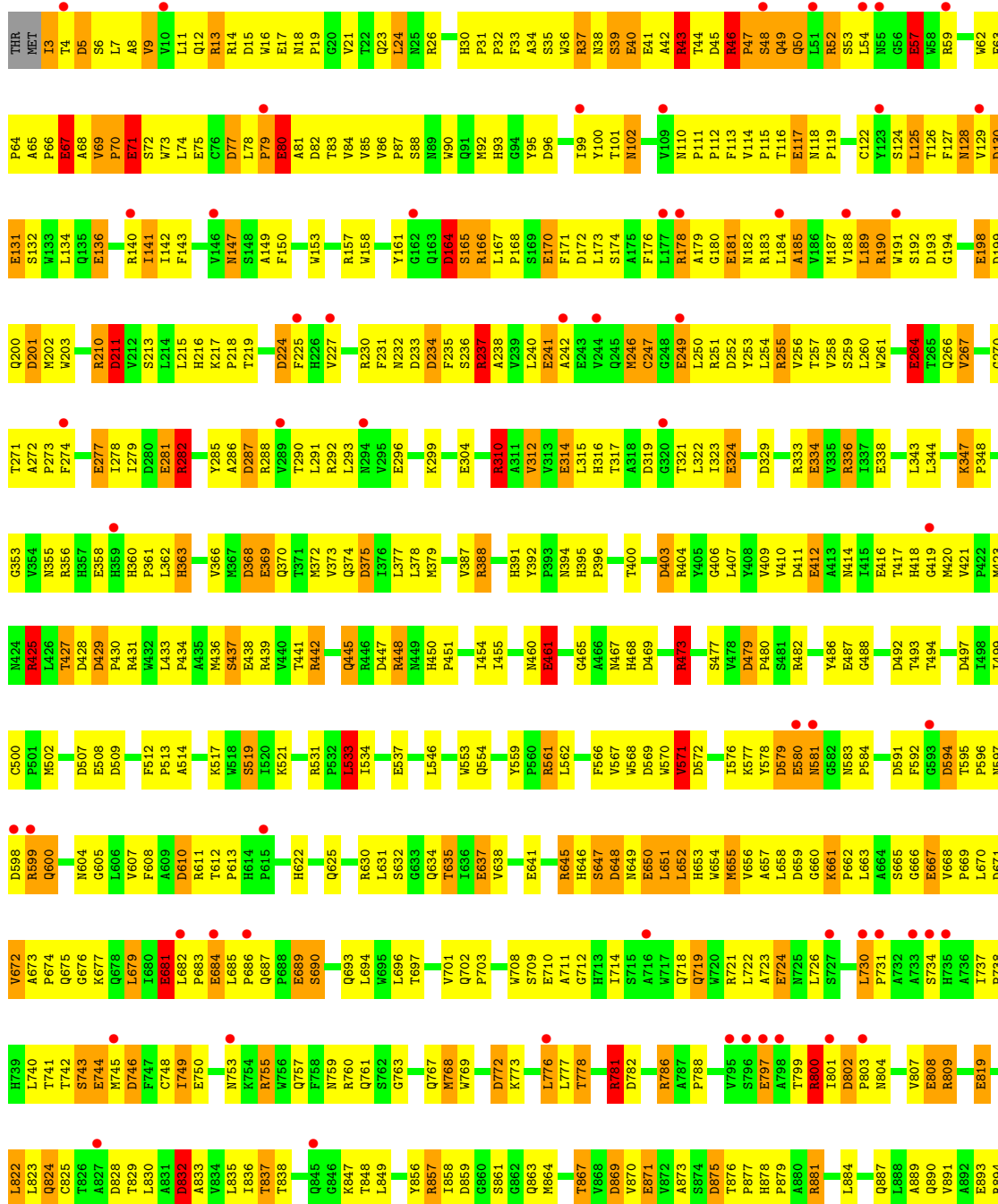






● Molecule 1: Beta-Galactosidase

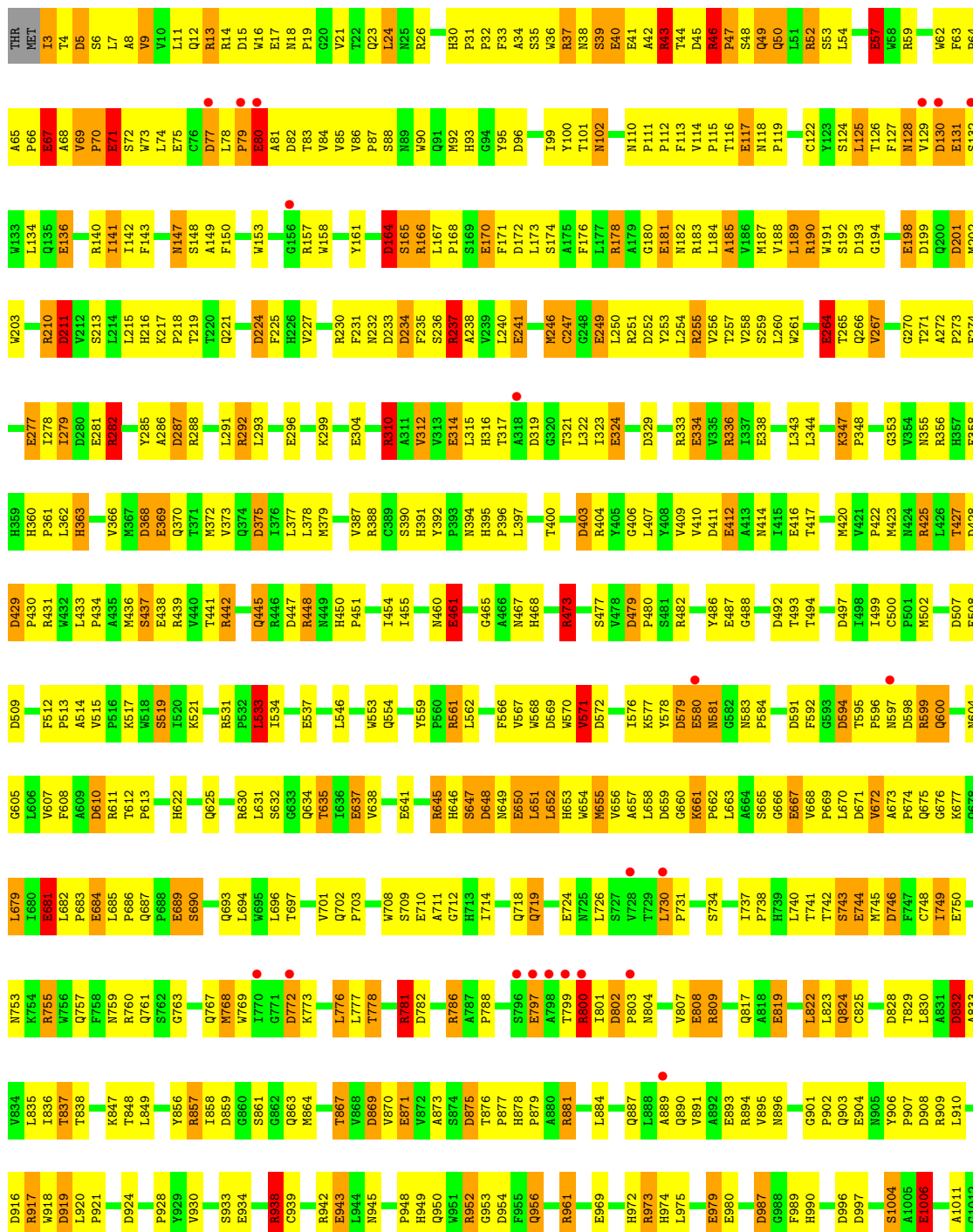
Chain M:





• Molecule 1: Beta-Galactosidase

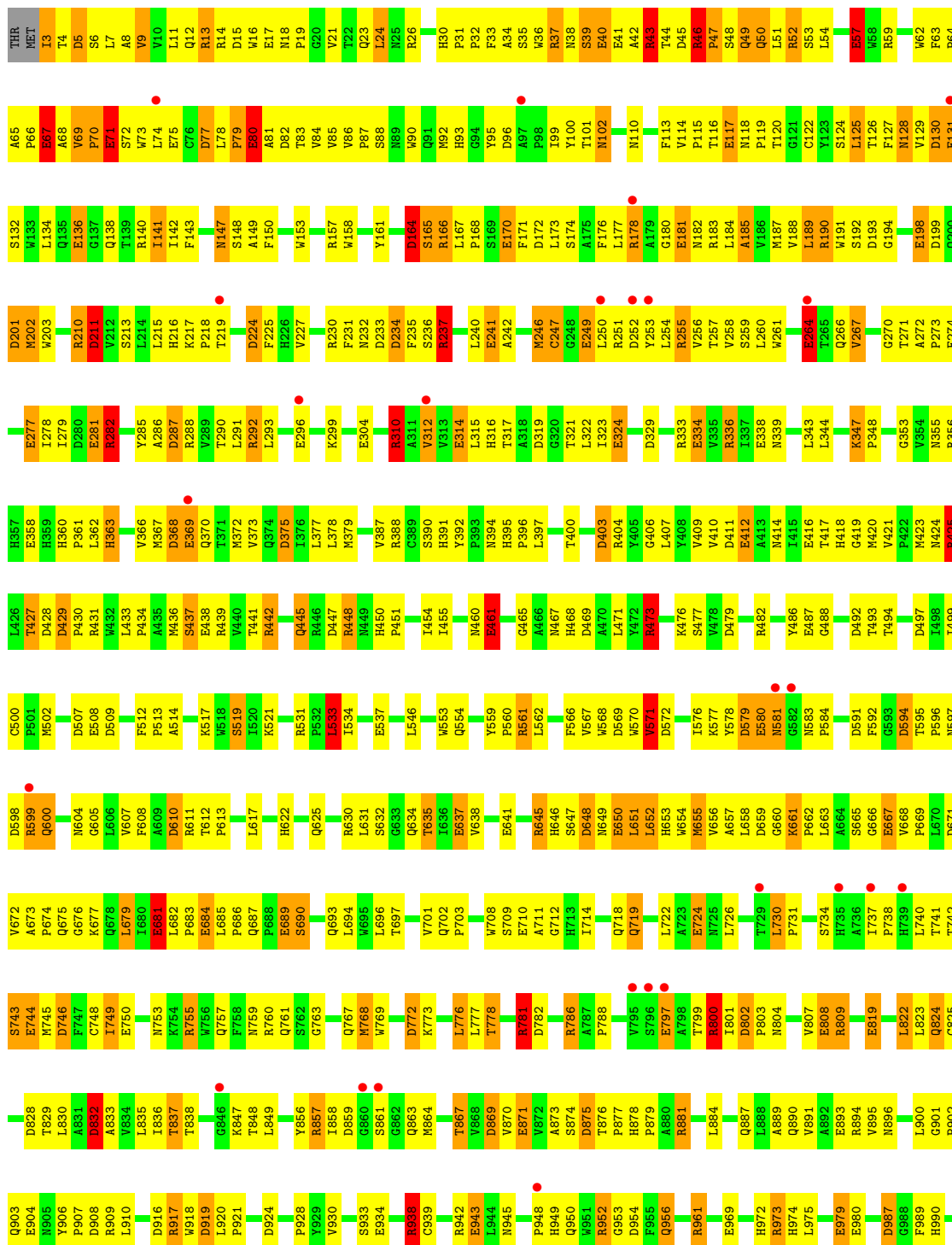
Chain N:



R1013
Y1014
H1015
Q1017
L1018
V1019
W1020
Q1022
K1023

• Molecule 1: Beta-Galactosidase

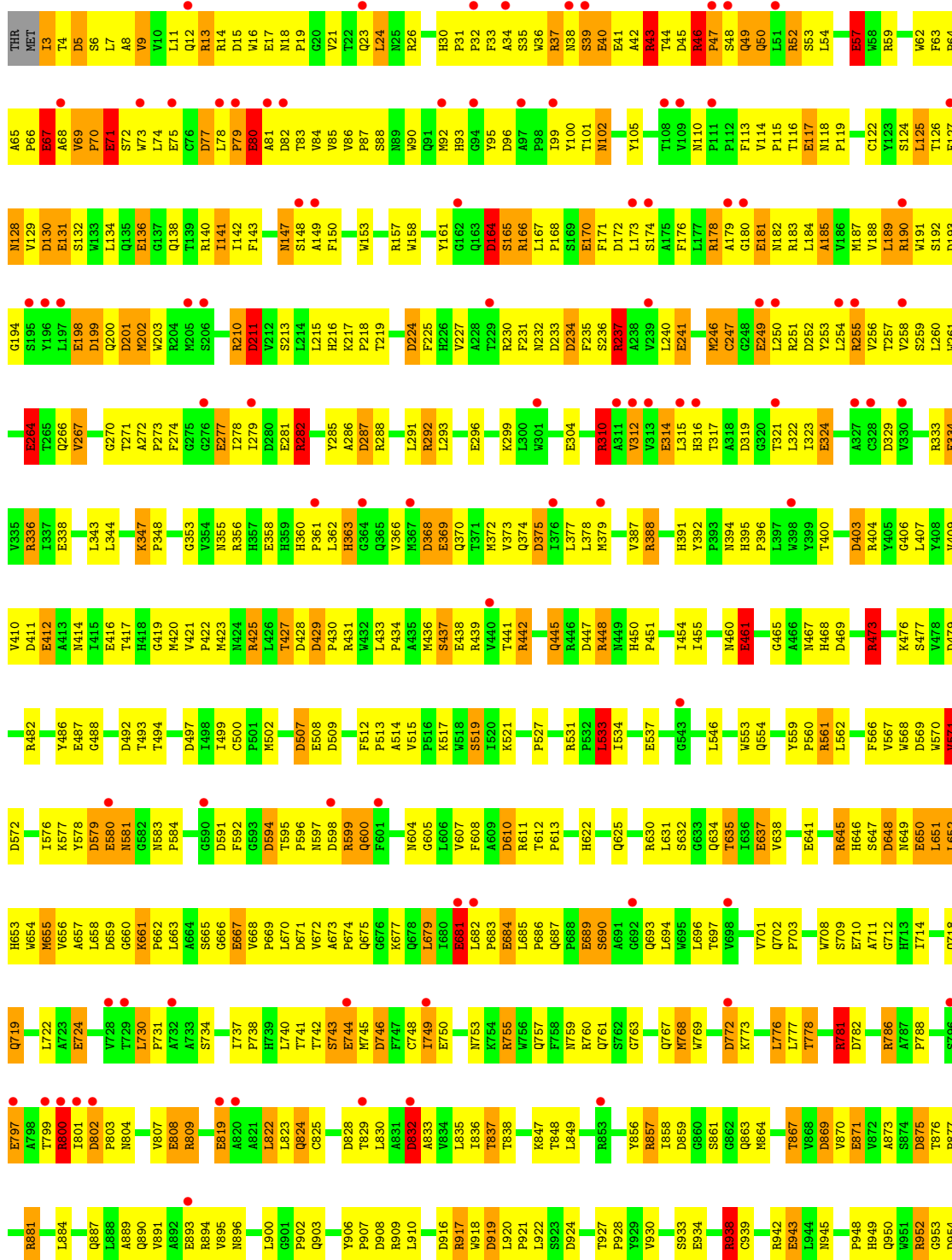
Chain O:





• Molecule 1: Beta-Galactosidase

Chain P:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.60Å 207.30Å 510.30Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 68.54 – 2.50	Depositor EDS
% Data completeness (in resolution range)	66.0 (20.00-2.70) 66.8 (68.54-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.51Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.234 , (Not available) 0.446 , 0.431	Depositor DCC
R_{free} test set	2111 reflections (0.48%)	DCC
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 54.3	EDS
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 523624 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.58	EDS
Total number of atoms	67264	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CME, MG, 2FL

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	I	1.11	56/8439 (0.7%)	1.47	141/11510 (1.2%)
1	J	1.11	56/8439 (0.7%)	1.47	139/11510 (1.2%)
1	K	1.11	55/8439 (0.7%)	1.47	139/11510 (1.2%)
1	L	1.11	56/8439 (0.7%)	1.47	139/11510 (1.2%)
1	M	1.11	56/8439 (0.7%)	1.47	141/11510 (1.2%)
1	N	1.11	56/8439 (0.7%)	1.47	141/11510 (1.2%)
1	O	1.11	56/8439 (0.7%)	1.47	140/11510 (1.2%)
1	P	1.11	55/8439 (0.7%)	1.47	143/11510 (1.2%)
All	All	1.11	446/67512 (0.7%)	1.47	1123/92080 (1.2%)

All (446) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	710	GLU	CD-OE2	7.97	1.34	1.25
1	N	710	GLU	CD-OE2	7.97	1.34	1.25
1	P	710	GLU	CD-OE2	7.94	1.34	1.25
1	K	710	GLU	CD-OE2	7.92	1.34	1.25
1	O	819	GLU	CD-OE2	7.91	1.34	1.25
1	P	744	GLU	CD-OE2	7.88	1.34	1.25
1	M	710	GLU	CD-OE2	7.88	1.34	1.25
1	N	819	GLU	CD-OE2	7.88	1.34	1.25
1	M	819	GLU	CD-OE2	7.87	1.34	1.25
1	I	710	GLU	CD-OE2	7.87	1.34	1.25
1	J	710	GLU	CD-OE2	7.86	1.34	1.25
1	K	744	GLU	CD-OE2	7.85	1.34	1.25
1	I	744	GLU	CD-OE2	7.84	1.34	1.25
1	M	744	GLU	CD-OE2	7.84	1.34	1.25
1	O	710	GLU	CD-OE2	7.84	1.34	1.25
1	J	744	GLU	CD-OE2	7.83	1.34	1.25
1	K	819	GLU	CD-OE2	7.82	1.34	1.25
1	I	819	GLU	CD-OE2	7.82	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	744	GLU	CD-OE2	7.80	1.34	1.25
1	P	819	GLU	CD-OE2	7.80	1.34	1.25
1	J	819	GLU	CD-OE2	7.79	1.34	1.25
1	L	819	GLU	CD-OE2	7.79	1.34	1.25
1	O	744	GLU	CD-OE2	7.77	1.34	1.25
1	N	744	GLU	CD-OE2	7.75	1.34	1.25
1	I	281	GLU	CD-OE2	7.70	1.34	1.25
1	M	281	GLU	CD-OE2	7.70	1.34	1.25
1	L	281	GLU	CD-OE2	7.69	1.34	1.25
1	N	281	GLU	CD-OE2	7.69	1.34	1.25
1	O	281	GLU	CD-OE2	7.69	1.34	1.25
1	K	281	GLU	CD-OE2	7.68	1.34	1.25
1	J	281	GLU	CD-OE2	7.67	1.34	1.25
1	P	281	GLU	CD-OE2	7.67	1.34	1.25
1	J	689	GLU	CD-OE2	7.55	1.33	1.25
1	N	689	GLU	CD-OE2	7.52	1.33	1.25
1	O	689	GLU	CD-OE2	7.51	1.33	1.25
1	P	689	GLU	CD-OE2	7.47	1.33	1.25
1	L	689	GLU	CD-OE2	7.47	1.33	1.25
1	K	689	GLU	CD-OE2	7.46	1.33	1.25
1	M	689	GLU	CD-OE2	7.45	1.33	1.25
1	M	249	GLU	CD-OE2	7.44	1.33	1.25
1	L	249	GLU	CD-OE2	7.42	1.33	1.25
1	N	249	GLU	CD-OE2	7.40	1.33	1.25
1	O	249	GLU	CD-OE2	7.40	1.33	1.25
1	I	689	GLU	CD-OE2	7.39	1.33	1.25
1	I	249	GLU	CD-OE2	7.38	1.33	1.25
1	J	249	GLU	CD-OE2	7.36	1.33	1.25
1	K	249	GLU	CD-OE2	7.33	1.33	1.25
1	P	249	GLU	CD-OE2	7.33	1.33	1.25
1	K	131	GLU	CD-OE2	7.29	1.33	1.25
1	I	131	GLU	CD-OE2	7.24	1.33	1.25
1	J	131	GLU	CD-OE2	7.24	1.33	1.25
1	O	131	GLU	CD-OE2	7.23	1.33	1.25
1	L	75	GLU	CD-OE2	7.23	1.33	1.25
1	M	131	GLU	CD-OE2	7.22	1.33	1.25
1	L	131	GLU	CD-OE2	7.21	1.33	1.25
1	P	131	GLU	CD-OE2	7.20	1.33	1.25
1	N	181	GLU	CD-OE2	7.19	1.33	1.25
1	N	131	GLU	CD-OE2	7.18	1.33	1.25
1	L	181	GLU	CD-OE2	7.17	1.33	1.25
1	I	75	GLU	CD-OE2	7.14	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	181	GLU	CD-OE2	7.14	1.33	1.25
1	K	75	GLU	CD-OE2	7.14	1.33	1.25
1	O	75	GLU	CD-OE2	7.13	1.33	1.25
1	M	181	GLU	CD-OE2	7.12	1.33	1.25
1	J	75	GLU	CD-OE2	7.11	1.33	1.25
1	K	580	GLU	CD-OE2	7.11	1.33	1.25
1	P	580	GLU	CD-OE2	7.11	1.33	1.25
1	K	181	GLU	CD-OE2	7.10	1.33	1.25
1	M	75	GLU	CD-OE2	7.10	1.33	1.25
1	I	580	GLU	CD-OE2	7.10	1.33	1.25
1	P	181	GLU	CD-OE2	7.09	1.33	1.25
1	J	181	GLU	CD-OE2	7.08	1.33	1.25
1	N	75	GLU	CD-OE2	7.08	1.33	1.25
1	M	580	GLU	CD-OE2	7.08	1.33	1.25
1	P	75	GLU	CD-OE2	7.07	1.33	1.25
1	L	580	GLU	CD-OE2	7.07	1.33	1.25
1	O	580	GLU	CD-OE2	7.07	1.33	1.25
1	I	181	GLU	CD-OE2	7.05	1.33	1.25
1	N	580	GLU	CD-OE2	7.05	1.33	1.25
1	J	580	GLU	CD-OE2	7.04	1.33	1.25
1	N	277	GLU	CD-OE2	7.02	1.33	1.25
1	O	277	GLU	CD-OE2	7.01	1.33	1.25
1	P	277	GLU	CD-OE2	6.98	1.33	1.25
1	M	277	GLU	CD-OE2	6.98	1.33	1.25
1	K	277	GLU	CD-OE2	6.95	1.33	1.25
1	J	277	GLU	CD-OE2	6.94	1.33	1.25
1	I	277	GLU	CD-OE2	6.94	1.33	1.25
1	L	277	GLU	CD-OE2	6.94	1.33	1.25
1	O	893	GLU	CD-OE2	6.94	1.33	1.25
1	M	893	GLU	CD-OE2	6.91	1.33	1.25
1	K	893	GLU	CD-OE2	6.90	1.33	1.25
1	P	893	GLU	CD-OE2	6.89	1.33	1.25
1	L	893	GLU	CD-OE2	6.88	1.33	1.25
1	I	893	GLU	CD-OE2	6.88	1.33	1.25
1	N	893	GLU	CD-OE2	6.86	1.33	1.25
1	O	684	GLU	CD-OE2	6.85	1.33	1.25
1	P	684	GLU	CD-OE2	6.83	1.33	1.25
1	K	136	GLU	CD-OE2	6.83	1.33	1.25
1	I	136	GLU	CD-OE2	6.83	1.33	1.25
1	M	684	GLU	CD-OE2	6.82	1.33	1.25
1	J	893	GLU	CD-OE2	6.82	1.33	1.25
1	P	136	GLU	CD-OE2	6.82	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	980	GLU	CD-OE2	6.79	1.33	1.25
1	N	980	GLU	CD-OE2	6.79	1.33	1.25
1	O	136	GLU	CD-OE2	6.79	1.33	1.25
1	I	684	GLU	CD-OE2	6.79	1.33	1.25
1	M	136	GLU	CD-OE2	6.78	1.33	1.25
1	J	684	GLU	CD-OE2	6.78	1.33	1.25
1	N	684	GLU	CD-OE2	6.78	1.33	1.25
1	L	684	GLU	CD-OE2	6.78	1.33	1.25
1	K	684	GLU	CD-OE2	6.77	1.33	1.25
1	M	980	GLU	CD-OE2	6.77	1.33	1.25
1	L	980	GLU	CD-OE2	6.77	1.33	1.25
1	L	136	GLU	CD-OE2	6.76	1.33	1.25
1	N	136	GLU	CD-OE2	6.76	1.33	1.25
1	J	136	GLU	CD-OE2	6.76	1.33	1.25
1	M	681	GLU	CD-OE2	6.76	1.33	1.25
1	K	667	GLU	CD-OE2	6.76	1.33	1.25
1	J	681	GLU	CD-OE2	6.75	1.33	1.25
1	O	681	GLU	CD-OE2	6.75	1.33	1.25
1	L	681	GLU	CD-OE2	6.74	1.33	1.25
1	N	667	GLU	CD-OE2	6.74	1.33	1.25
1	P	808	GLU	CD-OE2	6.74	1.33	1.25
1	J	667	GLU	CD-OE2	6.73	1.33	1.25
1	M	667	GLU	CD-OE2	6.73	1.33	1.25
1	M	808	GLU	CD-OE2	6.73	1.33	1.25
1	K	681	GLU	CD-OE2	6.73	1.33	1.25
1	K	980	GLU	CD-OE2	6.72	1.33	1.25
1	L	667	GLU	CD-OE2	6.72	1.33	1.25
1	J	980	GLU	CD-OE2	6.72	1.33	1.25
1	P	980	GLU	CD-OE2	6.72	1.33	1.25
1	P	667	GLU	CD-OE2	6.71	1.33	1.25
1	K	264	GLU	CD-OE2	6.71	1.33	1.25
1	N	264	GLU	CD-OE2	6.70	1.33	1.25
1	N	681	GLU	CD-OE2	6.70	1.33	1.25
1	I	980	GLU	CD-OE2	6.70	1.33	1.25
1	P	681	GLU	CD-OE2	6.70	1.33	1.25
1	I	681	GLU	CD-OE2	6.69	1.33	1.25
1	O	667	GLU	CD-OE2	6.69	1.33	1.25
1	L	264	GLU	CD-OE2	6.69	1.33	1.25
1	O	808	GLU	CD-OE2	6.69	1.33	1.25
1	I	667	GLU	CD-OE2	6.68	1.33	1.25
1	J	264	GLU	CD-OE2	6.68	1.33	1.25
1	I	808	GLU	CD-OE2	6.67	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	808	GLU	CD-OE2	6.67	1.32	1.25
1	L	808	GLU	CD-OE2	6.66	1.32	1.25
1	N	808	GLU	CD-OE2	6.66	1.32	1.25
1	O	264	GLU	CD-OE2	6.64	1.32	1.25
1	P	264	GLU	CD-OE2	6.64	1.32	1.25
1	J	808	GLU	CD-OE2	6.63	1.32	1.25
1	I	264	GLU	CD-OE2	6.62	1.32	1.25
1	M	264	GLU	CD-OE2	6.62	1.32	1.25
1	I	57	GLU	CD-OE2	6.61	1.32	1.25
1	P	57	GLU	CD-OE2	6.60	1.32	1.25
1	N	57	GLU	CD-OE2	6.60	1.32	1.25
1	M	57	GLU	CD-OE2	6.60	1.32	1.25
1	O	57	GLU	CD-OE2	6.58	1.32	1.25
1	K	57	GLU	CD-OE2	6.57	1.32	1.25
1	K	117	GLU	CD-OE2	6.56	1.32	1.25
1	L	57	GLU	CD-OE2	6.56	1.32	1.25
1	M	117	GLU	CD-OE2	6.54	1.32	1.25
1	J	57	GLU	CD-OE2	6.53	1.32	1.25
1	O	117	GLU	CD-OE2	6.53	1.32	1.25
1	P	117	GLU	CD-OE2	6.51	1.32	1.25
1	J	416	GLU	CD-OE2	6.50	1.32	1.25
1	K	416	GLU	CD-OE2	6.50	1.32	1.25
1	L	416	GLU	CD-OE2	6.50	1.32	1.25
1	I	296	GLU	CD-OE2	6.50	1.32	1.25
1	O	416	GLU	CD-OE2	6.50	1.32	1.25
1	N	416	GLU	CD-OE2	6.50	1.32	1.25
1	N	296	GLU	CD-OE2	6.48	1.32	1.25
1	I	117	GLU	CD-OE2	6.47	1.32	1.25
1	O	296	GLU	CD-OE2	6.47	1.32	1.25
1	J	117	GLU	CD-OE2	6.47	1.32	1.25
1	M	416	GLU	CD-OE2	6.47	1.32	1.25
1	L	198	GLU	CD-OE2	6.46	1.32	1.25
1	P	416	GLU	CD-OE2	6.46	1.32	1.25
1	P	979	GLU	CD-OE2	6.46	1.32	1.25
1	K	198	GLU	CD-OE2	6.46	1.32	1.25
1	P	296	GLU	CD-OE2	6.46	1.32	1.25
1	M	296	GLU	CD-OE2	6.46	1.32	1.25
1	N	117	GLU	CD-OE2	6.45	1.32	1.25
1	J	296	GLU	CD-OE2	6.44	1.32	1.25
1	K	296	GLU	CD-OE2	6.44	1.32	1.25
1	M	198	GLU	CD-OE2	6.44	1.32	1.25
1	I	416	GLU	CD-OE2	6.44	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	117	GLU	CD-OE2	6.44	1.32	1.25
1	L	979	GLU	CD-OE2	6.43	1.32	1.25
1	I	198	GLU	CD-OE2	6.43	1.32	1.25
1	N	979	GLU	CD-OE2	6.43	1.32	1.25
1	J	979	GLU	CD-OE2	6.41	1.32	1.25
1	P	198	GLU	CD-OE2	6.41	1.32	1.25
1	J	198	GLU	CD-OE2	6.41	1.32	1.25
1	L	296	GLU	CD-OE2	6.41	1.32	1.25
1	I	650	GLU	CD-OE2	6.38	1.32	1.25
1	K	650	GLU	CD-OE2	6.38	1.32	1.25
1	O	979	GLU	CD-OE2	6.38	1.32	1.25
1	K	508	GLU	CD-OE2	6.37	1.32	1.25
1	M	979	GLU	CD-OE2	6.37	1.32	1.25
1	O	198	GLU	CD-OE2	6.37	1.32	1.25
1	I	979	GLU	CD-OE2	6.36	1.32	1.25
1	L	650	GLU	CD-OE2	6.36	1.32	1.25
1	N	198	GLU	CD-OE2	6.35	1.32	1.25
1	I	508	GLU	CD-OE2	6.35	1.32	1.25
1	K	979	GLU	CD-OE2	6.34	1.32	1.25
1	N	67	GLU	CD-OE2	6.34	1.32	1.25
1	N	650	GLU	CD-OE2	6.34	1.32	1.25
1	P	650	GLU	CD-OE2	6.33	1.32	1.25
1	J	241	GLU	CD-OE2	6.33	1.32	1.25
1	L	508	GLU	CD-OE2	6.33	1.32	1.25
1	O	241	GLU	CD-OE2	6.33	1.32	1.25
1	K	67	GLU	CD-OE2	6.32	1.32	1.25
1	M	650	GLU	CD-OE2	6.32	1.32	1.25
1	N	508	GLU	CD-OE2	6.32	1.32	1.25
1	K	241	GLU	CD-OE2	6.31	1.32	1.25
1	L	67	GLU	CD-OE2	6.31	1.32	1.25
1	O	67	GLU	CD-OE2	6.31	1.32	1.25
1	O	508	GLU	CD-OE2	6.31	1.32	1.25
1	M	67	GLU	CD-OE2	6.31	1.32	1.25
1	M	508	GLU	CD-OE2	6.31	1.32	1.25
1	J	508	GLU	CD-OE2	6.31	1.32	1.25
1	I	241	GLU	CD-OE2	6.30	1.32	1.25
1	P	508	GLU	CD-OE2	6.30	1.32	1.25
1	N	241	GLU	CD-OE2	6.29	1.32	1.25
1	O	650	GLU	CD-OE2	6.29	1.32	1.25
1	J	67	GLU	CD-OE2	6.29	1.32	1.25
1	I	969	GLU	CD-OE2	6.28	1.32	1.25
1	P	67	GLU	CD-OE2	6.28	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	241	GLU	CD-OE2	6.28	1.32	1.25
1	K	969	GLU	CD-OE2	6.28	1.32	1.25
1	I	67	GLU	CD-OE2	6.27	1.32	1.25
1	P	969	GLU	CD-OE2	6.26	1.32	1.25
1	L	241	GLU	CD-OE2	6.25	1.32	1.25
1	J	650	GLU	CD-OE2	6.25	1.32	1.25
1	O	969	GLU	CD-OE2	6.25	1.32	1.25
1	J	1006	GLU	CD-OE2	6.25	1.32	1.25
1	P	1006	GLU	CD-OE2	6.25	1.32	1.25
1	J	969	GLU	CD-OE2	6.23	1.32	1.25
1	I	1006	GLU	CD-OE2	6.22	1.32	1.25
1	O	1006	GLU	CD-OE2	6.22	1.32	1.25
1	L	1006	GLU	CD-OE2	6.21	1.32	1.25
1	L	969	GLU	CD-OE2	6.19	1.32	1.25
1	M	241	GLU	CD-OE2	6.19	1.32	1.25
1	N	969	GLU	CD-OE2	6.19	1.32	1.25
1	O	934	GLU	CD-OE2	6.18	1.32	1.25
1	K	1006	GLU	CD-OE2	6.17	1.32	1.25
1	M	1006	GLU	CD-OE2	6.16	1.32	1.25
1	P	934	GLU	CD-OE2	6.16	1.32	1.25
1	N	1006	GLU	CD-OE2	6.16	1.32	1.25
1	I	934	GLU	CD-OE2	6.15	1.32	1.25
1	J	934	GLU	CD-OE2	6.14	1.32	1.25
1	M	969	GLU	CD-OE2	6.14	1.32	1.25
1	L	934	GLU	CD-OE2	6.13	1.32	1.25
1	M	934	GLU	CD-OE2	6.13	1.32	1.25
1	K	934	GLU	CD-OE2	6.12	1.32	1.25
1	M	637	GLU	CD-OE2	6.09	1.32	1.25
1	O	637	GLU	CD-OE2	6.09	1.32	1.25
1	N	637	GLU	CD-OE2	6.09	1.32	1.25
1	N	934	GLU	CD-OE2	6.08	1.32	1.25
1	L	797	GLU	CD-OE2	6.07	1.32	1.25
1	K	797	GLU	CD-OE2	6.07	1.32	1.25
1	I	797	GLU	CD-OE2	6.06	1.32	1.25
1	N	797	GLU	CD-OE2	6.05	1.32	1.25
1	P	797	GLU	CD-OE2	6.04	1.32	1.25
1	J	797	GLU	CD-OE2	6.04	1.32	1.25
1	P	637	GLU	CD-OE2	6.04	1.32	1.25
1	M	797	GLU	CD-OE2	6.03	1.32	1.25
1	L	637	GLU	CD-OE2	6.03	1.32	1.25
1	K	637	GLU	CD-OE2	6.02	1.32	1.25
1	I	637	GLU	CD-OE2	6.01	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	637	GLU	CD-OE2	6.00	1.32	1.25
1	O	797	GLU	CD-OE2	5.99	1.32	1.25
1	O	358	GLU	CD-OE2	5.98	1.32	1.25
1	N	358	GLU	CD-OE2	5.96	1.32	1.25
1	N	724	GLU	CD-OE2	5.96	1.32	1.25
1	K	358	GLU	CD-OE2	5.95	1.32	1.25
1	L	724	GLU	CD-OE2	5.95	1.32	1.25
1	K	724	GLU	CD-OE2	5.94	1.32	1.25
1	P	724	GLU	CD-OE2	5.94	1.32	1.25
1	O	724	GLU	CD-OE2	5.94	1.32	1.25
1	J	724	GLU	CD-OE2	5.93	1.32	1.25
1	J	438	GLU	CD-OE2	5.93	1.32	1.25
1	M	358	GLU	CD-OE2	5.93	1.32	1.25
1	P	358	GLU	CD-OE2	5.93	1.32	1.25
1	M	724	GLU	CD-OE2	5.92	1.32	1.25
1	J	358	GLU	CD-OE2	5.91	1.32	1.25
1	O	438	GLU	CD-OE2	5.90	1.32	1.25
1	I	724	GLU	CD-OE2	5.90	1.32	1.25
1	P	438	GLU	CD-OE2	5.89	1.32	1.25
1	L	358	GLU	CD-OE2	5.89	1.32	1.25
1	I	358	GLU	CD-OE2	5.88	1.32	1.25
1	K	438	GLU	CD-OE2	5.87	1.32	1.25
1	I	871	GLU	CD-OE2	5.83	1.32	1.25
1	I	438	GLU	CD-OE2	5.83	1.32	1.25
1	M	438	GLU	CD-OE2	5.83	1.32	1.25
1	K	750	GLU	CD-OE2	5.82	1.32	1.25
1	N	438	GLU	CD-OE2	5.81	1.32	1.25
1	L	487	GLU	CD-OE2	5.79	1.32	1.25
1	L	871	GLU	CD-OE2	5.79	1.32	1.25
1	N	750	GLU	CD-OE2	5.79	1.32	1.25
1	N	487	GLU	CD-OE2	5.78	1.32	1.25
1	L	438	GLU	CD-OE2	5.78	1.32	1.25
1	M	871	GLU	CD-OE2	5.77	1.31	1.25
1	O	871	GLU	CD-OE2	5.77	1.31	1.25
1	I	487	GLU	CD-OE2	5.76	1.31	1.25
1	I	750	GLU	CD-OE2	5.76	1.31	1.25
1	J	750	GLU	CD-OE2	5.75	1.31	1.25
1	K	487	GLU	CD-OE2	5.75	1.31	1.25
1	M	750	GLU	CD-OE2	5.75	1.31	1.25
1	J	871	GLU	CD-OE2	5.75	1.31	1.25
1	O	71	GLU	CD-OE2	5.74	1.31	1.25
1	I	71	GLU	CD-OE2	5.73	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	487	GLU	CD-OE2	5.73	1.31	1.25
1	N	871	GLU	CD-OE2	5.73	1.31	1.25
1	M	487	GLU	CD-OE2	5.72	1.31	1.25
1	J	487	GLU	CD-OE2	5.72	1.31	1.25
1	L	750	GLU	CD-OE2	5.72	1.31	1.25
1	J	71	GLU	CD-OE2	5.72	1.31	1.25
1	P	750	GLU	CD-OE2	5.72	1.31	1.25
1	K	871	GLU	CD-OE2	5.71	1.31	1.25
1	M	369	GLU	CD-OE2	5.71	1.31	1.25
1	L	71	GLU	CD-OE2	5.71	1.31	1.25
1	O	750	GLU	CD-OE2	5.71	1.31	1.25
1	N	369	GLU	CD-OE2	5.71	1.31	1.25
1	P	871	GLU	CD-OE2	5.71	1.31	1.25
1	M	71	GLU	CD-OE2	5.70	1.31	1.25
1	P	487	GLU	CD-OE2	5.69	1.31	1.25
1	K	71	GLU	CD-OE2	5.69	1.31	1.25
1	N	71	GLU	CD-OE2	5.68	1.31	1.25
1	O	369	GLU	CD-OE2	5.68	1.31	1.25
1	P	71	GLU	CD-OE2	5.67	1.31	1.25
1	K	369	GLU	CD-OE2	5.66	1.31	1.25
1	J	369	GLU	CD-OE2	5.65	1.31	1.25
1	M	304	GLU	CD-OE2	5.64	1.31	1.25
1	L	369	GLU	CD-OE2	5.64	1.31	1.25
1	I	369	GLU	CD-OE2	5.64	1.31	1.25
1	J	304	GLU	CD-OE2	5.64	1.31	1.25
1	J	40	GLU	CD-OE2	5.63	1.31	1.25
1	P	304	GLU	CD-OE2	5.63	1.31	1.25
1	P	369	GLU	CD-OE2	5.62	1.31	1.25
1	L	304	GLU	CD-OE2	5.62	1.31	1.25
1	N	304	GLU	CD-OE2	5.62	1.31	1.25
1	N	314	GLU	CD-OE2	5.61	1.31	1.25
1	L	338	GLU	CD-OE2	5.60	1.31	1.25
1	K	304	GLU	CD-OE2	5.60	1.31	1.25
1	K	40	GLU	CD-OE2	5.59	1.31	1.25
1	K	338	GLU	CD-OE2	5.58	1.31	1.25
1	N	338	GLU	CD-OE2	5.58	1.31	1.25
1	O	338	GLU	CD-OE2	5.58	1.31	1.25
1	P	314	GLU	CD-OE2	5.58	1.31	1.25
1	M	40	GLU	CD-OE2	5.58	1.31	1.25
1	I	304	GLU	CD-OE2	5.57	1.31	1.25
1	I	338	GLU	CD-OE2	5.57	1.31	1.25
1	N	334	GLU	CD-OE2	5.57	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	40	GLU	CD-OE2	5.57	1.31	1.25
1	M	338	GLU	CD-OE2	5.57	1.31	1.25
1	O	334	GLU	CD-OE2	5.57	1.31	1.25
1	J	338	GLU	CD-OE2	5.56	1.31	1.25
1	P	338	GLU	CD-OE2	5.56	1.31	1.25
1	I	40	GLU	CD-OE2	5.55	1.31	1.25
1	M	334	GLU	CD-OE2	5.55	1.31	1.25
1	O	304	GLU	CD-OE2	5.55	1.31	1.25
1	I	334	GLU	CD-OE2	5.54	1.31	1.25
1	L	40	GLU	CD-OE2	5.54	1.31	1.25
1	L	314	GLU	CD-OE2	5.54	1.31	1.25
1	K	314	GLU	CD-OE2	5.54	1.31	1.25
1	L	334	GLU	CD-OE2	5.54	1.31	1.25
1	P	40	GLU	CD-OE2	5.54	1.31	1.25
1	N	40	GLU	CD-OE2	5.53	1.31	1.25
1	K	334	GLU	CD-OE2	5.53	1.31	1.25
1	I	314	GLU	CD-OE2	5.51	1.31	1.25
1	J	314	GLU	CD-OE2	5.51	1.31	1.25
1	J	334	GLU	CD-OE2	5.51	1.31	1.25
1	O	170	GLU	CD-OE2	5.49	1.31	1.25
1	M	314	GLU	CD-OE2	5.49	1.31	1.25
1	O	314	GLU	CD-OE2	5.49	1.31	1.25
1	I	170	GLU	CD-OE2	5.48	1.31	1.25
1	P	334	GLU	CD-OE2	5.47	1.31	1.25
1	O	80	GLU	CD-OE2	5.47	1.31	1.25
1	I	80	GLU	CD-OE2	5.45	1.31	1.25
1	J	80	GLU	CD-OE2	5.44	1.31	1.25
1	K	170	GLU	CD-OE2	5.44	1.31	1.25
1	P	324	GLU	CD-OE2	5.44	1.31	1.25
1	J	170	GLU	CD-OE2	5.43	1.31	1.25
1	L	80	GLU	CD-OE2	5.43	1.31	1.25
1	M	80	GLU	CD-OE2	5.43	1.31	1.25
1	K	80	GLU	CD-OE2	5.43	1.31	1.25
1	M	170	GLU	CD-OE2	5.42	1.31	1.25
1	P	80	GLU	CD-OE2	5.41	1.31	1.25
1	K	324	GLU	CD-OE2	5.40	1.31	1.25
1	O	324	GLU	CD-OE2	5.39	1.31	1.25
1	M	324	GLU	CD-OE2	5.37	1.31	1.25
1	L	170	GLU	CD-OE2	5.37	1.31	1.25
1	J	943	GLU	CD-OE2	5.37	1.31	1.25
1	N	324	GLU	CD-OE2	5.36	1.31	1.25
1	N	80	GLU	CD-OE2	5.36	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	41	GLU	CD-OE2	5.36	1.31	1.25
1	O	41	GLU	CD-OE2	5.36	1.31	1.25
1	P	170	GLU	CD-OE2	5.36	1.31	1.25
1	L	943	GLU	CD-OE2	5.36	1.31	1.25
1	L	324	GLU	CD-OE2	5.35	1.31	1.25
1	P	41	GLU	CD-OE2	5.35	1.31	1.25
1	N	170	GLU	CD-OE2	5.35	1.31	1.25
1	K	943	GLU	CD-OE2	5.34	1.31	1.25
1	M	943	GLU	CD-OE2	5.34	1.31	1.25
1	P	943	GLU	CD-OE2	5.34	1.31	1.25
1	I	324	GLU	CD-OE2	5.34	1.31	1.25
1	J	324	GLU	CD-OE2	5.34	1.31	1.25
1	I	943	GLU	CD-OE2	5.33	1.31	1.25
1	O	943	GLU	CD-OE2	5.32	1.31	1.25
1	N	41	GLU	CD-OE2	5.31	1.31	1.25
1	I	41	GLU	CD-OE2	5.31	1.31	1.25
1	N	943	GLU	CD-OE2	5.30	1.31	1.25
1	K	41	GLU	CD-OE2	5.30	1.31	1.25
1	L	41	GLU	CD-OE2	5.29	1.31	1.25
1	M	41	GLU	CD-OE2	5.26	1.31	1.25
1	N	641	GLU	CD-OE2	5.21	1.31	1.25
1	P	641	GLU	CD-OE2	5.16	1.31	1.25
1	K	641	GLU	CD-OE2	5.15	1.31	1.25
1	M	641	GLU	CD-OE2	5.15	1.31	1.25
1	I	412	GLU	CD-OE2	5.13	1.31	1.25
1	J	641	GLU	CD-OE2	5.13	1.31	1.25
1	N	17	GLU	CD-OE2	5.13	1.31	1.25
1	O	641	GLU	CD-OE2	5.11	1.31	1.25
1	M	412	GLU	CD-OE2	5.10	1.31	1.25
1	L	412	GLU	CD-OE2	5.10	1.31	1.25
1	P	412	GLU	CD-OE2	5.09	1.31	1.25
1	I	641	GLU	CD-OE2	5.09	1.31	1.25
1	N	412	GLU	CD-OE2	5.09	1.31	1.25
1	O	17	GLU	CD-OE2	5.09	1.31	1.25
1	I	17	GLU	CD-OE2	5.09	1.31	1.25
1	L	641	GLU	CD-OE2	5.09	1.31	1.25
1	M	904	GLU	CD-OE2	5.08	1.31	1.25
1	L	17	GLU	CD-OE2	5.07	1.31	1.25
1	M	17	GLU	CD-OE2	5.06	1.31	1.25
1	J	412	GLU	CD-OE2	5.06	1.31	1.25
1	K	412	GLU	CD-OE2	5.06	1.31	1.25
1	L	904	GLU	CD-OE2	5.06	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	17	GLU	CD-OE2	5.04	1.31	1.25
1	N	904	GLU	CD-OE2	5.04	1.31	1.25
1	O	412	GLU	CD-OE2	5.04	1.31	1.25
1	J	17	GLU	CD-OE2	5.02	1.31	1.25
1	O	904	GLU	CD-OE2	5.02	1.31	1.25
1	I	537	GLU	CD-OE2	5.02	1.31	1.25
1	K	904	GLU	CD-OE2	5.02	1.31	1.25
1	J	904	GLU	CD-OE2	5.01	1.31	1.25

All (1123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	561	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	M	561	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	I	561	ARG	NE-CZ-NH1	10.71	125.65	120.30
1	N	561	ARG	NE-CZ-NH1	10.65	125.62	120.30
1	K	561	ARG	NE-CZ-NH1	10.61	125.61	120.30
1	O	561	ARG	NE-CZ-NH1	10.61	125.61	120.30
1	P	561	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	L	561	ARG	NE-CZ-NH1	10.57	125.59	120.30
1	K	429	ASP	CB-CG-OD2	-10.18	109.13	118.30
1	L	429	ASP	CB-CG-OD2	-10.17	109.14	118.30
1	P	429	ASP	CB-CG-OD2	-10.14	109.17	118.30
1	I	429	ASP	CB-CG-OD2	-10.13	109.18	118.30
1	O	429	ASP	CB-CG-OD2	-10.13	109.18	118.30
1	J	429	ASP	CB-CG-OD2	-10.13	109.18	118.30
1	M	429	ASP	CB-CG-OD2	-10.12	109.19	118.30
1	N	429	ASP	CB-CG-OD2	-10.09	109.22	118.30
1	J	46	ARG	C-N-CD	-9.74	99.18	120.60
1	M	46	ARG	C-N-CD	-9.74	99.18	120.60
1	I	46	ARG	C-N-CD	-9.73	99.19	120.60
1	N	46	ARG	C-N-CD	-9.73	99.19	120.60
1	O	46	ARG	C-N-CD	-9.73	99.20	120.60
1	P	46	ARG	C-N-CD	-9.72	99.22	120.60
1	L	46	ARG	C-N-CD	-9.72	99.22	120.60
1	K	46	ARG	C-N-CD	-9.71	99.23	120.60
1	I	809	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	P	69	VAL	C-N-CD	-9.06	100.67	120.60
1	M	69	VAL	C-N-CD	-9.06	100.68	120.60
1	N	69	VAL	C-N-CD	-9.05	100.68	120.60
1	I	69	VAL	C-N-CD	-9.05	100.69	120.60
1	K	69	VAL	C-N-CD	-9.05	100.69	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	69	VAL	C-N-CD	-9.04	100.71	120.60
1	O	809	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	J	69	VAL	C-N-CD	-9.04	100.72	120.60
1	O	69	VAL	C-N-CD	-9.03	100.74	120.60
1	M	809	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	J	809	ARG	NE-CZ-NH2	-8.99	115.81	120.30
1	K	809	ARG	NE-CZ-NH2	-8.99	115.81	120.30
1	L	809	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	P	809	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	N	809	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	L	429	ASP	CB-CG-OD1	8.69	126.12	118.30
1	I	429	ASP	CB-CG-OD1	8.66	126.10	118.30
1	K	429	ASP	CB-CG-OD1	8.66	126.09	118.30
1	O	429	ASP	CB-CG-OD1	8.65	126.08	118.30
1	J	429	ASP	CB-CG-OD1	8.65	126.08	118.30
1	P	429	ASP	CB-CG-OD1	8.61	126.05	118.30
1	N	429	ASP	CB-CG-OD1	8.60	126.04	118.30
1	M	429	ASP	CB-CG-OD1	8.58	126.02	118.30
1	J	356	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	K	356	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	P	356	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	O	356	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	N	356	ARG	NE-CZ-NH1	8.43	124.52	120.30
1	M	130	ASP	CB-CG-OD1	8.41	125.87	118.30
1	N	130	ASP	CB-CG-OD1	8.41	125.87	118.30
1	N	329	ASP	CB-CG-OD2	-8.40	110.74	118.30
1	K	130	ASP	CB-CG-OD1	8.40	125.86	118.30
1	I	356	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	O	130	ASP	CB-CG-OD1	8.40	125.86	118.30
1	L	130	ASP	CB-CG-OD1	8.39	125.85	118.30
1	L	329	ASP	CB-CG-OD2	-8.39	110.75	118.30
1	J	329	ASP	CB-CG-OD2	-8.38	110.75	118.30
1	M	356	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	L	356	ARG	NE-CZ-NH1	8.37	124.49	120.30
1	O	329	ASP	CB-CG-OD2	-8.37	110.77	118.30
1	P	130	ASP	CB-CG-OD1	8.37	125.83	118.30
1	J	130	ASP	CB-CG-OD1	8.36	125.82	118.30
1	P	329	ASP	CB-CG-OD2	-8.36	110.78	118.30
1	I	329	ASP	CB-CG-OD2	-8.35	110.79	118.30
1	I	130	ASP	CB-CG-OD1	8.33	125.80	118.30
1	K	329	ASP	CB-CG-OD2	-8.32	110.81	118.30
1	K	43	ARG	NE-CZ-NH1	8.31	124.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	329	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	M	43	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	L	43	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	J	43	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	N	746	ASP	CB-CG-OD2	-8.29	110.84	118.30
1	K	746	ASP	CB-CG-OD2	-8.29	110.84	118.30
1	N	43	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	I	43	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	M	746	ASP	CB-CG-OD2	-8.26	110.87	118.30
1	O	746	ASP	CB-CG-OD2	-8.25	110.87	118.30
1	J	746	ASP	CB-CG-OD2	-8.23	110.89	118.30
1	I	746	ASP	CB-CG-OD2	-8.23	110.89	118.30
1	O	43	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	P	746	ASP	CB-CG-OD2	-8.22	110.90	118.30
1	P	43	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	L	746	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	I	368	ASP	CB-CG-OD2	-8.07	111.03	118.30
1	O	368	ASP	CB-CG-OD2	-8.07	111.04	118.30
1	N	368	ASP	CB-CG-OD2	-8.06	111.04	118.30
1	L	368	ASP	CB-CG-OD2	-8.05	111.05	118.30
1	P	368	ASP	CB-CG-OD2	-8.04	111.07	118.30
1	K	368	ASP	CB-CG-OD2	-8.03	111.08	118.30
1	J	368	ASP	CB-CG-OD2	-8.03	111.08	118.30
1	M	368	ASP	CB-CG-OD2	-7.98	111.12	118.30
1	K	881	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	O	881	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	P	881	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	I	881	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	J	881	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	L	881	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	N	881	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	I	199	ASP	CB-CG-OD2	-7.65	111.42	118.30
1	L	199	ASP	CB-CG-OD2	-7.65	111.42	118.30
1	K	199	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	M	881	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	N	572	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	M	199	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	I	572	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	O	199	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	O	572	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	K	572	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	P	199	ASP	CB-CG-OD2	-7.59	111.46	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	572	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	J	572	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	J	199	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	N	130	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	L	572	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	M	572	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	O	448	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	N	199	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	P	448	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	P	130	ASP	CB-CG-OD2	-7.55	111.51	118.30
1	K	130	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	O	130	ASP	CB-CG-OD2	-7.54	111.52	118.30
1	L	130	ASP	CB-CG-OD2	-7.53	111.53	118.30
1	M	130	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	J	130	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	I	130	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	I	448	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	N	448	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	L	448	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	J	448	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	K	448	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	M	448	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	M	509	ASP	CB-CG-OD2	-7.36	111.67	118.30
1	N	594	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	O	594	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	J	594	ASP	CB-CG-OD2	-7.35	111.68	118.30
1	L	594	ASP	CB-CG-OD2	-7.35	111.68	118.30
1	L	509	ASP	CB-CG-OD2	-7.35	111.69	118.30
1	J	509	ASP	CB-CG-OD2	-7.35	111.69	118.30
1	K	594	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	O	428	ASP	CB-CG-OD2	-7.34	111.70	118.30
1	O	509	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	P	509	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	I	428	ASP	CB-CG-OD2	-7.33	111.71	118.30
1	P	571	VAL	CB-CA-C	-7.32	97.49	111.40
1	N	509	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	I	509	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	I	594	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	L	571	VAL	CB-CA-C	-7.30	97.52	111.40
1	O	571	VAL	CB-CA-C	-7.30	97.53	111.40
1	P	428	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	K	571	VAL	CB-CA-C	-7.30	97.53	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	594	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	N	571	VAL	CB-CA-C	-7.30	97.53	111.40
1	J	571	VAL	CB-CA-C	-7.30	97.54	111.40
1	K	509	ASP	CB-CG-OD2	-7.29	111.73	118.30
1	I	571	VAL	CB-CA-C	-7.29	97.55	111.40
1	M	571	VAL	CB-CA-C	-7.29	97.55	111.40
1	M	428	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	P	594	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	K	428	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	N	428	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	O	492	ASP	CB-CG-OD2	-7.26	111.76	118.30
1	J	428	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	L	428	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	J	492	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	K	492	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	I	492	ASP	CB-CG-OD2	-7.24	111.79	118.30
1	M	492	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	P	492	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	N	492	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	L	492	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	P	645	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	L	645	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	M	645	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	O	645	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	I	645	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	N	645	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	M	687	GLN	C-N-CD	-7.10	104.98	120.60
1	K	687	GLN	C-N-CD	-7.09	105.00	120.60
1	N	687	GLN	C-N-CD	-7.09	105.01	120.60
1	K	645	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	P	687	GLN	C-N-CD	-7.08	105.01	120.60
1	J	687	GLN	C-N-CD	-7.08	105.02	120.60
1	I	687	GLN	C-N-CD	-7.08	105.03	120.60
1	L	687	GLN	C-N-CD	-7.08	105.03	120.60
1	I	859	ASP	CB-CG-OD1	7.07	124.66	118.30
1	O	687	GLN	C-N-CD	-7.06	105.06	120.60
1	L	859	ASP	CB-CG-OD1	7.06	124.65	118.30
1	P	859	ASP	CB-CG-OD1	7.06	124.65	118.30
1	J	859	ASP	CB-CG-OD1	7.05	124.64	118.30
1	J	645	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	L	473	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	O	859	ASP	CB-CG-OD1	7.03	124.62	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	473	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	K	859	ASP	CB-CG-OD1	7.02	124.62	118.30
1	M	859	ASP	CB-CG-OD1	7.01	124.61	118.30
1	K	473	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	N	473	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	I	473	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	N	859	ASP	CB-CG-OD1	6.99	124.59	118.30
1	P	473	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	M	473	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	J	473	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	J	859	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	N	447	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	L	859	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	K	492	ASP	CB-CG-OD1	6.85	124.46	118.30
1	N	659	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	L	447	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	P	859	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	O	287	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	I	287	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	O	447	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	P	659	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	I	234	ASP	CB-CG-OD1	6.82	124.44	118.30
1	M	859	ASP	CB-CG-OD2	-6.82	112.17	118.30
1	J	287	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	M	659	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	O	859	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	L	1004	SER	N-CA-CB	6.81	120.71	110.50
1	P	492	ASP	CB-CG-OD1	6.80	124.42	118.30
1	J	1004	SER	N-CA-CB	6.80	120.70	110.50
1	P	447	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	M	447	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	J	447	ASP	CB-CG-OD2	-6.79	112.18	118.30
1	J	234	ASP	CB-CG-OD1	6.79	124.42	118.30
1	L	492	ASP	CB-CG-OD1	6.79	124.41	118.30
1	O	659	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	M	492	ASP	CB-CG-OD1	6.79	124.41	118.30
1	N	859	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	N	287	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	K	447	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	J	492	ASP	CB-CG-OD1	6.78	124.40	118.30
1	K	1004	SER	N-CA-CB	6.78	120.67	110.50
1	M	234	ASP	CB-CG-OD1	6.78	124.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	492	ASP	CB-CG-OD1	6.78	124.40	118.30
1	I	659	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	L	287	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	P	287	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	I	859	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	K	859	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	I	447	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	K	287	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	P	1004	SER	N-CA-CB	6.77	120.65	110.50
1	N	832	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	I	403	ASP	CB-CG-OD1	6.76	124.39	118.30
1	M	287	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	L	403	ASP	CB-CG-OD1	6.76	124.39	118.30
1	N	201	ASP	CB-CG-OD1	6.76	124.39	118.30
1	O	403	ASP	CB-CG-OD1	6.76	124.39	118.30
1	K	659	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	I	1004	SER	N-CA-CB	6.76	120.64	110.50
1	L	659	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	O	234	ASP	CB-CG-OD1	6.76	124.38	118.30
1	I	492	ASP	CB-CG-OD1	6.76	124.38	118.30
1	N	492	ASP	CB-CG-OD1	6.76	124.38	118.30
1	M	403	ASP	CB-CG-OD1	6.75	124.38	118.30
1	J	101	THR	N-CA-CB	6.75	123.13	110.30
1	N	1004	SER	N-CA-CB	6.75	120.63	110.50
1	L	101	THR	N-CA-CB	6.75	123.13	110.30
1	O	201	ASP	CB-CG-OD1	6.75	124.38	118.30
1	P	234	ASP	CB-CG-OD1	6.75	124.38	118.30
1	J	659	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	K	234	ASP	CB-CG-OD1	6.75	124.38	118.30
1	N	101	THR	N-CA-CB	6.75	123.12	110.30
1	O	1004	SER	N-CA-CB	6.75	120.62	110.50
1	K	101	THR	N-CA-CB	6.74	123.11	110.30
1	L	234	ASP	CB-CG-OD1	6.74	124.37	118.30
1	I	101	THR	N-CA-CB	6.74	123.11	110.30
1	M	832	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	P	403	ASP	CB-CG-OD1	6.74	124.36	118.30
1	P	201	ASP	CB-CG-OD1	6.74	124.36	118.30
1	N	403	ASP	CB-CG-OD1	6.73	124.36	118.30
1	K	832	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	M	101	THR	N-CA-CB	6.73	123.09	110.30
1	P	101	THR	N-CA-CB	6.73	123.09	110.30
1	L	832	ASP	CB-CG-OD2	-6.73	112.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	1004	SER	N-CA-CB	6.73	120.59	110.50
1	O	101	THR	N-CA-CB	6.72	123.08	110.30
1	I	201	ASP	CB-CG-OD1	6.72	124.35	118.30
1	J	832	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	N	234	ASP	CB-CG-OD1	6.72	124.35	118.30
1	J	201	ASP	CB-CG-OD1	6.72	124.35	118.30
1	P	832	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	I	832	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	K	403	ASP	CB-CG-OD1	6.70	124.33	118.30
1	P	648	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	J	403	ASP	CB-CG-OD1	6.69	124.32	118.30
1	K	201	ASP	CB-CG-OD1	6.68	124.31	118.30
1	L	201	ASP	CB-CG-OD1	6.68	124.31	118.30
1	O	832	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	I	648	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	O	648	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	L	648	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	P	786	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	M	201	ASP	CB-CG-OD1	6.65	124.28	118.30
1	J	786	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	K	648	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	M	166	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	M	648	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	J	648	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	N	648	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	J	166	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	J	234	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	I	199	ASP	CB-CG-OD1	6.59	124.23	118.30
1	I	809	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	K	786	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	O	809	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	M	234	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	I	786	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	K	199	ASP	CB-CG-OD1	6.58	124.22	118.30
1	P	234	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	L	166	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	L	234	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	I	234	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	M	809	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	M	786	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	P	199	ASP	CB-CG-OD1	6.56	124.21	118.30
1	O	166	ARG	NE-CZ-NH1	6.56	123.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	199	ASP	CB-CG-OD1	6.55	124.20	118.30
1	J	809	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	N	786	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	O	786	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	N	234	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	K	809	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	L	809	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	O	199	ASP	CB-CG-OD1	6.53	124.18	118.30
1	K	234	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	L	786	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	O	234	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	P	809	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	L	199	ASP	CB-CG-OD1	6.51	124.16	118.30
1	N	201	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	K	166	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	J	199	ASP	CB-CG-OD1	6.51	124.16	118.30
1	N	166	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	N	199	ASP	CB-CG-OD1	6.51	124.16	118.30
1	N	809	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	P	319	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	I	166	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	J	201	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	M	201	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	O	201	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	I	45	ASP	CB-CG-OD1	6.45	124.11	118.30
1	J	319	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	K	201	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	L	319	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	I	201	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	M	769	TRP	CB-CA-C	-6.44	97.52	110.40
1	P	201	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	J	769	TRP	CB-CA-C	-6.44	97.52	110.40
1	L	201	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	P	166	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	P	769	TRP	CB-CA-C	-6.43	97.54	110.40
1	L	769	TRP	CB-CA-C	-6.43	97.54	110.40
1	I	769	TRP	CB-CA-C	-6.43	97.55	110.40
1	K	769	TRP	CB-CA-C	-6.42	97.55	110.40
1	M	319	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	P	252	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	N	769	TRP	CB-CA-C	-6.42	97.55	110.40
1	O	769	TRP	CB-CA-C	-6.42	97.56	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	45	ASP	CB-CG-OD1	6.41	124.07	118.30
1	J	252	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	K	252	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	K	319	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	I	319	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	J	45	ASP	CB-CG-OD1	6.40	124.06	118.30
1	N	319	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	O	96	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	N	252	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	L	96	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	L	45	ASP	CB-CG-OD1	6.39	124.05	118.30
1	L	252	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	K	579	ASP	CB-CG-OD1	6.38	124.05	118.30
1	I	252	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	M	45	ASP	CB-CG-OD1	6.38	124.04	118.30
1	M	252	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	I	172	ASP	CB-CG-OD2	-6.37	112.56	118.30
1	J	579	ASP	CB-CG-OD1	6.37	124.04	118.30
1	N	5	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	N	579	ASP	CB-CG-OD1	6.37	124.03	118.30
1	K	45	ASP	CB-CG-OD1	6.37	124.03	118.30
1	P	5	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	P	579	ASP	CB-CG-OD1	6.37	124.03	118.30
1	O	45	ASP	CB-CG-OD1	6.36	124.03	118.30
1	O	252	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	O	319	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	I	579	ASP	CB-CG-OD1	6.36	124.03	118.30
1	L	598	ASP	CB-CG-OD1	6.36	124.03	118.30
1	O	5	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	N	96	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	O	598	ASP	CB-CG-OD1	6.35	124.02	118.30
1	I	96	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	M	5	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	N	45	ASP	CB-CG-OD1	6.35	124.02	118.30
1	L	579	ASP	CB-CG-OD1	6.35	124.02	118.30
1	P	96	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	O	579	ASP	CB-CG-OD1	6.35	124.01	118.30
1	M	579	ASP	CB-CG-OD1	6.34	124.01	118.30
1	I	5	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	I	553	TRP	CA-CB-CG	-6.34	101.66	113.70
1	O	172	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	J	96	ASP	CB-CG-OD2	-6.34	112.60	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	553	TRP	CA-CB-CG	-6.34	101.66	113.70
1	M	553	TRP	CA-CB-CG	-6.34	101.66	113.70
1	K	553	TRP	CA-CB-CG	-6.34	101.66	113.70
1	L	553	TRP	CA-CB-CG	-6.34	101.66	113.70
1	M	96	ASP	CB-CG-OD2	-6.34	112.60	118.30
1	O	553	TRP	CA-CB-CG	-6.34	101.66	113.70
1	J	598	ASP	CB-CG-OD1	6.33	124.00	118.30
1	K	193	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	K	96	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	N	553	TRP	CA-CB-CG	-6.33	101.68	113.70
1	P	193	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	P	598	ASP	CB-CG-OD1	6.33	123.99	118.30
1	N	193	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	P	553	TRP	CA-CB-CG	-6.32	101.69	113.70
1	K	598	ASP	CB-CG-OD1	6.32	123.98	118.30
1	L	46	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	J	5	ASP	CB-CG-OD2	-6.32	112.62	118.30
1	L	5	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	J	875	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	P	172	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	K	172	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	O	193	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	I	1018	LEU	N-CA-CB	-6.30	97.79	110.40
1	J	1018	LEU	N-CA-CB	-6.30	97.81	110.40
1	L	172	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	L	193	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	I	598	ASP	CB-CG-OD1	6.29	123.96	118.30
1	J	193	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	K	1018	LEU	N-CA-CB	-6.29	97.82	110.40
1	N	1018	LEU	N-CA-CB	-6.29	97.82	110.40
1	P	1018	LEU	N-CA-CB	-6.29	97.82	110.40
1	O	1018	LEU	N-CA-CB	-6.29	97.83	110.40
1	K	5	ASP	CB-CG-OD2	-6.28	112.64	118.30
1	M	1018	LEU	N-CA-CB	-6.28	97.83	110.40
1	L	1018	LEU	N-CA-CB	-6.28	97.84	110.40
1	M	598	ASP	CB-CG-OD1	6.28	123.95	118.30
1	I	875	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	J	172	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	N	172	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	O	875	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	N	598	ASP	CB-CG-OD1	6.28	123.95	118.30
1	M	193	ASP	CB-CG-OD2	-6.27	112.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	909	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	M	875	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	K	46	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	M	172	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	O	909	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	N	46	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	I	193	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	I	46	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	J	45	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	L	875	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	P	875	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	K	875	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	I	45	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	K	909	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	N	875	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	N	909	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	P	45	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	P	46	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	O	45	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	M	45	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	M	909	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	L	45	ASP	CB-CG-OD2	-6.21	112.72	118.30
1	O	579	ASP	CB-CG-OD2	-6.21	112.72	118.30
1	O	46	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	I	210	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	M	210	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	N	210	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	I	579	ASP	CB-CG-OD2	-6.18	112.73	118.30
1	L	579	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	L	909	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	M	579	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	N	45	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	J	579	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	N	193	ASP	CB-CG-OD1	6.17	123.86	118.30
1	K	579	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	N	579	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	K	45	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	M	46	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	O	210	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	K	52	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	P	356	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	J	210	ARG	NE-CZ-NH1	6.16	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	46	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	L	210	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	P	579	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	P	403	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	N	996	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	I	909	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	J	996	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	O	997	ASP	CB-CG-OD2	-6.13	112.79	118.30
1	O	403	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	I	996	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	K	356	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	P	193	ASP	CB-CG-OD1	6.12	123.81	118.30
1	J	403	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	N	403	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	I	52	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	P	996	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	I	193	ASP	CB-CG-OD1	6.11	123.80	118.30
1	J	916	ASP	CB-CG-OD1	6.11	123.80	118.30
1	K	996	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	O	193	ASP	CB-CG-OD1	6.11	123.80	118.30
1	J	193	ASP	CB-CG-OD1	6.10	123.79	118.30
1	M	996	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	L	193	ASP	CB-CG-OD1	6.10	123.79	118.30
1	M	916	ASP	CB-CG-OD1	6.10	123.79	118.30
1	P	997	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	L	52	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	P	210	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	I	403	ASP	CB-CG-OD2	-6.09	112.81	118.30
1	K	997	ASP	CB-CG-OD2	-6.09	112.81	118.30
1	M	403	ASP	CB-CG-OD2	-6.09	112.81	118.30
1	M	997	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	O	52	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	L	916	ASP	CB-CG-OD1	6.09	123.78	118.30
1	P	52	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	J	909	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	L	403	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	O	916	ASP	CB-CG-OD1	6.08	123.78	118.30
1	L	997	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	O	233	ASP	CB-CG-OD1	6.08	123.77	118.30
1	K	193	ASP	CB-CG-OD1	6.08	123.77	118.30
1	J	997	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	M	52	ARG	NE-CZ-NH1	6.08	123.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	916	ASP	CB-CG-OD1	6.08	123.77	118.30
1	O	356	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	P	916	ASP	CB-CG-OD1	6.08	123.77	118.30
1	K	403	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	I	645	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	P	645	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	L	996	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	M	193	ASP	CB-CG-OD1	6.06	123.75	118.30
1	N	233	ASP	CB-CG-OD1	6.06	123.75	118.30
1	L	233	ASP	CB-CG-OD1	6.06	123.75	118.30
1	N	997	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	K	210	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	J	52	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	L	356	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	N	356	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	I	916	ASP	CB-CG-OD1	6.04	123.74	118.30
1	K	363	HIS	CA-CB-CG	-6.04	103.33	113.60
1	O	996	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	I	233	ASP	CB-CG-OD1	6.04	123.73	118.30
1	L	363	HIS	CA-CB-CG	-6.03	103.34	113.60
1	J	363	HIS	CA-CB-CG	-6.03	103.35	113.60
1	N	52	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	O	363	HIS	CA-CB-CG	-6.03	103.35	113.60
1	M	356	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	O	645	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	I	997	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	J	233	ASP	CB-CG-OD1	6.02	123.72	118.30
1	L	598	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	K	233	ASP	CB-CG-OD1	6.02	123.72	118.30
1	M	363	HIS	CA-CB-CG	-6.02	103.37	113.60
1	J	356	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	P	363	HIS	CA-CB-CG	-6.01	103.38	113.60
1	M	233	ASP	CB-CG-OD1	6.01	123.71	118.30
1	L	645	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	K	916	ASP	CB-CG-OD1	6.01	123.71	118.30
1	P	233	ASP	CB-CG-OD1	6.01	123.71	118.30
1	I	363	HIS	CA-CB-CG	-6.00	103.40	113.60
1	N	363	HIS	CA-CB-CG	-6.00	103.40	113.60
1	M	645	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	M	598	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	N	645	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	O	594	ASP	CB-CG-OD1	5.98	123.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	375	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	J	594	ASP	CB-CG-OD1	5.98	123.68	118.30
1	P	598	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	I	375	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	J	598	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	I	356	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	N	594	ASP	CB-CG-OD1	5.96	123.67	118.30
1	L	594	ASP	CB-CG-OD1	5.96	123.67	118.30
1	I	598	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	M	594	ASP	CB-CG-OD1	5.96	123.66	118.30
1	N	598	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	I	594	ASP	CB-CG-OD1	5.96	123.66	118.30
1	O	598	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	K	594	ASP	CB-CG-OD1	5.95	123.65	118.30
1	I	233	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	K	645	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	P	375	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	O	375	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	K	598	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	J	375	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	K	802	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	J	645	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	P	594	ASP	CB-CG-OD1	5.92	123.62	118.30
1	J	802	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	M	375	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	L	908	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	N	375	ASP	CB-CG-OD2	-5.89	112.99	118.30
1	P	802	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	K	233	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	O	802	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	K	375	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	L	233	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	N	233	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	O	233	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	I	802	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	P	233	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	J	908	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	L	802	ASP	CB-CG-OD2	-5.86	113.02	118.30
1	O	908	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	J	233	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	M	802	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	M	908	ASP	CB-CG-OD2	-5.85	113.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	908	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	K	908	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	M	233	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	N	802	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	I	648	ASP	CB-CG-OD1	5.83	123.54	118.30
1	N	908	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	O	648	ASP	CB-CG-OD1	5.82	123.54	118.30
1	I	908	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	P	648	ASP	CB-CG-OD1	5.82	123.53	118.30
1	J	648	ASP	CB-CG-OD1	5.81	123.53	118.30
1	J	869	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	N	648	ASP	CB-CG-OD1	5.80	123.52	118.30
1	N	973	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	M	648	ASP	CB-CG-OD1	5.79	123.52	118.30
1	M	869	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	O	973	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	L	828	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	P	828	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	L	96	ASP	CB-CG-OD1	5.79	123.51	118.30
1	P	164	ASP	CB-CG-OD1	5.79	123.51	118.30
1	J	533	LEU	CB-CA-C	5.79	121.19	110.20
1	O	96	ASP	CB-CG-OD1	5.79	123.51	118.30
1	L	164	ASP	CB-CG-OD1	5.78	123.51	118.30
1	M	781	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	K	164	ASP	CB-CG-OD1	5.78	123.50	118.30
1	J	610	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	K	648	ASP	CB-CG-OD1	5.78	123.50	118.30
1	K	869	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	I	781	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	K	828	ASP	CB-CG-OD2	-5.77	113.10	118.30
1	L	648	ASP	CB-CG-OD1	5.77	123.50	118.30
1	O	533	LEU	CB-CA-C	5.77	121.17	110.20
1	I	533	LEU	CB-CA-C	5.77	121.16	110.20
1	K	533	LEU	CB-CA-C	5.77	121.16	110.20
1	M	908	ASP	CB-CG-OD1	5.77	123.49	118.30
1	M	533	LEU	CB-CA-C	5.77	121.16	110.20
1	M	610	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	N	533	LEU	CB-CA-C	5.77	121.16	110.20
1	O	781	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	I	828	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	P	533	LEU	CB-CA-C	5.76	121.15	110.20
1	O	610	ASP	CB-CG-OD2	-5.76	113.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	533	LEU	CB-CA-C	5.76	121.15	110.20
1	O	908	ASP	CB-CG-OD1	5.76	123.48	118.30
1	P	610	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	P	869	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	L	908	ASP	CB-CG-OD1	5.76	123.48	118.30
1	N	96	ASP	CB-CG-OD1	5.76	123.48	118.30
1	I	973	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	K	781	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	M	973	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	O	659	ASP	CB-CG-OD1	5.76	123.48	118.30
1	L	869	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	J	96	ASP	CB-CG-OD1	5.75	123.48	118.30
1	O	828	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	P	425	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	M	164	ASP	CB-CG-OD1	5.75	123.47	118.30
1	N	869	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	N	828	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	P	287	ASP	CB-CG-OD1	5.75	123.47	118.30
1	L	610	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	O	287	ASP	CB-CG-OD1	5.74	123.47	118.30
1	I	869	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	K	610	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	M	96	ASP	CB-CG-OD1	5.74	123.47	118.30
1	O	425	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	J	287	ASP	CB-CG-OD1	5.74	123.47	118.30
1	K	908	ASP	CB-CG-OD1	5.74	123.46	118.30
1	M	828	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	N	164	ASP	CB-CG-OD1	5.74	123.46	118.30
1	J	828	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	M	659	ASP	CB-CG-OD1	5.74	123.46	118.30
1	P	96	ASP	CB-CG-OD1	5.74	123.46	118.30
1	I	287	ASP	CB-CG-OD1	5.73	123.46	118.30
1	K	96	ASP	CB-CG-OD1	5.73	123.46	118.30
1	M	425	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	J	425	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	L	329	ASP	CB-CG-OD1	5.73	123.45	118.30
1	N	610	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	N	671	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	J	164	ASP	CB-CG-OD1	5.72	123.45	118.30
1	J	973	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	K	287	ASP	CB-CG-OD1	5.72	123.45	118.30
1	L	973	ARG	NE-CZ-NH1	5.72	123.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	671	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	P	908	ASP	CB-CG-OD1	5.72	123.45	118.30
1	N	425	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	P	659	ASP	CB-CG-OD1	5.72	123.44	118.30
1	I	96	ASP	CB-CG-OD1	5.71	123.44	118.30
1	N	659	ASP	CB-CG-OD1	5.71	123.44	118.30
1	L	671	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	O	164	ASP	CB-CG-OD1	5.71	123.44	118.30
1	I	164	ASP	CB-CG-OD1	5.71	123.44	118.30
1	K	973	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	O	869	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	I	659	ASP	CB-CG-OD1	5.71	123.44	118.30
1	I	908	ASP	CB-CG-OD1	5.71	123.44	118.30
1	K	671	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	L	781	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	L	425	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	I	610	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	L	659	ASP	CB-CG-OD1	5.70	123.43	118.30
1	P	781	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	M	287	ASP	CB-CG-OD1	5.70	123.42	118.30
1	J	781	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	P	973	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	N	287	ASP	CB-CG-OD1	5.69	123.42	118.30
1	L	287	ASP	CB-CG-OD1	5.69	123.42	118.30
1	M	671	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	J	659	ASP	CB-CG-OD1	5.68	123.42	118.30
1	K	425	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	J	908	ASP	CB-CG-OD1	5.68	123.41	118.30
1	I	679	LEU	CA-CB-CG	-5.68	102.24	115.30
1	P	679	LEU	CA-CB-CG	-5.67	102.25	115.30
1	I	425	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	J	329	ASP	CB-CG-OD1	5.67	123.41	118.30
1	I	671	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	L	679	LEU	CA-CB-CG	-5.67	102.25	115.30
1	N	908	ASP	CB-CG-OD1	5.67	123.41	118.30
1	N	781	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	K	659	ASP	CB-CG-OD1	5.67	123.40	118.30
1	N	679	LEU	CA-CB-CG	-5.67	102.27	115.30
1	N	329	ASP	CB-CG-OD1	5.66	123.40	118.30
1	P	671	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	O	679	LEU	CA-CB-CG	-5.66	102.29	115.30
1	J	679	LEU	CA-CB-CG	-5.66	102.29	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	679	LEU	CA-CB-CG	-5.66	102.29	115.30
1	M	679	LEU	CA-CB-CG	-5.66	102.29	115.30
1	P	329	ASP	CB-CG-OD1	5.66	123.39	118.30
1	P	954	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	I	329	ASP	CB-CG-OD1	5.65	123.39	118.30
1	J	671	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	L	954	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	O	329	ASP	CB-CG-OD1	5.64	123.38	118.30
1	M	211	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	O	211	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	J	497	ASP	CB-CG-OD2	-5.63	113.24	118.30
1	P	497	ASP	CB-CG-OD2	-5.63	113.24	118.30
1	M	329	ASP	CB-CG-OD1	5.62	123.36	118.30
1	K	954	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	J	211	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	K	497	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	K	828	ASP	CB-CG-OD1	5.60	123.34	118.30
1	O	954	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	N	497	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	L	211	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	P	211	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	N	954	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	J	954	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	N	211	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	K	329	ASP	CB-CG-OD1	5.58	123.32	118.30
1	L	828	ASP	CB-CG-OD1	5.58	123.32	118.30
1	M	497	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	I	954	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	I	211	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	L	375	ASP	CB-CG-OD1	5.57	123.31	118.30
1	O	800	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	K	211	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	O	497	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	L	497	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	I	828	ASP	CB-CG-OD1	5.55	123.30	118.30
1	K	43	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	O	828	ASP	CB-CG-OD1	5.55	123.29	118.30
1	L	952	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	P	375	ASP	CB-CG-OD1	5.55	123.29	118.30
1	I	497	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	M	375	ASP	CB-CG-OD1	5.54	123.29	118.30
1	P	952	ARG	NE-CZ-NH2	-5.54	117.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	954	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	J	952	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	M	952	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	N	375	ASP	CB-CG-OD1	5.53	123.28	118.30
1	M	43	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	O	952	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	P	828	ASP	CB-CG-OD1	5.53	123.27	118.30
1	O	375	ASP	CB-CG-OD1	5.52	123.27	118.30
1	M	828	ASP	CB-CG-OD1	5.52	123.27	118.30
1	J	828	ASP	CB-CG-OD1	5.51	123.26	118.30
1	I	375	ASP	CB-CG-OD1	5.50	123.25	118.30
1	J	800	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	K	800	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	N	43	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	M	987	ASP	CB-CG-OD1	5.50	123.25	118.30
1	N	828	ASP	CB-CG-OD1	5.50	123.25	118.30
1	I	43	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	P	800	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	I	952	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	M	800	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	J	375	ASP	CB-CG-OD1	5.49	123.24	118.30
1	I	987	ASP	CB-CG-OD1	5.48	123.23	118.30
1	P	987	ASP	CB-CG-OD1	5.48	123.23	118.30
1	J	43	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	K	375	ASP	CB-CG-OD1	5.47	123.23	118.30
1	K	952	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	I	800	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	L	282	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	L	916	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	O	591	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	N	952	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	P	916	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	L	800	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	P	43	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	L	43	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	O	43	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	L	427	THR	CA-CB-CG2	-5.44	104.78	112.40
1	M	916	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	N	427	THR	CA-CB-CG2	-5.44	104.78	112.40
1	L	82	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	P	591	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	I	591	ASP	CB-CG-OD2	-5.44	113.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	800	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	J	427	THR	CA-CB-CG2	-5.43	104.79	112.40
1	O	82	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	O	427	THR	CA-CB-CG2	-5.43	104.79	112.40
1	L	591	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	M	427	THR	CA-CB-CG2	-5.43	104.79	112.40
1	N	916	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	L	987	ASP	CB-CG-OD1	5.43	123.19	118.30
1	O	411	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	I	82	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	I	427	THR	CA-CB-CG2	-5.43	104.80	112.40
1	J	924	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	P	427	THR	CA-CB-CG2	-5.42	104.81	112.40
1	N	987	ASP	CB-CG-OD1	5.42	123.18	118.30
1	J	916	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	K	987	ASP	CB-CG-OD1	5.42	123.18	118.30
1	J	82	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	O	987	ASP	CB-CG-OD1	5.42	123.17	118.30
1	N	282	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	I	776	LEU	CB-CA-C	-5.41	99.92	110.20
1	K	427	THR	CA-CB-CG2	-5.41	104.82	112.40
1	K	591	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	L	776	LEU	CB-CA-C	-5.41	99.91	110.20
1	M	82	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	P	776	LEU	CB-CA-C	-5.41	99.92	110.20
1	N	591	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	O	916	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	J	987	ASP	CB-CG-OD1	5.41	123.17	118.30
1	M	411	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	N	82	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	J	591	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	J	776	LEU	CB-CA-C	-5.40	99.93	110.20
1	M	924	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	M	776	LEU	CB-CA-C	-5.40	99.94	110.20
1	N	237	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	I	916	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	O	776	LEU	CB-CA-C	-5.40	99.95	110.20
1	K	282	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	O	924	ASP	CB-CG-OD2	-5.39	113.44	118.30
1	K	776	LEU	CB-CA-C	-5.39	99.96	110.20
1	L	411	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	J	411	ASP	CB-CG-OD2	-5.39	113.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	776	LEU	CB-CA-C	-5.39	99.97	110.20
1	I	411	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	K	82	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	I	924	ASP	CB-CG-OD2	-5.37	113.46	118.30
1	K	237	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	K	916	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	I	282	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	L	924	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	N	411	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	O	237	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	M	591	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	P	411	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	J	282	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	L	237	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	P	282	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	K	411	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	P	924	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	N	924	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	P	82	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	K	924	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	N	938	ARG	N-CA-CB	5.35	120.22	110.60
1	M	282	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	I	237	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	L	746	ASP	CB-CG-OD1	5.34	123.11	118.30
1	I	938	ARG	N-CA-CB	5.34	120.21	110.60
1	P	938	ARG	N-CA-CB	5.34	120.21	110.60
1	K	938	ARG	N-CA-CB	5.34	120.21	110.60
1	M	164	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	O	746	ASP	CB-CG-OD1	5.34	123.10	118.30
1	M	237	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	O	938	ARG	N-CA-CB	5.33	120.19	110.60
1	M	938	ARG	N-CA-CB	5.33	120.18	110.60
1	L	938	ARG	N-CA-CB	5.32	120.17	110.60
1	O	442	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	J	746	ASP	CB-CG-OD1	5.31	123.08	118.30
1	K	919	ASP	CB-CG-OD1	5.31	123.08	118.30
1	N	746	ASP	CB-CG-OD1	5.31	123.08	118.30
1	P	772	ASP	CB-CG-OD1	5.31	123.08	118.30
1	J	938	ARG	N-CA-CB	5.30	120.15	110.60
1	K	746	ASP	CB-CG-OD1	5.30	123.07	118.30
1	P	802	ASP	CB-CG-OD1	5.30	123.07	118.30
1	I	772	ASP	CB-CG-OD1	5.30	123.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	802	ASP	CB-CG-OD1	5.30	123.07	118.30
1	J	919	ASP	CB-CG-OD1	5.30	123.07	118.30
1	M	746	ASP	CB-CG-OD1	5.29	123.06	118.30
1	M	772	ASP	CB-CG-OD1	5.29	123.06	118.30
1	M	802	ASP	CB-CG-OD1	5.29	123.06	118.30
1	I	746	ASP	CB-CG-OD1	5.29	123.06	118.30
1	L	919	ASP	CB-CG-OD1	5.29	123.06	118.30
1	P	746	ASP	CB-CG-OD1	5.29	123.06	118.30
1	J	442	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	P	164	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	L	164	ASP	CB-CG-OD2	-5.28	113.54	118.30
1	N	772	ASP	CB-CG-OD1	5.28	123.06	118.30
1	O	919	ASP	CB-CG-OD1	5.28	123.06	118.30
1	P	919	ASP	CB-CG-OD1	5.28	123.05	118.30
1	J	509	ASP	CB-CG-OD1	5.28	123.05	118.30
1	M	561	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	I	561	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	L	802	ASP	CB-CG-OD1	5.28	123.05	118.30
1	N	561	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	I	164	ASP	CB-CG-OD2	-5.27	113.55	118.30
1	L	772	ASP	CB-CG-OD1	5.27	123.04	118.30
1	M	919	ASP	CB-CG-OD1	5.27	123.04	118.30
1	N	164	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	N	919	ASP	CB-CG-OD1	5.26	123.04	118.30
1	J	772	ASP	CB-CG-OD1	5.26	123.03	118.30
1	P	509	ASP	CB-CG-OD1	5.26	123.03	118.30
1	K	772	ASP	CB-CG-OD1	5.26	123.03	118.30
1	I	919	ASP	CB-CG-OD1	5.26	123.03	118.30
1	L	509	ASP	CB-CG-OD1	5.26	123.03	118.30
1	O	282	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	M	509	ASP	CB-CG-OD1	5.25	123.03	118.30
1	O	509	ASP	CB-CG-OD1	5.25	123.03	118.30
1	J	802	ASP	CB-CG-OD1	5.24	123.02	118.30
1	K	802	ASP	CB-CG-OD1	5.24	123.02	118.30
1	O	772	ASP	CB-CG-OD1	5.24	123.02	118.30
1	J	164	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	N	442	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	O	164	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	J	561	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	N	509	ASP	CB-CG-OD1	5.24	123.01	118.30
1	P	442	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	P	561	ARG	NE-CZ-NH2	-5.23	117.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	164	ASP	CB-CG-OD2	-5.23	113.60	118.30
1	N	802	ASP	CB-CG-OD1	5.23	123.00	118.30
1	L	15	ASP	CB-CG-OD2	-5.23	113.60	118.30
1	I	442	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	I	509	ASP	CB-CG-OD1	5.22	123.00	118.30
1	I	802	ASP	CB-CG-OD1	5.22	123.00	118.30
1	J	996	ASP	CB-CG-OD1	5.22	123.00	118.30
1	K	561	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	N	15	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	I	15	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	K	15	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	M	996	ASP	CB-CG-OD1	5.21	122.99	118.30
1	I	996	ASP	CB-CG-OD1	5.21	122.99	118.30
1	P	439	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	K	442	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	N	224	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	P	15	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	K	919	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	J	15	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	L	224	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	L	919	ASP	CB-CG-OD2	-5.19	113.62	118.30
1	K	996	ASP	CB-CG-OD1	5.19	122.97	118.30
1	M	772	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	P	772	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	J	237	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	O	561	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	O	996	ASP	CB-CG-OD1	5.19	122.97	118.30
1	P	996	ASP	CB-CG-OD1	5.19	122.97	118.30
1	K	509	ASP	CB-CG-OD1	5.18	122.97	118.30
1	J	919	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	M	15	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	J	255	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	M	442	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	O	224	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	P	237	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	I	224	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	J	772	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	O	479	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	L	772	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	M	224	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	O	772	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	I	439	ARG	NE-CZ-NH1	5.16	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	919	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	L	996	ASP	CB-CG-OD1	5.16	122.94	118.30
1	I	772	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	N	255	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	O	255	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	N	996	ASP	CB-CG-OD1	5.15	122.94	118.30
1	P	881	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	K	772	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	K	800	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	M	919	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	P	224	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	J	800	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	M	479	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	I	800	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	P	255	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	J	479	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	N	292	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	P	919	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	J	224	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	N	919	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	O	15	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	L	561	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	K	224	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	N	772	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	K	439	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	N	479	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	K	479	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	I	919	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	M	255	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	I	987	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	K	255	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	L	442	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	N	185	ALA	N-CA-CB	5.10	117.24	110.10
1	J	881	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	P	479	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	L	185	ALA	N-CA-CB	5.10	117.24	110.10
1	I	255	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	L	479	ASP	CB-CG-OD2	-5.09	113.71	118.30
1	O	800	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	I	479	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	P	292	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	J	439	ARG	NE-CZ-NH1	5.09	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	185	ALA	N-CA-CB	5.09	117.22	110.10
1	I	881	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	J	417	THR	CA-CB-CG2	-5.08	105.29	112.40
1	L	255	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	N	439	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	O	881	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	O	147	ASN	N-CA-CB	-5.08	101.46	110.60
1	J	147	ASN	N-CA-CB	-5.08	101.46	110.60
1	K	881	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	L	147	ASN	N-CA-CB	-5.08	101.46	110.60
1	O	439	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	P	987	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	K	147	ASN	N-CA-CB	-5.08	101.46	110.60
1	P	147	ASN	N-CA-CB	-5.08	101.47	110.60
1	M	147	ASN	N-CA-CB	-5.07	101.47	110.60
1	M	987	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	O	185	ALA	N-CA-CB	5.07	117.20	110.10
1	N	147	ASN	N-CA-CB	-5.07	101.47	110.60
1	J	185	ALA	N-CA-CB	5.07	117.20	110.10
1	J	292	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	P	185	ALA	N-CA-CB	5.07	117.20	110.10
1	P	417	THR	CA-CB-CG2	-5.07	105.30	112.40
1	I	147	ASN	N-CA-CB	-5.07	101.48	110.60
1	L	800	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	M	439	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	N	417	THR	CA-CB-CG2	-5.06	105.31	112.40
1	L	447	ASP	CB-CG-OD1	5.06	122.85	118.30
1	O	417	THR	CA-CB-CG2	-5.06	105.32	112.40
1	I	292	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	I	417	THR	CA-CB-CG2	-5.05	105.33	112.40
1	I	441	THR	CA-CB-CG2	-5.05	105.32	112.40
1	L	417	THR	CA-CB-CG2	-5.05	105.33	112.40
1	L	987	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	P	800	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	I	185	ALA	N-CA-CB	5.05	117.17	110.10
1	M	185	ALA	N-CA-CB	5.05	117.17	110.10
1	M	447	ASP	CB-CG-OD1	5.05	122.84	118.30
1	N	800	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	P	447	ASP	CB-CG-OD1	5.05	122.84	118.30
1	I	447	ASP	CB-CG-OD1	5.05	122.84	118.30
1	M	417	THR	CA-CB-CG2	-5.05	105.33	112.40
1	O	441	THR	CA-CB-CG2	-5.04	105.34	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	987	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	J	987	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	K	987	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	M	881	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	L	292	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	K	417	THR	CA-CB-CG2	-5.04	105.35	112.40
1	J	388	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	L	439	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	O	310	ARG	N-CA-CB	5.03	119.66	110.60
1	J	441	THR	CA-CB-CG2	-5.03	105.36	112.40
1	M	800	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	K	292	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	O	252	ASP	CB-CG-OD1	5.03	122.83	118.30
1	P	441	THR	CA-CB-CG2	-5.03	105.36	112.40
1	N	881	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	P	388	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	O	987	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	L	310	ARG	N-CA-CB	5.02	119.64	110.60
1	I	310	ARG	N-CA-CB	5.02	119.64	110.60
1	K	441	THR	CA-CB-CG2	-5.02	105.37	112.40
1	K	447	ASP	CB-CG-OD1	5.02	122.82	118.30
1	N	1013	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	L	1013	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	M	310	ARG	N-CA-CB	5.02	119.63	110.60
1	M	441	THR	CA-CB-CG2	-5.02	105.38	112.40
1	P	252	ASP	CB-CG-OD1	5.02	122.82	118.30
1	P	507	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	N	310	ARG	N-CA-CB	5.02	119.63	110.60
1	L	441	THR	CA-CB-CG2	-5.01	105.38	112.40
1	I	1013	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	K	252	ASP	CB-CG-OD1	5.01	122.81	118.30
1	M	1013	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	N	447	ASP	CB-CG-OD1	5.01	122.81	118.30
1	P	310	ARG	N-CA-CB	5.01	119.62	110.60
1	M	252	ASP	CB-CG-OD1	5.01	122.81	118.30
1	I	507	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	J	310	ARG	N-CA-CB	5.01	119.61	110.60
1	M	388	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	O	1013	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	P	1013	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	N	441	THR	CA-CB-CG2	-5.00	105.39	112.40
1	N	252	ASP	CB-CG-OD1	5.00	122.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	292	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	8219	0	7811	573	0
1	J	8219	0	7811	566	0
1	K	8219	0	7811	561	0
1	L	8219	0	7811	574	0
1	M	8219	0	7811	566	0
1	N	8219	0	7811	566	0
1	O	8219	0	7811	575	0
1	P	8219	0	7811	576	0
2	I	23	0	21	0	0
2	J	23	0	21	0	0
2	K	23	0	21	0	0
2	L	23	0	21	0	0
2	M	23	0	21	0	0
2	N	23	0	21	0	0
2	O	23	0	21	0	0
2	P	23	0	21	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	2	0	0	0	0
4	L	2	0	0	0	0
4	M	2	0	0	0	0
4	N	2	0	0	0	0
4	O	2	0	0	0	0
4	P	2	0	0	0	0
5	I	162	0	0	6	0
5	J	162	0	0	6	0
5	K	162	0	0	6	0
5	L	162	0	0	6	0
5	M	161	0	0	6	0
5	N	163	0	0	6	0
5	O	161	0	0	6	0
5	P	163	0	0	6	0
All	All	67264	0	62656	4491	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 35.

All (4491) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:43:ARG:HH11	1:J:43:ARG:HG2	1.20	1.07
1:I:43:ARG:HH11	1:I:43:ARG:HG2	1.20	1.07
1:M:43:ARG:HH11	1:M:43:ARG:HG2	1.20	1.06
1:P:427:THR:HA	1:P:436:MET:HE1	1.39	1.04
1:P:43:ARG:HH11	1:P:43:ARG:HG2	1.20	1.02
1:O:43:ARG:HH11	1:O:43:ARG:HG2	1.20	1.02
1:L:43:ARG:HG2	1:L:43:ARG:HH11	1.20	1.02
1:N:43:ARG:HG2	1:N:43:ARG:HH11	1.20	1.02
1:K:43:ARG:HH11	1:K:43:ARG:HG2	1.20	1.01
1:M:777:LEU:HD11	1:M:889:ALA:HA	1.43	1.01
1:J:777:LEU:HD11	1:J:889:ALA:HA	1.43	1.01
1:J:427:THR:HA	1:J:436:MET:HE1	1.43	1.00
1:K:777:LEU:HD11	1:K:889:ALA:HA	1.43	1.00
1:J:744:GLU:HB3	1:J:745:MET:HE3	1.44	1.00
1:O:777:LEU:HD11	1:O:889:ALA:HA	1.43	0.99
1:I:744:GLU:HB3	1:I:745:MET:HE3	1.44	0.98
1:O:744:GLU:HB3	1:O:745:MET:HE3	1.44	0.98
1:K:740:LEU:HD12	1:K:741:THR:H	1.29	0.98
1:L:777:LEU:HD11	1:L:889:ALA:HA	1.43	0.98
1:P:777:LEU:HD11	1:P:889:ALA:HA	1.43	0.98
1:N:740:LEU:HD12	1:N:741:THR:H	1.29	0.98

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:740:LEU:HD12	1:L:741:THR:H	1.29	0.98
1:I:777:LEU:HD11	1:I:889:ALA:HA	1.43	0.97
1:K:744:GLU:HB3	1:K:745:MET:HE3	1.44	0.97
1:L:744:GLU:HB3	1:L:745:MET:HE3	1.46	0.97
1:J:740:LEU:HD12	1:J:741:THR:H	1.29	0.97
1:N:777:LEU:HD11	1:N:889:ALA:HA	1.43	0.97
1:N:744:GLU:HB3	1:N:745:MET:HE3	1.44	0.97
1:P:740:LEU:HD12	1:P:741:THR:H	1.29	0.96
1:I:427:THR:HA	1:I:436:MET:HE1	1.47	0.96
1:M:744:GLU:HB3	1:M:745:MET:HE3	1.44	0.96
1:O:740:LEU:HD12	1:O:741:THR:H	1.29	0.96
1:I:740:LEU:HD12	1:I:741:THR:H	1.29	0.96
1:L:427:THR:HA	1:L:436:MET:HE1	1.46	0.95
1:M:740:LEU:HD12	1:M:741:THR:H	1.29	0.95
1:P:744:GLU:HB3	1:P:745:MET:HE3	1.47	0.95
1:O:427:THR:HA	1:O:436:MET:HE1	1.50	0.94
1:K:427:THR:HA	1:K:436:MET:CE	1.98	0.94
1:J:427:THR:HA	1:J:436:MET:CE	1.98	0.93
1:P:436:MET:HE3	1:P:467:ASN:HD22	1.34	0.93
1:L:427:THR:HA	1:L:436:MET:CE	1.98	0.93
1:M:427:THR:HA	1:M:436:MET:CE	1.98	0.93
1:O:427:THR:HA	1:O:436:MET:CE	1.98	0.93
1:N:427:THR:HA	1:N:436:MET:CE	1.98	0.92
1:P:427:THR:HA	1:P:436:MET:CE	1.98	0.92
1:I:427:THR:HA	1:I:436:MET:CE	1.98	0.92
1:I:102:ASN:HD22	1:I:201:ASP:HB2	1.35	0.92
1:K:427:THR:HA	1:K:436:MET:HE1	1.51	0.91
1:J:102:ASN:HD22	1:J:201:ASP:HB2	1.35	0.91
1:M:427:THR:HA	1:M:436:MET:HE1	1.49	0.91
1:L:102:ASN:HD22	1:L:201:ASP:HB2	1.35	0.91
1:K:102:ASN:HD22	1:K:201:ASP:HB2	1.35	0.91
1:M:425:ARG:NH2	1:P:287:ASP:OD2	2.03	0.90
1:M:102:ASN:HD22	1:M:201:ASP:HB2	1.35	0.90
1:K:46:ARG:HH11	1:K:46:ARG:HG3	1.37	0.90
1:M:46:ARG:HG3	1:M:46:ARG:HH11	1.36	0.90
1:J:668:VAL:HG13	1:J:669:PRO:HD2	1.54	0.90
1:M:668:VAL:HG13	1:M:669:PRO:HD2	1.54	0.90
1:K:18:ASN:ND2	1:K:21:VAL:HG23	1.87	0.90
1:L:316:HIS:HA	1:L:323:ILE:HD13	1.55	0.90
1:J:18:ASN:ND2	1:J:21:VAL:HG23	1.87	0.90
1:N:18:ASN:ND2	1:N:21:VAL:HG23	1.87	0.90
1:L:18:ASN:ND2	1:L:21:VAL:HG23	1.87	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:668:VAL:HG13	1:N:669:PRO:HD2	1.54	0.89
1:M:18:ASN:ND2	1:M:21:VAL:HG23	1.87	0.89
1:I:316:HIS:HA	1:I:323:ILE:HD13	1.55	0.89
1:J:46:ARG:HH11	1:J:46:ARG:HG3	1.36	0.89
1:O:18:ASN:ND2	1:O:21:VAL:HG23	1.87	0.89
1:O:102:ASN:HD22	1:O:201:ASP:HB2	1.35	0.89
1:K:668:VAL:HG13	1:K:669:PRO:HD2	1.54	0.89
1:P:316:HIS:HA	1:P:323:ILE:HD13	1.54	0.89
1:O:316:HIS:HA	1:O:323:ILE:HD13	1.54	0.89
1:J:436:MET:HE3	1:J:467:ASN:HD22	1.37	0.89
1:I:668:VAL:HG13	1:I:669:PRO:HD2	1.54	0.89
1:L:668:VAL:HG13	1:L:669:PRO:HD2	1.54	0.89
1:M:57:GLU:HG2	1:M:83:THR:CG2	2.03	0.89
1:P:18:ASN:ND2	1:P:21:VAL:HG23	1.87	0.89
1:I:57:GLU:HG2	1:I:83:THR:CG2	2.03	0.89
1:P:57:GLU:HG2	1:P:83:THR:CG2	2.03	0.89
1:J:57:GLU:HG2	1:J:83:THR:CG2	2.03	0.89
1:N:316:HIS:HA	1:N:323:ILE:HD13	1.55	0.89
1:K:57:GLU:HG2	1:K:83:THR:CG2	2.03	0.88
1:K:316:HIS:HA	1:K:323:ILE:HD13	1.55	0.88
1:P:668:VAL:HG13	1:P:669:PRO:HD2	1.54	0.88
1:I:18:ASN:ND2	1:I:21:VAL:HG23	1.87	0.88
1:P:102:ASN:HD22	1:P:201:ASP:HB2	1.35	0.88
1:I:46:ARG:HG3	1:I:46:ARG:HH11	1.37	0.88
1:L:46:ARG:HG3	1:L:46:ARG:HH11	1.37	0.88
1:M:316:HIS:HA	1:M:323:ILE:HD13	1.54	0.88
1:N:57:GLU:HG2	1:N:83:THR:CG2	2.03	0.88
1:N:102:ASN:HD22	1:N:201:ASP:HB2	1.35	0.88
1:L:57:GLU:HG2	1:L:83:THR:CG2	2.03	0.88
1:O:46:ARG:HG3	1:O:46:ARG:HH11	1.36	0.88
1:P:46:ARG:HG3	1:P:46:ARG:HH11	1.37	0.88
1:N:46:ARG:HH11	1:N:46:ARG:HG3	1.37	0.87
1:O:7:LEU:HD13	1:O:74:LEU:HD11	1.57	0.87
1:J:7:LEU:HD13	1:J:74:LEU:HD11	1.57	0.87
1:P:360:HIS:CE1	1:P:362:LEU:HB2	2.10	0.87
1:O:57:GLU:HG2	1:O:83:THR:CG2	2.03	0.87
1:K:360:HIS:CE1	1:K:362:LEU:HB2	2.10	0.87
1:N:7:LEU:HD13	1:N:74:LEU:HD11	1.57	0.87
1:I:7:LEU:HD13	1:I:74:LEU:HD11	1.57	0.87
1:L:360:HIS:CE1	1:L:362:LEU:HB2	2.10	0.87
1:J:856:TYR:HD2	1:J:864:MET:HE2	1.37	0.87
1:N:427:THR:HA	1:N:436:MET:HE1	1.57	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:360:HIS:CE1	1:M:362:LEU:HB2	2.10	0.87
1:I:360:HIS:CE1	1:I:362:LEU:HB2	2.10	0.87
1:J:316:HIS:HA	1:J:323:ILE:HD13	1.54	0.87
1:O:360:HIS:CE1	1:O:362:LEU:HB2	2.10	0.86
1:K:7:LEU:HD13	1:K:74:LEU:HD11	1.57	0.86
1:I:436:MET:HE3	1:I:467:ASN:HD22	1.40	0.86
1:J:360:HIS:CE1	1:J:362:LEU:HB2	2.10	0.86
1:N:360:HIS:CE1	1:N:362:LEU:HB2	2.10	0.86
1:L:436:MET:HE3	1:L:467:ASN:HD22	1.39	0.86
1:L:781:ARG:HH11	1:L:781:ARG:HG3	1.41	0.86
1:O:668:VAL:HG13	1:O:669:PRO:HD2	1.54	0.86
1:P:7:LEU:HD13	1:P:74:LEU:HD11	1.57	0.86
1:J:781:ARG:HG3	1:J:781:ARG:HH11	1.41	0.86
1:M:436:MET:HE3	1:M:467:ASN:HD22	1.41	0.85
1:K:781:ARG:HH11	1:K:781:ARG:HG3	1.41	0.85
1:N:781:ARG:HH11	1:N:781:ARG:HG3	1.41	0.85
1:O:781:ARG:HG3	1:O:781:ARG:HH11	1.41	0.85
1:P:249:GLU:HG2	1:P:251:ARG:NH1	1.92	0.85
1:L:7:LEU:HD13	1:L:74:LEU:HD11	1.57	0.85
1:N:949:HIS:CD2	1:N:1020:TRP:HE1	1.95	0.85
1:L:949:HIS:CD2	1:L:1020:TRP:HE1	1.95	0.85
1:K:249:GLU:HG2	1:K:251:ARG:NH1	1.92	0.85
1:M:949:HIS:CD2	1:M:1020:TRP:HE1	1.95	0.84
1:I:249:GLU:HG2	1:I:251:ARG:NH1	1.92	0.84
1:K:360:HIS:ND1	1:K:361:PRO:HD2	1.92	0.84
1:L:249:GLU:HG2	1:L:251:ARG:NH1	1.92	0.84
1:I:949:HIS:CD2	1:I:1020:TRP:HE1	1.95	0.84
1:O:949:HIS:CD2	1:O:1020:TRP:HE1	1.95	0.84
1:O:436:MET:HE3	1:O:467:ASN:HD22	1.43	0.84
1:J:360:HIS:ND1	1:J:361:PRO:HD2	1.93	0.84
1:M:249:GLU:HG2	1:M:251:ARG:NH1	1.92	0.84
1:M:360:HIS:ND1	1:M:361:PRO:HD2	1.92	0.84
1:K:894:ARG:NH2	1:K:921:PRO:HD3	1.93	0.84
1:N:360:HIS:ND1	1:N:361:PRO:HD2	1.93	0.84
1:J:249:GLU:HG2	1:J:251:ARG:NH1	1.92	0.84
1:P:360:HIS:ND1	1:P:361:PRO:HD2	1.93	0.84
1:L:360:HIS:ND1	1:L:361:PRO:HD2	1.92	0.84
1:I:360:HIS:ND1	1:I:361:PRO:HD2	1.93	0.84
1:O:249:GLU:HG2	1:O:251:ARG:NH1	1.92	0.84
1:P:894:ARG:NH2	1:P:921:PRO:HD3	1.93	0.83
1:J:894:ARG:NH2	1:J:921:PRO:HD3	1.93	0.83
1:J:434:PRO:HB3	1:K:434:PRO:HB3	1.57	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:7:LEU:HD13	1:M:74:LEU:HD11	1.57	0.83
1:J:949:HIS:CD2	1:J:1020:TRP:HE1	1.95	0.83
1:P:949:HIS:CD2	1:P:1020:TRP:HE1	1.95	0.83
1:M:781:ARG:HH11	1:M:781:ARG:HG3	1.41	0.83
1:I:781:ARG:HH11	1:I:781:ARG:HG3	1.41	0.83
1:K:949:HIS:CD2	1:K:1020:TRP:HE1	1.95	0.83
1:L:894:ARG:NH2	1:L:921:PRO:HD3	1.93	0.83
1:M:894:ARG:NH2	1:M:921:PRO:HD3	1.93	0.83
1:K:436:MET:HE3	1:K:467:ASN:HD22	1.44	0.83
1:L:777:LEU:CD1	1:L:889:ALA:HA	2.09	0.83
1:P:777:LEU:CD1	1:P:889:ALA:HA	2.09	0.83
1:N:777:LEU:CD1	1:N:889:ALA:HA	2.09	0.83
1:O:360:HIS:ND1	1:O:361:PRO:HD2	1.93	0.83
1:L:949:HIS:HD2	1:L:1020:TRP:HE1	1.27	0.83
1:I:890:GLN:HG3	1:I:891:VAL:N	1.94	0.83
1:K:436:MET:CE	1:K:467:ASN:HD22	1.93	0.82
1:N:249:GLU:HG2	1:N:251:ARG:NH1	1.92	0.82
1:N:894:ARG:NH2	1:N:921:PRO:HD3	1.93	0.82
1:L:746:ASP:HA	1:L:760:ARG:HG3	1.61	0.82
1:O:894:ARG:NH2	1:O:921:PRO:HD3	1.93	0.82
1:N:890:GLN:HG3	1:N:891:VAL:N	1.94	0.82
1:O:240:LEU:HD12	1:O:241:GLU:N	1.95	0.82
1:I:777:LEU:CD1	1:I:889:ALA:HA	2.09	0.82
1:L:436:MET:CE	1:L:467:ASN:HD22	1.93	0.82
1:K:63:PHE:HB3	1:K:64:PRO:HD2	1.62	0.82
1:I:894:ARG:NH2	1:I:921:PRO:HD3	1.93	0.82
1:N:240:LEU:HD12	1:N:241:GLU:N	1.95	0.82
1:P:781:ARG:HG3	1:P:781:ARG:HH11	1.41	0.82
1:O:777:LEU:CD1	1:O:889:ALA:HA	2.09	0.82
1:M:240:LEU:HD12	1:M:241:GLU:N	1.95	0.82
1:P:240:LEU:HD12	1:P:241:GLU:N	1.95	0.82
1:P:436:MET:CE	1:P:467:ASN:HD22	1.93	0.82
1:J:436:MET:CE	1:J:467:ASN:HD22	1.93	0.82
1:I:746:ASP:HA	1:I:760:ARG:HG3	1.61	0.82
1:J:316:HIS:HA	1:J:323:ILE:CD1	2.10	0.82
1:O:63:PHE:HB3	1:O:64:PRO:HD2	1.62	0.82
1:P:316:HIS:HA	1:P:323:ILE:CD1	2.10	0.82
1:N:227:VAL:HG13	1:N:240:LEU:HD11	1.62	0.82
1:J:890:GLN:HG3	1:J:891:VAL:N	1.94	0.82
1:P:63:PHE:HB3	1:P:64:PRO:HD2	1.62	0.82
1:K:746:ASP:HA	1:K:760:ARG:HG3	1.61	0.81
1:P:746:ASP:HA	1:P:760:ARG:HG3	1.61	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:316:HIS:HA	1:M:323:ILE:CD1	2.10	0.81
1:O:949:HIS:HD2	1:O:1020:TRP:HE1	1.28	0.81
1:L:227:VAL:HG13	1:L:240:LEU:HD11	1.62	0.81
1:K:65:ALA:HB1	1:K:66:PRO:HD2	1.62	0.81
1:K:777:LEU:CD1	1:K:889:ALA:HA	2.09	0.81
1:N:436:MET:CE	1:N:467:ASN:HD22	1.93	0.81
1:L:255:ARG:HH11	1:L:255:ARG:HG2	1.45	0.81
1:I:227:VAL:HG13	1:I:240:LEU:HD11	1.62	0.81
1:I:240:LEU:HD12	1:I:241:GLU:N	1.95	0.81
1:J:240:LEU:HD12	1:J:241:GLU:N	1.95	0.81
1:M:777:LEU:CD1	1:M:889:ALA:HA	2.09	0.81
1:O:746:ASP:HA	1:O:760:ARG:HG3	1.61	0.81
1:O:316:HIS:HA	1:O:323:ILE:CD1	2.10	0.81
1:K:316:HIS:HA	1:K:323:ILE:CD1	2.10	0.81
1:L:240:LEU:HD12	1:L:241:GLU:N	1.95	0.81
1:I:65:ALA:HB1	1:I:66:PRO:HD2	1.63	0.81
1:K:240:LEU:HD12	1:K:241:GLU:N	1.95	0.81
1:J:777:LEU:CD1	1:J:889:ALA:HA	2.09	0.81
1:M:436:MET:CE	1:M:467:ASN:HD22	1.93	0.81
1:N:65:ALA:HB1	1:N:66:PRO:HD2	1.62	0.81
1:L:890:GLN:HG3	1:L:891:VAL:N	1.94	0.81
1:M:255:ARG:HG2	1:M:255:ARG:HH11	1.45	0.81
1:P:128:ASN:ND2	1:P:180:GLY:HA2	1.96	0.81
1:L:65:ALA:HB1	1:L:66:PRO:HD2	1.62	0.81
1:O:436:MET:CE	1:O:467:ASN:HD22	1.93	0.81
1:O:65:ALA:HB1	1:O:66:PRO:HD2	1.62	0.81
1:I:63:PHE:HB3	1:I:64:PRO:HD2	1.62	0.81
1:O:128:ASN:ND2	1:O:180:GLY:HA2	1.96	0.81
1:M:128:ASN:ND2	1:M:180:GLY:HA2	1.96	0.81
1:N:128:ASN:ND2	1:N:180:GLY:HA2	1.96	0.81
1:L:316:HIS:HA	1:L:323:ILE:CD1	2.10	0.81
1:N:316:HIS:HA	1:N:323:ILE:CD1	2.10	0.81
1:J:128:ASN:ND2	1:J:180:GLY:HA2	1.96	0.81
1:K:822:LEU:HD12	1:K:824:GLN:H	1.46	0.81
1:L:822:LEU:HD12	1:L:824:GLN:H	1.46	0.81
1:O:890:GLN:HG3	1:O:891:VAL:N	1.94	0.81
1:M:746:ASP:HA	1:M:760:ARG:HG3	1.61	0.80
1:M:65:ALA:HB1	1:M:66:PRO:HD2	1.62	0.80
1:J:822:LEU:HD12	1:J:824:GLN:H	1.46	0.80
1:N:255:ARG:HG2	1:N:255:ARG:HH11	1.45	0.80
1:I:436:MET:CE	1:I:467:ASN:HD22	1.93	0.80
1:I:316:HIS:HA	1:I:323:ILE:CD1	2.10	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:890:GLN:HG3	1:M:891:VAL:N	1.94	0.80
1:I:255:ARG:HH11	1:I:255:ARG:HG2	1.45	0.80
1:P:227:VAL:HG13	1:P:240:LEU:HD11	1.62	0.80
1:N:63:PHE:HB3	1:N:64:PRO:HD2	1.62	0.80
1:L:128:ASN:ND2	1:L:180:GLY:HA2	1.96	0.80
1:N:746:ASP:HA	1:N:760:ARG:HG3	1.61	0.80
1:O:227:VAL:HG13	1:O:240:LEU:HD11	1.62	0.80
1:I:128:ASN:ND2	1:I:180:GLY:HA2	1.96	0.80
1:O:822:LEU:HD12	1:O:824:GLN:H	1.46	0.80
1:P:822:LEU:HD12	1:P:824:GLN:H	1.46	0.80
1:K:255:ARG:HH11	1:K:255:ARG:HG2	1.45	0.80
1:P:890:GLN:HG3	1:P:891:VAL:N	1.94	0.80
1:J:7:LEU:CD1	1:J:74:LEU:HD11	2.12	0.80
1:K:7:LEU:CD1	1:K:74:LEU:HD11	2.12	0.80
1:K:227:VAL:HG13	1:K:240:LEU:HD11	1.62	0.80
1:K:890:GLN:HG3	1:K:891:VAL:N	1.94	0.80
1:M:7:LEU:CD1	1:M:74:LEU:HD11	2.12	0.80
1:P:255:ARG:HH11	1:P:255:ARG:HG2	1.45	0.80
1:K:128:ASN:ND2	1:K:180:GLY:HA2	1.96	0.80
1:L:63:PHE:HB3	1:L:64:PRO:HD2	1.62	0.80
1:P:65:ALA:HB1	1:P:66:PRO:HD2	1.62	0.80
1:J:949:HIS:HD2	1:J:1020:TRP:HE1	1.27	0.79
1:M:63:PHE:HB3	1:M:64:PRO:HD2	1.62	0.79
1:I:114:VAL:HG13	1:I:191:TRP:HB2	1.64	0.79
1:O:255:ARG:HG2	1:O:255:ARG:HH11	1.45	0.79
1:M:227:VAL:HG13	1:M:240:LEU:HD11	1.62	0.79
1:N:114:VAL:HG13	1:N:191:TRP:HB2	1.64	0.79
1:L:166:ARG:HD3	5:L:4035:HOH:O	1.83	0.79
1:N:7:LEU:CD1	1:N:74:LEU:HD11	2.12	0.79
1:J:65:ALA:HB1	1:J:66:PRO:HD2	1.62	0.79
1:J:114:VAL:HG13	1:J:191:TRP:HB2	1.64	0.79
1:I:949:HIS:HD2	1:I:1020:TRP:HE1	1.27	0.79
1:J:227:VAL:HG13	1:J:240:LEU:HD11	1.62	0.79
1:N:166:ARG:HD3	5:N:4210:HOH:O	1.83	0.79
1:P:114:VAL:HG13	1:P:191:TRP:HB2	1.64	0.79
1:O:166:ARG:HD3	5:O:4035:HOH:O	1.83	0.79
1:I:7:LEU:CD1	1:I:74:LEU:HD11	2.12	0.79
1:J:255:ARG:HH11	1:J:255:ARG:HG2	1.45	0.79
1:I:655:MET:HE2	1:I:656:VAL:N	1.98	0.79
1:M:822:LEU:HD12	1:M:824:GLN:H	1.46	0.79
1:K:166:ARG:HD3	5:K:4035:HOH:O	1.83	0.79
1:L:682:LEU:HD22	1:L:683:PRO:HD2	1.65	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:746:ASP:HA	1:J:760:ARG:HG3	1.61	0.79
1:P:102:ASN:ND2	1:P:201:ASP:HB2	1.98	0.79
1:P:655:MET:HE2	1:P:656:VAL:N	1.98	0.79
1:O:655:MET:HE2	1:O:656:VAL:N	1.98	0.79
1:O:7:LEU:CD1	1:O:74:LEU:HD11	2.12	0.79
1:P:7:LEU:CD1	1:P:74:LEU:HD11	2.12	0.79
1:L:7:LEU:CD1	1:L:74:LEU:HD11	2.12	0.79
1:J:63:PHE:HB3	1:J:64:PRO:HD2	1.62	0.79
1:L:114:VAL:HG13	1:L:191:TRP:HB2	1.64	0.79
1:J:655:MET:HE2	1:J:656:VAL:N	1.98	0.79
1:I:682:LEU:HD22	1:I:683:PRO:HD2	1.65	0.79
1:O:682:LEU:HD22	1:O:683:PRO:HD2	1.65	0.79
1:K:655:MET:HE2	1:K:656:VAL:N	1.99	0.79
1:P:682:LEU:HD22	1:P:683:PRO:HD2	1.65	0.79
1:J:102:ASN:ND2	1:J:201:ASP:HB2	1.98	0.78
1:J:651:LEU:HD12	1:J:652:LEU:H	1.48	0.78
1:N:102:ASN:ND2	1:N:201:ASP:HB2	1.98	0.78
1:N:655:MET:HE2	1:N:656:VAL:N	1.98	0.78
1:N:682:LEU:HD22	1:N:683:PRO:HD2	1.65	0.78
1:O:822:LEU:HD12	1:O:823:LEU:N	1.98	0.78
1:M:682:LEU:HD22	1:M:683:PRO:HD2	1.65	0.78
1:K:114:VAL:HG13	1:K:191:TRP:HB2	1.64	0.78
1:M:655:MET:HE2	1:M:656:VAL:N	1.98	0.78
1:K:43:ARG:NH1	1:K:43:ARG:HG2	1.94	0.78
1:K:651:LEU:HD12	1:K:652:LEU:H	1.48	0.78
1:K:822:LEU:HD12	1:K:823:LEU:N	1.98	0.78
1:N:822:LEU:HD12	1:N:823:LEU:N	1.98	0.78
1:J:166:ARG:HD3	5:J:4035:HOH:O	1.83	0.78
1:J:210:ARG:NH1	1:J:395:HIS:N	2.32	0.78
1:O:651:LEU:HD12	1:O:652:LEU:H	1.48	0.78
1:K:949:HIS:HD2	1:K:1020:TRP:HE1	1.27	0.78
1:M:949:HIS:HD2	1:M:1020:TRP:HE1	1.28	0.78
1:N:822:LEU:HD12	1:N:824:GLN:H	1.46	0.78
1:M:114:VAL:HG13	1:M:191:TRP:HB2	1.64	0.78
1:N:210:ARG:NH1	1:N:395:HIS:N	2.32	0.78
1:M:499:ILE:HB	1:M:533:LEU:HB2	1.66	0.78
1:I:210:ARG:NH1	1:I:395:HIS:N	2.32	0.78
1:P:210:ARG:NH1	1:P:395:HIS:N	2.32	0.78
1:L:102:ASN:ND2	1:L:201:ASP:HB2	1.98	0.78
1:M:651:LEU:HD12	1:M:652:LEU:H	1.49	0.78
1:M:822:LEU:HD12	1:M:823:LEU:N	1.98	0.78
1:M:434:PRO:HB3	1:P:434:PRO:HB3	1.65	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:166:ARG:HD3	5:P:4543:HOH:O	1.83	0.78
1:I:822:LEU:HD12	1:I:823:LEU:N	1.98	0.78
1:I:822:LEU:HD12	1:I:824:GLN:H	1.46	0.78
1:O:210:ARG:NH1	1:O:395:HIS:N	2.32	0.78
1:P:499:ILE:HB	1:P:533:LEU:HB2	1.66	0.78
1:K:682:LEU:HD22	1:K:683:PRO:HD2	1.65	0.78
1:I:166:ARG:HD3	5:I:4035:HOH:O	1.83	0.78
1:M:425:ARG:HH22	1:P:287:ASP:CG	1.87	0.78
1:J:822:LEU:HD12	1:J:823:LEU:N	1.98	0.78
1:J:682:LEU:HD22	1:J:683:PRO:HD2	1.65	0.78
1:L:499:ILE:HB	1:L:533:LEU:HB2	1.66	0.78
1:L:655:MET:HE2	1:L:656:VAL:N	1.98	0.78
1:I:102:ASN:ND2	1:I:201:ASP:HB2	1.98	0.78
1:O:102:ASN:ND2	1:O:201:ASP:HB2	1.98	0.78
1:O:114:VAL:HG13	1:O:191:TRP:HB2	1.64	0.78
1:N:949:HIS:HD2	1:N:1020:TRP:HE1	1.27	0.77
1:L:822:LEU:HD12	1:L:823:LEU:N	1.98	0.77
1:J:499:ILE:HB	1:J:533:LEU:HB2	1.66	0.77
1:K:499:ILE:HB	1:K:533:LEU:HB2	1.66	0.77
1:M:53:SER:C	1:M:54:LEU:HD23	2.04	0.77
1:L:43:ARG:HG2	1:L:43:ARG:NH1	1.94	0.77
1:P:360:HIS:CG	1:P:361:PRO:HD2	2.20	0.77
1:K:360:HIS:CG	1:K:361:PRO:HD2	2.20	0.77
1:M:166:ARG:HD3	5:M:4035:HOH:O	1.82	0.77
1:P:53:SER:C	1:P:54:LEU:HD23	2.04	0.77
1:J:53:SER:C	1:J:54:LEU:HD23	2.04	0.77
1:N:651:LEU:HD12	1:N:652:LEU:H	1.48	0.77
1:P:822:LEU:HD12	1:P:823:LEU:N	1.98	0.77
1:N:189:LEU:HD23	1:N:189:LEU:N	2.00	0.77
1:L:210:ARG:NH1	1:L:395:HIS:N	2.32	0.77
1:O:499:ILE:HB	1:O:533:LEU:HB2	1.66	0.77
1:L:189:LEU:HD23	1:L:189:LEU:N	2.00	0.77
1:K:53:SER:C	1:K:54:LEU:HD23	2.04	0.77
1:N:436:MET:HE3	1:N:467:ASN:HD22	1.48	0.77
1:M:210:ARG:NH1	1:M:395:HIS:N	2.32	0.77
1:I:53:SER:C	1:I:54:LEU:HD23	2.04	0.77
1:M:856:TYR:HD2	1:M:864:MET:HE2	1.48	0.77
1:P:651:LEU:HD12	1:P:652:LEU:H	1.48	0.77
1:I:360:HIS:CG	1:I:361:PRO:HD2	2.20	0.77
1:P:949:HIS:HD2	1:P:1020:TRP:HE1	1.28	0.77
1:N:395:HIS:CG	1:N:396:PRO:HD2	2.20	0.77
1:O:260:LEU:O	1:O:267:VAL:HG23	1.85	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:53:SER:C	1:N:54:LEU:HD23	2.04	0.77
1:K:260:LEU:O	1:K:267:VAL:HG23	1.85	0.77
1:L:53:SER:C	1:L:54:LEU:HD23	2.04	0.77
1:K:102:ASN:ND2	1:K:201:ASP:HB2	1.98	0.77
1:J:360:HIS:CG	1:J:361:PRO:HD2	2.20	0.77
1:L:395:HIS:CG	1:L:396:PRO:HD2	2.20	0.77
1:P:189:LEU:HD23	1:P:189:LEU:N	2.00	0.77
1:J:189:LEU:N	1:J:189:LEU:HD23	2.00	0.77
1:I:260:LEU:O	1:I:267:VAL:HG23	1.85	0.77
1:N:360:HIS:CG	1:N:361:PRO:HD2	2.20	0.77
1:P:260:LEU:O	1:P:267:VAL:HG23	1.85	0.77
1:L:360:HIS:CG	1:L:361:PRO:HD2	2.20	0.77
1:I:395:HIS:CG	1:I:396:PRO:HD2	2.20	0.77
1:L:654:TRP:CE2	1:L:666:GLY:HA3	2.20	0.77
1:K:210:ARG:NH1	1:K:395:HIS:N	2.32	0.77
1:K:395:HIS:CG	1:K:396:PRO:HD2	2.20	0.77
1:N:499:ILE:HB	1:N:533:LEU:HB2	1.66	0.77
1:O:395:HIS:CG	1:O:396:PRO:HD2	2.20	0.76
1:O:53:SER:C	1:O:54:LEU:HD23	2.04	0.76
1:M:423:MET:HB2	1:P:282:ARG:HG3	1.65	0.76
1:K:654:TRP:CE2	1:K:666:GLY:HA3	2.20	0.76
1:J:260:LEU:O	1:J:267:VAL:HG23	1.85	0.76
1:M:189:LEU:N	1:M:189:LEU:HD23	2.00	0.76
1:M:102:ASN:ND2	1:M:201:ASP:HB2	1.98	0.76
1:L:23:GLN:O	1:L:24:LEU:HD13	1.86	0.76
1:L:651:LEU:HD12	1:L:652:LEU:H	1.48	0.76
1:N:251:ARG:HB3	1:N:253:TYR:CE2	2.21	0.76
1:I:189:LEU:HD23	1:I:189:LEU:N	2.00	0.76
1:I:651:LEU:HD12	1:I:652:LEU:H	1.48	0.76
1:O:654:TRP:CE2	1:O:666:GLY:HA3	2.21	0.76
1:J:654:TRP:CE2	1:J:666:GLY:HA3	2.20	0.76
1:M:654:TRP:CE2	1:M:666:GLY:HA3	2.20	0.76
1:J:23:GLN:O	1:J:24:LEU:HD13	1.86	0.76
1:L:260:LEU:O	1:L:267:VAL:HG23	1.85	0.76
1:J:395:HIS:CG	1:J:396:PRO:HD2	2.20	0.76
1:K:189:LEU:HD23	1:K:189:LEU:N	2.00	0.76
1:I:654:TRP:CE2	1:I:666:GLY:HA3	2.20	0.76
1:M:360:HIS:CG	1:M:361:PRO:HD2	2.20	0.76
1:O:230:ARG:HH11	1:O:230:ARG:HG3	1.51	0.76
1:P:395:HIS:CG	1:P:396:PRO:HD2	2.20	0.76
1:O:189:LEU:N	1:O:189:LEU:HD23	2.00	0.76
1:P:23:GLN:O	1:P:24:LEU:HD13	1.86	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:595:THR:HG23	1:I:596:PRO:HA	1.68	0.76
1:I:499:ILE:HB	1:I:533:LEU:HB2	1.66	0.76
1:J:856:TYR:CD2	1:J:864:MET:HE2	2.20	0.76
1:O:360:HIS:CG	1:O:361:PRO:HD2	2.20	0.76
1:P:251:ARG:HB3	1:P:253:TYR:CE2	2.21	0.76
1:P:230:ARG:HH11	1:P:230:ARG:HG3	1.51	0.76
1:O:595:THR:HG23	1:O:596:PRO:HA	1.68	0.76
1:J:696:LEU:HD12	1:J:697:THR:N	2.01	0.76
1:K:595:THR:HG23	1:K:596:PRO:HA	1.68	0.76
1:M:251:ARG:HB3	1:M:253:TYR:CE2	2.21	0.75
1:L:230:ARG:HH11	1:L:230:ARG:HG3	1.51	0.75
1:N:654:TRP:CE2	1:N:666:GLY:HA3	2.21	0.75
1:O:696:LEU:HD12	1:O:697:THR:N	2.01	0.75
1:M:23:GLN:O	1:M:24:LEU:HD13	1.86	0.75
1:J:595:THR:HG23	1:J:596:PRO:HA	1.68	0.75
1:J:251:ARG:HB3	1:J:253:TYR:CE2	2.21	0.75
1:M:230:ARG:HG3	1:M:230:ARG:HH11	1.51	0.75
1:K:653[B]:HIS:CD2	1:K:667:GLU:HG3	2.22	0.75
1:M:653[B]:HIS:CD2	1:M:667:GLU:HG3	2.22	0.75
1:L:595:THR:HG23	1:L:596:PRO:HA	1.68	0.75
1:L:696:LEU:HD12	1:L:697:THR:N	2.02	0.75
1:N:260:LEU:O	1:N:267:VAL:HG23	1.85	0.75
1:P:43:ARG:NH1	1:P:43:ARG:HG2	1.94	0.75
1:P:654:TRP:CE2	1:P:666:GLY:HA3	2.20	0.75
1:N:653[B]:HIS:CD2	1:N:667:GLU:HG3	2.22	0.75
1:O:696:LEU:HD12	1:O:697:THR:H	1.51	0.75
1:M:696:LEU:HD12	1:M:697:THR:N	2.01	0.75
1:I:696:LEU:HD12	1:I:697:THR:H	1.51	0.75
1:I:251:ARG:HB3	1:I:253:TYR:CE2	2.21	0.75
1:L:251:ARG:HB3	1:L:253:TYR:CE2	2.21	0.75
1:J:230:ARG:HG3	1:J:230:ARG:HH11	1.51	0.75
1:I:653[B]:HIS:CD2	1:I:667:GLU:HG3	2.22	0.75
1:M:395:HIS:CG	1:M:396:PRO:HD2	2.20	0.75
1:I:434:PRO:HB3	1:L:434:PRO:HB3	1.66	0.75
1:M:260:LEU:O	1:M:267:VAL:HG23	1.85	0.75
1:O:653[B]:HIS:CD2	1:O:667:GLU:HG3	2.22	0.75
1:J:653[B]:HIS:CD2	1:J:667:GLU:HG3	2.22	0.75
1:L:653[B]:HIS:CD2	1:L:667:GLU:HG3	2.22	0.75
1:K:696:LEU:HD12	1:K:697:THR:H	1.51	0.75
1:K:251:ARG:HB3	1:K:253:TYR:CE2	2.21	0.75
1:P:653[B]:HIS:CD2	1:P:667:GLU:HG3	2.22	0.75
1:I:696:LEU:HD12	1:I:697:THR:N	2.01	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:23:GLN:O	1:K:24:LEU:HD13	1.86	0.75
1:P:696:LEU:HD12	1:P:697:THR:N	2.02	0.75
1:K:437:SER:HB2	5:K:7508:HOH:O	1.87	0.75
1:N:292:ARG:C	1:N:293:LEU:HD23	2.08	0.75
1:K:654:TRP:NE1	1:K:666:GLY:HA3	2.02	0.74
1:M:654:TRP:NE1	1:M:666:GLY:HA3	2.02	0.74
1:P:128:ASN:HD21	1:P:180:GLY:HA2	1.52	0.74
1:M:128:ASN:HD21	1:M:180:GLY:HA2	1.52	0.74
1:N:696:LEU:HD12	1:N:697:THR:N	2.01	0.74
1:N:23:GLN:O	1:N:24:LEU:HD13	1.86	0.74
1:K:230:ARG:HH11	1:K:230:ARG:HG3	1.51	0.74
1:N:654:TRP:NE1	1:N:666:GLY:HA3	2.02	0.74
1:M:418:HIS:O	1:P:282:ARG:HD3	1.86	0.74
1:O:23:GLN:O	1:O:24:LEU:HD13	1.86	0.74
1:N:595:THR:HG23	1:N:596:PRO:HA	1.68	0.74
1:L:292:ARG:C	1:L:293:LEU:HD23	2.08	0.74
1:N:43:ARG:NH1	1:N:43:ARG:HG2	1.94	0.74
1:I:654:TRP:NE1	1:I:666:GLY:HA3	2.02	0.74
1:J:654:TRP:NE1	1:J:666:GLY:HA3	2.02	0.74
1:J:696:LEU:HD12	1:J:697:THR:H	1.51	0.74
1:N:696:LEU:HD12	1:N:697:THR:H	1.51	0.74
1:P:595:THR:HG23	1:P:596:PRO:HA	1.68	0.74
1:N:434:PRO:HB3	1:O:434:PRO:HB3	1.68	0.74
1:N:427:THR:HA	1:N:436:MET:HE2	1.68	0.74
1:P:654:TRP:NE1	1:P:666:GLY:HA3	2.02	0.74
1:L:696:LEU:HD12	1:L:697:THR:H	1.51	0.74
1:I:23:GLN:O	1:I:24:LEU:HD13	1.86	0.74
1:O:292:ARG:C	1:O:293:LEU:HD23	2.08	0.74
1:P:822:LEU:HD12	1:P:824:GLN:N	2.03	0.74
1:N:662:PRO:C	1:N:663:LEU:HD23	2.08	0.74
1:M:336:ARG:HG2	1:M:336:ARG:HH11	1.52	0.74
1:I:336:ARG:HG2	1:I:336:ARG:HH11	1.52	0.74
1:J:43:ARG:NH1	1:J:43:ARG:HG2	1.94	0.74
1:M:696:LEU:HD12	1:M:697:THR:H	1.51	0.74
1:M:662:PRO:C	1:M:663:LEU:HD23	2.08	0.74
1:P:292:ARG:C	1:P:293:LEU:HD23	2.08	0.74
1:M:595:THR:HG23	1:M:596:PRO:HA	1.68	0.74
1:O:251:ARG:HB3	1:O:253:TYR:CE2	2.21	0.74
1:N:230:ARG:HH11	1:N:230:ARG:HG3	1.51	0.74
1:O:662:PRO:C	1:O:663:LEU:HD23	2.08	0.74
1:L:662:PRO:C	1:L:663:LEU:HD23	2.08	0.74
1:J:128:ASN:HD21	1:J:180:GLY:HA2	1.52	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:696:LEU:HD12	1:K:697:THR:N	2.02	0.74
1:P:701:VAL:O	1:P:703:PRO:HD3	1.88	0.74
1:I:292:ARG:C	1:I:293:LEU:HD23	2.08	0.74
1:J:292:ARG:C	1:J:293:LEU:HD23	2.08	0.74
1:N:336:ARG:HH11	1:N:336:ARG:HG2	1.52	0.74
1:M:822:LEU:HD12	1:M:824:GLN:N	2.03	0.74
1:J:701:VAL:O	1:J:703:PRO:HD3	1.88	0.74
1:O:701:VAL:O	1:O:703:PRO:HD3	1.88	0.74
1:I:701:VAL:O	1:I:703:PRO:HD3	1.88	0.74
1:K:46:ARG:NH1	1:K:46:ARG:HG3	2.02	0.73
1:M:419:GLY:HA2	1:P:282:ARG:NH1	2.02	0.73
1:O:654:TRP:NE1	1:O:666:GLY:HA3	2.02	0.73
1:O:856:TYR:HD2	1:O:864:MET:HE2	1.53	0.73
1:N:701:VAL:O	1:N:703:PRO:HD3	1.88	0.73
1:M:46:ARG:HG3	1:M:46:ARG:NH1	2.02	0.73
1:I:230:ARG:HG3	1:I:230:ARG:HH11	1.51	0.73
1:L:654:TRP:NE1	1:L:666:GLY:HA3	2.02	0.73
1:L:701:VAL:O	1:L:703:PRO:HD3	1.88	0.73
1:I:423:MET:HB2	1:L:282:ARG:HG3	1.70	0.73
1:K:662:PRO:C	1:K:663:LEU:HD23	2.08	0.73
1:J:336:ARG:HH11	1:J:336:ARG:HG2	1.52	0.73
1:O:128:ASN:HD21	1:O:180:GLY:HA2	1.52	0.73
1:N:856:TYR:HD2	1:N:864:MET:HE2	1.52	0.73
1:M:292:ARG:C	1:M:293:LEU:HD23	2.08	0.73
1:K:822:LEU:HD12	1:K:824:GLN:N	2.03	0.73
1:I:822:LEU:HD12	1:I:824:GLN:N	2.03	0.73
1:N:437:SER:HB2	5:N:4350:HOH:O	1.88	0.73
1:K:701:VAL:O	1:K:703:PRO:HD3	1.88	0.73
1:P:662:PRO:C	1:P:663:LEU:HD23	2.08	0.73
1:J:662:PRO:C	1:J:663:LEU:HD23	2.08	0.73
1:N:128:ASN:HD21	1:N:180:GLY:HA2	1.52	0.73
1:I:128:ASN:HD21	1:I:180:GLY:HA2	1.52	0.73
1:P:696:LEU:HD12	1:P:697:THR:H	1.52	0.73
1:I:662:PRO:C	1:I:663:LEU:HD23	2.08	0.73
1:O:822:LEU:HD12	1:O:824:GLN:N	2.03	0.73
1:P:748:CME:C	1:P:749:ILE:HD13	2.19	0.73
1:K:128:ASN:HD21	1:K:180:GLY:HA2	1.52	0.73
1:O:46:ARG:HG3	1:O:46:ARG:NH1	2.02	0.73
1:N:822:LEU:HD12	1:N:824:GLN:N	2.03	0.73
1:I:43:ARG:NH1	1:I:43:ARG:HG2	1.94	0.72
1:J:748:CME:C	1:J:749:ILE:HD13	2.19	0.72
1:L:128:ASN:HD21	1:L:180:GLY:HA2	1.52	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:49:GLN:NE2	1:K:49:GLN:H	1.87	0.72
1:O:748:CME:C	1:O:749:ILE:HD13	2.19	0.72
1:M:748:CME:C	1:M:749:ILE:HD13	2.19	0.72
1:I:651:LEU:HD12	1:I:652:LEU:N	2.04	0.72
1:K:292:ARG:C	1:K:293:LEU:HD23	2.08	0.72
1:K:748:CME:C	1:K:749:ILE:HD13	2.19	0.72
1:O:49:GLN:NE2	1:O:49:GLN:H	1.87	0.72
1:J:49:GLN:NE2	1:J:49:GLN:H	1.87	0.72
1:L:336:ARG:HG2	1:L:336:ARG:HH11	1.52	0.72
1:M:651:LEU:HD12	1:M:652:LEU:N	2.05	0.72
1:M:49:GLN:H	1:M:49:GLN:NE2	1.87	0.72
1:L:748:CME:C	1:L:749:ILE:HD13	2.19	0.72
1:J:822:LEU:HD12	1:J:824:GLN:N	2.03	0.72
1:M:701:VAL:O	1:M:703:PRO:HD3	1.88	0.72
1:N:748:CME:C	1:N:749:ILE:HD13	2.19	0.72
1:M:188:VAL:C	1:M:189:LEU:HD23	2.10	0.72
1:M:11:LEU:N	1:M:11:LEU:HD23	2.05	0.72
1:I:748:CME:C	1:I:749:ILE:HD13	2.19	0.72
1:L:651:LEU:HD12	1:L:652:LEU:N	2.04	0.72
1:O:651:LEU:HD12	1:O:652:LEU:N	2.04	0.72
1:L:822:LEU:HD12	1:L:824:GLN:N	2.03	0.72
1:P:188:VAL:C	1:P:189:LEU:HD23	2.10	0.72
1:P:49:GLN:H	1:P:49:GLN:NE2	1.87	0.72
1:N:49:GLN:NE2	1:N:49:GLN:H	1.87	0.72
1:J:651:LEU:HD12	1:J:652:LEU:N	2.04	0.72
1:K:651:LEU:HD12	1:K:652:LEU:N	2.04	0.72
1:K:188:VAL:C	1:K:189:LEU:HD23	2.10	0.72
1:N:11:LEU:HD23	1:N:11:LEU:N	2.05	0.72
1:I:188:VAL:C	1:I:189:LEU:HD23	2.10	0.71
1:K:11:LEU:N	1:K:11:LEU:HD23	2.05	0.71
1:L:49:GLN:H	1:L:49:GLN:NE2	1.87	0.71
1:J:188:VAL:C	1:J:189:LEU:HD23	2.10	0.71
1:N:651:LEU:HD12	1:N:652:LEU:N	2.04	0.71
1:J:240:LEU:HD12	1:J:241:GLU:H	1.56	0.71
1:K:336:ARG:HG2	1:K:336:ARG:HH11	1.52	0.71
1:L:856:TYR:HD2	1:L:864:MET:HE2	1.55	0.71
1:P:240:LEU:HD12	1:P:241:GLU:H	1.56	0.71
1:L:188:VAL:C	1:L:189:LEU:HD23	2.10	0.71
1:J:46:ARG:NH1	1:J:46:ARG:HG3	2.02	0.71
1:P:651:LEU:HD12	1:P:652:LEU:N	2.04	0.71
1:M:230:ARG:HG3	1:M:230:ARG:NH1	2.06	0.71
1:I:278:ILE:H	1:I:278:ILE:HD12	1.56	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:230:ARG:NH1	1:L:230:ARG:HG3	2.06	0.71
1:O:188:VAL:C	1:O:189:LEU:HD23	2.10	0.71
1:P:336:ARG:HH11	1:P:336:ARG:HG2	1.52	0.71
1:N:282:ARG:NH1	1:O:419:GLY:HA2	2.05	0.71
1:L:681:GLU:HA	1:L:681:GLU:OE2	1.90	0.71
1:I:49:GLN:NE2	1:I:49:GLN:H	1.87	0.71
1:O:43:ARG:HG2	1:O:43:ARG:NH1	1.94	0.71
1:I:46:ARG:HG3	1:I:46:ARG:NH1	2.02	0.71
1:P:278:ILE:H	1:P:278:ILE:HD12	1.56	0.71
1:K:278:ILE:HD12	1:K:278:ILE:H	1.56	0.71
1:O:11:LEU:N	1:O:11:LEU:HD23	2.05	0.71
1:P:681:GLU:OE2	1:P:681:GLU:HA	1.90	0.71
1:O:336:ARG:HG2	1:O:336:ARG:HH11	1.52	0.71
1:K:681:GLU:OE2	1:K:681:GLU:HA	1.90	0.71
1:J:437:SER:HB2	5:J:7508:HOH:O	1.90	0.70
1:P:230:ARG:HG3	1:P:230:ARG:NH1	2.05	0.70
1:N:188:VAL:C	1:N:189:LEU:HD23	2.10	0.70
1:I:11:LEU:N	1:I:11:LEU:HD23	2.05	0.70
1:K:622:HIS:O	1:K:625:GLN:HG2	1.91	0.70
1:I:856:TYR:HD2	1:I:864:MET:HE2	1.54	0.70
1:N:740:LEU:HD12	1:N:741:THR:N	2.06	0.70
1:L:920:LEU:HB3	1:L:921:PRO:HD2	1.73	0.70
1:O:920:LEU:HB3	1:O:921:PRO:HD2	1.73	0.70
1:O:278:ILE:H	1:O:278:ILE:HD12	1.56	0.70
1:M:681:GLU:OE2	1:M:681:GLU:HA	1.90	0.70
1:N:622:HIS:O	1:N:625:GLN:HG2	1.91	0.70
1:I:740:LEU:HD12	1:I:741:THR:N	2.06	0.70
1:P:46:ARG:HG3	1:P:46:ARG:NH1	2.02	0.70
1:M:920:LEU:HB3	1:M:921:PRO:HD2	1.73	0.70
1:P:622:HIS:O	1:P:625:GLN:HG2	1.91	0.70
1:L:11:LEU:HD23	1:L:11:LEU:N	2.05	0.70
1:P:11:LEU:N	1:P:11:LEU:HD23	2.05	0.70
1:J:11:LEU:HD23	1:J:11:LEU:N	2.05	0.70
1:I:681:GLU:OE2	1:I:681:GLU:HA	1.90	0.70
1:I:240:LEU:HD12	1:I:241:GLU:H	1.56	0.70
1:K:240:LEU:HD12	1:K:241:GLU:H	1.56	0.70
1:J:278:ILE:HD12	1:J:278:ILE:H	1.56	0.70
1:N:278:ILE:HD12	1:N:278:ILE:H	1.56	0.70
1:P:1017:GLN:HB3	5:P:4679:HOH:O	1.92	0.70
1:M:622:HIS:O	1:M:625:GLN:HG2	1.91	0.70
1:K:1017:GLN:HB3	5:K:7510:HOH:O	1.92	0.70
1:O:622:HIS:O	1:O:625:GLN:HG2	1.91	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:230:ARG:NH1	1:O:230:ARG:HG3	2.05	0.70
1:N:230:ARG:NH1	1:N:230:ARG:HG3	2.06	0.70
1:L:278:ILE:HD12	1:L:278:ILE:H	1.56	0.70
1:I:577:LYS:O	1:I:584:PRO:HA	1.92	0.70
1:J:622:HIS:O	1:J:625:GLN:HG2	1.91	0.70
1:J:78:LEU:HB3	1:J:79:PRO:HD2	1.74	0.70
1:M:577:LYS:O	1:M:584:PRO:HA	1.92	0.70
1:L:240:LEU:HD12	1:L:241:GLU:H	1.56	0.70
1:I:622:HIS:O	1:I:625:GLN:HG2	1.91	0.70
1:L:622:HIS:O	1:L:625:GLN:HG2	1.91	0.70
1:O:681:GLU:HA	1:O:681:GLU:OE2	1.90	0.70
1:P:78:LEU:HB3	1:P:79:PRO:HD2	1.74	0.70
1:M:278:ILE:HD12	1:M:278:ILE:H	1.56	0.69
1:N:681:GLU:HA	1:N:681:GLU:OE2	1.90	0.69
1:I:78:LEU:HB3	1:I:79:PRO:HD2	1.74	0.69
1:J:681:GLU:OE2	1:J:681:GLU:HA	1.90	0.69
1:P:920:LEU:HB3	1:P:921:PRO:HD2	1.73	0.69
1:K:293:LEU:N	1:K:293:LEU:HD23	2.07	0.69
1:M:1017:GLN:HB3	5:M:7510:HOH:O	1.92	0.69
1:I:1017:GLN:HB3	5:I:7510:HOH:O	1.92	0.69
1:L:1017:GLN:HB3	5:L:7510:HOH:O	1.92	0.69
1:K:920:LEU:HB3	1:K:921:PRO:HD2	1.73	0.69
1:N:577:LYS:O	1:N:584:PRO:HA	1.92	0.69
1:N:920:LEU:HB3	1:N:921:PRO:HD2	1.73	0.69
1:P:293:LEU:HD23	1:P:293:LEU:N	2.07	0.69
1:K:78:LEU:HB3	1:K:79:PRO:HD2	1.74	0.69
1:M:43:ARG:HG2	1:M:43:ARG:NH1	1.94	0.69
1:O:740:LEU:HD12	1:O:741:THR:N	2.06	0.69
1:O:240:LEU:HD12	1:O:241:GLU:H	1.56	0.69
1:P:856:TYR:HD2	1:P:864:MET:HE2	1.55	0.69
1:M:658:LEU:O	1:M:661:LYS:HD3	1.93	0.69
1:P:577:LYS:O	1:P:584:PRO:HA	1.92	0.69
1:M:293:LEU:N	1:M:293:LEU:HD23	2.07	0.69
1:M:861:SER:OG	1:M:863:GLN:HG3	1.93	0.69
1:I:861:SER:OG	1:I:863:GLN:HG3	1.93	0.69
1:J:577:LYS:O	1:J:584:PRO:HA	1.92	0.69
1:N:240:LEU:HD12	1:N:241:GLU:H	1.56	0.69
1:I:230:ARG:HG3	1:I:230:ARG:NH1	2.05	0.69
1:K:658:LEU:O	1:K:661:LYS:HD3	1.93	0.69
1:I:658:LEU:O	1:I:661:LYS:HD3	1.93	0.69
1:L:78:LEU:HB3	1:L:79:PRO:HD2	1.74	0.69
1:O:78:LEU:HB3	1:O:79:PRO:HD2	1.74	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:861:SER:OG	1:O:863:GLN:HG3	1.93	0.69
1:O:577:LYS:O	1:O:584:PRO:HA	1.92	0.69
1:J:920:LEU:HB3	1:J:921:PRO:HD2	1.73	0.69
1:O:1017:GLN:HB3	5:O:7510:HOH:O	1.92	0.69
1:N:129:VAL:HG23	1:N:182:ASN:ND2	2.08	0.69
1:I:673:ALA:HB1	1:I:674:PRO:HD2	1.75	0.69
1:M:129:VAL:HG23	1:M:182:ASN:ND2	2.08	0.69
1:N:658:LEU:O	1:N:661:LYS:HD3	1.93	0.69
1:N:861:SER:OG	1:N:863:GLN:HG3	1.93	0.69
1:P:861:SER:OG	1:P:863:GLN:HG3	1.93	0.69
1:J:129:VAL:HG23	1:J:182:ASN:ND2	2.08	0.69
1:K:577:LYS:O	1:K:584:PRO:HA	1.92	0.69
1:M:240:LEU:HD12	1:M:241:GLU:H	1.55	0.68
1:M:322:LEU:HD11	1:M:324:GLU:O	1.94	0.68
1:O:658:LEU:O	1:O:661:LYS:HD3	1.93	0.68
1:J:861:SER:OG	1:J:863:GLN:HG3	1.93	0.68
1:M:78:LEU:HB3	1:M:79:PRO:HD2	1.74	0.68
1:I:920:LEU:HB3	1:I:921:PRO:HD2	1.73	0.68
1:J:230:ARG:HG3	1:J:230:ARG:NH1	2.06	0.68
1:M:856:TYR:CD2	1:M:864:MET:HE2	2.28	0.68
1:J:322:LEU:HD11	1:J:324:GLU:O	1.94	0.68
1:N:1017:GLN:HB3	5:N:4346:HOH:O	1.92	0.68
1:N:673:ALA:HB1	1:N:674:PRO:HD2	1.75	0.68
1:N:423:MET:HB2	1:O:282:ARG:HG3	1.73	0.68
1:K:673:ALA:HB1	1:K:674:PRO:HD2	1.75	0.68
1:P:322:LEU:HD11	1:P:324:GLU:O	1.94	0.68
1:L:658:LEU:O	1:L:661:LYS:HD3	1.93	0.68
1:P:658:LEU:O	1:P:661:LYS:HD3	1.93	0.68
1:J:1017:GLN:HB3	5:J:7510:HOH:O	1.92	0.68
1:M:745:MET:HA	1:M:745:MET:HE2	1.76	0.68
1:N:293:LEU:HD23	1:N:293:LEU:N	2.07	0.68
1:I:293:LEU:N	1:I:293:LEU:HD23	2.07	0.68
1:O:129:VAL:HG23	1:O:182:ASN:ND2	2.08	0.68
1:J:282:ARG:HG3	1:K:423:MET:HB2	1.74	0.68
1:L:673:ALA:HB1	1:L:674:PRO:HD2	1.75	0.68
1:K:230:ARG:HG3	1:K:230:ARG:NH1	2.06	0.68
1:K:3:ILE:HG13	1:K:4:THR:N	2.09	0.68
1:K:861:SER:OG	1:K:863:GLN:HG3	1.93	0.68
1:L:577:LYS:O	1:L:584:PRO:HA	1.92	0.68
1:O:322:LEU:HD11	1:O:324:GLU:O	1.94	0.68
1:I:282:ARG:HG3	1:L:423:MET:HB2	1.75	0.68
1:J:673:ALA:HB1	1:J:674:PRO:HD2	1.75	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:46:ARG:HG3	1:N:46:ARG:NH1	2.02	0.68
1:K:322:LEU:HD11	1:K:324:GLU:O	1.94	0.68
1:L:293:LEU:HD23	1:L:293:LEU:N	2.07	0.68
1:J:293:LEU:HD23	1:J:293:LEU:N	2.07	0.68
1:I:322:LEU:HD11	1:I:324:GLU:O	1.93	0.68
1:N:78:LEU:HB3	1:N:79:PRO:HD2	1.74	0.68
1:N:210:ARG:HH12	1:N:395:HIS:N	1.92	0.68
1:P:210:ARG:HH12	1:P:395:HIS:N	1.92	0.68
1:M:673:ALA:HB1	1:M:674:PRO:HD2	1.75	0.68
1:P:740:LEU:HD12	1:P:741:THR:N	2.06	0.67
1:N:322:LEU:HD11	1:N:324:GLU:O	1.94	0.67
1:K:427:THR:HA	1:K:436:MET:HE2	1.74	0.67
1:P:36:TRP:CE2	1:P:42:ALA:HA	2.30	0.67
1:O:293:LEU:N	1:O:293:LEU:HD23	2.07	0.67
1:N:278:ILE:N	1:N:278:ILE:HD12	2.10	0.67
1:K:129:VAL:HG23	1:K:182:ASN:ND2	2.08	0.67
1:K:740:LEU:HD12	1:K:741:THR:N	2.06	0.67
1:J:336:ARG:HG2	1:J:336:ARG:NH1	2.09	0.67
1:O:278:ILE:N	1:O:278:ILE:HD12	2.10	0.67
1:K:77:ASP:C	1:K:78:LEU:HD23	2.15	0.67
1:L:129:VAL:HG23	1:L:182:ASN:ND2	2.08	0.67
1:P:129:VAL:HG23	1:P:182:ASN:ND2	2.08	0.67
1:P:749:ILE:HD13	1:P:749:ILE:N	2.10	0.67
1:I:129:VAL:HG23	1:I:182:ASN:ND2	2.08	0.67
1:P:437:SER:HB2	5:P:4520:HOH:O	1.94	0.67
1:P:217:LYS:HG2	1:P:218:PRO:HD2	1.77	0.67
1:O:673:ALA:HB1	1:O:674:PRO:HD2	1.75	0.67
1:J:740:LEU:HD12	1:J:741:THR:N	2.06	0.67
1:I:1021:CME:CZ	1:I:1021:CME:HB3	2.21	0.67
1:K:42:ALA:O	1:K:310:ARG:NH1	2.28	0.67
1:I:36:TRP:CE2	1:I:42:ALA:HA	2.30	0.67
1:P:24:LEU:HB2	1:P:161:TYR:HB3	1.77	0.67
1:M:24:LEU:HB2	1:M:161:TYR:HB3	1.77	0.67
1:M:217:LYS:HG2	1:M:218:PRO:HD2	1.76	0.67
1:M:42:ALA:O	1:M:310:ARG:NH1	2.28	0.67
1:O:336:ARG:HG2	1:O:336:ARG:NH1	2.09	0.67
1:J:278:ILE:HD12	1:J:278:ILE:N	2.10	0.67
1:M:77:ASP:C	1:M:78:LEU:HD23	2.15	0.67
1:I:3:ILE:HG13	1:I:4:THR:N	2.09	0.67
1:P:673:ALA:HB1	1:P:674:PRO:HD2	1.75	0.67
1:K:210:ARG:HH12	1:K:395:HIS:N	1.92	0.67
1:L:322:LEU:HD11	1:L:324:GLU:O	1.94	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:42:ALA:O	1:N:310:ARG:NH1	2.28	0.67
1:L:278:ILE:HD12	1:L:278:ILE:N	2.10	0.67
1:J:658:LEU:O	1:J:661:LYS:HD3	1.93	0.67
1:N:749:ILE:N	1:N:749:ILE:HD13	2.10	0.67
1:O:427:THR:HA	1:O:436:MET:HE2	1.75	0.67
1:L:42:ALA:O	1:L:310:ARG:NH1	2.28	0.67
1:M:36:TRP:CE2	1:M:42:ALA:HA	2.30	0.67
1:P:77:ASP:C	1:P:78:LEU:HD23	2.15	0.67
1:L:77:ASP:C	1:L:78:LEU:HD23	2.15	0.67
1:O:77:ASP:C	1:O:78:LEU:HD23	2.15	0.67
1:O:377:LEU:HD22	1:O:708:TRP:HA	1.77	0.67
1:M:210:ARG:HH12	1:M:395:HIS:N	1.92	0.67
1:L:36:TRP:CE2	1:L:42:ALA:HA	2.30	0.67
1:N:36:TRP:CE2	1:N:42:ALA:HA	2.30	0.67
1:L:336:ARG:HG2	1:L:336:ARG:NH1	2.09	0.67
1:I:278:ILE:N	1:I:278:ILE:HD12	2.10	0.67
1:I:77:ASP:C	1:I:78:LEU:HD23	2.15	0.67
1:K:856:TYR:HD2	1:K:864:MET:HE2	1.60	0.67
1:K:749:ILE:N	1:K:749:ILE:HD13	2.10	0.67
1:L:740:LEU:HD12	1:L:741:THR:N	2.06	0.67
1:I:217:LYS:HG2	1:I:218:PRO:HD2	1.76	0.67
1:I:24:LEU:HB2	1:I:161:TYR:HB3	1.77	0.67
1:N:77:ASP:C	1:N:78:LEU:HD23	2.15	0.67
1:L:861:SER:OG	1:L:863:GLN:HG3	1.93	0.67
1:I:59:ARG:NH2	1:I:81:ALA:O	2.28	0.67
1:P:377:LEU:HD22	1:P:708:TRP:HA	1.77	0.67
1:M:427:THR:HA	1:M:436:MET:HE2	1.77	0.66
1:L:24:LEU:HB2	1:L:161:TYR:HB3	1.77	0.66
1:J:24:LEU:HB2	1:J:161:TYR:HB3	1.77	0.66
1:K:278:ILE:HD12	1:K:278:ILE:N	2.10	0.66
1:M:939:CYS:HA	1:M:956:GLN:HB3	1.78	0.66
1:N:682:LEU:CD2	1:N:683:PRO:HD2	2.26	0.66
1:O:36:TRP:CE2	1:O:42:ALA:HA	2.30	0.66
1:J:42:ALA:O	1:J:310:ARG:NH1	2.28	0.66
1:L:217:LYS:HG2	1:L:218:PRO:HD2	1.76	0.66
1:P:278:ILE:N	1:P:278:ILE:HD12	2.10	0.66
1:P:117:GLU:N	1:P:117:GLU:OE1	2.27	0.66
1:K:377:LEU:HD22	1:K:708:TRP:HA	1.77	0.66
1:P:114:VAL:HG13	1:P:115:PRO:HD2	1.78	0.66
1:J:36:TRP:CE2	1:J:42:ALA:HA	2.30	0.66
1:N:282:ARG:HG3	1:O:423:MET:HB2	1.77	0.66
1:N:377:LEU:HD22	1:N:708:TRP:HA	1.77	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:433:LEU:HB3	1:J:434:PRO:HD3	1.77	0.66
1:P:433:LEU:HB3	1:P:434:PRO:HD3	1.77	0.66
1:J:77:ASP:C	1:J:78:LEU:HD23	2.15	0.66
1:K:454:ILE:HG13	1:K:455:ILE:HG13	1.78	0.66
1:K:30:HIS:HB2	1:K:31:PRO:HD2	1.78	0.66
1:M:30:HIS:HB2	1:M:31:PRO:HD2	1.78	0.66
1:M:377:LEU:HD22	1:M:708:TRP:HA	1.77	0.66
1:L:46:ARG:HG3	1:L:46:ARG:NH1	2.02	0.66
1:N:114:VAL:HG13	1:N:115:PRO:HD2	1.78	0.66
1:K:682:LEU:CD2	1:K:683:PRO:HD2	2.26	0.66
1:P:42:ALA:O	1:P:310:ARG:NH1	2.28	0.66
1:N:24:LEU:HB2	1:N:161:TYR:HB3	1.77	0.66
1:M:278:ILE:HD12	1:M:278:ILE:N	2.10	0.66
1:I:454:ILE:HG13	1:I:455:ILE:HG13	1.78	0.66
1:J:377:LEU:HD22	1:J:708:TRP:HA	1.77	0.66
1:L:59:ARG:NH2	1:L:81:ALA:O	2.28	0.66
1:I:114:VAL:HG13	1:I:115:PRO:HD2	1.78	0.66
1:J:114:VAL:HG13	1:J:115:PRO:HD2	1.78	0.66
1:P:682:LEU:CD2	1:P:683:PRO:HD2	2.26	0.66
1:I:917:ARG:NH2	1:I:943:GLU:OE1	2.29	0.66
1:I:117:GLU:N	1:I:117:GLU:OE1	2.27	0.66
1:J:30:HIS:HB2	1:J:31:PRO:HD2	1.78	0.66
1:O:917:ARG:NH2	1:O:943:GLU:OE1	2.29	0.66
1:M:59:ARG:NH2	1:M:81:ALA:O	2.29	0.66
1:N:917:ARG:NH2	1:N:943:GLU:OE1	2.29	0.66
1:I:745:MET:HA	1:I:745:MET:HE2	1.78	0.66
1:N:360:HIS:HE1	1:N:362:LEU:HB2	1.61	0.66
1:K:114:VAL:HG13	1:K:115:PRO:HD2	1.78	0.66
1:M:433:LEU:HB3	1:M:434:PRO:HD3	1.77	0.66
1:I:42:ALA:O	1:I:310:ARG:NH1	2.28	0.66
1:N:282:ARG:HD3	1:O:418:HIS:O	1.96	0.66
1:P:917:ARG:NH2	1:P:943:GLU:OE1	2.29	0.66
1:J:917:ARG:NH2	1:J:943:GLU:OE1	2.29	0.66
1:J:3:ILE:HG13	1:J:4:THR:N	2.09	0.66
1:L:30:HIS:HB2	1:L:31:PRO:HD2	1.78	0.66
1:J:939:CYS:HA	1:J:956:GLN:HB3	1.77	0.66
1:J:59:ARG:NH2	1:J:81:ALA:O	2.28	0.66
1:I:749:ILE:N	1:I:749:ILE:HD13	2.10	0.66
1:K:36:TRP:CE2	1:K:42:ALA:HA	2.30	0.66
1:O:24:LEU:HB2	1:O:161:TYR:HB3	1.77	0.66
1:M:336:ARG:NH1	1:M:336:ARG:HG2	2.09	0.66
1:P:59:ARG:NH2	1:P:81:ALA:O	2.29	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:454:ILE:HG13	1:L:455:ILE:HG13	1.78	0.66
1:M:454:ILE:HG13	1:M:455:ILE:HG13	1.78	0.66
1:K:59:ARG:NH2	1:K:81:ALA:O	2.28	0.66
1:L:749:ILE:HD13	1:L:749:ILE:N	2.10	0.66
1:M:749:ILE:HD13	1:M:749:ILE:N	2.10	0.66
1:O:360:HIS:HE1	1:O:362:LEU:HB2	1.61	0.66
1:M:1021:CME:HB3	1:M:1021:CME:CZ	2.21	0.66
1:K:433:LEU:HB3	1:K:434:PRO:HD3	1.77	0.66
1:J:114:VAL:CG1	1:J:191:TRP:HB2	2.26	0.66
1:O:682:LEU:CD2	1:O:683:PRO:HD2	2.26	0.66
1:L:210:ARG:HH12	1:L:395:HIS:N	1.92	0.66
1:I:360:HIS:HE1	1:I:362:LEU:HB2	1.61	0.66
1:J:1021:CME:HB3	1:J:1021:CME:CZ	2.21	0.66
1:L:682:LEU:CD2	1:L:683:PRO:HD2	2.26	0.66
1:O:114:VAL:HG13	1:O:115:PRO:HD2	1.78	0.66
1:K:217:LYS:HG2	1:K:218:PRO:HD2	1.76	0.66
1:N:217:LYS:HG2	1:N:218:PRO:HD2	1.76	0.66
1:K:336:ARG:HG2	1:K:336:ARG:NH1	2.09	0.66
1:J:423:MET:HB2	1:K:282:ARG:HG3	1.77	0.66
1:I:939:CYS:HA	1:I:956:GLN:HB3	1.78	0.66
1:P:246:MET:HG2	1:P:274:PHE:CE2	2.31	0.66
1:O:745:MET:HE2	1:O:745:MET:HA	1.77	0.65
1:N:336:ARG:NH1	1:N:336:ARG:HG2	2.09	0.65
1:O:246:MET:HG2	1:O:274:PHE:CE2	2.31	0.65
1:M:753:ASN:OD1	1:M:753:ASN:N	2.30	0.65
1:I:377:LEU:HD22	1:I:708:TRP:HA	1.77	0.65
1:N:59:ARG:NH2	1:N:81:ALA:O	2.29	0.65
1:N:246:MET:HG2	1:N:274:PHE:CE2	2.31	0.65
1:I:246:MET:HG2	1:I:274:PHE:CE2	2.31	0.65
1:K:1021:CME:HB3	1:K:1021:CME:CZ	2.21	0.65
1:L:114:VAL:CG1	1:L:191:TRP:HB2	2.26	0.65
1:J:217:LYS:HG2	1:J:218:PRO:HD2	1.76	0.65
1:I:433:LEU:HB3	1:I:434:PRO:HD3	1.77	0.65
1:L:939:CYS:HA	1:L:956:GLN:HB3	1.78	0.65
1:L:917:ARG:NH2	1:L:943:GLU:OE1	2.29	0.65
1:P:114:VAL:CG1	1:P:191:TRP:HB2	2.26	0.65
1:K:24:LEU:HB2	1:K:161:TYR:HB3	1.77	0.65
1:N:745:MET:HA	1:N:745:MET:HE2	1.78	0.65
1:O:42:ALA:O	1:O:310:ARG:NH1	2.28	0.65
1:I:703:PRO:O	1:I:711:ALA:HB1	1.97	0.65
1:N:703:PRO:O	1:N:711:ALA:HB1	1.97	0.65
1:N:939:CYS:HA	1:N:956:GLN:HB3	1.78	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:246:MET:HG2	1:K:274:PHE:CE2	2.31	0.65
1:N:232:ASN:ND2	1:N:234:ASP:OD1	2.30	0.65
1:O:59:ARG:NH2	1:O:81:ALA:O	2.29	0.65
1:L:3:ILE:HG13	1:L:4:THR:N	2.09	0.65
1:J:237:ARG:HH11	1:J:237:ARG:CB	2.10	0.65
1:P:360:HIS:HE1	1:P:362:LEU:HB2	1.61	0.65
1:O:217:LYS:HG2	1:O:218:PRO:HD2	1.76	0.65
1:O:433:LEU:HB3	1:O:434:PRO:HD3	1.77	0.65
1:M:917:ARG:NH2	1:M:943:GLU:OE1	2.29	0.65
1:N:454:ILE:HG13	1:N:455:ILE:HG13	1.78	0.65
1:P:30:HIS:HB2	1:P:31:PRO:HD2	1.78	0.65
1:J:749:ILE:N	1:J:749:ILE:HD13	2.10	0.65
1:P:347:LYS:HB3	1:P:348:PRO:HD2	1.79	0.65
1:N:800:ARG:HB3	1:N:800:ARG:NH1	2.12	0.65
1:K:939:CYS:HA	1:K:956:GLN:HB3	1.77	0.65
1:L:237:ARG:HH11	1:L:237:ARG:CB	2.10	0.65
1:N:30:HIS:HB2	1:N:31:PRO:HD2	1.78	0.65
1:M:360:HIS:HE1	1:M:362:LEU:HB2	1.61	0.65
1:I:114:VAL:CG1	1:I:191:TRP:HB2	2.26	0.65
1:M:682:LEU:CD2	1:M:683:PRO:HD2	2.26	0.65
1:J:210:ARG:HH12	1:J:395:HIS:N	1.92	0.65
1:J:682:LEU:CD2	1:J:683:PRO:HD2	2.26	0.65
1:N:856:TYR:CD2	1:N:864:MET:HE2	2.31	0.65
1:O:3:ILE:HG13	1:O:4:THR:N	2.09	0.65
1:O:749:ILE:HD13	1:O:749:ILE:N	2.10	0.65
1:I:336:ARG:HG2	1:I:336:ARG:NH1	2.09	0.65
1:O:703:PRO:O	1:O:711:ALA:HB1	1.97	0.65
1:L:703:PRO:O	1:L:711:ALA:HB1	1.97	0.65
1:K:703:PRO:O	1:K:711:ALA:HB1	1.97	0.65
1:J:800:ARG:NH1	1:J:800:ARG:HB3	2.12	0.65
1:P:3:ILE:HG13	1:P:4:THR:N	2.09	0.65
1:P:454:ILE:HG13	1:P:455:ILE:HG13	1.78	0.65
1:K:347:LYS:HB3	1:K:348:PRO:HD2	1.79	0.65
1:I:682:LEU:CD2	1:I:683:PRO:HD2	2.26	0.65
1:M:114:VAL:CG1	1:M:191:TRP:HB2	2.26	0.65
1:O:114:VAL:CG1	1:O:191:TRP:HB2	2.26	0.65
1:L:433:LEU:HB3	1:L:434:PRO:HD3	1.77	0.65
1:J:246:MET:HG2	1:J:274:PHE:CE2	2.31	0.65
1:K:237:ARG:CB	1:K:237:ARG:HH11	2.10	0.65
1:I:800:ARG:NH1	1:I:800:ARG:HB3	2.12	0.65
1:M:114:VAL:HG13	1:M:115:PRO:HD2	1.78	0.65
1:I:210:ARG:HH12	1:I:395:HIS:N	1.92	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:210:ARG:HH12	1:O:395:HIS:N	1.92	0.65
1:J:217:LYS:HE3	1:J:324:GLU:OE1	1.98	0.65
1:L:36:TRP:C	1:L:37:ARG:HD3	2.18	0.65
1:P:703:PRO:O	1:P:711:ALA:HB1	1.97	0.65
1:J:703:PRO:O	1:J:711:ALA:HB1	1.97	0.65
1:N:237:ARG:HH11	1:N:237:ARG:CB	2.10	0.65
1:J:454:ILE:HG13	1:J:455:ILE:HG13	1.78	0.65
1:O:30:HIS:HB2	1:O:31:PRO:HD2	1.78	0.65
1:I:30:HIS:HB2	1:I:31:PRO:HD2	1.78	0.65
1:L:246:MET:HG2	1:L:274:PHE:CE2	2.31	0.65
1:O:939:CYS:HA	1:O:956:GLN:HB3	1.78	0.65
1:P:232:ASN:ND2	1:P:234:ASP:OD1	2.30	0.65
1:N:114:VAL:CG1	1:N:191:TRP:HB2	2.26	0.64
1:L:114:VAL:HG13	1:L:115:PRO:HD2	1.78	0.64
1:L:232:ASN:ND2	1:L:234:ASP:OD1	2.30	0.64
1:M:759:ASN:OD1	1:M:761:GLN:N	2.30	0.64
1:K:753:ASN:OD1	1:K:753:ASN:N	2.30	0.64
1:L:377:LEU:HD22	1:L:708:TRP:HA	1.77	0.64
1:P:939:CYS:HA	1:P:956:GLN:HB3	1.77	0.64
1:K:917:ARG:NH2	1:K:943:GLU:OE1	2.29	0.64
1:L:759:ASN:OD1	1:L:761:GLN:N	2.30	0.64
1:K:114:VAL:CG1	1:K:191:TRP:HB2	2.26	0.64
1:K:36:TRP:C	1:K:37:ARG:HD3	2.18	0.64
1:M:419:GLY:HA2	1:P:282:ARG:HH11	1.63	0.64
1:M:800:ARG:NH1	1:M:800:ARG:HB3	2.12	0.64
1:O:759:ASN:OD1	1:O:761:GLN:N	2.30	0.64
1:M:3:ILE:HG13	1:M:4:THR:N	2.09	0.64
1:N:1021:CME:HB3	1:N:1021:CME:CZ	2.21	0.64
1:N:433:LEU:HB3	1:N:434:PRO:HD3	1.78	0.64
1:K:800:ARG:HB3	1:K:800:ARG:NH1	2.12	0.64
1:O:800:ARG:NH1	1:O:800:ARG:HB3	2.12	0.64
1:P:800:ARG:NH1	1:P:800:ARG:HB3	2.12	0.64
1:I:347:LYS:HB3	1:I:348:PRO:HD2	1.79	0.64
1:O:36:TRP:C	1:O:37:ARG:HD3	2.18	0.64
1:K:217:LYS:HE3	1:K:324:GLU:OE1	1.98	0.64
1:O:454:ILE:HG13	1:O:455:ILE:HG13	1.78	0.64
1:N:759:ASN:OD1	1:N:761:GLN:N	2.30	0.64
1:L:800:ARG:NH1	1:L:800:ARG:HB3	2.12	0.64
1:M:237:ARG:HH11	1:M:237:ARG:CB	2.10	0.64
1:M:246:MET:HG2	1:M:274:PHE:CE2	2.31	0.64
1:I:237:ARG:CB	1:I:237:ARG:HH11	2.10	0.64
1:M:437:SER:HB2	5:M:7508:HOH:O	1.98	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:282:ARG:HH11	1:O:419:GLY:HA2	1.61	0.64
1:N:377:LEU:CD2	1:N:708:TRP:HA	2.28	0.64
1:J:232:ASN:ND2	1:J:234:ASP:OD1	2.30	0.64
1:N:117:GLU:OE1	1:N:117:GLU:N	2.27	0.64
1:O:753:ASN:OD1	1:O:753:ASN:N	2.30	0.64
1:O:237:ARG:HH11	1:O:237:ARG:CB	2.10	0.64
1:L:427:THR:HA	1:L:436:MET:HE2	1.80	0.64
1:N:894:ARG:HD3	1:N:919:ASP:OD2	1.98	0.64
1:O:217:LYS:HE3	1:O:324:GLU:OE1	1.98	0.64
1:M:217:LYS:HE3	1:M:324:GLU:OE1	1.98	0.64
1:K:759:ASN:OD1	1:K:761:GLN:N	2.30	0.64
1:M:740:LEU:HD12	1:M:741:THR:N	2.06	0.64
1:P:36:TRP:C	1:P:37:ARG:HD3	2.18	0.64
1:I:437:SER:HB2	5:I:7508:HOH:O	1.97	0.64
1:M:36:TRP:C	1:M:37:ARG:HD3	2.18	0.64
1:K:377:LEU:CD2	1:K:708:TRP:HA	2.28	0.64
1:I:232:ASN:ND2	1:I:234:ASP:OD1	2.30	0.64
1:L:117:GLU:OE1	1:L:117:GLU:N	2.27	0.64
1:J:36:TRP:C	1:J:37:ARG:HD3	2.18	0.64
1:O:377:LEU:CD2	1:O:708:TRP:HA	2.28	0.64
1:M:377:LEU:CD2	1:M:708:TRP:HA	2.28	0.64
1:I:377:LEU:CD2	1:I:708:TRP:HA	2.28	0.64
1:P:237:ARG:CB	1:P:237:ARG:HH11	2.10	0.64
1:L:377:LEU:CD2	1:L:708:TRP:HA	2.28	0.64
1:J:347:LYS:HB3	1:J:348:PRO:HD2	1.79	0.64
1:J:701:VAL:HG12	1:J:702:GLN:N	2.13	0.64
1:M:701:VAL:HG12	1:M:702:GLN:N	2.13	0.64
1:P:377:LEU:CD2	1:P:708:TRP:HA	2.28	0.64
1:I:753:ASN:OD1	1:I:753:ASN:N	2.30	0.64
1:P:753:ASN:N	1:P:753:ASN:OD1	2.30	0.64
1:J:894:ARG:HD3	1:J:919:ASP:OD2	1.98	0.64
1:P:128:ASN:HA	1:P:180:GLY:O	1.98	0.64
1:I:36:TRP:C	1:I:37:ARG:HD3	2.18	0.64
1:P:217:LYS:HE3	1:P:324:GLU:OE1	1.98	0.64
1:K:701:VAL:HG12	1:K:702:GLN:N	2.13	0.64
1:O:117:GLU:OE1	1:O:117:GLU:N	2.27	0.64
1:O:856:TYR:CD2	1:O:864:MET:HE2	2.32	0.63
1:M:703:PRO:O	1:M:711:ALA:HB1	1.97	0.63
1:P:336:ARG:NH1	1:P:336:ARG:HG2	2.09	0.63
1:K:902:PRO:O	1:K:938:ARG:NH1	2.32	0.63
1:L:347:LYS:HB3	1:L:348:PRO:HD2	1.79	0.63
1:K:894:ARG:HD3	1:K:919:ASP:OD2	1.98	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:894:ARG:NH1	1:P:919:ASP:OD2	2.30	0.63
1:J:377:LEU:CD2	1:J:708:TRP:HA	2.28	0.63
1:M:232:ASN:ND2	1:M:234:ASP:OD1	2.30	0.63
1:N:945:ASN:OD1	1:N:950:GLN:NE2	2.30	0.63
1:N:128:ASN:HA	1:N:180:GLY:O	1.99	0.63
1:K:232:ASN:ND2	1:K:234:ASP:OD1	2.30	0.63
1:N:568:TRP:HE1	1:N:604:ASN:HD22	1.47	0.63
1:I:759:ASN:OD1	1:I:761:GLN:N	2.30	0.63
1:M:347:LYS:HB3	1:M:348:PRO:HD2	1.79	0.63
1:O:347:LYS:HB3	1:O:348:PRO:HD2	1.79	0.63
1:I:427:THR:HA	1:I:436:MET:HE2	1.78	0.63
1:P:894:ARG:HD3	1:P:919:ASP:OD2	1.98	0.63
1:N:36:TRP:C	1:N:37:ARG:HD3	2.18	0.63
1:O:917:ARG:HH22	1:O:943:GLU:CD	2.02	0.63
1:N:902:PRO:O	1:N:938:ARG:NH1	2.31	0.63
1:P:902:PRO:O	1:P:938:ARG:NH1	2.31	0.63
1:M:902:PRO:O	1:M:938:ARG:NH1	2.31	0.63
1:K:128:ASN:HA	1:K:180:GLY:O	1.98	0.63
1:I:217:LYS:HE3	1:I:324:GLU:OE1	1.98	0.63
1:N:217:LYS:HE3	1:N:324:GLU:OE1	1.98	0.63
1:I:856:TYR:CD2	1:I:864:MET:HE2	2.33	0.63
1:P:856:TYR:CD2	1:P:864:MET:HE2	2.33	0.63
1:J:579:ASP:CG	1:J:583:ASN:HB2	2.19	0.63
1:M:894:ARG:NH1	1:M:919:ASP:OD2	2.30	0.63
1:I:894:ARG:HD3	1:I:919:ASP:OD2	1.98	0.63
1:L:128:ASN:HA	1:L:180:GLY:O	1.98	0.63
1:J:37:ARG:HG3	1:J:37:ARG:HH11	1.64	0.63
1:I:701:VAL:HG12	1:I:702:GLN:N	2.13	0.63
1:K:30:HIS:ND1	1:K:31:PRO:O	2.26	0.63
1:L:917:ARG:HH22	1:L:943:GLU:CD	2.02	0.63
1:J:759:ASN:OD1	1:J:761:GLN:N	2.30	0.63
1:J:18:ASN:HD22	1:J:21:VAL:HG23	1.64	0.63
1:N:579:ASP:CG	1:N:583:ASN:HB2	2.19	0.63
1:I:128:ASN:HA	1:I:180:GLY:O	1.98	0.63
1:J:395:HIS:ND1	1:J:396:PRO:HD2	2.14	0.63
1:K:395:HIS:ND1	1:K:396:PRO:HD2	2.14	0.63
1:I:917:ARG:HH22	1:I:943:GLU:CD	2.02	0.63
1:O:232:ASN:ND2	1:O:234:ASP:OD1	2.30	0.63
1:O:902:PRO:O	1:O:938:ARG:NH1	2.31	0.63
1:K:117:GLU:OE1	1:K:117:GLU:N	2.27	0.63
1:I:599:ARG:HB2	1:I:600:GLN:OE1	1.99	0.63
1:K:599:ARG:HB2	1:K:600:GLN:OE1	1.99	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:945:ASN:OD1	1:L:950:GLN:NE2	2.30	0.63
1:O:128:ASN:HA	1:O:180:GLY:O	1.98	0.63
1:O:255:ARG:HG2	1:O:255:ARG:NH1	2.14	0.63
1:J:255:ARG:NH1	1:J:255:ARG:HG2	2.14	0.63
1:O:395:HIS:ND1	1:O:396:PRO:HD2	2.14	0.63
1:L:701:VAL:HG12	1:L:702:GLN:N	2.13	0.63
1:M:917:ARG:HH22	1:M:943:GLU:CD	2.02	0.63
1:K:917:ARG:HH22	1:K:943:GLU:CD	2.02	0.63
1:O:847:LYS:HG3	1:O:848:THR:N	2.14	0.63
1:J:902:PRO:O	1:J:938:ARG:NH1	2.32	0.63
1:M:724:GLU:O	1:N:847:LYS:NZ	2.23	0.63
1:J:128:ASN:HA	1:J:180:GLY:O	1.98	0.63
1:L:217:LYS:HE3	1:L:324:GLU:OE1	1.98	0.63
1:K:579:ASP:CG	1:K:583:ASN:HB2	2.19	0.63
1:M:847:LYS:HG3	1:M:848:THR:N	2.14	0.63
1:J:117:GLU:OE1	1:J:117:GLU:N	2.27	0.63
1:M:599:ARG:HB2	1:M:600:GLN:OE1	1.99	0.63
1:J:894:ARG:NH1	1:J:919:ASP:OD2	2.30	0.62
1:L:894:ARG:HD3	1:L:919:ASP:OD2	1.98	0.62
1:M:894:ARG:HD3	1:M:919:ASP:OD2	1.98	0.62
1:M:128:ASN:HA	1:M:180:GLY:O	1.98	0.62
1:O:190:ARG:HD3	1:O:191:TRP:CZ2	2.34	0.62
1:M:395:HIS:ND1	1:M:396:PRO:HD2	2.14	0.62
1:L:37:ARG:HH11	1:L:37:ARG:HG3	1.64	0.62
1:P:701:VAL:HG12	1:P:702:GLN:N	2.13	0.62
1:N:847:LYS:HG3	1:N:848:THR:N	2.14	0.62
1:L:753:ASN:N	1:L:753:ASN:OD1	2.30	0.62
1:P:759:ASN:OD1	1:P:761:GLN:N	2.30	0.62
1:N:347:LYS:HB3	1:N:348:PRO:HD2	1.79	0.62
1:L:894:ARG:NH1	1:L:919:ASP:OD2	2.30	0.62
1:O:894:ARG:HD3	1:O:919:ASP:OD2	1.98	0.62
1:M:37:ARG:HG3	1:M:37:ARG:HH11	1.64	0.62
1:K:742:THR:HG22	1:K:743:SER:N	2.14	0.62
1:L:742:THR:HG22	1:L:743:SER:N	2.14	0.62
1:M:742:THR:HG22	1:M:743:SER:N	2.14	0.62
1:I:579:ASP:CG	1:I:583:ASN:HB2	2.19	0.62
1:M:190:ARG:HD3	1:M:191:TRP:CZ2	2.34	0.62
1:N:395:HIS:ND1	1:N:396:PRO:HD2	2.14	0.62
1:I:395:HIS:ND1	1:I:396:PRO:HD2	2.14	0.62
1:K:37:ARG:HH11	1:K:37:ARG:HG3	1.64	0.62
1:J:742:THR:HG22	1:J:743:SER:N	2.14	0.62
1:I:255:ARG:HG2	1:I:255:ARG:NH1	2.14	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:395:HIS:ND1	1:P:396:PRO:HD2	2.14	0.62
1:O:37:ARG:HH11	1:O:37:ARG:HG3	1.64	0.62
1:L:902:PRO:O	1:L:938:ARG:NH1	2.31	0.62
1:P:599:ARG:HB2	1:P:600:GLN:OE1	1.99	0.62
1:N:287:ASP:OD2	1:O:425:ARG:NH2	2.31	0.62
1:I:18:ASN:HD22	1:I:21:VAL:HG23	1.64	0.62
1:L:360:HIS:HE1	1:L:362:LEU:HB2	1.61	0.62
1:P:37:ARG:HG3	1:P:37:ARG:HH11	1.64	0.62
1:O:701:VAL:HG12	1:O:702:GLN:N	2.13	0.62
1:P:917:ARG:HH22	1:P:943:GLU:CD	2.02	0.62
1:N:3:ILE:HG13	1:N:4:THR:N	2.09	0.62
1:J:847:LYS:HG3	1:J:848:THR:N	2.14	0.62
1:L:568:TRP:HE1	1:L:604:ASN:HD22	1.47	0.62
1:I:742:THR:HG22	1:I:743:SER:N	2.14	0.62
1:M:919:ASP:O	1:M:920:LEU:HD23	2.00	0.62
1:I:190:ARG:HD3	1:I:191:TRP:CZ2	2.35	0.62
1:J:190:ARG:HD3	1:J:191:TRP:CZ2	2.35	0.62
1:N:701:VAL:HG12	1:N:702:GLN:N	2.13	0.62
1:L:856:TYR:CD2	1:L:864:MET:HE2	2.33	0.62
1:J:753:ASN:N	1:J:753:ASN:OD1	2.30	0.62
1:I:568:TRP:HE1	1:I:604:ASN:HD22	1.47	0.62
1:J:599:ARG:HB2	1:J:600:GLN:OE1	1.99	0.62
1:N:742:THR:HG22	1:N:743:SER:N	2.14	0.62
1:N:190:ARG:HD3	1:N:191:TRP:CZ2	2.35	0.62
1:P:190:ARG:HD3	1:P:191:TRP:CZ2	2.35	0.62
1:L:395:HIS:ND1	1:L:396:PRO:HD2	2.14	0.62
1:N:599:ARG:HB2	1:N:600:GLN:OE1	1.99	0.62
1:I:945:ASN:OD1	1:I:950:GLN:NE2	2.30	0.62
1:O:579:ASP:CG	1:O:583:ASN:HB2	2.19	0.62
1:K:255:ARG:HG2	1:K:255:ARG:NH1	2.14	0.62
1:L:190:ARG:HD3	1:L:191:TRP:CZ2	2.34	0.62
1:K:190:ARG:HD3	1:K:191:TRP:CZ2	2.35	0.62
1:J:917:ARG:HH22	1:J:943:GLU:CD	2.02	0.62
1:P:568:TRP:HE1	1:P:604:ASN:HD22	1.47	0.62
1:M:127:PHE:HE2	1:M:184:LEU:HG	1.65	0.62
1:P:578:TYR:HA	1:P:583:ASN:O	2.00	0.62
1:P:579:ASP:CG	1:P:583:ASN:HB2	2.19	0.62
1:K:919:ASP:O	1:K:920:LEU:HD23	2.00	0.62
1:L:579:ASP:CG	1:L:583:ASN:HB2	2.19	0.62
1:N:917:ARG:HH22	1:N:943:GLU:CD	2.02	0.62
1:M:579:ASP:CG	1:M:583:ASN:HB2	2.19	0.62
1:M:194:GLY:O	1:M:198:GLU:HG3	2.00	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:360:HIS:HE1	1:J:362:LEU:HB2	1.61	0.62
1:O:4:THR:HA	1:O:9:VAL:HG11	1.82	0.62
1:I:902:PRO:O	1:I:938:ARG:NH1	2.32	0.62
1:O:568:TRP:HE1	1:O:604:ASN:HD22	1.47	0.62
1:N:753:ASN:N	1:N:753:ASN:OD1	2.30	0.62
1:P:178:ARG:NH1	1:P:181:GLU:O	2.33	0.62
1:P:742:THR:HG22	1:P:743:SER:N	2.14	0.61
1:N:18:ASN:HD22	1:N:21:VAL:HG23	1.64	0.61
1:P:4:THR:HA	1:P:9:VAL:HG11	1.82	0.61
1:O:599:ARG:HB2	1:O:600:GLN:OE1	1.99	0.61
1:K:651:LEU:HD13	1:K:669:PRO:HA	1.82	0.61
1:I:578:TYR:HA	1:I:583:ASN:O	2.00	0.61
1:I:194:GLY:O	1:I:198:GLU:HG3	2.00	0.61
1:J:745:MET:HA	1:J:745:MET:HE2	1.80	0.61
1:N:578:TYR:HA	1:N:583:ASN:O	2.00	0.61
1:M:1020:TRP:HD1	1:M:1021:CME:N	1.99	0.61
1:I:1020:TRP:HD1	1:I:1021:CME:N	1.99	0.61
1:L:30:HIS:ND1	1:L:31:PRO:O	2.26	0.61
1:K:786:ARG:HH11	1:K:990:HIS:CE1	2.18	0.61
1:J:127:PHE:HE2	1:J:184:LEU:HG	1.65	0.61
1:M:786:ARG:HH11	1:M:990:HIS:CE1	2.18	0.61
1:J:568:TRP:HE1	1:J:604:ASN:HD22	1.47	0.61
1:O:742:THR:HG22	1:O:743:SER:N	2.14	0.61
1:K:745:MET:HE2	1:K:745:MET:HA	1.82	0.61
1:J:651:LEU:HD13	1:J:669:PRO:HA	1.83	0.61
1:O:782:ASP:HA	1:O:884:LEU:HD23	1.83	0.61
1:O:127:PHE:HE2	1:O:184:LEU:HG	1.65	0.61
1:I:127:PHE:HE2	1:I:184:LEU:HG	1.65	0.61
1:O:945:ASN:OD1	1:O:950:GLN:NE2	2.30	0.61
1:K:847:LYS:HG3	1:K:848:THR:N	2.14	0.61
1:O:360:HIS:CE1	1:O:361:PRO:HD2	2.36	0.61
1:O:578:TYR:HA	1:O:583:ASN:O	2.00	0.61
1:P:1020:TRP:HD1	1:P:1021:CME:N	1.99	0.61
1:N:919:ASP:O	1:N:920:LEU:HD23	2.00	0.61
1:O:437:SER:HB2	5:O:7508:HOH:O	2.01	0.61
1:K:568:TRP:HE1	1:K:604:ASN:HD22	1.47	0.61
1:L:323:ILE:HD12	1:L:323:ILE:N	2.16	0.61
1:P:323:ILE:N	1:P:323:ILE:HD12	2.16	0.61
1:M:323:ILE:HD12	1:M:323:ILE:N	2.16	0.61
1:J:919:ASP:O	1:J:920:LEU:HD23	2.00	0.61
1:I:919:ASP:O	1:I:920:LEU:HD23	2.00	0.61
1:N:37:ARG:HH11	1:N:37:ARG:HG3	1.64	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:578:TYR:HA	1:L:583:ASN:O	2.00	0.61
1:P:689:GLU:OE2	1:P:689:GLU:HA	2.01	0.61
1:I:847:LYS:HG3	1:I:848:THR:N	2.14	0.61
1:M:568:TRP:HE1	1:M:604:ASN:HD22	1.47	0.61
1:N:323:ILE:HD12	1:N:323:ILE:N	2.16	0.61
1:K:578:TYR:HA	1:K:583:ASN:O	2.00	0.61
1:K:4:THR:HA	1:K:9:VAL:HG11	1.82	0.61
1:P:30:HIS:ND1	1:P:31:PRO:O	2.26	0.61
1:P:847:LYS:HG3	1:P:848:THR:N	2.14	0.61
1:N:224:ASP:OD2	1:N:225:PHE:N	2.34	0.61
1:L:847:LYS:HG3	1:L:848:THR:N	2.14	0.61
1:I:323:ILE:HD12	1:I:323:ILE:N	2.16	0.61
1:J:1020:TRP:HD1	1:J:1021:CME:N	1.99	0.61
1:I:37:ARG:HG3	1:I:37:ARG:HH11	1.64	0.61
1:N:662:PRO:O	1:N:663:LEU:HD23	2.01	0.61
1:I:4:THR:HA	1:I:9:VAL:HG11	1.82	0.61
1:M:4:THR:HA	1:M:9:VAL:HG11	1.82	0.61
1:L:224:ASP:OD2	1:L:225:PHE:N	2.34	0.61
1:I:689:GLU:OE2	1:I:689:GLU:HA	2.01	0.61
1:L:599:ARG:HB2	1:L:600:GLN:OE1	1.99	0.61
1:M:651:LEU:HD13	1:M:669:PRO:HA	1.82	0.61
1:P:18:ASN:HD22	1:P:21:VAL:HG23	1.64	0.61
1:K:323:ILE:N	1:K:323:ILE:HD12	2.16	0.61
1:O:1020:TRP:HD1	1:O:1021:CME:N	1.98	0.61
1:N:30:HIS:ND1	1:N:31:PRO:O	2.26	0.61
1:N:194:GLY:O	1:N:198:GLU:HG3	2.00	0.61
1:P:786:ARG:HH11	1:P:990:HIS:CE1	2.18	0.61
1:M:117:GLU:OE1	1:M:117:GLU:N	2.27	0.61
1:K:194:GLY:O	1:K:198:GLU:HG3	2.00	0.61
1:I:224:ASP:OD2	1:I:225:PHE:N	2.34	0.61
1:K:127:PHE:HE2	1:K:184:LEU:HG	1.65	0.61
1:P:919:ASP:O	1:P:920:LEU:HD23	2.00	0.61
1:M:782:ASP:HA	1:M:884:LEU:HD23	1.83	0.61
1:O:894:ARG:NH1	1:O:919:ASP:OD2	2.30	0.61
1:O:919:ASP:O	1:O:920:LEU:HD23	2.00	0.61
1:M:54:LEU:HD23	1:M:54:LEU:N	2.15	0.61
1:P:54:LEU:N	1:P:54:LEU:HD23	2.15	0.61
1:P:662:PRO:O	1:P:663:LEU:HD23	2.01	0.61
1:N:125:LEU:HG	1:N:126:THR:N	2.16	0.61
1:I:30:HIS:ND1	1:I:31:PRO:O	2.26	0.61
1:J:194:GLY:O	1:J:198:GLU:HG3	2.00	0.61
1:L:786:ARG:HH11	1:L:990:HIS:CE1	2.18	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:127:PHE:HE2	1:P:184:LEU:HG	1.65	0.61
1:L:18:ASN:HD22	1:L:21:VAL:HG23	1.64	0.60
1:O:1021:CME:HB3	1:O:1021:CME:CZ	2.21	0.60
1:L:919:ASP:O	1:L:920:LEU:HD23	2.00	0.60
1:I:662:PRO:O	1:I:663:LEU:HD23	2.01	0.60
1:J:689:GLU:HA	1:J:689:GLU:OE2	2.01	0.60
1:L:178:ARG:NH1	1:L:181:GLU:O	2.33	0.60
1:O:224:ASP:OD2	1:O:225:PHE:N	2.34	0.60
1:J:945:ASN:OD1	1:J:950:GLN:NE2	2.30	0.60
1:O:786:ARG:HH11	1:O:990:HIS:CE1	2.18	0.60
1:P:360:HIS:CE1	1:P:361:PRO:HD2	2.36	0.60
1:O:651:LEU:HD13	1:O:669:PRO:HA	1.83	0.60
1:N:782:ASP:HA	1:N:884:LEU:HD23	1.83	0.60
1:P:249:GLU:HG2	1:P:251:ARG:HH12	1.67	0.60
1:N:894:ARG:NH1	1:N:919:ASP:OD2	2.30	0.60
1:K:662:PRO:O	1:K:663:LEU:HD23	2.01	0.60
1:J:662:PRO:O	1:J:663:LEU:HD23	2.01	0.60
1:J:786:ARG:HH11	1:J:990:HIS:CE1	2.18	0.60
1:K:460:ASN:ND2	1:K:461:GLU:HG3	2.17	0.60
1:L:194:GLY:O	1:L:198:GLU:HG3	2.00	0.60
1:J:224:ASP:OD2	1:J:225:PHE:N	2.34	0.60
1:N:127:PHE:HE2	1:N:184:LEU:HG	1.65	0.60
1:N:651:LEU:HD13	1:N:669:PRO:HA	1.83	0.60
1:J:323:ILE:HD12	1:J:323:ILE:N	2.16	0.60
1:L:782:ASP:HA	1:L:884:LEU:HD23	1.83	0.60
1:L:1021:CME:HZ3	1:L:1021:CME:HB3	1.84	0.60
1:P:782:ASP:HA	1:P:884:LEU:HD23	1.83	0.60
1:K:689:GLU:HA	1:K:689:GLU:OE2	2.01	0.60
1:L:127:PHE:HE2	1:L:184:LEU:HG	1.65	0.60
1:M:1021:CME:HZ3	1:M:1021:CME:HB3	1.84	0.60
1:P:194:GLY:O	1:P:198:GLU:HG3	2.00	0.60
1:I:786:ARG:HH11	1:I:990:HIS:CE1	2.18	0.60
1:K:1011:ALA:HB3	1:K:1014:TYR:CZ	2.37	0.60
1:J:130:ASP:OD1	1:J:132:SER:N	2.29	0.60
1:I:360:HIS:CE1	1:I:361:PRO:HD2	2.36	0.60
1:J:578:TYR:HA	1:J:583:ASN:O	2.00	0.60
1:P:7:LEU:N	1:P:71:GLU:OE2	2.35	0.60
1:L:7:LEU:N	1:L:71:GLU:OE2	2.35	0.60
1:I:249:GLU:HG2	1:I:251:ARG:HH12	1.67	0.60
1:O:125:LEU:HG	1:O:126:THR:N	2.16	0.60
1:K:125:LEU:HG	1:K:126:THR:N	2.16	0.60
1:J:4:THR:HA	1:J:9:VAL:HG11	1.82	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:224:ASP:OD2	1:M:225:PHE:N	2.34	0.60
1:L:14:ARG:HA	1:L:16:TRP:CZ3	2.37	0.60
1:J:1011:ALA:HB3	1:J:1014:TYR:CZ	2.37	0.60
1:P:224:ASP:OD2	1:P:225:PHE:N	2.34	0.60
1:K:224:ASP:OD2	1:K:225:PHE:N	2.34	0.60
1:I:651:LEU:HD13	1:I:669:PRO:HA	1.82	0.60
1:L:651:LEU:HD13	1:L:669:PRO:HA	1.83	0.60
1:J:360:HIS:CE1	1:J:361:PRO:HD2	2.36	0.60
1:L:1020:TRP:HD1	1:L:1021:CME:N	1.99	0.60
1:I:1021:CME:HB3	1:I:1021:CME:HZ3	1.84	0.60
1:O:662:PRO:O	1:O:663:LEU:HD23	2.01	0.60
1:M:125:LEU:HG	1:M:126:THR:N	2.16	0.60
1:N:689:GLU:OE2	1:N:689:GLU:HA	2.01	0.60
1:P:1011:ALA:HB3	1:P:1014:TYR:CZ	2.37	0.60
1:J:782:ASP:HA	1:J:884:LEU:HD23	1.83	0.60
1:N:1021:CME:HB3	1:N:1021:CME:HZ3	1.84	0.60
1:O:249:GLU:HG2	1:O:251:ARG:HH12	1.67	0.60
1:P:1021:CME:HB3	1:P:1021:CME:HZ3	1.84	0.60
1:K:1020:TRP:HD1	1:K:1021:CME:N	1.99	0.60
1:N:533:LEU:C	1:N:533:LEU:HD12	2.22	0.60
1:J:36:TRP:O	1:J:37:ARG:HD3	2.02	0.60
1:M:662:PRO:O	1:M:663:LEU:HD23	2.01	0.60
1:M:578:TYR:HA	1:M:583:ASN:O	2.00	0.60
1:M:1011:ALA:HB3	1:M:1014:TYR:CZ	2.37	0.60
1:M:689:GLU:OE2	1:M:689:GLU:HA	2.01	0.60
1:I:460:ASN:ND2	1:I:461:GLU:HG3	2.17	0.60
1:L:460:ASN:ND2	1:L:461:GLU:HG3	2.17	0.60
1:O:323:ILE:N	1:O:323:ILE:HD12	2.16	0.60
1:P:651:LEU:HD13	1:P:669:PRO:HA	1.82	0.60
1:N:7:LEU:N	1:N:71:GLU:OE2	2.35	0.60
1:L:360:HIS:CE1	1:L:361:PRO:HD2	2.36	0.60
1:M:360:HIS:CE1	1:M:361:PRO:HD2	2.36	0.60
1:N:1020:TRP:HD1	1:N:1021:CME:N	1.99	0.60
1:L:36:TRP:O	1:L:37:ARG:HD3	2.02	0.60
1:I:533:LEU:HD12	1:I:533:LEU:C	2.22	0.60
1:N:4:THR:HA	1:N:9:VAL:HG11	1.82	0.60
1:O:460:ASN:ND2	1:O:461:GLU:HG3	2.17	0.60
1:N:786:ARG:HH11	1:N:990:HIS:CE1	2.18	0.60
1:O:194:GLY:O	1:O:198:GLU:HG3	2.00	0.60
1:J:7:LEU:N	1:J:71:GLU:OE2	2.35	0.60
1:K:360:HIS:CE1	1:K:361:PRO:HD2	2.36	0.60
1:N:372:MET:HE1	1:N:395:HIS:HB3	1.84	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:533:LEU:HD12	1:L:533:LEU:C	2.22	0.60
1:O:36:TRP:O	1:O:37:ARG:HD3	2.02	0.60
1:M:36:TRP:O	1:M:37:ARG:HD3	2.02	0.60
1:L:662:PRO:O	1:L:663:LEU:HD23	2.01	0.60
1:P:261:TRP:CH2	1:P:266:GLN:HB2	2.37	0.60
1:M:502:MET:HB2	1:M:537:GLU:HB2	1.84	0.60
1:K:178:ARG:NH1	1:K:181:GLU:O	2.33	0.60
1:N:502:MET:HB2	1:N:537:GLU:HB2	1.84	0.60
1:N:14:ARG:HA	1:N:16:TRP:CZ3	2.37	0.60
1:N:360:HIS:CE1	1:N:361:PRO:HD2	2.36	0.60
1:K:782:ASP:HA	1:K:884:LEU:HD23	1.83	0.60
1:P:1021:CME:CZ	1:P:1021:CME:HB3	2.21	0.60
1:I:782:ASP:HA	1:I:884:LEU:HD23	1.83	0.60
1:J:533:LEU:C	1:J:533:LEU:HD12	2.22	0.60
1:K:533:LEU:HD12	1:K:533:LEU:C	2.22	0.60
1:K:36:TRP:O	1:K:37:ARG:HD3	2.02	0.60
1:L:37:ARG:NH2	1:L:218:PRO:HD3	2.17	0.60
1:I:261:TRP:CH2	1:I:266:GLN:HB2	2.37	0.60
1:P:14:ARG:HA	1:P:16:TRP:CZ3	2.37	0.60
1:L:689:GLU:OE2	1:L:689:GLU:HA	2.01	0.60
1:N:873:ALA:O	1:N:876:THR:HG22	2.02	0.60
1:P:945:ASN:OD1	1:P:950:GLN:NE2	2.30	0.60
1:N:261:TRP:CH2	1:N:266:GLN:HB2	2.37	0.60
1:O:18:ASN:HD22	1:O:21:VAL:HG23	1.64	0.59
1:P:533:LEU:C	1:P:533:LEU:HD12	2.22	0.59
1:O:37:ARG:NH2	1:O:218:PRO:HD3	2.17	0.59
1:J:125:LEU:HG	1:J:126:THR:N	2.16	0.59
1:K:579:ASP:OD1	1:K:583:ASN:HB2	2.03	0.59
1:I:125:LEU:HG	1:I:126:THR:N	2.16	0.59
1:M:579:ASP:OD1	1:M:583:ASN:HB2	2.02	0.59
1:I:502:MET:HB2	1:I:537:GLU:HB2	1.84	0.59
1:J:873:ALA:O	1:J:876:THR:HG22	2.02	0.59
1:M:460:ASN:ND2	1:M:461:GLU:HG3	2.17	0.59
1:J:57:GLU:HG2	1:J:83:THR:HG23	1.85	0.59
1:O:7:LEU:N	1:O:71:GLU:OE2	2.35	0.59
1:O:1021:CME:HB3	1:O:1021:CME:HZ3	1.84	0.59
1:M:7:LEU:N	1:M:71:GLU:OE2	2.35	0.59
1:O:533:LEU:HD12	1:O:533:LEU:C	2.22	0.59
1:J:23:GLN:OE1	1:J:26:ARG:HB3	2.03	0.59
1:I:23:GLN:OE1	1:I:26:ARG:HB3	2.02	0.59
1:M:30:HIS:HB2	1:M:31:PRO:CD	2.33	0.59
1:J:261:TRP:CH2	1:J:266:GLN:HB2	2.37	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:849:LEU:N	1:I:849:LEU:HD23	2.17	0.59
1:K:873:ALA:O	1:K:876:THR:HG22	2.02	0.59
1:O:57:GLU:HG2	1:O:83:THR:HG23	1.85	0.59
1:J:579:ASP:OD1	1:J:583:ASN:HB2	2.03	0.59
1:M:1021:CME:OH	1:M:1023:LYS:HG2	2.03	0.59
1:I:1021:CME:OH	1:I:1023:LYS:HG2	2.03	0.59
1:K:1021:CME:HZ3	1:K:1021:CME:HB3	1.84	0.59
1:L:822:LEU:CD1	1:L:824:GLN:H	2.16	0.59
1:M:822:LEU:CD1	1:M:824:GLN:H	2.16	0.59
1:M:23:GLN:OE1	1:M:26:ARG:HB3	2.02	0.59
1:J:14:ARG:HA	1:J:16:TRP:CZ3	2.37	0.59
1:J:502:MET:HB2	1:J:537:GLU:HB2	1.84	0.59
1:K:261:TRP:CH2	1:K:266:GLN:HB2	2.37	0.59
1:J:460:ASN:ND2	1:J:461:GLU:HG3	2.17	0.59
1:I:1011:ALA:HB3	1:I:1014:TYR:CZ	2.37	0.59
1:M:14:ARG:HA	1:M:16:TRP:CZ3	2.37	0.59
1:M:18:ASN:HD22	1:M:21:VAL:HG23	1.64	0.59
1:J:1021:CME:OH	1:J:1023:LYS:HG2	2.03	0.59
1:O:23:GLN:OE1	1:O:26:ARG:HB3	2.02	0.59
1:N:460:ASN:ND2	1:N:461:GLU:HG3	2.17	0.59
1:O:178:ARG:NH1	1:O:181:GLU:O	2.33	0.59
1:O:689:GLU:OE2	1:O:689:GLU:HA	2.01	0.59
1:L:1011:ALA:HB3	1:L:1014:TYR:CZ	2.37	0.59
1:P:873:ALA:O	1:P:876:THR:HG22	2.02	0.59
1:I:14:ARG:HA	1:I:16:TRP:CZ3	2.37	0.59
1:M:57:GLU:HG2	1:M:83:THR:HG23	1.85	0.59
1:K:856:TYR:CD2	1:K:864:MET:HE2	2.38	0.59
1:L:30:HIS:HB2	1:L:31:PRO:CD	2.33	0.59
1:N:849:LEU:N	1:N:849:LEU:HD23	2.17	0.59
1:M:873:ALA:O	1:M:876:THR:HG22	2.02	0.59
1:M:178:ARG:NH1	1:M:181:GLU:O	2.33	0.59
1:O:14:ARG:HA	1:O:16:TRP:CZ3	2.37	0.59
1:K:7:LEU:N	1:K:71:GLU:OE2	2.35	0.59
1:N:249:GLU:HG2	1:N:251:ARG:HH12	1.67	0.59
1:M:533:LEU:HD12	1:M:533:LEU:C	2.22	0.59
1:K:30:HIS:HB2	1:K:31:PRO:CD	2.33	0.59
1:L:4:THR:HA	1:L:9:VAL:HG11	1.82	0.59
1:I:30:HIS:HB2	1:I:31:PRO:CD	2.32	0.59
1:L:849:LEU:HD23	1:L:849:LEU:N	2.17	0.59
1:L:272:ALA:HB1	1:L:273:PRO:HD2	1.85	0.59
1:O:873:ALA:O	1:O:876:THR:HG22	2.02	0.59
1:K:14:ARG:HA	1:K:16:TRP:CZ3	2.37	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:7:LEU:N	1:I:71:GLU:OE2	2.35	0.59
1:J:37:ARG:NH2	1:J:218:PRO:HD3	2.17	0.59
1:L:437:SER:HB2	5:L:7508:HOH:O	2.01	0.59
1:O:261:TRP:CH2	1:O:266:GLN:HB2	2.37	0.59
1:I:178:ARG:NH1	1:I:181:GLU:O	2.33	0.59
1:P:502:MET:HB2	1:P:537:GLU:HB2	1.84	0.59
1:J:272:ALA:HB1	1:J:273:PRO:HD2	1.85	0.59
1:O:1011:ALA:HB3	1:O:1014:TYR:CZ	2.37	0.59
1:I:493:THR:HG23	5:I:4020:HOH:O	2.03	0.59
1:I:873:ALA:O	1:I:876:THR:HG22	2.02	0.59
1:N:178:ARG:NH1	1:N:181:GLU:O	2.33	0.59
1:P:1021:CME:OH	1:P:1023:LYS:HG2	2.03	0.59
1:M:255:ARG:NH1	1:M:255:ARG:HG2	2.14	0.59
1:N:763:GLY:HA3	1:N:822:LEU:CD2	2.33	0.59
1:I:763:GLY:HA3	1:I:822:LEU:CD2	2.33	0.59
1:I:54:LEU:N	1:I:54:LEU:HD23	2.15	0.59
1:P:125:LEU:HG	1:P:126:THR:N	2.16	0.59
1:J:30:HIS:HB2	1:J:31:PRO:CD	2.33	0.59
1:N:30:HIS:HB2	1:N:31:PRO:CD	2.33	0.59
1:O:30:HIS:HB2	1:O:31:PRO:CD	2.33	0.59
1:P:261:TRP:CZ3	1:P:266:GLN:HB2	2.38	0.59
1:O:261:TRP:CZ3	1:O:266:GLN:HB2	2.38	0.59
1:O:849:LEU:HD23	1:O:849:LEU:N	2.17	0.59
1:K:849:LEU:N	1:K:849:LEU:HD23	2.17	0.59
1:J:906:TYR:HB3	1:J:907:PRO:HD2	1.85	0.59
1:M:261:TRP:CH2	1:M:266:GLN:HB2	2.37	0.59
1:P:473:ARG:HD3	1:P:473:ARG:O	2.03	0.59
1:J:427:THR:HA	1:J:436:MET:HE2	1.83	0.59
1:L:166:ARG:HG3	1:L:392:TYR:HB2	1.85	0.59
1:N:166:ARG:HG3	1:N:392:TYR:HB2	1.85	0.59
1:O:54:LEU:HD23	1:O:54:LEU:N	2.15	0.59
1:N:473:ARG:HD3	1:N:473:ARG:O	2.03	0.59
1:M:493:THR:HG23	5:M:4020:HOH:O	2.03	0.59
1:O:473:ARG:HD3	1:O:473:ARG:O	2.03	0.59
1:P:730:LEU:HB3	1:P:731:PRO:HD2	1.85	0.59
1:M:473:ARG:O	1:M:473:ARG:HD3	2.03	0.59
1:P:906:TYR:HB3	1:P:907:PRO:HD2	1.85	0.59
1:L:502:MET:HB2	1:L:537:GLU:HB2	1.84	0.59
1:P:493:THR:HG23	5:P:4536:HOH:O	2.03	0.59
1:L:57:GLU:HG2	1:L:83:THR:HG23	1.84	0.59
1:K:763:GLY:HA3	1:K:822:LEU:CD2	2.33	0.59
1:P:763:GLY:HA3	1:P:822:LEU:CD2	2.33	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:36:TRP:O	1:N:37:ARG:HD3	2.02	0.59
1:N:261:TRP:CZ3	1:N:266:GLN:HB2	2.38	0.59
1:M:945:ASN:OD1	1:M:950:GLN:NE2	2.30	0.59
1:L:873:ALA:O	1:L:876:THR:HG22	2.02	0.59
1:O:730:LEU:HB3	1:O:731:PRO:HD2	1.85	0.59
1:I:473:ARG:HD3	1:I:473:ARG:O	2.03	0.59
1:I:287:ASP:OD2	1:L:425:ARG:NH2	2.36	0.59
1:L:261:TRP:CH2	1:L:266:GLN:HB2	2.37	0.59
1:K:473:ARG:O	1:K:473:ARG:HD3	2.03	0.59
1:N:1011:ALA:HB3	1:N:1014:TYR:CZ	2.37	0.59
1:K:945:ASN:OD1	1:K:950:GLN:NE2	2.30	0.59
1:K:493:THR:HG23	5:K:4020:HOH:O	2.03	0.59
1:N:272:ALA:HB1	1:N:273:PRO:HD2	1.85	0.59
1:P:579:ASP:OD1	1:P:583:ASN:HB2	2.03	0.58
1:N:54:LEU:HD23	1:N:54:LEU:N	2.15	0.58
1:N:23:GLN:OE1	1:N:26:ARG:HB3	2.02	0.58
1:K:261:TRP:CZ3	1:K:266:GLN:HB2	2.38	0.58
1:K:778:THR:HB	1:K:887:GLN:HB3	1.85	0.58
1:P:291:LEU:HD12	1:P:291:LEU:N	2.18	0.58
1:M:291:LEU:HD12	1:M:291:LEU:N	2.18	0.58
1:P:460:ASN:ND2	1:P:461:GLU:HG3	2.17	0.58
1:I:7:LEU:HD13	1:I:74:LEU:CD1	2.32	0.58
1:O:579:ASP:OD1	1:O:583:ASN:HB2	2.03	0.58
1:N:579:ASP:OD1	1:N:583:ASN:HB2	2.03	0.58
1:O:166:ARG:HG3	1:O:392:TYR:HB2	1.85	0.58
1:I:166:ARG:HG3	1:I:392:TYR:HB2	1.85	0.58
1:J:54:LEU:HD23	1:J:54:LEU:N	2.15	0.58
1:P:37:ARG:NH2	1:P:218:PRO:HD3	2.17	0.58
1:L:125:LEU:HG	1:L:126:THR:N	2.16	0.58
1:L:261:TRP:CZ3	1:L:266:GLN:HB2	2.38	0.58
1:L:778:THR:HB	1:L:887:GLN:HB3	1.85	0.58
1:I:645:ARG:NH2	1:I:650:GLU:OE1	2.37	0.58
1:M:772:ASP:N	1:M:772:ASP:OD1	2.30	0.58
1:N:493:THR:HG23	5:N:4203:HOH:O	2.03	0.58
1:O:502:MET:HB2	1:O:537:GLU:HB2	1.84	0.58
1:K:18:ASN:HD22	1:K:21:VAL:HG23	1.64	0.58
1:P:57:GLU:HG2	1:P:83:THR:HG23	1.85	0.58
1:K:7:LEU:HD13	1:K:74:LEU:CD1	2.32	0.58
1:J:763:GLY:HA3	1:J:822:LEU:CD2	2.33	0.58
1:M:730:LEU:HB3	1:M:731:PRO:HD2	1.85	0.58
1:K:54:LEU:HD23	1:K:54:LEU:N	2.15	0.58
1:K:37:ARG:NH2	1:K:218:PRO:HD3	2.17	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:36:TRP:O	1:I:37:ARG:HD3	2.02	0.58
1:N:37:ARG:NH2	1:N:218:PRO:HD3	2.17	0.58
1:M:37:ARG:NH2	1:M:218:PRO:HD3	2.17	0.58
1:P:30:HIS:HB2	1:P:31:PRO:CD	2.33	0.58
1:O:291:LEU:N	1:O:291:LEU:HD12	2.18	0.58
1:N:291:LEU:HD12	1:N:291:LEU:N	2.18	0.58
1:L:473:ARG:HD3	1:L:473:ARG:O	2.03	0.58
1:K:906:TYR:HB3	1:K:907:PRO:HD2	1.85	0.58
1:M:429:ASP:OD1	1:M:430:PRO:HD2	2.03	0.58
1:J:493:THR:HG23	5:J:4020:HOH:O	2.03	0.58
1:N:1021:CME:OH	1:N:1023:LYS:HG2	2.03	0.58
1:K:894:ARG:NH1	1:K:919:ASP:OD2	2.30	0.58
1:L:763:GLY:HA3	1:L:822:LEU:CD2	2.33	0.58
1:P:23:GLN:OE1	1:P:26:ARG:HB3	2.02	0.58
1:I:282:ARG:NH1	1:L:419:GLY:HA2	2.18	0.58
1:M:261:TRP:CZ3	1:M:266:GLN:HB2	2.38	0.58
1:L:291:LEU:HD12	1:L:291:LEU:N	2.18	0.58
1:P:645:ARG:NH2	1:P:650:GLU:OE1	2.37	0.58
1:N:906:TYR:HB3	1:N:907:PRO:HD2	1.85	0.58
1:N:730:LEU:HB3	1:N:731:PRO:HD2	1.85	0.58
1:M:166:ARG:HG3	1:M:392:TYR:HB2	1.85	0.58
1:P:36:TRP:O	1:P:37:ARG:HD3	2.02	0.58
1:O:272:ALA:HB1	1:O:273:PRO:HD2	1.85	0.58
1:I:291:LEU:N	1:I:291:LEU:HD12	2.18	0.58
1:M:130:ASP:OD1	1:M:132:SER:N	2.29	0.58
1:K:730:LEU:HB3	1:K:731:PRO:HD2	1.85	0.58
1:K:57:GLU:HG2	1:K:83:THR:HG23	1.84	0.58
1:J:249:GLU:HG2	1:J:251:ARG:HH12	1.67	0.58
1:O:822:LEU:CD1	1:O:824:GLN:H	2.15	0.58
1:L:23:GLN:OE1	1:L:26:ARG:HB3	2.02	0.58
1:K:23:GLN:OE1	1:K:26:ARG:HB3	2.02	0.58
1:N:645:ARG:NH2	1:N:650:GLU:OE1	2.37	0.58
1:P:849:LEU:HD23	1:P:849:LEU:N	2.17	0.58
1:M:849:LEU:N	1:M:849:LEU:HD23	2.17	0.58
1:N:668:VAL:CG1	1:N:669:PRO:HD2	2.31	0.58
1:O:1021:CME:OH	1:O:1023:LYS:HG2	2.03	0.58
1:J:1021:CME:HB3	1:J:1021:CME:HZ3	1.84	0.58
1:J:822:LEU:CD1	1:J:824:GLN:H	2.16	0.58
1:L:54:LEU:HD23	1:L:54:LEU:N	2.15	0.58
1:L:579:ASP:OD1	1:L:583:ASN:HB2	2.03	0.58
1:K:502:MET:HB2	1:K:537:GLU:HB2	1.84	0.58
1:I:272:ALA:HB1	1:I:273:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:291:LEU:HD12	1:K:291:LEU:N	2.18	0.58
1:N:580:GLU:H	1:N:580:GLU:CD	2.07	0.58
1:M:272:ALA:HB1	1:M:273:PRO:HD2	1.85	0.58
1:K:580:GLU:HG2	1:K:581:ASN:OD1	2.04	0.58
1:P:740:LEU:CD1	1:P:741:THR:H	2.12	0.58
1:I:668:VAL:CG1	1:I:669:PRO:HD2	2.31	0.58
1:N:57:GLU:HG2	1:N:83:THR:HG23	1.84	0.58
1:L:1021:CME:OH	1:L:1023:LYS:HG2	2.03	0.58
1:J:372:MET:HE1	1:J:395:HIS:HB3	1.84	0.58
1:I:261:TRP:CZ3	1:I:266:GLN:HB2	2.38	0.58
1:J:261:TRP:CZ3	1:J:266:GLN:HB2	2.38	0.58
1:K:580:GLU:CD	1:K:580:GLU:H	2.07	0.58
1:J:291:LEU:HD12	1:J:291:LEU:N	2.18	0.58
1:J:645:ARG:NH2	1:J:650:GLU:OE1	2.37	0.58
1:K:645:ARG:NH2	1:K:650:GLU:OE1	2.37	0.58
1:L:645:ARG:NH2	1:L:650:GLU:OE1	2.37	0.58
1:O:645:ARG:NH2	1:O:650:GLU:OE1	2.37	0.58
1:M:645:ARG:NH2	1:M:650:GLU:OE1	2.37	0.58
1:M:30:HIS:ND1	1:M:31:PRO:O	2.26	0.58
1:M:580:GLU:CD	1:M:580:GLU:H	2.07	0.58
1:M:580:GLU:HG2	1:M:581:ASN:OD1	2.04	0.58
1:K:153:TRP:CD1	1:K:158:TRP:HA	2.39	0.58
1:N:778:THR:HB	1:N:887:GLN:HB3	1.85	0.58
1:I:429:ASP:OD1	1:I:430:PRO:HD2	2.03	0.58
1:I:153:TRP:CD1	1:I:158:TRP:HA	2.39	0.58
1:L:493:THR:HG23	5:L:4020:HOH:O	2.03	0.58
1:M:316:HIS:CA	1:M:323:ILE:HD13	2.32	0.58
1:N:7:LEU:HD13	1:N:74:LEU:CD1	2.32	0.58
1:I:579:ASP:OD1	1:I:583:ASN:HB2	2.03	0.58
1:K:1021:CME:OH	1:K:1023:LYS:HG2	2.03	0.58
1:I:166:ARG:HG3	1:I:392:TYR:CB	2.34	0.58
1:N:580:GLU:HG2	1:N:581:ASN:OD1	2.04	0.58
1:J:473:ARG:HD3	1:J:473:ARG:O	2.03	0.58
1:L:730:LEU:HB3	1:L:731:PRO:HD2	1.85	0.58
1:J:778:THR:HB	1:J:887:GLN:HB3	1.85	0.58
1:J:429:ASP:OD1	1:J:430:PRO:HD2	2.03	0.58
1:M:316:HIS:HD2	1:M:317:THR:O	1.87	0.57
1:O:7:LEU:HD13	1:O:74:LEU:CD1	2.32	0.57
1:N:166:ARG:HG3	1:N:392:TYR:CB	2.34	0.57
1:L:153:TRP:CD1	1:L:158:TRP:HA	2.39	0.57
1:O:493:THR:HG23	5:O:4020:HOH:O	2.03	0.57
1:I:580:GLU:HG2	1:I:581:ASN:OD1	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:355:ASN:OD1	1:N:388:ARG:HD3	2.04	0.57
1:P:429:ASP:OD1	1:P:430:PRO:HD2	2.03	0.57
1:P:153:TRP:CD1	1:P:158:TRP:HA	2.39	0.57
1:N:316:HIS:HD2	1:N:317:THR:O	1.87	0.57
1:O:166:ARG:HG3	1:O:392:TYR:CB	2.34	0.57
1:I:37:ARG:NH2	1:I:218:PRO:HD3	2.17	0.57
1:J:849:LEU:N	1:J:849:LEU:HD23	2.17	0.57
1:J:355:ASN:OD1	1:J:388:ARG:HD3	2.04	0.57
1:O:130:ASP:OD1	1:O:132:SER:N	2.30	0.57
1:M:355:ASN:OD1	1:M:388:ARG:HD3	2.04	0.57
1:M:668:VAL:CG1	1:M:669:PRO:HD2	2.31	0.57
1:K:360:HIS:HE1	1:K:362:LEU:HB2	1.61	0.57
1:P:7:LEU:HD13	1:P:74:LEU:CD1	2.32	0.57
1:L:255:ARG:NH1	1:L:255:ARG:HG2	2.14	0.57
1:J:166:ARG:HG3	1:J:392:TYR:CB	2.34	0.57
1:N:701:VAL:HG22	1:N:714:ILE:HD12	1.87	0.57
1:K:714:ILE:N	1:K:714:ILE:HD13	2.20	0.57
1:M:153:TRP:CD1	1:M:158:TRP:HA	2.39	0.57
1:K:429:ASP:OD1	1:K:430:PRO:HD2	2.03	0.57
1:N:429:ASP:OD1	1:N:430:PRO:HD2	2.03	0.57
1:M:906:TYR:HB3	1:M:907:PRO:HD2	1.85	0.57
1:O:429:ASP:OD1	1:O:430:PRO:HD2	2.03	0.57
1:O:316:HIS:CA	1:O:323:ILE:HD13	2.32	0.57
1:J:7:LEU:HD13	1:J:74:LEU:CD1	2.32	0.57
1:K:166:ARG:HG3	1:K:392:TYR:CB	2.34	0.57
1:P:166:ARG:HG3	1:P:392:TYR:CB	2.34	0.57
1:J:153:TRP:CD1	1:J:158:TRP:HA	2.39	0.57
1:I:906:TYR:HB3	1:I:907:PRO:HD2	1.85	0.57
1:O:778:THR:HB	1:O:887:GLN:HB3	1.85	0.57
1:P:580:GLU:CD	1:P:580:GLU:H	2.07	0.57
1:J:580:GLU:HG2	1:J:581:ASN:OD1	2.04	0.57
1:P:272:ALA:HB1	1:P:273:PRO:HD2	1.85	0.57
1:L:355:ASN:OD1	1:L:388:ARG:HD3	2.04	0.57
1:L:580:GLU:HG2	1:L:581:ASN:OD1	2.04	0.57
1:I:316:HIS:HD2	1:I:317:THR:O	1.87	0.57
1:J:316:HIS:HD2	1:J:317:THR:O	1.87	0.57
1:O:763:GLY:HA3	1:O:822:LEU:CD2	2.33	0.57
1:J:166:ARG:HG3	1:J:392:TYR:HB2	1.85	0.57
1:P:372:MET:HE1	1:P:395:HIS:HB3	1.86	0.57
1:P:166:ARG:HG3	1:P:392:TYR:HB2	1.85	0.57
1:L:701:VAL:HG22	1:L:714:ILE:HD12	1.87	0.57
1:L:714:ILE:N	1:L:714:ILE:HD13	2.20	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:580:GLU:CD	1:J:580:GLU:H	2.07	0.57
1:L:580:GLU:CD	1:L:580:GLU:H	2.07	0.57
1:M:403:ASP:OD1	1:M:451:PRO:HD2	2.05	0.57
1:L:429:ASP:OD1	1:L:430:PRO:HD2	2.03	0.57
1:J:730:LEU:HB3	1:J:731:PRO:HD2	1.85	0.57
1:K:835:LEU:C	1:K:836:ILE:HD13	2.25	0.57
1:P:778:THR:HB	1:P:887:GLN:HB3	1.85	0.57
1:P:403:ASP:OD1	1:P:451:PRO:HD2	2.05	0.57
1:O:153:TRP:CD1	1:O:158:TRP:HA	2.39	0.57
1:I:425:ARG:NH2	1:L:287:ASP:OD2	2.36	0.57
1:L:166:ARG:HG3	1:L:392:TYR:CB	2.34	0.57
1:K:372:MET:HE1	1:K:395:HIS:HB3	1.85	0.57
1:O:3:ILE:HG23	1:O:4:THR:H	1.69	0.57
1:K:403:ASP:OD1	1:K:451:PRO:HD2	2.05	0.57
1:J:403:ASP:OD1	1:J:451:PRO:HD2	2.05	0.57
1:L:316:HIS:CA	1:L:323:ILE:HD13	2.32	0.57
1:O:316:HIS:HD2	1:O:317:THR:O	1.87	0.57
1:I:894:ARG:NH1	1:I:919:ASP:OD2	2.30	0.57
1:P:781:ARG:HG3	1:P:781:ARG:NH1	2.17	0.57
1:K:166:ARG:HG3	1:K:392:TYR:HB2	1.85	0.57
1:M:166:ARG:HG3	1:M:392:TYR:CB	2.34	0.57
1:M:778:THR:HB	1:M:887:GLN:HB3	1.85	0.57
1:J:835:LEU:C	1:J:836:ILE:HD13	2.25	0.57
1:N:153:TRP:CD1	1:N:158:TRP:HA	2.39	0.57
1:O:355:ASN:OD1	1:O:388:ARG:HD3	2.04	0.57
1:L:1021:CME:CZ	1:L:1021:CME:HB3	2.21	0.57
1:M:763:GLY:HA3	1:M:822:LEU:CD2	2.33	0.57
1:I:3:ILE:HG23	1:I:4:THR:H	1.70	0.57
1:I:580:GLU:CD	1:I:580:GLU:H	2.07	0.57
1:O:906:TYR:HB3	1:O:907:PRO:HD2	1.85	0.57
1:K:355:ASN:OD1	1:K:388:ARG:HD3	2.04	0.57
1:O:580:GLU:H	1:O:580:GLU:CD	2.07	0.57
1:O:767:GLN:HG3	1:O:768:MET:N	2.20	0.57
1:I:778:THR:HB	1:I:887:GLN:HB3	1.85	0.57
1:P:316:HIS:HD2	1:P:317:THR:O	1.87	0.57
1:O:71:GLU:HB2	5:O:7512:HOH:O	2.05	0.57
1:K:781:ARG:HG3	1:K:781:ARG:NH1	2.17	0.57
1:L:249:GLU:HG2	1:L:251:ARG:HH12	1.67	0.57
1:P:66:PRO:HB3	1:P:187:MET:CE	2.35	0.57
1:J:66:PRO:HB3	1:J:187:MET:CE	2.35	0.57
1:J:3:ILE:HG23	1:J:4:THR:H	1.69	0.57
1:M:3:ILE:HG23	1:M:4:THR:H	1.70	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:580:GLU:HG2	1:P:581:ASN:OD1	2.04	0.57
1:I:835:LEU:C	1:I:836:ILE:HD13	2.25	0.57
1:L:130:ASP:OD1	1:L:132:SER:N	2.29	0.57
1:K:272:ALA:HB1	1:K:273:PRO:HD2	1.85	0.57
1:O:403:ASP:OD1	1:O:451:PRO:HD2	2.05	0.57
1:I:316:HIS:CA	1:I:323:ILE:HD13	2.32	0.57
1:N:316:HIS:CA	1:N:323:ILE:HD13	2.33	0.57
1:K:66:PRO:HB3	1:K:187:MET:CE	2.35	0.57
1:I:66:PRO:HB3	1:I:187:MET:CE	2.35	0.57
1:N:66:PRO:HB3	1:N:187:MET:CE	2.35	0.57
1:P:822:LEU:CD1	1:P:824:GLN:H	2.16	0.57
1:M:701:VAL:HG22	1:M:714:ILE:HD12	1.87	0.57
1:N:287:ASP:N	1:N:287:ASP:OD1	2.29	0.57
1:O:580:GLU:HG2	1:O:581:ASN:OD1	2.04	0.57
1:M:84:VAL:HG12	1:M:85:VAL:N	2.20	0.57
1:O:66:PRO:HB3	1:O:187:MET:CE	2.35	0.56
1:L:654:TRP:CE3	1:L:655:MET:HA	2.40	0.56
1:O:701:VAL:HG22	1:O:714:ILE:HD12	1.87	0.56
1:K:3:ILE:HG23	1:K:4:THR:H	1.70	0.56
1:J:30:HIS:ND1	1:J:31:PRO:O	2.26	0.56
1:P:355:ASN:OD1	1:P:388:ARG:HD3	2.04	0.56
1:J:767:GLN:HG3	1:J:768:MET:N	2.20	0.56
1:K:84:VAL:HG12	1:K:85:VAL:N	2.20	0.56
1:K:822:LEU:CD1	1:K:824:GLN:H	2.15	0.56
1:N:654:TRP:CE3	1:N:655:MET:HA	2.40	0.56
1:P:714:ILE:N	1:P:714:ILE:HD13	2.20	0.56
1:L:3:ILE:HG23	1:L:4:THR:H	1.69	0.56
1:I:355:ASN:OD1	1:I:388:ARG:HD3	2.04	0.56
1:I:730:LEU:HB3	1:I:731:PRO:HD2	1.85	0.56
1:J:84:VAL:HG12	1:J:85:VAL:N	2.20	0.56
1:K:740:LEU:CD1	1:K:741:THR:H	2.12	0.56
1:M:249:GLU:HG2	1:M:251:ARG:HH12	1.67	0.56
1:P:894:ARG:HH22	1:P:921:PRO:HD3	1.71	0.56
1:N:255:ARG:HG2	1:N:255:ARG:NH1	2.14	0.56
1:J:654:TRP:CE3	1:J:655:MET:HA	2.40	0.56
1:O:800:ARG:CZ	1:O:800:ARG:HB3	2.36	0.56
1:O:767:GLN:HA	1:O:776:LEU:HD12	1.88	0.56
1:L:84:VAL:HG12	1:L:85:VAL:N	2.20	0.56
1:O:287:ASP:N	1:O:287:ASP:OD1	2.29	0.56
1:N:140:ARG:HB2	1:N:171:PHE:O	2.06	0.56
1:M:767:GLN:HA	1:M:776:LEU:HD12	1.88	0.56
1:P:140:ARG:HB2	1:P:171:PHE:O	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:767:GLN:HG3	1:I:768:MET:N	2.20	0.56
1:L:906:TYR:HB3	1:L:907:PRO:HD2	1.85	0.56
1:I:140:ARG:HB2	1:I:171:PHE:O	2.06	0.56
1:O:835:LEU:C	1:O:836:ILE:HD13	2.25	0.56
1:L:767:GLN:HG3	1:L:768:MET:N	2.20	0.56
1:P:668:VAL:CG1	1:P:669:PRO:HD2	2.31	0.56
1:N:71:GLU:HB2	5:N:4348:HOH:O	2.05	0.56
1:I:654:TRP:CE3	1:I:655:MET:HA	2.40	0.56
1:J:714:ILE:N	1:J:714:ILE:HD13	2.20	0.56
1:J:800:ARG:CZ	1:J:800:ARG:HB3	2.36	0.56
1:O:724:GLU:O	1:P:847:LYS:NZ	2.27	0.56
1:N:786:ARG:HH11	1:N:990:HIS:HE1	1.54	0.56
1:P:835:LEU:C	1:P:836:ILE:HD13	2.25	0.56
1:M:740:LEU:CD1	1:M:741:THR:H	2.12	0.56
1:M:71:GLU:HB2	5:M:7512:HOH:O	2.05	0.56
1:M:894:ARG:HH22	1:M:921:PRO:HD3	1.71	0.56
1:O:894:ARG:HH22	1:O:921:PRO:HD3	1.71	0.56
1:M:66:PRO:HB3	1:M:187:MET:CE	2.35	0.56
1:O:654:TRP:CE3	1:O:655:MET:HA	2.40	0.56
1:K:654:TRP:CE3	1:K:655:MET:HA	2.40	0.56
1:I:372:MET:HE1	1:I:395:HIS:HB3	1.87	0.56
1:P:701:VAL:HG22	1:P:714:ILE:HD12	1.87	0.56
1:I:800:ARG:HB3	1:I:800:ARG:CZ	2.36	0.56
1:N:3:ILE:HG23	1:N:4:THR:H	1.69	0.56
1:O:786:ARG:HH11	1:O:990:HIS:HE1	1.54	0.56
1:O:84:VAL:HG12	1:O:85:VAL:N	2.20	0.56
1:K:71:GLU:HB2	5:K:7512:HOH:O	2.05	0.56
1:K:894:ARG:HH22	1:K:921:PRO:HD3	1.71	0.56
1:P:654:TRP:CE3	1:P:655:MET:HA	2.40	0.56
1:N:822:LEU:CD1	1:N:824:GLN:H	2.16	0.56
1:M:166:ARG:HG2	1:M:414:ASN:ND2	2.21	0.56
1:I:334:GLU:OE1	1:I:336:ARG:NH1	2.39	0.56
1:J:334:GLU:OE1	1:J:336:ARG:NH1	2.39	0.56
1:M:714:ILE:HD13	1:M:714:ILE:N	2.20	0.56
1:N:403:ASP:OD1	1:N:451:PRO:HD2	2.05	0.56
1:P:427:THR:HA	1:P:436:MET:HE2	1.87	0.56
1:L:316:HIS:HD2	1:L:317:THR:O	1.87	0.56
1:K:316:HIS:HD2	1:K:317:THR:O	1.87	0.56
1:I:71:GLU:HB2	5:I:7512:HOH:O	2.05	0.56
1:K:166:ARG:HG2	1:K:414:ASN:ND2	2.21	0.56
1:M:654:TRP:CE3	1:M:655:MET:HA	2.40	0.56
1:L:372:MET:HE1	1:L:395:HIS:HB3	1.88	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:334:GLU:OE1	1:M:336:ARG:NH1	2.39	0.56
1:I:701:VAL:HG22	1:I:714:ILE:HD12	1.87	0.56
1:P:3:ILE:HG23	1:P:4:THR:H	1.69	0.56
1:I:786:ARG:HH11	1:I:990:HIS:HE1	1.54	0.56
1:J:767:GLN:HA	1:J:776:LEU:HD12	1.88	0.56
1:N:767:GLN:HA	1:N:776:LEU:HD12	1.88	0.56
1:J:781:ARG:NH1	1:J:781:ARG:HG3	2.17	0.56
1:J:166:ARG:HG2	1:J:414:ASN:ND2	2.21	0.56
1:I:166:ARG:HG2	1:I:414:ASN:ND2	2.21	0.56
1:I:714:ILE:N	1:I:714:ILE:HD13	2.20	0.56
1:I:767:GLN:HA	1:I:776:LEU:HD12	1.88	0.56
1:K:140:ARG:HB2	1:K:171:PHE:O	2.06	0.56
1:M:869:ASP:OD2	1:M:1015:HIS:ND1	2.33	0.56
1:P:84:VAL:HG12	1:P:85:VAL:N	2.20	0.56
1:P:71:GLU:HB2	5:P:4681:HOH:O	2.05	0.56
1:K:334:GLU:OE1	1:K:336:ARG:NH1	2.39	0.56
1:N:800:ARG:CZ	1:N:800:ARG:HB3	2.36	0.56
1:L:800:ARG:CZ	1:L:800:ARG:HB3	2.36	0.56
1:N:287:ASP:CG	1:O:425:ARG:HH22	2.09	0.56
1:L:767:GLN:HA	1:L:776:LEU:HD12	1.88	0.56
1:I:403:ASP:OD1	1:I:451:PRO:HD2	2.05	0.56
1:J:975:LEU:N	1:J:975:LEU:HD23	2.21	0.56
1:M:835:LEU:C	1:M:836:ILE:HD13	2.25	0.56
1:L:894:ARG:HH22	1:L:921:PRO:HD3	1.71	0.56
1:J:701:VAL:HG22	1:J:714:ILE:HD12	1.87	0.56
1:O:334:GLU:OE1	1:O:336:ARG:NH1	2.39	0.56
1:M:786:ARG:HH11	1:M:990:HIS:HE1	1.54	0.56
1:M:767:GLN:HG3	1:M:768:MET:N	2.20	0.56
1:M:140:ARG:HB2	1:M:171:PHE:O	2.06	0.56
1:L:140:ARG:HB2	1:L:171:PHE:O	2.06	0.56
1:J:869:ASP:OD2	1:J:1015:HIS:ND1	2.33	0.56
1:K:767:GLN:HA	1:K:776:LEU:HD12	1.88	0.56
1:K:767:GLN:HG3	1:K:768:MET:N	2.20	0.56
1:L:166:ARG:HG2	1:L:414:ASN:ND2	2.21	0.55
1:L:334:GLU:OE1	1:L:336:ARG:NH1	2.39	0.55
1:M:800:ARG:CZ	1:M:800:ARG:HB3	2.36	0.55
1:K:800:ARG:CZ	1:K:800:ARG:HB3	2.36	0.55
1:N:989:PHE:CE1	1:N:1014:TYR:HB3	2.42	0.55
1:N:84:VAL:HG12	1:N:85:VAL:N	2.20	0.55
1:I:84:VAL:HG12	1:I:85:VAL:N	2.20	0.55
1:P:767:GLN:HA	1:P:776:LEU:HD12	1.88	0.55
1:P:316:HIS:CA	1:P:323:ILE:HD13	2.32	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:166:ARG:HG2	1:O:414:ASN:ND2	2.21	0.55
1:N:714:ILE:HD13	1:N:714:ILE:N	2.20	0.55
1:L:403:ASP:OD1	1:L:451:PRO:HD2	2.05	0.55
1:J:71:GLU:HB2	5:J:7512:HOH:O	2.05	0.55
1:K:249:GLU:HG2	1:K:251:ARG:HH12	1.67	0.55
1:M:372:MET:HE1	1:M:395:HIS:HB3	1.87	0.55
1:N:334:GLU:OE1	1:N:336:ARG:NH1	2.39	0.55
1:O:714:ILE:HD13	1:O:714:ILE:N	2.20	0.55
1:K:701:VAL:HG22	1:K:714:ILE:HD12	1.87	0.55
1:M:78:LEU:HD23	1:M:78:LEU:N	2.21	0.55
1:P:786:ARG:HH11	1:P:990:HIS:HE1	1.54	0.55
1:K:989:PHE:CE1	1:K:1014:TYR:HB3	2.42	0.55
1:P:767:GLN:HG3	1:P:768:MET:N	2.20	0.55
1:P:772:ASP:N	1:P:772:ASP:OD1	2.30	0.55
1:I:975:LEU:N	1:I:975:LEU:HD23	2.21	0.55
1:L:71:GLU:HB2	5:L:7512:HOH:O	2.05	0.55
1:M:781:ARG:HG3	1:M:781:ARG:NH1	2.17	0.55
1:L:66:PRO:HB3	1:L:187:MET:CE	2.35	0.55
1:N:166:ARG:HG2	1:N:414:ASN:ND2	2.21	0.55
1:O:372:MET:HE1	1:O:395:HIS:HB3	1.87	0.55
1:N:767:GLN:HG3	1:N:768:MET:N	2.20	0.55
1:O:975:LEU:HD23	1:O:975:LEU:N	2.21	0.55
1:L:835:LEU:C	1:L:836:ILE:HD13	2.25	0.55
1:M:282:ARG:HB2	1:P:422:PRO:HA	1.87	0.55
1:N:78:LEU:N	1:N:78:LEU:HD23	2.21	0.55
1:P:800:ARG:CZ	1:P:800:ARG:HB3	2.36	0.55
1:K:975:LEU:HD23	1:K:975:LEU:N	2.21	0.55
1:N:835:LEU:C	1:N:836:ILE:HD13	2.25	0.55
1:O:5:ASP:OD2	1:O:157:ARG:HA	2.07	0.55
1:P:258:VAL:HA	1:P:312:VAL:O	2.07	0.55
1:J:140:ARG:HB2	1:J:171:PHE:O	2.06	0.55
1:L:668:VAL:CG1	1:L:669:PRO:HD2	2.31	0.55
1:I:57:GLU:HG2	1:I:83:THR:HG23	1.84	0.55
1:M:7:LEU:HD13	1:M:74:LEU:CD1	2.32	0.55
1:P:334:GLU:OE1	1:P:336:ARG:NH1	2.39	0.55
1:I:282:ARG:HD3	1:L:418:HIS:O	2.06	0.55
1:O:30:HIS:ND1	1:O:31:PRO:O	2.26	0.55
1:K:786:ARG:HH11	1:K:990:HIS:HE1	1.54	0.55
1:O:50:GLN:O	1:O:215:LEU:HA	2.07	0.55
1:O:140:ARG:HB2	1:O:171:PHE:O	2.06	0.55
1:M:989:PHE:CE1	1:M:1014:TYR:HB3	2.42	0.55
1:I:989:PHE:CE1	1:I:1014:TYR:HB3	2.42	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:5:ASP:OD2	1:J:157:ARG:HA	2.07	0.55
1:P:50:GLN:O	1:P:215:LEU:HA	2.07	0.55
1:M:5:ASP:OD2	1:M:157:ARG:HA	2.07	0.55
1:N:258:VAL:HA	1:N:312:VAL:O	2.07	0.55
1:O:258:VAL:HA	1:O:312:VAL:O	2.07	0.55
1:N:436:MET:HE1	1:N:467:ASN:HD22	1.69	0.55
1:I:37:ARG:CG	1:I:37:ARG:HH11	2.20	0.55
1:M:37:ARG:CG	1:M:37:ARG:HH11	2.20	0.55
1:M:246:MET:HE3	1:M:247:CYS:C	2.27	0.55
1:J:989:PHE:CE1	1:J:1014:TYR:HB3	2.42	0.55
1:O:989:PHE:CE1	1:O:1014:TYR:HB3	2.42	0.55
1:M:975:LEU:HD23	1:M:975:LEU:N	2.21	0.55
1:J:50:GLN:O	1:J:215:LEU:HA	2.07	0.55
1:P:595:THR:HG23	1:P:596:PRO:CA	2.37	0.55
1:L:989:PHE:CE1	1:L:1014:TYR:HB3	2.42	0.55
1:J:178:ARG:NH1	1:J:181:GLU:O	2.33	0.55
1:L:50:GLN:O	1:L:215:LEU:HA	2.07	0.55
1:K:130:ASP:OD1	1:K:132:SER:N	2.30	0.55
1:O:740:LEU:CD1	1:O:741:THR:H	2.12	0.55
1:M:92:MET:HE3	1:M:362:LEU:O	2.07	0.55
1:P:166:ARG:HG2	1:P:414:ASN:ND2	2.21	0.55
1:L:37:ARG:HH11	1:L:37:ARG:CG	2.20	0.55
1:N:403:ASP:OD2	1:N:450:HIS:ND1	2.34	0.55
1:N:39:SER:OG	1:N:40:GLU:N	2.40	0.55
1:J:258:VAL:HA	1:J:312:VAL:O	2.07	0.55
1:M:258:VAL:HA	1:M:312:VAL:O	2.07	0.55
1:P:975:LEU:N	1:P:975:LEU:HD23	2.21	0.55
1:I:258:VAL:HA	1:I:312:VAL:O	2.07	0.55
1:P:5:ASP:OD2	1:P:157:ARG:HA	2.07	0.55
1:O:37:ARG:HH11	1:O:37:ARG:CG	2.20	0.54
1:J:37:ARG:CG	1:J:37:ARG:HH11	2.20	0.54
1:P:78:LEU:HD23	1:P:78:LEU:N	2.21	0.54
1:L:287:ASP:N	1:L:287:ASP:OD1	2.29	0.54
1:P:39:SER:OG	1:P:40:GLU:N	2.40	0.54
1:I:50:GLN:O	1:I:215:LEU:HA	2.07	0.54
1:L:975:LEU:HD23	1:L:975:LEU:N	2.21	0.54
1:N:5:ASP:OD2	1:N:157:ARG:HA	2.07	0.54
1:M:50:GLN:O	1:M:215:LEU:HA	2.07	0.54
1:P:37:ARG:CG	1:P:37:ARG:HH11	2.20	0.54
1:L:78:LEU:N	1:L:78:LEU:HD23	2.21	0.54
1:O:78:LEU:N	1:O:78:LEU:HD23	2.21	0.54
1:O:246:MET:HE3	1:O:247:CYS:C	2.27	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:282:ARG:HG3	1:P:423:MET:HB2	1.88	0.54
1:P:952:ARG:O	1:P:1018:LEU:HD23	2.08	0.54
1:K:5:ASP:OD2	1:K:157:ARG:HA	2.07	0.54
1:N:742:THR:HG22	1:N:743:SER:H	1.73	0.54
1:O:668:VAL:CG1	1:O:669:PRO:HD2	2.32	0.54
1:M:66:PRO:HB3	1:M:187:MET:HE1	1.90	0.54
1:J:66:PRO:HB3	1:J:187:MET:HE1	1.90	0.54
1:N:130:ASP:OD1	1:N:132:SER:N	2.29	0.54
1:I:869:ASP:OD2	1:I:1015:HIS:ND1	2.33	0.54
1:K:50:GLN:O	1:K:215:LEU:HA	2.07	0.54
1:L:745:MET:HE2	1:L:745:MET:HA	1.89	0.54
1:J:668:VAL:CG1	1:J:669:PRO:HD2	2.31	0.54
1:I:66:PRO:HB3	1:I:187:MET:HE1	1.89	0.54
1:I:822:LEU:CD1	1:I:824:GLN:H	2.16	0.54
1:K:634:GLN:O	1:K:682:LEU:HB2	2.07	0.54
1:I:127:PHE:CE2	1:I:184:LEU:HG	2.42	0.54
1:P:989:PHE:CE1	1:P:1014:TYR:HB3	2.42	0.54
1:L:5:ASP:OD2	1:L:157:ARG:HA	2.07	0.54
1:P:127:PHE:CE2	1:P:184:LEU:HG	2.42	0.54
1:L:952:ARG:O	1:L:1018:LEU:HD23	2.08	0.54
1:K:920:LEU:HB3	1:K:921:PRO:CD	2.38	0.54
1:N:894:ARG:HH22	1:N:921:PRO:HD3	1.71	0.54
1:I:894:ARG:HH22	1:I:921:PRO:HD3	1.71	0.54
1:M:634:GLN:O	1:M:682:LEU:HB2	2.07	0.54
1:M:876:THR:OG1	1:M:877:PRO:HD2	2.08	0.54
1:O:876:THR:OG1	1:O:877:PRO:HD2	2.08	0.54
1:L:258:VAL:HA	1:L:312:VAL:O	2.07	0.54
1:N:515:VAL:HG21	1:O:281:GLU:HG3	1.90	0.54
1:N:50:GLN:O	1:N:215:LEU:HA	2.07	0.54
1:J:952:ARG:O	1:J:1018:LEU:HD23	2.08	0.54
1:I:5:ASP:OD2	1:I:157:ARG:HA	2.07	0.54
1:L:920:LEU:HB3	1:L:921:PRO:CD	2.38	0.54
1:P:278:ILE:H	1:P:278:ILE:CD1	2.21	0.54
1:N:737:ILE:HB	1:N:738:PRO:HD2	1.90	0.54
1:I:737:ILE:HB	1:I:738:PRO:HD2	1.90	0.54
1:P:737:ILE:HB	1:P:738:PRO:HD2	1.90	0.54
1:K:869:ASP:OD2	1:K:1015:HIS:ND1	2.33	0.54
1:K:433:LEU:HD12	1:K:433:LEU:C	2.28	0.54
1:O:634:GLN:O	1:O:682:LEU:HB2	2.07	0.54
1:P:634:GLN:O	1:P:682:LEU:HB2	2.07	0.54
1:L:786:ARG:HH11	1:L:990:HIS:HE1	1.54	0.54
1:N:127:PHE:CE2	1:N:184:LEU:HG	2.42	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:130:ASP:OD1	1:J:131:GLU:N	2.41	0.54
1:I:876:THR:OG1	1:I:877:PRO:HD2	2.08	0.54
1:O:130:ASP:OD1	1:O:131:GLU:N	2.41	0.54
1:P:808:GLU:OE1	1:P:808:GLU:HA	2.08	0.54
1:K:952:ARG:O	1:K:1018:LEU:HD23	2.08	0.54
1:J:433:LEU:HD12	1:J:433:LEU:C	2.28	0.54
1:N:634:GLN:O	1:N:682:LEU:HB2	2.07	0.54
1:K:37:ARG:CG	1:K:37:ARG:HH11	2.20	0.54
1:M:595:THR:HG23	1:M:596:PRO:CA	2.37	0.54
1:J:786:ARG:HH11	1:J:990:HIS:HE1	1.54	0.54
1:O:952:ARG:O	1:O:1018:LEU:HD23	2.08	0.54
1:N:975:LEU:HD23	1:N:975:LEU:N	2.21	0.54
1:O:39:SER:OG	1:O:40:GLU:N	2.40	0.54
1:P:130:ASP:OD1	1:P:131:GLU:N	2.41	0.54
1:I:742:THR:HG22	1:I:743:SER:H	1.73	0.54
1:K:742:THR:HG22	1:K:743:SER:H	1.73	0.54
1:I:254:LEU:C	1:I:255:ARG:HG2	2.28	0.54
1:O:254:LEU:C	1:O:255:ARG:HG2	2.28	0.54
1:P:433:LEU:C	1:P:433:LEU:HD12	2.28	0.54
1:L:433:LEU:HD12	1:L:433:LEU:C	2.28	0.54
1:N:876:THR:OG1	1:N:877:PRO:HD2	2.08	0.54
1:O:737:ILE:HB	1:O:738:PRO:HD2	1.90	0.54
1:J:39:SER:OG	1:J:40:GLU:N	2.40	0.54
1:L:737:ILE:HB	1:L:738:PRO:HD2	1.90	0.54
1:M:737:ILE:HB	1:M:738:PRO:HD2	1.90	0.54
1:K:258:VAL:HA	1:K:312:VAL:O	2.07	0.54
1:L:254:LEU:C	1:L:255:ARG:HG2	2.28	0.53
1:L:66:PRO:HB3	1:L:187:MET:HE1	1.90	0.53
1:P:254:LEU:C	1:P:255:ARG:HG2	2.28	0.53
1:L:631:LEU:HD12	1:L:632:SER:N	2.24	0.53
1:K:14:ARG:HG2	1:K:16:TRP:CZ2	2.43	0.53
1:M:130:ASP:OD1	1:M:131:GLU:N	2.41	0.53
1:L:645:ARG:HH22	1:L:650:GLU:CD	2.12	0.53
1:P:920:LEU:HB3	1:P:921:PRO:CD	2.38	0.53
1:P:66:PRO:HB3	1:P:187:MET:HE1	1.89	0.53
1:N:37:ARG:HH11	1:N:37:ARG:CG	2.20	0.53
1:J:631:LEU:HD12	1:J:632:SER:N	2.24	0.53
1:P:246:MET:HE3	1:P:247:CYS:C	2.28	0.53
1:K:246:MET:HE3	1:K:247:CYS:C	2.29	0.53
1:M:236:SER:OG	1:M:237:ARG:HD3	2.09	0.53
1:K:127:PHE:CE2	1:K:184:LEU:HG	2.42	0.53
1:J:876:THR:OG1	1:J:877:PRO:HD2	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:876:THR:OG1	1:K:877:PRO:HD2	2.08	0.53
1:K:645:ARG:HH22	1:K:650:GLU:CD	2.12	0.53
1:O:645:ARG:HH22	1:O:650:GLU:CD	2.12	0.53
1:N:130:ASP:OD1	1:N:131:GLU:N	2.41	0.53
1:K:808:GLU:HA	1:K:808:GLU:OE1	2.08	0.53
1:I:952:ARG:O	1:I:1018:LEU:HD23	2.08	0.53
1:O:141:ILE:HG12	1:O:142:ILE:N	2.24	0.53
1:J:742:THR:HG22	1:J:743:SER:H	1.73	0.53
1:I:634:GLN:O	1:I:682:LEU:HB2	2.07	0.53
1:J:634:GLN:O	1:J:682:LEU:HB2	2.07	0.53
1:N:433:LEU:C	1:N:433:LEU:HD12	2.28	0.53
1:I:14:ARG:HG2	1:I:16:TRP:CZ2	2.43	0.53
1:L:876:THR:OG1	1:L:877:PRO:HD2	2.08	0.53
1:M:952:ARG:O	1:M:1018:LEU:HD23	2.08	0.53
1:O:910:LEU:HD12	1:O:910:LEU:C	2.29	0.53
1:J:737:ILE:HB	1:J:738:PRO:HD2	1.90	0.53
1:K:737:ILE:HB	1:K:738:PRO:HD2	1.90	0.53
1:N:638:VAL:O	1:N:677:LYS:HA	2.09	0.53
1:P:745:MET:HE2	1:P:745:MET:HA	1.91	0.53
1:M:254:LEU:C	1:M:255:ARG:HG2	2.28	0.53
1:O:127:PHE:CE2	1:O:184:LEU:HG	2.42	0.53
1:N:14:ARG:HG2	1:N:16:TRP:CZ2	2.43	0.53
1:L:130:ASP:OD1	1:L:131:GLU:N	2.41	0.53
1:P:130:ASP:OD1	1:P:132:SER:N	2.30	0.53
1:K:910:LEU:C	1:K:910:LEU:HD12	2.29	0.53
1:M:808:GLU:OE1	1:M:808:GLU:HA	2.08	0.53
1:P:141:ILE:HG12	1:P:142:ILE:N	2.24	0.53
1:I:651:LEU:CD1	1:I:669:PRO:HA	2.39	0.53
1:L:7:LEU:HD13	1:L:74:LEU:CD1	2.32	0.53
1:J:920:LEU:HB3	1:J:921:PRO:CD	2.38	0.53
1:L:649:ASN:OD1	1:L:703:PRO:HD2	2.09	0.53
1:N:278:ILE:CD1	1:N:278:ILE:H	2.21	0.53
1:P:236:SER:OG	1:P:237:ARG:HD3	2.09	0.53
1:O:236:SER:OG	1:O:237:ARG:HD3	2.09	0.53
1:J:127:PHE:CE2	1:J:184:LEU:HG	2.42	0.53
1:L:14:ARG:HG2	1:L:16:TRP:CZ2	2.44	0.53
1:M:282:ARG:HB3	1:P:421:VAL:HG22	1.91	0.53
1:P:910:LEU:HD12	1:P:910:LEU:C	2.29	0.53
1:N:808:GLU:OE1	1:N:808:GLU:HA	2.08	0.53
1:L:742:THR:HG22	1:L:743:SER:H	1.73	0.53
1:K:316:HIS:CA	1:K:323:ILE:HD13	2.32	0.53
1:P:649:ASN:OD1	1:P:703:PRO:HD2	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:649:ASN:OD1	1:K:703:PRO:HD2	2.09	0.53
1:O:631:LEU:HD12	1:O:632:SER:N	2.24	0.53
1:I:78:LEU:HD23	1:I:78:LEU:N	2.21	0.53
1:K:473:ARG:C	1:K:473:ARG:HD3	2.29	0.53
1:J:645:ARG:HH22	1:J:650:GLU:CD	2.12	0.53
1:P:974:HIS:NE2	1:P:975:LEU:HD21	2.24	0.53
1:J:910:LEU:HD12	1:J:910:LEU:C	2.29	0.53
1:M:651:LEU:CD1	1:M:669:PRO:HA	2.39	0.53
1:N:651:LEU:CD1	1:N:669:PRO:HA	2.39	0.53
1:L:651:LEU:CD1	1:L:669:PRO:HA	2.39	0.53
1:J:316:HIS:CA	1:J:323:ILE:HD13	2.32	0.53
1:L:634:GLN:O	1:L:682:LEU:HB2	2.07	0.53
1:O:433:LEU:C	1:O:433:LEU:HD12	2.28	0.53
1:N:649:ASN:OD1	1:N:703:PRO:HD2	2.09	0.53
1:N:631:LEU:HD12	1:N:632:SER:N	2.24	0.53
1:L:236:SER:OG	1:L:237:ARG:HD3	2.09	0.53
1:M:14:ARG:HG2	1:M:16:TRP:CZ2	2.43	0.53
1:I:974:HIS:NE2	1:I:975:LEU:HD21	2.24	0.53
1:I:638:VAL:O	1:I:677:LYS:HA	2.09	0.53
1:J:287:ASP:OD2	1:K:425:ARG:NH2	2.41	0.53
1:M:73:TRP:CE2	1:M:122:CYS:HB3	2.44	0.53
1:I:39:SER:OG	1:I:40:GLU:N	2.40	0.53
1:L:141:ILE:HG12	1:L:142:ILE:N	2.24	0.53
1:K:73:TRP:CE2	1:K:122:CYS:HB3	2.44	0.53
1:P:255:ARG:HG2	1:P:255:ARG:NH1	2.14	0.53
1:M:127:PHE:CE2	1:M:184:LEU:HG	2.42	0.53
1:N:645:ARG:HH22	1:N:650:GLU:CD	2.12	0.53
1:J:835:LEU:O	1:J:836:ILE:HD13	2.09	0.53
1:J:974:HIS:NE2	1:J:975:LEU:HD21	2.24	0.53
1:L:403:ASP:OD2	1:L:450:HIS:ND1	2.34	0.53
1:M:974:HIS:NE2	1:M:975:LEU:HD21	2.24	0.53
1:K:130:ASP:OD1	1:K:131:GLU:N	2.41	0.53
1:L:974:HIS:NE2	1:L:975:LEU:HD21	2.24	0.53
1:J:808:GLU:HA	1:J:808:GLU:OE1	2.08	0.53
1:N:867:THR:HG22	1:N:867:THR:O	2.09	0.53
1:N:952:ARG:O	1:N:1018:LEU:HD23	2.08	0.53
1:K:287:ASP:N	1:K:287:ASP:OD1	2.29	0.53
1:I:73:TRP:CE2	1:I:122:CYS:HB3	2.44	0.53
1:J:73:TRP:CE2	1:J:122:CYS:HB3	2.44	0.53
1:I:141:ILE:HG12	1:I:142:ILE:N	2.24	0.53
1:O:808:GLU:OE1	1:O:808:GLU:HA	2.08	0.53
1:O:742:THR:HG22	1:O:743:SER:H	1.73	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:740:LEU:CD1	1:L:741:THR:H	2.12	0.53
1:K:651:LEU:CD1	1:K:669:PRO:HA	2.39	0.53
1:I:433:LEU:C	1:I:433:LEU:HD12	2.28	0.53
1:O:649:ASN:OD1	1:O:703:PRO:HD2	2.09	0.53
1:J:78:LEU:N	1:J:78:LEU:HD23	2.21	0.53
1:J:236:SER:OG	1:J:237:ARG:HD3	2.09	0.53
1:J:14:ARG:HG2	1:J:16:TRP:CZ2	2.43	0.53
1:P:876:THR:OG1	1:P:877:PRO:HD2	2.08	0.53
1:O:403:ASP:OD2	1:O:450:HIS:ND1	2.34	0.53
1:L:835:LEU:O	1:L:836:ILE:HD13	2.09	0.53
1:L:910:LEU:HD12	1:L:910:LEU:C	2.29	0.53
1:M:141:ILE:HG12	1:M:142:ILE:N	2.24	0.53
1:L:638:VAL:O	1:L:677:LYS:HA	2.09	0.53
1:P:69:VAL:HG13	1:P:70:PRO:HD2	1.91	0.53
1:I:579:ASP:N	1:I:583:ASN:O	2.40	0.53
1:K:254:LEU:C	1:K:255:ARG:HG2	2.28	0.53
1:K:631:LEU:HD12	1:K:632:SER:N	2.24	0.53
1:O:278:ILE:H	1:O:278:ILE:CD1	2.21	0.53
1:M:631:LEU:HD12	1:M:632:SER:N	2.24	0.53
1:M:278:ILE:CD1	1:M:278:ILE:H	2.21	0.53
1:K:78:LEU:N	1:K:78:LEU:HD23	2.21	0.53
1:M:987:ASP:OD2	1:M:990:HIS:HD2	1.92	0.53
1:J:473:ARG:HD3	1:J:473:ARG:C	2.29	0.53
1:I:819:GLU:HA	1:I:819:GLU:OE2	2.09	0.53
1:L:808:GLU:OE1	1:L:808:GLU:HA	2.08	0.53
1:K:39:SER:OG	1:K:40:GLU:N	2.40	0.53
1:P:651:LEU:CD1	1:P:669:PRO:HA	2.39	0.52
1:O:595:THR:HG23	1:O:596:PRO:CA	2.38	0.52
1:J:595:THR:HG23	1:J:596:PRO:CA	2.37	0.52
1:I:236:SER:OG	1:I:237:ARG:HD3	2.09	0.52
1:L:597:ASN:HD22	1:L:599:ARG:H	1.57	0.52
1:L:987:ASP:OD2	1:L:990:HIS:HD2	1.92	0.52
1:N:987:ASP:OD2	1:N:990:HIS:HD2	1.92	0.52
1:O:14:ARG:HG2	1:O:16:TRP:CZ2	2.43	0.52
1:M:645:ARG:HH22	1:M:650:GLU:CD	2.12	0.52
1:M:835:LEU:O	1:M:836:ILE:HD13	2.09	0.52
1:N:974:HIS:NE2	1:N:975:LEU:HD21	2.24	0.52
1:K:69:VAL:HG13	1:K:70:PRO:HD2	1.91	0.52
1:J:425:ARG:NH2	1:K:287:ASP:OD2	2.42	0.52
1:K:638:VAL:O	1:K:677:LYS:HA	2.09	0.52
1:I:130:ASP:OD1	1:I:131:GLU:N	2.41	0.52
1:I:808:GLU:OE1	1:I:808:GLU:HA	2.08	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:742:THR:HG22	1:P:743:SER:H	1.73	0.52
1:K:634:GLN:HE22	1:K:685:LEU:H	1.57	0.52
1:M:423:MET:HE2	1:P:282:ARG:HG2	1.90	0.52
1:I:631:LEU:HD12	1:I:632:SER:N	2.24	0.52
1:I:282:ARG:HH11	1:L:419:GLY:HA2	1.74	0.52
1:I:69:VAL:HG13	1:I:70:PRO:HD2	1.91	0.52
1:J:819:GLU:OE2	1:J:819:GLU:HA	2.09	0.52
1:L:819:GLU:HA	1:L:819:GLU:OE2	2.09	0.52
1:M:910:LEU:HD12	1:M:910:LEU:C	2.29	0.52
1:N:910:LEU:HD12	1:N:910:LEU:C	2.29	0.52
1:O:68:ALA:O	1:O:70:PRO:HD3	2.10	0.52
1:M:638:VAL:O	1:M:677:LYS:HA	2.09	0.52
1:J:141:ILE:HG12	1:J:142:ILE:N	2.24	0.52
1:M:742:THR:HG22	1:M:743:SER:H	1.73	0.52
1:J:894:ARG:HH22	1:J:921:PRO:HD3	1.71	0.52
1:J:246:MET:HE3	1:J:247:CYS:C	2.30	0.52
1:I:597:ASN:HD22	1:I:599:ARG:H	1.57	0.52
1:P:68:ALA:O	1:P:70:PRO:HD3	2.10	0.52
1:L:68:ALA:O	1:L:70:PRO:HD3	2.10	0.52
1:O:638:VAL:O	1:O:677:LYS:HA	2.09	0.52
1:M:867:THR:HG22	1:M:867:THR:O	2.09	0.52
1:P:819:GLU:HA	1:P:819:GLU:OE2	2.09	0.52
1:N:73:TRP:CE2	1:N:122:CYS:HB3	2.44	0.52
1:L:39:SER:OG	1:L:40:GLU:N	2.40	0.52
1:N:254:LEU:C	1:N:255:ARG:HG2	2.28	0.52
1:J:653[A]:HIS:HD2	1:J:666:GLY:O	1.93	0.52
1:K:653[A]:HIS:HD2	1:K:666:GLY:O	1.93	0.52
1:P:634:GLN:HE22	1:P:685:LEU:H	1.57	0.52
1:L:595:THR:HG23	1:L:596:PRO:CA	2.38	0.52
1:M:649:ASN:OD1	1:M:703:PRO:HD2	2.09	0.52
1:N:236:SER:OG	1:N:237:ARG:HD3	2.09	0.52
1:K:987:ASP:OD2	1:K:990:HIS:HD2	1.93	0.52
1:I:473:ARG:HD3	1:I:473:ARG:C	2.29	0.52
1:I:910:LEU:C	1:I:910:LEU:HD12	2.29	0.52
1:J:638:VAL:O	1:J:677:LYS:HA	2.09	0.52
1:J:651:LEU:CD1	1:J:669:PRO:HA	2.39	0.52
1:P:653[A]:HIS:HD2	1:P:666:GLY:O	1.93	0.52
1:M:433:LEU:HD12	1:M:433:LEU:C	2.28	0.52
1:N:595:THR:HG23	1:N:596:PRO:CA	2.37	0.52
1:K:663:LEU:N	1:K:663:LEU:HD23	2.24	0.52
1:N:246:MET:HE3	1:N:247:CYS:CA	2.39	0.52
1:P:987:ASP:OD2	1:P:990:HIS:HD2	1.93	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:127:PHE:CE2	1:L:184:LEU:HG	2.42	0.52
1:J:403:ASP:OD2	1:J:450:HIS:ND1	2.34	0.52
1:P:73:TRP:CE2	1:P:122:CYS:HB3	2.44	0.52
1:O:69:VAL:HG13	1:O:70:PRO:HD2	1.91	0.52
1:L:73:TRP:CE2	1:L:122:CYS:HB3	2.44	0.52
1:N:69:VAL:HG13	1:N:70:PRO:HD2	1.91	0.52
1:M:39:SER:OG	1:M:40:GLU:N	2.40	0.52
1:J:433:LEU:N	1:J:434:PRO:CD	2.73	0.52
1:K:433:LEU:N	1:K:434:PRO:CD	2.73	0.52
1:I:634:GLN:HE22	1:I:685:LEU:H	1.57	0.52
1:N:653[A]:HIS:HD2	1:N:666:GLY:O	1.93	0.52
1:M:634:GLN:HE22	1:M:685:LEU:H	1.57	0.52
1:M:653[A]:HIS:HD2	1:M:666:GLY:O	1.93	0.52
1:I:433:LEU:N	1:I:434:PRO:CD	2.73	0.52
1:I:278:ILE:H	1:I:278:ILE:CD1	2.21	0.52
1:K:6:SER:O	1:K:9:VAL:HG12	2.10	0.52
1:J:6:SER:O	1:J:9:VAL:HG12	2.10	0.52
1:L:69:VAL:HG13	1:L:70:PRO:HD2	1.91	0.52
1:M:68:ALA:O	1:M:70:PRO:HD3	2.10	0.52
1:N:819:GLU:HA	1:N:819:GLU:OE2	2.09	0.52
1:O:869:ASP:OD2	1:O:1015:HIS:ND1	2.33	0.52
1:N:740:LEU:CD1	1:N:741:THR:H	2.12	0.52
1:J:254:LEU:C	1:J:255:ARG:HG2	2.28	0.52
1:K:595:THR:HG23	1:K:596:PRO:CA	2.37	0.52
1:K:9:VAL:O	1:K:12:GLN:HB3	2.10	0.52
1:I:6:SER:O	1:I:9:VAL:HG12	2.10	0.52
1:K:30:HIS:CE1	1:K:33:PHE:CD1	2.98	0.52
1:I:246:MET:HE3	1:I:247:CYS:C	2.30	0.52
1:L:6:SER:O	1:L:9:VAL:HG12	2.10	0.52
1:P:9:VAL:O	1:P:12:GLN:HB3	2.10	0.52
1:N:9:VAL:O	1:N:12:GLN:HB3	2.10	0.52
1:N:597:ASN:HD22	1:N:599:ARG:H	1.57	0.52
1:P:14:ARG:HG2	1:P:16:TRP:CZ2	2.43	0.52
1:I:645:ARG:HH22	1:I:650:GLU:CD	2.12	0.52
1:P:645:ARG:HH22	1:P:650:GLU:CD	2.12	0.52
1:P:835:LEU:O	1:P:836:ILE:HD13	2.09	0.52
1:O:974:HIS:NE2	1:O:975:LEU:HD21	2.24	0.52
1:K:974:HIS:NE2	1:K:975:LEU:HD21	2.24	0.52
1:N:835:LEU:O	1:N:836:ILE:HD13	2.09	0.52
1:J:68:ALA:O	1:J:70:PRO:HD3	2.10	0.52
1:L:610:ASP:O	1:L:611:ARG:HB2	2.10	0.52
1:M:610:ASP:O	1:M:611:ARG:HB2	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:638:VAL:O	1:P:677:LYS:HA	2.09	0.52
1:J:512:PHE:HE1	1:J:517:LYS:HG3	1.75	0.52
1:I:65:ALA:HB1	1:I:66:PRO:CD	2.39	0.52
1:I:653[A]:HIS:HD2	1:I:666:GLY:O	1.93	0.52
1:L:433:LEU:N	1:L:434:PRO:CD	2.73	0.52
1:I:649:ASN:OD1	1:I:703:PRO:HD2	2.09	0.52
1:J:278:ILE:CD1	1:J:278:ILE:H	2.21	0.52
1:L:278:ILE:CD1	1:L:278:ILE:H	2.21	0.52
1:I:30:HIS:CE1	1:I:33:PHE:CD1	2.98	0.52
1:I:987:ASP:OD2	1:I:990:HIS:HD2	1.93	0.52
1:N:473:ARG:HD3	1:N:473:ARG:C	2.29	0.52
1:P:403:ASP:OD2	1:P:450:HIS:ND1	2.34	0.52
1:I:68:ALA:O	1:I:70:PRO:HD3	2.10	0.52
1:K:819:GLU:HA	1:K:819:GLU:OE2	2.09	0.52
1:N:610:ASP:O	1:N:611:ARG:HB2	2.10	0.52
1:J:781:ARG:HH11	1:J:781:ARG:CG	2.19	0.52
1:N:781:ARG:HG3	1:N:781:ARG:NH1	2.17	0.52
1:P:500:CYS:HA	1:P:534:ILE:O	2.10	0.52
1:N:53:SER:O	1:N:54:LEU:HD23	2.10	0.52
1:P:631:LEU:HD12	1:P:632:SER:N	2.24	0.52
1:I:246:MET:HE3	1:I:247:CYS:CA	2.40	0.52
1:K:597:ASN:HD22	1:K:599:ARG:H	1.57	0.52
1:N:6:SER:O	1:N:9:VAL:HG12	2.10	0.52
1:O:597:ASN:HD22	1:O:599:ARG:H	1.57	0.52
1:I:867:THR:HG22	1:I:867:THR:O	2.09	0.52
1:M:819:GLU:OE2	1:M:819:GLU:HA	2.10	0.52
1:L:832:ASP:OD1	1:L:832:ASP:N	2.43	0.52
1:N:832:ASP:OD1	1:N:832:ASP:N	2.43	0.52
1:M:870:VAL:HG12	1:M:871:GLU:N	2.25	0.52
1:N:141:ILE:HG12	1:N:142:ILE:N	2.24	0.52
1:O:651:LEU:CD1	1:O:669:PRO:HA	2.39	0.52
1:I:53:SER:O	1:I:54:LEU:HD23	2.10	0.52
1:L:53:SER:O	1:L:54:LEU:HD23	2.10	0.52
1:O:9:VAL:O	1:O:12:GLN:HB3	2.10	0.52
1:L:246:MET:HE3	1:L:247:CYS:CA	2.40	0.52
1:M:473:ARG:C	1:M:473:ARG:HD3	2.29	0.52
1:O:835:LEU:O	1:O:836:ILE:HD13	2.09	0.52
1:K:867:THR:O	1:K:867:THR:HG22	2.09	0.52
1:O:819:GLU:OE2	1:O:819:GLU:HA	2.09	0.52
1:K:141:ILE:HG12	1:K:142:ILE:N	2.24	0.52
1:P:512:PHE:HE1	1:P:517:LYS:HG3	1.75	0.52
1:K:668:VAL:CG1	1:K:669:PRO:HD2	2.31	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:781:ARG:HH11	1:N:781:ARG:CG	2.19	0.51
1:N:65:ALA:HB1	1:N:66:PRO:CD	2.39	0.51
1:N:634:GLN:HE22	1:N:685:LEU:H	1.57	0.51
1:J:500:CYS:HA	1:J:534:ILE:O	2.11	0.51
1:I:500:CYS:HA	1:I:534:ILE:O	2.11	0.51
1:I:9:VAL:O	1:I:12:GLN:HB3	2.10	0.51
1:K:708:TRP:CE3	1:K:709:SER:HB3	2.45	0.51
1:N:708:TRP:CE3	1:N:709:SER:HB3	2.45	0.51
1:J:30:HIS:CE1	1:J:33:PHE:CD1	2.98	0.51
1:N:237:ARG:CG	1:N:237:ARG:HH11	2.23	0.51
1:J:237:ARG:CG	1:J:237:ARG:HH11	2.23	0.51
1:P:30:HIS:CE1	1:P:33:PHE:CD1	2.98	0.51
1:L:237:ARG:HH11	1:L:237:ARG:CG	2.24	0.51
1:P:473:ARG:HD3	1:P:473:ARG:C	2.29	0.51
1:K:835:LEU:O	1:K:836:ILE:HD13	2.09	0.51
1:I:835:LEU:O	1:I:836:ILE:HD13	2.09	0.51
1:K:512:PHE:HE1	1:K:517:LYS:HG3	1.75	0.51
1:N:176:PHE:CD1	1:N:176:PHE:N	2.78	0.51
1:P:870:VAL:HG12	1:P:871:GLU:N	2.25	0.51
1:K:870:VAL:HG12	1:K:871:GLU:N	2.25	0.51
1:K:781:ARG:HH11	1:K:781:ARG:CG	2.19	0.51
1:N:920:LEU:HB3	1:N:921:PRO:CD	2.38	0.51
1:J:634:GLN:HE22	1:J:685:LEU:H	1.57	0.51
1:N:500:CYS:HA	1:N:534:ILE:O	2.11	0.51
1:N:433:LEU:N	1:N:434:PRO:CD	2.73	0.51
1:J:649:ASN:OD1	1:J:703:PRO:HD2	2.09	0.51
1:J:9:VAL:O	1:J:12:GLN:HB3	2.10	0.51
1:N:30:HIS:CE1	1:N:33:PHE:CD1	2.98	0.51
1:O:30:HIS:CE1	1:O:33:PHE:CD1	2.98	0.51
1:O:568:TRP:HE1	1:O:604:ASN:ND2	2.09	0.51
1:K:568:TRP:HE1	1:K:604:ASN:ND2	2.08	0.51
1:I:287:ASP:CG	1:L:425:ARG:HH22	2.13	0.51
1:O:73:TRP:CE2	1:O:122:CYS:HB3	2.44	0.51
1:O:832:ASP:OD1	1:O:832:ASP:N	2.43	0.51
1:M:176:PHE:CD1	1:M:176:PHE:N	2.78	0.51
1:J:867:THR:O	1:J:867:THR:HG22	2.09	0.51
1:M:920:LEU:HB3	1:M:921:PRO:CD	2.38	0.51
1:M:500:CYS:HA	1:M:534:ILE:O	2.10	0.51
1:L:500:CYS:HA	1:L:534:ILE:O	2.10	0.51
1:P:53:SER:O	1:P:54:LEU:HD23	2.10	0.51
1:O:433:LEU:N	1:O:434:PRO:CD	2.73	0.51
1:I:663:LEU:HD23	1:I:663:LEU:N	2.24	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:236:SER:OG	1:K:237:ARG:HD3	2.09	0.51
1:J:597:ASN:HD22	1:J:599:ARG:H	1.57	0.51
1:O:987:ASP:OD2	1:O:990:HIS:HD2	1.93	0.51
1:O:473:ARG:HD3	1:O:473:ARG:C	2.29	0.51
1:M:69:VAL:HG13	1:M:70:PRO:HD2	1.91	0.51
1:O:867:THR:HG22	1:O:867:THR:O	2.09	0.51
1:N:512:PHE:HE1	1:N:517:LYS:HG3	1.75	0.51
1:O:781:ARG:HG3	1:O:781:ARG:NH1	2.17	0.51
1:M:822:LEU:HD11	1:M:824:GLN:O	2.11	0.51
1:J:53:SER:O	1:J:54:LEU:HD23	2.10	0.51
1:O:53:SER:O	1:O:54:LEU:HD23	2.10	0.51
1:P:6:SER:O	1:P:9:VAL:HG12	2.10	0.51
1:O:237:ARG:HH11	1:O:237:ARG:CG	2.23	0.51
1:K:68:ALA:O	1:K:70:PRO:HD3	2.10	0.51
1:J:176:PHE:CD1	1:J:176:PHE:N	2.79	0.51
1:I:832:ASP:N	1:I:832:ASP:OD1	2.43	0.51
1:L:211:ASP:N	1:L:211:ASP:OD1	2.42	0.51
1:I:512:PHE:HE1	1:I:517:LYS:HG3	1.75	0.51
1:L:92:MET:HE3	1:L:362:LEU:O	2.10	0.51
1:I:781:ARG:HH11	1:I:781:ARG:CG	2.19	0.51
1:K:822:LEU:HD11	1:K:824:GLN:O	2.11	0.51
1:O:822:LEU:HD11	1:O:824:GLN:O	2.11	0.51
1:O:653[A]:HIS:HD2	1:O:666:GLY:O	1.93	0.51
1:L:653[A]:HIS:HD2	1:L:666:GLY:O	1.93	0.51
1:I:419:GLY:HA2	1:L:282:ARG:NH1	2.25	0.51
1:O:708:TRP:CE3	1:O:709:SER:HB3	2.45	0.51
1:I:708:TRP:CE3	1:I:709:SER:HB3	2.45	0.51
1:L:568:TRP:HE1	1:L:604:ASN:ND2	2.08	0.51
1:J:987:ASP:OD2	1:J:990:HIS:HD2	1.92	0.51
1:L:867:THR:HG22	1:L:867:THR:O	2.09	0.51
1:L:512:PHE:HE1	1:L:517:LYS:HG3	1.75	0.51
1:J:579:ASP:OD2	1:J:583:ASN:HB2	2.11	0.51
1:N:579:ASP:OD2	1:N:583:ASN:HB2	2.11	0.51
1:L:822:LEU:HD11	1:L:824:GLN:O	2.11	0.51
1:L:634:GLN:HE22	1:L:685:LEU:H	1.57	0.51
1:O:500:CYS:HA	1:O:534:ILE:O	2.10	0.51
1:L:708:TRP:CE3	1:L:709:SER:HB3	2.45	0.51
1:P:597:ASN:HD22	1:P:599:ARG:H	1.57	0.51
1:M:127:PHE:N	1:M:127:PHE:CD2	2.79	0.51
1:J:568:TRP:HE1	1:J:604:ASN:ND2	2.08	0.51
1:P:211:ASP:N	1:P:211:ASP:OD1	2.42	0.51
1:M:211:ASP:N	1:M:211:ASP:OD1	2.42	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:610:ASP:O	1:K:611:ARG:HB2	2.10	0.51
1:O:512:PHE:HE1	1:O:517:LYS:HG3	1.75	0.51
1:J:870:VAL:HG12	1:J:871:GLU:N	2.25	0.51
1:P:433:LEU:N	1:P:434:PRO:CD	2.73	0.51
1:O:434:PRO:HA	1:O:437:SER:OG	2.11	0.51
1:N:663:LEU:HD23	1:N:663:LEU:N	2.24	0.51
1:P:663:LEU:N	1:P:663:LEU:HD23	2.24	0.51
1:M:708:TRP:CE3	1:M:709:SER:HB3	2.45	0.51
1:K:246:MET:HE3	1:K:247:CYS:CA	2.41	0.51
1:J:127:PHE:CD2	1:J:127:PHE:N	2.79	0.51
1:M:568:TRP:HE1	1:M:604:ASN:ND2	2.09	0.51
1:N:68:ALA:O	1:N:70:PRO:HD3	2.10	0.51
1:K:176:PHE:N	1:K:176:PHE:CD1	2.78	0.51
1:I:176:PHE:N	1:I:176:PHE:CD1	2.79	0.51
1:J:610:ASP:O	1:J:611:ARG:HB2	2.10	0.51
1:K:436:MET:HE1	1:K:467:ASN:HD22	1.74	0.51
1:K:53:SER:O	1:K:54:LEU:HD23	2.10	0.51
1:N:282:ARG:HH11	1:O:419:GLY:CA	2.23	0.51
1:K:278:ILE:H	1:K:278:ILE:CD1	2.21	0.51
1:L:579:ASP:OD2	1:L:583:ASN:HB2	2.11	0.51
1:P:246:MET:HE3	1:P:247:CYS:CA	2.41	0.51
1:M:6:SER:O	1:M:9:VAL:HG12	2.10	0.51
1:M:9:VAL:O	1:M:12:GLN:HB3	2.10	0.51
1:M:237:ARG:CG	1:M:237:ARG:HH11	2.23	0.51
1:L:176:PHE:N	1:L:176:PHE:CD1	2.79	0.51
1:N:870:VAL:HG12	1:N:871:GLU:N	2.25	0.51
1:M:512:PHE:HE1	1:M:517:LYS:HG3	1.75	0.51
1:P:436:MET:HE3	1:P:467:ASN:ND2	2.15	0.51
1:P:579:ASP:OD2	1:P:583:ASN:HB2	2.11	0.51
1:M:433:LEU:N	1:M:434:PRO:CD	2.73	0.51
1:I:822:LEU:HD11	1:I:824:GLN:O	2.11	0.51
1:N:434:PRO:HA	1:N:437:SER:OG	2.11	0.51
1:M:30:HIS:CE1	1:M:33:PHE:CD1	2.98	0.51
1:J:708:TRP:CE3	1:J:709:SER:HB3	2.45	0.51
1:O:6:SER:O	1:O:9:VAL:HG12	2.10	0.51
1:L:473:ARG:HD3	1:L:473:ARG:C	2.29	0.51
1:I:833:ALA:HB1	1:I:858:ILE:O	2.11	0.51
1:P:832:ASP:OD1	1:P:832:ASP:N	2.43	0.51
1:O:176:PHE:CD1	1:O:176:PHE:N	2.78	0.51
1:P:961:ARG:NH2	1:P:979:GLU:O	2.37	0.51
1:N:579:ASP:N	1:N:583:ASN:O	2.40	0.51
1:J:822:LEU:HD11	1:J:824:GLN:O	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:822:LEU:HD11	1:P:824:GLN:O	2.11	0.51
1:M:833:ALA:HB1	1:M:858:ILE:O	2.11	0.51
1:L:9:VAL:O	1:L:12:GLN:HB3	2.10	0.51
1:K:178:ARG:HH11	1:K:178:ARG:HB2	1.76	0.51
1:L:581:ASN:OD1	1:L:581:ASN:N	2.44	0.51
1:P:131:GLU:HG3	1:P:132:SER:N	2.26	0.51
1:K:73:TRP:CZ2	1:K:185:ALA:HB1	2.46	0.51
1:I:130:ASP:OD1	1:I:132:SER:N	2.30	0.51
1:L:833:ALA:HB1	1:L:858:ILE:O	2.11	0.51
1:I:595:THR:HG23	1:I:596:PRO:CA	2.37	0.50
1:K:579:ASP:OD2	1:K:583:ASN:HB2	2.11	0.50
1:P:708:TRP:CE3	1:P:709:SER:HB3	2.45	0.50
1:J:246:MET:HE3	1:J:247:CYS:CA	2.40	0.50
1:N:127:PHE:CD2	1:N:127:PHE:N	2.79	0.50
1:M:178:ARG:HB2	1:M:178:ARG:HH11	1.77	0.50
1:J:178:ARG:HB2	1:J:178:ARG:HH11	1.76	0.50
1:J:69:VAL:HG13	1:J:70:PRO:HD2	1.91	0.50
1:N:73:TRP:CZ2	1:N:185:ALA:HB1	2.47	0.50
1:M:436:MET:HE1	1:M:467:ASN:HD22	1.76	0.50
1:I:92:MET:HE3	1:I:362:LEU:O	2.11	0.50
1:L:433:LEU:N	1:L:434:PRO:HD2	2.26	0.50
1:O:49:GLN:HE21	1:O:49:GLN:H	1.59	0.50
1:L:30:HIS:CE1	1:L:33:PHE:CD1	2.98	0.50
1:M:579:ASP:OD2	1:M:583:ASN:HB2	2.11	0.50
1:I:127:PHE:CD2	1:I:127:PHE:N	2.79	0.50
1:O:178:ARG:HB2	1:O:178:ARG:HH11	1.76	0.50
1:I:73:TRP:CZ2	1:I:185:ALA:HB1	2.47	0.50
1:L:73:TRP:CZ2	1:L:185:ALA:HB1	2.47	0.50
1:L:870:VAL:HG12	1:L:871:GLU:N	2.25	0.50
1:P:867:THR:O	1:P:867:THR:HG22	2.09	0.50
1:P:592:PHE:CD1	1:P:592:PHE:N	2.79	0.50
1:N:869:ASP:OD2	1:N:1015:HIS:ND1	2.33	0.50
1:O:610:ASP:O	1:O:611:ARG:HB2	2.10	0.50
1:K:65:ALA:HB1	1:K:66:PRO:CD	2.38	0.50
1:P:433:LEU:N	1:P:434:PRO:HD2	2.26	0.50
1:P:434:PRO:HA	1:P:437:SER:OG	2.11	0.50
1:M:53:SER:O	1:M:54:LEU:HD23	2.10	0.50
1:K:36:TRP:CD2	1:K:42:ALA:HA	2.47	0.50
1:I:433:LEU:N	1:I:434:PRO:HD2	2.26	0.50
1:M:36:TRP:CD2	1:M:42:ALA:HA	2.47	0.50
1:I:660:GLY:O	1:I:662:PRO:HD3	2.12	0.50
1:K:49:GLN:HE21	1:K:49:GLN:H	1.59	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:568:TRP:HE1	1:I:604:ASN:ND2	2.09	0.50
1:J:581:ASN:N	1:J:581:ASN:OD1	2.44	0.50
1:P:570:TRP:CD1	1:P:571:VAL:HG22	2.47	0.50
1:I:579:ASP:OD2	1:I:583:ASN:HB2	2.11	0.50
1:K:433:LEU:N	1:K:434:PRO:HD2	2.26	0.50
1:O:920:LEU:HB3	1:O:921:PRO:CD	2.38	0.50
1:I:920:LEU:HB3	1:I:921:PRO:CD	2.38	0.50
1:N:36:TRP:CD2	1:N:42:ALA:HA	2.47	0.50
1:I:434:PRO:HA	1:I:437:SER:OG	2.11	0.50
1:O:660:GLY:O	1:O:662:PRO:HD3	2.12	0.50
1:N:833:ALA:HB1	1:N:858:ILE:O	2.11	0.50
1:N:246:MET:HE3	1:N:247:CYS:C	2.31	0.50
1:P:237:ARG:CG	1:P:237:ARG:HH11	2.23	0.50
1:K:127:PHE:N	1:K:127:PHE:CD2	2.79	0.50
1:L:131:GLU:HG3	1:L:132:SER:N	2.26	0.50
1:I:403:ASP:OD2	1:I:450:HIS:ND1	2.34	0.50
1:K:131:GLU:HG3	1:K:132:SER:N	2.26	0.50
1:N:131:GLU:HG3	1:N:132:SER:N	2.26	0.50
1:J:73:TRP:CZ2	1:J:185:ALA:HB1	2.46	0.50
1:O:833:ALA:HB1	1:O:858:ILE:O	2.11	0.50
1:K:833:ALA:HB1	1:K:858:ILE:O	2.11	0.50
1:P:869:ASP:OD2	1:P:1015:HIS:ND1	2.33	0.50
1:O:579:ASP:OD2	1:O:583:ASN:HB2	2.11	0.50
1:J:433:LEU:N	1:J:434:PRO:HD2	2.26	0.50
1:M:433:LEU:N	1:M:434:PRO:HD2	2.26	0.50
1:K:500:CYS:HA	1:K:534:ILE:O	2.11	0.50
1:J:36:TRP:CD2	1:J:42:ALA:HA	2.47	0.50
1:L:23:GLN:HB3	1:L:26:ARG:NH2	2.27	0.50
1:L:434:PRO:HA	1:L:437:SER:OG	2.11	0.50
1:O:23:GLN:HB3	1:O:26:ARG:NH2	2.27	0.50
1:K:660:GLY:O	1:K:662:PRO:HD3	2.12	0.50
1:P:660:GLY:O	1:P:662:PRO:HD3	2.12	0.50
1:L:635:THR:HG23	1:L:681:GLU:OE2	2.12	0.50
1:I:635:THR:HG23	1:I:681:GLU:OE2	2.12	0.50
1:P:568:TRP:HE1	1:P:604:ASN:ND2	2.08	0.50
1:M:767:GLN:CG	1:M:768:MET:N	2.75	0.50
1:L:767:GLN:CG	1:L:768:MET:N	2.75	0.50
1:M:570:TRP:CD1	1:M:571:VAL:HG22	2.47	0.50
1:N:570:TRP:CD1	1:N:571:VAL:HG22	2.47	0.50
1:K:592:PHE:CD1	1:K:592:PHE:N	2.79	0.50
1:O:870:VAL:HG12	1:O:871:GLU:N	2.25	0.50
1:J:434:PRO:HA	1:J:437:SER:OG	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:66:PRO:HB3	1:N:187:MET:HE1	1.93	0.50
1:O:36:TRP:CD2	1:O:42:ALA:HA	2.47	0.50
1:M:23:GLN:HB3	1:M:26:ARG:NH2	2.27	0.50
1:N:660:GLY:O	1:N:662:PRO:HD3	2.12	0.50
1:O:635:THR:HG23	1:O:681:GLU:OE2	2.12	0.50
1:L:178:ARG:HH11	1:L:178:ARG:HB2	1.76	0.50
1:N:473:ARG:HD2	1:O:469:ASP:HB3	1.94	0.50
1:M:832:ASP:OD1	1:M:832:ASP:N	2.43	0.50
1:J:833:ALA:HB1	1:J:858:ILE:O	2.11	0.50
1:I:870:VAL:HG12	1:I:871:GLU:N	2.25	0.50
1:P:635:THR:HG23	1:P:681:GLU:OE2	2.12	0.50
1:L:31:PRO:CB	1:L:32:PRO:HD2	2.42	0.50
1:O:246:MET:HE3	1:O:247:CYS:CA	2.42	0.50
1:N:31:PRO:CB	1:N:32:PRO:HD2	2.42	0.50
1:K:237:ARG:CG	1:K:237:ARG:HH11	2.23	0.50
1:K:237:ARG:HB3	1:K:237:ARG:HH11	1.77	0.50
1:I:31:PRO:CB	1:I:32:PRO:HD2	2.42	0.50
1:L:246:MET:HE3	1:L:247:CYS:C	2.31	0.50
1:O:127:PHE:N	1:O:127:PHE:CD2	2.79	0.50
1:O:73:TRP:CZ2	1:O:185:ALA:HB1	2.47	0.50
1:J:832:ASP:N	1:J:832:ASP:OD1	2.43	0.50
1:O:592:PHE:CD1	1:O:592:PHE:N	2.79	0.50
1:P:559:TYR:HB2	1:P:562:LEU:HD12	1.94	0.50
1:M:465:GLY:O	1:M:468:HIS:HB2	2.12	0.50
1:K:434:PRO:HA	1:K:437:SER:OG	2.11	0.50
1:K:66:PRO:HB3	1:K:187:MET:HE1	1.93	0.50
1:O:634:GLN:HE22	1:O:685:LEU:H	1.57	0.50
1:N:822:LEU:HD11	1:N:824:GLN:O	2.11	0.50
1:L:36:TRP:CD2	1:L:42:ALA:HA	2.47	0.50
1:N:23:GLN:HB3	1:N:26:ARG:NH2	2.27	0.50
1:O:433:LEU:N	1:O:434:PRO:HD2	2.26	0.50
1:I:23:GLN:HB3	1:I:26:ARG:NH2	2.27	0.50
1:L:579:ASP:N	1:L:583:ASN:O	2.40	0.50
1:N:237:ARG:HH11	1:N:237:ARG:HB3	1.77	0.50
1:I:237:ARG:CG	1:I:237:ARG:HH11	2.23	0.50
1:P:767:GLN:CG	1:P:768:MET:N	2.75	0.50
1:N:592:PHE:N	1:N:592:PHE:CD1	2.79	0.50
1:K:832:ASP:N	1:K:832:ASP:OD1	2.43	0.50
1:O:420:MET:HA	1:O:420:MET:HE3	1.93	0.50
1:J:559:TYR:HB2	1:J:562:LEU:HD12	1.94	0.50
1:K:465:GLY:O	1:K:468:HIS:HB2	2.12	0.50
1:P:748:CME:SD	1:P:755:ARG:HG2	2.52	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:663:LEU:HD23	1:J:663:LEU:N	2.24	0.50
1:K:579:ASP:N	1:K:583:ASN:O	2.40	0.50
1:P:73:TRP:CZ2	1:P:185:ALA:HB1	2.47	0.50
1:N:465:GLY:O	1:N:468:HIS:HB2	2.12	0.50
1:K:570:TRP:CD1	1:K:571:VAL:HG22	2.47	0.50
1:I:610:ASP:O	1:I:611:ARG:HB2	2.10	0.50
1:O:1020:TRP:CD1	1:O:1021:CME:N	2.80	0.49
1:J:660:GLY:O	1:J:662:PRO:HD3	2.12	0.49
1:P:49:GLN:H	1:P:49:GLN:HE21	1.59	0.49
1:M:597:ASN:HD22	1:M:599:ARG:H	1.57	0.49
1:O:767:GLN:CG	1:O:768:MET:N	2.75	0.49
1:P:420:MET:HA	1:P:420:MET:HE3	1.94	0.49
1:O:961:ARG:NH2	1:O:979:GLU:O	2.37	0.49
1:M:65:ALA:HB1	1:M:66:PRO:CD	2.38	0.49
1:P:23:GLN:HB3	1:P:26:ARG:NH2	2.27	0.49
1:L:660:GLY:O	1:L:662:PRO:HD3	2.12	0.49
1:M:567:VAL:HG12	1:M:568:TRP:N	2.27	0.49
1:M:282:ARG:NH1	1:P:419:GLY:O	2.45	0.49
1:L:570:TRP:CD1	1:L:571:VAL:HG22	2.47	0.49
1:J:635:THR:HG23	1:J:681:GLU:OE2	2.12	0.49
1:M:237:ARG:HH11	1:M:237:ARG:HB3	1.77	0.49
1:N:567:VAL:HG12	1:N:568:TRP:N	2.27	0.49
1:I:567:VAL:HG12	1:I:568:TRP:N	2.27	0.49
1:J:567:VAL:HG12	1:J:568:TRP:N	2.27	0.49
1:N:178:ARG:HH11	1:N:178:ARG:HB2	1.76	0.49
1:N:581:ASN:N	1:N:581:ASN:OD1	2.44	0.49
1:N:767:GLN:CG	1:N:768:MET:N	2.75	0.49
1:P:833:ALA:HB1	1:P:858:ILE:O	2.11	0.49
1:J:740:LEU:CD1	1:J:741:THR:H	2.12	0.49
1:O:65:ALA:HB1	1:O:66:PRO:CD	2.38	0.49
1:I:36:TRP:CD2	1:I:42:ALA:HA	2.47	0.49
1:J:23:GLN:HB3	1:J:26:ARG:NH2	2.27	0.49
1:J:49:GLN:HE21	1:J:49:GLN:H	1.59	0.49
1:P:178:ARG:HB2	1:P:178:ARG:HH11	1.76	0.49
1:M:131:GLU:HG3	1:M:132:SER:N	2.26	0.49
1:I:767:GLN:CG	1:I:768:MET:N	2.75	0.49
1:P:610:ASP:O	1:P:611:ARG:HB2	2.10	0.49
1:M:592:PHE:N	1:M:592:PHE:CD1	2.79	0.49
1:J:592:PHE:CD1	1:J:592:PHE:N	2.79	0.49
1:I:570:TRP:CD1	1:I:571:VAL:HG22	2.47	0.49
1:J:824:GLN:HG3	1:J:825:CYS:N	2.28	0.49
1:M:434:PRO:HA	1:M:437:SER:OG	2.11	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:635:THR:HG23	1:N:681:GLU:OE2	2.12	0.49
1:M:246:MET:HE3	1:M:247:CYS:CA	2.42	0.49
1:P:127:PHE:CD2	1:P:127:PHE:N	2.79	0.49
1:K:581:ASN:OD1	1:K:581:ASN:N	2.44	0.49
1:I:581:ASN:N	1:I:581:ASN:OD1	2.44	0.49
1:O:131:GLU:HG3	1:O:132:SER:N	2.26	0.49
1:O:581:ASN:N	1:O:581:ASN:OD1	2.44	0.49
1:J:767:GLN:CG	1:J:768:MET:N	2.75	0.49
1:N:559:TYR:HB2	1:N:562:LEU:HD12	1.94	0.49
1:J:211:ASP:OD1	1:J:211:ASP:N	2.42	0.49
1:N:961:ARG:NH2	1:N:979:GLU:O	2.38	0.49
1:I:961:ARG:NH2	1:I:979:GLU:O	2.37	0.49
1:O:559:TYR:HB2	1:O:562:LEU:HD12	1.94	0.49
1:M:748:CME:SD	1:M:755:ARG:HG2	2.52	0.49
1:L:317:THR:HG23	1:L:323:ILE:HD11	1.95	0.49
1:J:317:THR:HG23	1:J:323:ILE:HD11	1.95	0.49
1:N:894:ARG:NH1	1:N:920:LEU:HA	2.28	0.49
1:I:894:ARG:NH1	1:I:920:LEU:HA	2.28	0.49
1:I:673:ALA:O	1:I:674:PRO:C	2.51	0.49
1:L:127:PHE:CD2	1:L:127:PHE:N	2.79	0.49
1:K:131:GLU:O	1:K:134:LEU:N	2.46	0.49
1:I:131:GLU:HG3	1:I:132:SER:N	2.26	0.49
1:J:465:GLY:O	1:J:468:HIS:HB2	2.12	0.49
1:P:928:PRO:HB2	1:P:973:ARG:HH11	1.78	0.49
1:L:961:ARG:NH2	1:L:979:GLU:O	2.37	0.49
1:M:317:THR:HG23	1:M:323:ILE:HD11	1.95	0.49
1:L:894:ARG:NH1	1:L:920:LEU:HA	2.28	0.49
1:M:894:ARG:NH1	1:M:920:LEU:HA	2.28	0.49
1:O:894:ARG:NH1	1:O:920:LEU:HA	2.28	0.49
1:P:781:ARG:CG	1:P:781:ARG:HH11	2.19	0.49
1:K:230:ARG:HH11	1:K:230:ARG:CG	2.24	0.49
1:K:23:GLN:HB3	1:K:26:ARG:NH2	2.27	0.49
1:I:856:TYR:HD2	1:I:864:MET:CE	2.25	0.49
1:K:31:PRO:CB	1:K:32:PRO:HD2	2.42	0.49
1:J:131:GLU:O	1:J:134:LEU:N	2.46	0.49
1:P:131:GLU:O	1:P:134:LEU:N	2.46	0.49
1:I:131:GLU:O	1:I:134:LEU:N	2.46	0.49
1:O:211:ASP:OD1	1:O:211:ASP:N	2.42	0.49
1:L:592:PHE:CD1	1:L:592:PHE:N	2.79	0.49
1:P:176:PHE:N	1:P:176:PHE:CD1	2.79	0.49
1:O:570:TRP:CD1	1:O:571:VAL:HG22	2.47	0.49
1:K:559:TYR:HB2	1:K:562:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:748:CME:SD	1:K:755:ARG:HG2	2.52	0.49
1:K:894:ARG:NH1	1:K:920:LEU:HA	2.28	0.49
1:J:230:ARG:CG	1:J:230:ARG:HH11	2.24	0.49
1:P:65:ALA:HB1	1:P:66:PRO:CD	2.39	0.49
1:K:260:LEU:HA	1:K:260:LEU:HD12	1.61	0.49
1:J:315:LEU:O	1:J:322:LEU:HD12	2.13	0.49
1:M:635:THR:HG23	1:M:681:GLU:OE2	2.12	0.49
1:J:673:ALA:O	1:J:674:PRO:C	2.51	0.49
1:M:31:PRO:CB	1:M:32:PRO:HD2	2.42	0.49
1:P:31:PRO:CB	1:P:32:PRO:HD2	2.42	0.49
1:N:568:TRP:HE1	1:N:604:ASN:ND2	2.09	0.49
1:P:581:ASN:OD1	1:P:581:ASN:N	2.44	0.49
1:N:928:PRO:HB2	1:N:973:ARG:HH11	1.78	0.49
1:P:465:GLY:O	1:P:468:HIS:HB2	2.12	0.49
1:J:570:TRP:CD1	1:J:571:VAL:HG22	2.47	0.49
1:N:317:THR:HG23	1:N:323:ILE:HD11	1.95	0.49
1:O:92:MET:HE3	1:O:362:LEU:O	2.13	0.49
1:N:1020:TRP:CD1	1:N:1021:CME:N	2.80	0.49
1:N:824:GLN:HG3	1:N:825:CYS:N	2.28	0.49
1:M:423:MET:HE2	1:P:282:ARG:CG	2.42	0.49
1:J:631:LEU:HD12	1:J:632:SER:H	1.78	0.49
1:O:673:ALA:O	1:O:674:PRO:C	2.51	0.49
1:L:237:ARG:HH11	1:L:237:ARG:HB3	1.77	0.49
1:I:344:LEU:HD23	1:I:344:LEU:C	2.33	0.49
1:M:579:ASP:N	1:M:583:ASN:O	2.40	0.49
1:N:131:GLU:O	1:N:134:LEU:N	2.46	0.49
1:M:73:TRP:CZ2	1:M:185:ALA:HB1	2.47	0.49
1:I:748:CME:SD	1:I:755:ARG:HG2	2.52	0.49
1:K:317:THR:HG23	1:K:323:ILE:HD11	1.95	0.49
1:J:1020:TRP:CD1	1:J:1021:CME:N	2.80	0.49
1:M:660:GLY:O	1:M:662:PRO:HD3	2.12	0.49
1:K:673:ALA:O	1:K:674:PRO:C	2.51	0.49
1:J:31:PRO:CB	1:J:32:PRO:HD2	2.42	0.49
1:L:567:VAL:HG12	1:L:568:TRP:N	2.27	0.49
1:K:567:VAL:HG12	1:K:568:TRP:N	2.27	0.49
1:K:403:ASP:OD2	1:K:450:HIS:ND1	2.34	0.49
1:L:465:GLY:O	1:L:468:HIS:HB2	2.12	0.49
1:J:928:PRO:HB2	1:J:973:ARG:HH11	1.78	0.49
1:L:746:ASP:HA	1:L:760:ARG:CG	2.39	0.48
1:J:748:CME:SD	1:J:755:ARG:HG2	2.52	0.48
1:P:315:LEU:O	1:P:322:LEU:HD12	2.13	0.48
1:N:433:LEU:N	1:N:434:PRO:HD2	2.26	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:631:LEU:HD12	1:P:632:SER:H	1.78	0.48
1:K:631:LEU:HD12	1:K:632:SER:H	1.78	0.48
1:P:237:ARG:HB3	1:P:237:ARG:HH11	1.77	0.48
1:P:567:VAL:HG12	1:P:568:TRP:N	2.27	0.48
1:J:131:GLU:HG3	1:J:132:SER:N	2.26	0.48
1:I:178:ARG:HH11	1:I:178:ARG:HB2	1.76	0.48
1:M:86:VAL:HG13	1:M:87:PRO:HA	1.95	0.48
1:K:767:GLN:CG	1:K:768:MET:N	2.75	0.48
1:N:1018:LEU:HD23	1:N:1018:LEU:HA	1.51	0.48
1:P:167:LEU:HB3	1:P:168:PRO:HD2	1.95	0.48
1:K:772:ASP:OD1	1:K:772:ASP:N	2.30	0.48
1:J:420:MET:HE3	1:J:420:MET:HA	1.95	0.48
1:I:465:GLY:O	1:I:468:HIS:HB2	2.12	0.48
1:L:802:ASP:OD1	1:L:803:PRO:HD2	2.13	0.48
1:L:928:PRO:HB2	1:L:973:ARG:HH11	1.78	0.48
1:J:961:ARG:NH2	1:J:979:GLU:O	2.37	0.48
1:I:167:LEU:HB3	1:I:168:PRO:HD2	1.95	0.48
1:L:748:CME:SD	1:L:755:ARG:HG2	2.52	0.48
1:O:748:CME:SD	1:O:755:ARG:HG2	2.53	0.48
1:P:742:THR:CG2	1:P:743:SER:N	2.76	0.48
1:L:824:GLN:O	1:L:838:THR:HA	2.14	0.48
1:P:824:GLN:HG3	1:P:825:CYS:N	2.28	0.48
1:M:433:LEU:HD12	1:M:433:LEU:O	2.13	0.48
1:P:36:TRP:CD2	1:P:42:ALA:HA	2.46	0.48
1:I:418:HIS:O	1:L:282:ARG:HD3	2.12	0.48
1:K:635:THR:HG23	1:K:681:GLU:OE2	2.12	0.48
1:O:631:LEU:HD12	1:O:632:SER:H	1.78	0.48
1:I:79:PRO:HG2	1:I:80:GLU:OE2	2.13	0.48
1:O:237:ARG:HB3	1:O:237:ARG:HH11	1.77	0.48
1:O:567:VAL:HG12	1:O:568:TRP:N	2.27	0.48
1:L:86:VAL:HG13	1:L:87:PRO:HA	1.96	0.48
1:K:73:TRP:CH2	1:K:185:ALA:HB1	2.49	0.48
1:P:442:ARG:HA	1:P:445:GLN:HG3	1.95	0.48
1:P:344:LEU:C	1:P:344:LEU:HD23	2.34	0.48
1:M:167:LEU:HB3	1:M:168:PRO:HD2	1.95	0.48
1:J:742:THR:CG2	1:J:743:SER:N	2.76	0.48
1:N:748:CME:SD	1:N:755:ARG:HG2	2.52	0.48
1:J:894:ARG:NH1	1:J:920:LEU:HA	2.28	0.48
1:J:189:LEU:N	1:J:189:LEU:CD2	2.75	0.48
1:N:79:PRO:HG2	1:N:80:GLU:OE2	2.13	0.48
1:M:673:ALA:O	1:M:674:PRO:C	2.51	0.48
1:M:131:GLU:O	1:M:134:LEU:N	2.46	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:131:GLU:O	1:L:134:LEU:N	2.46	0.48
1:I:442:ARG:HA	1:I:445:GLN:HG3	1.95	0.48
1:I:757:GLN:HG2	1:I:757:GLN:O	2.12	0.48
1:J:757:GLN:HG2	1:J:757:GLN:O	2.12	0.48
1:K:211:ASP:N	1:K:211:ASP:OD1	2.42	0.48
1:M:928:PRO:HB2	1:M:973:ARG:HH11	1.78	0.48
1:M:802:ASP:OD1	1:M:803:PRO:HD2	2.13	0.48
1:L:559:TYR:HB2	1:L:562:LEU:HD12	1.94	0.48
1:M:559:TYR:HB2	1:M:562:LEU:HD12	1.94	0.48
1:L:742:THR:CG2	1:L:743:SER:N	2.76	0.48
1:O:824:GLN:O	1:O:838:THR:HA	2.14	0.48
1:M:824:GLN:HG3	1:M:825:CYS:N	2.28	0.48
1:O:685:LEU:HA	1:O:686:PRO:HD3	1.70	0.48
1:N:433:LEU:O	1:N:433:LEU:HD12	2.13	0.48
1:O:433:LEU:HD12	1:O:433:LEU:O	2.13	0.48
1:L:663:LEU:HD23	1:L:663:LEU:N	2.24	0.48
1:P:79:PRO:HG2	1:P:80:GLU:OE2	2.13	0.48
1:N:631:LEU:HD12	1:N:632:SER:H	1.79	0.48
1:N:344:LEU:C	1:N:344:LEU:HD23	2.33	0.48
1:P:778:THR:HG22	1:P:887:GLN:H	1.79	0.48
1:M:612:THR:HB	1:M:613:PRO:HD2	1.95	0.48
1:O:612:THR:HB	1:O:613:PRO:HD2	1.96	0.48
1:P:612:THR:HB	1:P:613:PRO:HD2	1.95	0.48
1:O:465:GLY:O	1:O:468:HIS:HB2	2.12	0.48
1:M:344:LEU:C	1:M:344:LEU:HD23	2.34	0.48
1:I:559:TYR:HB2	1:I:562:LEU:HD12	1.94	0.48
1:I:592:PHE:N	1:I:592:PHE:CD1	2.79	0.48
1:N:420:MET:HA	1:N:420:MET:HE3	1.95	0.48
1:K:802:ASP:OD1	1:K:803:PRO:HD2	2.13	0.48
1:N:167:LEU:HB3	1:N:168:PRO:HD2	1.96	0.48
1:N:442:ARG:HA	1:N:445:GLN:HG3	1.96	0.48
1:I:745:MET:HA	1:I:745:MET:CE	2.43	0.48
1:M:742:THR:CG2	1:M:743:SER:H	2.27	0.48
1:M:652:LEU:HB3	1:M:668:VAL:O	2.14	0.48
1:J:433:LEU:O	1:J:433:LEU:HD12	2.13	0.48
1:I:781:ARG:HG3	1:I:781:ARG:NH1	2.17	0.48
1:M:79:PRO:HG2	1:M:80:GLU:OE2	2.13	0.48
1:J:237:ARG:HH11	1:J:237:ARG:HB3	1.77	0.48
1:O:31:PRO:CB	1:O:32:PRO:HD2	2.42	0.48
1:I:425:ARG:HH22	1:L:287:ASP:CG	2.15	0.48
1:N:86:VAL:HG13	1:N:87:PRO:HA	1.95	0.48
1:K:928:PRO:HB2	1:K:973:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:961:ARG:NH2	1:M:979:GLU:O	2.37	0.48
1:L:442:ARG:HA	1:L:445:GLN:HG3	1.95	0.48
1:I:928:PRO:HB2	1:I:973:ARG:HH11	1.78	0.48
1:I:317:THR:HG23	1:I:323:ILE:HD11	1.95	0.48
1:K:652:LEU:HB3	1:K:668:VAL:O	2.14	0.48
1:P:579:ASP:N	1:P:583:ASN:O	2.40	0.48
1:O:652:LEU:HB3	1:O:668:VAL:O	2.14	0.48
1:M:230:ARG:CG	1:M:230:ARG:HH11	2.24	0.48
1:P:63:PHE:CB	1:P:64:PRO:HD2	2.32	0.48
1:K:824:GLN:O	1:K:838:THR:HA	2.13	0.48
1:P:824:GLN:O	1:P:838:THR:HA	2.14	0.48
1:J:65:ALA:HB1	1:J:66:PRO:CD	2.38	0.48
1:J:702:GLN:O	1:J:712:GLY:N	2.45	0.48
1:O:126:THR:HA	1:O:182:ASN:O	2.14	0.48
1:K:856:TYR:HD2	1:K:864:MET:CE	2.25	0.48
1:M:778:THR:HG22	1:M:887:GLN:H	1.79	0.48
1:I:73:TRP:CH2	1:I:185:ALA:HB1	2.49	0.48
1:J:802:ASP:OD1	1:J:803:PRO:HD2	2.13	0.48
1:K:442:ARG:HA	1:K:445:GLN:HG3	1.96	0.48
1:O:802:ASP:OD1	1:O:803:PRO:HD2	2.13	0.48
1:J:745:MET:HA	1:J:745:MET:CE	2.44	0.48
1:O:742:THR:CG2	1:O:743:SER:N	2.76	0.48
1:N:742:THR:CG2	1:N:743:SER:N	2.76	0.48
1:K:1020:TRP:CD1	1:K:1021:CME:N	2.80	0.48
1:J:79:PRO:HG2	1:J:80:GLU:OE2	2.13	0.48
1:P:673:ALA:O	1:P:674:PRO:C	2.51	0.48
1:L:30:HIS:ND1	1:L:33:PHE:CE1	2.82	0.48
1:O:131:GLU:O	1:O:134:LEU:N	2.46	0.48
1:M:73:TRP:CH2	1:M:185:ALA:HB1	2.49	0.48
1:P:73:TRP:CH2	1:P:185:ALA:HB1	2.49	0.48
1:N:612:THR:HB	1:N:613:PRO:HD2	1.95	0.48
1:N:612:THR:HA	1:N:613:PRO:HD3	1.68	0.48
1:I:211:ASP:OD1	1:I:211:ASP:N	2.42	0.48
1:J:344:LEU:C	1:J:344:LEU:HD23	2.34	0.48
1:L:167:LEU:HB3	1:L:168:PRO:HD2	1.96	0.48
1:O:442:ARG:HA	1:O:445:GLN:HG3	1.96	0.48
1:O:742:THR:CG2	1:O:743:SER:H	2.27	0.48
1:L:742:THR:CG2	1:L:743:SER:H	2.27	0.48
1:J:253:TYR:N	1:J:253:TYR:CD2	2.82	0.48
1:P:894:ARG:NH1	1:P:920:LEU:HA	2.28	0.48
1:N:66:PRO:HD2	1:N:67:GLU:OE2	2.14	0.48
1:M:824:GLN:O	1:M:838:THR:HA	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:824:GLN:O	1:N:838:THR:HA	2.14	0.48
1:I:824:GLN:O	1:I:838:THR:HA	2.14	0.48
1:L:315:LEU:O	1:L:322:LEU:HD12	2.13	0.48
1:I:631:LEU:HD12	1:I:632:SER:H	1.78	0.48
1:K:79:PRO:HG2	1:K:80:GLU:OE2	2.13	0.48
1:I:237:ARG:HB3	1:I:237:ARG:HH11	1.77	0.48
1:P:599:ARG:HB2	1:P:600:GLN:H	1.40	0.48
1:L:271:THR:HG22	1:L:272:ALA:N	2.29	0.48
1:J:778:THR:HG22	1:J:887:GLN:H	1.79	0.48
1:O:73:TRP:CH2	1:O:185:ALA:HB1	2.49	0.48
1:N:73:TRP:CH2	1:N:185:ALA:HB1	2.48	0.48
1:L:869:ASP:OD2	1:L:1015:HIS:ND1	2.33	0.48
1:L:772:ASP:OD1	1:L:772:ASP:N	2.30	0.48
1:O:928:PRO:HB2	1:O:973:ARG:HH11	1.78	0.48
1:I:742:THR:CG2	1:I:743:SER:N	2.76	0.48
1:O:436:MET:HE1	1:O:467:ASN:HD22	1.75	0.48
1:O:317:THR:HG23	1:O:323:ILE:HD11	1.95	0.48
1:M:1020:TRP:CD1	1:M:1021:CME:N	2.80	0.48
1:K:66:PRO:HD2	1:K:67:GLU:OE2	2.14	0.48
1:O:824:GLN:HG3	1:O:825:CYS:N	2.28	0.48
1:P:433:LEU:O	1:P:433:LEU:HD12	2.13	0.48
1:O:315:LEU:O	1:O:322:LEU:HD12	2.13	0.48
1:I:315:LEU:O	1:I:322:LEU:HD12	2.13	0.48
1:P:24:LEU:HD12	1:P:24:LEU:HA	1.62	0.48
1:N:315:LEU:O	1:N:322:LEU:HD12	2.13	0.48
1:M:315:LEU:O	1:M:322:LEU:HD12	2.13	0.48
1:M:702:GLN:O	1:M:712:GLY:N	2.45	0.48
1:N:126:THR:HA	1:N:182:ASN:O	2.14	0.48
1:O:344:LEU:C	1:O:344:LEU:HD23	2.34	0.48
1:I:778:THR:HG22	1:I:887:GLN:H	1.79	0.48
1:P:86:VAL:HG13	1:P:87:PRO:HA	1.96	0.48
1:J:73:TRP:CH2	1:J:185:ALA:HB1	2.49	0.48
1:J:167:LEU:HB3	1:J:168:PRO:HD2	1.95	0.48
1:J:118:ASN:HA	1:J:119:PRO:HD2	1.60	0.48
1:N:802:ASP:OD1	1:N:803:PRO:HD2	2.13	0.48
1:K:742:THR:CG2	1:K:743:SER:H	2.27	0.48
1:P:317:THR:HG23	1:P:323:ILE:HD11	1.95	0.48
1:L:781:ARG:NH1	1:L:781:ARG:HG3	2.17	0.48
1:P:253:TYR:CD2	1:P:253:TYR:N	2.82	0.48
1:L:66:PRO:HD2	1:L:67:GLU:OE2	2.14	0.48
1:J:631:LEU:HD12	1:J:635:THR:O	2.14	0.48
1:L:79:PRO:HG2	1:L:80:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:129:VAL:CG2	1:M:182:ASN:ND2	2.77	0.48
1:L:673:ALA:O	1:L:674:PRO:C	2.51	0.48
1:I:126:THR:HA	1:I:182:ASN:O	2.14	0.48
1:K:30:HIS:ND1	1:K:33:PHE:CE1	2.82	0.48
1:K:344:LEU:HD23	1:K:344:LEU:C	2.34	0.48
1:L:73:TRP:CH2	1:L:185:ALA:HB1	2.49	0.48
1:J:612:THR:HB	1:J:613:PRO:HD2	1.96	0.48
1:K:409:VAL:HG12	1:K:410:VAL:N	2.29	0.48
1:K:742:THR:CG2	1:K:743:SER:N	2.76	0.47
1:M:742:THR:CG2	1:M:743:SER:N	2.76	0.47
1:L:652:LEU:HB3	1:L:668:VAL:O	2.14	0.47
1:P:652:LEU:HB3	1:P:668:VAL:O	2.14	0.47
1:N:948:PRO:O	1:N:1022:GLN:HA	2.14	0.47
1:I:253:TYR:CD2	1:I:253:TYR:N	2.82	0.47
1:I:948:PRO:O	1:I:1022:GLN:HA	2.14	0.47
1:O:66:PRO:HB3	1:O:187:MET:HE1	1.96	0.47
1:O:856:TYR:CD2	1:O:864:MET:CE	2.97	0.47
1:L:126:THR:HA	1:L:182:ASN:O	2.14	0.47
1:I:84:VAL:CG1	1:I:85:VAL:N	2.77	0.47
1:M:878:HIS:HA	1:M:879:PRO:HD3	1.66	0.47
1:J:409:VAL:HG12	1:J:410:VAL:N	2.29	0.47
1:I:802:ASP:OD1	1:I:803:PRO:HD2	2.13	0.47
1:N:742:THR:CG2	1:N:743:SER:H	2.27	0.47
1:N:745:MET:CE	1:N:745:MET:HA	2.44	0.47
1:J:652:LEU:HB3	1:J:668:VAL:O	2.14	0.47
1:I:652:LEU:HB3	1:I:668:VAL:O	2.14	0.47
1:O:948:PRO:O	1:O:1022:GLN:HA	2.14	0.47
1:K:433:LEU:HD12	1:K:433:LEU:O	2.13	0.47
1:N:253:TYR:CD2	1:N:253:TYR:N	2.82	0.47
1:K:824:GLN:HG3	1:K:825:CYS:N	2.28	0.47
1:L:824:GLN:HG3	1:L:825:CYS:N	2.28	0.47
1:J:824:GLN:O	1:J:838:THR:HA	2.14	0.47
1:O:395:HIS:HA	1:O:396:PRO:HD3	1.48	0.47
1:K:315:LEU:O	1:K:322:LEU:HD12	2.13	0.47
1:L:24:LEU:HD12	1:L:24:LEU:HA	1.62	0.47
1:O:11:LEU:N	1:O:11:LEU:CD2	2.76	0.47
1:N:30:HIS:ND1	1:N:33:PHE:CE1	2.82	0.47
1:O:30:HIS:ND1	1:O:33:PHE:CE1	2.82	0.47
1:N:84:VAL:CG1	1:N:85:VAL:N	2.78	0.47
1:L:420:MET:HE3	1:L:420:MET:HA	1.96	0.47
1:K:253:TYR:N	1:K:253:TYR:CD2	2.82	0.47
1:P:66:PRO:HD2	1:P:67:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:730:LEU:HA	1:M:731:PRO:HD3	1.74	0.47
1:I:824:GLN:HG3	1:I:825:CYS:N	2.28	0.47
1:M:856:TYR:CD2	1:M:864:MET:CE	2.97	0.47
1:L:702:GLN:O	1:L:712:GLY:N	2.45	0.47
1:N:856:TYR:CD2	1:N:864:MET:CE	2.97	0.47
1:K:631:LEU:HD12	1:K:635:THR:O	2.14	0.47
1:M:126:THR:HA	1:M:182:ASN:O	2.14	0.47
1:M:30:HIS:ND1	1:M:33:PHE:CE1	2.82	0.47
1:L:344:LEU:C	1:L:344:LEU:HD23	2.34	0.47
1:N:778:THR:HG22	1:N:887:GLN:H	1.79	0.47
1:J:142:ILE:HG12	1:J:170:GLU:HG2	1.97	0.47
1:J:610:ASP:OD2	1:J:612:THR:HG23	2.15	0.47
1:O:610:ASP:OD2	1:O:612:THR:HG23	2.15	0.47
1:L:875:ASP:N	1:L:875:ASP:OD2	2.47	0.47
1:N:93:HIS:HB3	1:N:95:TYR:CE1	2.50	0.47
1:L:57:GLU:HG2	1:L:83:THR:HG21	1.93	0.47
1:L:253:TYR:N	1:L:253:TYR:CD2	2.82	0.47
1:K:66:PRO:CB	1:K:187:MET:HE1	2.45	0.47
1:M:66:PRO:CB	1:M:187:MET:HE1	2.45	0.47
1:J:66:PRO:CB	1:J:187:MET:HE1	2.44	0.47
1:O:663:LEU:N	1:O:663:LEU:HD23	2.24	0.47
1:K:661:LYS:HA	1:K:662:PRO:HD3	1.63	0.47
1:O:631:LEU:HD12	1:O:635:THR:O	2.14	0.47
1:I:30:HIS:ND1	1:I:33:PHE:CE1	2.82	0.47
1:L:347:LYS:CB	1:L:348:PRO:HD2	2.43	0.47
1:K:86:VAL:HG13	1:K:87:PRO:HA	1.95	0.47
1:L:612:THR:HB	1:L:613:PRO:HD2	1.96	0.47
1:J:88:SER:HA	1:J:366:VAL:HG21	1.97	0.47
1:J:442:ARG:HA	1:J:445:GLN:HG3	1.96	0.47
1:P:409:VAL:HG12	1:P:410:VAL:N	2.29	0.47
1:K:167:LEU:HB3	1:K:168:PRO:HD2	1.95	0.47
1:L:745:MET:HA	1:L:745:MET:CE	2.44	0.47
1:J:579:ASP:OD1	1:J:583:ASN:N	2.43	0.47
1:O:781:ARG:HH11	1:O:781:ARG:CG	2.19	0.47
1:J:948:PRO:O	1:J:1022:GLN:HA	2.14	0.47
1:I:856:TYR:CD2	1:I:864:MET:CE	2.97	0.47
1:I:631:LEU:HD12	1:I:635:THR:O	2.14	0.47
1:K:129:VAL:CG2	1:K:182:ASN:ND2	2.77	0.47
1:K:856:TYR:CD2	1:K:864:MET:CE	2.97	0.47
1:M:274:PHE:HB3	1:M:286:ALA:O	2.15	0.47
1:M:73:TRP:CZ2	1:M:122:CYS:HB3	2.50	0.47
1:I:142:ILE:HG12	1:I:170:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:142:ILE:HG12	1:M:170:GLU:HG2	1.97	0.47
1:L:610:ASP:OD2	1:L:612:THR:HG23	2.15	0.47
1:N:142:ILE:HG12	1:N:170:GLU:HG2	1.97	0.47
1:L:757:GLN:O	1:L:757:GLN:HG2	2.12	0.47
1:M:88:SER:HA	1:M:366:VAL:HG21	1.97	0.47
1:J:93:HIS:HB3	1:J:95:TYR:CE1	2.50	0.47
1:J:742:THR:CG2	1:J:743:SER:H	2.27	0.47
1:O:745:MET:CE	1:O:745:MET:HA	2.44	0.47
1:I:436:MET:HE1	1:I:467:ASN:HD22	1.77	0.47
1:L:1020:TRP:CD1	1:L:1021:CME:N	2.80	0.47
1:M:948:PRO:O	1:M:1022:GLN:HA	2.14	0.47
1:O:253:TYR:CD2	1:O:253:TYR:N	2.82	0.47
1:I:433:LEU:O	1:I:433:LEU:HD12	2.13	0.47
1:P:856:TYR:CD2	1:P:864:MET:CE	2.97	0.47
1:J:30:HIS:ND1	1:J:33:PHE:CE1	2.82	0.47
1:I:377:LEU:HD22	1:I:708:TRP:CA	2.44	0.47
1:I:274:PHE:HB3	1:I:286:ALA:O	2.15	0.47
1:J:469:ASP:HB3	1:K:473:ARG:HD2	1.95	0.47
1:P:142:ILE:HG12	1:P:170:GLU:HG2	1.97	0.47
1:P:802:ASP:OD1	1:P:803:PRO:HD2	2.14	0.47
1:P:531:ARG:O	1:P:561:ARG:NH1	2.46	0.47
1:I:694:LEU:HA	1:I:694:LEU:HD12	1.69	0.47
1:O:88:SER:HA	1:O:366:VAL:HG21	1.96	0.47
1:I:93:HIS:HB3	1:I:95:TYR:CE1	2.49	0.47
1:O:167:LEU:HB3	1:O:168:PRO:HD2	1.95	0.47
1:L:740:LEU:HD13	1:L:749:ILE:CD1	2.45	0.47
1:P:740:LEU:HD13	1:P:749:ILE:CD1	2.45	0.47
1:P:745:MET:HA	1:P:745:MET:CE	2.44	0.47
1:P:746:ASP:HA	1:P:760:ARG:CG	2.39	0.47
1:P:92:MET:HE3	1:P:362:LEU:O	2.15	0.47
1:N:579:ASP:OD1	1:N:583:ASN:N	2.43	0.47
1:O:1021:CME:HE2	1:O:1021:CME:HB3	1.41	0.47
1:P:230:ARG:HH11	1:P:230:ARG:CG	2.24	0.47
1:O:66:PRO:HD2	1:O:67:GLU:OE2	2.14	0.47
1:P:66:PRO:CB	1:P:187:MET:HE1	2.45	0.47
1:N:395:HIS:HA	1:N:396:PRO:HD3	1.48	0.47
1:O:260:LEU:HA	1:O:260:LEU:HD12	1.61	0.47
1:M:663:LEU:N	1:M:663:LEU:HD23	2.24	0.47
1:L:631:LEU:HD12	1:L:632:SER:H	1.78	0.47
1:M:77:ASP:O	1:M:78:LEU:HD23	2.15	0.47
1:N:673:ALA:O	1:N:674:PRO:C	2.51	0.47
1:O:377:LEU:HD22	1:O:708:TRP:CA	2.44	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:377:LEU:HD22	1:J:708:TRP:CA	2.44	0.47
1:N:274:PHE:HB3	1:N:286:ALA:O	2.15	0.47
1:P:30:HIS:ND1	1:P:33:PHE:CE1	2.82	0.47
1:I:473:ARG:HD2	1:L:469:ASP:HB3	1.96	0.47
1:K:778:THR:HG22	1:K:887:GLN:H	1.79	0.47
1:L:778:THR:HG22	1:L:887:GLN:H	1.79	0.47
1:I:271:THR:HG22	1:I:272:ALA:N	2.29	0.47
1:O:778:THR:HG22	1:O:887:GLN:H	1.79	0.47
1:M:84:VAL:CG1	1:M:85:VAL:N	2.78	0.47
1:J:86:VAL:HG13	1:J:87:PRO:HA	1.96	0.47
1:L:84:VAL:CG1	1:L:85:VAL:N	2.77	0.47
1:O:86:VAL:HG13	1:O:87:PRO:HA	1.96	0.47
1:P:84:VAL:CG1	1:P:85:VAL:N	2.78	0.47
1:P:73:TRP:CZ2	1:P:122:CYS:HB3	2.50	0.47
1:O:73:TRP:CZ2	1:O:122:CYS:HB3	2.50	0.47
1:K:608:PHE:O	1:K:611:ARG:N	2.41	0.47
1:M:420:MET:HE3	1:M:420:MET:HA	1.96	0.47
1:O:875:ASP:N	1:O:875:ASP:OD2	2.47	0.47
1:K:420:MET:HE3	1:K:420:MET:HA	1.97	0.47
1:M:409:VAL:HG12	1:M:410:VAL:N	2.29	0.47
1:N:409:VAL:HG12	1:N:410:VAL:N	2.29	0.47
1:M:646:HIS:O	1:M:648:ASP:N	2.47	0.47
1:P:93:HIS:HB3	1:P:95:TYR:CE1	2.50	0.47
1:P:147:ASN:HA	1:P:148:SER:HA	1.54	0.47
1:K:88:SER:HA	1:K:366:VAL:HG21	1.97	0.47
1:N:740:LEU:HD13	1:N:749:ILE:CD1	2.45	0.47
1:J:740:LEU:HD13	1:J:749:ILE:CD1	2.45	0.47
1:M:253:TYR:CD2	1:M:253:TYR:N	2.82	0.47
1:K:948:PRO:O	1:K:1022:GLN:HA	2.14	0.47
1:I:66:PRO:CB	1:I:187:MET:HE1	2.45	0.47
1:N:66:PRO:CB	1:N:187:MET:HE1	2.45	0.47
1:J:66:PRO:HD2	1:J:67:GLU:OE2	2.14	0.47
1:P:278:ILE:CD1	1:P:278:ILE:N	2.78	0.47
1:M:631:LEU:HD12	1:M:635:THR:O	2.14	0.47
1:K:77:ASP:O	1:K:78:LEU:HD23	2.15	0.47
1:O:79:PRO:HG2	1:O:80:GLU:OE2	2.13	0.47
1:N:129:VAL:CG2	1:N:182:ASN:ND2	2.77	0.47
1:P:274:PHE:HB3	1:P:286:ALA:O	2.15	0.47
1:O:274:PHE:HB3	1:O:286:ALA:O	2.15	0.47
1:I:347:LYS:CB	1:I:348:PRO:HD2	2.43	0.47
1:O:271:THR:HG22	1:O:272:ALA:N	2.29	0.47
1:M:271:THR:HG22	1:M:272:ALA:N	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:271:THR:HG22	1:K:272:ALA:N	2.29	0.47
1:L:142:ILE:HG12	1:L:170:GLU:HG2	1.97	0.47
1:N:73:TRP:CZ2	1:N:122:CYS:HB3	2.50	0.47
1:K:142:ILE:HG12	1:K:170:GLU:HG2	1.97	0.47
1:K:612:THR:HB	1:K:613:PRO:HD2	1.95	0.47
1:I:612:THR:HB	1:I:613:PRO:HD2	1.96	0.47
1:L:93:HIS:HB3	1:L:95:TYR:CE1	2.49	0.47
1:J:875:ASP:OD2	1:J:875:ASP:N	2.47	0.47
1:J:942:ARG:HA	1:J:953:GLY:O	2.15	0.47
1:L:749:ILE:N	1:L:749:ILE:CD1	2.78	0.47
1:O:740:LEU:HD13	1:O:749:ILE:CD1	2.45	0.47
1:I:740:LEU:HD13	1:I:749:ILE:CD1	2.45	0.47
1:M:740:LEU:HD13	1:M:749:ILE:CD1	2.45	0.47
1:O:579:ASP:N	1:O:583:ASN:O	2.40	0.47
1:L:948:PRO:O	1:L:1022:GLN:HA	2.14	0.47
1:I:66:PRO:HD2	1:I:67:GLU:OE2	2.14	0.47
1:L:66:PRO:CB	1:L:187:MET:HE1	2.45	0.47
1:O:654:TRP:O	1:O:655:MET:HB3	2.15	0.47
1:L:210:ARG:NH1	1:L:395:HIS:CA	2.78	0.47
1:M:210:ARG:NH1	1:M:395:HIS:CA	2.78	0.47
1:K:210:ARG:NH1	1:K:395:HIS:CA	2.78	0.47
1:L:433:LEU:HD12	1:L:433:LEU:O	2.13	0.47
1:P:631:LEU:HD12	1:P:635:THR:O	2.14	0.47
1:I:78:LEU:CB	1:I:79:PRO:HD2	2.44	0.47
1:O:77:ASP:O	1:O:78:LEU:HD23	2.15	0.47
1:J:126:THR:HA	1:J:182:ASN:O	2.14	0.47
1:J:73:TRP:CZ2	1:J:122:CYS:HB3	2.50	0.47
1:L:73:TRP:CZ2	1:L:122:CYS:HB3	2.50	0.47
1:I:610:ASP:OD2	1:I:612:THR:HG23	2.15	0.47
1:K:930:VAL:HA	1:K:973:ARG:HD3	1.97	0.47
1:M:942:ARG:HA	1:M:953:GLY:O	2.15	0.47
1:J:531:ARG:O	1:J:561:ARG:NH1	2.46	0.47
1:N:942:ARG:HA	1:N:953:GLY:O	2.15	0.47
1:K:679:LEU:HA	1:K:679:LEU:HD23	1.26	0.47
1:O:942:ARG:HA	1:O:953:GLY:O	2.15	0.47
1:K:646:HIS:O	1:K:648:ASP:N	2.47	0.47
1:I:742:THR:CG2	1:I:743:SER:H	2.27	0.47
1:K:745:MET:HA	1:K:745:MET:CE	2.44	0.47
1:J:57:GLU:HG2	1:J:83:THR:HG21	1.93	0.47
1:L:65:ALA:HB1	1:L:66:PRO:CD	2.39	0.47
1:O:66:PRO:CB	1:O:187:MET:HE1	2.45	0.47
1:O:210:ARG:NH1	1:O:395:HIS:CA	2.78	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:395:HIS:HA	1:L:396:PRO:HD3	1.48	0.47
1:M:581:ASN:N	1:M:581:ASN:OD1	2.44	0.47
1:I:86:VAL:HG13	1:I:87:PRO:HA	1.95	0.47
1:N:610:ASP:OD2	1:N:612:THR:HG23	2.15	0.47
1:N:930:VAL:HA	1:N:973:ARG:HD3	1.97	0.47
1:L:930:VAL:HA	1:L:973:ARG:HD3	1.97	0.47
1:K:875:ASP:OD2	1:K:875:ASP:N	2.47	0.47
1:I:118:ASN:HA	1:I:119:PRO:HD2	1.60	0.47
1:L:88:SER:HA	1:L:366:VAL:HG21	1.97	0.47
1:O:93:HIS:HB3	1:O:95:TYR:CE1	2.50	0.47
1:L:942:ARG:HA	1:L:953:GLY:O	2.15	0.47
1:K:740:LEU:HD13	1:K:749:ILE:CD1	2.45	0.46
1:L:740:LEU:HD13	1:L:749:ILE:HD12	1.97	0.46
1:M:745:MET:CE	1:M:745:MET:HA	2.43	0.46
1:M:749:ILE:N	1:M:749:ILE:CD1	2.78	0.46
1:P:744:GLU:C	1:P:745:MET:HE3	2.35	0.46
1:N:652:LEU:HB3	1:N:668:VAL:O	2.14	0.46
1:I:316:HIS:HB2	1:I:321:THR:O	2.15	0.46
1:P:316:HIS:HB2	1:P:321:THR:O	2.15	0.46
1:M:576:ILE:CG2	1:M:577:LYS:N	2.78	0.46
1:L:682:LEU:HD23	1:L:682:LEU:HA	1.67	0.46
1:K:654:TRP:O	1:K:655:MET:HB3	2.15	0.46
1:M:654:TRP:O	1:M:655:MET:HB3	2.15	0.46
1:J:210:ARG:NH1	1:J:395:HIS:CA	2.78	0.46
1:L:654:TRP:O	1:L:655:MET:HB3	2.15	0.46
1:I:702:GLN:O	1:I:712:GLY:N	2.45	0.46
1:K:126:THR:HA	1:K:182:ASN:O	2.14	0.46
1:I:129:VAL:CG2	1:I:182:ASN:ND2	2.77	0.46
1:J:274:PHE:HB3	1:J:286:ALA:O	2.15	0.46
1:K:569:ASP:O	1:K:605:GLY:HA2	2.15	0.46
1:M:569:ASP:O	1:M:605:GLY:HA2	2.16	0.46
1:J:84:VAL:CG1	1:J:85:VAL:N	2.77	0.46
1:M:610:ASP:OD2	1:M:612:THR:HG23	2.15	0.46
1:P:610:ASP:OD2	1:P:612:THR:HG23	2.15	0.46
1:K:93:HIS:HB3	1:K:95:TYR:CE1	2.50	0.46
1:P:942:ARG:HA	1:P:953:GLY:O	2.15	0.46
1:I:409:VAL:HG12	1:I:410:VAL:N	2.29	0.46
1:M:442:ARG:HA	1:M:445:GLN:HG3	1.96	0.46
1:L:646:HIS:O	1:L:648:ASP:N	2.47	0.46
1:J:740:LEU:HD13	1:J:749:ILE:HD12	1.97	0.46
1:O:316:HIS:HB2	1:O:321:THR:O	2.16	0.46
1:M:316:HIS:HB2	1:M:321:THR:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:579:ASP:OD1	1:I:583:ASN:N	2.43	0.46
1:O:63:PHE:CB	1:O:64:PRO:HD2	2.32	0.46
1:K:702:GLN:O	1:K:712:GLY:N	2.45	0.46
1:L:631:LEU:HD12	1:L:635:THR:O	2.14	0.46
1:P:126:THR:HA	1:P:182:ASN:O	2.14	0.46
1:L:569:ASP:O	1:L:605:GLY:HA2	2.15	0.46
1:J:569:ASP:O	1:J:605:GLY:HA2	2.15	0.46
1:N:271:THR:HG22	1:N:272:ALA:N	2.29	0.46
1:O:84:VAL:CG1	1:O:85:VAL:N	2.77	0.46
1:K:73:TRP:CZ2	1:K:122:CYS:HB3	2.50	0.46
1:I:608:PHE:O	1:I:611:ARG:N	2.41	0.46
1:O:445:GLN:HE21	1:O:445:GLN:HB3	1.54	0.46
1:N:830:LEU:CD1	1:N:830:LEU:N	2.78	0.46
1:I:875:ASP:N	1:I:875:ASP:OD2	2.47	0.46
1:L:378:LEU:HA	1:L:378:LEU:HD23	1.53	0.46
1:J:830:LEU:CD1	1:J:830:LEU:N	2.78	0.46
1:M:93:HIS:HB3	1:M:95:TYR:CE1	2.50	0.46
1:O:100:TYR:HB2	1:O:203:TRP:CE3	2.51	0.46
1:O:830:LEU:CD1	1:O:830:LEU:N	2.78	0.46
1:K:147:ASN:HA	1:K:148:SER:HA	1.55	0.46
1:L:486:TYR:CZ	1:L:488:GLY:HA3	2.51	0.46
1:J:147:ASN:HA	1:J:148:SER:HA	1.54	0.46
1:N:88:SER:HA	1:N:366:VAL:HG21	1.97	0.46
1:K:878:HIS:HA	1:K:879:PRO:HD3	1.66	0.46
1:I:746:ASP:HA	1:I:760:ARG:CG	2.39	0.46
1:K:740:LEU:HD13	1:K:749:ILE:HD12	1.97	0.46
1:I:230:ARG:CG	1:I:230:ARG:HH11	2.24	0.46
1:N:210:ARG:NH1	1:N:395:HIS:CA	2.78	0.46
1:K:278:ILE:N	1:K:278:ILE:CD1	2.78	0.46
1:N:631:LEU:HD12	1:N:635:THR:O	2.14	0.46
1:J:129:VAL:CG2	1:J:182:ASN:ND2	2.77	0.46
1:L:274:PHE:HB3	1:L:286:ALA:O	2.15	0.46
1:P:13:ARG:O	1:P:14:ARG:HB2	2.16	0.46
1:K:84:VAL:CG1	1:K:85:VAL:N	2.78	0.46
1:I:930:VAL:HA	1:I:973:ARG:HD3	1.97	0.46
1:O:930:VAL:HA	1:O:973:ARG:HD3	1.97	0.46
1:M:100:TYR:HB2	1:M:203:TRP:CE3	2.51	0.46
1:K:743:SER:O	1:K:760:ARG:NH1	2.49	0.46
1:P:740:LEU:HD13	1:P:749:ILE:HD12	1.97	0.46
1:K:316:HIS:HB2	1:K:321:THR:O	2.16	0.46
1:N:781:ARG:O	1:N:884:LEU:HA	2.16	0.46
1:O:37:ARG:NH1	1:O:37:ARG:CG	2.79	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:856:TYR:HD2	1:L:864:MET:CE	2.25	0.46
1:M:631:LEU:HD12	1:M:632:SER:H	1.78	0.46
1:P:129:VAL:CG2	1:P:182:ASN:ND2	2.77	0.46
1:P:377:LEU:HD22	1:P:708:TRP:CA	2.44	0.46
1:O:429:ASP:HA	1:O:430:PRO:HD3	1.51	0.46
1:O:142:ILE:HG12	1:O:170:GLU:HG2	1.97	0.46
1:N:608:PHE:O	1:N:611:ARG:N	2.41	0.46
1:J:930:VAL:HA	1:J:973:ARG:HD3	1.97	0.46
1:I:100:TYR:HB2	1:I:203:TRP:CE3	2.51	0.46
1:J:100:TYR:HB2	1:J:203:TRP:CE3	2.51	0.46
1:O:409:VAL:HG12	1:O:410:VAL:N	2.29	0.46
1:O:147:ASN:HA	1:O:148:SER:HA	1.54	0.46
1:P:88:SER:HA	1:P:366:VAL:HG21	1.97	0.46
1:O:339:ASN:O	1:P:527:PRO:HB3	2.15	0.46
1:P:391:HIS:ND1	1:P:412:GLU:OE1	2.44	0.46
1:L:743:SER:O	1:L:760:ARG:NH1	2.49	0.46
1:N:316:HIS:HB2	1:N:321:THR:O	2.16	0.46
1:O:576:ILE:CG2	1:O:577:LYS:N	2.78	0.46
1:P:781:ARG:O	1:P:884:LEU:HA	2.16	0.46
1:P:37:ARG:CG	1:P:37:ARG:NH1	2.79	0.46
1:K:395:HIS:HA	1:K:396:PRO:HD3	1.48	0.46
1:J:260:LEU:HD12	1:J:260:LEU:HA	1.61	0.46
1:P:702:GLN:O	1:P:712:GLY:N	2.45	0.46
1:N:856:TYR:HD2	1:N:864:MET:CE	2.25	0.46
1:I:77:ASP:O	1:I:78:LEU:HD23	2.15	0.46
1:N:78:LEU:CB	1:N:79:PRO:HD2	2.44	0.46
1:M:900:LEU:HA	1:M:900:LEU:HD23	1.75	0.46
1:K:377:LEU:HD22	1:K:708:TRP:CA	2.44	0.46
1:N:569:ASP:O	1:N:605:GLY:HA2	2.15	0.46
1:I:569:ASP:O	1:I:605:GLY:HA2	2.15	0.46
1:N:599:ARG:HB2	1:N:600:GLN:H	1.41	0.46
1:O:13:ARG:O	1:O:14:ARG:HB2	2.15	0.46
1:J:512:PHE:CE1	1:J:517:LYS:HG3	2.51	0.46
1:P:930:VAL:HA	1:P:973:ARG:HD3	1.97	0.46
1:M:930:VAL:HA	1:M:973:ARG:HD3	1.97	0.46
1:L:400:THR:O	1:L:404:ARG:HD2	2.16	0.46
1:J:670:LEU:HD23	1:J:670:LEU:HA	1.67	0.46
1:K:486:TYR:CZ	1:K:488:GLY:HA3	2.51	0.46
1:K:99:ILE:HG23	1:K:594:ASP:HB2	1.98	0.46
1:K:400:THR:O	1:K:404:ARG:HD2	2.16	0.46
1:P:743:SER:O	1:P:760:ARG:NH1	2.49	0.46
1:J:316:HIS:HB2	1:J:321:THR:O	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:781:ARG:O	1:K:884:LEU:HA	2.16	0.46
1:P:948:PRO:O	1:P:1022:GLN:HA	2.14	0.46
1:L:37:ARG:NH1	1:L:37:ARG:CG	2.79	0.46
1:L:856:TYR:CD2	1:L:864:MET:CE	2.97	0.46
1:K:274:PHE:HB3	1:K:286:ALA:O	2.15	0.46
1:O:569:ASP:O	1:O:605:GLY:HA2	2.15	0.46
1:O:974:HIS:C	1:O:975:LEU:HD23	2.36	0.46
1:K:610:ASP:OD2	1:K:612:THR:HG23	2.15	0.46
1:I:612:THR:HA	1:I:613:PRO:HD3	1.68	0.46
1:L:409:VAL:HG12	1:L:410:VAL:N	2.29	0.46
1:I:646:HIS:O	1:I:648:ASP:N	2.47	0.46
1:J:772:ASP:OD1	1:J:772:ASP:N	2.30	0.46
1:I:420:MET:HE3	1:I:420:MET:HA	1.97	0.46
1:N:486:TYR:CZ	1:N:488:GLY:HA3	2.51	0.46
1:J:486:TYR:CZ	1:J:488:GLY:HA3	2.51	0.46
1:J:99:ILE:HG23	1:J:594:ASP:HB2	1.98	0.46
1:I:147:ASN:HA	1:I:148:SER:HA	1.55	0.46
1:J:400:THR:O	1:J:404:ARG:HD2	2.16	0.46
1:L:118:ASN:HA	1:L:119:PRO:HD2	1.60	0.46
1:L:744:GLU:C	1:L:745:MET:HE3	2.36	0.46
1:P:742:THR:CG2	1:P:743:SER:H	2.27	0.46
1:J:576:ILE:CG2	1:J:577:LYS:N	2.78	0.46
1:I:1020:TRP:CD1	1:I:1021:CME:N	2.80	0.46
1:M:781:ARG:O	1:M:884:LEU:HA	2.16	0.46
1:N:230:ARG:CG	1:N:230:ARG:HH11	2.24	0.46
1:M:260:LEU:HA	1:M:260:LEU:HD12	1.61	0.46
1:L:49:GLN:H	1:L:49:GLN:HE21	1.59	0.46
1:N:77:ASP:O	1:N:78:LEU:HD23	2.15	0.46
1:I:13:ARG:O	1:I:14:ARG:HB2	2.16	0.46
1:P:271:THR:HG22	1:P:272:ALA:N	2.29	0.46
1:P:512:PHE:CE1	1:P:517:LYS:HG3	2.51	0.46
1:I:88:SER:HA	1:I:366:VAL:HG21	1.97	0.46
1:N:211:ASP:N	1:N:211:ASP:OD1	2.42	0.46
1:J:646:HIS:O	1:J:648:ASP:N	2.47	0.46
1:O:99:ILE:HG23	1:O:594:ASP:HB2	1.98	0.46
1:K:830:LEU:N	1:K:830:LEU:CD1	2.78	0.46
1:L:830:LEU:CD1	1:L:830:LEU:N	2.78	0.46
1:P:99:ILE:HG23	1:P:594:ASP:HB2	1.98	0.46
1:O:743:SER:O	1:O:760:ARG:NH1	2.49	0.46
1:N:749:ILE:N	1:N:749:ILE:CD1	2.78	0.46
1:I:749:ILE:N	1:I:749:ILE:CD1	2.78	0.46
1:I:576:ILE:CG2	1:I:577:LYS:N	2.78	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:251:ARG:CB	1:L:253:TYR:CE2	2.98	0.46
1:N:894:ARG:HH12	1:N:920:LEU:HA	1.81	0.46
1:M:66:PRO:HD2	1:M:67:GLU:OE2	2.14	0.46
1:J:655:MET:HE3	1:J:655:MET:HB2	1.92	0.46
1:N:49:GLN:H	1:N:49:GLN:HE21	1.59	0.46
1:L:78:LEU:HB3	1:L:79:PRO:CD	2.45	0.46
1:L:583:ASN:HA	1:L:584:PRO:HD3	1.80	0.46
1:P:708:TRP:N	1:P:708:TRP:CD1	2.84	0.46
1:O:272:ALA:HA	1:O:273:PRO:HD3	1.76	0.46
1:M:403:ASP:OD2	1:M:450:HIS:ND1	2.34	0.46
1:K:974:HIS:C	1:K:975:LEU:HD23	2.36	0.46
1:L:70:PRO:O	1:L:73:TRP:N	2.45	0.46
1:L:486:TYR:CE2	1:L:488:GLY:HA3	2.51	0.46
1:L:409:VAL:CG1	1:L:410:VAL:N	2.79	0.46
1:N:486:TYR:CE2	1:N:488:GLY:HA3	2.51	0.46
1:J:486:TYR:CE2	1:J:488:GLY:HA3	2.51	0.46
1:M:486:TYR:CZ	1:M:488:GLY:HA3	2.51	0.46
1:P:830:LEU:CD1	1:P:830:LEU:N	2.78	0.46
1:O:486:TYR:CZ	1:O:488:GLY:HA3	2.51	0.46
1:N:400:THR:O	1:N:404:ARG:HD2	2.16	0.46
1:P:486:TYR:CZ	1:P:488:GLY:HA3	2.51	0.46
1:L:99:ILE:HG23	1:L:594:ASP:HB2	1.98	0.46
1:N:100:TYR:HB2	1:N:203:TRP:CE3	2.51	0.46
1:J:743:SER:OG	1:J:744:GLU:N	2.49	0.46
1:K:743:SER:OG	1:K:744:GLU:N	2.49	0.46
1:K:57:GLU:HG2	1:K:83:THR:HG21	1.93	0.46
1:K:67:GLU:HG2	1:K:67:GLU:H	1.30	0.46
1:K:254:LEU:HD23	1:K:254:LEU:HA	1.62	0.46
1:I:210:ARG:HH11	1:I:395:HIS:HB2	1.81	0.46
1:N:11:LEU:N	1:N:11:LEU:CD2	2.76	0.46
1:O:278:ILE:N	1:O:278:ILE:CD1	2.78	0.46
1:P:78:LEU:CB	1:P:79:PRO:HD2	2.44	0.46
1:L:576:ILE:CG2	1:L:577:LYS:N	2.78	0.46
1:M:708:TRP:CD1	1:M:708:TRP:N	2.84	0.46
1:N:512:PHE:CE1	1:N:517:LYS:HG3	2.51	0.46
1:O:512:PHE:CE1	1:O:517:LYS:HG3	2.51	0.46
1:M:486:TYR:CE2	1:M:488:GLY:HA3	2.51	0.46
1:P:646:HIS:O	1:P:648:ASP:N	2.47	0.46
1:M:830:LEU:N	1:M:830:LEU:CD1	2.78	0.46
1:J:743:SER:O	1:J:760:ARG:NH1	2.49	0.46
1:N:740:LEU:HD13	1:N:749:ILE:HD12	1.97	0.46
1:N:743:SER:O	1:N:760:ARG:NH1	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:740:LEU:HD13	1:O:749:ILE:HD12	1.97	0.46
1:I:740:LEU:HD13	1:I:749:ILE:HD12	1.97	0.46
1:L:436:MET:HE3	1:L:467:ASN:ND2	2.21	0.46
1:L:781:ARG:O	1:L:884:LEU:HA	2.16	0.46
1:P:1020:TRP:CD1	1:P:1021:CME:N	2.80	0.46
1:I:781:ARG:O	1:I:884:LEU:HA	2.16	0.46
1:O:894:ARG:HH12	1:O:920:LEU:HA	1.81	0.46
1:N:255:ARG:NH1	1:N:255:ARG:CG	2.79	0.46
1:J:254:LEU:HA	1:J:254:LEU:HD23	1.62	0.46
1:I:654:TRP:O	1:I:655:MET:HB3	2.15	0.46
1:N:210:ARG:HH12	1:N:394:ASN:C	2.20	0.46
1:L:655:MET:HB2	1:L:655:MET:HE3	1.92	0.46
1:O:78:LEU:HB3	1:O:79:PRO:CD	2.45	0.46
1:K:708:TRP:N	1:K:708:TRP:CD1	2.84	0.46
1:J:900:LEU:HD23	1:J:900:LEU:HA	1.75	0.46
1:M:473:ARG:HD2	1:P:469:ASP:HB3	1.96	0.46
1:M:111:PRO:HA	1:M:112:PRO:HA	1.57	0.46
1:N:726:LEU:HA	1:N:726:LEU:HD23	1.65	0.46
1:N:391:HIS:ND1	1:N:412:GLU:OE1	2.44	0.46
1:N:99:ILE:HG23	1:N:594:ASP:HB2	1.98	0.46
1:K:942:ARG:HA	1:K:953:GLY:O	2.15	0.46
1:K:746:ASP:HA	1:K:760:ARG:CG	2.39	0.45
1:M:743:SER:OG	1:M:744:GLU:N	2.49	0.45
1:M:740:LEU:HD13	1:M:749:ILE:HD12	1.97	0.45
1:J:822:LEU:C	1:J:822:LEU:HD12	2.37	0.45
1:O:822:LEU:HD12	1:O:822:LEU:C	2.36	0.45
1:N:654:TRP:O	1:N:655:MET:HB3	2.15	0.45
1:I:37:ARG:CG	1:I:37:ARG:NH1	2.79	0.45
1:P:77:ASP:O	1:P:78:LEU:HD23	2.15	0.45
1:I:974:HIS:C	1:I:975:LEU:HD23	2.36	0.45
1:M:974:HIS:C	1:M:975:LEU:HD23	2.36	0.45
1:N:807:VAL:CG1	1:N:808:GLU:N	2.80	0.45
1:K:70:PRO:O	1:K:73:TRP:N	2.45	0.45
1:I:73:TRP:CZ2	1:I:122:CYS:HB3	2.50	0.45
1:M:445:GLN:HB3	1:M:445:GLN:HE21	1.54	0.45
1:O:726:LEU:HD23	1:O:726:LEU:HA	1.65	0.45
1:I:479:ASP:HA	1:I:480:PRO:HD2	1.61	0.45
1:I:486:TYR:CZ	1:I:488:GLY:HA3	2.51	0.45
1:I:942:ARG:HA	1:I:953:GLY:O	2.15	0.45
1:P:100:TYR:HB2	1:P:203:TRP:CE3	2.51	0.45
1:P:400:THR:O	1:P:404:ARG:HD2	2.16	0.45
1:J:749:ILE:CD1	1:J:749:ILE:N	2.78	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:856:TYR:CD2	1:J:864:MET:CE	2.97	0.45
1:J:781:ARG:O	1:J:884:LEU:HA	2.16	0.45
1:P:894:ARG:HH12	1:P:920:LEU:HA	1.81	0.45
1:L:894:ARG:HH12	1:L:920:LEU:HA	1.81	0.45
1:P:685:LEU:HA	1:P:686:PRO:HD3	1.70	0.45
1:I:210:ARG:NH1	1:I:395:HIS:CA	2.78	0.45
1:P:210:ARG:NH1	1:P:395:HIS:CA	2.78	0.45
1:J:682:LEU:HD23	1:J:682:LEU:HA	1.67	0.45
1:I:79:PRO:HD2	1:I:80:GLU:OE2	2.17	0.45
1:N:78:LEU:HB3	1:N:79:PRO:CD	2.45	0.45
1:J:271:THR:HG22	1:J:272:ALA:N	2.29	0.45
1:K:409:VAL:CG1	1:K:410:VAL:N	2.79	0.45
1:P:409:VAL:CG1	1:P:410:VAL:N	2.79	0.45
1:O:486:TYR:CE2	1:O:488:GLY:HA3	2.51	0.45
1:L:670:LEU:HA	1:L:670:LEU:HD23	1.67	0.45
1:J:173:LEU:HA	1:J:173:LEU:HD23	1.69	0.45
1:O:391:HIS:ND1	1:O:412:GLU:OE1	2.44	0.45
1:N:875:ASP:OD2	1:N:875:ASP:N	2.47	0.45
1:M:746:ASP:HA	1:M:760:ARG:CG	2.39	0.45
1:L:316:HIS:HB2	1:L:321:THR:O	2.16	0.45
1:P:46:ARG:CG	1:P:46:ARG:NH1	2.78	0.45
1:J:579:ASP:N	1:J:583:ASN:O	2.40	0.45
1:O:781:ARG:O	1:O:884:LEU:HA	2.16	0.45
1:K:894:ARG:HH12	1:K:920:LEU:HA	1.81	0.45
1:I:63:PHE:CB	1:I:64:PRO:HD2	2.32	0.45
1:P:825:CYS:HA	1:P:837:THR:O	2.17	0.45
1:M:825:CYS:HA	1:M:837:THR:O	2.17	0.45
1:N:210:ARG:HH11	1:N:395:HIS:HB2	1.82	0.45
1:I:210:ARG:HH12	1:I:394:ASN:C	2.19	0.45
1:J:37:ARG:NH1	1:J:37:ARG:CG	2.79	0.45
1:L:77:ASP:O	1:L:78:LEU:HD23	2.15	0.45
1:L:129:VAL:CG2	1:L:182:ASN:ND2	2.77	0.45
1:I:4:THR:CA	1:I:9:VAL:HG11	2.47	0.45
1:N:347:LYS:HA	1:N:348:PRO:HD3	1.77	0.45
1:J:599:ARG:HB2	1:J:600:GLN:H	1.41	0.45
1:L:13:ARG:O	1:L:14:ARG:HB2	2.15	0.45
1:N:974:HIS:C	1:N:975:LEU:HD23	2.36	0.45
1:K:807:VAL:CG1	1:K:808:GLU:N	2.80	0.45
1:K:512:PHE:CE1	1:K:517:LYS:HG3	2.51	0.45
1:P:608:PHE:O	1:P:611:ARG:N	2.41	0.45
1:L:363:HIS:CD2	1:L:363:HIS:N	2.81	0.45
1:O:400:THR:O	1:O:404:ARG:HD2	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:830:LEU:N	1:I:830:LEU:CD1	2.78	0.45
1:I:46:ARG:CG	1:I:46:ARG:NH1	2.78	0.45
1:L:230:ARG:HH11	1:L:230:ARG:CG	2.24	0.45
1:M:822:LEU:C	1:M:822:LEU:HD12	2.37	0.45
1:J:654:TRP:O	1:J:655:MET:HB3	2.15	0.45
1:M:210:ARG:HH11	1:M:395:HIS:HB2	1.81	0.45
1:I:260:LEU:HA	1:I:260:LEU:HD12	1.61	0.45
1:K:210:ARG:HH11	1:K:395:HIS:HB2	1.81	0.45
1:O:702:GLN:HA	1:O:703:PRO:HD2	1.84	0.45
1:M:49:GLN:H	1:M:49:GLN:HE21	1.59	0.45
1:O:79:PRO:HD2	1:O:80:GLU:OE2	2.17	0.45
1:O:343:LEU:HD23	1:O:348:PRO:HA	1.99	0.45
1:P:569:ASP:O	1:P:605:GLY:HA2	2.15	0.45
1:M:13:ARG:O	1:M:14:ARG:HB2	2.16	0.45
1:L:387:VAL:CG2	1:L:388:ARG:N	2.80	0.45
1:J:409:VAL:CG1	1:J:410:VAL:N	2.79	0.45
1:I:486:TYR:CE2	1:I:488:GLY:HA3	2.51	0.45
1:M:875:ASP:OD2	1:M:875:ASP:N	2.47	0.45
1:P:875:ASP:OD2	1:P:875:ASP:N	2.47	0.45
1:K:100:TYR:HB2	1:K:203:TRP:CE3	2.51	0.45
1:M:743:SER:O	1:M:760:ARG:NH1	2.49	0.45
1:N:436:MET:HE1	1:N:467:ASN:HB2	1.97	0.45
1:K:46:ARG:NH1	1:K:46:ARG:CG	2.78	0.45
1:J:651:LEU:HD13	1:J:651:LEU:HA	1.51	0.45
1:N:576:ILE:CG2	1:N:577:LYS:N	2.78	0.45
1:O:255:ARG:CG	1:O:255:ARG:NH1	2.79	0.45
1:O:210:ARG:HH11	1:O:395:HIS:HB2	1.82	0.45
1:M:79:PRO:HD2	1:M:80:GLU:OE2	2.16	0.45
1:L:377:LEU:HD22	1:L:708:TRP:CA	2.44	0.45
1:J:347:LYS:CB	1:J:348:PRO:HD2	2.43	0.45
1:K:13:ARG:O	1:K:14:ARG:HB2	2.16	0.45
1:P:807:VAL:CG1	1:P:808:GLU:N	2.80	0.45
1:J:807:VAL:CG1	1:J:808:GLU:N	2.79	0.45
1:I:807:VAL:CG1	1:I:808:GLU:N	2.80	0.45
1:M:512:PHE:CE1	1:M:517:LYS:HG3	2.51	0.45
1:M:723:ALA:HB1	1:N:875:ASP:OD1	2.16	0.45
1:I:391:HIS:ND1	1:I:412:GLU:OE1	2.44	0.45
1:I:400:THR:O	1:I:404:ARG:HD2	2.16	0.45
1:I:743:SER:O	1:I:760:ARG:NH1	2.49	0.45
1:L:668:VAL:HG13	1:L:669:PRO:CD	2.38	0.45
1:N:57:GLU:HG2	1:N:83:THR:HG21	1.93	0.45
1:N:7:LEU:O	1:N:8:ALA:C	2.55	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:825:CYS:HA	1:K:837:THR:O	2.17	0.45
1:L:210:ARG:HH11	1:L:395:HIS:HB2	1.81	0.45
1:M:210:ARG:HH12	1:M:394:ASN:C	2.19	0.45
1:I:12:GLN:HA	1:I:12:GLN:OE1	2.17	0.45
1:J:708:TRP:CD1	1:J:708:TRP:N	2.84	0.45
1:J:343:LEU:HD23	1:J:348:PRO:HA	1.99	0.45
1:L:343:LEU:HD23	1:L:348:PRO:HA	1.99	0.45
1:L:974:HIS:C	1:L:975:LEU:HD23	2.36	0.45
1:I:409:VAL:CG1	1:I:410:VAL:N	2.79	0.45
1:M:400:THR:O	1:M:404:ARG:HD2	2.16	0.45
1:M:118:ASN:HA	1:M:119:PRO:HD2	1.60	0.45
1:P:363:HIS:CD2	1:P:363:HIS:N	2.81	0.45
1:K:757:GLN:O	1:K:757:GLN:HG2	2.12	0.45
1:M:99:ILE:HG23	1:M:594:ASP:HB2	1.98	0.45
1:N:531:ARG:O	1:N:561:ARG:NH1	2.46	0.45
1:L:637:GLU:HA	1:L:679:LEU:CD2	2.47	0.45
1:P:743:SER:OG	1:P:744:GLU:N	2.49	0.45
1:P:254:LEU:HD23	1:P:254:LEU:HA	1.62	0.45
1:N:377:LEU:HD22	1:N:708:TRP:CA	2.44	0.45
1:M:377:LEU:HD22	1:M:708:TRP:CA	2.44	0.45
1:L:12:GLN:HA	1:L:12:GLN:OE1	2.17	0.45
1:M:12:GLN:OE1	1:M:12:GLN:HA	2.17	0.45
1:N:13:ARG:O	1:N:14:ARG:HB2	2.16	0.45
1:J:974:HIS:C	1:J:975:LEU:HD23	2.36	0.45
1:I:512:PHE:CE1	1:I:517:LYS:HG3	2.51	0.45
1:N:409:VAL:CG1	1:N:410:VAL:N	2.79	0.45
1:O:637:GLU:HA	1:O:679:LEU:CD2	2.47	0.45
1:N:147:ASN:HA	1:N:148:SER:HA	1.55	0.45
1:N:479:ASP:HA	1:N:480:PRO:HD2	1.61	0.45
1:J:637:GLU:HA	1:J:679:LEU:CD2	2.47	0.45
1:L:67:GLU:H	1:L:67:GLU:HG2	1.31	0.45
1:J:210:ARG:HH11	1:J:395:HIS:HB2	1.81	0.45
1:P:210:ARG:HH12	1:P:394:ASN:C	2.20	0.45
1:I:24:LEU:HA	1:I:24:LEU:HD12	1.62	0.45
1:P:702:GLN:HA	1:P:703:PRO:HD2	1.84	0.45
1:O:702:GLN:O	1:O:712:GLY:N	2.45	0.45
1:P:79:PRO:HD2	1:P:80:GLU:OE2	2.17	0.45
1:O:129:VAL:CG2	1:O:182:ASN:ND2	2.77	0.45
1:O:708:TRP:CD1	1:O:708:TRP:N	2.84	0.45
1:O:4:THR:CA	1:O:9:VAL:HG11	2.47	0.45
1:M:343:LEU:HD23	1:M:348:PRO:HA	1.99	0.45
1:L:272:ALA:HB1	1:L:273:PRO:CD	2.47	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:429:ASP:HA	1:P:430:PRO:HD3	1.51	0.45
1:M:637:GLU:HA	1:M:679:LEU:CD2	2.47	0.45
1:M:173:LEU:HD23	1:M:173:LEU:HA	1.69	0.45
1:J:92:MET:HE3	1:J:362:LEU:O	2.16	0.45
1:M:251:ARG:CB	1:M:253:TYR:CE2	2.98	0.45
1:J:894:ARG:HH12	1:J:920:LEU:HA	1.81	0.45
1:L:825:CYS:HA	1:L:837:THR:O	2.17	0.45
1:J:210:ARG:HH12	1:J:394:ASN:C	2.20	0.45
1:I:395:HIS:HA	1:I:396:PRO:HD3	1.48	0.45
1:O:210:ARG:HH12	1:O:394:ASN:C	2.19	0.45
1:I:49:GLN:H	1:I:49:GLN:HE21	1.59	0.45
1:J:77:ASP:O	1:J:78:LEU:HD23	2.15	0.45
1:J:79:PRO:HD2	1:J:80:GLU:OE2	2.17	0.45
1:L:79:PRO:HD2	1:L:80:GLU:OE2	2.17	0.45
1:K:576:ILE:CG2	1:K:577:LYS:N	2.78	0.45
1:K:12:GLN:HA	1:K:12:GLN:OE1	2.17	0.45
1:N:79:PRO:HD2	1:N:80:GLU:OE2	2.17	0.45
1:P:12:GLN:HA	1:P:12:GLN:OE1	2.17	0.45
1:L:347:LYS:HA	1:L:348:PRO:HD3	1.77	0.45
1:M:599:ARG:HB2	1:M:600:GLN:H	1.41	0.45
1:O:272:ALA:HB1	1:O:273:PRO:CD	2.47	0.45
1:J:387:VAL:CG2	1:J:388:ARG:N	2.80	0.45
1:K:272:ALA:HA	1:K:273:PRO:HD3	1.76	0.45
1:P:974:HIS:C	1:P:975:LEU:HD23	2.36	0.45
1:M:807:VAL:CG1	1:M:808:GLU:N	2.80	0.45
1:I:131:GLU:HA	1:I:134:LEU:HB2	1.99	0.45
1:O:409:VAL:CG1	1:O:410:VAL:N	2.79	0.45
1:N:646:HIS:O	1:N:648:ASP:N	2.47	0.45
1:L:878:HIS:HA	1:L:879:PRO:HD3	1.66	0.45
1:O:363:HIS:N	1:O:363:HIS:CD2	2.81	0.45
1:I:740:LEU:CD1	1:I:741:THR:H	2.12	0.45
1:J:583:ASN:HA	1:J:584:PRO:HD3	1.79	0.45
1:P:227:VAL:CG1	1:P:240:LEU:HD11	2.42	0.45
1:P:822:LEU:HD12	1:P:823:LEU:H	1.81	0.45
1:P:654:TRP:O	1:P:655:MET:HB3	2.15	0.45
1:N:682:LEU:HA	1:N:682:LEU:HD23	1.67	0.45
1:K:37:ARG:CG	1:K:37:ARG:NH1	2.79	0.45
1:N:702:GLN:O	1:N:712:GLY:N	2.45	0.45
1:N:234:ASP:O	1:N:235:PHE:HB2	2.17	0.45
1:P:234:ASP:O	1:P:235:PHE:HB2	2.17	0.45
1:P:900:LEU:HA	1:P:900:LEU:HD23	1.75	0.45
1:L:272:ALA:HA	1:L:273:PRO:HD3	1.77	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:272:ALA:HB1	1:N:273:PRO:CD	2.47	0.45
1:M:409:VAL:CG1	1:M:410:VAL:N	2.79	0.45
1:I:531:ARG:O	1:I:561:ARG:NH1	2.46	0.45
1:I:637:GLU:HA	1:I:679:LEU:CD2	2.47	0.45
1:I:878:HIS:HA	1:I:879:PRO:HD3	1.66	0.45
1:P:722:LEU:HA	1:P:722:LEU:HD23	1.75	0.45
1:I:1021:CME:HB3	1:I:1021:CME:HE2	1.41	0.44
1:J:395:HIS:HA	1:J:396:PRO:HD3	1.48	0.44
1:L:210:ARG:HH12	1:L:394:ASN:C	2.20	0.44
1:O:49:GLN:CD	1:O:49:GLN:H	2.20	0.44
1:M:78:LEU:HB3	1:M:79:PRO:CD	2.45	0.44
1:J:12:GLN:HA	1:J:12:GLN:OE1	2.17	0.44
1:J:4:THR:CA	1:J:9:VAL:HG11	2.47	0.44
1:K:343:LEU:HD23	1:K:348:PRO:HA	1.99	0.44
1:L:708:TRP:CD1	1:L:708:TRP:N	2.84	0.44
1:M:234:ASP:O	1:M:235:PHE:HB2	2.17	0.44
1:O:645:ARG:NH2	1:O:650:GLU:OE2	2.48	0.44
1:O:387:VAL:CG2	1:O:388:ARG:N	2.80	0.44
1:I:1018:LEU:HD23	1:I:1018:LEU:HA	1.51	0.44
1:P:571:VAL:HG13	1:P:607:VAL:HG23	1.99	0.44
1:O:202:MET:HE3	1:O:202:MET:HB3	1.86	0.44
1:L:173:LEU:HA	1:L:173:LEU:HD23	1.69	0.44
1:L:202:MET:HB3	1:L:202:MET:HE3	1.84	0.44
1:P:264:GLU:OE2	1:P:264:GLU:HA	2.17	0.44
1:I:743:SER:OG	1:I:744:GLU:N	2.49	0.44
1:N:746:ASP:HA	1:N:760:ARG:CG	2.39	0.44
1:M:894:ARG:HH12	1:M:920:LEU:HA	1.81	0.44
1:N:230:ARG:NH2	1:N:241:GLU:OE2	2.51	0.44
1:M:254:LEU:HD23	1:M:254:LEU:HA	1.62	0.44
1:J:685:LEU:HA	1:J:686:PRO:HD3	1.70	0.44
1:N:260:LEU:HD12	1:N:260:LEU:HA	1.61	0.44
1:M:34:ALA:HB3	1:M:36:TRP:CZ3	2.53	0.44
1:J:701:VAL:CG1	1:J:702:GLN:N	2.81	0.44
1:K:701:VAL:HG12	1:K:702:GLN:H	1.83	0.44
1:K:79:PRO:HD2	1:K:80:GLU:OE2	2.17	0.44
1:L:4:THR:CA	1:L:9:VAL:HG11	2.47	0.44
1:N:343:LEU:HD23	1:N:348:PRO:HA	1.99	0.44
1:N:4:THR:CA	1:N:9:VAL:HG11	2.47	0.44
1:J:13:ARG:O	1:J:14:ARG:HB2	2.16	0.44
1:I:287:ASP:N	1:I:287:ASP:OD1	2.29	0.44
1:M:131:GLU:HA	1:M:134:LEU:HB2	2.00	0.44
1:K:387:VAL:CG2	1:K:388:ARG:N	2.80	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:272:ALA:HB1	1:K:273:PRO:CD	2.47	0.44
1:P:387:VAL:CG2	1:P:388:ARG:N	2.80	0.44
1:L:1018:LEU:HA	1:L:1018:LEU:HD23	1.51	0.44
1:O:807:VAL:CG1	1:O:808:GLU:N	2.79	0.44
1:L:807:VAL:CG1	1:L:808:GLU:N	2.79	0.44
1:K:571:VAL:HG13	1:K:607:VAL:HG23	1.99	0.44
1:N:118:ASN:HA	1:N:119:PRO:HD2	1.60	0.44
1:N:757:GLN:HG2	1:N:757:GLN:O	2.12	0.44
1:I:99:ILE:HG23	1:I:594:ASP:HB2	1.98	0.44
1:L:100:TYR:HB2	1:L:203:TRP:CE3	2.51	0.44
1:M:479:ASP:HA	1:M:480:PRO:HD2	1.61	0.44
1:L:743:SER:OG	1:L:744:GLU:N	2.49	0.44
1:I:781:ARG:CG	1:I:781:ARG:NH1	2.79	0.44
1:J:230:ARG:NH2	1:J:241:GLU:OE2	2.51	0.44
1:O:825:CYS:HA	1:O:837:THR:O	2.17	0.44
1:L:685:LEU:HB3	1:L:686:PRO:HD2	1.99	0.44
1:K:682:LEU:HD23	1:K:682:LEU:HA	1.67	0.44
1:K:685:LEU:HB3	1:K:686:PRO:HD2	1.99	0.44
1:K:210:ARG:HH12	1:K:394:ASN:C	2.19	0.44
1:O:3:ILE:O	1:O:6:SER:HB3	2.18	0.44
1:O:347:LYS:CB	1:O:348:PRO:HD2	2.43	0.44
1:N:287:ASP:CG	1:O:425:ARG:NH2	2.71	0.44
1:N:12:GLN:HA	1:N:12:GLN:OE1	2.17	0.44
1:P:730:LEU:HA	1:P:731:PRO:HD3	1.74	0.44
1:P:645:ARG:NH2	1:P:650:GLU:OE2	2.48	0.44
1:K:637:GLU:HA	1:K:679:LEU:CD2	2.47	0.44
1:P:486:TYR:CE2	1:P:488:GLY:HA3	2.51	0.44
1:N:670:LEU:HD23	1:N:670:LEU:HA	1.67	0.44
1:K:378:LEU:HA	1:K:378:LEU:HD23	1.53	0.44
1:I:772:ASP:OD1	1:I:772:ASP:N	2.30	0.44
1:K:749:ILE:N	1:K:749:ILE:CD1	2.78	0.44
1:N:743:SER:OG	1:N:744:GLU:N	2.49	0.44
1:L:230:ARG:NH2	1:L:241:GLU:OE2	2.51	0.44
1:N:825:CYS:HA	1:N:837:THR:O	2.17	0.44
1:I:701:VAL:HG12	1:I:702:GLN:H	1.83	0.44
1:I:658:LEU:HD12	1:I:693:GLN:O	2.18	0.44
1:I:78:LEU:HB3	1:I:79:PRO:CD	2.45	0.44
1:J:3:ILE:O	1:J:6:SER:HB3	2.18	0.44
1:P:343:LEU:HD23	1:P:348:PRO:HA	1.99	0.44
1:O:12:GLN:OE1	1:O:12:GLN:HA	2.17	0.44
1:K:131:GLU:HA	1:K:134:LEU:HB2	1.99	0.44
1:I:571:VAL:HG13	1:I:607:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:378:LEU:HD23	1:P:378:LEU:HA	1.53	0.44
1:N:637:GLU:HA	1:N:679:LEU:CD2	2.47	0.44
1:O:788:PRO:O	1:O:933:SER:HB2	2.18	0.44
1:N:878:HIS:HA	1:N:879:PRO:HD3	1.66	0.44
1:O:743:SER:OG	1:O:744:GLU:N	2.49	0.44
1:I:7:LEU:O	1:I:8:ALA:C	2.55	0.44
1:M:7:LEU:O	1:M:8:ALA:C	2.55	0.44
1:K:230:ARG:NH2	1:K:241:GLU:OE2	2.51	0.44
1:L:34:ALA:HB3	1:L:36:TRP:CZ3	2.53	0.44
1:L:658:LEU:HD12	1:L:693:GLN:O	2.18	0.44
1:M:701:VAL:CG1	1:M:702:GLN:N	2.81	0.44
1:I:49:GLN:CD	1:I:49:GLN:H	2.20	0.44
1:J:419:GLY:HA2	1:K:282:ARG:NH1	2.33	0.44
1:L:3:ILE:O	1:L:6:SER:HB3	2.18	0.44
1:M:3:ILE:O	1:M:6:SER:HB3	2.18	0.44
1:I:343:LEU:HD23	1:I:348:PRO:HA	1.99	0.44
1:L:344:LEU:N	1:L:347:LYS:O	2.36	0.44
1:N:344:LEU:N	1:N:347:LYS:O	2.36	0.44
1:N:387:VAL:CG2	1:N:388:ARG:N	2.80	0.44
1:O:50:GLN:HB3	1:O:216:HIS:HB3	2.00	0.44
1:K:486:TYR:CE2	1:K:488:GLY:HA3	2.51	0.44
1:J:264:GLU:HA	1:J:264:GLU:OE2	2.17	0.44
1:L:43:ARG:NH1	1:L:44:THR:CG2	2.81	0.44
1:L:781:ARG:CG	1:L:781:ARG:NH1	2.79	0.44
1:O:251:ARG:CB	1:O:253:TYR:CE2	2.98	0.44
1:J:894:ARG:NH1	1:J:920:LEU:CA	2.81	0.44
1:L:894:ARG:NH1	1:L:920:LEU:CA	2.81	0.44
1:J:825:CYS:HA	1:J:837:THR:O	2.17	0.44
1:N:685:LEU:HA	1:N:686:PRO:HD3	1.70	0.44
1:O:34:ALA:HB3	1:O:36:TRP:CZ3	2.53	0.44
1:O:856:TYR:HD2	1:O:864:MET:CE	2.25	0.44
1:M:658:LEU:HD12	1:M:693:GLN:O	2.18	0.44
1:J:234:ASP:O	1:J:235:PHE:HB2	2.17	0.44
1:M:4:THR:CA	1:M:9:VAL:HG11	2.47	0.44
1:I:234:ASP:O	1:I:235:PHE:HB2	2.17	0.44
1:M:429:ASP:HA	1:M:430:PRO:HD3	1.51	0.44
1:P:272:ALA:HB1	1:P:273:PRO:CD	2.47	0.44
1:I:730:LEU:HA	1:I:731:PRO:HD3	1.74	0.44
1:P:164:ASP:OD2	1:P:167:LEU:HD12	2.18	0.44
1:N:164:ASP:OD2	1:N:167:LEU:HD12	2.18	0.44
1:N:264:GLU:HA	1:N:264:GLU:OE2	2.17	0.44
1:K:788:PRO:O	1:K:933:SER:HB2	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:43:ARG:NH1	1:M:44:THR:CG2	2.81	0.44
1:P:7:LEU:O	1:P:8:ALA:C	2.55	0.44
1:L:7:LEU:O	1:L:8:ALA:C	2.55	0.44
1:O:254:LEU:HA	1:O:254:LEU:HD23	1.62	0.44
1:I:825:CYS:HA	1:I:837:THR:O	2.17	0.44
1:M:419:GLY:CA	1:P:282:ARG:HH11	2.30	0.44
1:O:234:ASP:O	1:O:235:PHE:HB2	2.17	0.44
1:O:730:LEU:HA	1:O:731:PRO:HD3	1.74	0.44
1:N:50:GLN:HB3	1:N:216:HIS:HB3	2.00	0.44
1:M:73:TRP:O	1:M:183:ARG:NH1	2.48	0.44
1:M:378:LEU:HA	1:M:378:LEU:HD23	1.53	0.44
1:N:788:PRO:O	1:N:933:SER:HB2	2.18	0.44
1:P:637:GLU:HA	1:P:679:LEU:CD2	2.47	0.44
1:O:43:ARG:NH1	1:O:44:THR:CG2	2.81	0.44
1:P:287:ASP:OD1	1:P:287:ASP:N	2.29	0.44
1:K:894:ARG:NH1	1:K:920:LEU:CA	2.81	0.44
1:I:894:ARG:HH12	1:I:920:LEU:HA	1.81	0.44
1:M:230:ARG:NH2	1:M:241:GLU:OE2	2.51	0.44
1:J:822:LEU:HD12	1:J:823:LEU:H	1.80	0.44
1:I:822:LEU:C	1:I:822:LEU:HD12	2.37	0.44
1:N:34:ALA:HB3	1:N:36:TRP:CZ3	2.53	0.44
1:K:78:LEU:CB	1:K:79:PRO:HD2	2.44	0.44
1:K:673:ALA:O	1:K:676:GLY:N	2.47	0.44
1:P:658:LEU:HD12	1:P:693:GLN:O	2.18	0.44
1:M:272:ALA:HB1	1:M:273:PRO:CD	2.47	0.44
1:L:645:ARG:NH2	1:L:650:GLU:OE2	2.48	0.44
1:M:387:VAL:CG2	1:M:388:ARG:N	2.80	0.44
1:O:429:ASP:OD1	1:O:431:ARG:HD3	2.18	0.44
1:M:50:GLN:HB3	1:M:216:HIS:HB3	2.00	0.44
1:J:70:PRO:O	1:J:73:TRP:N	2.45	0.44
1:O:571:VAL:HG13	1:O:607:VAL:HG23	1.99	0.44
1:O:164:ASP:OD2	1:O:167:LEU:HD12	2.18	0.44
1:L:406:GLY:O	1:L:407:LEU:HD23	2.18	0.44
1:O:173:LEU:HD23	1:O:173:LEU:HA	1.69	0.44
1:I:111:PRO:HA	1:I:112:PRO:HA	1.57	0.44
1:O:406:GLY:O	1:O:407:LEU:HD23	2.18	0.44
1:K:111:PRO:HA	1:K:112:PRO:HA	1.57	0.44
1:J:406:GLY:O	1:J:407:LEU:HD23	2.18	0.44
1:K:406:GLY:O	1:K:407:LEU:HD23	2.18	0.44
1:O:583:ASN:HA	1:O:584:PRO:HD3	1.79	0.44
1:J:781:ARG:NH1	1:J:781:ARG:CG	2.79	0.44
1:P:894:ARG:NH1	1:P:920:LEU:CA	2.81	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:894:ARG:NH1	1:O:920:LEU:CA	2.81	0.44
1:I:894:ARG:NH1	1:I:920:LEU:CA	2.81	0.44
1:O:67:GLU:H	1:O:67:GLU:HG2	1.30	0.44
1:N:254:LEU:HD23	1:N:254:LEU:HA	1.62	0.44
1:J:63:PHE:CB	1:J:64:PRO:HD2	2.32	0.44
1:L:533:LEU:HD12	1:L:534:ILE:N	2.33	0.44
1:O:533:LEU:HD12	1:O:534:ILE:N	2.33	0.44
1:K:34:ALA:HB3	1:K:36:TRP:CZ3	2.53	0.44
1:J:24:LEU:HD12	1:J:24:LEU:HA	1.62	0.44
1:O:701:VAL:CG1	1:O:702:GLN:N	2.81	0.44
1:K:658:LEU:HD12	1:K:693:GLN:O	2.18	0.44
1:I:708:TRP:CD1	1:I:708:TRP:N	2.84	0.44
1:L:234:ASP:O	1:L:235:PHE:HB2	2.17	0.44
1:P:272:ALA:HA	1:P:273:PRO:HD3	1.76	0.44
1:I:387:VAL:CG2	1:I:388:ARG:N	2.80	0.44
1:M:35:SER:O	1:M:50:GLN:HG3	2.18	0.44
1:N:131:GLU:HA	1:N:134:LEU:HB2	1.99	0.44
1:N:35:SER:O	1:N:50:GLN:HG3	2.18	0.44
1:P:870:VAL:CG1	1:P:871:GLU:N	2.81	0.44
1:K:870:VAL:CG1	1:K:871:GLU:N	2.81	0.44
1:P:559:TYR:HA	1:P:560:PRO:HD2	1.73	0.44
1:M:757:GLN:O	1:M:757:GLN:HG2	2.12	0.44
1:L:507:ASP:C	1:L:519:SER:HB2	2.39	0.44
1:M:972:HIS:HB3	5:M:4095:HOH:O	2.18	0.44
1:P:118:ASN:HA	1:P:119:PRO:HD2	1.60	0.44
1:L:788:PRO:O	1:L:933:SER:HB2	2.18	0.44
1:P:576:ILE:CG2	1:P:577:LYS:N	2.78	0.43
1:N:360:HIS:HA	1:N:361:PRO:HD3	1.86	0.43
1:I:685:LEU:HB3	1:I:686:PRO:HD2	1.99	0.43
1:P:685:LEU:HB3	1:P:686:PRO:HD2	1.99	0.43
1:P:210:ARG:HH11	1:P:395:HIS:HB2	1.82	0.43
1:P:260:LEU:HA	1:P:260:LEU:HD12	1.61	0.43
1:J:34:ALA:HB3	1:J:36:TRP:CZ3	2.53	0.43
1:L:260:LEU:HD12	1:L:260:LEU:HA	1.61	0.43
1:L:661:LYS:HA	1:L:662:PRO:HD3	1.63	0.43
1:K:3:ILE:O	1:K:6:SER:HB3	2.18	0.43
1:J:658:LEU:HD12	1:J:693:GLN:O	2.18	0.43
1:K:234:ASP:O	1:K:235:PHE:HB2	2.17	0.43
1:N:3:ILE:O	1:N:6:SER:HB3	2.18	0.43
1:L:50:GLN:HB3	1:L:216:HIS:HB3	2.00	0.43
1:P:131:GLU:HA	1:P:134:LEU:HB2	2.00	0.43
1:N:70:PRO:O	1:N:73:TRP:N	2.45	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:571:VAL:HG13	1:N:607:VAL:HG23	2.00	0.43
1:K:164:ASP:OD2	1:K:167:LEU:HD12	2.18	0.43
1:K:507:ASP:C	1:K:519:SER:HB2	2.39	0.43
1:P:200:GLN:N	1:P:200:GLN:OE1	2.44	0.43
1:M:670:LEU:HD23	1:M:670:LEU:HA	1.67	0.43
1:L:972:HIS:HB3	5:L:4095:HOH:O	2.18	0.43
1:L:149:ALA:O	1:L:150:PHE:HB3	2.18	0.43
1:J:43:ARG:NH1	1:J:44:THR:CG2	2.81	0.43
1:J:46:ARG:HB3	1:J:47:PRO:HD2	2.01	0.43
1:P:46:ARG:HB3	1:P:47:PRO:HD2	2.00	0.43
1:M:894:ARG:NH1	1:M:920:LEU:CA	2.81	0.43
1:K:63:PHE:N	1:K:63:PHE:CD1	2.86	0.43
1:P:63:PHE:CD1	1:P:63:PHE:N	2.86	0.43
1:N:63:PHE:N	1:N:63:PHE:CD1	2.86	0.43
1:L:63:PHE:N	1:L:63:PHE:CD1	2.86	0.43
1:K:533:LEU:HD12	1:K:534:ILE:N	2.33	0.43
1:N:533:LEU:HD12	1:N:534:ILE:N	2.33	0.43
1:I:533:LEU:HD12	1:I:534:ILE:N	2.33	0.43
1:I:419:GLY:HA2	1:L:282:ARG:HH11	1.83	0.43
1:L:49:GLN:CD	1:L:49:GLN:H	2.20	0.43
1:N:658:LEU:HD12	1:N:693:GLN:O	2.18	0.43
1:P:347:LYS:CB	1:P:348:PRO:HD2	2.43	0.43
1:P:3:ILE:O	1:P:6:SER:HB3	2.18	0.43
1:K:237:ARG:NH1	1:K:237:ARG:CG	2.82	0.43
1:M:645:ARG:NH2	1:M:650:GLU:OE2	2.48	0.43
1:J:429:ASP:OD1	1:J:431:ARG:HD3	2.18	0.43
1:O:73:TRP:O	1:O:183:ARG:NH1	2.48	0.43
1:L:512:PHE:CE1	1:L:517:LYS:HG3	2.51	0.43
1:J:870:VAL:CG1	1:J:871:GLU:N	2.81	0.43
1:P:637:GLU:HA	1:P:679:LEU:HD23	2.01	0.43
1:N:378:LEU:HD23	1:N:378:LEU:HA	1.53	0.43
1:M:149:ALA:O	1:M:150:PHE:HB3	2.18	0.43
1:P:406:GLY:O	1:P:407:LEU:HD23	2.18	0.43
1:P:507:ASP:C	1:P:519:SER:HB2	2.39	0.43
1:K:668:VAL:HG13	1:K:669:PRO:CD	2.38	0.43
1:O:1021:CME:HZ3	1:O:1022:GLN:O	2.19	0.43
1:O:230:ARG:NH2	1:O:241:GLU:OE2	2.51	0.43
1:K:763:GLY:HA3	1:K:822:LEU:HD22	2.01	0.43
1:M:63:PHE:CD1	1:M:63:PHE:N	2.86	0.43
1:M:685:LEU:HB3	1:M:686:PRO:HD2	1.99	0.43
1:I:34:ALA:HB3	1:I:36:TRP:CZ3	2.53	0.43
1:M:189:LEU:N	1:M:189:LEU:CD2	2.75	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:4:THR:CA	1:K:9:VAL:HG11	2.47	0.43
1:I:3:ILE:O	1:I:6:SER:HB3	2.18	0.43
1:N:237:ARG:NH1	1:N:237:ARG:CG	2.82	0.43
1:K:778:THR:HB	1:K:887:GLN:CB	2.48	0.43
1:I:50:GLN:HB3	1:I:216:HIS:HB3	2.00	0.43
1:K:35:SER:O	1:K:50:GLN:HG3	2.18	0.43
1:M:1018:LEU:HA	1:M:1018:LEU:HD23	1.51	0.43
1:K:961:ARG:NH2	1:K:979:GLU:O	2.37	0.43
1:I:726:LEU:HA	1:I:726:LEU:HD23	1.66	0.43
1:I:363:HIS:N	1:I:363:HIS:CD2	2.81	0.43
1:J:507:ASP:C	1:J:519:SER:HB2	2.39	0.43
1:K:694:LEU:HA	1:K:694:LEU:HD12	1.69	0.43
1:N:43:ARG:NH1	1:N:44:THR:CG2	2.81	0.43
1:M:57:GLU:HG2	1:M:83:THR:HG21	1.93	0.43
1:N:1021:CME:HB3	1:N:1021:CME:HE2	1.41	0.43
1:J:210:ARG:HH11	1:J:395:HIS:CA	2.32	0.43
1:M:533:LEU:HD12	1:M:534:ILE:N	2.33	0.43
1:I:138:GLN:N	1:I:217:LYS:O	2.36	0.43
1:N:37:ARG:NH1	1:N:37:ARG:CG	2.79	0.43
1:K:701:VAL:CG1	1:K:702:GLN:N	2.81	0.43
1:N:422:PRO:HA	1:O:282:ARG:HB2	1.99	0.43
1:M:347:LYS:CB	1:M:348:PRO:HD2	2.43	0.43
1:K:50:GLN:HB3	1:K:216:HIS:HB3	2.00	0.43
1:M:870:VAL:CG1	1:M:871:GLU:N	2.81	0.43
1:M:164:ASP:OD2	1:M:167:LEU:HD12	2.18	0.43
1:J:637:GLU:HA	1:J:679:LEU:HD23	2.01	0.43
1:K:722:LEU:HA	1:K:722:LEU:HD23	1.75	0.43
1:O:757:GLN:HG2	1:O:757:GLN:O	2.12	0.43
1:K:647:SER:OG	1:K:672:VAL:N	2.35	0.43
1:N:149:ALA:O	1:N:150:PHE:HB3	2.18	0.43
1:P:788:PRO:O	1:P:933:SER:HB2	2.18	0.43
1:N:46:ARG:HB3	1:N:47:PRO:HD2	2.00	0.43
1:J:533:LEU:HD12	1:J:534:ILE:N	2.33	0.43
1:I:336:ARG:CG	1:I:336:ARG:HH11	2.26	0.43
1:N:701:VAL:HG12	1:N:702:GLN:H	1.83	0.43
1:N:49:GLN:CD	1:N:49:GLN:H	2.20	0.43
1:I:429:ASP:HA	1:I:430:PRO:HD3	1.51	0.43
1:N:429:ASP:OD1	1:N:431:ARG:HD3	2.18	0.43
1:L:870:VAL:CG1	1:L:871:GLU:N	2.81	0.43
1:O:637:GLU:HA	1:O:679:LEU:HD23	2.01	0.43
1:N:173:LEU:HA	1:N:173:LEU:HD23	1.69	0.43
1:M:287:ASP:N	1:M:287:ASP:OD1	2.29	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:375:ASP:O	1:P:379:MET:HG3	2.19	0.43
1:O:149:ALA:O	1:O:150:PHE:HB3	2.18	0.43
1:J:788:PRO:O	1:J:933:SER:HB2	2.18	0.43
1:J:149:ALA:O	1:J:150:PHE:HB3	2.18	0.43
1:K:436:MET:HE1	1:K:467:ASN:HB2	2.00	0.43
1:K:46:ARG:HB3	1:K:47:PRO:HD2	2.00	0.43
1:I:895:VAL:O	1:I:919:ASP:HA	2.19	0.43
1:O:63:PHE:CD1	1:O:63:PHE:N	2.86	0.43
1:L:823:LEU:HA	1:L:823:LEU:HD23	1.73	0.43
1:J:823:LEU:HD23	1:J:823:LEU:HA	1.73	0.43
1:J:63:PHE:CD1	1:J:63:PHE:N	2.86	0.43
1:O:682:LEU:HD23	1:O:682:LEU:HA	1.67	0.43
1:J:685:LEU:HB3	1:J:686:PRO:HD2	1.99	0.43
1:L:673:ALA:O	1:L:676:GLY:N	2.47	0.43
1:N:708:TRP:CD1	1:N:708:TRP:N	2.84	0.43
1:L:778:THR:HB	1:L:887:GLN:CB	2.49	0.43
1:J:778:THR:HB	1:J:887:GLN:CB	2.48	0.43
1:K:429:ASP:OD1	1:K:431:ARG:HD3	2.18	0.43
1:N:807:VAL:HG13	1:N:808:GLU:N	2.34	0.43
1:I:70:PRO:O	1:I:73:TRP:N	2.45	0.43
1:M:571:VAL:HG13	1:M:607:VAL:HG23	1.99	0.43
1:I:870:VAL:CG1	1:I:871:GLU:N	2.81	0.43
1:O:559:TYR:HA	1:O:560:PRO:HD2	1.73	0.43
1:J:164:ASP:OD2	1:J:167:LEU:HD12	2.18	0.43
1:M:637:GLU:HA	1:M:679:LEU:HD23	2.01	0.43
1:O:646:HIS:O	1:O:648:ASP:N	2.48	0.43
1:M:406:GLY:O	1:M:407:LEU:HD23	2.18	0.43
1:J:375:ASP:O	1:J:379:MET:HG3	2.19	0.43
1:O:507:ASP:C	1:O:519:SER:HB2	2.39	0.43
1:I:507:ASP:C	1:I:519:SER:HB2	2.38	0.43
1:P:43:ARG:NH1	1:P:44:THR:CG2	2.81	0.43
1:K:43:ARG:NH1	1:K:44:THR:CG2	2.81	0.43
1:O:436:MET:HE1	1:O:467:ASN:HB2	2.01	0.43
1:J:651:LEU:HD12	1:J:668:VAL:O	2.19	0.43
1:N:651:LEU:HD12	1:N:668:VAL:O	2.19	0.43
1:L:895:VAL:O	1:L:919:ASP:HA	2.19	0.43
1:I:63:PHE:N	1:I:63:PHE:CD1	2.86	0.43
1:K:255:ARG:CG	1:K:255:ARG:NH1	2.79	0.43
1:P:210:ARG:HH11	1:P:395:HIS:CA	2.32	0.43
1:L:210:ARG:HH11	1:L:395:HIS:CA	2.32	0.43
1:P:34:ALA:HB3	1:P:36:TRP:CZ3	2.53	0.43
1:O:658:LEU:HD12	1:O:693:GLN:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:778:THR:HB	1:N:887:GLN:CB	2.48	0.43
1:M:778:THR:HB	1:M:887:GLN:CB	2.48	0.43
1:L:131:GLU:HA	1:L:134:LEU:HB2	2.00	0.43
1:P:50:GLN:HB3	1:P:216:HIS:HB3	2.00	0.43
1:M:608:PHE:O	1:M:611:ARG:N	2.41	0.43
1:J:570:TRP:HD1	1:J:571:VAL:HG22	1.84	0.43
1:P:679:LEU:HD23	1:P:679:LEU:HA	1.26	0.43
1:P:718:GLN:HG3	1:P:719:GLN:N	2.33	0.43
1:P:670:LEU:HA	1:P:670:LEU:HD23	1.67	0.43
1:J:308:LEU:HA	1:J:308:LEU:HD23	1.80	0.43
1:J:110:ASN:O	1:J:113:PHE:HB2	2.19	0.43
1:O:694:LEU:O	1:O:722:LEU:N	2.51	0.43
1:L:479:ASP:HA	1:L:480:PRO:HD2	1.61	0.43
1:L:436:MET:HE1	1:L:467:ASN:HD22	1.79	0.43
1:K:651:LEU:HD12	1:K:668:VAL:O	2.19	0.43
1:O:46:ARG:HB3	1:O:47:PRO:HD2	2.00	0.43
1:N:92:MET:HE3	1:N:362:LEU:O	2.18	0.43
1:P:1021:CME:HZ3	1:P:1022:GLN:O	2.19	0.43
1:M:895:VAL:O	1:M:919:ASP:HA	2.19	0.43
1:P:822:LEU:C	1:P:822:LEU:HD12	2.37	0.43
1:O:685:LEU:HB3	1:O:686:PRO:HD2	1.99	0.43
1:P:682:LEU:HD23	1:P:682:LEU:HA	1.67	0.43
1:M:682:LEU:HA	1:M:682:LEU:HD23	1.67	0.43
1:K:260:LEU:HD12	1:K:310:ARG:O	2.19	0.43
1:M:260:LEU:HD12	1:M:310:ARG:O	2.19	0.43
1:L:579:ASP:OD1	1:L:583:ASN:N	2.43	0.43
1:O:708:TRP:CZ3	1:O:709:SER:HB3	2.54	0.43
1:M:708:TRP:CZ3	1:M:709:SER:HB3	2.54	0.43
1:I:708:TRP:CZ3	1:I:709:SER:HB3	2.54	0.43
1:P:568:TRP:CD2	1:P:569:ASP:HB3	2.54	0.43
1:I:778:THR:HB	1:I:887:GLN:CB	2.48	0.43
1:L:35:SER:O	1:L:50:GLN:HG3	2.18	0.43
1:P:1018:LEU:HD23	1:P:1018:LEU:HA	1.51	0.43
1:J:287:ASP:N	1:J:287:ASP:OD1	2.29	0.43
1:P:73:TRP:O	1:P:183:ARG:NH1	2.48	0.43
1:K:637:GLU:HA	1:K:679:LEU:HD23	2.01	0.43
1:K:93:HIS:HB3	1:K:95:TYR:HE1	1.84	0.43
1:N:637:GLU:HA	1:N:679:LEU:HD23	2.01	0.43
1:I:718:GLN:HG3	1:I:719:GLN:N	2.34	0.43
1:N:375:ASP:O	1:N:379:MET:HG3	2.19	0.43
1:M:110:ASN:O	1:M:113:PHE:HB2	2.19	0.43
1:K:264:GLU:OE2	1:K:264:GLU:HA	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:694:LEU:HD12	1:M:694:LEU:HA	1.69	0.43
1:M:694:LEU:O	1:M:722:LEU:N	2.51	0.43
1:M:507:ASP:C	1:M:519:SER:HB2	2.39	0.43
1:K:375:ASP:O	1:K:379:MET:HG3	2.19	0.43
1:O:718:GLN:HG3	1:O:719:GLN:N	2.34	0.43
1:O:43:ARG:NH1	1:O:44:THR:HG23	2.34	0.43
1:O:781:ARG:NH1	1:O:781:ARG:CG	2.79	0.43
1:I:251:ARG:CB	1:I:253:TYR:CE2	2.98	0.43
1:J:920:LEU:CB	1:J:921:PRO:CD	2.97	0.43
1:L:63:PHE:CB	1:L:64:PRO:HD2	2.32	0.43
1:O:210:ARG:HH11	1:O:395:HIS:CA	2.32	0.43
1:I:260:LEU:HD12	1:I:310:ARG:O	2.19	0.43
1:N:708:TRP:CZ3	1:N:709:SER:HB3	2.54	0.43
1:L:237:ARG:CG	1:L:237:ARG:NH1	2.82	0.43
1:P:237:ARG:CG	1:P:237:ARG:NH1	2.82	0.43
1:O:421:VAL:O	1:O:425:ARG:NH1	2.46	0.43
1:J:568:TRP:CD2	1:J:569:ASP:HB3	2.54	0.43
1:K:568:TRP:CD2	1:K:569:ASP:HB3	2.54	0.43
1:M:429:ASP:OD1	1:M:431:ARG:HD3	2.18	0.43
1:N:778:THR:CG2	1:N:887:GLN:H	2.32	0.43
1:J:287:ASP:CG	1:K:425:ARG:HH22	2.22	0.43
1:K:612:THR:HA	1:K:613:PRO:HD3	1.68	0.43
1:P:445:GLN:HB3	1:P:445:GLN:HE21	1.54	0.43
1:I:93:HIS:HB3	1:I:95:TYR:HE1	1.84	0.43
1:O:285:TYR:HB3	1:O:288:ARG:HG3	2.01	0.43
1:M:264:GLU:OE2	1:M:264:GLU:HA	2.17	0.43
1:M:726:LEU:HA	1:M:726:LEU:HD23	1.66	0.43
1:O:264:GLU:OE2	1:O:264:GLU:HA	2.17	0.43
1:I:369:GLU:O	1:I:373:VAL:HG23	2.19	0.43
1:P:285:TYR:HB3	1:P:288:ARG:HG3	2.01	0.43
1:I:375:ASP:O	1:I:379:MET:HG3	2.19	0.43
1:N:406:GLY:O	1:N:407:LEU:HD23	2.18	0.43
1:L:531:ARG:O	1:L:561:ARG:NH1	2.46	0.43
1:J:972:HIS:HB3	5:J:4095:HOH:O	2.18	0.43
1:N:1021:CME:HZ3	1:N:1022:GLN:O	2.19	0.43
1:L:1021:CME:HZ3	1:L:1022:GLN:O	2.19	0.43
1:N:894:ARG:NH1	1:N:920:LEU:CA	2.81	0.43
1:N:210:ARG:HH11	1:N:395:HIS:CA	2.32	0.43
1:M:395:HIS:HA	1:M:396:PRO:HD3	1.48	0.43
1:O:138:GLN:N	1:O:217:LYS:O	2.36	0.43
1:N:260:LEU:HD12	1:N:310:ARG:O	2.19	0.43
1:I:701:VAL:CG1	1:I:702:GLN:N	2.81	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:657:ALA:HA	1:N:661:LYS:O	2.19	0.43
1:O:344:LEU:N	1:O:347:LYS:O	2.36	0.43
1:I:568:TRP:CD2	1:I:569:ASP:HB3	2.54	0.43
1:O:597:ASN:ND2	1:O:599:ARG:H	2.17	0.43
1:J:473:ARG:HD2	1:K:469:ASP:HB3	1.99	0.43
1:M:778:THR:CG2	1:M:887:GLN:H	2.32	0.43
1:M:807:VAL:HG13	1:M:808:GLU:N	2.34	0.43
1:O:870:VAL:CG1	1:O:871:GLU:N	2.81	0.43
1:L:571:VAL:HG13	1:L:607:VAL:HG23	1.99	0.43
1:M:788:PRO:O	1:M:933:SER:HB2	2.18	0.43
1:O:110:ASN:O	1:O:113:PHE:HB2	2.19	0.43
1:I:788:PRO:O	1:I:933:SER:HB2	2.18	0.43
1:M:647:SER:OG	1:M:672:VAL:N	2.35	0.43
1:L:110:ASN:O	1:L:113:PHE:HB2	2.19	0.43
1:I:43:ARG:NH1	1:I:44:THR:HG23	2.34	0.42
1:M:651:LEU:HD12	1:M:668:VAL:O	2.19	0.42
1:P:251:ARG:CB	1:P:253:TYR:CE2	2.98	0.42
1:I:1021:CME:HZ3	1:I:1022:GLN:O	2.19	0.42
1:K:895:VAL:O	1:K:919:ASP:HA	2.19	0.42
1:O:230:ARG:HH11	1:O:230:ARG:CG	2.24	0.42
1:L:254:LEU:HA	1:L:254:LEU:HD23	1.62	0.42
1:L:685:LEU:HA	1:L:686:PRO:HD3	1.70	0.42
1:P:533:LEU:HD12	1:P:534:ILE:N	2.33	0.42
1:J:34:ALA:HB3	1:J:36:TRP:CE3	2.54	0.42
1:I:661:LYS:HA	1:I:662:PRO:HD3	1.63	0.42
1:M:49:GLN:CD	1:M:49:GLN:H	2.20	0.42
1:L:900:LEU:HD23	1:L:900:LEU:HA	1.75	0.42
1:I:237:ARG:CG	1:I:237:ARG:NH1	2.82	0.42
1:J:272:ALA:HB1	1:J:273:PRO:CD	2.47	0.42
1:I:429:ASP:OD1	1:I:431:ARG:HD3	2.18	0.42
1:J:85:VAL:HG12	1:J:86:VAL:N	2.34	0.42
1:I:807:VAL:HG13	1:I:808:GLU:N	2.34	0.42
1:I:164:ASP:OD2	1:I:167:LEU:HD12	2.18	0.42
1:L:164:ASP:OD2	1:L:167:LEU:HD12	2.18	0.42
1:O:93:HIS:HB3	1:O:95:TYR:HE1	1.84	0.42
1:I:353:GLY:C	1:I:566:PHE:HA	2.40	0.42
1:N:110:ASN:O	1:N:113:PHE:HB2	2.19	0.42
1:K:972:HIS:HB3	5:K:4095:HOH:O	2.18	0.42
1:J:369:GLU:O	1:J:373:VAL:HG23	2.19	0.42
1:P:369:GLU:O	1:P:373:VAL:HG23	2.19	0.42
1:L:353:GLY:C	1:L:566:PHE:HA	2.40	0.42
1:N:369:GLU:O	1:N:373:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:43:ARG:NH1	1:I:44:THR:CG2	2.81	0.42
1:P:43:ARG:NH1	1:P:44:THR:HG23	2.34	0.42
1:O:746:ASP:HA	1:O:760:ARG:CG	2.39	0.42
1:L:651:LEU:HD12	1:L:668:VAL:O	2.19	0.42
1:N:240:LEU:HD12	1:N:240:LEU:C	2.36	0.42
1:J:114:VAL:HG21	1:J:192:SER:N	2.35	0.42
1:L:114:VAL:HG21	1:L:192:SER:N	2.35	0.42
1:N:685:LEU:HB3	1:N:686:PRO:HD2	1.99	0.42
1:P:395:HIS:HA	1:P:396:PRO:HD3	1.48	0.42
1:P:260:LEU:HD12	1:P:310:ARG:O	2.19	0.42
1:L:260:LEU:HD12	1:L:310:ARG:O	2.19	0.42
1:L:34:ALA:HB3	1:L:36:TRP:CE3	2.54	0.42
1:O:657:ALA:HA	1:O:661:LYS:O	2.19	0.42
1:O:800:ARG:CZ	1:O:800:ARG:CB	2.98	0.42
1:K:645:ARG:NH2	1:K:650:GLU:OE2	2.48	0.42
1:J:778:THR:CG2	1:J:887:GLN:H	2.32	0.42
1:O:778:THR:HB	1:O:887:GLN:CB	2.49	0.42
1:L:429:ASP:OD1	1:L:431:ARG:HD3	2.18	0.42
1:I:85:VAL:HG12	1:I:86:VAL:N	2.34	0.42
1:K:73:TRP:O	1:K:183:ARG:NH1	2.48	0.42
1:M:141:ILE:HD13	1:M:143:PHE:CE1	2.55	0.42
1:P:927:THR:HA	1:P:928:PRO:HD3	1.62	0.42
1:L:93:HIS:HB3	1:L:95:TYR:HE1	1.84	0.42
1:J:373:VAL:O	1:J:374:GLN:C	2.57	0.42
1:I:264:GLU:HA	1:I:264:GLU:OE2	2.17	0.42
1:I:285:TYR:HB3	1:I:288:ARG:HG3	2.01	0.42
1:L:718:GLN:HG3	1:L:719:GLN:N	2.34	0.42
1:M:353:GLY:C	1:M:566:PHE:HA	2.40	0.42
1:O:1004:SER:HB2	1:O:1006:GLU:OE2	2.19	0.42
1:P:972:HIS:HB3	5:P:4578:HOH:O	2.18	0.42
1:J:43:ARG:NH1	1:J:44:THR:HG23	2.34	0.42
1:M:43:ARG:NH1	1:M:44:THR:HG23	2.34	0.42
1:O:7:LEU:O	1:O:8:ALA:C	2.55	0.42
1:K:7:LEU:O	1:K:8:ALA:C	2.55	0.42
1:J:251:ARG:CB	1:J:253:TYR:CE2	2.98	0.42
1:J:895:VAL:O	1:J:919:ASP:HA	2.19	0.42
1:J:1021:CME:HB3	1:J:1021:CME:HE2	1.41	0.42
1:I:210:ARG:HH11	1:I:395:HIS:CA	2.32	0.42
1:M:657:ALA:HA	1:M:661:LYS:O	2.19	0.42
1:J:708:TRP:CZ3	1:J:709:SER:HB3	2.54	0.42
1:M:597:ASN:ND2	1:M:599:ARG:H	2.17	0.42
1:J:272:ALA:HA	1:J:273:PRO:HD3	1.76	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:836:ILE:HD13	1:K:836:ILE:N	2.34	0.42
1:P:778:THR:CG2	1:P:887:GLN:H	2.32	0.42
1:J:50:GLN:HB3	1:J:216:HIS:HB3	2.00	0.42
1:P:807:VAL:HG13	1:P:808:GLU:N	2.34	0.42
1:M:1018:LEU:HD22	1:M:1019:VAL:N	2.35	0.42
1:N:1018:LEU:HD22	1:N:1019:VAL:N	2.35	0.42
1:K:141:ILE:HD13	1:K:143:PHE:CE1	2.55	0.42
1:I:637:GLU:HA	1:I:679:LEU:HD23	2.01	0.42
1:N:353:GLY:C	1:N:566:PHE:HA	2.40	0.42
1:P:353:GLY:C	1:P:566:PHE:HA	2.40	0.42
1:J:378:LEU:HD23	1:J:378:LEU:HA	1.53	0.42
1:O:367:MET:HE2	1:O:367:MET:HB3	1.88	0.42
1:N:507:ASP:C	1:N:519:SER:HB2	2.39	0.42
1:I:406:GLY:O	1:I:407:LEU:HD23	2.18	0.42
1:O:972:HIS:HB3	5:O:4095:HOH:O	2.18	0.42
1:K:43:ARG:NH1	1:K:44:THR:HG23	2.34	0.42
1:M:46:ARG:HB3	1:M:47:PRO:HD2	2.00	0.42
1:I:651:LEU:HD12	1:I:668:VAL:O	2.19	0.42
1:L:46:ARG:HB3	1:L:47:PRO:HD2	2.00	0.42
1:L:46:ARG:CG	1:L:46:ARG:NH1	2.78	0.42
1:K:1021:CME:HZ3	1:K:1022:GLN:O	2.19	0.42
1:O:895:VAL:O	1:O:919:ASP:HA	2.19	0.42
1:I:230:ARG:NH2	1:I:241:GLU:OE2	2.51	0.42
1:P:823:LEU:HA	1:P:823:LEU:HD23	1.73	0.42
1:M:210:ARG:HH11	1:M:395:HIS:CA	2.32	0.42
1:K:78:LEU:HB3	1:K:79:PRO:CD	2.45	0.42
1:P:657:ALA:HA	1:P:661:LYS:O	2.19	0.42
1:J:657:ALA:HA	1:J:661:LYS:O	2.19	0.42
1:L:708:TRP:CZ3	1:L:709:SER:HB3	2.54	0.42
1:M:237:ARG:NH1	1:M:237:ARG:CG	2.82	0.42
1:L:568:TRP:CD2	1:L:569:ASP:HB3	2.54	0.42
1:L:184:LEU:HA	1:L:184:LEU:HD23	1.83	0.42
1:P:429:ASP:OD1	1:P:431:ARG:HD3	2.18	0.42
1:P:35:SER:O	1:P:50:GLN:HG3	2.18	0.42
1:I:35:SER:O	1:I:50:GLN:HG3	2.18	0.42
1:O:807:VAL:HG13	1:O:808:GLU:N	2.34	0.42
1:J:141:ILE:HD13	1:J:143:PHE:CE1	2.55	0.42
1:J:571:VAL:HG13	1:J:607:VAL:HG23	1.99	0.42
1:M:679:LEU:HA	1:M:679:LEU:HD23	1.26	0.42
1:K:149:ALA:O	1:K:150:PHE:HB3	2.18	0.42
1:N:1004:SER:HB2	1:N:1006:GLU:OE2	2.20	0.42
1:O:375:ASP:O	1:O:379:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:476:LYS:HD2	1:O:476:LYS:HA	1.81	0.42
1:L:391:HIS:ND1	1:L:412:GLU:OE1	2.44	0.42
1:J:1004:SER:HB2	1:J:1006:GLU:OE2	2.19	0.42
1:P:110:ASN:O	1:P:113:PHE:HB2	2.19	0.42
1:L:285:TYR:HB3	1:L:288:ARG:HG3	2.01	0.42
1:L:1004:SER:HB2	1:L:1006:GLU:OE2	2.20	0.42
1:K:110:ASN:O	1:K:113:PHE:HB2	2.19	0.42
1:N:718:GLN:HG3	1:N:719:GLN:N	2.34	0.42
1:O:257:THR:OG1	1:O:316:HIS:HE1	2.03	0.42
1:P:57:GLU:HG2	1:P:83:THR:HG21	1.93	0.42
1:J:257:THR:OG1	1:J:316:HIS:HE1	2.03	0.42
1:N:781:ARG:CG	1:N:781:ARG:NH1	2.79	0.42
1:N:701:VAL:CG1	1:N:702:GLN:N	2.81	0.42
1:L:701:VAL:CG1	1:L:702:GLN:N	2.81	0.42
1:P:377:LEU:HA	1:P:377:LEU:HD23	1.91	0.42
1:K:708:TRP:CZ3	1:K:709:SER:HB3	2.54	0.42
1:K:800:ARG:CZ	1:K:800:ARG:CB	2.98	0.42
1:I:347:LYS:HA	1:I:348:PRO:HD3	1.77	0.42
1:L:597:ASN:ND2	1:L:599:ARG:H	2.17	0.42
1:M:469:ASP:HB3	1:P:473:ARG:HD2	2.02	0.42
1:K:778:THR:CG2	1:K:887:GLN:H	2.32	0.42
1:L:730:LEU:HA	1:L:731:PRO:HD3	1.74	0.42
1:O:131:GLU:HA	1:O:134:LEU:HB2	1.99	0.42
1:J:35:SER:O	1:J:50:GLN:HG3	2.18	0.42
1:P:1018:LEU:HD22	1:P:1019:VAL:N	2.34	0.42
1:L:1018:LEU:HD22	1:L:1019:VAL:N	2.35	0.42
1:J:1018:LEU:HD22	1:J:1019:VAL:N	2.35	0.42
1:I:69:VAL:HA	1:I:70:PRO:HD2	1.77	0.42
1:I:73:TRP:O	1:I:183:ARG:NH1	2.48	0.42
1:L:612:THR:HA	1:L:613:PRO:HD3	1.68	0.42
1:O:353:GLY:C	1:O:566:PHE:HA	2.40	0.42
1:I:722:LEU:HD23	1:I:722:LEU:HA	1.75	0.42
1:L:694:LEU:HA	1:L:694:LEU:HD12	1.69	0.42
1:P:1004:SER:HB2	1:P:1006:GLU:OE2	2.20	0.42
1:K:1004:SER:HB2	1:K:1006:GLU:OE2	2.20	0.42
1:L:375:ASP:O	1:L:379:MET:HG3	2.19	0.42
1:P:149:ALA:O	1:P:150:PHE:HB3	2.18	0.42
1:L:43:ARG:HH11	1:L:43:ARG:CG	2.10	0.42
1:N:43:ARG:NH1	1:N:44:THR:HG23	2.34	0.42
1:J:746:ASP:HA	1:J:760:ARG:CG	2.39	0.42
1:L:18:ASN:OD1	1:L:19:PRO:HD2	2.20	0.42
1:M:18:ASN:OD1	1:M:19:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:651:LEU:HD12	1:P:668:VAL:O	2.19	0.42
1:P:230:ARG:NH2	1:P:241:GLU:OE2	2.50	0.42
1:M:823:LEU:HA	1:M:823:LEU:HD23	1.73	0.42
1:I:34:ALA:HB3	1:I:36:TRP:CE3	2.54	0.42
1:K:210:ARG:HH11	1:K:395:HIS:CA	2.32	0.42
1:N:568:TRP:CD2	1:N:569:ASP:HB3	2.54	0.42
1:O:568:TRP:CD2	1:O:569:ASP:HB3	2.54	0.42
1:M:568:TRP:CD2	1:M:569:ASP:HB3	2.54	0.42
1:J:131:GLU:HA	1:J:134:LEU:HB2	2.00	0.42
1:I:469:ASP:HB3	1:L:473:ARG:HD2	2.01	0.42
1:I:272:ALA:HB1	1:I:273:PRO:CD	2.47	0.42
1:O:85:VAL:HG12	1:O:86:VAL:N	2.35	0.42
1:O:1018:LEU:HD22	1:O:1019:VAL:N	2.35	0.42
1:I:141:ILE:HD13	1:I:143:PHE:CE1	2.55	0.42
1:N:141:ILE:HD13	1:N:143:PHE:CE1	2.55	0.42
1:L:445:GLN:HB3	1:L:445:GLN:HE21	1.54	0.42
1:P:373:VAL:O	1:P:374:GLN:C	2.57	0.42
1:K:718:GLN:HG3	1:K:719:GLN:N	2.33	0.42
1:K:531:ARG:O	1:K:561:ARG:NH1	2.46	0.42
1:K:285:TYR:HB3	1:K:288:ARG:HG3	2.01	0.42
1:L:369:GLU:O	1:L:373:VAL:HG23	2.19	0.42
1:K:18:ASN:OD1	1:K:19:PRO:HD2	2.20	0.42
1:M:257:THR:OG1	1:M:316:HIS:HE1	2.03	0.42
1:J:1021:CME:HZ3	1:J:1022:GLN:O	2.19	0.42
1:K:62:TRP:C	1:K:63:PHE:CD1	2.93	0.42
1:I:62:TRP:C	1:I:63:PHE:CD1	2.93	0.42
1:N:114:VAL:HG21	1:N:192:SER:N	2.35	0.42
1:O:34:ALA:HB3	1:O:36:TRP:CE3	2.54	0.42
1:O:189:LEU:N	1:O:189:LEU:CD2	2.75	0.42
1:J:78:LEU:HB3	1:J:79:PRO:CD	2.45	0.42
1:J:78:LEU:CB	1:J:79:PRO:HD2	2.44	0.42
1:P:708:TRP:CZ3	1:P:709:SER:HB3	2.54	0.42
1:I:344:LEU:N	1:I:347:LYS:O	2.36	0.42
1:O:35:SER:O	1:O:50:GLN:HG3	2.18	0.42
1:K:807:VAL:HG13	1:K:808:GLU:N	2.34	0.42
1:L:608:PHE:O	1:L:611:ARG:N	2.41	0.42
1:N:870:VAL:CG1	1:N:871:GLU:N	2.81	0.42
1:P:93:HIS:HB3	1:P:95:TYR:HE1	1.84	0.42
1:J:829:THR:C	1:J:830:LEU:HD12	2.40	0.42
1:M:93:HIS:HB3	1:M:95:TYR:HE1	1.84	0.42
1:K:147:ASN:HB2	1:K:165:SER:HB3	2.01	0.42
1:M:829:THR:C	1:M:830:LEU:HD12	2.40	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:285:TYR:HB3	1:N:288:ARG:HG3	2.01	0.42
1:I:476:LYS:HA	1:I:476:LYS:HD2	1.81	0.42
1:N:694:LEU:HD12	1:N:694:LEU:HA	1.69	0.42
1:I:221:GLN:HG2	1:I:221:GLN:H	1.70	0.42
1:K:369:GLU:O	1:K:373:VAL:HG23	2.19	0.42
1:K:353:GLY:C	1:K:566:PHE:HA	2.40	0.42
1:I:149:ALA:O	1:I:150:PHE:HB3	2.18	0.42
1:J:436:MET:HE3	1:J:467:ASN:ND2	2.18	0.42
1:I:436:MET:HE3	1:I:467:ASN:ND2	2.22	0.42
1:I:57:GLU:HG2	1:I:83:THR:HG21	1.93	0.42
1:I:46:ARG:HB3	1:I:47:PRO:HD2	2.00	0.42
1:N:583:ASN:HA	1:N:584:PRO:HD3	1.79	0.42
1:P:62:TRP:C	1:P:63:PHE:CD1	2.93	0.42
1:J:763:GLY:HA3	1:J:822:LEU:HD22	2.01	0.42
1:J:62:TRP:C	1:J:63:PHE:CD1	2.93	0.42
1:I:260:LEU:C	1:I:267:VAL:HG23	2.40	0.42
1:P:138:GLN:N	1:P:217:LYS:O	2.36	0.42
1:P:78:LEU:HB3	1:P:79:PRO:CD	2.45	0.42
1:M:673:ALA:O	1:M:676:GLY:N	2.47	0.42
1:J:418:HIS:O	1:K:282:ARG:HD3	2.20	0.42
1:J:800:ARG:CZ	1:J:800:ARG:CB	2.98	0.42
1:M:800:ARG:CZ	1:M:800:ARG:CB	2.98	0.42
1:J:256:VAL:O	1:J:271:THR:HA	2.20	0.42
1:L:778:THR:O	1:L:778:THR:HG22	2.20	0.42
1:I:645:ARG:NH2	1:I:650:GLU:OE2	2.48	0.42
1:P:256:VAL:O	1:P:271:THR:HA	2.20	0.42
1:I:778:THR:HG22	1:I:778:THR:O	2.20	0.42
1:J:178:ARG:CB	1:J:178:ARG:HH11	2.33	0.42
1:O:141:ILE:HD13	1:O:143:PHE:CE1	2.55	0.42
1:P:141:ILE:HD13	1:P:143:PHE:CE1	2.55	0.42
1:P:70:PRO:O	1:P:73:TRP:N	2.45	0.42
1:K:829:THR:C	1:K:830:LEU:HD12	2.40	0.42
1:L:637:GLU:HA	1:L:679:LEU:HD23	2.01	0.42
1:N:221:GLN:HG2	1:N:221:GLN:H	1.70	0.42
1:O:118:ASN:HA	1:O:119:PRO:HD2	1.60	0.42
1:N:972:HIS:HB3	5:N:4245:HOH:O	2.18	0.42
1:I:972:HIS:HB3	5:I:4095:HOH:O	2.18	0.42
1:M:375:ASP:O	1:M:379:MET:HG3	2.19	0.42
1:M:1004:SER:HB2	1:M:1006:GLU:OE2	2.20	0.42
1:M:281:GLU:HG3	1:P:515:VAL:HG21	2.02	0.42
1:N:111:PRO:HA	1:N:112:PRO:HA	1.57	0.42
1:K:257:THR:OG1	1:K:316:HIS:HE1	2.03	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:360:HIS:ND1	1:I:362:LEU:HB2	2.35	0.42
1:O:579:ASP:OD1	1:O:583:ASN:N	2.43	0.42
1:M:781:ARG:HH11	1:M:781:ARG:CG	2.19	0.42
1:N:895:VAL:O	1:N:919:ASP:HA	2.19	0.42
1:O:62:TRP:C	1:O:63:PHE:CD1	2.93	0.42
1:I:114:VAL:HG21	1:I:192:SER:N	2.35	0.42
1:O:114:VAL:HG21	1:O:192:SER:N	2.34	0.42
1:L:657:ALA:HA	1:L:661:LYS:O	2.19	0.42
1:N:234:ASP:OD1	1:N:236:SER:HB3	2.20	0.42
1:O:234:ASP:OD1	1:O:236:SER:HB3	2.20	0.42
1:J:597:ASN:ND2	1:J:599:ARG:H	2.17	0.42
1:O:184:LEU:HA	1:O:184:LEU:HD23	1.84	0.42
1:N:256:VAL:O	1:N:271:THR:HA	2.20	0.42
1:O:256:VAL:O	1:O:271:THR:HA	2.20	0.42
1:M:256:VAL:O	1:M:271:THR:HA	2.20	0.42
1:L:807:VAL:HG13	1:L:808:GLU:N	2.34	0.42
1:P:147:ASN:HB2	1:P:165:SER:HB3	2.02	0.42
1:O:829:THR:C	1:O:830:LEU:HD12	2.40	0.42
1:N:147:ASN:HB2	1:N:165:SER:HB3	2.02	0.42
1:I:1004:SER:HB2	1:I:1006:GLU:OE2	2.20	0.42
1:J:726:LEU:HD23	1:J:726:LEU:HA	1.65	0.42
1:N:772:ASP:N	1:N:772:ASP:OD1	2.30	0.42
1:L:264:GLU:OE2	1:L:264:GLU:HA	2.17	0.42
1:K:214:LEU:HA	1:K:214:LEU:HD23	1.84	0.42
1:P:173:LEU:HD23	1:P:173:LEU:HA	1.69	0.42
1:M:718:GLN:HG3	1:M:719:GLN:N	2.34	0.42
1:L:43:ARG:NH1	1:L:44:THR:HG23	2.34	0.42
1:L:257:THR:OG1	1:L:316:HIS:HE1	2.03	0.42
1:O:18:ASN:OD1	1:O:19:PRO:HD2	2.20	0.42
1:L:46:ARG:HB3	1:L:47:PRO:CD	2.50	0.42
1:M:360:HIS:ND1	1:M:362:LEU:HB2	2.35	0.42
1:O:360:HIS:ND1	1:O:362:LEU:HB2	2.35	0.42
1:P:895:VAL:O	1:P:919:ASP:HA	2.19	0.42
1:O:120:THR:HG21	1:O:187:MET:HE3	2.01	0.42
1:N:763:GLY:HA3	1:N:822:LEU:HD22	2.01	0.42
1:O:260:LEU:HD12	1:O:310:ARG:O	2.19	0.42
1:M:37:ARG:CG	1:M:37:ARG:NH1	2.79	0.42
1:K:657:ALA:HA	1:K:661:LYS:O	2.19	0.42
1:P:49:GLN:H	1:P:49:GLN:CD	2.20	0.42
1:P:4:THR:CA	1:P:9:VAL:HG11	2.47	0.42
1:P:597:ASN:ND2	1:P:599:ARG:H	2.17	0.42
1:I:502:MET:HA	1:I:537:GLU:O	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:178:ARG:CB	1:O:178:ARG:HH11	2.33	0.42
1:L:778:THR:CG2	1:L:887:GLN:H	2.32	0.42
1:N:906:TYR:HB3	1:N:907:PRO:CD	2.50	0.42
1:K:256:VAL:O	1:K:271:THR:HA	2.20	0.42
1:P:85:VAL:HG12	1:P:86:VAL:N	2.34	0.42
1:L:141:ILE:HD13	1:L:143:PHE:CE1	2.55	0.42
1:N:69:VAL:HG12	1:N:70:PRO:N	2.35	0.42
1:J:93:HIS:HB3	1:J:95:TYR:HE1	1.84	0.42
1:L:829:THR:C	1:L:830:LEU:HD12	2.40	0.42
1:P:829:THR:C	1:P:830:LEU:HD12	2.40	0.42
1:I:829:THR:C	1:I:830:LEU:HD12	2.40	0.42
1:P:476:LYS:HD2	1:P:476:LYS:HA	1.81	0.42
1:K:670:LEU:HD23	1:K:670:LEU:HA	1.67	0.42
1:L:513:PRO:O	1:L:514:ALA:HB3	2.20	0.42
1:J:285:TYR:HB3	1:J:288:ARG:HG3	2.01	0.42
1:J:513:PRO:O	1:J:514:ALA:HB3	2.20	0.42
1:I:257:THR:HA	1:I:270:GLY:O	2.20	0.41
1:I:651:LEU:HA	1:I:651:LEU:HD13	1.51	0.41
1:P:114:VAL:HG21	1:P:192:SER:N	2.34	0.41
1:M:114:VAL:HG21	1:M:192:SER:N	2.34	0.41
1:P:34:ALA:HB3	1:P:36:TRP:CE3	2.54	0.41
1:J:138:GLN:N	1:J:217:LYS:O	2.36	0.41
1:N:34:ALA:HB3	1:N:36:TRP:CE3	2.54	0.41
1:K:24:LEU:HA	1:K:24:LEU:HD12	1.62	0.41
1:J:336:ARG:HH11	1:J:336:ARG:CG	2.26	0.41
1:K:579:ASP:OD1	1:K:583:ASN:N	2.43	0.41
1:O:673:ALA:O	1:O:676:GLY:N	2.47	0.41
1:L:900:LEU:HB2	1:L:939:CYS:O	2.20	0.41
1:P:800:ARG:CB	1:P:800:ARG:CZ	2.98	0.41
1:L:800:ARG:CZ	1:L:800:ARG:CB	2.98	0.41
1:P:178:ARG:CB	1:P:178:ARG:HH11	2.33	0.41
1:M:502:MET:HA	1:M:537:GLU:O	2.20	0.41
1:J:502:MET:HA	1:J:537:GLU:O	2.20	0.41
1:I:178:ARG:HH11	1:I:178:ARG:CB	2.33	0.41
1:P:502:MET:HA	1:P:537:GLU:O	2.20	0.41
1:K:502:MET:HA	1:K:537:GLU:O	2.20	0.41
1:J:645:ARG:NH2	1:J:650:GLU:OE2	2.48	0.41
1:N:73:TRP:O	1:N:183:ARG:NH1	2.48	0.41
1:I:570:TRP:HD1	1:I:571:VAL:HG22	1.84	0.41
1:J:718:GLN:HG3	1:J:719:GLN:N	2.34	0.41
1:K:350:LEU:HA	1:K:350:LEU:HD12	1.78	0.41
1:M:231:PHE:N	1:M:231:PHE:CD1	2.88	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:757:GLN:HG2	1:P:757:GLN:O	2.12	0.41
1:J:214:LEU:HA	1:J:214:LEU:HD23	1.84	0.41
1:K:202:MET:HE3	1:K:202:MET:HB3	1.85	0.41
1:M:200:GLN:OE1	1:M:200:GLN:N	2.44	0.41
1:O:378:LEU:HA	1:O:378:LEU:HD23	1.53	0.41
1:I:110:ASN:O	1:I:113:PHE:HB2	2.19	0.41
1:K:46:ARG:HB3	1:K:47:PRO:CD	2.50	0.41
1:O:46:ARG:HB3	1:O:47:PRO:CD	2.50	0.41
1:P:67:GLU:HG2	1:P:67:GLU:H	1.31	0.41
1:J:255:ARG:CG	1:J:255:ARG:NH1	2.79	0.41
1:K:685:LEU:HA	1:K:686:PRO:HD3	1.70	0.41
1:J:260:LEU:HD12	1:J:310:ARG:O	2.19	0.41
1:J:260:LEU:C	1:J:267:VAL:HG23	2.40	0.41
1:I:900:LEU:HD23	1:I:900:LEU:HA	1.75	0.41
1:J:237:ARG:NH1	1:J:237:ARG:CG	2.81	0.41
1:I:800:ARG:CB	1:I:800:ARG:CZ	2.98	0.41
1:M:234:ASP:OD1	1:M:236:SER:HB3	2.20	0.41
1:N:730:LEU:HA	1:N:731:PRO:HD3	1.74	0.41
1:M:778:THR:HG22	1:M:778:THR:O	2.20	0.41
1:I:1018:LEU:HD22	1:I:1019:VAL:N	2.35	0.41
1:J:425:ARG:HH22	1:K:287:ASP:CG	2.23	0.41
1:I:69:VAL:HG12	1:I:70:PRO:N	2.35	0.41
1:M:69:VAL:HA	1:M:70:PRO:HD2	1.77	0.41
1:O:147:ASN:HB2	1:O:165:SER:HB3	2.02	0.41
1:N:390:SER:HA	1:N:391:HIS:HA	1.91	0.41
1:J:368:ASP:O	1:J:369:GLU:C	2.58	0.41
1:J:363:HIS:N	1:J:363:HIS:CD2	2.81	0.41
1:L:617:LEU:HA	1:L:617:LEU:HD12	1.88	0.41
1:O:231:PHE:N	1:O:231:PHE:CD1	2.88	0.41
1:P:896:ASN:HA	1:P:918:TRP:O	2.21	0.41
1:I:257:THR:OG1	1:I:316:HIS:HE1	2.03	0.41
1:P:257:THR:HA	1:P:270:GLY:O	2.20	0.41
1:K:257:THR:HA	1:K:270:GLY:O	2.20	0.41
1:K:323:ILE:CD1	1:K:323:ILE:N	2.82	0.41
1:P:360:HIS:HA	1:P:361:PRO:HD3	1.86	0.41
1:O:668:VAL:HG13	1:O:669:PRO:CD	2.38	0.41
1:M:781:ARG:CG	1:M:781:ARG:NH1	2.79	0.41
1:O:822:LEU:HD12	1:O:823:LEU:H	1.80	0.41
1:M:62:TRP:C	1:M:63:PHE:CD1	2.93	0.41
1:I:655:MET:HE2	1:I:655:MET:C	2.41	0.41
1:I:763:GLY:HA3	1:I:822:LEU:HD22	2.01	0.41
1:O:24:LEU:HA	1:O:24:LEU:HD12	1.62	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:234:ASP:OD1	1:L:236:SER:HB3	2.20	0.41
1:P:900:LEU:HB2	1:P:939:CYS:O	2.21	0.41
1:O:237:ARG:CG	1:O:237:ARG:NH1	2.82	0.41
1:O:901:GLY:HA3	1:O:902:PRO:HA	1.86	0.41
1:K:597:ASN:ND2	1:K:599:ARG:H	2.17	0.41
1:L:256:VAL:O	1:L:271:THR:HA	2.20	0.41
1:P:778:THR:O	1:P:778:THR:HG22	2.20	0.41
1:I:778:THR:CG2	1:I:887:GLN:H	2.32	0.41
1:K:85:VAL:HG12	1:K:86:VAL:N	2.34	0.41
1:O:570:TRP:HD1	1:O:571:VAL:HG22	1.84	0.41
1:K:694:LEU:O	1:K:722:LEU:N	2.51	0.41
1:N:368:ASP:O	1:N:369:GLU:C	2.58	0.41
1:O:369:GLU:O	1:O:373:VAL:HG23	2.19	0.41
1:M:363:HIS:N	1:M:363:HIS:CD2	2.81	0.41
1:O:617:LEU:HD12	1:O:617:LEU:HA	1.88	0.41
1:J:353:GLY:C	1:J:566:PHE:HA	2.40	0.41
1:M:531:ARG:O	1:M:561:ARG:NH1	2.46	0.41
1:I:896:ASN:HA	1:I:918:TRP:O	2.21	0.41
1:M:285:TYR:HB3	1:M:288:ARG:HG3	2.01	0.41
1:M:421:VAL:O	1:M:425:ARG:NH1	2.46	0.41
1:P:18:ASN:OD1	1:P:19:PRO:HD2	2.20	0.41
1:N:46:ARG:HB3	1:N:47:PRO:CD	2.50	0.41
1:O:57:GLU:HG2	1:O:83:THR:HG21	1.94	0.41
1:I:583:ASN:HA	1:I:584:PRO:HD3	1.80	0.41
1:J:323:ILE:CD1	1:J:323:ILE:N	2.82	0.41
1:O:651:LEU:HD12	1:O:668:VAL:O	2.19	0.41
1:K:251:ARG:CB	1:K:253:TYR:CE2	2.98	0.41
1:M:1021:CME:HZ3	1:M:1022:GLN:O	2.19	0.41
1:O:763:GLY:HA3	1:O:822:LEU:HD22	2.01	0.41
1:L:62:TRP:C	1:L:63:PHE:CD1	2.93	0.41
1:K:114:VAL:HG21	1:K:192:SER:N	2.34	0.41
1:M:730:LEU:HD21	1:N:823:LEU:O	2.19	0.41
1:I:658:LEU:O	1:I:659:ASP:C	2.58	0.41
1:I:657:ALA:HA	1:I:661:LYS:O	2.19	0.41
1:O:49:GLN:NE2	1:O:49:GLN:N	2.64	0.41
1:O:78:LEU:HA	1:O:79:PRO:HD3	1.94	0.41
1:O:900:LEU:HB2	1:O:939:CYS:O	2.21	0.41
1:K:429:ASP:O	1:K:432:TRP:N	2.44	0.41
1:M:85:VAL:HG12	1:M:86:VAL:N	2.34	0.41
1:L:85:VAL:HG12	1:L:86:VAL:N	2.34	0.41
1:L:69:VAL:HG12	1:L:70:PRO:N	2.35	0.41
1:P:694:LEU:O	1:P:722:LEU:N	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:368:ASP:O	1:K:369:GLU:C	2.58	0.41
1:K:513:PRO:O	1:K:514:ALA:HB3	2.20	0.41
1:M:391:HIS:ND1	1:M:412:GLU:OE1	2.44	0.41
1:O:874:SER:HB3	1:P:724:GLU:OE1	2.20	0.41
1:M:368:ASP:O	1:M:369:GLU:C	2.58	0.41
1:J:391:HIS:ND1	1:J:412:GLU:OE1	2.44	0.41
1:P:668:VAL:HG13	1:P:669:PRO:CD	2.38	0.41
1:P:361:PRO:HB2	1:P:576:ILE:HD12	2.03	0.41
1:N:822:LEU:C	1:N:822:LEU:HD12	2.37	0.41
1:K:260:LEU:C	1:K:267:VAL:HG23	2.40	0.41
1:L:260:LEU:C	1:L:267:VAL:HG23	2.40	0.41
1:K:696:LEU:CD1	1:K:697:THR:N	2.80	0.41
1:L:49:GLN:N	1:L:49:GLN:NE2	2.64	0.41
1:L:78:LEU:CB	1:L:79:PRO:CD	2.99	0.41
1:K:583:ASN:HA	1:K:584:PRO:HD3	1.79	0.41
1:J:658:LEU:O	1:J:659:ASP:C	2.58	0.41
1:P:234:ASP:OD1	1:P:236:SER:HB3	2.20	0.41
1:N:597:ASN:ND2	1:N:599:ARG:H	2.17	0.41
1:L:178:ARG:HH11	1:L:178:ARG:CB	2.33	0.41
1:P:645:ARG:NH2	1:P:650:GLU:CD	2.74	0.41
1:O:645:ARG:NH2	1:O:650:GLU:CD	2.74	0.41
1:J:778:THR:O	1:J:778:THR:HG22	2.20	0.41
1:P:69:VAL:HG12	1:P:70:PRO:N	2.35	0.41
1:O:608:PHE:O	1:O:611:ARG:N	2.41	0.41
1:I:679:LEU:HA	1:I:679:LEU:HD23	1.26	0.41
1:M:369:GLU:O	1:M:373:VAL:HG23	2.19	0.41
1:K:391:HIS:ND1	1:K:412:GLU:OE1	2.44	0.41
1:I:378:LEU:HA	1:I:378:LEU:HD23	1.53	0.41
1:P:922:LEU:HD12	1:P:922:LEU:HA	1.87	0.41
1:K:363:HIS:CD2	1:K:363:HIS:N	2.81	0.41
1:J:857:ARG:HG2	1:J:857:ARG:HH11	1.86	0.41
1:J:740:LEU:CD1	1:J:741:THR:N	2.80	0.41
1:I:740:LEU:CD1	1:I:741:THR:N	2.80	0.41
1:P:745:MET:HE3	1:P:745:MET:N	2.35	0.41
1:M:436:MET:HE1	1:M:467:ASN:HB2	2.02	0.41
1:N:18:ASN:OD1	1:N:19:PRO:HD2	2.20	0.41
1:I:323:ILE:N	1:I:323:ILE:CD1	2.82	0.41
1:I:361:PRO:HB2	1:I:576:ILE:HD12	2.03	0.41
1:L:763:GLY:HA3	1:L:822:LEU:HD22	2.01	0.41
1:N:62:TRP:C	1:N:63:PHE:CD1	2.93	0.41
1:P:655:MET:C	1:P:655:MET:HE2	2.41	0.41
1:M:24:LEU:HA	1:M:24:LEU:HD12	1.62	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:34:ALA:HB3	1:M:36:TRP:CE3	2.54	0.41
1:P:595:THR:CG2	1:P:596:PRO:HA	2.46	0.41
1:M:347:LYS:HA	1:M:348:PRO:HD3	1.77	0.41
1:I:597:ASN:ND2	1:I:599:ARG:H	2.17	0.41
1:L:502:MET:HA	1:L:537:GLU:O	2.20	0.41
1:M:134:LEU:CD1	1:M:179:ALA:HA	2.51	0.41
1:I:906:TYR:HB3	1:I:907:PRO:CD	2.50	0.41
1:L:134:LEU:CD1	1:L:179:ALA:HA	2.51	0.41
1:J:69:VAL:HG12	1:J:70:PRO:N	2.35	0.41
1:J:922:LEU:HA	1:J:922:LEU:HD12	1.87	0.41
1:O:857:ARG:HG2	1:O:857:ARG:HH11	1.86	0.41
1:I:231:PHE:CD1	1:I:231:PHE:N	2.88	0.41
1:M:513:PRO:O	1:M:514:ALA:HB3	2.20	0.41
1:J:668:VAL:HG13	1:J:669:PRO:CD	2.38	0.41
1:I:46:ARG:HB3	1:I:47:PRO:CD	2.50	0.41
1:O:361:PRO:HB2	1:O:576:ILE:HD12	2.03	0.41
1:N:251:ARG:CB	1:N:253:TYR:CE2	2.98	0.41
1:M:227:VAL:CG1	1:M:240:LEU:HD11	2.42	0.41
1:I:822:LEU:HD12	1:I:823:LEU:H	1.80	0.41
1:K:658:LEU:O	1:K:659:ASP:C	2.58	0.41
1:K:49:GLN:NE2	1:K:49:GLN:N	2.64	0.41
1:M:78:LEU:CB	1:M:79:PRO:CD	2.99	0.41
1:M:900:LEU:HB2	1:M:939:CYS:O	2.21	0.41
1:I:900:LEU:HB2	1:I:939:CYS:O	2.20	0.41
1:N:347:LYS:CB	1:N:348:PRO:HD2	2.43	0.41
1:O:502:MET:HA	1:O:537:GLU:O	2.20	0.41
1:N:85:VAL:HG12	1:N:86:VAL:N	2.34	0.41
1:J:807:VAL:HG13	1:J:808:GLU:N	2.34	0.41
1:J:608:PHE:O	1:J:611:ARG:N	2.41	0.41
1:J:559:TYR:HA	1:J:560:PRO:HD2	1.73	0.41
1:L:570:TRP:HD1	1:L:571:VAL:HG22	1.84	0.41
1:P:612:THR:HA	1:P:613:PRO:HD3	1.68	0.41
1:N:93:HIS:HB3	1:N:95:TYR:HE1	1.84	0.41
1:N:647:SER:OG	1:N:672:VAL:N	2.35	0.41
1:O:51:LEU:HA	1:O:51:LEU:HD12	1.84	0.41
1:P:231:PHE:N	1:P:231:PHE:CD1	2.88	0.41
1:L:147:ASN:HB2	1:L:165:SER:HB3	2.01	0.41
1:N:896:ASN:HA	1:N:918:TRP:O	2.21	0.41
1:J:46:ARG:HB3	1:J:47:PRO:CD	2.50	0.41
1:P:323:ILE:CD1	1:P:323:ILE:N	2.82	0.41
1:O:257:THR:HA	1:O:270:GLY:O	2.20	0.41
1:L:227:VAL:CG1	1:L:240:LEU:HD11	2.42	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:65:ALA:CB	1:K:66:PRO:CD	2.99	0.41
1:J:282:ARG:NH1	1:K:419:GLY:HA2	2.36	0.41
1:M:31:PRO:HA	1:M:32:PRO:HD3	1.88	0.41
1:K:344:LEU:N	1:K:347:LYS:O	2.36	0.41
1:N:502:MET:HA	1:N:537:GLU:O	2.20	0.41
1:I:256:VAL:O	1:I:271:THR:HA	2.20	0.41
1:K:429:ASP:OD2	1:K:431:ARG:NH1	2.54	0.41
1:O:429:ASP:OD1	1:O:431:ARG:N	2.51	0.41
1:P:570:TRP:HD1	1:P:571:VAL:HG22	1.84	0.41
1:N:445:GLN:HE21	1:N:445:GLN:HB3	1.54	0.41
1:J:147:ASN:HB2	1:J:165:SER:HB3	2.02	0.41
1:I:147:ASN:HB2	1:I:165:SER:HB3	2.02	0.41
1:I:368:ASP:O	1:I:369:GLU:C	2.58	0.41
1:L:373:VAL:O	1:L:374:GLN:C	2.57	0.41
1:O:772:ASP:N	1:O:772:ASP:OD1	2.30	0.41
1:P:202:MET:HB3	1:P:202:MET:HE3	1.84	0.41
1:O:745:MET:CE	1:O:745:MET:CA	2.99	0.41
1:M:668:VAL:HG13	1:M:669:PRO:CD	2.38	0.41
1:J:18:ASN:OD1	1:J:19:PRO:HD2	2.20	0.41
1:P:257:THR:OG1	1:P:316:HIS:HE1	2.03	0.41
1:N:257:THR:HA	1:N:270:GLY:O	2.20	0.41
1:J:7:LEU:O	1:J:8:ALA:C	2.55	0.41
1:J:257:THR:HA	1:J:270:GLY:O	2.20	0.41
1:J:361:PRO:HB2	1:J:576:ILE:HD12	2.03	0.41
1:N:361:PRO:HB2	1:N:576:ILE:HD12	2.03	0.41
1:N:360:HIS:ND1	1:N:362:LEU:HB2	2.35	0.41
1:P:255:ARG:CG	1:P:255:ARG:NH1	2.79	0.41
1:J:655:MET:HG3	1:J:655:MET:O	2.21	0.41
1:N:655:MET:HE2	1:N:655:MET:C	2.41	0.41
1:I:823:LEU:HA	1:I:823:LEU:HD23	1.73	0.41
1:L:655:MET:C	1:L:655:MET:HE2	2.42	0.41
1:L:655:MET:O	1:L:655:MET:HG3	2.21	0.41
1:K:34:ALA:HB3	1:K:36:TRP:CE3	2.54	0.41
1:M:260:LEU:C	1:M:267:VAL:HG23	2.40	0.41
1:L:702:GLN:HA	1:L:703:PRO:HD2	1.84	0.41
1:N:673:ALA:O	1:N:676:GLY:N	2.47	0.41
1:M:377:LEU:HA	1:M:377:LEU:HD23	1.90	0.41
1:J:234:ASP:OD1	1:J:236:SER:HB3	2.20	0.41
1:N:800:ARG:CZ	1:N:800:ARG:CB	2.98	0.41
1:I:234:ASP:OD1	1:I:236:SER:HB3	2.20	0.41
1:P:184:LEU:HA	1:P:184:LEU:HD23	1.84	0.41
1:I:265:THR:HG22	1:I:266:GLN:N	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:906:TYR:HB3	1:J:907:PRO:CD	2.50	0.41
1:L:645:ARG:NH2	1:L:650:GLU:CD	2.74	0.41
1:O:778:THR:CG2	1:O:887:GLN:H	2.32	0.41
1:P:403:ASP:CG	1:P:451:PRO:HD2	2.41	0.41
1:L:429:ASP:OD1	1:L:431:ARG:N	2.51	0.41
1:K:403:ASP:CG	1:K:451:PRO:HD2	2.41	0.41
1:J:1018:LEU:HD23	1:J:1018:LEU:HA	1.51	0.41
1:K:1018:LEU:HD22	1:K:1019:VAL:N	2.35	0.41
1:J:141:ILE:HG12	1:J:142:ILE:H	1.86	0.41
1:M:69:VAL:HG12	1:M:70:PRO:N	2.35	0.41
1:K:141:ILE:HG12	1:K:142:ILE:H	1.86	0.41
1:N:570:TRP:HD1	1:N:571:VAL:HG22	1.84	0.41
1:J:445:GLN:HB3	1:J:445:GLN:HE21	1.54	0.41
1:N:829:THR:C	1:N:830:LEU:HD12	2.40	0.41
1:L:231:PHE:N	1:L:231:PHE:CD1	2.88	0.41
1:L:546:LEU:HD12	1:L:546:LEU:HA	1.84	0.41
1:K:857:ARG:HG2	1:K:857:ARG:HH11	1.86	0.41
1:O:471:LEU:HA	1:O:471:LEU:HD23	1.85	0.41
1:J:202:MET:HE3	1:J:202:MET:HB3	1.82	0.41
1:N:363:HIS:N	1:N:363:HIS:CD2	2.81	0.41
1:M:857:ARG:HG2	1:M:857:ARG:HH11	1.86	0.41
1:L:896:ASN:HA	1:L:918:TRP:O	2.21	0.41
1:I:647:SER:OG	1:I:672:VAL:N	2.35	0.41
1:I:745:MET:CA	1:I:745:MET:CE	2.99	0.41
1:L:745:MET:CA	1:L:745:MET:CE	2.99	0.41
1:L:102:ASN:ND2	1:L:201:ASP:CB	2.78	0.41
1:N:257:THR:OG1	1:N:316:HIS:HE1	2.03	0.41
1:M:257:THR:HA	1:M:270:GLY:O	2.20	0.41
1:P:46:ARG:HB3	1:P:47:PRO:CD	2.50	0.41
1:K:66:PRO:CB	1:K:187:MET:CE	2.99	0.41
1:K:230:ARG:O	1:K:238:ALA:HA	2.21	0.41
1:L:822:LEU:C	1:L:822:LEU:HD12	2.37	0.41
1:P:701:VAL:CG1	1:P:702:GLN:N	2.81	0.41
1:O:78:LEU:CB	1:O:79:PRO:CD	2.99	0.41
1:P:658:LEU:HA	1:P:658:LEU:HD12	1.83	0.41
1:N:31:PRO:HA	1:N:32:PRO:HD3	1.88	0.41
1:K:234:ASP:OD1	1:K:236:SER:HB3	2.20	0.41
1:O:234:ASP:OD1	1:O:236:SER:N	2.54	0.41
1:L:265:THR:HG22	1:L:266:GLN:N	2.36	0.41
1:N:429:ASP:OD2	1:N:431:ARG:NH1	2.54	0.41
1:J:403:ASP:CG	1:J:451:PRO:HD2	2.41	0.41
1:K:69:VAL:HG12	1:K:70:PRO:N	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:70:PRO:O	1:O:73:TRP:N	2.45	0.41
1:M:407:LEU:HA	1:M:407:LEU:HD23	1.89	0.41
1:M:373:VAL:O	1:M:374:GLN:C	2.57	0.41
1:J:694:LEU:HD12	1:J:694:LEU:HA	1.69	0.41
1:L:105:TYR:CE2	1:L:199:ASP:HB2	2.56	0.41
1:P:513:PRO:O	1:P:514:ALA:HB3	2.20	0.41
1:P:745:MET:CE	1:P:745:MET:CA	2.99	0.40
1:N:316:HIS:HA	1:N:323:ILE:HD12	1.99	0.40
1:I:18:ASN:OD1	1:I:19:PRO:HD2	2.20	0.40
1:P:360:HIS:ND1	1:P:362:LEU:HB2	2.35	0.40
1:M:230:ARG:O	1:M:238:ALA:HA	2.22	0.40
1:J:66:PRO:CB	1:J:187:MET:CE	2.99	0.40
1:O:655:MET:O	1:O:655:MET:HG3	2.21	0.40
1:J:395:HIS:CE1	1:J:397:LEU:HB3	2.57	0.40
1:M:858:ILE:HG12	1:M:864:MET:HG3	2.03	0.40
1:O:701:VAL:HG12	1:O:702:GLN:H	1.83	0.40
1:K:49:GLN:CD	1:K:49:GLN:H	2.20	0.40
1:P:856:TYR:HD2	1:P:864:MET:CE	2.25	0.40
1:J:900:LEU:HB2	1:J:939:CYS:O	2.21	0.40
1:I:599:ARG:HB2	1:I:600:GLN:H	1.40	0.40
1:K:178:ARG:HH11	1:K:178:ARG:CB	2.33	0.40
1:L:429:ASP:OD2	1:L:431:ARG:NH1	2.54	0.40
1:I:403:ASP:CG	1:I:451:PRO:HD2	2.41	0.40
1:I:134:LEU:HD21	1:I:177:LEU:HB2	2.03	0.40
1:O:69:VAL:HG12	1:O:70:PRO:N	2.35	0.40
1:L:679:LEU:HD23	1:L:679:LEU:HA	1.26	0.40
1:L:147:ASN:HA	1:L:148:SER:HA	1.54	0.40
1:P:857:ARG:HH11	1:P:857:ARG:HG2	1.86	0.40
1:K:482:ARG:HH11	1:K:482:ARG:HD2	1.71	0.40
1:N:513:PRO:O	1:N:514:ALA:HB3	2.20	0.40
1:O:878:HIS:HA	1:O:879:PRO:HD3	1.66	0.40
1:N:279:ILE:HD11	1:O:424:ASN:OD1	2.21	0.40
1:O:242:ALA:O	1:O:290:THR:HA	2.22	0.40
1:P:749:ILE:CD1	1:P:749:ILE:N	2.78	0.40
1:I:436:MET:HE1	1:I:467:ASN:HB2	2.03	0.40
1:M:323:ILE:N	1:M:323:ILE:CD1	2.82	0.40
1:L:360:HIS:ND1	1:L:362:LEU:HB2	2.35	0.40
1:O:227:VAL:CG1	1:O:240:LEU:HD11	2.42	0.40
1:L:230:ARG:O	1:L:238:ALA:HA	2.21	0.40
1:I:655:MET:HG3	1:I:655:MET:O	2.21	0.40
1:N:822:LEU:HD12	1:N:823:LEU:H	1.80	0.40
1:L:395:HIS:CE1	1:L:397:LEU:HB3	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:631:LEU:HA	1:P:631:LEU:HD12	1.81	0.40
1:K:246:MET:HB3	1:K:274:PHE:CZ	2.57	0.40
1:L:234:ASP:OD1	1:L:236:SER:N	2.54	0.40
1:J:246:MET:HB3	1:J:274:PHE:CZ	2.57	0.40
1:J:134:LEU:CD1	1:J:179:ALA:HA	2.51	0.40
1:N:265:THR:HG22	1:N:266:GLN:N	2.36	0.40
1:M:272:ALA:HA	1:M:273:PRO:HD3	1.76	0.40
1:P:429:ASP:OD2	1:P:431:ARG:NH1	2.54	0.40
1:O:134:LEU:HD21	1:O:177:LEU:HB2	2.04	0.40
1:O:906:TYR:HB3	1:O:907:PRO:CD	2.50	0.40
1:L:134:LEU:HD21	1:L:177:LEU:HB2	2.04	0.40
1:P:134:LEU:CD1	1:P:179:ALA:HA	2.51	0.40
1:I:134:LEU:CD1	1:I:179:ALA:HA	2.51	0.40
1:O:69:VAL:HA	1:O:70:PRO:HD2	1.77	0.40
1:K:570:TRP:HD1	1:K:571:VAL:HG22	1.84	0.40
1:I:373:VAL:O	1:I:374:GLN:C	2.57	0.40
1:N:407:LEU:HA	1:N:407:LEU:HD23	1.89	0.40
1:O:368:ASP:O	1:O:369:GLU:C	2.58	0.40
1:K:896:ASN:HA	1:K:918:TRP:O	2.21	0.40
1:N:857:ARG:HG2	1:N:857:ARG:HH11	1.86	0.40
1:J:896:ASN:HA	1:J:918:TRP:O	2.21	0.40
1:P:105:TYR:CE2	1:P:199:ASP:HB2	2.57	0.40
1:J:479:ASP:HA	1:J:480:PRO:HD2	1.61	0.40
1:O:513:PRO:O	1:O:514:ALA:HB3	2.20	0.40
1:O:531:ARG:O	1:O:561:ARG:NH1	2.46	0.40
1:N:745:MET:CE	1:N:745:MET:CA	2.99	0.40
1:M:745:MET:CA	1:M:745:MET:CE	2.99	0.40
1:M:46:ARG:HB3	1:M:47:PRO:CD	2.50	0.40
1:P:583:ASN:HA	1:P:584:PRO:HD3	1.79	0.40
1:M:361:PRO:HB2	1:M:576:ILE:HD12	2.03	0.40
1:I:67:GLU:H	1:I:67:GLU:HG2	1.31	0.40
1:P:655:MET:HB2	1:P:655:MET:HE3	1.94	0.40
1:O:655:MET:HE2	1:O:655:MET:C	2.41	0.40
1:M:655:MET:O	1:M:655:MET:HG3	2.21	0.40
1:N:395:HIS:CE1	1:N:397:LEU:HB3	2.56	0.40
1:I:395:HIS:CE1	1:I:397:LEU:HB3	2.56	0.40
1:I:702:GLN:HA	1:I:703:PRO:HD2	1.84	0.40
1:N:858:ILE:HG12	1:N:864:MET:HG3	2.03	0.40
1:I:282:ARG:HH11	1:L:419:GLY:CA	2.34	0.40
1:N:246:MET:HB3	1:N:274:PHE:CZ	2.57	0.40
1:P:6:SER:OG	1:P:9:VAL:HB	2.22	0.40
1:L:272:ALA:CB	1:L:273:PRO:CD	2.99	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:178:ARG:HH11	1:N:178:ARG:CB	2.33	0.40
1:P:778:THR:HB	1:P:887:GLN:CB	2.48	0.40
1:J:73:TRP:O	1:J:183:ARG:NH1	2.48	0.40
1:O:390:SER:HA	1:O:391:HIS:HA	1.91	0.40
1:N:679:LEU:HD23	1:N:679:LEU:HA	1.26	0.40
1:J:231:PHE:N	1:J:231:PHE:CD1	2.88	0.40
1:K:740:LEU:CD1	1:K:741:THR:N	2.80	0.40
1:N:102:ASN:ND2	1:N:201:ASP:CB	2.78	0.40
1:K:360:HIS:HA	1:K:361:PRO:HD3	1.86	0.40
1:K:92:MET:HE3	1:K:362:LEU:O	2.21	0.40
1:J:240:LEU:HD12	1:J:240:LEU:C	2.36	0.40
1:K:254:LEU:O	1:K:255:ARG:NH1	2.54	0.40
1:M:763:GLY:HA3	1:M:822:LEU:HD22	2.01	0.40
1:I:685:LEU:HA	1:I:686:PRO:HD3	1.70	0.40
1:O:395:HIS:CE1	1:O:397:LEU:HB3	2.56	0.40
1:I:37:ARG:HD3	1:I:37:ARG:N	2.36	0.40
1:M:6:SER:OG	1:M:9:VAL:HB	2.22	0.40
1:N:901:GLY:HA3	1:N:902:PRO:HA	1.86	0.40
1:N:6:SER:OG	1:N:9:VAL:HB	2.22	0.40
1:L:421:VAL:O	1:L:425:ARG:NH1	2.46	0.40
1:K:645:ARG:NH2	1:K:650:GLU:CD	2.74	0.40
1:N:778:THR:HG22	1:N:778:THR:O	2.20	0.40
1:M:282:ARG:HD3	1:P:420:MET:O	2.21	0.40
1:K:134:LEU:CD1	1:K:179:ALA:HA	2.51	0.40
1:I:390:SER:HA	1:I:391:HIS:HA	1.91	0.40
1:O:722:LEU:HA	1:O:722:LEU:HD23	1.75	0.40
1:O:896:ASN:HA	1:O:918:TRP:O	2.21	0.40
1:L:817:GLN:HE21	1:L:817:GLN:HB3	1.63	0.40
1:L:728:VAL:HG22	1:L:728:VAL:H	1.62	0.40
1:K:231:PHE:CD1	1:K:231:PHE:N	2.88	0.40
1:J:242:ALA:O	1:J:290:THR:HA	2.22	0.40
1:K:745:MET:CE	1:K:745:MET:CA	2.99	0.40
1:J:102:ASN:ND2	1:J:201:ASP:CB	2.78	0.40
1:K:651:LEU:HA	1:K:651:LEU:HD13	1.51	0.40
1:N:230:ARG:O	1:N:238:ALA:HA	2.21	0.40
1:I:66:PRO:CB	1:I:187:MET:CE	2.99	0.40
1:L:66:PRO:CB	1:L:187:MET:CE	2.99	0.40
1:O:66:PRO:CB	1:O:187:MET:CE	2.99	0.40
1:K:822:LEU:HD12	1:K:822:LEU:C	2.37	0.40
1:K:822:LEU:HD12	1:K:823:LEU:H	1.80	0.40
1:I:254:LEU:O	1:I:255:ARG:NH1	2.54	0.40
1:L:37:ARG:N	1:L:37:ARG:HD3	2.36	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:377:LEU:HD23	1:J:377:LEU:HA	1.90	0.40
1:K:900:LEU:HB2	1:K:939:CYS:O	2.21	0.40
1:M:246:MET:HB3	1:M:274:PHE:CZ	2.57	0.40
1:M:178:ARG:CB	1:M:178:ARG:HH11	2.33	0.40
1:J:429:ASP:O	1:J:432:TRP:N	2.44	0.40
1:J:429:ASP:OD2	1:J:431:ARG:NH1	2.54	0.40
1:L:906:TYR:HB3	1:L:907:PRO:CD	2.50	0.40
1:M:48:SER:OG	1:M:50:GLN:HG2	2.22	0.40
1:M:570:TRP:HD1	1:M:571:VAL:HG22	1.84	0.40
1:P:368:ASP:O	1:P:369:GLU:C	2.58	0.40
1:J:722:LEU:HA	1:J:722:LEU:HD23	1.75	0.40
1:J:817:GLN:HE21	1:J:817:GLN:HB3	1.63	0.40
1:I:202:MET:HB3	1:I:202:MET:HE3	1.85	0.40
1:N:231:PHE:N	1:N:231:PHE:CD1	2.88	0.40
1:M:721:ARG:HB3	1:M:721:ARG:HE	1.69	0.40
1:N:817:GLN:HE21	1:N:817:GLN:HB3	1.63	0.40
1:M:147:ASN:HB2	1:M:165:SER:HB3	2.02	0.40
1:M:242:ALA:O	1:M:290:THR:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	25	55
1	J	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	25	55
1	K	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	25	55
1	L	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	25	55
1	M	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	25	55
1	N	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	25	55
1	O	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	25	55
1	P	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	25	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	8144/8184 (100%)	7648 (94%)	424 (5%)	72 (1%)	25	55

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	174	SER
1	J	174	SER
1	K	174	SER
1	L	174	SER
1	M	174	SER
1	N	174	SER
1	O	174	SER
1	P	174	SER
1	I	46	ARG
1	I	164	ASP
1	I	461	GLU
1	J	46	ARG
1	J	164	ASP
1	J	461	GLU
1	K	46	ARG
1	K	164	ASP
1	K	461	GLU
1	L	46	ARG
1	L	164	ASP
1	L	461	GLU
1	M	46	ARG
1	M	164	ASP
1	M	461	GLU
1	N	46	ARG
1	N	164	ASP
1	N	461	GLU
1	O	46	ARG
1	O	164	ASP
1	O	461	GLU
1	P	46	ARG
1	P	164	ASP
1	P	461	GLU
1	I	647	SER
1	J	647	SER
1	K	647	SER
1	L	647	SER
1	M	647	SER

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Mol	Chain	Res	Type
1	M	690	SER
1	N	647	SER
1	O	647	SER
1	P	647	SER
1	I	47	PRO
1	I	70	PRO
1	I	690	SER
1	J	47	PRO
1	J	70	PRO
1	J	690	SER
1	K	47	PRO
1	K	70	PRO
1	K	690	SER
1	L	47	PRO
1	L	70	PRO
1	L	690	SER
1	M	47	PRO
1	M	70	PRO
1	N	47	PRO
1	N	70	PRO
1	N	690	SER
1	O	47	PRO
1	O	70	PRO
1	O	690	SER
1	P	47	PRO
1	P	70	PRO
1	P	690	SER
1	I	79	PRO
1	J	79	PRO
1	K	79	PRO
1	L	79	PRO
1	M	79	PRO
1	N	79	PRO
1	O	79	PRO
1	P	79	PRO

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	I	872/872 (100%)	759 (87%)	113 (13%)	6	15
1	J	872/872 (100%)	759 (87%)	113 (13%)	6	15
1	K	872/872 (100%)	759 (87%)	113 (13%)	6	15
1	L	872/872 (100%)	759 (87%)	113 (13%)	6	15
1	M	872/872 (100%)	759 (87%)	113 (13%)	6	15
1	N	872/872 (100%)	759 (87%)	113 (13%)	6	15
1	O	872/872 (100%)	759 (87%)	113 (13%)	6	15
1	P	872/872 (100%)	759 (87%)	113 (13%)	6	15
All	All	6976/6976 (100%)	6072 (87%)	904 (13%)	6	15

All (904) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	3	ILE
1	I	9	VAL
1	I	13	ARG
1	I	24	LEU
1	I	37	ARG
1	I	38	ASN
1	I	39	SER
1	I	43	ARG
1	I	48	SER
1	I	49	GLN
1	I	50	GLN
1	I	52	ARG
1	I	57	GLU
1	I	67	GLU
1	I	71	GLU
1	I	72	SER
1	I	77	ASP
1	I	80	GLU
1	I	90	TRP
1	I	102	ASN
1	I	116	THR
1	I	124	SER
1	I	125	LEU
1	I	128	ASN
1	I	136	GLU
1	I	141	ILE
1	I	165	SER

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Mol	Chain	Res	Type
1	I	178	ARG
1	I	189	LEU
1	I	190	ARG
1	I	202	MET
1	I	211	ASP
1	I	213	SER
1	I	219	THR
1	I	237	ARG
1	I	246	MET
1	I	247	CYS
1	I	250	LEU
1	I	259	SER
1	I	264	GLU
1	I	267	VAL
1	I	277	GLU
1	I	279	ILE
1	I	282	ARG
1	I	299	LYS
1	I	310	ARG
1	I	312	VAL
1	I	314	GLU
1	I	333	ARG
1	I	336	ARG
1	I	347	LYS
1	I	370	GLN
1	I	425	ARG
1	I	437	SER
1	I	445	GLN
1	I	448	ARG
1	I	461	GLU
1	I	473	ARG
1	I	477	SER
1	I	482	ARG
1	I	494	THR
1	I	519	SER
1	I	521	LYS
1	I	533	LEU
1	I	546	LEU
1	I	554	GLN
1	I	571	VAL
1	I	581	ASN
1	I	599	ARG

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Mol	Chain	Res	Type
1	I	600	GLN
1	I	630	ARG
1	I	635	THR
1	I	651	LEU
1	I	652	LEU
1	I	655	MET
1	I	661	LYS
1	I	665	SER
1	I	672	VAL
1	I	675	GLN
1	I	681	GLU
1	I	684	GLU
1	I	690	SER
1	I	719	GLN
1	I	730	LEU
1	I	734	SER
1	I	743	SER
1	I	749	ILE
1	I	755	ARG
1	I	768	MET
1	I	773	LYS
1	I	778	THR
1	I	781	ARG
1	I	797	GLU
1	I	799	THR
1	I	800	ARG
1	I	801	ILE
1	I	804	ASN
1	I	809	ARG
1	I	822	LEU
1	I	824	GLN
1	I	832	ASP
1	I	837	THR
1	I	857	ARG
1	I	867	THR
1	I	881	ARG
1	I	903[A]	GLN
1	I	903[B]	GLN
1	I	917	ARG
1	I	938	ARG
1	I	956	GLN
1	I	961	ARG

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Mol	Chain	Res	Type
1	I	1006	GLU
1	I	1018	LEU
1	J	3	ILE
1	J	9	VAL
1	J	13	ARG
1	J	24	LEU
1	J	37	ARG
1	J	38	ASN
1	J	39	SER
1	J	43	ARG
1	J	48	SER
1	J	49	GLN
1	J	50	GLN
1	J	52	ARG
1	J	57	GLU
1	J	67	GLU
1	J	71	GLU
1	J	72	SER
1	J	77	ASP
1	J	80	GLU
1	J	90	TRP
1	J	102	ASN
1	J	116	THR
1	J	124	SER
1	J	125	LEU
1	J	128	ASN
1	J	136	GLU
1	J	141	ILE
1	J	165	SER
1	J	178	ARG
1	J	189	LEU
1	J	190	ARG
1	J	202	MET
1	J	211	ASP
1	J	213	SER
1	J	219	THR
1	J	237	ARG
1	J	246	MET
1	J	247	CYS
1	J	250	LEU
1	J	259	SER
1	J	264	GLU

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Mol	Chain	Res	Type
1	J	267	VAL
1	J	277	GLU
1	J	279	ILE
1	J	282	ARG
1	J	299	LYS
1	J	310	ARG
1	J	312	VAL
1	J	314	GLU
1	J	333	ARG
1	J	336	ARG
1	J	347	LYS
1	J	370	GLN
1	J	425	ARG
1	J	437	SER
1	J	445	GLN
1	J	448	ARG
1	J	461	GLU
1	J	473	ARG
1	J	477	SER
1	J	482	ARG
1	J	494	THR
1	J	519	SER
1	J	521	LYS
1	J	533	LEU
1	J	546	LEU
1	J	554	GLN
1	J	571	VAL
1	J	581	ASN
1	J	599	ARG
1	J	600	GLN
1	J	630	ARG
1	J	635	THR
1	J	651	LEU
1	J	652	LEU
1	J	655	MET
1	J	661	LYS
1	J	665	SER
1	J	672	VAL
1	J	675	GLN
1	J	681	GLU
1	J	684	GLU
1	J	690	SER

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Mol	Chain	Res	Type
1	J	719	GLN
1	J	730	LEU
1	J	734	SER
1	J	743	SER
1	J	749	ILE
1	J	755	ARG
1	J	768	MET
1	J	773	LYS
1	J	778	THR
1	J	781	ARG
1	J	797	GLU
1	J	799	THR
1	J	800	ARG
1	J	801	ILE
1	J	804	ASN
1	J	809	ARG
1	J	822	LEU
1	J	824	GLN
1	J	832	ASP
1	J	837	THR
1	J	857	ARG
1	J	867	THR
1	J	881	ARG
1	J	903[A]	GLN
1	J	903[B]	GLN
1	J	917	ARG
1	J	938	ARG
1	J	956	GLN
1	J	961	ARG
1	J	1006	GLU
1	J	1018	LEU
1	K	3	ILE
1	K	9	VAL
1	K	13	ARG
1	K	24	LEU
1	K	37	ARG
1	K	38	ASN
1	K	39	SER
1	K	43	ARG
1	K	48	SER
1	K	49	GLN
1	K	50	GLN

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Mol	Chain	Res	Type
1	K	52	ARG
1	K	57	GLU
1	K	67	GLU
1	K	71	GLU
1	K	72	SER
1	K	77	ASP
1	K	80	GLU
1	K	90	TRP
1	K	102	ASN
1	K	116	THR
1	K	124	SER
1	K	125	LEU
1	K	128	ASN
1	K	136	GLU
1	K	141	ILE
1	K	165	SER
1	K	178	ARG
1	K	189	LEU
1	K	190	ARG
1	K	202	MET
1	K	211	ASP
1	K	213	SER
1	K	219	THR
1	K	237	ARG
1	K	246	MET
1	K	247	CYS
1	K	250	LEU
1	K	259	SER
1	K	264	GLU
1	K	267	VAL
1	K	277	GLU
1	K	279	ILE
1	K	282	ARG
1	K	299	LYS
1	K	310	ARG
1	K	312	VAL
1	K	314	GLU
1	K	333	ARG
1	K	336	ARG
1	K	347	LYS
1	K	370	GLN
1	K	425	ARG

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Mol	Chain	Res	Type
1	K	437	SER
1	K	445	GLN
1	K	448	ARG
1	K	461	GLU
1	K	473	ARG
1	K	477	SER
1	K	482	ARG
1	K	494	THR
1	K	519	SER
1	K	521	LYS
1	K	533	LEU
1	K	546	LEU
1	K	554	GLN
1	K	571	VAL
1	K	581	ASN
1	K	599	ARG
1	K	600	GLN
1	K	630	ARG
1	K	635	THR
1	K	651	LEU
1	K	652	LEU
1	K	655	MET
1	K	661	LYS
1	K	665	SER
1	K	672	VAL
1	K	675	GLN
1	K	681	GLU
1	K	684	GLU
1	K	690	SER
1	K	719	GLN
1	K	730	LEU
1	K	734	SER
1	K	743	SER
1	K	749	ILE
1	K	755	ARG
1	K	768	MET
1	K	773	LYS
1	K	778	THR
1	K	781	ARG
1	K	797	GLU
1	K	799	THR
1	K	800	ARG

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Mol	Chain	Res	Type
1	K	801	ILE
1	K	804	ASN
1	K	809	ARG
1	K	822	LEU
1	K	824	GLN
1	K	832	ASP
1	K	837	THR
1	K	857	ARG
1	K	867	THR
1	K	881	ARG
1	K	903[A]	GLN
1	K	903[B]	GLN
1	K	917	ARG
1	K	938	ARG
1	K	956	GLN
1	K	961	ARG
1	K	1006	GLU
1	K	1018	LEU
1	L	3	ILE
1	L	9	VAL
1	L	13	ARG
1	L	24	LEU
1	L	37	ARG
1	L	38	ASN
1	L	39	SER
1	L	43	ARG
1	L	48	SER
1	L	49	GLN
1	L	50	GLN
1	L	52	ARG
1	L	57	GLU
1	L	67	GLU
1	L	71	GLU
1	L	72	SER
1	L	77	ASP
1	L	80	GLU
1	L	90	TRP
1	L	102	ASN
1	L	116	THR
1	L	124	SER
1	L	125	LEU
1	L	128	ASN

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Mol	Chain	Res	Type
1	L	136	GLU
1	L	141	ILE
1	L	165	SER
1	L	178	ARG
1	L	189	LEU
1	L	190	ARG
1	L	202	MET
1	L	211	ASP
1	L	213	SER
1	L	219	THR
1	L	237	ARG
1	L	246	MET
1	L	247	CYS
1	L	250	LEU
1	L	259	SER
1	L	264	GLU
1	L	267	VAL
1	L	277	GLU
1	L	279	ILE
1	L	282	ARG
1	L	299	LYS
1	L	310	ARG
1	L	312	VAL
1	L	314	GLU
1	L	333	ARG
1	L	336	ARG
1	L	347	LYS
1	L	370	GLN
1	L	425	ARG
1	L	437	SER
1	L	445	GLN
1	L	448	ARG
1	L	461	GLU
1	L	473	ARG
1	L	477	SER
1	L	482	ARG
1	L	494	THR
1	L	519	SER
1	L	521	LYS
1	L	533	LEU
1	L	546	LEU
1	L	554	GLN

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Mol	Chain	Res	Type
1	L	571	VAL
1	L	581	ASN
1	L	599	ARG
1	L	600	GLN
1	L	630	ARG
1	L	635	THR
1	L	651	LEU
1	L	652	LEU
1	L	655	MET
1	L	661	LYS
1	L	665	SER
1	L	672	VAL
1	L	675	GLN
1	L	681	GLU
1	L	684	GLU
1	L	690	SER
1	L	719	GLN
1	L	730	LEU
1	L	734	SER
1	L	743	SER
1	L	749	ILE
1	L	755	ARG
1	L	768	MET
1	L	773	LYS
1	L	778	THR
1	L	781	ARG
1	L	797	GLU
1	L	799	THR
1	L	800	ARG
1	L	801	ILE
1	L	804	ASN
1	L	809	ARG
1	L	822	LEU
1	L	824	GLN
1	L	832	ASP
1	L	837	THR
1	L	857	ARG
1	L	867	THR
1	L	881	ARG
1	L	903[A]	GLN
1	L	903[B]	GLN
1	L	917	ARG

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Mol	Chain	Res	Type
1	L	938	ARG
1	L	956	GLN
1	L	961	ARG
1	L	1006	GLU
1	L	1018	LEU
1	M	3	ILE
1	M	9	VAL
1	M	13	ARG
1	M	24	LEU
1	M	37	ARG
1	M	38	ASN
1	M	39	SER
1	M	43	ARG
1	M	48	SER
1	M	49	GLN
1	M	50	GLN
1	M	52	ARG
1	M	57	GLU
1	M	67	GLU
1	M	71	GLU
1	M	72	SER
1	M	77	ASP
1	M	80	GLU
1	M	90	TRP
1	M	102	ASN
1	M	116	THR
1	M	124	SER
1	M	125	LEU
1	M	128	ASN
1	M	136	GLU
1	M	141	ILE
1	M	165	SER
1	M	178	ARG
1	M	189	LEU
1	M	190	ARG
1	M	202	MET
1	M	211	ASP
1	M	213	SER
1	M	219	THR
1	M	237	ARG
1	M	246	MET
1	M	247	CYS

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Mol	Chain	Res	Type
1	M	250	LEU
1	M	259	SER
1	M	264	GLU
1	M	267	VAL
1	M	277	GLU
1	M	279	ILE
1	M	282	ARG
1	M	299	LYS
1	M	310	ARG
1	M	312	VAL
1	M	314	GLU
1	M	333	ARG
1	M	336	ARG
1	M	347	LYS
1	M	370	GLN
1	M	425	ARG
1	M	437	SER
1	M	445	GLN
1	M	448	ARG
1	M	461	GLU
1	M	473	ARG
1	M	477	SER
1	M	482	ARG
1	M	494	THR
1	M	519	SER
1	M	521	LYS
1	M	533	LEU
1	M	546	LEU
1	M	554	GLN
1	M	571	VAL
1	M	581	ASN
1	M	599	ARG
1	M	600	GLN
1	M	630	ARG
1	M	635	THR
1	M	651	LEU
1	M	652	LEU
1	M	655	MET
1	M	661	LYS
1	M	665	SER
1	M	672	VAL
1	M	675	GLN

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Mol	Chain	Res	Type
1	M	681	GLU
1	M	684	GLU
1	M	690	SER
1	M	719	GLN
1	M	730	LEU
1	M	734	SER
1	M	743	SER
1	M	749	ILE
1	M	755	ARG
1	M	768	MET
1	M	773	LYS
1	M	778	THR
1	M	781	ARG
1	M	797	GLU
1	M	799	THR
1	M	800	ARG
1	M	801	ILE
1	M	804	ASN
1	M	809	ARG
1	M	822	LEU
1	M	824	GLN
1	M	832	ASP
1	M	837	THR
1	M	857	ARG
1	M	867	THR
1	M	881	ARG
1	M	903[A]	GLN
1	M	903[B]	GLN
1	M	917	ARG
1	M	938	ARG
1	M	956	GLN
1	M	961	ARG
1	M	1006	GLU
1	M	1018	LEU
1	N	3	ILE
1	N	9	VAL
1	N	13	ARG
1	N	24	LEU
1	N	37	ARG
1	N	38	ASN
1	N	39	SER
1	N	43	ARG

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Mol	Chain	Res	Type
1	N	48	SER
1	N	49	GLN
1	N	50	GLN
1	N	52	ARG
1	N	57	GLU
1	N	67	GLU
1	N	71	GLU
1	N	72	SER
1	N	77	ASP
1	N	80	GLU
1	N	90	TRP
1	N	102	ASN
1	N	116	THR
1	N	124	SER
1	N	125	LEU
1	N	128	ASN
1	N	136	GLU
1	N	141	ILE
1	N	165	SER
1	N	178	ARG
1	N	189	LEU
1	N	190	ARG
1	N	202	MET
1	N	211	ASP
1	N	213	SER
1	N	219	THR
1	N	237	ARG
1	N	246	MET
1	N	247	CYS
1	N	250	LEU
1	N	259	SER
1	N	264	GLU
1	N	267	VAL
1	N	277	GLU
1	N	279	ILE
1	N	282	ARG
1	N	299	LYS
1	N	310	ARG
1	N	312	VAL
1	N	314	GLU
1	N	333	ARG
1	N	336	ARG

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Mol	Chain	Res	Type
1	N	347	LYS
1	N	370	GLN
1	N	425	ARG
1	N	437	SER
1	N	445	GLN
1	N	448	ARG
1	N	461	GLU
1	N	473	ARG
1	N	477	SER
1	N	482	ARG
1	N	494	THR
1	N	519	SER
1	N	521	LYS
1	N	533	LEU
1	N	546	LEU
1	N	554	GLN
1	N	571	VAL
1	N	581	ASN
1	N	599	ARG
1	N	600	GLN
1	N	630	ARG
1	N	635	THR
1	N	651	LEU
1	N	652	LEU
1	N	655	MET
1	N	661	LYS
1	N	665	SER
1	N	672	VAL
1	N	675	GLN
1	N	681	GLU
1	N	684	GLU
1	N	690	SER
1	N	719	GLN
1	N	730	LEU
1	N	734	SER
1	N	743	SER
1	N	749	ILE
1	N	755	ARG
1	N	768	MET
1	N	773	LYS
1	N	778	THR
1	N	781	ARG

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Mol	Chain	Res	Type
1	N	797	GLU
1	N	799	THR
1	N	800	ARG
1	N	801	ILE
1	N	804	ASN
1	N	809	ARG
1	N	822	LEU
1	N	824	GLN
1	N	832	ASP
1	N	837	THR
1	N	857	ARG
1	N	867	THR
1	N	881	ARG
1	N	903[A]	GLN
1	N	903[B]	GLN
1	N	917	ARG
1	N	938	ARG
1	N	956	GLN
1	N	961	ARG
1	N	1006	GLU
1	N	1018	LEU
1	O	3	ILE
1	O	9	VAL
1	O	13	ARG
1	O	24	LEU
1	O	37	ARG
1	O	38	ASN
1	O	39	SER
1	O	43	ARG
1	O	48	SER
1	O	49	GLN
1	O	50	GLN
1	O	52	ARG
1	O	57	GLU
1	O	67	GLU
1	O	71	GLU
1	O	72	SER
1	O	77	ASP
1	O	80	GLU
1	O	90	TRP
1	O	102	ASN
1	O	116	THR

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Mol	Chain	Res	Type
1	O	124	SER
1	O	125	LEU
1	O	128	ASN
1	O	136	GLU
1	O	141	ILE
1	O	165	SER
1	O	178	ARG
1	O	189	LEU
1	O	190	ARG
1	O	202	MET
1	O	211	ASP
1	O	213	SER
1	O	219	THR
1	O	237	ARG
1	O	246	MET
1	O	247	CYS
1	O	250	LEU
1	O	259	SER
1	O	264	GLU
1	O	267	VAL
1	O	277	GLU
1	O	279	ILE
1	O	282	ARG
1	O	299	LYS
1	O	310	ARG
1	O	312	VAL
1	O	314	GLU
1	O	333	ARG
1	O	336	ARG
1	O	347	LYS
1	O	370	GLN
1	O	425	ARG
1	O	437	SER
1	O	445	GLN
1	O	448	ARG
1	O	461	GLU
1	O	473	ARG
1	O	477	SER
1	O	482	ARG
1	O	494	THR
1	O	519	SER
1	O	521	LYS

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Mol	Chain	Res	Type
1	O	533	LEU
1	O	546	LEU
1	O	554	GLN
1	O	571	VAL
1	O	581	ASN
1	O	599	ARG
1	O	600	GLN
1	O	630	ARG
1	O	635	THR
1	O	651	LEU
1	O	652	LEU
1	O	655	MET
1	O	661	LYS
1	O	665	SER
1	O	672	VAL
1	O	675	GLN
1	O	681	GLU
1	O	684	GLU
1	O	690	SER
1	O	719	GLN
1	O	730	LEU
1	O	734	SER
1	O	743	SER
1	O	749	ILE
1	O	755	ARG
1	O	768	MET
1	O	773	LYS
1	O	778	THR
1	O	781	ARG
1	O	797	GLU
1	O	799	THR
1	O	800	ARG
1	O	801	ILE
1	O	804	ASN
1	O	809	ARG
1	O	822	LEU
1	O	824	GLN
1	O	832	ASP
1	O	837	THR
1	O	857	ARG
1	O	867	THR
1	O	881	ARG

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Mol	Chain	Res	Type
1	O	903[A]	GLN
1	O	903[B]	GLN
1	O	917	ARG
1	O	938	ARG
1	O	956	GLN
1	O	961	ARG
1	O	1006	GLU
1	O	1018	LEU
1	P	3	ILE
1	P	9	VAL
1	P	13	ARG
1	P	24	LEU
1	P	37	ARG
1	P	38	ASN
1	P	39	SER
1	P	43	ARG
1	P	48	SER
1	P	49	GLN
1	P	50	GLN
1	P	52	ARG
1	P	57	GLU
1	P	67	GLU
1	P	71	GLU
1	P	72	SER
1	P	77	ASP
1	P	80	GLU
1	P	90	TRP
1	P	102	ASN
1	P	116	THR
1	P	124	SER
1	P	125	LEU
1	P	128	ASN
1	P	136	GLU
1	P	141	ILE
1	P	165	SER
1	P	178	ARG
1	P	189	LEU
1	P	190	ARG
1	P	202	MET
1	P	211	ASP
1	P	213	SER
1	P	219	THR

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Mol	Chain	Res	Type
1	P	237	ARG
1	P	246	MET
1	P	247	CYS
1	P	250	LEU
1	P	259	SER
1	P	264	GLU
1	P	267	VAL
1	P	277	GLU
1	P	279	ILE
1	P	282	ARG
1	P	299	LYS
1	P	310	ARG
1	P	312	VAL
1	P	314	GLU
1	P	333	ARG
1	P	336	ARG
1	P	347	LYS
1	P	370	GLN
1	P	425	ARG
1	P	437	SER
1	P	445	GLN
1	P	448	ARG
1	P	461	GLU
1	P	473	ARG
1	P	477	SER
1	P	482	ARG
1	P	494	THR
1	P	519	SER
1	P	521	LYS
1	P	533	LEU
1	P	546	LEU
1	P	554	GLN
1	P	571	VAL
1	P	581	ASN
1	P	599	ARG
1	P	600	GLN
1	P	630	ARG
1	P	635	THR
1	P	651	LEU
1	P	652	LEU
1	P	655	MET
1	P	661	LYS

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Mol	Chain	Res	Type
1	P	665	SER
1	P	672	VAL
1	P	675	GLN
1	P	681	GLU
1	P	684	GLU
1	P	690	SER
1	P	719	GLN
1	P	730	LEU
1	P	734	SER
1	P	743	SER
1	P	749	ILE
1	P	755	ARG
1	P	768	MET
1	P	773	LYS
1	P	778	THR
1	P	781	ARG
1	P	797	GLU
1	P	799	THR
1	P	800	ARG
1	P	801	ILE
1	P	804	ASN
1	P	809	ARG
1	P	822	LEU
1	P	824	GLN
1	P	832	ASP
1	P	837	THR
1	P	857	ARG
1	P	867	THR
1	P	881	ARG
1	P	903[A]	GLN
1	P	903[B]	GLN
1	P	917	ARG
1	P	938	ARG
1	P	956	GLN
1	P	961	ARG
1	P	1006	GLU
1	P	1018	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (159) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	49	GLN

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Mol	Chain	Res	Type
1	I	102	ASN
1	I	128	ASN
1	I	221	GLN
1	I	226	HIS
1	I	316	HIS
1	I	363	HIS
1	I	394	ASN
1	I	445	GLN
1	I	467	ASN
1	I	597	ASN
1	I	624	GLN
1	I	634	GLN
1	I	739	HIS
1	I	761	GLN
1	I	817	GLN
1	I	949	HIS
1	I	977	HIS
1	I	990	HIS
1	I	1017	GLN
1	J	49	GLN
1	J	102	ASN
1	J	128	ASN
1	J	221	GLN
1	J	226	HIS
1	J	316	HIS
1	J	363	HIS
1	J	394	ASN
1	J	445	GLN
1	J	467	ASN
1	J	597	ASN
1	J	624	GLN
1	J	634	GLN
1	J	739	HIS
1	J	761	GLN
1	J	817	GLN
1	J	949	HIS
1	J	977	HIS
1	J	990	HIS
1	J	1017	GLN
1	K	49	GLN
1	K	102	ASN
1	K	128	ASN

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Mol	Chain	Res	Type
1	K	221	GLN
1	K	226	HIS
1	K	316	HIS
1	K	363	HIS
1	K	394	ASN
1	K	445	GLN
1	K	467	ASN
1	K	597	ASN
1	K	624	GLN
1	K	634	GLN
1	K	739	HIS
1	K	761	GLN
1	K	817	GLN
1	K	949	HIS
1	K	977	HIS
1	K	990	HIS
1	K	1017	GLN
1	L	49	GLN
1	L	102	ASN
1	L	128	ASN
1	L	221	GLN
1	L	226	HIS
1	L	316	HIS
1	L	363	HIS
1	L	394	ASN
1	L	445	GLN
1	L	467	ASN
1	L	597	ASN
1	L	624	GLN
1	L	634	GLN
1	L	739	HIS
1	L	761	GLN
1	L	817	GLN
1	L	949	HIS
1	L	977	HIS
1	L	990	HIS
1	L	1017	GLN
1	M	49	GLN
1	M	102	ASN
1	M	128	ASN
1	M	221	GLN
1	M	226	HIS

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Mol	Chain	Res	Type
1	M	316	HIS
1	M	363	HIS
1	M	394	ASN
1	M	445	GLN
1	M	467	ASN
1	M	597	ASN
1	M	624	GLN
1	M	634	GLN
1	M	739	HIS
1	M	761	GLN
1	M	817	GLN
1	M	949	HIS
1	M	977	HIS
1	M	990	HIS
1	M	1017	GLN
1	N	49	GLN
1	N	102	ASN
1	N	128	ASN
1	N	221	GLN
1	N	226	HIS
1	N	316	HIS
1	N	363	HIS
1	N	394	ASN
1	N	445	GLN
1	N	467	ASN
1	N	597	ASN
1	N	624	GLN
1	N	634	GLN
1	N	739	HIS
1	N	761	GLN
1	N	817	GLN
1	N	949	HIS
1	N	977	HIS
1	N	990	HIS
1	N	1017	GLN
1	O	49	GLN
1	O	102	ASN
1	O	128	ASN
1	O	221	GLN
1	O	226	HIS
1	O	316	HIS
1	O	363	HIS

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Mol	Chain	Res	Type
1	O	394	ASN
1	O	445	GLN
1	O	467	ASN
1	O	597	ASN
1	O	624	GLN
1	O	634	GLN
1	O	739	HIS
1	O	761	GLN
1	O	817	GLN
1	O	949	HIS
1	O	977	HIS
1	O	990	HIS
1	O	1017	GLN
1	P	49	GLN
1	P	102	ASN
1	P	128	ASN
1	P	221	GLN
1	P	226	HIS
1	P	316	HIS
1	P	363	HIS
1	P	394	ASN
1	P	445	GLN
1	P	467	ASN
1	P	597	ASN
1	P	634	GLN
1	P	739	HIS
1	P	761	GLN
1	P	817	GLN
1	P	949	HIS
1	P	977	HIS
1	P	990	HIS
1	P	1017	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

24 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	CME	I	1021	1	9,9,10	4.84	1 (11%)	7,9,11	1.30	0
1	CME	I	748	1	9,9,10	5.78	1 (11%)	7,9,11	2.67	4 (57%)
1	CME	I	914	1	9,9,10	6.34	1 (11%)	7,9,11	1.95	2 (28%)
1	CME	J	1021	1	9,9,10	4.88	1 (11%)	7,9,11	1.30	0
1	CME	J	748	1	9,9,10	5.77	1 (11%)	7,9,11	2.67	4 (57%)
1	CME	J	914	1	9,9,10	6.38	1 (11%)	7,9,11	1.95	2 (28%)
1	CME	K	1021	1	9,9,10	4.87	1 (11%)	7,9,11	1.31	0
1	CME	K	748	1	9,9,10	5.79	1 (11%)	7,9,11	2.67	4 (57%)
1	CME	K	914	1	9,9,10	6.41	1 (11%)	7,9,11	1.95	2 (28%)
1	CME	L	1021	1	9,9,10	4.88	1 (11%)	7,9,11	1.31	0
1	CME	L	748	1	9,9,10	5.77	1 (11%)	7,9,11	2.66	4 (57%)
1	CME	L	914	1	9,9,10	6.36	1 (11%)	7,9,11	1.95	2 (28%)
1	CME	M	1021	1	9,9,10	4.86	1 (11%)	7,9,11	1.30	0
1	CME	M	748	1	9,9,10	5.79	1 (11%)	7,9,11	2.67	4 (57%)
1	CME	M	914	1	9,9,10	6.36	1 (11%)	7,9,11	1.96	2 (28%)
1	CME	N	1021	1	9,9,10	4.85	1 (11%)	7,9,11	1.30	0
1	CME	N	748	1	9,9,10	5.75	1 (11%)	7,9,11	2.68	4 (57%)
1	CME	N	914	1	9,9,10	6.40	1 (11%)	7,9,11	1.95	2 (28%)
1	CME	O	1021	1	9,9,10	4.90	1 (11%)	7,9,11	1.31	0
1	CME	O	748	1	9,9,10	5.79	1 (11%)	7,9,11	2.68	4 (57%)
1	CME	O	914	1	9,9,10	6.36	1 (11%)	7,9,11	1.95	2 (28%)
1	CME	P	1021	1	9,9,10	4.88	1 (11%)	7,9,11	1.30	0
1	CME	P	748	1	9,9,10	5.81	1 (11%)	7,9,11	2.67	4 (57%)
1	CME	P	914	1	9,9,10	6.37	1 (11%)	7,9,11	1.95	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	I	1021	1	-	0/6/8/10	0/0/0/0
1	CME	I	748	1	-	0/6/8/10	0/0/0/0
1	CME	I	914	1	-	0/6/8/10	0/0/0/0
1	CME	J	1021	1	-	0/6/8/10	0/0/0/0
1	CME	J	748	1	-	0/6/8/10	0/0/0/0
1	CME	J	914	1	-	0/6/8/10	0/0/0/0
1	CME	K	1021	1	-	0/6/8/10	0/0/0/0
1	CME	K	748	1	-	0/6/8/10	0/0/0/0
1	CME	K	914	1	-	0/6/8/10	0/0/0/0
1	CME	L	1021	1	-	0/6/8/10	0/0/0/0
1	CME	L	748	1	-	0/6/8/10	0/0/0/0
1	CME	L	914	1	-	0/6/8/10	0/0/0/0
1	CME	M	1021	1	-	0/6/8/10	0/0/0/0
1	CME	M	748	1	-	0/6/8/10	0/0/0/0
1	CME	M	914	1	-	0/6/8/10	0/0/0/0
1	CME	N	1021	1	-	0/6/8/10	0/0/0/0
1	CME	N	748	1	-	0/6/8/10	0/0/0/0
1	CME	N	914	1	-	0/6/8/10	0/0/0/0
1	CME	O	1021	1	-	0/6/8/10	0/0/0/0
1	CME	O	748	1	-	0/6/8/10	0/0/0/0
1	CME	O	914	1	-	0/6/8/10	0/0/0/0
1	CME	P	1021	1	-	0/6/8/10	0/0/0/0
1	CME	P	748	1	-	0/6/8/10	0/0/0/0
1	CME	P	914	1	-	0/6/8/10	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	914	CME	O-C	19.16	1.24	1.11
1	N	914	CME	O-C	19.13	1.24	1.11
1	J	914	CME	O-C	19.08	1.24	1.11
1	P	914	CME	O-C	19.05	1.24	1.11
1	L	914	CME	O-C	19.03	1.24	1.11
1	O	914	CME	O-C	19.02	1.24	1.11
1	M	914	CME	O-C	19.01	1.24	1.11
1	I	914	CME	O-C	18.95	1.24	1.11
1	P	748	CME	O-C	17.29	1.23	1.11
1	K	748	CME	O-C	17.25	1.23	1.11
1	M	748	CME	O-C	17.24	1.23	1.11
1	O	748	CME	O-C	17.23	1.23	1.11
1	I	748	CME	O-C	17.20	1.23	1.11
1	L	748	CME	O-C	17.18	1.23	1.11
1	J	748	CME	O-C	17.17	1.23	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	748	CME	O-C	17.12	1.23	1.11
1	O	1021	CME	O-C	14.57	1.21	1.11
1	J	1021	CME	O-C	14.53	1.21	1.11
1	P	1021	CME	O-C	14.52	1.21	1.11
1	L	1021	CME	O-C	14.51	1.21	1.11
1	K	1021	CME	O-C	14.49	1.21	1.11
1	M	1021	CME	O-C	14.45	1.21	1.11
1	N	1021	CME	O-C	14.44	1.21	1.11
1	I	1021	CME	O-C	14.40	1.21	1.11

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	748	CME	CB-CA-N	4.88	118.54	110.27
1	O	748	CME	CB-CA-N	4.87	118.53	110.27
1	P	748	CME	CB-CA-N	4.85	118.49	110.27
1	I	748	CME	CB-CA-N	4.84	118.48	110.27
1	K	748	CME	CB-CA-N	4.84	118.47	110.27
1	M	748	CME	CB-CA-N	4.83	118.47	110.27
1	J	748	CME	CB-CA-N	4.83	118.47	110.27
1	L	748	CME	CB-CA-N	4.83	118.46	110.27
1	I	914	CME	CB-SG-SD	-4.47	94.95	103.87
1	K	914	CME	CB-SG-SD	-4.47	94.95	103.87
1	P	914	CME	CB-SG-SD	-4.47	94.96	103.87
1	M	914	CME	CB-SG-SD	-4.47	94.96	103.87
1	L	914	CME	CB-SG-SD	-4.46	94.97	103.87
1	O	914	CME	CB-SG-SD	-4.46	94.97	103.87
1	J	914	CME	CB-SG-SD	-4.46	94.98	103.87
1	N	914	CME	CB-SG-SD	-4.46	94.98	103.87
1	K	748	CME	C-CA-N	3.27	117.09	113.83
1	O	748	CME	C-CA-N	3.27	117.09	113.83
1	I	748	CME	C-CA-N	3.26	117.09	113.83
1	J	748	CME	C-CA-N	3.26	117.09	113.83
1	N	748	CME	C-CA-N	3.25	117.07	113.83
1	M	748	CME	C-CA-N	3.24	117.07	113.83
1	P	748	CME	C-CA-N	3.24	117.06	113.83
1	L	748	CME	C-CA-N	3.24	117.06	113.83
1	M	748	CME	CA-CB-SG	-2.73	104.79	113.36
1	P	748	CME	CA-CB-SG	-2.73	104.80	113.36
1	L	748	CME	CA-CB-SG	-2.73	104.82	113.36
1	J	748	CME	CA-CB-SG	-2.72	104.83	113.36
1	N	748	CME	CA-CB-SG	-2.72	104.83	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	748	CME	CA-CB-SG	-2.72	104.84	113.36
1	K	748	CME	CA-CB-SG	-2.72	104.84	113.36
1	I	748	CME	CA-CB-SG	-2.72	104.85	113.36
1	K	748	CME	CB-SG-SD	2.33	108.52	103.87
1	I	748	CME	CB-SG-SD	2.33	108.51	103.87
1	M	748	CME	CB-SG-SD	2.32	108.51	103.87
1	J	748	CME	CB-SG-SD	2.32	108.50	103.87
1	N	748	CME	CB-SG-SD	2.32	108.50	103.87
1	P	748	CME	CB-SG-SD	2.32	108.50	103.87
1	O	748	CME	CB-SG-SD	2.32	108.49	103.87
1	L	748	CME	CB-SG-SD	2.31	108.47	103.87
1	M	914	CME	CB-CA-N	2.08	113.80	110.27
1	L	914	CME	CB-CA-N	2.06	113.77	110.27
1	P	914	CME	CB-CA-N	2.06	113.76	110.27
1	N	914	CME	CB-CA-N	2.06	113.76	110.27
1	O	914	CME	CB-CA-N	2.05	113.75	110.27
1	K	914	CME	CB-CA-N	2.04	113.73	110.27
1	J	914	CME	CB-CA-N	2.04	113.72	110.27
1	I	914	CME	CB-CA-N	2.03	113.72	110.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 40 ligands modelled in this entry, 32 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2FL	I	2001	4	24,24,24	0.56	0	35,35,35	1.43	3 (8%)
2	2FL	J	2001	4	24,24,24	0.57	0	35,35,35	1.43	3 (8%)
2	2FL	K	2001	4	24,24,24	0.56	0	35,35,35	1.43	3 (8%)
2	2FL	L	2001	4	24,24,24	0.56	0	35,35,35	1.43	3 (8%)
2	2FL	M	2001	4	24,24,24	0.56	0	35,35,35	1.43	3 (8%)
2	2FL	N	2001	4	24,24,24	0.57	0	35,35,35	1.43	3 (8%)
2	2FL	O	2001	4	24,24,24	0.56	0	35,35,35	1.43	3 (8%)
2	2FL	P	2001	4	24,24,24	0.57	0	35,35,35	1.43	3 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2FL	I	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	J	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	K	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	L	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	M	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	N	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	O	2001	4	-	0/8/48/48	0/2/2/2
2	2FL	P	2001	4	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	2001	2FL	F2-C2-C3	6.08	113.39	108.55
2	M	2001	2FL	F2-C2-C3	6.07	113.38	108.55
2	L	2001	2FL	F2-C2-C3	6.07	113.38	108.55
2	J	2001	2FL	F2-C2-C3	6.07	113.38	108.55
2	K	2001	2FL	F2-C2-C3	6.06	113.37	108.55
2	I	2001	2FL	F2-C2-C3	6.06	113.37	108.55
2	P	2001	2FL	F2-C2-C3	6.06	113.37	108.55
2	O	2001	2FL	F2-C2-C3	6.04	113.36	108.55
2	I	2001	2FL	C2-C3-C4	-3.17	105.39	109.40
2	O	2001	2FL	C2-C3-C4	-3.16	105.40	109.40
2	M	2001	2FL	C2-C3-C4	-3.14	105.42	109.40
2	P	2001	2FL	C2-C3-C4	-3.13	105.44	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	2001	2FL	C2-C3-C4	-3.13	105.44	109.40
2	N	2001	2FL	C2-C3-C4	-3.13	105.44	109.40
2	J	2001	2FL	C2-C3-C4	-3.13	105.45	109.40
2	K	2001	2FL	C2-C3-C4	-3.12	105.45	109.40
2	O	2001	2FL	C1-C2-C3	2.53	114.69	111.18
2	L	2001	2FL	C1-C2-C3	2.51	114.67	111.18
2	I	2001	2FL	C1-C2-C3	2.50	114.66	111.18
2	K	2001	2FL	C1-C2-C3	2.49	114.65	111.18
2	M	2001	2FL	C1-C2-C3	2.49	114.64	111.18
2	P	2001	2FL	C1-C2-C3	2.49	114.64	111.18
2	J	2001	2FL	C1-C2-C3	2.48	114.63	111.18
2	N	2001	2FL	C1-C2-C3	2.46	114.61	111.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	I	1021/1023 (99%)	-0.00	23 (2%)	57	64	11, 32, 70, 100	0
1	J	1021/1023 (99%)	-0.09	18 (1%)	65	71	10, 30, 69, 100	0
1	K	1021/1023 (99%)	0.31	48 (4%)	30	34	24, 45, 81, 100	0
1	L	1021/1023 (99%)	0.36	47 (4%)	31	35	25, 45, 81, 100	0
1	M	1021/1023 (99%)	0.45	60 (5%)	22	23	27, 48, 83, 100	0
1	N	1021/1023 (99%)	0.05	22 (2%)	59	65	16, 36, 74, 100	0
1	O	1021/1023 (99%)	0.22	27 (2%)	53	59	21, 42, 78, 100	0
1	P	1021/1023 (99%)	0.76	91 (8%)	10	10	39, 60, 91, 100	0
All	All	8168/8184 (99%)	0.26	336 (4%)	35	40	10, 43, 80, 100	0

All (336) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	801	ILE	9.6
1	O	796	SER	7.8
1	P	797	GLU	7.0
1	O	1023	LYS	6.9
1	N	799	THR	6.7
1	I	730	LEU	6.7
1	O	582	GLY	6.3
1	M	177	LEU	6.2
1	N	1023	LYS	6.1
1	P	68	ALA	6.0
1	K	276	GLY	6.0
1	M	734	SER	6.0
1	N	797	GLU	5.9
1	P	796	SER	5.6
1	M	79	PRO	5.5
1	P	799	THR	5.4

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Mol	Chain	Res	Type	RSRZ
1	N	796	SER	5.4
1	M	51	LEU	5.3
1	P	81	ALA	5.3
1	K	796	SER	5.2
1	L	733	ALA	5.1
1	L	130	ASP	5.1
1	J	93	HIS	4.8
1	K	801	ILE	4.8
1	I	732	ALA	4.7
1	L	732	ALA	4.6
1	L	370	GLN	4.6
1	P	398	TRP	4.5
1	P	312	VAL	4.5
1	K	731	PRO	4.4
1	P	78	LEU	4.3
1	P	728	VAL	4.2
1	O	797	GLU	4.1
1	L	161	TYR	4.1
1	P	47	PRO	4.1
1	K	578	TYR	4.1
1	P	732	ALA	4.0
1	M	798	ALA	4.0
1	M	796	SER	4.0
1	L	798	ALA	4.0
1	P	162	GLY	4.0
1	P	801	ILE	4.0
1	P	313	VAL	3.9
1	M	162	GLY	3.9
1	N	130	ASP	3.8
1	L	81	ALA	3.8
1	M	320	GLY	3.8
1	P	99	ILE	3.8
1	I	249	GLU	3.7
1	M	580	GLU	3.7
1	M	682	LEU	3.7
1	M	731	PRO	3.7
1	I	683	PRO	3.7
1	N	730	LEU	3.7
1	L	269	SER	3.6
1	M	123	TYR	3.6
1	N	77	ASP	3.6
1	K	799	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	P	174	SER	3.5
1	N	772	ASP	3.5
1	P	698	VAL	3.5
1	P	179	ALA	3.4
1	K	137	GLY	3.4
1	P	34	ALA	3.4
1	P	254	LEU	3.4
1	L	128	ASN	3.4
1	M	599	ARG	3.3
1	L	597	ASN	3.3
1	O	250	LEU	3.3
1	P	180	GLY	3.3
1	P	316	HIS	3.3
1	M	225	PHE	3.3
1	M	274	PHE	3.3
1	N	798	ALA	3.3
1	P	32	PRO	3.3
1	L	284	GLY	3.2
1	P	729	THR	3.2
1	P	379	MET	3.2
1	P	692	GLY	3.2
1	O	948	PRO	3.2
1	N	889	ALA	3.2
1	L	123	TYR	3.2
1	K	321	THR	3.1
1	O	178	ARG	3.1
1	K	580	GLU	3.1
1	I	129	VAL	3.1
1	M	129	VAL	3.1
1	M	242	ALA	3.1
1	M	827	ALA	3.1
1	N	80	GLU	3.1
1	I	795	VAL	3.0
1	M	803	PRO	3.0
1	P	108	THR	3.0
1	P	819	GLU	3.0
1	O	97	ALA	3.0
1	K	733	ALA	3.0
1	J	800	ARG	3.0
1	L	590	GLY	3.0
1	J	83	THR	3.0
1	N	318	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	N	800	ARG	3.0
1	L	172	ASP	2.9
1	L	173	LEU	2.9
1	P	92	MET	2.9
1	K	734	SER	2.9
1	P	601	PHE	2.9
1	L	4	THR	2.9
1	P	772	ASP	2.9
1	N	156	GLY	2.9
1	M	730	LEU	2.9
1	P	173	LEU	2.9
1	K	771	GLY	2.9
1	L	735	HIS	2.9
1	M	598	ASP	2.9
1	N	79	PRO	2.9
1	L	796	SER	2.8
1	J	728	VAL	2.8
1	M	227	VAL	2.8
1	N	770	ILE	2.8
1	O	219	THR	2.8
1	P	853	ARG	2.8
1	K	798	ALA	2.8
1	M	593	GLY	2.8
1	K	829	THR	2.8
1	P	681	GLU	2.8
1	L	374	GLN	2.8
1	P	327	ALA	2.8
1	K	136	GLU	2.7
1	M	745	MET	2.7
1	I	771	GLY	2.7
1	M	797	GLU	2.7
1	M	55	ASN	2.7
1	K	131	GLU	2.7
1	P	893	GLU	2.7
1	J	801	ILE	2.7
1	P	229	THR	2.7
1	M	10	VAL	2.7
1	M	419	GLY	2.7
1	P	364	GLY	2.7
1	L	653[A]	HIS	2.7
1	L	581	ASN	2.7
1	M	727	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	76	CYS	2.6
1	M	48	SER	2.6
1	M	992	GLY	2.6
1	N	129	VAL	2.6
1	L	799	THR	2.6
1	P	440	VAL	2.6
1	O	735	HIS	2.6
1	I	801	ILE	2.6
1	P	149	ALA	2.6
1	K	224	ASP	2.6
1	L	283	GLY	2.6
1	M	59	ARG	2.6
1	P	315	LEU	2.6
1	K	64	PRO	2.6
1	M	615	PRO	2.6
1	O	739	HIS	2.6
1	P	311	ALA	2.6
1	L	138	GLN	2.6
1	P	276	GLY	2.6
1	K	653[A]	HIS	2.6
1	P	205	MET	2.6
1	P	580	GLU	2.6
1	P	744	GLU	2.6
1	K	127	PHE	2.5
1	K	49	GLN	2.5
1	M	99	ILE	2.5
1	O	861	SER	2.5
1	P	206	SER	2.5
1	L	49	GLN	2.5
1	I	250	LEU	2.5
1	P	832	ASP	2.5
1	K	601	PHE	2.5
1	P	829	THR	2.5
1	I	727	SER	2.5
1	O	264	GLU	2.5
1	K	60	PHE	2.5
1	K	102	ASN	2.5
1	P	109	VAL	2.5
1	L	801	ILE	2.5
1	O	729	THR	2.5
1	M	109	VAL	2.5
1	M	188	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	178	ARG	2.5
1	K	452	SER	2.4
1	M	733	ALA	2.4
1	P	196	TYR	2.4
1	J	735	HIS	2.4
1	P	800	ARG	2.4
1	P	301	TRP	2.4
1	N	132	SER	2.4
1	L	237	ARG	2.4
1	N	580	GLU	2.4
1	J	795	VAL	2.4
1	N	728	VAL	2.4
1	P	682	LEU	2.4
1	P	38	ASN	2.4
1	K	250	LEU	2.4
1	M	146	VAL	2.4
1	I	593	GLY	2.4
1	P	48	SER	2.4
1	L	730	LEU	2.4
1	J	81	ALA	2.3
1	L	129	VAL	2.3
1	P	376	ILE	2.3
1	K	860	GLY	2.3
1	L	57	GLU	2.3
1	L	687	GLN	2.3
1	M	289	VAL	2.3
1	I	130	ASP	2.3
1	M	686	PRO	2.3
1	P	82	ASP	2.3
1	O	846	GLY	2.3
1	P	51	LEU	2.3
1	P	749	ILE	2.3
1	O	131	GLU	2.3
1	J	734	SER	2.3
1	I	421	VAL	2.3
1	J	179	ALA	2.3
1	N	803	PRO	2.3
1	P	988	GLY	2.3
1	P	258	VAL	2.3
1	M	735	HIS	2.3
1	I	74	LEU	2.3
1	K	108	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	238	ALA	2.3
1	I	578	TYR	2.3
1	L	1023	LYS	2.3
1	O	253	TYR	2.3
1	P	321	THR	2.2
1	M	845	GLN	2.2
1	P	239	VAL	2.2
1	K	154	CYS	2.2
1	L	259	SER	2.2
1	M	140	ARG	2.2
1	P	39	SER	2.2
1	K	253	TYR	2.2
1	J	797	GLU	2.2
1	P	75	GLU	2.2
1	P	12	GLN	2.2
1	P	23	GLN	2.2
1	O	795	VAL	2.2
1	K	252	ASP	2.2
1	N	597	ASN	2.2
1	K	747	PHE	2.2
1	L	39	SER	2.2
1	P	195	SER	2.2
1	L	832	ASP	2.2
1	J	8	ALA	2.2
1	M	753	ASN	2.2
1	P	148	SER	2.2
1	K	260	LEU	2.2
1	I	581	ASN	2.2
1	K	587	ALA	2.2
1	L	180	GLY	2.2
1	O	737	ILE	2.2
1	L	189	LEU	2.2
1	P	250	LEU	2.2
1	J	581	ASN	2.2
1	J	977	HIS	2.2
1	M	249	GLU	2.2
1	L	160	GLY	2.2
1	P	598	ASP	2.2
1	O	599	ARG	2.2
1	L	139	THR	2.2
1	M	54	LEU	2.2
1	P	249	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	4	THR	2.1
1	K	728	VAL	2.1
1	P	820	ALA	2.1
1	K	70	PRO	2.1
1	K	251	ARG	2.1
1	P	190	ARG	2.1
1	J	82	ASP	2.1
1	K	980	GLU	2.1
1	O	860	GLY	2.1
1	P	94	GLY	2.1
1	K	61	ALA	2.1
1	L	373	VAL	2.1
1	P	79	PRO	2.1
1	O	369	GLU	2.1
1	O	252	ASP	2.1
1	L	34	ALA	2.1
1	M	684	GLU	2.1
1	P	111	PRO	2.1
1	M	184	LEU	2.1
1	P	73	TRP	2.1
1	L	61	ALA	2.1
1	L	716	ALA	2.1
1	O	312	VAL	2.1
1	P	279	ILE	2.1
1	J	753	ASN	2.1
1	O	581	ASN	2.1
1	I	760	ARG	2.1
1	I	582	GLY	2.1
1	O	74	LEU	2.1
1	L	40	GLU	2.1
1	P	590	GLY	2.1
1	P	97	ALA	2.1
1	K	50	GLN	2.1
1	P	328	CYS	2.1
1	K	248	GLY	2.1
1	M	716	ALA	2.1
1	J	890	GLN	2.1
1	K	687	GLN	2.1
1	L	36	TRP	2.1
1	M	244	VAL	2.1
1	M	930	VAL	2.1
1	M	178	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	255	ARG	2.1
1	M	581	ASN	2.1
1	M	776	LEU	2.1
1	P	197	LEU	2.1
1	M	359	HIS	2.0
1	M	294	ASN	2.0
1	I	733	ALA	2.0
1	L	390	SER	2.0
1	P	802	ASP	2.0
1	I	73	TRP	2.0
1	K	98	PRO	2.0
1	M	191	TRP	2.0
1	P	330	VAL	2.0
1	P	361	PRO	2.0
1	P	367	MET	2.0
1	K	51	LEU	2.0
1	O	296	GLU	2.0
1	K	738	PRO	2.0
1	K	720	TRP	2.0
1	M	795	VAL	2.0
1	P	543	GLY	2.0
1	P	127	PHE	2.0
1	I	735	HIS	2.0
1	L	779	PRO	2.0
1	I	84	VAL	2.0
1	K	109	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CME	O	914	10/11	0.20	1.89	36,44,80,86	0
1	CME	M	748	10/11	0.26	1.45	56,68,100,100	0
1	CME	L	748	10/11	0.26	1.00	53,65,99,100	0
1	CME	K	1021	10/11	0.27	0.96	57,73,100,100	0
1	CME	I	1021	10/11	0.20	0.57	44,60,94,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	CME	K	748	10/11	0.24	0.53	53,65,98,100	0
1	CME	N	914	10/11	0.20	0.48	31,38,75,81	0
1	CME	L	1021	10/11	0.24	0.33	57,73,100,100	0
1	CME	N	748	10/11	0.20	0.23	44,56,90,100	0
1	CME	J	1021	10/11	0.22	0.19	42,58,93,100	0
1	CME	N	1021	10/11	0.24	0.17	48,64,99,100	0
1	CME	I	914	10/11	0.18	0.11	26,34,70,76	0
1	CME	J	914	10/11	0.16	0.05	25,32,69,75	0
1	CME	M	1021	10/11	0.23	-0.11	60,75,100,100	0
1	CME	L	914	10/11	0.19	-0.15	40,47,84,89	0
1	CME	J	748	10/11	0.18	-0.20	38,50,84,95	0
1	CME	I	748	10/11	0.17	-0.27	40,52,85,97	0
1	CME	P	748	10/11	0.21	-0.32	68,80,100,100	0
1	CME	P	1021	10/11	0.23	-0.46	72,87,100,100	0
1	CME	O	1021	10/11	0.17	-0.52	54,69,100,100	0
1	CME	M	914	10/11	0.17	-0.59	42,50,86,92	0
1	CME	K	914	10/11	0.13	-0.79	40,47,84,89	0
1	CME	P	914	10/11	0.16	-0.98	54,62,98,100	0
1	CME	O	748	10/11	0.17	-1.14	50,62,95,100	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	2FL	M	2001	23/23	0.63	8.39	65,77,93,100	0
2	2FL	N	2001	23/23	0.42	6.03	54,65,82,100	0
2	2FL	O	2001	23/23	0.46	5.15	59,70,87,100	0
4	NA	N	3101	1/1	0.39	4.60	44,44,44,44	0
4	NA	K	3102	1/1	0.29	4.25	40,40,40,40	0
2	2FL	L	2001	23/23	0.41	3.99	63,74,91,100	0
2	2FL	J	2001	23/23	0.39	3.39	48,59,76,99	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	2FL	K	2001	23/23	0.40	2.96	63,74,91,100	0
3	MG	N	3001	1/1	0.28	2.77	37,37,37,37	0
2	2FL	P	2001	23/23	0.38	2.51	77,89,100,100	0
3	MG	O	3001	1/1	0.29	2.40	42,42,42,42	0
4	NA	J	3102	1/1	0.18	2.15	25,25,25,25	0
4	NA	K	3101	1/1	0.30	1.63	53,53,53,53	0
4	NA	O	3101	1/1	0.26	1.22	49,49,49,49	0
4	NA	I	3102	1/1	0.16	1.19	27,27,27,27	0
3	MG	P	3001	1/1	0.28	1.08	60,60,60,60	0
2	2FL	I	2001	23/23	0.26	0.92	49,61,78,100	0
4	NA	I	3101	1/1	0.23	0.63	39,39,39,39	0
4	NA	M	3101	1/1	0.20	0.51	55,55,55,55	0
3	MG	O	3002	1/1	0.21	0.35	35,35,35,35	0
3	MG	I	3001	1/1	0.17	0.30	32,32,32,32	0
4	NA	P	3101	1/1	0.25	0.10	67,67,67,67	0
4	NA	L	3101	1/1	0.20	0.08	53,53,53,53	0
4	NA	P	3102	1/1	0.21	0.05	55,55,55,55	0
4	NA	O	3102	1/1	0.18	-0.20	37,37,37,37	0
4	NA	M	3102	1/1	0.19	-0.22	43,43,43,43	0
4	NA	N	3102	1/1	0.15	-0.55	31,31,31,31	0
3	MG	N	3002	1/1	0.17	-0.63	30,30,30,30	0
3	MG	K	3001	1/1	0.16	-0.77	45,45,45,45	0
3	MG	K	3002	1/1	0.16	-0.93	39,39,39,39	0
3	MG	L	3002	1/1	0.15	-1.00	39,39,39,39	0
3	MG	J	3001	1/1	0.06	-1.85	31,31,31,31	0
4	NA	J	3101	1/1	0.10	-1.91	38,38,38,38	0
3	MG	L	3001	1/1	0.10	-2.03	46,46,46,46	0
3	MG	M	3001	1/1	0.13	-2.36	48,48,48,48	0
3	MG	I	3002	1/1	0.06	-2.76	26,26,26,26	0
3	MG	P	3002	1/1	0.10	-3.48	53,53,53,53	0
3	MG	J	3002	1/1	0.08	-3.54	24,24,24,24	0
3	MG	M	3002	1/1	0.10	-3.73	41,41,41,41	0
4	NA	L	3102	1/1	0.10	-3.74	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.