



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:25 PM UTC

PDB ID : 4V44 / pdb_00004v44
Title : E. COLI (lacZ) BETA-GALACTOSIDASE IN COMPLEX WITH 2-F-LACTOSE
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 X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

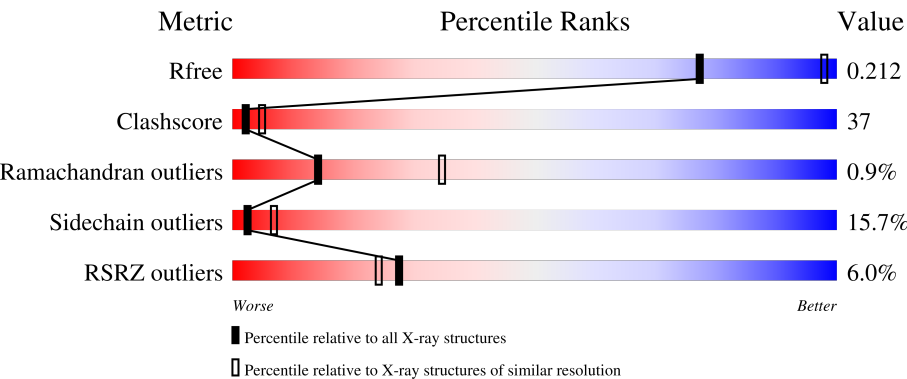
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1023	2% 43%41%14%
1	B	1023	% 43%41%14%
1	C	1023	2% 45%40%14%
1	D	1023	4% 43%42%14%
1	E	1023	12% 43%41%14%

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Mol	Chain	Length	Quality of chain
1	F	1023	2% 44% 41% 14%
1	G	1023	% 43% 42% 13%
1	H	1023	5% 44% 41% 13%
1	I	1023	2% 44% 40% 14%
1	J	1023	2% 44% 41% 13%
1	K	1023	2% 44% 40% 14%
1	L	1023	4% 43% 41% 14%
1	M	1023	16% 43% 41% 14%
1	N	1023	3% 44% 40% 14%
1	O	1023	2% 43% 42% 14%
1	P	1023	35% 43% 42% 14%
2	Q	2	50% 50%
2	R	2	50% 50%
2	S	2	50% 50%
2	T	2	50% 50%
2	U	2	50% 50%
2	V	2	50% 50%
2	W	2	50% 50%
2	X	2	50% 50%
2	Y	2	50% 50%
2	Z	2	50% 50%
2	a	2	50% 50%
2	b	2	50% 50%
2	c	2	50% 50%
2	d	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	e	2	 50% 50%
2	f	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CME	A	1021	-	-	X	-
1	CME	B	1021	-	-	X	-
1	CME	C	1021	-	-	X	-
1	CME	D	1021	-	-	X	-
1	CME	E	1021	-	-	X	-
1	CME	F	1021	-	-	X	-
1	CME	G	1021	-	-	X	-
1	CME	H	1021	-	-	X	-
1	CME	I	1021	-	-	X	-
1	CME	J	1021	-	-	X	-
1	CME	K	1021	-	-	X	-
1	CME	L	1021	-	-	X	-
1	CME	M	1021	-	-	X	-
1	CME	N	1021	-	-	X	-
1	CME	O	1021	-	-	X	-
1	CME	P	1021	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 134528 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-Galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	B	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	C	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	D	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	E	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	F	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	G	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
1	H	1021	Total	C	N	O	S	0	2	0
			8219	5196	1454	1528	41			
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 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	748	CME	CYS	modified residue	UNP P00722
A	914	CME	CYS	modified residue	UNP P00722
A	1021	CME	CYS	modified residue	UNP P00722
B	748	CME	CYS	modified residue	UNP P00722
B	914	CME	CYS	modified residue	UNP P00722
B	1021	CME	CYS	modified residue	UNP P00722
C	748	CME	CYS	modified residue	UNP P00722
C	914	CME	CYS	modified residue	UNP P00722
C	1021	CME	CYS	modified residue	UNP P00722
D	748	CME	CYS	modified residue	UNP P00722
D	914	CME	CYS	modified residue	UNP P00722
D	1021	CME	CYS	modified residue	UNP P00722
E	748	CME	CYS	modified residue	UNP P00722
E	914	CME	CYS	modified residue	UNP P00722
E	1021	CME	CYS	modified residue	UNP P00722
F	748	CME	CYS	modified residue	UNP P00722
F	914	CME	CYS	modified residue	UNP P00722
F	1021	CME	CYS	modified residue	UNP P00722
G	748	CME	CYS	modified residue	UNP P00722
G	914	CME	CYS	modified residue	UNP P00722
G	1021	CME	CYS	modified residue	UNP P00722
H	748	CME	CYS	modified residue	UNP P00722
H	914	CME	CYS	modified residue	UNP P00722
H	1021	CME	CYS	modified residue	UNP P00722
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 an oligosaccharide called 2-deoxy-2-fluoro-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	2	Total	C	F	O	0	0	0
			23	12	1	10			
2	R	2	Total	C	F	O	0	0	0
			23	12	1	10			
2	S	2	Total	C	F	O	0	0	0
			23	12	1	10			
2	T	2	Total	C	F	O	0	0	0
			23	12	1	10			
2	U	2	Total	C	F	O	0	0	0
			23	12	1	10			
2	V	2	Total	C	F	O	0	0	0
			23	12	1	10			
2	W	2	Total	C	F	O	0	0	0
			23	12	1	10			
2	X	2	Total	C	F	O	0	0	0
			23	12	1	10			
2	Y	2	Total	C	F	O	0	0	0
			23	12	1	10			
2	Z	2	Total	C	F	O	0	0	0
			23	12	1	10			
2	a	2	Total	C	F	O	0	0	0
			23	12	1	10			
2	b	2	Total	C	F	O	0	0	0
			23	12	1	10			
2	c	2	Total	C	F	O	0	0	0
			23	12	1	10			
2	d	2	Total	C	F	O	0	0	0
			23	12	1	10			
2	e	2	Total	C	F	O	0	0	0
			23	12	1	10			
2	f	2	Total	C	F	O	0	0	0
			23	12	1	10			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Mg 2	0	0
3	B	2	Total 2	Mg 2	0	0
3	C	2	Total 2	Mg 2	0	0
3	D	2	Total 2	Mg 2	0	0
3	E	2	Total 2	Mg 2	0	0
3	F	2	Total 2	Mg 2	0	0
3	G	2	Total 2	Mg 2	0	0
3	H	2	Total 2	Mg 2	0	0
3	I	2	Total 2	Mg 2	0	0
3	J	2	Total 2	Mg 2	0	0
3	K	2	Total 2	Mg 2	0	0
3	L	2	Total 2	Mg 2	0	0
3	M	2	Total 2	Mg 2	0	0
3	N	2	Total 2	Mg 2	0	0
3	O	2	Total 2	Mg 2	0	0
3	P	2	Total 2	Mg 2	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Na 2	0	0
4	B	2	Total 2	Na 2	0	0
4	C	2	Total 2	Na 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total 2	Na 2	0	0
4	E	2	Total 2	Na 2	0	0
4	F	2	Total 2	Na 2	0	0
4	G	2	Total 2	Na 2	0	0
4	H	2	Total 2	Na 2	0	0
4	I	2	Total 2	Na 2	0	0
4	J	2	Total 2	Na 2	0	0
4	K	2	Total 2	Na 2	0	0
4	L	2	Total 2	Na 2	0	0
4	M	2	Total 2	Na 2	0	0
4	N	2	Total 2	Na 2	0	0
4	O	2	Total 2	Na 2	0	0
4	P	2	Total 2	Na 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	160	Total 160	O 160	0	0
5	B	163	Total 163	O 163	0	0
5	C	162	Total 162	O 162	0	0
5	D	163	Total 163	O 163	0	0
5	E	162	Total 162	O 162	0	0
5	F	162	Total 162	O 162	0	0

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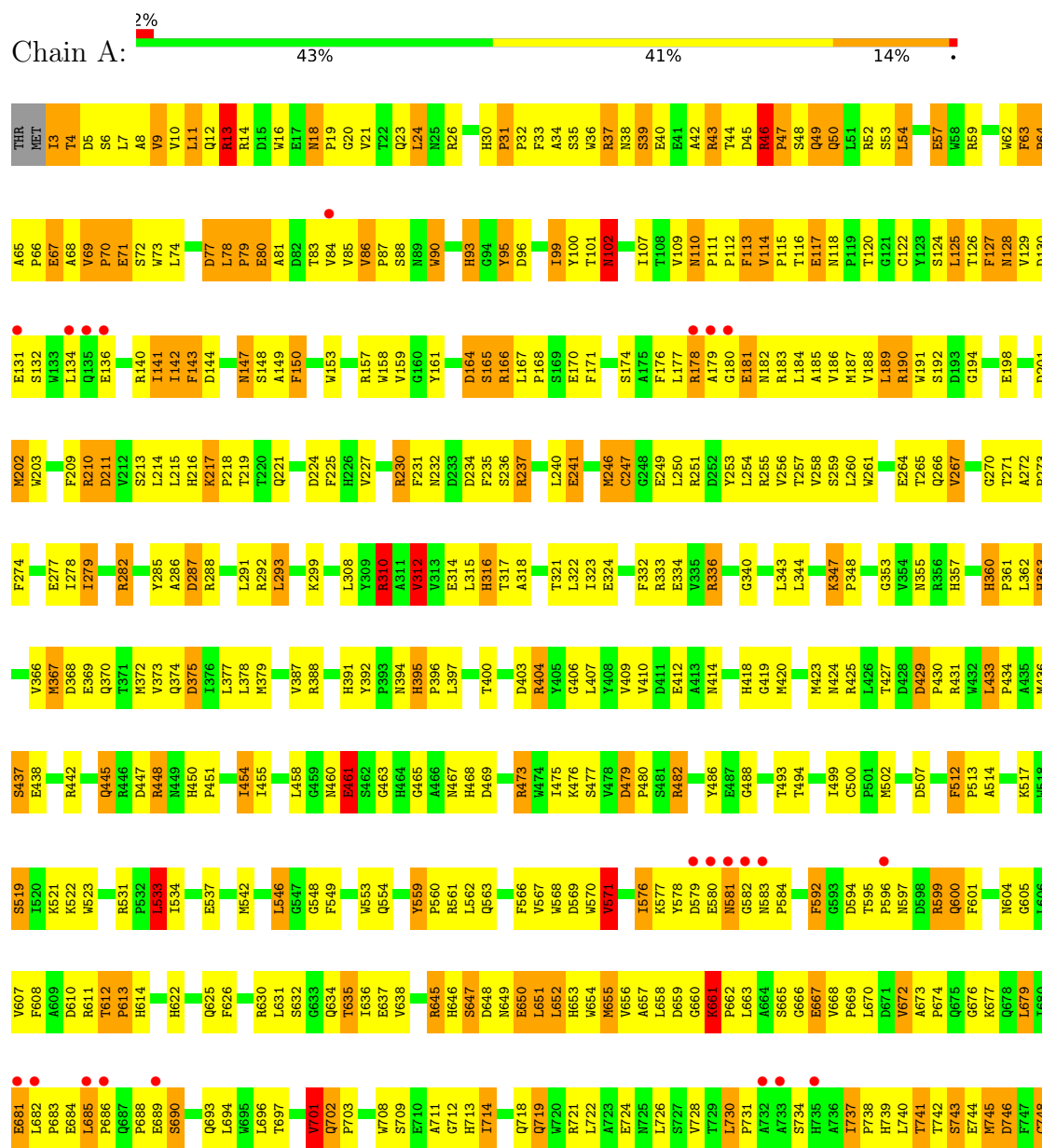
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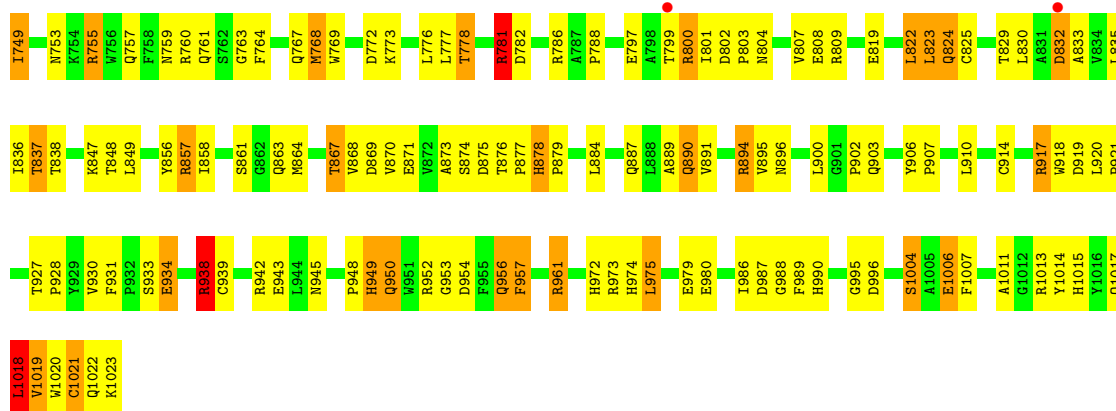
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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5	H	162	Total 162	O 162	0	0
5	I	162	Total 162	O 162	0	0
5	J	162	Total 162	O 162	0	0
5	K	162	Total 162	O 162	0	0
5	L	162	Total 162	O 162	0	0
5	M	161	Total 161	O 161	0	0
5	N	163	Total 163	O 163	0	0
5	O	161	Total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

3 Residue-property plots

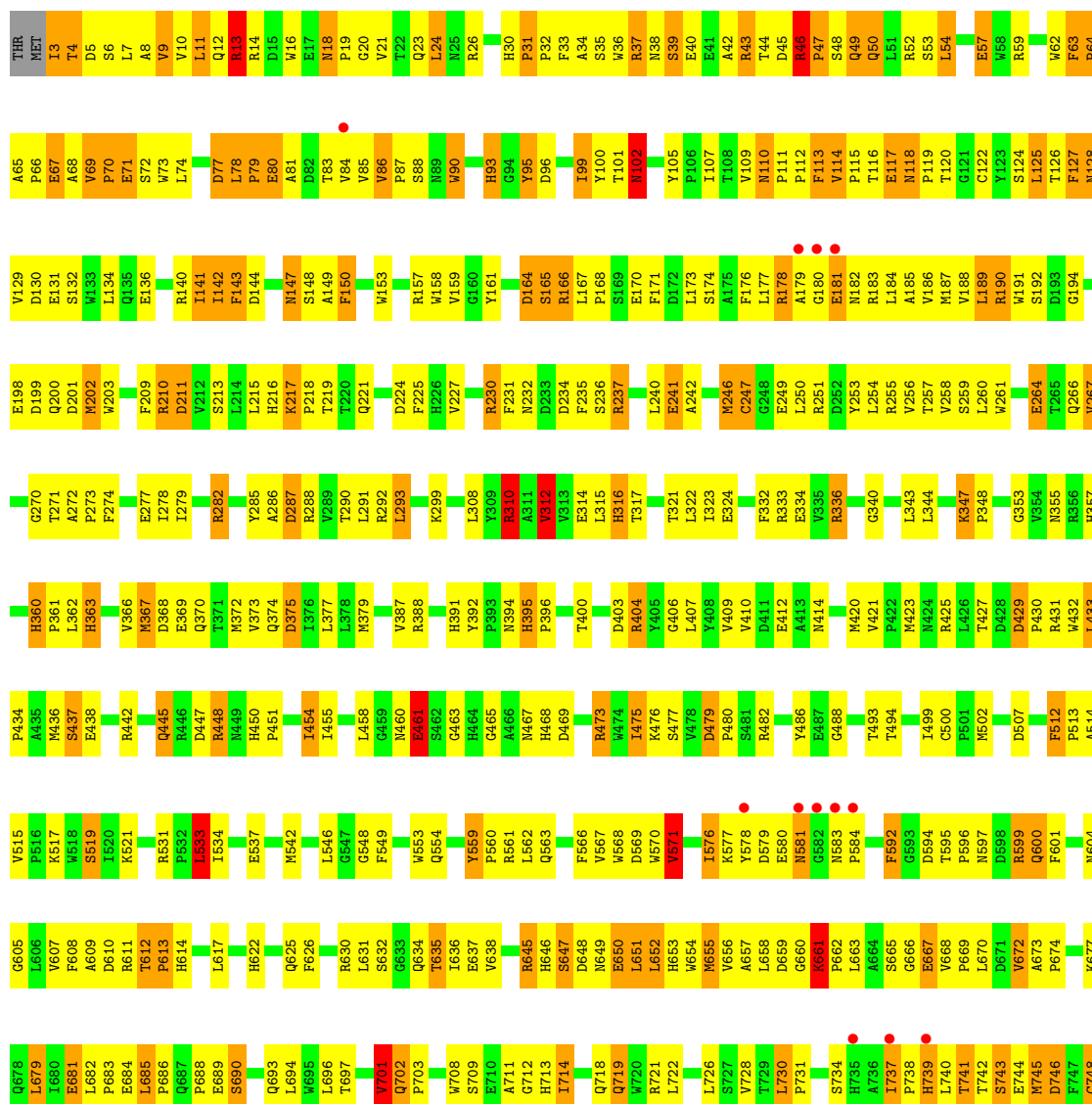
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

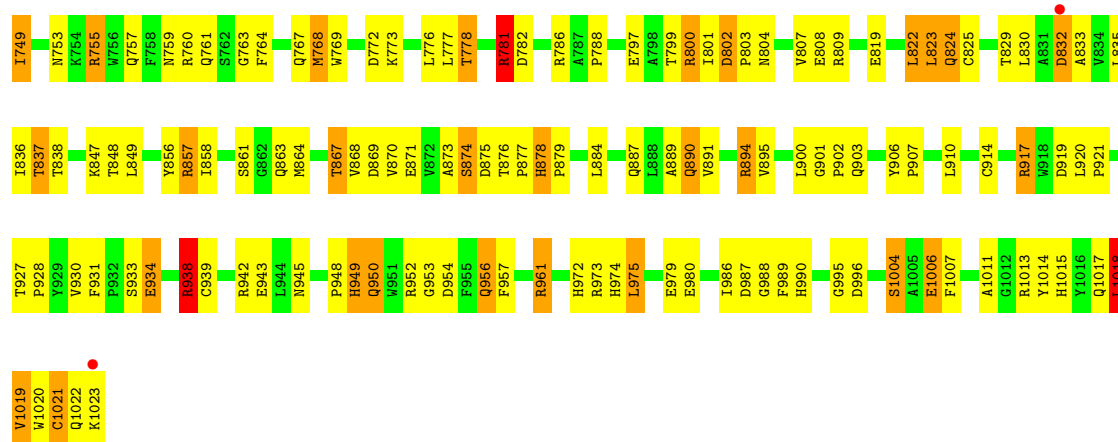
• Molecule 1: Beta-Galactosidase



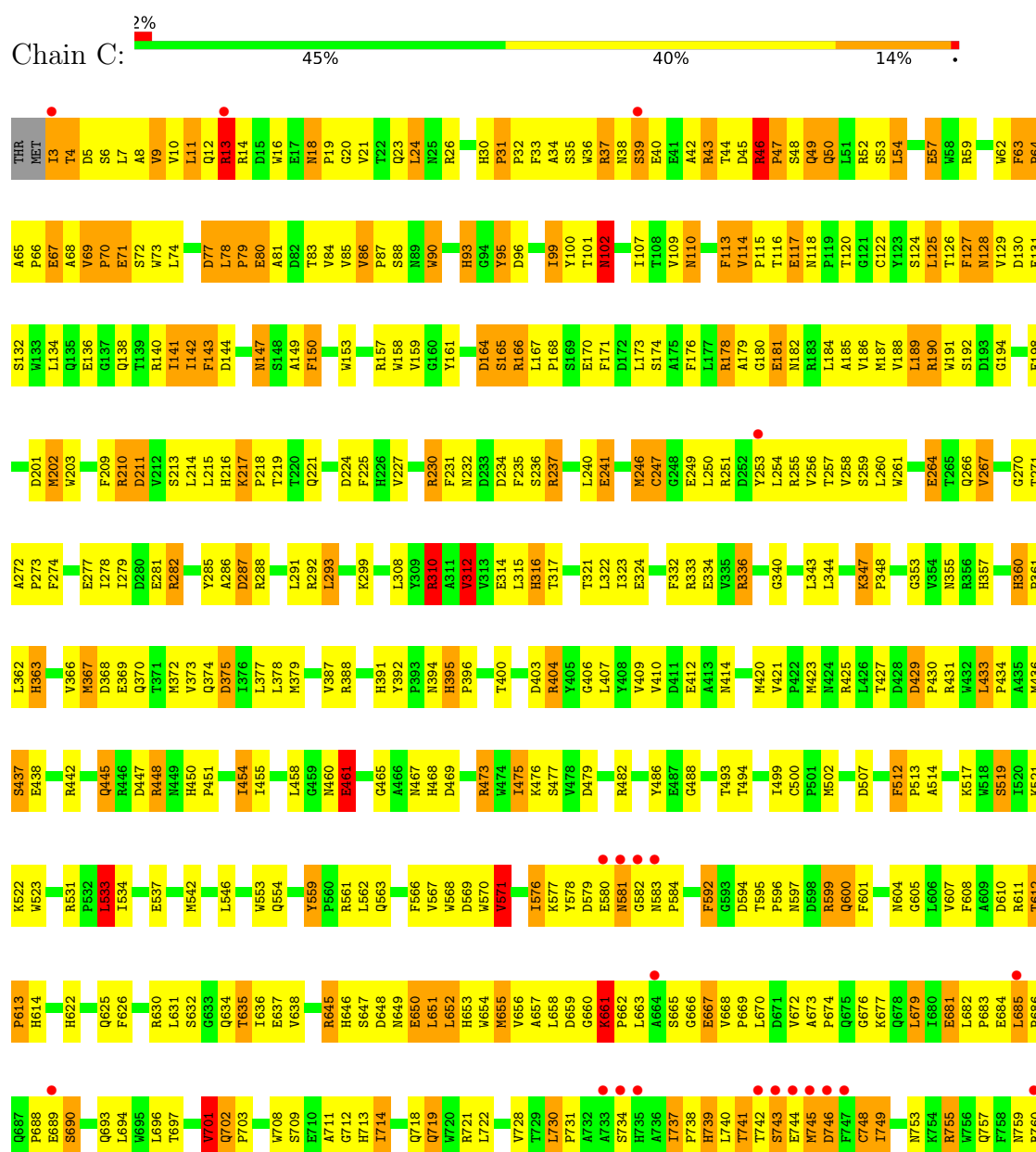


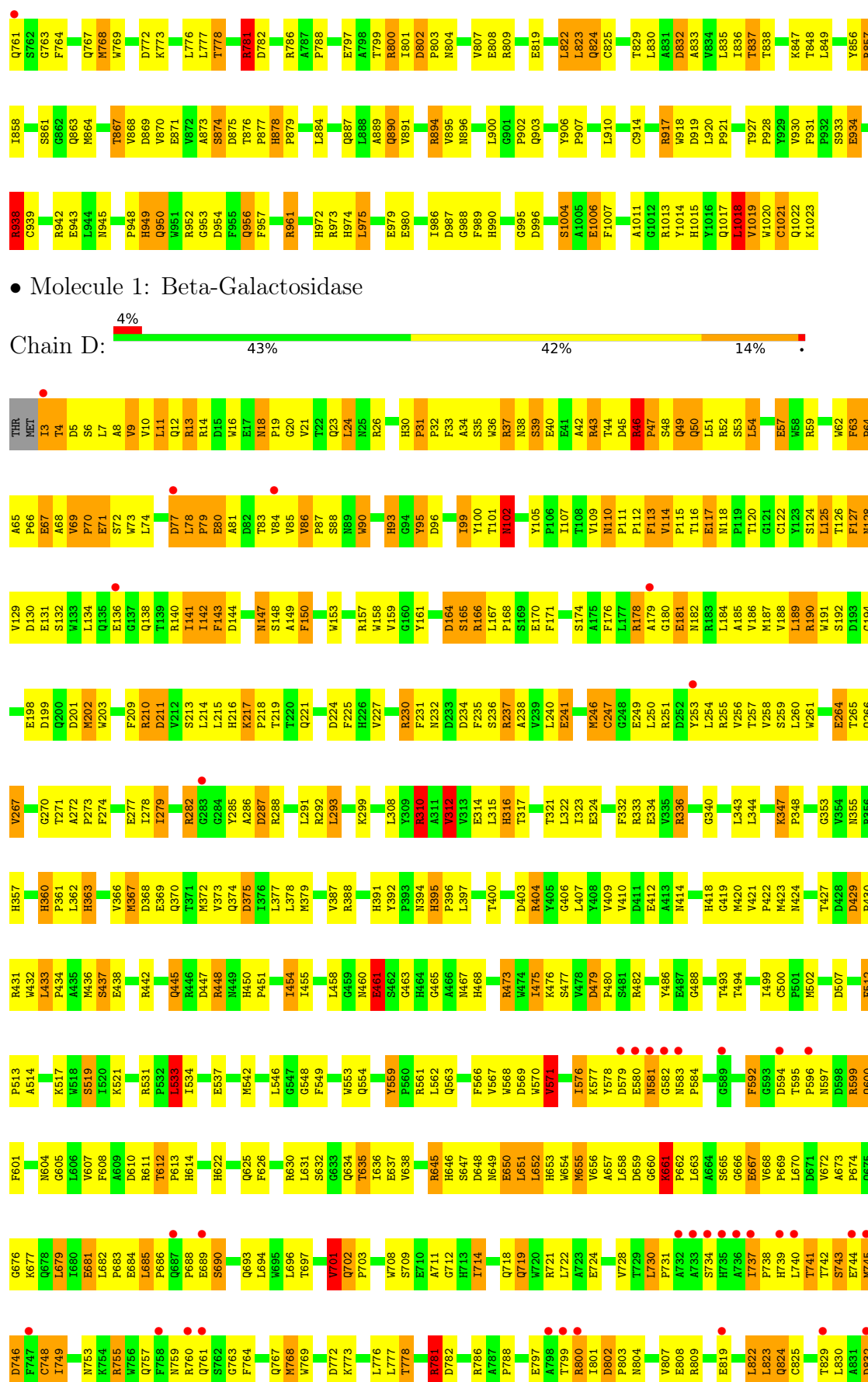
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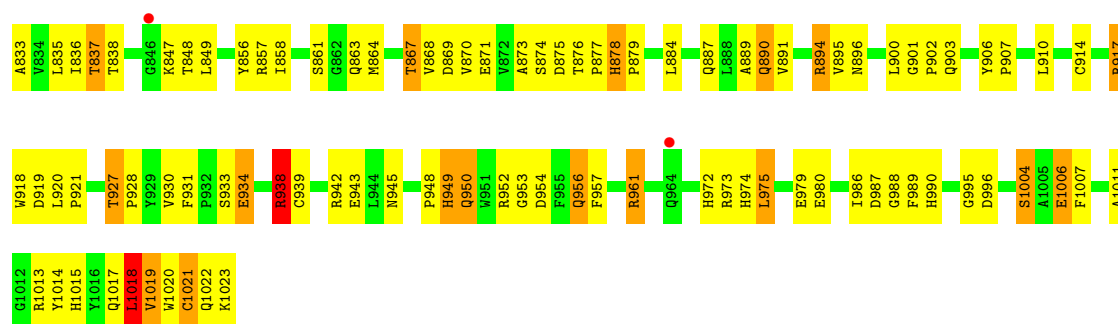




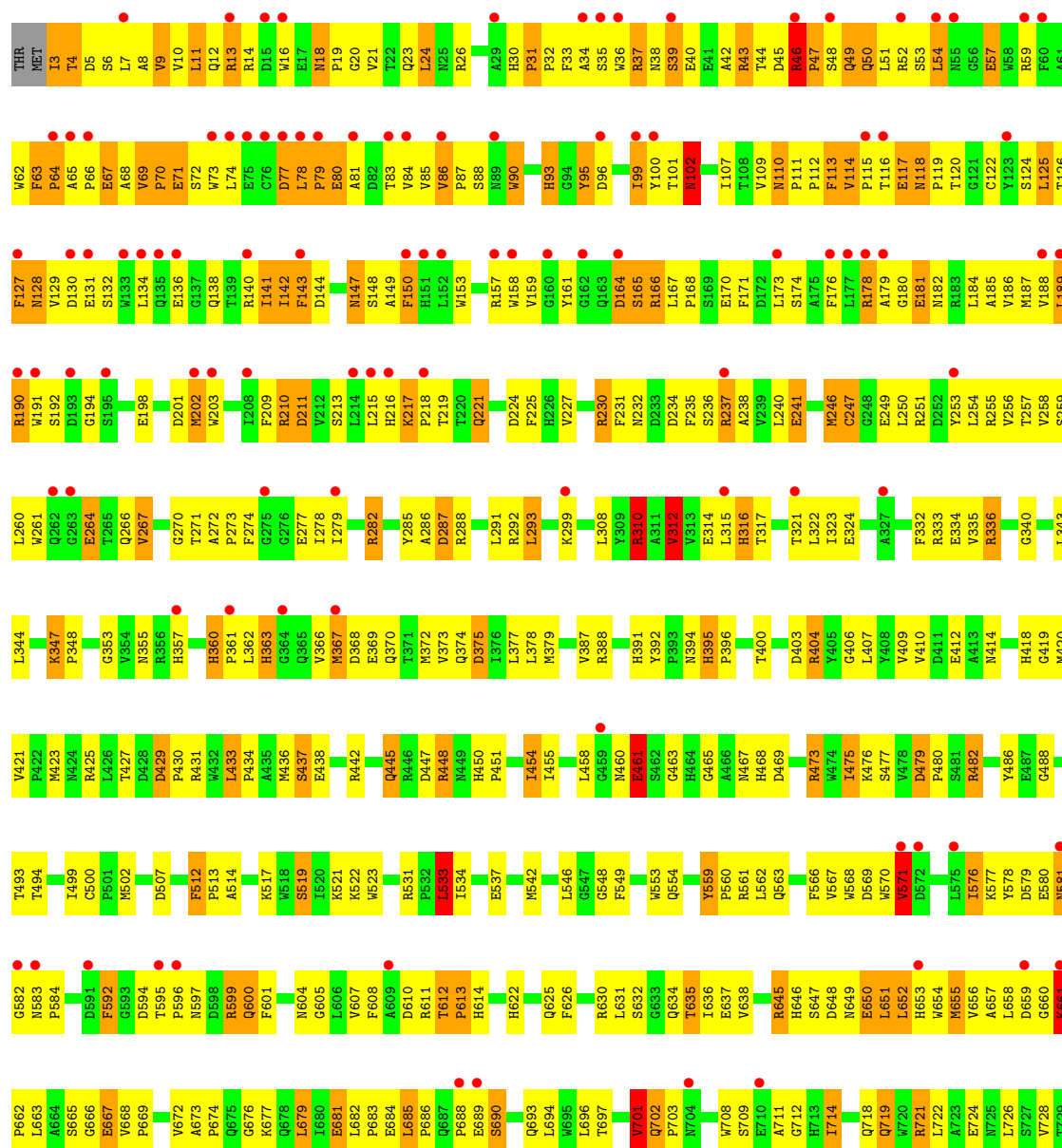
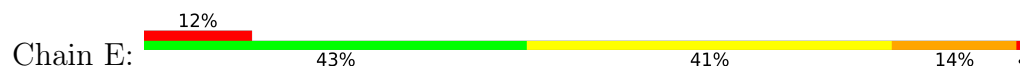
● Molecule 1: Beta-Galactosidase

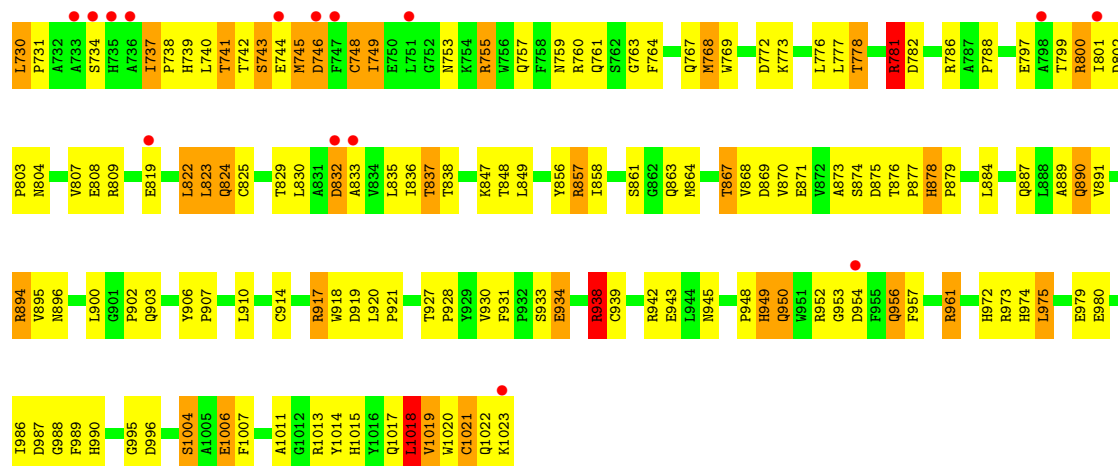




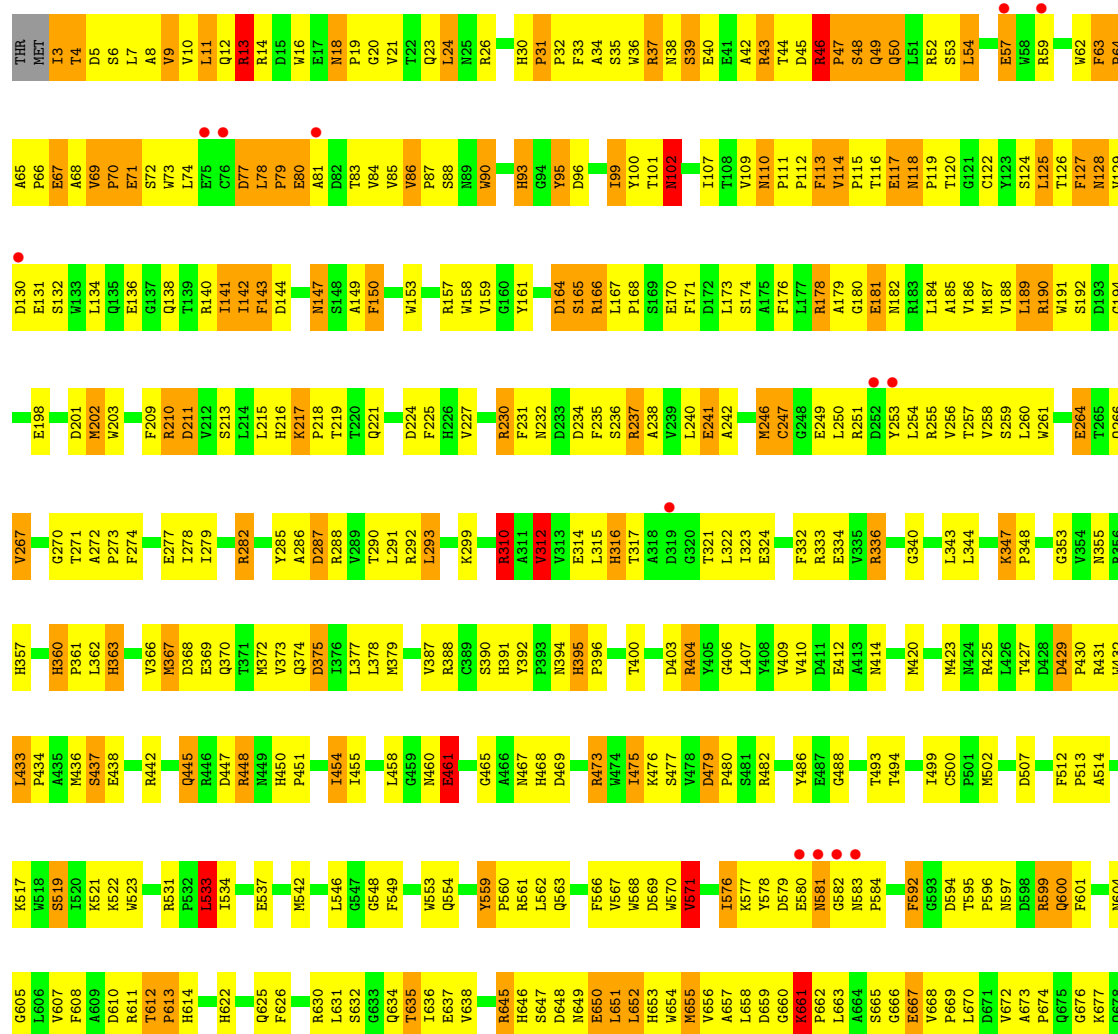
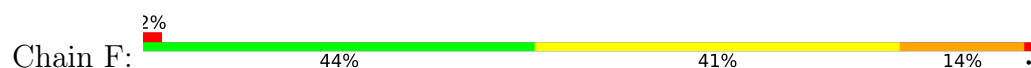


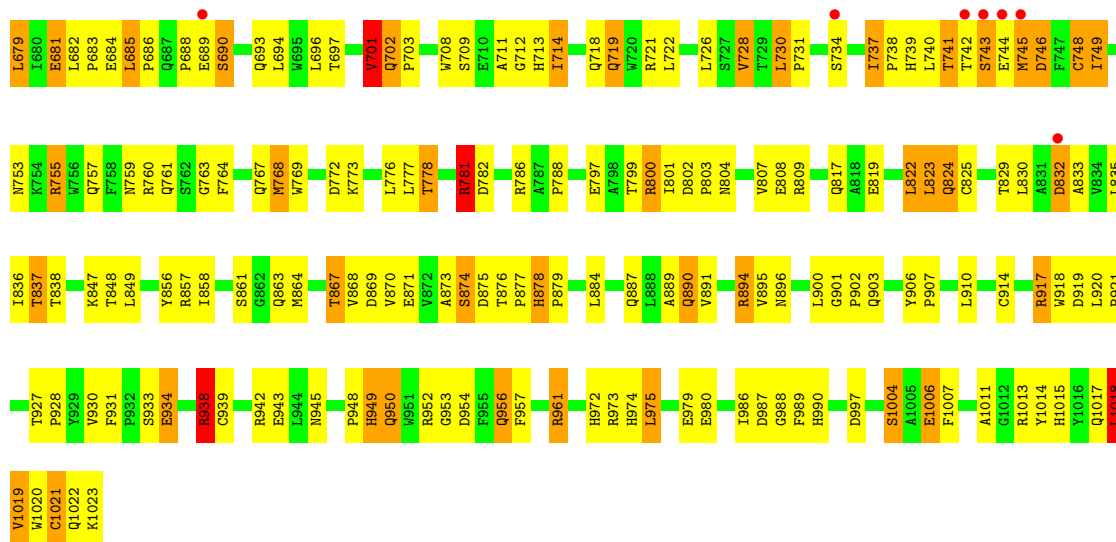
• Molecule 1: Beta-Galactosidase



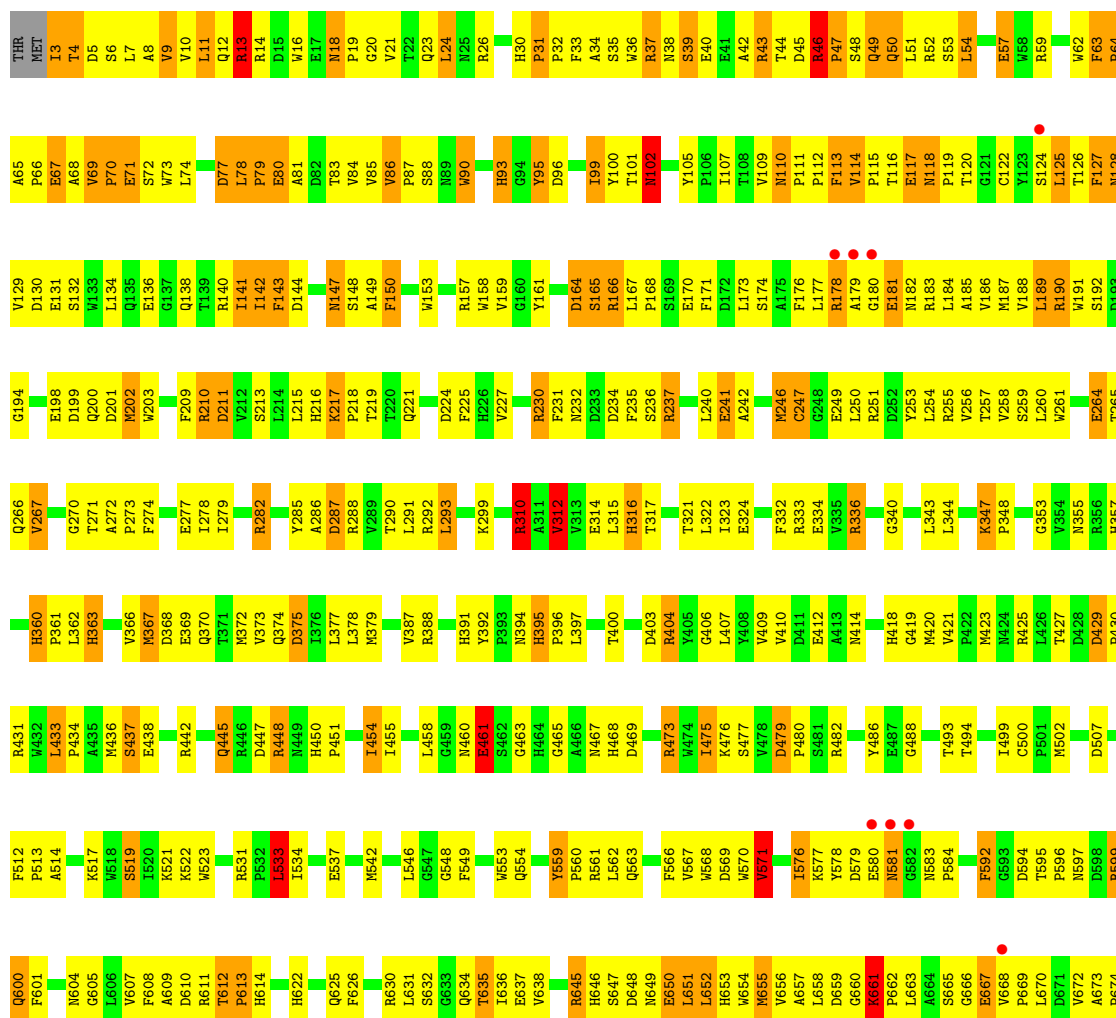
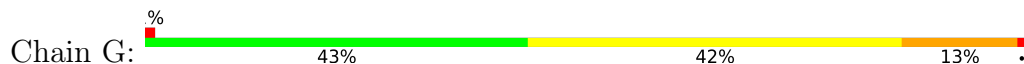


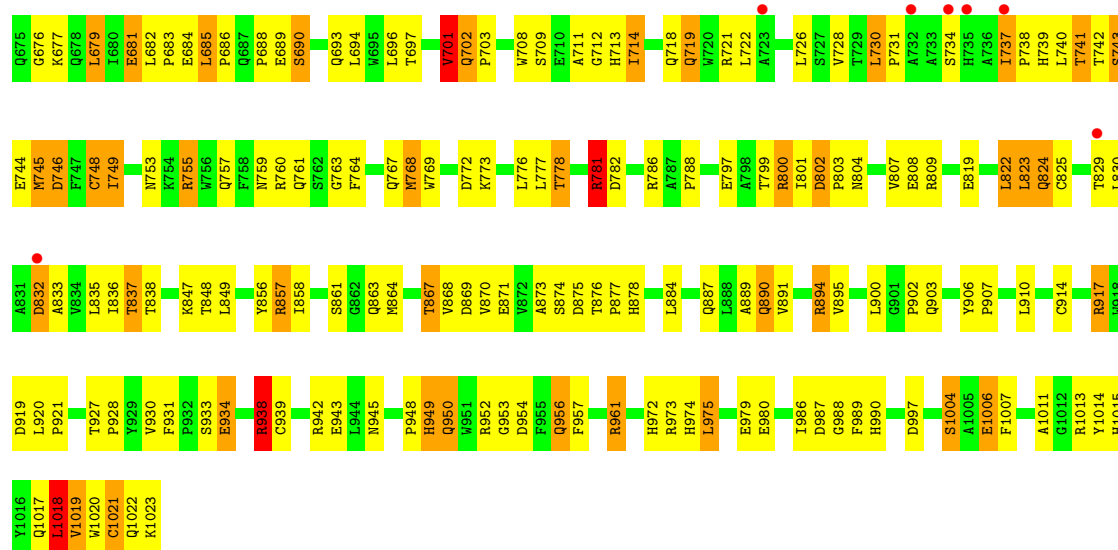
• Molecule 1: Beta-Galactosidase



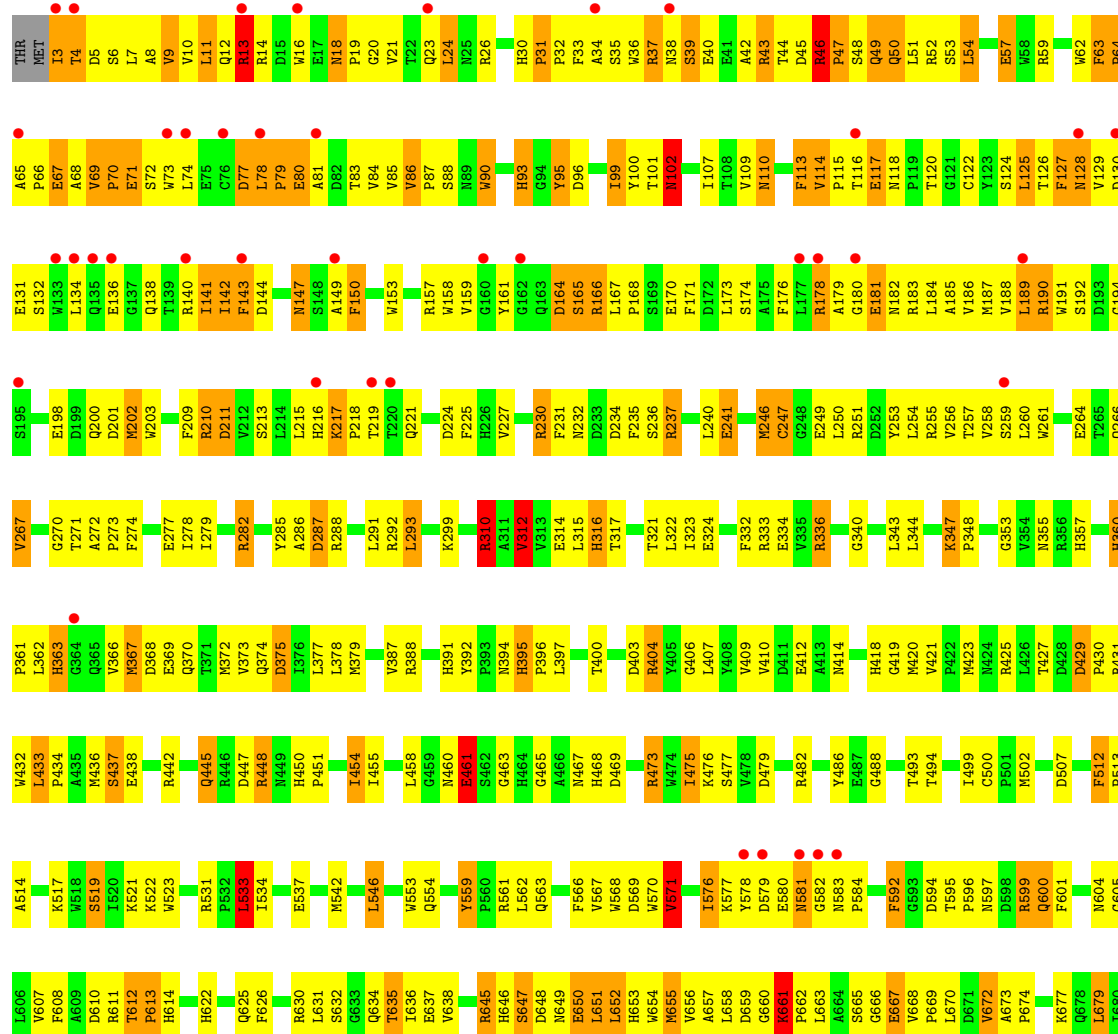
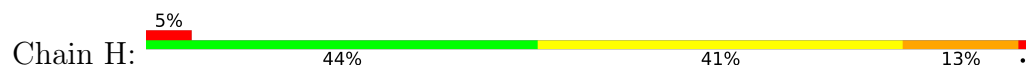


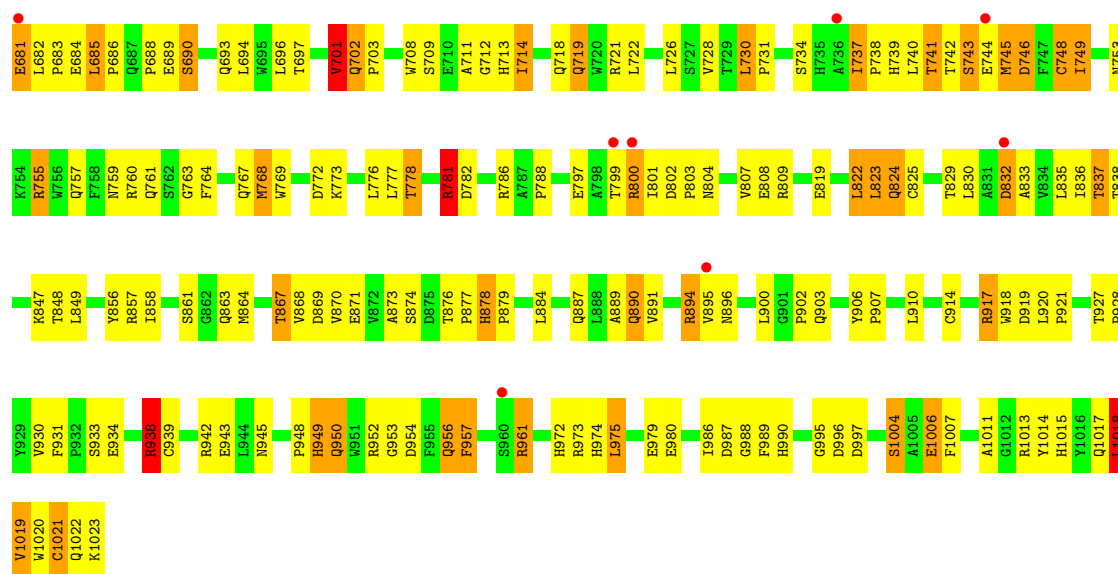
• Molecule 1: Beta-Galactosidase



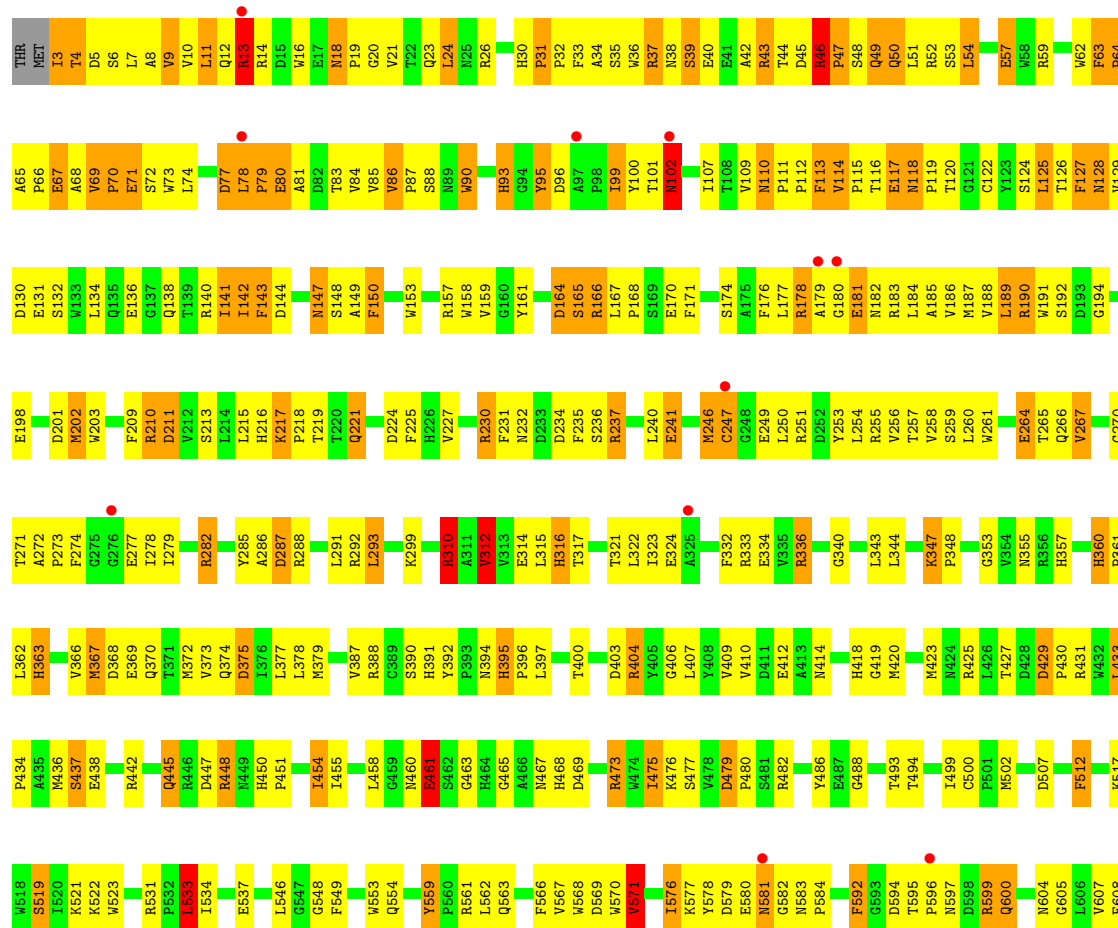
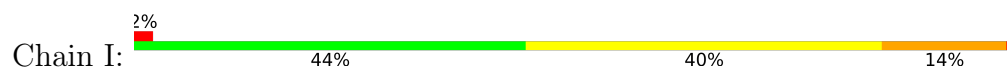


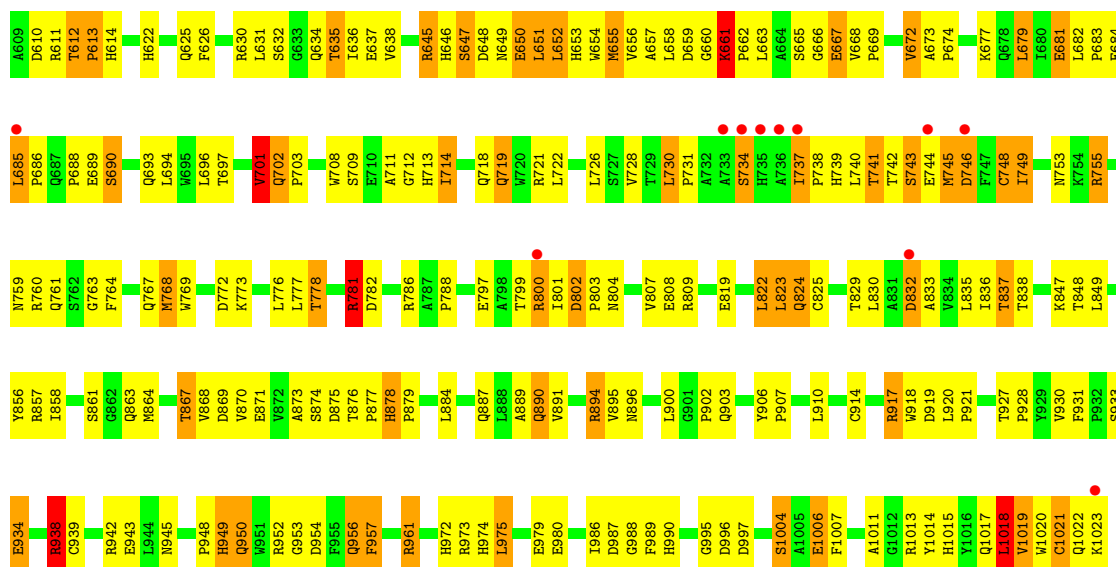
• Molecule 1: Beta-Galactosidase



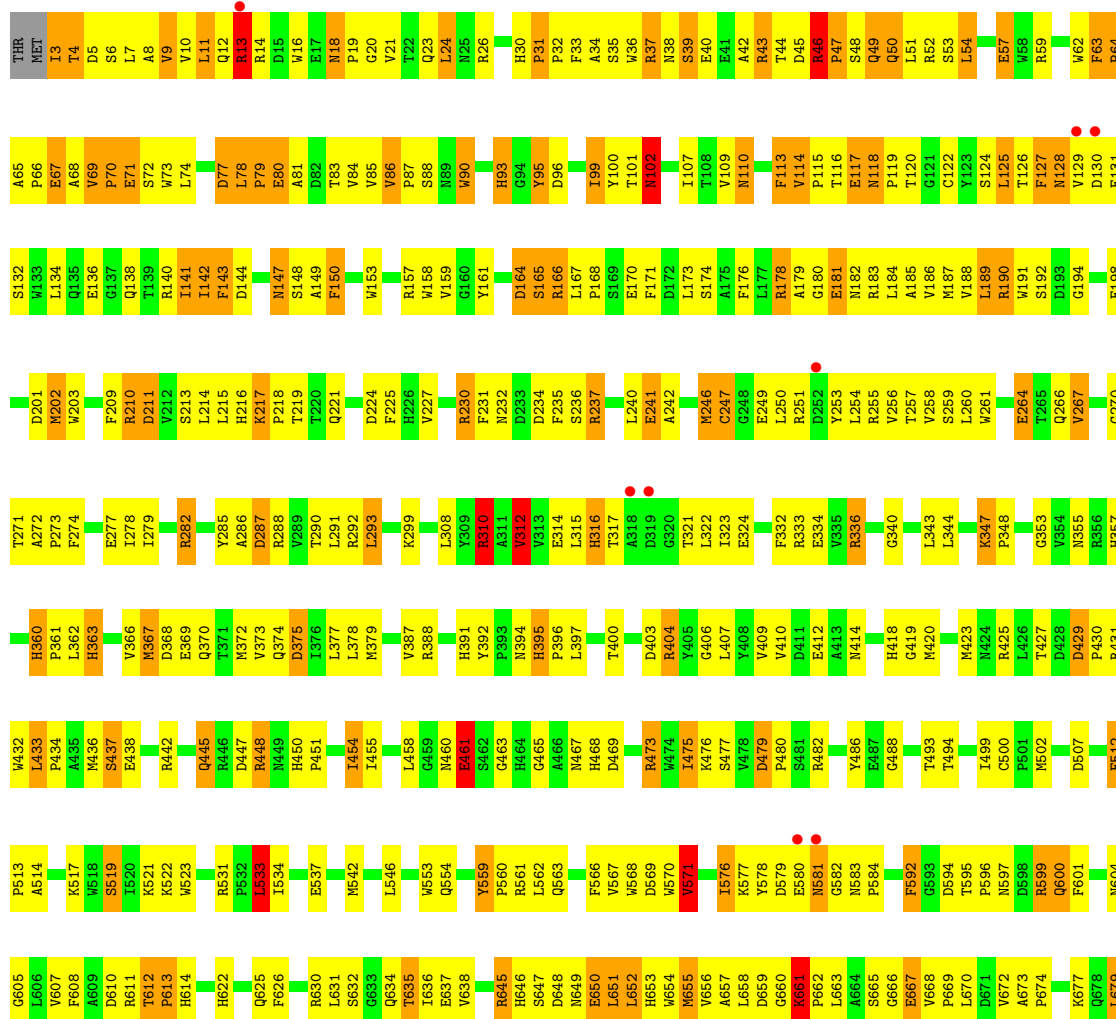
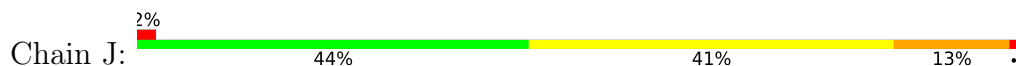


• Molecule 1: Beta-Galactosidase



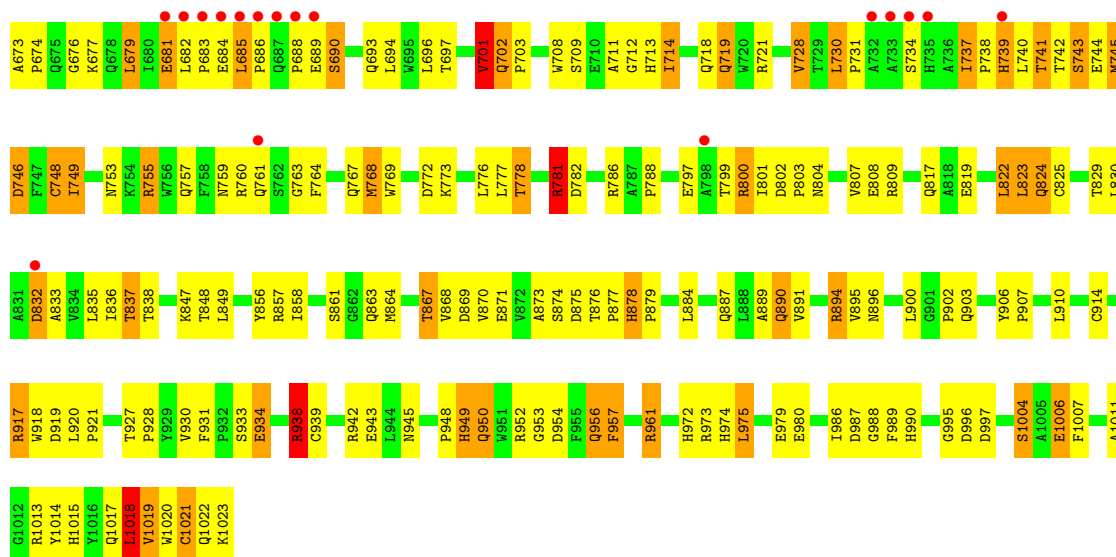


• Molecule 1: Beta-Galactosidase

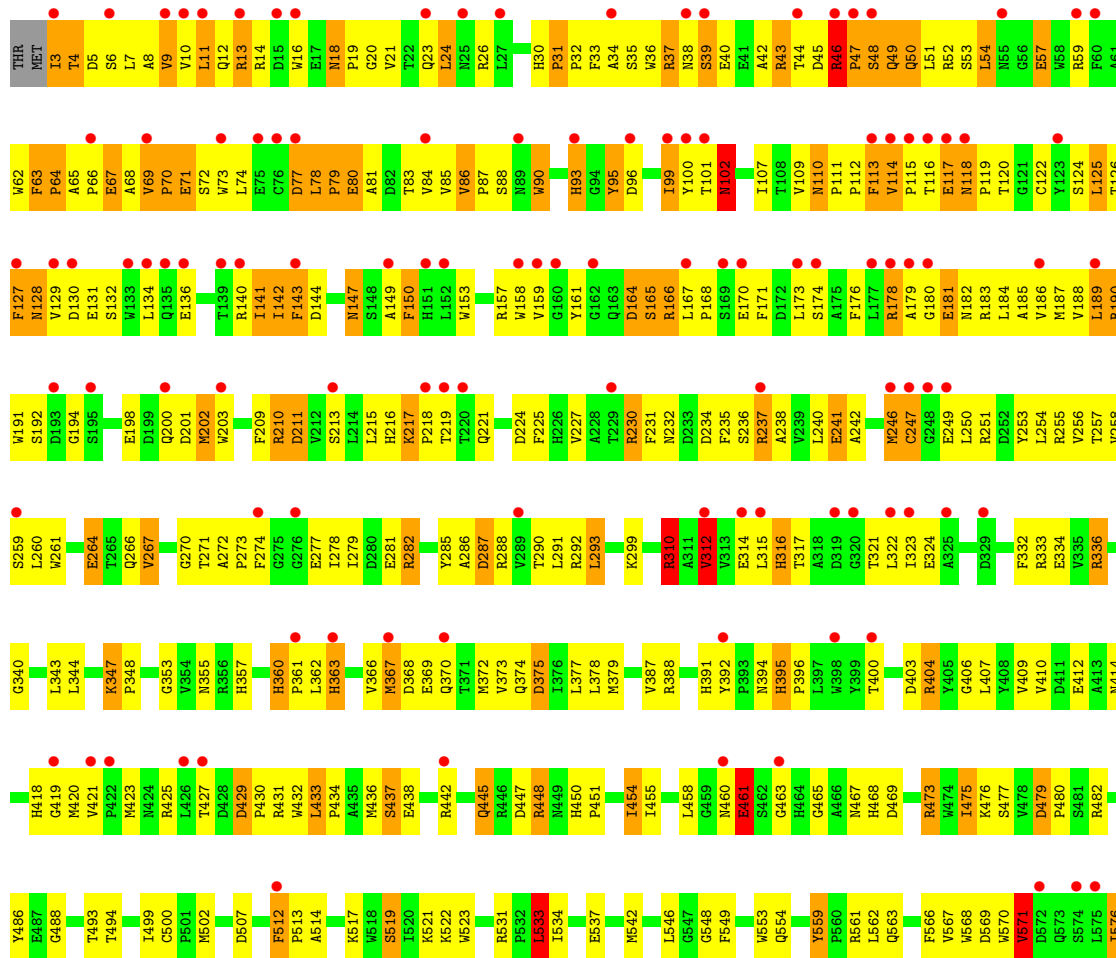
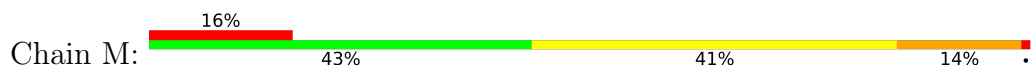


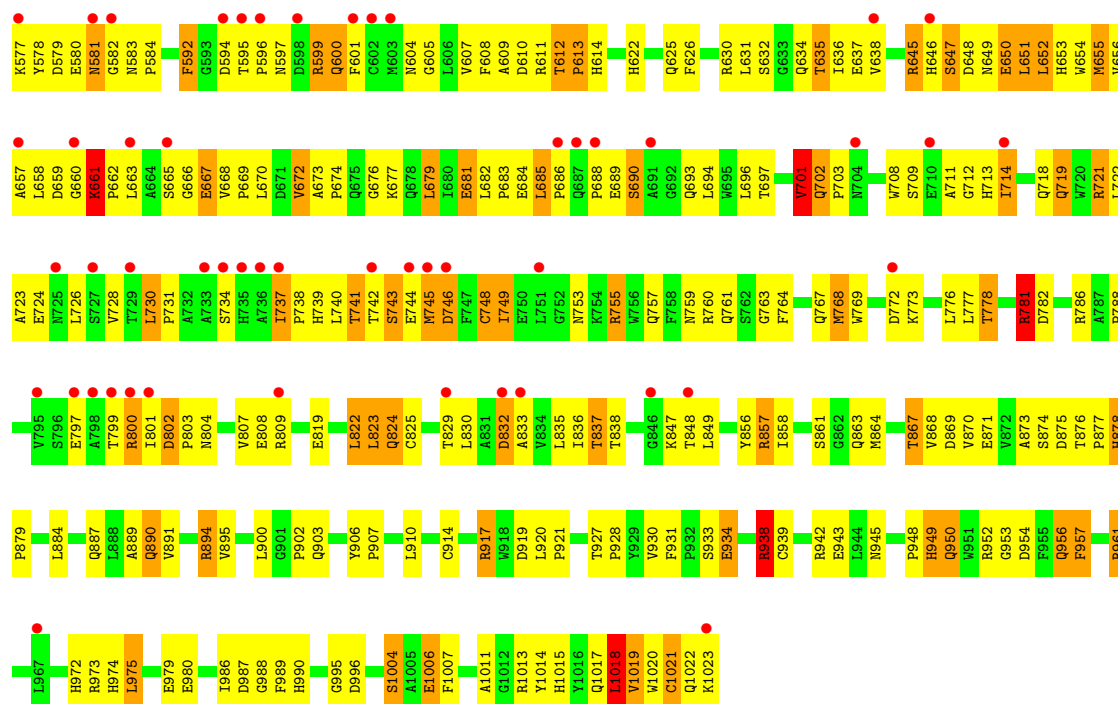




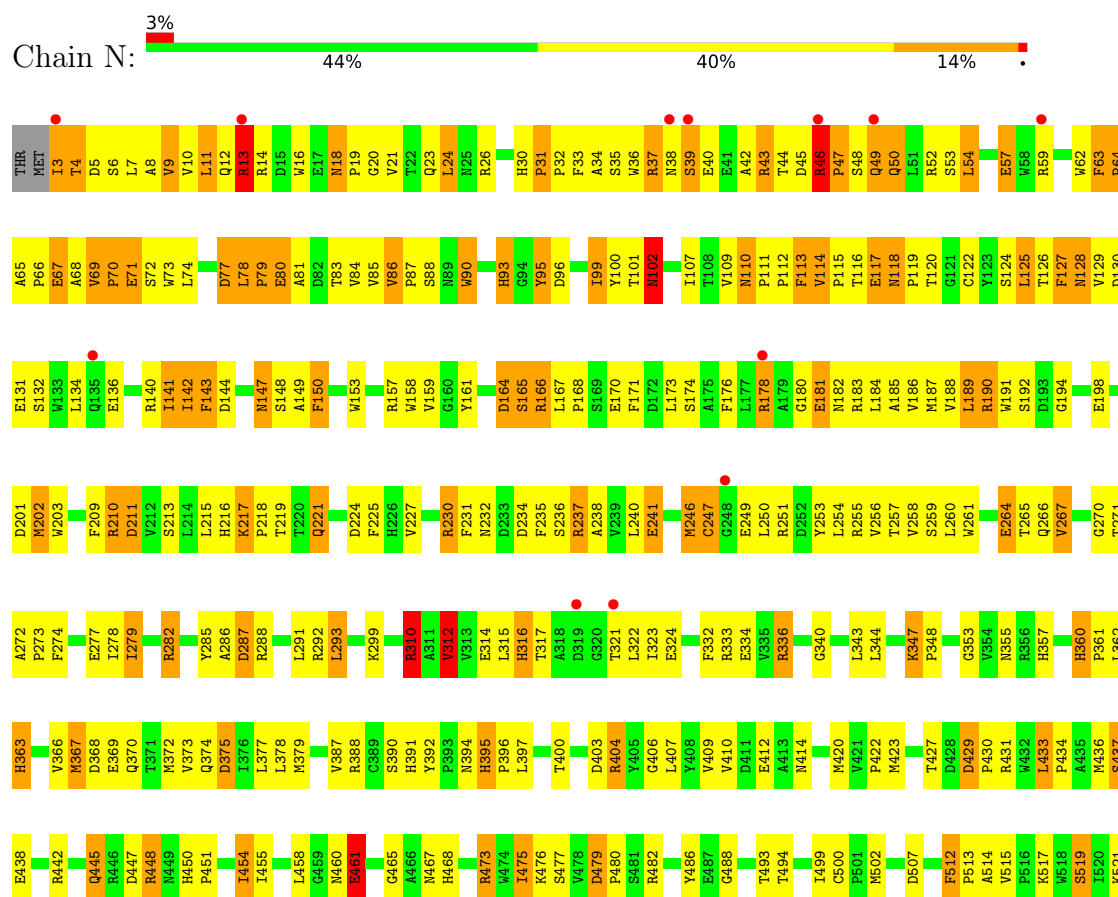


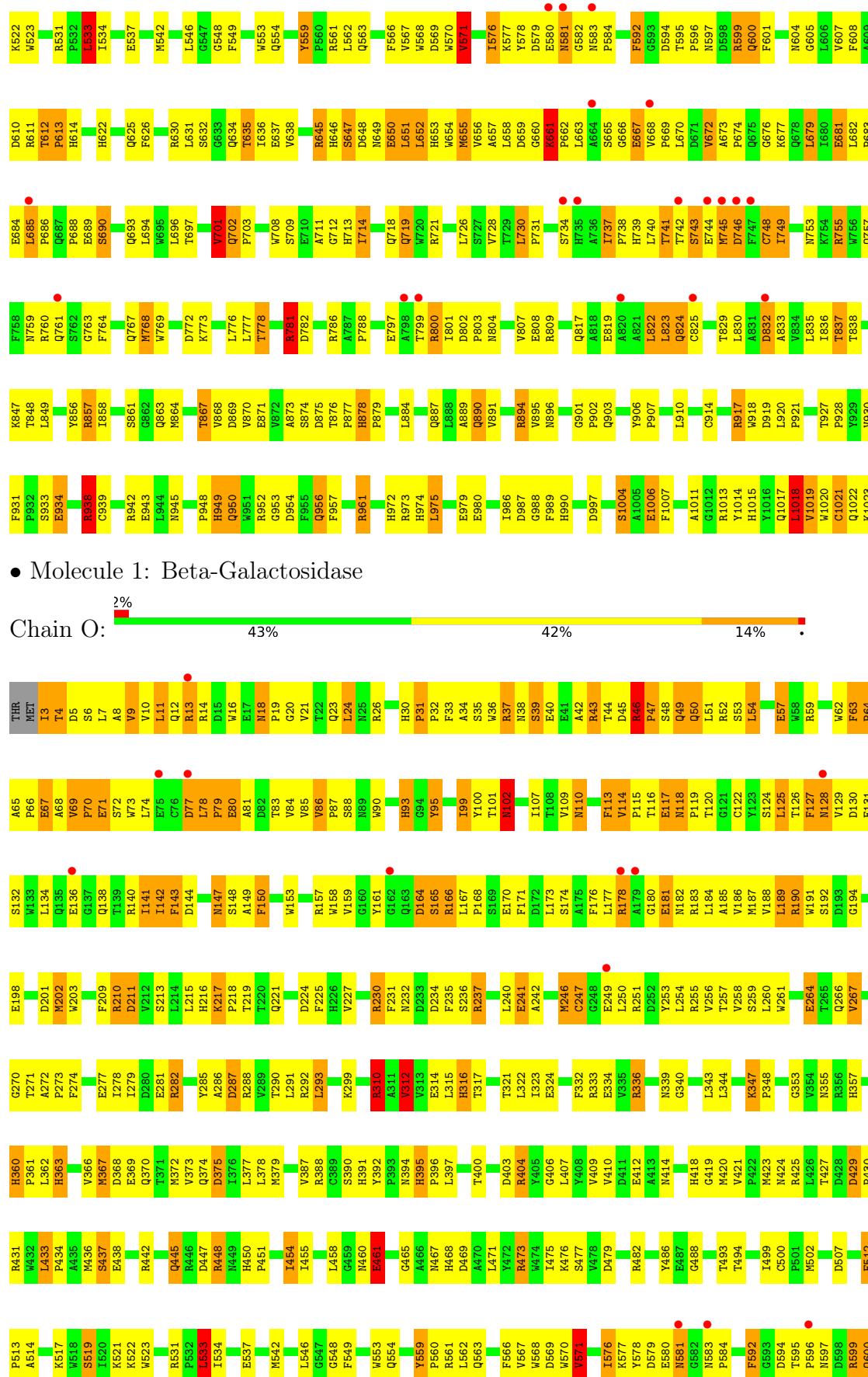
• Molecule 1: Beta-Galactosidase



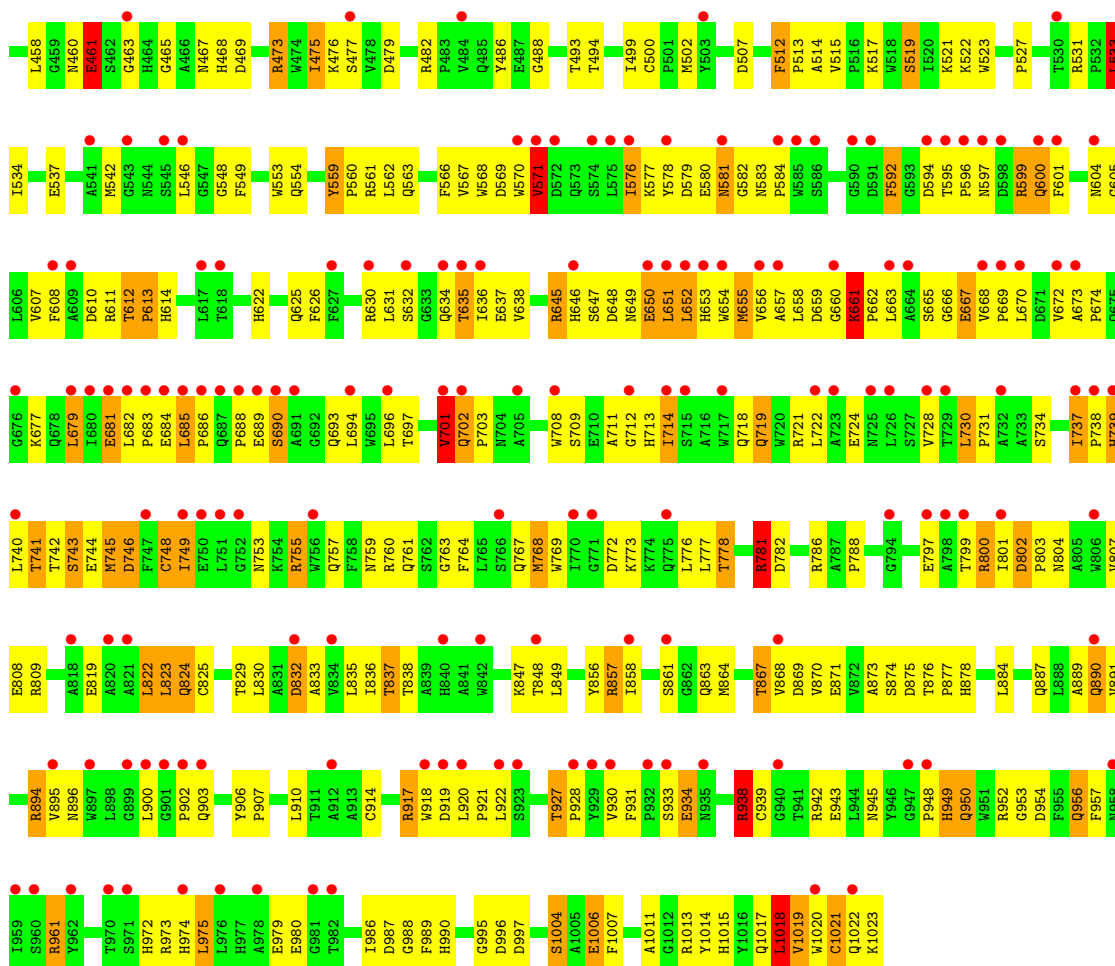


• Molecule 1: Beta-Galactosidase









- Molecule 2: 2-deoxy-2-fluoro-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain Q: 50% 50%



- Molecule 2: 2-deoxy-2-fluoro-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain R: 50% 50%



- Molecule 2: 2-deoxy-2-fluoro-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain S: 50% 50%



- Molecule 2: 2-deoxy-2-fluoro-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain T:  50% 50%



- Molecule 2: 2-deoxy-2-fluoro-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain U:  50% 50%



- Molecule 2: 2-deoxy-2-fluoro-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain V:  50% 50%



- Molecule 2: 2-deoxy-2-fluoro-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain W:  50% 50%



- Molecule 2: 2-deoxy-2-fluoro-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain X:  50% 50%



- Molecule 2: 2-deoxy-2-fluoro-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain Y:  50% 50%



- Molecule 2: 2-deoxy-2-fluoro-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain Z:  50% 50%



- Molecule 2: 2-deoxy-2-fluoro-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain a:  50% 50%



- Molecule 2: 2-deoxy-2-fluoro-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain b:



- Molecule 2: 2-deoxy-2-fluoro-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain c:



- Molecule 2: 2-deoxy-2-fluoro-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain d:



- Molecule 2: 2-deoxy-2-fluoro-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain e:



- Molecule 2: 2-deoxy-2-fluoro-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain f:



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 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	66.0 (20.00-2.70) 65.8 (20.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.71Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.234 , (Not available) 0.211 , 0.212	Depositor DCC
R_{free} test set	1909 reflections (0.47%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 95.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	134528	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.37	5/8439 (0.1%)	1.70	117/11510 (1.0%)
1	B	1.37	5/8439 (0.1%)	1.70	119/11510 (1.0%)
1	C	1.37	5/8439 (0.1%)	1.70	119/11510 (1.0%)
1	D	1.37	6/8439 (0.1%)	1.70	117/11510 (1.0%)
1	E	1.37	5/8439 (0.1%)	1.70	117/11510 (1.0%)
1	F	1.37	5/8439 (0.1%)	1.70	117/11510 (1.0%)
1	G	1.37	5/8439 (0.1%)	1.70	119/11510 (1.0%)
1	H	1.37	5/8439 (0.1%)	1.70	118/11510 (1.0%)
1	I	1.37	5/8439 (0.1%)	1.70	120/11510 (1.0%)
1	J	1.37	5/8439 (0.1%)	1.70	117/11510 (1.0%)
1	K	1.37	5/8439 (0.1%)	1.70	118/11510 (1.0%)
1	L	1.37	5/8439 (0.1%)	1.70	119/11510 (1.0%)
1	M	1.37	5/8439 (0.1%)	1.70	118/11510 (1.0%)
1	N	1.37	5/8439 (0.1%)	1.70	118/11510 (1.0%)
1	O	1.37	5/8439 (0.1%)	1.70	119/11510 (1.0%)
1	P	1.37	6/8439 (0.1%)	1.70	118/11510 (1.0%)
All	All	1.37	82/135024 (0.1%)	1.70	1890/184160 (1.0%)

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	479	ASP	C-N	-6.90	1.27	1.33
1	P	479	ASP	C-N	-6.85	1.27	1.33
1	C	479	ASP	C-N	-6.83	1.27	1.33
1	E	479	ASP	C-N	-6.83	1.27	1.33
1	M	479	ASP	C-N	-6.83	1.27	1.33
1	D	479	ASP	C-N	-6.82	1.27	1.33
1	I	479	ASP	C-N	-6.82	1.27	1.33
1	F	479	ASP	C-N	-6.82	1.27	1.33
1	B	479	ASP	C-N	-6.79	1.27	1.33
1	O	479	ASP	C-N	-6.79	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	ASP	C-N	-6.78	1.27	1.33
1	K	479	ASP	C-N	-6.78	1.27	1.33
1	L	479	ASP	C-N	-6.75	1.27	1.33
1	H	479	ASP	C-N	-6.74	1.27	1.33
1	G	479	ASP	C-N	-6.73	1.27	1.33
1	N	479	ASP	C-N	-6.70	1.27	1.33
1	O	118	ASN	N-CA	-6.27	1.40	1.46
1	P	118	ASN	N-CA	-6.25	1.40	1.46
1	H	118	ASN	N-CA	-6.25	1.40	1.46
1	L	118	ASN	N-CA	-6.24	1.40	1.46
1	C	118	ASN	N-CA	-6.24	1.40	1.46
1	B	118	ASN	N-CA	-6.23	1.40	1.46
1	D	118	ASN	N-CA	-6.23	1.40	1.46
1	J	118	ASN	N-CA	-6.23	1.40	1.46
1	G	118	ASN	N-CA	-6.22	1.40	1.46
1	F	118	ASN	N-CA	-6.22	1.40	1.46
1	E	118	ASN	N-CA	-6.21	1.40	1.46
1	K	118	ASN	N-CA	-6.21	1.40	1.46
1	A	118	ASN	N-CA	-6.21	1.40	1.46
1	M	118	ASN	N-CA	-6.19	1.40	1.46
1	N	118	ASN	N-CA	-6.19	1.40	1.46
1	I	118	ASN	N-CA	-6.16	1.40	1.46
1	P	31	PRO	C-N	-5.85	1.27	1.33
1	K	31	PRO	C-N	-5.81	1.27	1.33
1	G	31	PRO	C-N	-5.81	1.27	1.33
1	D	31	PRO	C-N	-5.81	1.27	1.33
1	I	31	PRO	C-N	-5.78	1.27	1.33
1	J	31	PRO	C-N	-5.78	1.27	1.33
1	H	31	PRO	C-N	-5.78	1.27	1.33
1	B	31	PRO	C-N	-5.77	1.27	1.33
1	M	31	PRO	C-N	-5.77	1.27	1.33
1	N	31	PRO	C-N	-5.76	1.27	1.33
1	O	31	PRO	C-N	-5.76	1.27	1.33
1	A	31	PRO	C-N	-5.75	1.27	1.33
1	E	31	PRO	C-N	-5.75	1.27	1.33
1	L	31	PRO	C-N	-5.73	1.27	1.33
1	C	31	PRO	C-N	-5.73	1.27	1.33
1	F	31	PRO	C-N	-5.72	1.27	1.33
1	C	454	ILE	CA-CB	-5.71	1.48	1.54
1	M	454	ILE	CA-CB	-5.69	1.48	1.54
1	H	454	ILE	CA-CB	-5.69	1.48	1.54
1	G	454	ILE	CA-CB	-5.68	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	454	ILE	CA-CB	-5.66	1.48	1.54
1	O	454	ILE	CA-CB	-5.65	1.48	1.54
1	D	454	ILE	CA-CB	-5.65	1.48	1.54
1	A	454	ILE	CA-CB	-5.64	1.48	1.54
1	B	454	ILE	CA-CB	-5.64	1.48	1.54
1	E	454	ILE	CA-CB	-5.64	1.48	1.54
1	J	454	ILE	CA-CB	-5.64	1.48	1.54
1	L	454	ILE	CA-CB	-5.64	1.48	1.54
1	N	454	ILE	CA-CB	-5.63	1.48	1.54
1	B	636	ILE	CA-CB	-5.63	1.47	1.54
1	F	454	ILE	CA-CB	-5.63	1.48	1.54
1	H	636	ILE	CA-CB	-5.63	1.47	1.54
1	M	636	ILE	CA-CB	-5.61	1.47	1.54
1	J	636	ILE	CA-CB	-5.61	1.47	1.54
1	I	636	ILE	CA-CB	-5.61	1.47	1.54
1	K	454	ILE	CA-CB	-5.61	1.48	1.54
1	I	454	ILE	CA-CB	-5.60	1.48	1.54
1	K	636	ILE	CA-CB	-5.59	1.47	1.54
1	P	636	ILE	CA-CB	-5.59	1.47	1.54
1	E	636	ILE	CA-CB	-5.58	1.47	1.54
1	N	636	ILE	CA-CB	-5.57	1.47	1.54
1	C	636	ILE	CA-CB	-5.57	1.47	1.54
1	F	636	ILE	CA-CB	-5.56	1.47	1.54
1	A	636	ILE	CA-CB	-5.56	1.47	1.54
1	D	636	ILE	CA-CB	-5.53	1.47	1.54
1	G	636	ILE	CA-CB	-5.53	1.47	1.54
1	L	636	ILE	CA-CB	-5.52	1.47	1.54
1	O	636	ILE	CA-CB	-5.52	1.47	1.54
1	D	1019	VAL	CA-CB	-5.03	1.48	1.54
1	P	1019	VAL	CA-CB	-5.02	1.48	1.54

All (1890) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	363	HIS	CA-CB-CG	-10.47	103.33	113.80
1	L	363	HIS	CA-CB-CG	-10.46	103.34	113.80
1	J	363	HIS	CA-CB-CG	-10.45	103.35	113.80
1	O	363	HIS	CA-CB-CG	-10.45	103.35	113.80
1	E	363	HIS	CA-CB-CG	-10.43	103.37	113.80
1	M	363	HIS	CA-CB-CG	-10.43	103.37	113.80
1	B	363	HIS	CA-CB-CG	-10.43	103.37	113.80
1	P	363	HIS	CA-CB-CG	-10.42	103.38	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	HIS	CA-CB-CG	-10.42	103.38	113.80
1	C	363	HIS	CA-CB-CG	-10.41	103.39	113.80
1	F	363	HIS	CA-CB-CG	-10.41	103.39	113.80
1	H	363	HIS	CA-CB-CG	-10.41	103.39	113.80
1	D	363	HIS	CA-CB-CG	-10.40	103.39	113.80
1	I	363	HIS	CA-CB-CG	-10.40	103.40	113.80
1	N	363	HIS	CA-CB-CG	-10.40	103.40	113.80
1	G	363	HIS	CA-CB-CG	-10.39	103.41	113.80
1	P	571	VAL	CB-CA-C	-9.31	97.49	110.90
1	D	571	VAL	CB-CA-C	-9.31	97.50	110.90
1	C	571	VAL	CB-CA-C	-9.30	97.51	110.90
1	G	571	VAL	CB-CA-C	-9.29	97.52	110.90
1	L	571	VAL	CB-CA-C	-9.29	97.52	110.90
1	O	571	VAL	CB-CA-C	-9.29	97.53	110.90
1	H	571	VAL	CB-CA-C	-9.29	97.53	110.90
1	K	571	VAL	CB-CA-C	-9.28	97.53	110.90
1	N	571	VAL	CB-CA-C	-9.28	97.53	110.90
1	J	571	VAL	CB-CA-C	-9.28	97.54	110.90
1	B	571	VAL	CB-CA-C	-9.28	97.54	110.90
1	F	571	VAL	CB-CA-C	-9.28	97.54	110.90
1	I	571	VAL	CB-CA-C	-9.27	97.55	110.90
1	M	571	VAL	CB-CA-C	-9.27	97.55	110.90
1	A	571	VAL	CB-CA-C	-9.26	97.56	110.90
1	E	571	VAL	CB-CA-C	-9.25	97.58	110.90
1	J	949	HIS	CA-CB-CG	-8.38	105.42	113.80
1	K	949	HIS	CA-CB-CG	-8.36	105.44	113.80
1	B	949	HIS	CA-CB-CG	-8.35	105.45	113.80
1	H	949	HIS	CA-CB-CG	-8.35	105.45	113.80
1	A	949	HIS	CA-CB-CG	-8.35	105.45	113.80
1	L	949	HIS	CA-CB-CG	-8.35	105.45	113.80
1	O	949	HIS	CA-CB-CG	-8.35	105.45	113.80
1	I	949	HIS	CA-CB-CG	-8.35	105.45	113.80
1	N	949	HIS	CA-CB-CG	-8.35	105.45	113.80
1	C	949	HIS	CA-CB-CG	-8.33	105.47	113.80
1	E	949	HIS	CA-CB-CG	-8.33	105.47	113.80
1	P	949	HIS	CA-CB-CG	-8.32	105.47	113.80
1	F	949	HIS	CA-CB-CG	-8.31	105.49	113.80
1	I	1018	LEU	N-CA-CB	-8.30	97.79	111.66
1	M	949	HIS	CA-CB-CG	-8.30	105.50	113.80
1	J	1018	LEU	N-CA-CB	-8.30	97.81	111.66
1	A	1018	LEU	N-CA-CB	-8.29	97.81	111.66
1	G	949	HIS	CA-CB-CG	-8.29	105.51	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1018	LEU	N-CA-CB	-8.29	97.82	111.66
1	K	1018	LEU	N-CA-CB	-8.29	97.82	111.66
1	N	1018	LEU	N-CA-CB	-8.29	97.82	111.66
1	P	1018	LEU	N-CA-CB	-8.29	97.82	111.66
1	O	1018	LEU	N-CA-CB	-8.28	97.83	111.66
1	C	1018	LEU	N-CA-CB	-8.28	97.83	111.66
1	D	1018	LEU	N-CA-CB	-8.28	97.83	111.66
1	F	1018	LEU	N-CA-CB	-8.28	97.83	111.66
1	M	1018	LEU	N-CA-CB	-8.28	97.83	111.66
1	L	1018	LEU	N-CA-CB	-8.28	97.84	111.66
1	D	949	HIS	CA-CB-CG	-8.27	105.53	113.80
1	H	1018	LEU	N-CA-CB	-8.27	97.85	111.66
1	E	1018	LEU	N-CA-CB	-8.26	97.86	111.66
1	D	18	ASN	O-C-N	8.26	126.22	121.27
1	C	18	ASN	O-C-N	8.24	126.21	121.27
1	K	18	ASN	O-C-N	8.23	126.21	121.27
1	M	18	ASN	O-C-N	8.23	126.21	121.27
1	B	1018	LEU	N-CA-CB	-8.23	97.91	111.66
1	J	18	ASN	O-C-N	8.22	126.20	121.27
1	E	18	ASN	O-C-N	8.21	126.19	121.27
1	P	18	ASN	O-C-N	8.19	126.18	121.27
1	N	18	ASN	O-C-N	8.18	126.18	121.27
1	B	18	ASN	O-C-N	8.17	126.17	121.27
1	G	18	ASN	O-C-N	8.17	126.17	121.27
1	I	18	ASN	O-C-N	8.15	126.16	121.27
1	A	18	ASN	O-C-N	8.12	126.14	121.27
1	E	927	THR	CA-C-N	8.11	129.98	119.84
1	E	927	THR	C-N-CA	8.11	129.98	119.84
1	L	18	ASN	O-C-N	8.11	126.14	121.27
1	K	927	THR	CA-C-N	8.10	129.97	119.84
1	K	927	THR	C-N-CA	8.10	129.97	119.84
1	J	927	THR	CA-C-N	8.10	129.96	119.84
1	J	927	THR	C-N-CA	8.10	129.96	119.84
1	O	927	THR	CA-C-N	8.09	129.96	119.84
1	O	927	THR	C-N-CA	8.09	129.96	119.84
1	H	927	THR	CA-C-N	8.09	129.95	119.84
1	H	927	THR	C-N-CA	8.09	129.95	119.84
1	M	927	THR	CA-C-N	8.08	129.94	119.84
1	M	927	THR	C-N-CA	8.08	129.94	119.84
1	O	18	ASN	O-C-N	8.08	126.12	121.27
1	C	927	THR	CA-C-N	8.08	129.94	119.84
1	C	927	THR	C-N-CA	8.08	129.94	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	927	THR	CA-C-N	8.08	129.94	119.84
1	F	927	THR	C-N-CA	8.08	129.94	119.84
1	F	18	ASN	O-C-N	8.07	126.11	121.27
1	L	927	THR	CA-C-N	8.07	129.93	119.84
1	L	927	THR	C-N-CA	8.07	129.93	119.84
1	H	18	ASN	O-C-N	8.07	126.11	121.27
1	P	927	THR	CA-C-N	8.07	129.93	119.84
1	P	927	THR	C-N-CA	8.07	129.93	119.84
1	N	927	THR	CA-C-N	8.07	129.93	119.84
1	N	927	THR	C-N-CA	8.07	129.93	119.84
1	A	927	THR	CA-C-N	8.06	129.92	119.84
1	A	927	THR	C-N-CA	8.06	129.92	119.84
1	B	927	THR	CA-C-N	8.05	129.90	119.84
1	B	927	THR	C-N-CA	8.05	129.90	119.84
1	G	927	THR	CA-C-N	8.05	129.90	119.84
1	G	927	THR	C-N-CA	8.05	129.90	119.84
1	I	927	THR	CA-C-N	8.04	129.89	119.84
1	I	927	THR	C-N-CA	8.04	129.89	119.84
1	D	927	THR	CA-C-N	8.04	129.89	119.84
1	D	927	THR	C-N-CA	8.04	129.89	119.84
1	A	4	THR	N-CA-C	-7.85	103.68	113.18
1	M	4	THR	N-CA-C	-7.85	103.68	113.18
1	D	4	THR	N-CA-C	-7.85	103.69	113.18
1	N	147	ASN	CA-CB-CG	7.84	120.44	112.60
1	F	4	THR	N-CA-C	-7.84	103.70	113.18
1	G	147	ASN	CA-CB-CG	7.83	120.44	112.60
1	P	147	ASN	CA-CB-CG	7.83	120.43	112.60
1	K	4	THR	N-CA-C	-7.83	103.71	113.18
1	B	4	THR	N-CA-C	-7.83	103.71	113.18
1	I	4	THR	N-CA-C	-7.82	103.72	113.18
1	K	147	ASN	CA-CB-CG	7.82	120.42	112.60
1	G	4	THR	N-CA-C	-7.82	103.72	113.18
1	C	4	THR	N-CA-C	-7.82	103.72	113.18
1	F	147	ASN	CA-CB-CG	7.82	120.42	112.60
1	H	4	THR	N-CA-C	-7.82	103.72	113.18
1	J	147	ASN	CA-CB-CG	7.82	120.42	112.60
1	O	4	THR	N-CA-C	-7.82	103.72	113.18
1	E	147	ASN	CA-CB-CG	7.81	120.41	112.60
1	E	4	THR	N-CA-C	-7.81	103.73	113.18
1	L	4	THR	N-CA-C	-7.80	103.74	113.18
1	M	147	ASN	CA-CB-CG	7.80	120.41	112.60
1	J	4	THR	N-CA-C	-7.80	103.74	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	4	THR	N-CA-C	-7.80	103.74	113.18
1	N	4	THR	N-CA-C	-7.80	103.74	113.18
1	A	147	ASN	CA-CB-CG	7.80	120.40	112.60
1	B	147	ASN	CA-CB-CG	7.80	120.40	112.60
1	I	147	ASN	CA-CB-CG	7.79	120.39	112.60
1	C	147	ASN	CA-CB-CG	7.79	120.39	112.60
1	H	147	ASN	CA-CB-CG	7.79	120.39	112.60
1	O	147	ASN	CA-CB-CG	7.79	120.39	112.60
1	D	147	ASN	CA-CB-CG	7.79	120.39	112.60
1	L	147	ASN	CA-CB-CG	7.77	120.37	112.60
1	G	150	PHE	CA-CB-CG	-7.58	106.22	113.80
1	B	150	PHE	CA-CB-CG	-7.57	106.23	113.80
1	H	150	PHE	CA-CB-CG	-7.57	106.23	113.80
1	M	150	PHE	CA-CB-CG	-7.56	106.24	113.80
1	N	150	PHE	CA-CB-CG	-7.56	106.24	113.80
1	C	150	PHE	CA-CB-CG	-7.56	106.24	113.80
1	P	150	PHE	CA-CB-CG	-7.56	106.24	113.80
1	L	150	PHE	CA-CB-CG	-7.55	106.25	113.80
1	K	150	PHE	CA-CB-CG	-7.55	106.25	113.80
1	F	150	PHE	CA-CB-CG	-7.55	106.25	113.80
1	I	150	PHE	CA-CB-CG	-7.55	106.25	113.80
1	J	150	PHE	CA-CB-CG	-7.55	106.25	113.80
1	A	150	PHE	CA-CB-CG	-7.54	106.26	113.80
1	O	150	PHE	CA-CB-CG	-7.54	106.26	113.80
1	D	150	PHE	CA-CB-CG	-7.53	106.27	113.80
1	E	150	PHE	CA-CB-CG	-7.53	106.28	113.80
1	G	1007	PHE	CA-CB-CG	-7.50	106.30	113.80
1	O	1007	PHE	CA-CB-CG	-7.49	106.31	113.80
1	C	1007	PHE	CA-CB-CG	-7.48	106.32	113.80
1	J	1007	PHE	CA-CB-CG	-7.48	106.32	113.80
1	L	1007	PHE	CA-CB-CG	-7.47	106.33	113.80
1	I	1007	PHE	CA-CB-CG	-7.47	106.33	113.80
1	A	1007	PHE	CA-CB-CG	-7.47	106.33	113.80
1	P	1007	PHE	CA-CB-CG	-7.46	106.34	113.80
1	K	1007	PHE	CA-CB-CG	-7.46	106.34	113.80
1	D	1007	PHE	CA-CB-CG	-7.45	106.35	113.80
1	N	1007	PHE	CA-CB-CG	-7.45	106.35	113.80
1	B	1007	PHE	CA-CB-CG	-7.45	106.35	113.80
1	M	1007	PHE	CA-CB-CG	-7.44	106.36	113.80
1	H	1007	PHE	CA-CB-CG	-7.44	106.36	113.80
1	F	1007	PHE	CA-CB-CG	-7.43	106.37	113.80
1	E	1007	PHE	CA-CB-CG	-7.42	106.38	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	102	ASN	CA-CB-CG	7.39	119.99	112.60
1	C	101	THR	N-CA-CB	7.38	123.16	111.20
1	D	101	THR	N-CA-CB	7.38	123.15	111.20
1	J	101	THR	N-CA-CB	7.37	123.13	111.20
1	E	101	THR	N-CA-CB	7.36	123.13	111.20
1	L	101	THR	N-CA-CB	7.36	123.13	111.20
1	H	980	GLU	N-CA-C	7.36	119.94	111.11
1	N	101	THR	N-CA-CB	7.36	123.12	111.20
1	D	395	HIS	CA-C-O	7.36	126.72	119.51
1	O	102	ASN	CA-CB-CG	7.36	119.96	112.60
1	F	101	THR	N-CA-CB	7.35	123.11	111.20
1	I	980	GLU	N-CA-C	7.35	119.94	111.11
1	K	101	THR	N-CA-CB	7.35	123.11	111.20
1	K	980	GLU	N-CA-C	7.35	119.93	111.11
1	N	980	GLU	N-CA-C	7.35	119.93	111.11
1	P	980	GLU	N-CA-C	7.35	119.93	111.11
1	N	102	ASN	CA-CB-CG	7.35	119.95	112.60
1	N	395	HIS	CA-C-O	7.35	126.71	119.51
1	H	101	THR	N-CA-CB	7.35	123.10	111.20
1	I	101	THR	N-CA-CB	7.35	123.11	111.20
1	J	980	GLU	N-CA-C	7.35	119.93	111.11
1	A	101	THR	N-CA-CB	7.34	123.10	111.20
1	B	101	THR	N-CA-CB	7.34	123.10	111.20
1	P	395	HIS	CA-C-O	7.34	126.71	119.51
1	A	102	ASN	CA-CB-CG	7.34	119.94	112.60
1	H	102	ASN	CA-CB-CG	7.34	119.94	112.60
1	M	101	THR	N-CA-CB	7.34	123.09	111.20
1	F	395	HIS	CA-C-O	7.34	126.70	119.51
1	G	101	THR	N-CA-CB	7.34	123.08	111.20
1	K	102	ASN	CA-CB-CG	7.34	119.94	112.60
1	P	101	THR	N-CA-CB	7.34	123.09	111.20
1	H	395	HIS	CA-C-O	7.33	126.70	119.51
1	G	980	GLU	N-CA-C	7.33	119.91	111.11
1	L	980	GLU	N-CA-C	7.33	119.91	111.11
1	O	101	THR	N-CA-CB	7.33	123.08	111.20
1	B	102	ASN	CA-CB-CG	7.33	119.93	112.60
1	D	102	ASN	CA-CB-CG	7.33	119.93	112.60
1	I	395	HIS	CA-C-O	7.33	126.69	119.51
1	A	980	GLU	N-CA-C	7.33	119.90	111.11
1	E	395	HIS	CA-C-O	7.33	126.69	119.51
1	C	102	ASN	CA-CB-CG	7.32	119.92	112.60
1	D	980	GLU	N-CA-C	7.32	119.90	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	980	GLU	N-CA-C	7.32	119.90	111.11
1	L	1004	SER	N-CA-CB	7.32	120.71	110.17
1	M	395	HIS	CA-C-O	7.32	126.68	119.51
1	J	395	HIS	CA-C-O	7.32	126.68	119.51
1	C	395	HIS	CA-C-O	7.31	126.68	119.51
1	O	395	HIS	CA-C-O	7.31	126.68	119.51
1	G	102	ASN	CA-CB-CG	7.31	119.91	112.60
1	J	1004	SER	N-CA-CB	7.31	120.70	110.17
1	L	395	HIS	CA-C-O	7.31	126.67	119.51
1	A	1004	SER	N-CA-CB	7.31	120.70	110.17
1	F	102	ASN	CA-CB-CG	7.31	119.91	112.60
1	M	102	ASN	CA-CB-CG	7.31	119.91	112.60
1	I	102	ASN	CA-CB-CG	7.31	119.91	112.60
1	C	980	GLU	N-CA-C	7.30	119.88	111.11
1	P	102	ASN	CA-CB-CG	7.30	119.90	112.60
1	B	395	HIS	CA-C-O	7.30	126.67	119.51
1	K	395	HIS	CA-C-O	7.30	126.66	119.51
1	J	102	ASN	CA-CB-CG	7.30	119.90	112.60
1	M	980	GLU	N-CA-C	7.30	119.87	111.11
1	G	395	HIS	CA-C-O	7.29	126.66	119.51
1	F	980	GLU	N-CA-C	7.29	119.86	111.11
1	K	1004	SER	N-CA-CB	7.29	120.67	110.17
1	B	980	GLU	N-CA-C	7.29	119.86	111.11
1	O	980	GLU	N-CA-C	7.28	119.85	111.11
1	E	102	ASN	CA-CB-CG	7.28	119.88	112.60
1	P	1004	SER	N-CA-CB	7.28	120.65	110.17
1	D	1004	SER	N-CA-CB	7.28	120.65	110.17
1	G	1004	SER	N-CA-CB	7.28	120.65	110.17
1	A	395	HIS	CA-C-O	7.27	126.64	119.51
1	E	1004	SER	N-CA-CB	7.27	120.64	110.17
1	I	1004	SER	N-CA-CB	7.27	120.64	110.17
1	N	1004	SER	N-CA-CB	7.26	120.63	110.17
1	O	1004	SER	N-CA-CB	7.25	120.62	110.17
1	B	1004	SER	N-CA-CB	7.25	120.61	110.17
1	C	1004	SER	N-CA-CB	7.25	120.60	110.17
1	F	1004	SER	N-CA-CB	7.24	120.60	110.17
1	H	1004	SER	N-CA-CB	7.24	120.60	110.17
1	M	1004	SER	N-CA-CB	7.24	120.59	110.17
1	E	614	HIS	N-CA-C	-7.22	100.94	110.40
1	K	614	HIS	N-CA-C	-7.21	100.95	110.40
1	G	614	HIS	N-CA-C	-7.21	100.96	110.40
1	I	614	HIS	N-CA-C	-7.21	100.96	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	614	HIS	N-CA-C	-7.20	100.97	110.40
1	L	614	HIS	N-CA-C	-7.20	100.97	110.40
1	M	614	HIS	N-CA-C	-7.20	100.97	110.40
1	B	614	HIS	N-CA-C	-7.19	100.98	110.40
1	J	614	HIS	N-CA-C	-7.19	100.98	110.40
1	C	614	HIS	N-CA-C	-7.19	100.98	110.40
1	H	614	HIS	N-CA-C	-7.19	100.99	110.40
1	N	614	HIS	N-CA-C	-7.18	100.99	110.40
1	D	614	HIS	N-CA-C	-7.17	101.01	110.40
1	F	614	HIS	N-CA-C	-7.16	101.02	110.40
1	J	781	ARG	N-CA-C	7.16	120.05	109.24
1	P	614	HIS	N-CA-C	-7.16	101.02	110.40
1	A	614	HIS	N-CA-C	-7.16	101.03	110.40
1	D	781	ARG	N-CA-C	7.16	120.04	109.24
1	M	781	ARG	N-CA-C	7.15	120.04	109.24
1	O	781	ARG	N-CA-C	7.15	120.04	109.24
1	N	781	ARG	N-CA-C	7.14	120.03	109.24
1	A	781	ARG	N-CA-C	7.14	120.03	109.24
1	P	781	ARG	N-CA-C	7.14	120.02	109.24
1	F	781	ARG	N-CA-C	7.14	120.02	109.24
1	I	781	ARG	N-CA-C	7.14	120.02	109.24
1	G	781	ARG	N-CA-C	7.13	120.01	109.24
1	L	781	ARG	N-CA-C	7.13	120.01	109.24
1	H	781	ARG	N-CA-C	7.13	120.00	109.24
1	K	781	ARG	N-CA-C	7.13	120.00	109.24
1	B	781	ARG	N-CA-C	7.11	119.98	109.24
1	E	781	ARG	N-CA-C	7.11	119.98	109.24
1	C	781	ARG	N-CA-C	7.10	119.96	109.24
1	E	113	PHE	CA-CB-CG	-7.06	106.74	113.80
1	O	113	PHE	CA-CB-CG	-7.06	106.74	113.80
1	A	113	PHE	CA-CB-CG	-7.05	106.75	113.80
1	B	113	PHE	CA-CB-CG	-7.03	106.77	113.80
1	F	113	PHE	CA-CB-CG	-7.03	106.77	113.80
1	J	113	PHE	CA-CB-CG	-7.03	106.77	113.80
1	C	113	PHE	CA-CB-CG	-7.02	106.78	113.80
1	G	429	ASP	CA-C-O	7.02	125.06	119.59
1	H	113	PHE	CA-CB-CG	-7.02	106.78	113.80
1	K	113	PHE	CA-CB-CG	-7.02	106.78	113.80
1	N	429	ASP	CA-C-O	7.02	125.06	119.59
1	K	429	ASP	CA-C-O	7.01	125.06	119.59
1	P	113	PHE	CA-CB-CG	-7.01	106.79	113.80
1	G	113	PHE	CA-CB-CG	-7.00	106.80	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	113	PHE	CA-CB-CG	-7.00	106.80	113.80
1	I	113	PHE	CA-CB-CG	-6.99	106.81	113.80
1	E	429	ASP	CA-C-O	6.98	125.04	119.59
1	M	113	PHE	CA-CB-CG	-6.98	106.82	113.80
1	N	113	PHE	CA-CB-CG	-6.98	106.82	113.80
1	I	429	ASP	CA-C-O	6.98	125.03	119.59
1	B	429	ASP	CA-C-O	6.97	125.03	119.59
1	L	113	PHE	CA-CB-CG	-6.97	106.83	113.80
1	C	429	ASP	CA-C-O	6.96	125.02	119.59
1	M	429	ASP	CA-C-O	6.96	125.02	119.59
1	P	429	ASP	CA-C-O	6.95	125.01	119.59
1	J	429	ASP	CA-C-O	6.94	125.00	119.59
1	F	429	ASP	CA-C-O	6.93	125.00	119.59
1	A	429	ASP	CA-C-O	6.92	124.99	119.59
1	L	429	ASP	CA-C-O	6.92	124.98	119.59
1	O	429	ASP	CA-C-O	6.91	124.98	119.59
1	D	429	ASP	CA-C-O	6.91	124.98	119.59
1	H	429	ASP	CA-C-O	6.89	124.97	119.59
1	A	650	GLU	N-CA-C	6.62	119.94	108.76
1	O	650	GLU	N-CA-C	6.62	119.94	108.76
1	P	650	GLU	N-CA-C	6.61	119.94	108.76
1	M	650	GLU	N-CA-C	6.61	119.93	108.76
1	D	650	GLU	N-CA-C	6.60	119.92	108.76
1	L	650	GLU	N-CA-C	6.60	119.92	108.76
1	I	650	GLU	N-CA-C	6.60	119.91	108.76
1	E	650	GLU	N-CA-C	6.59	119.90	108.76
1	N	650	GLU	N-CA-C	6.59	119.90	108.76
1	G	650	GLU	N-CA-C	6.59	119.89	108.76
1	J	650	GLU	N-CA-C	6.58	119.88	108.76
1	C	650	GLU	N-CA-C	6.57	119.87	108.76
1	H	650	GLU	N-CA-C	6.57	119.87	108.76
1	F	650	GLU	N-CA-C	6.56	119.85	108.76
1	K	650	GLU	N-CA-C	6.56	119.85	108.76
1	B	650	GLU	N-CA-C	6.55	119.83	108.76
1	O	93	HIS	CA-CB-CG	-6.52	107.28	113.80
1	N	109	VAL	N-CA-C	6.51	116.62	107.37
1	C	109	VAL	N-CA-C	6.51	116.61	107.37
1	E	93	HIS	CA-CB-CG	-6.50	107.30	113.80
1	G	109	VAL	N-CA-C	6.50	116.61	107.37
1	I	109	VAL	N-CA-C	6.50	116.60	107.37
1	A	63	PHE	CA-C-N	6.50	126.19	119.56
1	A	63	PHE	C-N-CA	6.50	126.19	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	93	HIS	CA-CB-CG	-6.50	107.31	113.80
1	C	63	PHE	CA-C-N	6.49	126.18	119.56
1	C	63	PHE	C-N-CA	6.49	126.18	119.56
1	F	93	HIS	CA-CB-CG	-6.49	107.31	113.80
1	G	93	HIS	CA-CB-CG	-6.49	107.31	113.80
1	J	142	ILE	N-CA-C	6.49	117.46	107.78
1	N	93	HIS	CA-CB-CG	-6.49	107.31	113.80
1	P	109	VAL	N-CA-C	6.49	116.59	107.37
1	A	109	VAL	N-CA-C	6.49	116.58	107.37
1	F	109	VAL	N-CA-C	6.49	116.58	107.37
1	E	142	ILE	N-CA-C	6.49	117.44	107.78
1	L	109	VAL	N-CA-C	6.49	116.58	107.37
1	H	93	HIS	CA-CB-CG	-6.49	107.31	113.80
1	K	109	VAL	N-CA-C	6.49	116.58	107.37
1	M	109	VAL	N-CA-C	6.49	116.58	107.37
1	O	142	ILE	N-CA-C	6.49	117.44	107.78
1	D	93	HIS	CA-CB-CG	-6.48	107.32	113.80
1	F	142	ILE	N-CA-C	6.48	117.44	107.78
1	C	447	ASP	N-CA-C	6.48	121.35	113.38
1	J	93	HIS	CA-CB-CG	-6.48	107.32	113.80
1	B	109	VAL	N-CA-C	6.48	116.57	107.37
1	B	142	ILE	N-CA-C	6.48	117.44	107.78
1	L	93	HIS	CA-CB-CG	-6.48	107.32	113.80
1	M	142	ILE	N-CA-C	6.48	117.43	107.78
1	B	93	HIS	CA-CB-CG	-6.48	107.32	113.80
1	P	142	ILE	N-CA-C	6.48	117.43	107.78
1	G	447	ASP	N-CA-C	6.48	121.34	113.38
1	O	109	VAL	N-CA-C	6.47	116.56	107.37
1	E	63	PHE	CA-C-N	6.47	126.16	119.56
1	E	63	PHE	C-N-CA	6.47	126.16	119.56
1	E	447	ASP	N-CA-C	6.47	121.34	113.38
1	G	142	ILE	N-CA-C	6.47	117.42	107.78
1	H	447	ASP	N-CA-C	6.47	121.34	113.38
1	I	142	ILE	N-CA-C	6.47	117.42	107.78
1	N	142	ILE	N-CA-C	6.47	117.42	107.78
1	A	142	ILE	N-CA-C	6.47	117.42	107.78
1	D	109	VAL	N-CA-C	6.47	116.56	107.37
1	D	142	ILE	N-CA-C	6.47	117.42	107.78
1	H	142	ILE	N-CA-C	6.47	117.41	107.78
1	H	109	VAL	N-CA-C	6.46	116.55	107.37
1	H	63	PHE	CA-C-N	6.46	126.15	119.56
1	H	63	PHE	C-N-CA	6.46	126.15	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	93	HIS	CA-CB-CG	-6.46	107.34	113.80
1	C	142	ILE	N-CA-C	6.46	117.41	107.78
1	O	447	ASP	N-CA-C	6.46	121.33	113.38
1	K	142	ILE	N-CA-C	6.46	117.41	107.78
1	M	447	ASP	N-CA-C	6.46	121.33	113.38
1	D	447	ASP	N-CA-C	6.46	121.32	113.38
1	E	109	VAL	N-CA-C	6.46	116.54	107.37
1	G	63	PHE	CA-C-N	6.46	126.15	119.56
1	G	63	PHE	C-N-CA	6.46	126.15	119.56
1	N	447	ASP	N-CA-C	6.46	121.32	113.38
1	I	93	HIS	CA-CB-CG	-6.46	107.34	113.80
1	J	63	PHE	CA-C-N	6.45	126.14	119.56
1	J	63	PHE	C-N-CA	6.45	126.14	119.56
1	K	63	PHE	CA-C-N	6.45	126.14	119.56
1	K	63	PHE	C-N-CA	6.45	126.14	119.56
1	J	109	VAL	N-CA-C	6.45	116.53	107.37
1	H	679	LEU	CA-C-N	-6.45	114.52	123.10
1	H	679	LEU	C-N-CA	-6.45	114.52	123.10
1	M	63	PHE	CA-C-N	6.45	126.14	119.56
1	M	63	PHE	C-N-CA	6.45	126.14	119.56
1	O	63	PHE	CA-C-N	6.45	126.14	119.56
1	O	63	PHE	C-N-CA	6.45	126.14	119.56
1	I	63	PHE	CA-C-N	6.45	126.14	119.56
1	I	63	PHE	C-N-CA	6.45	126.14	119.56
1	L	142	ILE	N-CA-C	6.45	117.39	107.78
1	L	447	ASP	N-CA-C	6.45	121.31	113.38
1	B	447	ASP	N-CA-C	6.44	121.31	113.38
1	J	447	ASP	N-CA-C	6.44	121.30	113.38
1	K	93	HIS	CA-CB-CG	-6.44	107.36	113.80
1	F	447	ASP	N-CA-C	6.44	121.30	113.38
1	M	93	HIS	CA-CB-CG	-6.43	107.37	113.80
1	L	63	PHE	CA-C-N	6.43	126.12	119.56
1	L	63	PHE	C-N-CA	6.43	126.12	119.56
1	G	679	LEU	CA-C-N	-6.43	114.55	123.10
1	G	679	LEU	C-N-CA	-6.43	114.55	123.10
1	B	63	PHE	CA-C-N	6.42	126.11	119.56
1	B	63	PHE	C-N-CA	6.42	126.11	119.56
1	O	679	LEU	CA-C-N	-6.42	114.56	123.10
1	O	679	LEU	C-N-CA	-6.42	114.56	123.10
1	P	447	ASP	N-CA-C	6.42	121.28	113.38
1	K	447	ASP	N-CA-C	6.42	121.28	113.38
1	E	679	LEU	CA-C-N	-6.42	114.56	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	679	LEU	C-N-CA	-6.42	114.56	123.10
1	P	63	PHE	CA-C-N	6.42	126.11	119.56
1	P	63	PHE	C-N-CA	6.42	126.11	119.56
1	A	93	HIS	CA-CB-CG	-6.42	107.38	113.80
1	F	63	PHE	CA-C-N	6.42	126.11	119.56
1	F	63	PHE	C-N-CA	6.42	126.11	119.56
1	P	679	LEU	CA-C-N	-6.42	114.56	123.10
1	P	679	LEU	C-N-CA	-6.42	114.56	123.10
1	L	679	LEU	CA-C-N	-6.42	114.57	123.10
1	L	679	LEU	C-N-CA	-6.42	114.57	123.10
1	D	63	PHE	CA-C-N	6.41	126.10	119.56
1	D	63	PHE	C-N-CA	6.41	126.10	119.56
1	J	679	LEU	CA-C-N	-6.41	114.57	123.10
1	J	679	LEU	C-N-CA	-6.41	114.57	123.10
1	C	679	LEU	CA-C-N	-6.41	114.57	123.10
1	C	679	LEU	C-N-CA	-6.41	114.57	123.10
1	N	63	PHE	CA-C-N	6.41	126.10	119.56
1	N	63	PHE	C-N-CA	6.41	126.10	119.56
1	I	447	ASP	N-CA-C	6.41	121.26	113.38
1	D	679	LEU	CA-C-N	-6.40	114.59	123.10
1	D	679	LEU	C-N-CA	-6.40	114.59	123.10
1	A	447	ASP	N-CA-C	6.40	121.25	113.38
1	F	679	LEU	CA-C-N	-6.39	114.59	123.10
1	F	679	LEU	C-N-CA	-6.39	114.59	123.10
1	M	679	LEU	CA-C-N	-6.39	114.60	123.10
1	M	679	LEU	C-N-CA	-6.39	114.60	123.10
1	N	679	LEU	CA-C-N	-6.39	114.60	123.10
1	N	679	LEU	C-N-CA	-6.39	114.60	123.10
1	I	679	LEU	CA-C-N	-6.39	114.60	123.10
1	I	679	LEU	C-N-CA	-6.39	114.60	123.10
1	A	679	LEU	CA-C-N	-6.38	114.61	123.10
1	A	679	LEU	C-N-CA	-6.38	114.61	123.10
1	K	679	LEU	CA-C-N	-6.38	114.61	123.10
1	K	679	LEU	C-N-CA	-6.38	114.61	123.10
1	B	679	LEU	CA-C-N	-6.38	114.62	123.10
1	B	679	LEU	C-N-CA	-6.38	114.62	123.10
1	J	181	GLU	N-CA-C	6.34	118.95	109.25
1	G	181	GLU	N-CA-C	6.33	118.93	109.25
1	L	181	GLU	N-CA-C	6.33	118.93	109.25
1	N	181	GLU	N-CA-C	6.33	118.93	109.25
1	F	181	GLU	N-CA-C	6.32	118.93	109.25
1	H	181	GLU	N-CA-C	6.32	118.92	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	181	GLU	N-CA-C	6.32	118.92	109.25
1	A	181	GLU	N-CA-C	6.32	118.92	109.25
1	E	143	PHE	CA-CB-CG	-6.32	107.48	113.80
1	O	181	GLU	N-CA-C	6.31	118.91	109.25
1	E	181	GLU	N-CA-C	6.31	118.91	109.25
1	I	181	GLU	N-CA-C	6.31	118.91	109.25
1	P	181	GLU	N-CA-C	6.31	118.91	109.25
1	J	143	PHE	CA-CB-CG	-6.31	107.49	113.80
1	A	143	PHE	CA-CB-CG	-6.31	107.49	113.80
1	C	181	GLU	N-CA-C	6.31	118.90	109.25
1	O	143	PHE	CA-CB-CG	-6.30	107.50	113.80
1	B	181	GLU	N-CA-C	6.30	118.89	109.25
1	K	181	GLU	N-CA-C	6.30	118.89	109.25
1	P	143	PHE	CA-CB-CG	-6.30	107.50	113.80
1	H	159	VAL	N-CA-C	6.30	116.60	111.62
1	I	143	PHE	CA-CB-CG	-6.30	107.50	113.80
1	M	143	PHE	CA-CB-CG	-6.30	107.50	113.80
1	J	46	ARG	C-N-CD	-6.30	99.18	125.00
1	M	46	ARG	C-N-CD	-6.30	99.18	125.00
1	G	46	ARG	C-N-CD	-6.30	99.19	125.00
1	I	46	ARG	C-N-CD	-6.30	99.19	125.00
1	N	143	PHE	CA-CB-CG	-6.30	107.50	113.80
1	D	181	GLU	N-CA-C	6.29	118.88	109.25
1	L	143	PHE	CA-CB-CG	-6.29	107.50	113.80
1	N	46	ARG	C-N-CD	-6.29	99.19	125.00
1	E	46	ARG	C-N-CD	-6.29	99.20	125.00
1	O	46	ARG	C-N-CD	-6.29	99.20	125.00
1	D	46	ARG	C-N-CD	-6.29	99.20	125.00
1	E	612	THR	CA-C-N	6.29	126.26	119.78
1	E	612	THR	C-N-CA	6.29	126.26	119.78
1	G	553	TRP	CA-CB-CG	-6.29	101.65	113.60
1	A	46	ARG	C-N-CD	-6.29	99.21	125.00
1	D	159	VAL	N-CA-C	6.29	116.59	111.62
1	H	46	ARG	C-N-CD	-6.29	99.21	125.00
1	J	118	ASN	CA-C-O	6.29	125.97	119.49
1	P	46	ARG	C-N-CD	-6.29	99.22	125.00
1	B	46	ARG	C-N-CD	-6.29	99.22	125.00
1	I	612	THR	CA-C-N	6.29	126.26	119.78
1	I	612	THR	C-N-CA	6.29	126.26	119.78
1	L	46	ARG	C-N-CD	-6.29	99.22	125.00
1	I	553	TRP	CA-CB-CG	-6.29	101.66	113.60
1	J	553	TRP	CA-CB-CG	-6.29	101.66	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	46	ARG	C-N-CD	-6.29	99.23	125.00
1	L	553	TRP	CA-CB-CG	-6.29	101.66	113.60
1	M	553	TRP	CA-CB-CG	-6.29	101.66	113.60
1	K	553	TRP	CA-CB-CG	-6.28	101.66	113.60
1	O	553	TRP	CA-CB-CG	-6.28	101.66	113.60
1	F	46	ARG	C-N-CD	-6.28	99.25	125.00
1	A	118	ASN	CA-C-O	6.28	125.96	119.49
1	E	159	VAL	N-CA-C	6.28	116.58	111.62
1	N	159	VAL	N-CA-C	6.28	116.58	111.62
1	C	46	ARG	C-N-CD	-6.28	99.26	125.00
1	G	612	THR	CA-C-N	6.28	126.25	119.78
1	G	612	THR	C-N-CA	6.28	126.25	119.78
1	H	553	TRP	CA-CB-CG	-6.28	101.67	113.60
1	C	553	TRP	CA-CB-CG	-6.28	101.68	113.60
1	F	553	TRP	CA-CB-CG	-6.28	101.68	113.60
1	N	553	TRP	CA-CB-CG	-6.28	101.68	113.60
1	H	143	PHE	CA-CB-CG	-6.27	107.53	113.80
1	J	533	LEU	CB-CA-C	6.27	121.19	109.71
1	C	143	PHE	CA-CB-CG	-6.27	107.53	113.80
1	C	533	LEU	CB-CA-C	6.27	121.18	109.71
1	D	143	PHE	CA-CB-CG	-6.27	107.53	113.80
1	D	553	TRP	CA-CB-CG	-6.27	101.69	113.60
1	P	553	TRP	CA-CB-CG	-6.27	101.69	113.60
1	E	553	TRP	CA-CB-CG	-6.27	101.69	113.60
1	G	118	ASN	CA-C-O	6.27	125.95	119.49
1	B	143	PHE	CA-CB-CG	-6.26	107.53	113.80
1	F	533	LEU	CB-CA-C	6.26	121.17	109.71
1	K	143	PHE	CA-CB-CG	-6.26	107.54	113.80
1	L	118	ASN	CA-C-O	6.26	125.94	119.49
1	L	878	HIS	CA-CB-CG	-6.26	107.54	113.80
1	O	533	LEU	CB-CA-C	6.26	121.17	109.71
1	A	533	LEU	CB-CA-C	6.26	121.16	109.71
1	H	533	LEU	CB-CA-C	6.26	121.16	109.71
1	B	553	TRP	CA-CB-CG	-6.26	101.71	113.60
1	F	143	PHE	CA-CB-CG	-6.26	107.54	113.80
1	I	118	ASN	CA-C-O	6.26	125.94	119.49
1	I	533	LEU	CB-CA-C	6.26	121.16	109.71
1	K	533	LEU	CB-CA-C	6.26	121.16	109.71
1	N	533	LEU	CB-CA-C	6.26	121.16	109.71
1	M	533	LEU	CB-CA-C	6.25	121.16	109.71
1	A	553	TRP	CA-CB-CG	-6.25	101.72	113.60
1	P	533	LEU	CB-CA-C	6.25	121.15	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	118	ASN	CA-C-O	6.25	125.93	119.49
1	B	612	THR	CA-C-N	6.25	126.22	119.78
1	B	612	THR	C-N-CA	6.25	126.22	119.78
1	E	533	LEU	CB-CA-C	6.25	121.14	109.71
1	G	533	LEU	CB-CA-C	6.25	121.15	109.71
1	L	533	LEU	CB-CA-C	6.25	121.15	109.71
1	M	118	ASN	CA-C-O	6.25	125.93	119.49
1	M	878	HIS	CA-CB-CG	-6.25	107.55	113.80
1	H	118	ASN	CA-C-O	6.25	125.92	119.49
1	F	159	VAL	N-CA-C	6.25	116.55	111.62
1	O	612	THR	CA-C-N	6.24	126.21	119.78
1	O	612	THR	C-N-CA	6.24	126.21	119.78
1	P	612	THR	CA-C-N	6.24	126.20	119.78
1	P	612	THR	C-N-CA	6.24	126.20	119.78
1	A	612	THR	CA-C-N	6.24	126.20	119.78
1	A	612	THR	C-N-CA	6.24	126.20	119.78
1	F	612	THR	CA-C-N	6.24	126.20	119.78
1	F	612	THR	C-N-CA	6.24	126.20	119.78
1	B	533	LEU	CB-CA-C	6.23	121.11	109.71
1	G	143	PHE	CA-CB-CG	-6.23	107.57	113.80
1	D	533	LEU	CB-CA-C	6.23	121.11	109.71
1	H	878	HIS	CA-CB-CG	-6.23	107.57	113.80
1	M	159	VAL	N-CA-C	6.23	116.54	111.62
1	M	612	THR	CA-C-N	6.23	126.20	119.78
1	M	612	THR	C-N-CA	6.23	126.20	119.78
1	J	159	VAL	N-CA-C	6.23	116.54	111.62
1	N	118	ASN	CA-C-O	6.23	125.90	119.49
1	L	612	THR	CA-C-N	6.23	126.19	119.78
1	L	612	THR	C-N-CA	6.23	126.19	119.78
1	E	118	ASN	CA-C-O	6.22	125.90	119.49
1	B	159	VAL	N-CA-C	6.22	116.54	111.62
1	P	118	ASN	CA-C-O	6.22	125.90	119.49
1	O	159	VAL	N-CA-C	6.22	116.53	111.62
1	P	159	VAL	N-CA-C	6.22	116.53	111.62
1	B	118	ASN	CA-C-O	6.21	125.89	119.49
1	D	612	THR	CA-C-N	6.21	126.18	119.78
1	D	612	THR	C-N-CA	6.21	126.18	119.78
1	F	118	ASN	CA-C-O	6.21	125.89	119.49
1	E	878	HIS	CA-CB-CG	-6.21	107.59	113.80
1	L	159	VAL	N-CA-C	6.21	116.53	111.62
1	K	118	ASN	CA-C-O	6.21	125.89	119.49
1	N	878	HIS	CA-CB-CG	-6.21	107.59	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	118	ASN	CA-C-O	6.21	125.89	119.49
1	G	159	VAL	N-CA-C	6.21	116.53	111.62
1	I	159	VAL	N-CA-C	6.21	116.52	111.62
1	K	159	VAL	N-CA-C	6.21	116.52	111.62
1	C	612	THR	CA-C-N	6.21	126.17	119.78
1	C	612	THR	C-N-CA	6.21	126.17	119.78
1	I	878	HIS	CA-CB-CG	-6.20	107.60	113.80
1	A	95	TYR	N-CA-C	6.20	118.04	111.28
1	A	159	VAL	N-CA-C	6.20	116.52	111.62
1	P	95	TYR	N-CA-C	6.20	118.04	111.28
1	P	878	HIS	CA-CB-CG	-6.20	107.60	113.80
1	F	95	TYR	N-CA-C	6.20	118.03	111.28
1	K	612	THR	CA-C-N	6.19	126.16	119.78
1	K	612	THR	C-N-CA	6.19	126.16	119.78
1	C	159	VAL	N-CA-C	6.19	116.51	111.62
1	J	612	THR	CA-C-N	6.19	126.16	119.78
1	J	612	THR	C-N-CA	6.19	126.16	119.78
1	N	612	THR	CA-C-N	6.19	126.16	119.78
1	N	612	THR	C-N-CA	6.19	126.16	119.78
1	H	612	THR	CA-C-N	6.19	126.16	119.78
1	H	612	THR	C-N-CA	6.19	126.16	119.78
1	J	878	HIS	CA-CB-CG	-6.19	107.61	113.80
1	B	878	HIS	CA-CB-CG	-6.19	107.61	113.80
1	C	118	ASN	CA-C-O	6.19	125.86	119.49
1	O	95	TYR	N-CA-C	6.19	118.03	111.28
1	C	20	GLY	CA-C-N	-6.18	114.87	123.10
1	C	20	GLY	C-N-CA	-6.18	114.87	123.10
1	C	878	HIS	CA-CB-CG	-6.18	107.62	113.80
1	K	878	HIS	CA-CB-CG	-6.18	107.61	113.80
1	B	95	TYR	N-CA-C	6.18	118.02	111.28
1	D	878	HIS	CA-CB-CG	-6.18	107.62	113.80
1	G	878	HIS	CA-CB-CG	-6.18	107.62	113.80
1	A	878	HIS	CA-CB-CG	-6.18	107.62	113.80
1	I	95	TYR	N-CA-C	6.17	118.01	111.28
1	B	20	GLY	CA-C-N	-6.17	114.89	123.10
1	B	20	GLY	C-N-CA	-6.17	114.89	123.10
1	O	878	HIS	CA-CB-CG	-6.17	107.63	113.80
1	I	20	GLY	CA-C-N	-6.17	114.90	123.10
1	I	20	GLY	C-N-CA	-6.17	114.90	123.10
1	H	20	GLY	CA-C-N	-6.16	114.90	123.10
1	H	20	GLY	C-N-CA	-6.16	114.90	123.10
1	N	20	GLY	CA-C-N	-6.16	114.90	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	20	GLY	C-N-CA	-6.16	114.90	123.10
1	C	95	TYR	N-CA-C	6.16	118.00	111.28
1	B	563	GLN	N-CA-C	6.16	119.74	112.72
1	D	95	TYR	N-CA-C	6.16	117.99	111.28
1	F	878	HIS	CA-CB-CG	-6.16	107.64	113.80
1	P	20	GLY	CA-C-N	-6.16	114.91	123.10
1	P	20	GLY	C-N-CA	-6.16	114.91	123.10
1	E	95	TYR	N-CA-C	6.15	117.98	111.28
1	F	20	GLY	CA-C-N	-6.15	114.92	123.10
1	F	20	GLY	C-N-CA	-6.15	114.92	123.10
1	L	20	GLY	CA-C-N	-6.15	114.92	123.10
1	L	20	GLY	C-N-CA	-6.15	114.92	123.10
1	D	20	GLY	CA-C-N	-6.15	114.92	123.10
1	D	20	GLY	C-N-CA	-6.15	114.92	123.10
1	M	95	TYR	N-CA-C	6.15	117.98	111.28
1	J	20	GLY	CA-C-N	-6.15	114.92	123.10
1	J	20	GLY	C-N-CA	-6.15	114.92	123.10
1	B	110	ASN	CA-CB-CG	-6.15	106.45	112.60
1	H	95	TYR	N-CA-C	6.14	117.98	111.28
1	M	20	GLY	CA-C-N	-6.14	114.93	123.10
1	M	20	GLY	C-N-CA	-6.14	114.93	123.10
1	M	110	ASN	CA-CB-CG	-6.14	106.46	112.60
1	J	95	TYR	N-CA-C	6.14	117.97	111.28
1	L	95	TYR	N-CA-C	6.13	117.97	111.28
1	K	20	GLY	CA-C-N	-6.13	114.94	123.10
1	K	20	GLY	C-N-CA	-6.13	114.94	123.10
1	M	563	GLN	N-CA-C	6.13	119.71	112.72
1	J	110	ASN	CA-CB-CG	-6.13	106.47	112.60
1	L	479	ASP	CA-C-O	6.13	127.33	120.34
1	K	95	TYR	N-CA-C	6.13	117.96	111.28
1	G	563	GLN	N-CA-C	6.13	119.70	112.72
1	E	563	GLN	N-CA-C	6.12	119.70	112.72
1	F	563	GLN	N-CA-C	6.12	119.70	112.72
1	G	20	GLY	CA-C-N	-6.12	114.96	123.10
1	G	20	GLY	C-N-CA	-6.12	114.96	123.10
1	G	95	TYR	N-CA-C	6.12	117.95	111.28
1	K	110	ASN	CA-CB-CG	-6.12	106.48	112.60
1	A	20	GLY	CA-C-N	-6.12	114.97	123.10
1	A	20	GLY	C-N-CA	-6.12	114.97	123.10
1	D	563	GLN	N-CA-C	6.12	119.69	112.72
1	L	563	GLN	N-CA-C	6.12	119.69	112.72
1	M	479	ASP	CA-C-O	6.12	127.31	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	563	GLN	N-CA-C	6.11	119.69	112.72
1	D	553	TRP	CA-C-N	-6.11	111.61	120.29
1	D	553	TRP	C-N-CA	-6.11	111.61	120.29
1	G	110	ASN	CA-CB-CG	-6.11	106.49	112.60
1	I	563	GLN	N-CA-C	6.11	119.69	112.72
1	O	563	GLN	N-CA-C	6.11	119.69	112.72
1	A	110	ASN	CA-CB-CG	-6.11	106.49	112.60
1	B	448	ARG	N-CA-C	6.11	120.20	112.87
1	O	479	ASP	CA-C-O	6.11	127.31	120.34
1	E	20	GLY	CA-C-N	-6.11	114.98	123.10
1	E	20	GLY	C-N-CA	-6.11	114.98	123.10
1	O	20	GLY	CA-C-N	-6.11	114.98	123.10
1	O	20	GLY	C-N-CA	-6.11	114.98	123.10
1	H	563	GLN	N-CA-C	6.10	119.68	112.72
1	G	746	ASP	N-CA-C	6.10	115.91	107.73
1	H	553	TRP	CA-C-N	-6.10	111.62	120.29
1	H	553	TRP	C-N-CA	-6.10	111.62	120.29
1	F	110	ASN	CA-CB-CG	-6.10	106.50	112.60
1	H	110	ASN	CA-CB-CG	-6.10	106.50	112.60
1	J	563	GLN	N-CA-C	6.10	119.67	112.72
1	N	95	TYR	N-CA-C	6.10	117.93	111.28
1	N	563	GLN	N-CA-C	6.10	119.67	112.72
1	E	448	ARG	N-CA-C	6.10	120.19	112.87
1	F	448	ARG	N-CA-C	6.10	120.19	112.87
1	D	110	ASN	CA-CB-CG	-6.10	106.50	112.60
1	H	746	ASP	N-CA-C	6.10	115.90	107.73
1	E	553	TRP	CA-C-N	-6.09	111.64	120.29
1	E	553	TRP	C-N-CA	-6.09	111.64	120.29
1	F	746	ASP	N-CA-C	6.09	115.89	107.73
1	O	110	ASN	CA-CB-CG	-6.09	106.51	112.60
1	G	479	ASP	CA-C-O	6.09	127.28	120.34
1	I	110	ASN	CA-CB-CG	-6.09	106.51	112.60
1	I	479	ASP	CA-C-O	6.09	127.28	120.34
1	N	479	ASP	CA-C-O	6.09	127.28	120.34
1	P	110	ASN	CA-CB-CG	-6.09	106.51	112.60
1	H	448	ARG	N-CA-C	6.09	120.18	112.87
1	P	479	ASP	CA-C-O	6.09	127.28	120.34
1	A	746	ASP	N-CA-C	6.09	115.89	107.73
1	C	479	ASP	CA-C-O	6.09	127.28	120.34
1	D	448	ARG	N-CA-C	6.09	120.17	112.87
1	K	563	GLN	N-CA-C	6.09	119.66	112.72
1	O	448	ARG	N-CA-C	6.08	120.17	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	553	TRP	CA-C-N	-6.08	111.65	120.29
1	O	553	TRP	C-N-CA	-6.08	111.65	120.29
1	A	448	ARG	N-CA-C	6.08	120.17	112.87
1	F	479	ASP	CA-C-O	6.08	127.27	120.34
1	G	553	TRP	CA-C-N	-6.08	111.65	120.29
1	G	553	TRP	C-N-CA	-6.08	111.65	120.29
1	H	479	ASP	CA-C-O	6.08	127.27	120.34
1	L	553	TRP	CA-C-N	-6.08	111.65	120.29
1	L	553	TRP	C-N-CA	-6.08	111.65	120.29
1	P	563	GLN	N-CA-C	6.08	119.65	112.72
1	B	479	ASP	CA-C-O	6.08	127.27	120.34
1	C	110	ASN	CA-CB-CG	-6.08	106.52	112.60
1	L	110	ASN	CA-CB-CG	-6.08	106.52	112.60
1	N	553	TRP	CA-C-N	-6.08	111.66	120.29
1	N	553	TRP	C-N-CA	-6.08	111.66	120.29
1	G	448	ARG	N-CA-C	6.08	120.16	112.87
1	K	479	ASP	CA-C-O	6.08	127.27	120.34
1	M	746	ASP	N-CA-C	6.08	115.88	107.73
1	O	746	ASP	N-CA-C	6.08	115.88	107.73
1	P	746	ASP	N-CA-C	6.08	115.88	107.73
1	I	448	ARG	N-CA-C	6.08	120.16	112.87
1	C	746	ASP	N-CA-C	6.08	115.87	107.73
1	F	553	TRP	CA-C-N	-6.08	111.66	120.29
1	F	553	TRP	C-N-CA	-6.08	111.66	120.29
1	J	448	ARG	N-CA-C	6.08	120.16	112.87
1	K	316	HIS	CA-CB-CG	-6.08	107.72	113.80
1	K	746	ASP	N-CA-C	6.08	115.87	107.73
1	N	746	ASP	N-CA-C	6.08	115.87	107.73
1	M	448	ARG	N-CA-C	6.07	120.16	112.87
1	L	448	ARG	N-CA-C	6.07	120.15	112.87
1	C	316	HIS	CA-CB-CG	-6.07	107.73	113.80
1	E	316	HIS	CA-CB-CG	-6.07	107.73	113.80
1	I	316	HIS	CA-CB-CG	-6.07	107.73	113.80
1	K	553	TRP	CA-C-N	-6.07	111.67	120.29
1	K	553	TRP	C-N-CA	-6.07	111.67	120.29
1	N	110	ASN	CA-CB-CG	-6.07	106.53	112.60
1	D	746	ASP	N-CA-C	6.07	115.86	107.73
1	I	553	TRP	CA-C-N	-6.07	111.68	120.29
1	I	553	TRP	C-N-CA	-6.07	111.68	120.29
1	J	553	TRP	CA-C-N	-6.07	111.68	120.29
1	J	553	TRP	C-N-CA	-6.07	111.68	120.29
1	K	448	ARG	N-CA-C	6.07	120.15	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	746	ASP	N-CA-C	6.06	115.86	107.73
1	N	316	HIS	CA-CB-CG	-6.06	107.74	113.80
1	L	746	ASP	N-CA-C	6.06	115.85	107.73
1	J	316	HIS	CA-CB-CG	-6.06	107.74	113.80
1	M	553	TRP	CA-C-N	-6.06	111.68	120.29
1	M	553	TRP	C-N-CA	-6.06	111.68	120.29
1	A	479	ASP	CA-C-O	6.06	127.25	120.34
1	C	553	TRP	CA-C-N	-6.06	111.69	120.29
1	C	553	TRP	C-N-CA	-6.06	111.69	120.29
1	A	553	TRP	CA-C-N	-6.06	111.69	120.29
1	A	553	TRP	C-N-CA	-6.06	111.69	120.29
1	E	110	ASN	CA-CB-CG	-6.06	106.54	112.60
1	E	479	ASP	CA-C-O	6.06	127.24	120.34
1	P	316	HIS	CA-CB-CG	-6.06	107.74	113.80
1	B	746	ASP	N-CA-C	6.05	115.84	107.73
1	C	563	GLN	N-CA-C	6.05	119.62	112.72
1	G	316	HIS	CA-CB-CG	-6.05	107.75	113.80
1	B	553	TRP	CA-C-N	-6.05	111.70	120.29
1	B	553	TRP	C-N-CA	-6.05	111.70	120.29
1	E	746	ASP	N-CA-C	6.05	115.83	107.73
1	F	316	HIS	CA-CB-CG	-6.04	107.75	113.80
1	N	448	ARG	N-CA-C	6.04	120.12	112.87
1	C	448	ARG	N-CA-C	6.04	120.12	112.87
1	B	988	GLY	N-CA-C	-6.04	104.80	113.86
1	J	746	ASP	N-CA-C	6.04	115.83	107.73
1	P	553	TRP	CA-C-N	-6.04	111.71	120.29
1	P	553	TRP	C-N-CA	-6.04	111.71	120.29
1	F	988	GLY	N-CA-C	-6.04	104.80	113.86
1	H	316	HIS	CA-CB-CG	-6.04	107.76	113.80
1	P	448	ARG	N-CA-C	6.04	120.12	112.87
1	A	988	GLY	N-CA-C	-6.04	104.81	113.86
1	M	988	GLY	N-CA-C	-6.04	104.81	113.86
1	E	988	GLY	N-CA-C	-6.03	104.81	113.86
1	J	479	ASP	CA-C-O	6.03	127.22	120.34
1	A	316	HIS	CA-CB-CG	-6.03	107.77	113.80
1	B	316	HIS	CA-CB-CG	-6.03	107.77	113.80
1	D	316	HIS	CA-CB-CG	-6.03	107.77	113.80
1	D	479	ASP	CA-C-O	6.03	127.21	120.34
1	J	988	GLY	N-CA-C	-6.02	104.82	113.86
1	M	592	PHE	CA-CB-CG	-6.02	107.78	113.80
1	M	316	HIS	CA-CB-CG	-6.02	107.78	113.80
1	G	988	GLY	N-CA-C	-6.02	104.83	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	988	GLY	N-CA-C	-6.02	104.84	113.86
1	H	988	GLY	N-CA-C	-6.01	104.84	113.86
1	L	316	HIS	CA-CB-CG	-6.01	107.78	113.80
1	N	988	GLY	N-CA-C	-6.01	104.84	113.86
1	I	988	GLY	N-CA-C	-6.01	104.84	113.86
1	O	988	GLY	N-CA-C	-6.01	104.84	113.86
1	L	988	GLY	N-CA-C	-6.01	104.85	113.86
1	A	592	PHE	CA-CB-CG	-6.01	107.79	113.80
1	K	592	PHE	CA-CB-CG	-6.01	107.79	113.80
1	O	316	HIS	CA-CB-CG	-6.00	107.80	113.80
1	G	592	PHE	CA-CB-CG	-6.00	107.80	113.80
1	K	626	PHE	CA-CB-CG	-6.00	107.80	113.80
1	E	626	PHE	CA-CB-CG	-6.00	107.80	113.80
1	L	592	PHE	CA-CB-CG	-6.00	107.80	113.80
1	M	626	PHE	CA-CB-CG	-6.00	107.80	113.80
1	C	988	GLY	N-CA-C	-5.99	104.87	113.86
1	D	988	GLY	N-CA-C	-5.99	104.87	113.86
1	G	701	VAL	N-CA-C	5.99	118.08	108.85
1	H	626	PHE	CA-CB-CG	-5.99	107.81	113.80
1	P	988	GLY	N-CA-C	-5.99	104.88	113.86
1	K	701	VAL	N-CA-C	5.99	118.07	108.85
1	C	701	VAL	N-CA-C	5.99	118.07	108.85
1	D	592	PHE	CA-CB-CG	-5.99	107.81	113.80
1	E	745	MET	CA-C-N	-5.99	112.00	122.84
1	E	745	MET	C-N-CA	-5.99	112.00	122.84
1	P	592	PHE	CA-CB-CG	-5.98	107.82	113.80
1	C	592	PHE	CA-CB-CG	-5.98	107.82	113.80
1	C	626	PHE	CA-CB-CG	-5.98	107.82	113.80
1	N	626	PHE	CA-CB-CG	-5.98	107.82	113.80
1	B	626	PHE	CA-CB-CG	-5.97	107.83	113.80
1	D	626	PHE	CA-CB-CG	-5.97	107.83	113.80
1	J	701	VAL	N-CA-C	5.97	118.05	108.85
1	L	701	VAL	N-CA-C	5.97	118.05	108.85
1	N	592	PHE	CA-CB-CG	-5.97	107.83	113.80
1	O	701	VAL	N-CA-C	5.97	118.05	108.85
1	A	701	VAL	N-CA-C	5.97	118.05	108.85
1	I	745	MET	CA-C-N	-5.97	112.03	122.84
1	I	745	MET	C-N-CA	-5.97	112.03	122.84
1	O	592	PHE	CA-CB-CG	-5.97	107.83	113.80
1	B	701	VAL	N-CA-C	5.97	118.04	108.85
1	I	592	PHE	CA-CB-CG	-5.97	107.83	113.80
1	I	701	VAL	N-CA-C	5.97	118.04	108.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	745	MET	CA-C-N	-5.97	112.04	122.84
1	M	745	MET	C-N-CA	-5.97	112.04	122.84
1	E	701	VAL	N-CA-C	5.97	118.04	108.85
1	I	626	PHE	CA-CB-CG	-5.97	107.83	113.80
1	P	745	MET	CA-C-N	-5.96	112.04	122.84
1	P	745	MET	C-N-CA	-5.96	112.04	122.84
1	D	745	MET	CA-C-N	-5.96	112.05	122.84
1	D	745	MET	C-N-CA	-5.96	112.05	122.84
1	F	701	VAL	N-CA-C	5.96	118.03	108.85
1	H	701	VAL	N-CA-C	5.96	118.03	108.85
1	H	745	MET	CA-C-N	-5.96	112.05	122.84
1	H	745	MET	C-N-CA	-5.96	112.05	122.84
1	J	745	MET	CA-C-N	-5.96	112.05	122.84
1	J	745	MET	C-N-CA	-5.96	112.05	122.84
1	F	745	MET	CA-C-N	-5.96	112.05	122.84
1	F	745	MET	C-N-CA	-5.96	112.05	122.84
1	D	701	VAL	N-CA-C	5.96	118.03	108.85
1	K	745	MET	CA-C-N	-5.96	112.05	122.84
1	K	745	MET	C-N-CA	-5.96	112.05	122.84
1	L	626	PHE	CA-CB-CG	-5.96	107.84	113.80
1	F	592	PHE	CA-CB-CG	-5.96	107.84	113.80
1	B	592	PHE	CA-CB-CG	-5.96	107.84	113.80
1	B	745	MET	CA-C-N	-5.95	112.07	122.84
1	B	745	MET	C-N-CA	-5.95	112.07	122.84
1	N	701	VAL	N-CA-C	5.95	118.02	108.85
1	A	626	PHE	CA-CB-CG	-5.95	107.85	113.80
1	L	745	MET	CA-C-N	-5.95	112.07	122.84
1	L	745	MET	C-N-CA	-5.95	112.07	122.84
1	O	626	PHE	CA-CB-CG	-5.95	107.85	113.80
1	G	745	MET	CA-C-N	-5.95	112.07	122.84
1	G	745	MET	C-N-CA	-5.95	112.07	122.84
1	P	626	PHE	CA-CB-CG	-5.95	107.85	113.80
1	P	701	VAL	N-CA-C	5.95	118.01	108.85
1	J	592	PHE	CA-CB-CG	-5.95	107.85	113.80
1	M	701	VAL	N-CA-C	5.95	118.01	108.85
1	J	626	PHE	CA-CB-CG	-5.95	107.86	113.80
1	C	745	MET	CA-C-N	-5.94	112.08	122.84
1	C	745	MET	C-N-CA	-5.94	112.08	122.84
1	O	745	MET	CA-C-N	-5.94	112.08	122.84
1	O	745	MET	C-N-CA	-5.94	112.08	122.84
1	A	745	MET	CA-C-N	-5.94	112.09	122.84
1	A	745	MET	C-N-CA	-5.94	112.09	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	592	PHE	CA-CB-CG	-5.94	107.86	113.80
1	F	626	PHE	CA-CB-CG	-5.94	107.86	113.80
1	N	745	MET	CA-C-N	-5.93	112.10	122.84
1	N	745	MET	C-N-CA	-5.93	112.10	122.84
1	P	69	VAL	C-N-CD	-5.93	100.67	125.00
1	G	626	PHE	CA-CB-CG	-5.93	107.87	113.80
1	M	69	VAL	C-N-CD	-5.93	100.68	125.00
1	N	69	VAL	C-N-CD	-5.93	100.68	125.00
1	A	69	VAL	C-N-CD	-5.93	100.69	125.00
1	C	69	VAL	C-N-CD	-5.93	100.69	125.00
1	I	69	VAL	C-N-CD	-5.93	100.69	125.00
1	K	69	VAL	C-N-CD	-5.93	100.69	125.00
1	H	592	PHE	CA-CB-CG	-5.93	107.87	113.80
1	H	69	VAL	C-N-CD	-5.93	100.70	125.00
1	B	69	VAL	C-N-CD	-5.92	100.71	125.00
1	L	69	VAL	C-N-CD	-5.92	100.71	125.00
1	J	69	VAL	C-N-CD	-5.92	100.72	125.00
1	E	69	VAL	C-N-CD	-5.92	100.72	125.00
1	G	69	VAL	C-N-CD	-5.92	100.72	125.00
1	D	69	VAL	C-N-CD	-5.92	100.73	125.00
1	O	69	VAL	C-N-CD	-5.92	100.74	125.00
1	F	69	VAL	C-N-CD	-5.91	100.76	125.00
1	F	764	PHE	CA-CB-CG	-5.91	107.89	113.80
1	E	764	PHE	CA-CB-CG	-5.89	107.91	113.80
1	L	764	PHE	CA-CB-CG	-5.89	107.91	113.80
1	P	764	PHE	CA-CB-CG	-5.87	107.93	113.80
1	G	764	PHE	CA-CB-CG	-5.87	107.93	113.80
1	M	764	PHE	CA-CB-CG	-5.87	107.93	113.80
1	A	764	PHE	CA-CB-CG	-5.86	107.94	113.80
1	H	764	PHE	CA-CB-CG	-5.85	107.95	113.80
1	I	764	PHE	CA-CB-CG	-5.85	107.95	113.80
1	K	764	PHE	CA-CB-CG	-5.85	107.95	113.80
1	J	764	PHE	CA-CB-CG	-5.84	107.96	113.80
1	O	764	PHE	CA-CB-CG	-5.84	107.96	113.80
1	C	764	PHE	CA-CB-CG	-5.84	107.96	113.80
1	K	209	PHE	CA-CB-CG	-5.83	107.97	113.80
1	O	209	PHE	CA-CB-CG	-5.82	107.98	113.80
1	D	209	PHE	CA-CB-CG	-5.82	107.98	113.80
1	F	209	PHE	CA-CB-CG	-5.82	107.98	113.80
1	B	764	PHE	CA-CB-CG	-5.82	107.98	113.80
1	N	764	PHE	CA-CB-CG	-5.82	107.98	113.80
1	D	764	PHE	CA-CB-CG	-5.81	107.99	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	PHE	CA-CB-CG	-5.81	107.99	113.80
1	M	209	PHE	CA-CB-CG	-5.80	108.00	113.80
1	N	209	PHE	CA-CB-CG	-5.80	108.00	113.80
1	E	209	PHE	CA-CB-CG	-5.80	108.00	113.80
1	I	209	PHE	CA-CB-CG	-5.80	108.00	113.80
1	H	209	PHE	CA-CB-CG	-5.79	108.01	113.80
1	J	209	PHE	CA-CB-CG	-5.79	108.01	113.80
1	P	209	PHE	CA-CB-CG	-5.79	108.01	113.80
1	A	209	PHE	CA-CB-CG	-5.79	108.01	113.80
1	L	209	PHE	CA-CB-CG	-5.79	108.01	113.80
1	C	209	PHE	CA-CB-CG	-5.77	108.03	113.80
1	G	209	PHE	CA-CB-CG	-5.76	108.03	113.80
1	P	166	ARG	N-CA-C	5.74	120.41	113.17
1	D	166	ARG	N-CA-C	5.74	120.40	113.17
1	I	166	ARG	N-CA-C	5.73	120.39	113.17
1	L	166	ARG	N-CA-C	5.73	120.39	113.17
1	N	166	ARG	N-CA-C	5.72	120.38	113.17
1	M	166	ARG	N-CA-C	5.72	120.38	113.17
1	F	166	ARG	N-CA-C	5.71	120.37	113.17
1	L	728	VAL	CB-CA-C	-5.71	104.87	112.46
1	C	166	ARG	N-CA-C	5.70	120.36	113.17
1	D	612	THR	N-CA-CB	5.70	119.63	109.94
1	N	612	THR	N-CA-CB	5.70	119.63	109.94
1	A	166	ARG	N-CA-C	5.70	120.35	113.17
1	H	612	THR	N-CA-CB	5.70	119.63	109.94
1	P	612	THR	N-CA-CB	5.70	119.63	109.94
1	B	612	THR	N-CA-CB	5.70	119.62	109.94
1	K	166	ARG	N-CA-C	5.70	120.35	113.17
1	N	728	VAL	CB-CA-C	-5.70	104.89	112.46
1	O	612	THR	N-CA-CB	5.69	119.62	109.94
1	K	612	THR	N-CA-CB	5.69	119.62	109.94
1	B	166	ARG	N-CA-C	5.69	120.34	113.17
1	C	769	TRP	CB-CA-C	-5.69	97.49	109.38
1	G	612	THR	N-CA-CB	5.69	119.61	109.94
1	A	612	THR	N-CA-CB	5.69	119.61	109.94
1	J	612	THR	N-CA-CB	5.69	119.61	109.94
1	M	221	GLN	N-CA-CB	-5.69	102.41	111.62
1	G	728	VAL	CB-CA-C	-5.68	104.90	112.46
1	B	728	VAL	CB-CA-C	-5.68	104.90	112.46
1	G	166	ARG	N-CA-C	5.68	120.33	113.17
1	H	166	ARG	N-CA-C	5.68	120.33	113.17
1	O	728	VAL	CB-CA-C	-5.68	104.91	112.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	612	THR	N-CA-CB	5.68	119.59	109.94
1	M	612	THR	N-CA-CB	5.68	119.59	109.94
1	C	221	GLN	N-CA-CB	-5.68	102.42	111.62
1	E	769	TRP	CB-CA-C	-5.67	97.52	109.38
1	L	221	GLN	N-CA-CB	-5.67	102.43	111.62
1	M	769	TRP	CB-CA-C	-5.67	97.52	109.38
1	A	221	GLN	N-CA-CB	-5.67	102.43	111.62
1	E	612	THR	N-CA-CB	5.67	119.58	109.94
1	F	769	TRP	CB-CA-C	-5.67	97.52	109.38
1	H	769	TRP	CB-CA-C	-5.67	97.52	109.38
1	J	769	TRP	CB-CA-C	-5.67	97.52	109.38
1	O	166	ARG	N-CA-C	5.67	120.32	113.17
1	C	612	THR	N-CA-CB	5.67	119.58	109.94
1	D	221	GLN	N-CA-CB	-5.67	102.43	111.62
1	F	221	GLN	N-CA-CB	-5.67	102.43	111.62
1	H	221	GLN	N-CA-CB	-5.67	102.43	111.62
1	J	166	ARG	N-CA-C	5.67	120.32	113.17
1	C	728	VAL	CB-CA-C	-5.67	104.92	112.46
1	E	166	ARG	N-CA-C	5.67	120.31	113.17
1	G	769	TRP	CB-CA-C	-5.67	97.53	109.38
1	J	728	VAL	CB-CA-C	-5.67	104.92	112.46
1	P	769	TRP	CB-CA-C	-5.67	97.54	109.38
1	B	769	TRP	CB-CA-C	-5.67	97.54	109.38
1	D	728	VAL	CB-CA-C	-5.67	104.92	112.46
1	L	769	TRP	CB-CA-C	-5.67	97.54	109.38
1	I	769	TRP	CB-CA-C	-5.66	97.55	109.38
1	O	221	GLN	N-CA-CB	-5.66	102.45	111.62
1	E	221	GLN	N-CA-CB	-5.66	102.45	111.62
1	F	312	VAL	N-CA-C	5.66	116.03	108.11
1	K	769	TRP	CB-CA-C	-5.66	97.55	109.38
1	N	221	GLN	N-CA-CB	-5.66	102.45	111.62
1	B	221	GLN	N-CA-CB	-5.66	102.45	111.62
1	F	612	THR	N-CA-CB	5.66	119.56	109.94
1	I	221	GLN	N-CA-CB	-5.66	102.45	111.62
1	I	728	VAL	CB-CA-C	-5.66	104.93	112.46
1	N	769	TRP	CB-CA-C	-5.66	97.55	109.38
1	O	769	TRP	CB-CA-C	-5.66	97.56	109.38
1	D	769	TRP	CB-CA-C	-5.66	97.56	109.38
1	A	769	TRP	CB-CA-C	-5.66	97.56	109.38
1	I	612	THR	N-CA-CB	5.66	119.55	109.94
1	J	221	GLN	N-CA-CB	-5.66	102.46	111.62
1	A	728	VAL	CB-CA-C	-5.65	104.94	112.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	728	VAL	CB-CA-C	-5.65	104.94	112.46
1	P	221	GLN	N-CA-CB	-5.65	102.46	111.62
1	B	312	VAL	N-CA-C	5.65	116.02	108.11
1	P	728	VAL	CB-CA-C	-5.65	104.95	112.46
1	D	312	VAL	N-CA-C	5.65	116.02	108.11
1	E	728	VAL	CB-CA-C	-5.65	104.95	112.46
1	K	221	GLN	N-CA-CB	-5.65	102.47	111.62
1	K	728	VAL	CB-CA-C	-5.64	104.95	112.46
1	F	728	VAL	CB-CA-C	-5.64	104.96	112.46
1	G	221	GLN	N-CA-CB	-5.64	102.48	111.62
1	M	728	VAL	CB-CA-C	-5.64	104.96	112.46
1	J	312	VAL	N-CA-C	5.64	116.00	108.11
1	M	312	VAL	N-CA-C	5.64	116.00	108.11
1	N	458	LEU	CA-C-N	-5.62	114.77	122.42
1	N	458	LEU	C-N-CA	-5.62	114.77	122.42
1	K	312	VAL	N-CA-C	5.62	115.98	108.11
1	C	312	VAL	N-CA-C	5.62	115.98	108.11
1	G	312	VAL	N-CA-C	5.62	115.98	108.11
1	D	661	LYS	CA-C-N	5.62	125.80	119.90
1	D	661	LYS	C-N-CA	5.62	125.80	119.90
1	L	312	VAL	N-CA-C	5.62	115.98	108.11
1	A	312	VAL	N-CA-C	5.62	115.97	108.11
1	J	661	LYS	CA-C-N	5.62	125.80	119.90
1	J	661	LYS	C-N-CA	5.62	125.80	119.90
1	A	661	LYS	CA-C-N	5.62	125.80	119.90
1	A	661	LYS	C-N-CA	5.62	125.80	119.90
1	E	312	VAL	N-CA-C	5.62	115.97	108.11
1	B	458	LEU	CA-C-N	-5.61	114.79	122.42
1	B	458	LEU	C-N-CA	-5.61	114.79	122.42
1	P	312	VAL	N-CA-C	5.61	115.96	108.11
1	O	312	VAL	N-CA-C	5.61	115.96	108.11
1	H	661	LYS	CA-C-N	5.60	125.78	119.90
1	H	661	LYS	C-N-CA	5.60	125.78	119.90
1	N	312	VAL	N-CA-C	5.60	115.95	108.11
1	G	458	LEU	CA-C-N	-5.60	114.80	122.42
1	G	458	LEU	C-N-CA	-5.60	114.80	122.42
1	O	458	LEU	CA-C-N	-5.60	114.81	122.42
1	O	458	LEU	C-N-CA	-5.60	114.81	122.42
1	H	312	VAL	N-CA-C	5.59	115.94	108.11
1	P	661	LYS	CA-C-N	5.59	125.77	119.90
1	P	661	LYS	C-N-CA	5.59	125.77	119.90
1	B	661	LYS	CA-C-N	5.59	125.77	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	661	LYS	C-N-CA	5.59	125.77	119.90
1	D	954	ASP	CA-CB-CG	-5.59	107.01	112.60
1	H	458	LEU	CA-C-N	-5.59	114.82	122.42
1	H	458	LEU	C-N-CA	-5.59	114.82	122.42
1	G	661	LYS	CA-C-N	5.58	125.76	119.90
1	G	661	LYS	C-N-CA	5.58	125.76	119.90
1	M	458	LEU	CA-C-N	-5.58	114.83	122.42
1	M	458	LEU	C-N-CA	-5.58	114.83	122.42
1	A	458	LEU	CA-C-N	-5.58	114.83	122.42
1	A	458	LEU	C-N-CA	-5.58	114.83	122.42
1	D	458	LEU	CA-C-N	-5.58	114.83	122.42
1	D	458	LEU	C-N-CA	-5.58	114.83	122.42
1	E	458	LEU	CA-C-N	-5.58	114.83	122.42
1	E	458	LEU	C-N-CA	-5.58	114.83	122.42
1	G	954	ASP	CA-CB-CG	-5.58	107.02	112.60
1	I	312	VAL	N-CA-C	5.58	115.93	108.11
1	L	458	LEU	CA-C-N	-5.58	114.83	122.42
1	L	458	LEU	C-N-CA	-5.58	114.83	122.42
1	M	954	ASP	CA-CB-CG	-5.58	107.02	112.60
1	P	458	LEU	CA-C-N	-5.58	114.83	122.42
1	P	458	LEU	C-N-CA	-5.58	114.83	122.42
1	J	458	LEU	CA-C-N	-5.58	114.83	122.42
1	J	458	LEU	C-N-CA	-5.58	114.83	122.42
1	J	954	ASP	CA-CB-CG	-5.58	107.02	112.60
1	K	458	LEU	CA-C-N	-5.58	114.84	122.42
1	K	458	LEU	C-N-CA	-5.58	114.84	122.42
1	C	458	LEU	CA-C-N	-5.57	114.84	122.42
1	C	458	LEU	C-N-CA	-5.57	114.84	122.42
1	C	661	LYS	CA-C-N	5.57	125.75	119.90
1	C	661	LYS	C-N-CA	5.57	125.75	119.90
1	E	661	LYS	CA-C-N	5.57	125.75	119.90
1	E	661	LYS	C-N-CA	5.57	125.75	119.90
1	F	458	LEU	CA-C-N	-5.57	114.84	122.42
1	F	458	LEU	C-N-CA	-5.57	114.84	122.42
1	N	954	ASP	CA-CB-CG	-5.57	107.03	112.60
1	I	661	LYS	CA-C-N	5.57	125.75	119.90
1	I	661	LYS	C-N-CA	5.57	125.75	119.90
1	L	954	ASP	CA-CB-CG	-5.57	107.03	112.60
1	B	954	ASP	CA-CB-CG	-5.56	107.04	112.60
1	L	661	LYS	CA-C-N	5.56	125.74	119.90
1	L	661	LYS	C-N-CA	5.56	125.74	119.90
1	M	661	LYS	CA-C-N	5.56	125.74	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	661	LYS	C-N-CA	5.56	125.74	119.90
1	F	661	LYS	CA-C-N	5.56	125.74	119.90
1	F	661	LYS	C-N-CA	5.56	125.74	119.90
1	K	661	LYS	CA-C-N	5.56	125.73	119.90
1	K	661	LYS	C-N-CA	5.56	125.73	119.90
1	C	954	ASP	CA-CB-CG	-5.55	107.05	112.60
1	A	954	ASP	CA-CB-CG	-5.55	107.05	112.60
1	I	458	LEU	CA-C-N	-5.55	114.87	122.42
1	I	458	LEU	C-N-CA	-5.55	114.87	122.42
1	O	661	LYS	CA-C-N	5.55	125.73	119.90
1	O	661	LYS	C-N-CA	5.55	125.73	119.90
1	N	661	LYS	CA-C-N	5.55	125.72	119.90
1	N	661	LYS	C-N-CA	5.55	125.72	119.90
1	P	954	ASP	CA-CB-CG	-5.54	107.06	112.60
1	O	954	ASP	CA-CB-CG	-5.54	107.06	112.60
1	E	954	ASP	CA-CB-CG	-5.53	107.07	112.60
1	F	954	ASP	CA-CB-CG	-5.52	107.08	112.60
1	I	954	ASP	CA-CB-CG	-5.52	107.08	112.60
1	K	954	ASP	CA-CB-CG	-5.51	107.08	112.60
1	B	147	ASN	N-CA-CB	-5.50	101.43	110.68
1	E	147	ASN	N-CA-CB	-5.50	101.43	110.68
1	M	878	HIS	CA-C-N	5.50	125.41	119.85
1	M	878	HIS	C-N-CA	5.50	125.41	119.85
1	E	127	PHE	CA-CB-CG	-5.50	108.30	113.80
1	H	954	ASP	CA-CB-CG	-5.50	107.10	112.60
1	M	127	PHE	CA-CB-CG	-5.49	108.31	113.80
1	O	147	ASN	N-CA-CB	-5.49	101.46	110.68
1	I	739	HIS	CA-CB-CG	-5.49	108.31	113.80
1	J	147	ASN	N-CA-CB	-5.49	101.46	110.68
1	L	147	ASN	N-CA-CB	-5.49	101.46	110.68
1	L	739	HIS	CA-CB-CG	-5.49	108.31	113.80
1	I	127	PHE	CA-CB-CG	-5.49	108.31	113.80
1	K	147	ASN	N-CA-CB	-5.49	101.46	110.68
1	K	739	HIS	CA-CB-CG	-5.49	108.31	113.80
1	P	147	ASN	N-CA-CB	-5.49	101.47	110.68
1	C	147	ASN	N-CA-CB	-5.48	101.47	110.68
1	A	739	HIS	CA-CB-CG	-5.48	108.32	113.80
1	M	147	ASN	N-CA-CB	-5.48	101.47	110.68
1	N	147	ASN	N-CA-CB	-5.48	101.47	110.68
1	A	147	ASN	N-CA-CB	-5.48	101.47	110.68
1	I	878	HIS	CA-C-N	5.48	125.39	119.85
1	I	878	HIS	C-N-CA	5.48	125.39	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	147	ASN	N-CA-CB	-5.48	101.48	110.68
1	D	147	ASN	N-CA-CB	-5.48	101.48	110.68
1	F	147	ASN	N-CA-CB	-5.47	101.49	110.68
1	N	739	HIS	CA-CB-CG	-5.47	108.33	113.80
1	G	147	ASN	N-CA-CB	-5.47	101.49	110.68
1	H	147	ASN	N-CA-CB	-5.47	101.49	110.68
1	N	127	PHE	CA-CB-CG	-5.46	108.34	113.80
1	D	878	HIS	CA-C-N	5.46	125.36	119.85
1	D	878	HIS	C-N-CA	5.46	125.36	119.85
1	E	878	HIS	CA-C-N	5.46	125.36	119.85
1	E	878	HIS	C-N-CA	5.46	125.36	119.85
1	C	127	PHE	CA-CB-CG	-5.45	108.35	113.80
1	L	878	HIS	CA-C-N	5.45	125.36	119.85
1	L	878	HIS	C-N-CA	5.45	125.36	119.85
1	N	878	HIS	CA-C-N	5.45	125.36	119.85
1	N	878	HIS	C-N-CA	5.45	125.36	119.85
1	A	878	HIS	CA-C-N	5.45	125.36	119.85
1	A	878	HIS	C-N-CA	5.45	125.36	119.85
1	P	127	PHE	CA-CB-CG	-5.45	108.35	113.80
1	C	878	HIS	CA-C-N	5.45	125.35	119.85
1	C	878	HIS	C-N-CA	5.45	125.35	119.85
1	F	127	PHE	CA-CB-CG	-5.45	108.35	113.80
1	J	127	PHE	CA-CB-CG	-5.45	108.35	113.80
1	N	938	ARG	N-CA-CB	5.45	120.22	110.80
1	C	739	HIS	CA-CB-CG	-5.45	108.35	113.80
1	C	938	ARG	N-CA-CB	5.45	120.22	110.80
1	J	739	HIS	CA-CB-CG	-5.45	108.36	113.80
1	B	127	PHE	CA-CB-CG	-5.44	108.36	113.80
1	F	878	HIS	CA-C-N	5.44	125.35	119.85
1	F	878	HIS	C-N-CA	5.44	125.35	119.85
1	B	938	ARG	N-CA-CB	5.44	120.21	110.80
1	L	340	GLY	CA-C-N	-5.44	114.78	122.94
1	L	340	GLY	C-N-CA	-5.44	114.78	122.94
1	M	739	HIS	CA-CB-CG	-5.44	108.36	113.80
1	D	739	HIS	CA-CB-CG	-5.44	108.36	113.80
1	E	340	GLY	CA-C-N	-5.44	114.78	122.94
1	E	340	GLY	C-N-CA	-5.44	114.78	122.94
1	F	938	ARG	N-CA-CB	5.44	120.21	110.80
1	I	938	ARG	N-CA-CB	5.44	120.21	110.80
1	K	938	ARG	N-CA-CB	5.44	120.21	110.80
1	P	938	ARG	N-CA-CB	5.44	120.21	110.80
1	B	878	HIS	CA-C-N	5.43	125.34	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	878	HIS	C-N-CA	5.43	125.34	119.85
1	C	340	GLY	CA-C-N	-5.43	114.79	122.94
1	C	340	GLY	C-N-CA	-5.43	114.79	122.94
1	G	127	PHE	CA-CB-CG	-5.43	108.36	113.80
1	H	340	GLY	CA-C-N	-5.43	114.79	122.94
1	H	340	GLY	C-N-CA	-5.43	114.79	122.94
1	H	938	ARG	N-CA-CB	5.43	120.20	110.80
1	O	878	HIS	CA-C-N	5.43	125.34	119.85
1	O	878	HIS	C-N-CA	5.43	125.34	119.85
1	G	938	ARG	N-CA-CB	5.43	120.20	110.80
1	O	127	PHE	CA-CB-CG	-5.43	108.37	113.80
1	M	340	GLY	CA-C-N	-5.43	114.80	122.94
1	M	340	GLY	C-N-CA	-5.43	114.80	122.94
1	O	938	ARG	N-CA-CB	5.43	120.19	110.80
1	B	340	GLY	CA-C-N	-5.43	114.80	122.94
1	B	340	GLY	C-N-CA	-5.43	114.80	122.94
1	E	739	HIS	CA-CB-CG	-5.43	108.37	113.80
1	K	127	PHE	CA-CB-CG	-5.43	108.37	113.80
1	A	127	PHE	CA-CB-CG	-5.42	108.38	113.80
1	D	127	PHE	CA-CB-CG	-5.42	108.38	113.80
1	F	340	GLY	CA-C-N	-5.42	114.80	122.94
1	F	340	GLY	C-N-CA	-5.42	114.80	122.94
1	G	878	HIS	CA-C-N	5.42	125.33	119.85
1	G	878	HIS	C-N-CA	5.42	125.33	119.85
1	J	340	GLY	CA-C-N	-5.42	114.80	122.94
1	J	340	GLY	C-N-CA	-5.42	114.80	122.94
1	M	938	ARG	N-CA-CB	5.42	120.18	110.80
1	P	739	HIS	CA-CB-CG	-5.42	108.38	113.80
1	A	340	GLY	CA-C-N	-5.42	114.81	122.94
1	A	340	GLY	C-N-CA	-5.42	114.81	122.94
1	E	938	ARG	N-CA-CB	5.42	120.18	110.80
1	J	878	HIS	CA-C-N	5.42	125.33	119.85
1	J	878	HIS	C-N-CA	5.42	125.33	119.85
1	K	878	HIS	CA-C-N	5.42	125.33	119.85
1	K	878	HIS	C-N-CA	5.42	125.33	119.85
1	O	340	GLY	CA-C-N	-5.42	114.81	122.94
1	O	340	GLY	C-N-CA	-5.42	114.81	122.94
1	L	938	ARG	N-CA-CB	5.42	120.17	110.80
1	H	127	PHE	CA-CB-CG	-5.42	108.38	113.80
1	L	127	PHE	CA-CB-CG	-5.42	108.38	113.80
1	H	739	HIS	CA-CB-CG	-5.42	108.39	113.80
1	D	340	GLY	CA-C-N	-5.41	114.82	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	340	GLY	C-N-CA	-5.41	114.82	122.94
1	K	340	GLY	CA-C-N	-5.41	114.82	122.94
1	K	340	GLY	C-N-CA	-5.41	114.82	122.94
1	P	340	GLY	CA-C-N	-5.41	114.82	122.94
1	P	340	GLY	C-N-CA	-5.41	114.82	122.94
1	A	938	ARG	N-CA-CB	5.41	120.16	110.80
1	N	340	GLY	CA-C-N	-5.41	114.83	122.94
1	N	340	GLY	C-N-CA	-5.41	114.83	122.94
1	P	878	HIS	CA-C-N	5.41	125.32	119.85
1	P	878	HIS	C-N-CA	5.41	125.32	119.85
1	F	739	HIS	CA-CB-CG	-5.41	108.39	113.80
1	O	739	HIS	CA-CB-CG	-5.41	108.39	113.80
1	J	938	ARG	N-CA-CB	5.40	120.15	110.80
1	D	938	ARG	N-CA-CB	5.40	120.14	110.80
1	I	340	GLY	CA-C-N	-5.40	114.84	122.94
1	I	340	GLY	C-N-CA	-5.40	114.84	122.94
1	G	739	HIS	CA-CB-CG	-5.40	108.40	113.80
1	G	340	GLY	CA-C-N	-5.40	114.84	122.94
1	G	340	GLY	C-N-CA	-5.40	114.84	122.94
1	B	739	HIS	CA-CB-CG	-5.39	108.41	113.80
1	H	878	HIS	CA-C-N	5.39	125.30	119.85
1	H	878	HIS	C-N-CA	5.39	125.30	119.85
1	I	287	ASP	CA-CB-CG	-5.38	107.22	112.60
1	J	78	LEU	N-CA-CB	5.38	115.98	109.74
1	J	957	PHE	CA-CB-CG	-5.37	108.43	113.80
1	P	78	LEU	N-CA-CB	5.37	115.97	109.74
1	L	78	LEU	N-CA-CB	5.36	115.96	109.74
1	O	287	ASP	CA-CB-CG	-5.36	107.24	112.60
1	C	957	PHE	CA-CB-CG	-5.36	108.44	113.80
1	G	957	PHE	CA-CB-CG	-5.36	108.44	113.80
1	M	957	PHE	CA-CB-CG	-5.36	108.44	113.80
1	O	957	PHE	CA-CB-CG	-5.36	108.44	113.80
1	I	957	PHE	CA-CB-CG	-5.35	108.45	113.80
1	K	287	ASP	CA-CB-CG	-5.35	107.25	112.60
1	N	957	PHE	CA-CB-CG	-5.35	108.45	113.80
1	K	78	LEU	N-CA-CB	5.35	115.95	109.74
1	K	957	PHE	CA-CB-CG	-5.35	108.45	113.80
1	H	18	ASN	CA-C-N	5.35	126.53	119.84
1	H	18	ASN	C-N-CA	5.35	126.53	119.84
1	L	957	PHE	CA-CB-CG	-5.35	108.45	113.80
1	B	287	ASP	CA-CB-CG	-5.35	107.25	112.60
1	L	18	ASN	CA-C-N	5.35	126.53	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	18	ASN	C-N-CA	5.35	126.53	119.84
1	O	18	ASN	CA-C-N	5.35	126.52	119.84
1	O	18	ASN	C-N-CA	5.35	126.52	119.84
1	B	78	LEU	N-CA-CB	5.34	115.94	109.74
1	A	18	ASN	CA-C-N	5.34	126.52	119.84
1	A	18	ASN	C-N-CA	5.34	126.52	119.84
1	F	18	ASN	CA-C-N	5.34	126.52	119.84
1	F	18	ASN	C-N-CA	5.34	126.52	119.84
1	F	957	PHE	CA-CB-CG	-5.34	108.46	113.80
1	N	18	ASN	CA-C-N	5.34	126.52	119.84
1	N	18	ASN	C-N-CA	5.34	126.52	119.84
1	N	287	ASP	CA-CB-CG	-5.34	107.26	112.60
1	P	957	PHE	CA-CB-CG	-5.34	108.46	113.80
1	L	287	ASP	CA-CB-CG	-5.34	107.26	112.60
1	I	144	ASP	CA-CB-CG	-5.34	107.26	112.60
1	M	78	LEU	N-CA-CB	5.34	115.93	109.74
1	B	957	PHE	CA-CB-CG	-5.33	108.47	113.80
1	I	78	LEU	N-CA-CB	5.33	115.93	109.74
1	N	78	LEU	N-CA-CB	5.33	115.93	109.74
1	A	957	PHE	CA-CB-CG	-5.33	108.47	113.80
1	E	78	LEU	N-CA-CB	5.33	115.92	109.74
1	E	957	PHE	CA-CB-CG	-5.33	108.47	113.80
1	A	78	LEU	N-CA-CB	5.33	115.92	109.74
1	C	78	LEU	N-CA-CB	5.33	115.92	109.74
1	J	287	ASP	CA-CB-CG	-5.33	107.27	112.60
1	D	78	LEU	N-CA-CB	5.33	115.92	109.74
1	F	287	ASP	CA-CB-CG	-5.33	107.28	112.60
1	M	18	ASN	CA-C-N	5.33	126.50	119.84
1	M	18	ASN	C-N-CA	5.33	126.50	119.84
1	A	287	ASP	CA-CB-CG	-5.32	107.28	112.60
1	O	78	LEU	N-CA-CB	5.32	115.91	109.74
1	P	18	ASN	CA-C-N	5.32	126.49	119.84
1	P	18	ASN	C-N-CA	5.32	126.49	119.84
1	P	287	ASP	CA-CB-CG	-5.32	107.28	112.60
1	E	18	ASN	CA-C-N	5.32	126.48	119.84
1	E	18	ASN	C-N-CA	5.32	126.48	119.84
1	H	78	LEU	N-CA-CB	5.32	115.91	109.74
1	G	144	ASP	CA-CB-CG	-5.31	107.29	112.60
1	B	144	ASP	CA-CB-CG	-5.31	107.29	112.60
1	G	287	ASP	CA-CB-CG	-5.31	107.29	112.60
1	F	78	LEU	N-CA-CB	5.31	115.90	109.74
1	H	957	PHE	CA-CB-CG	-5.31	108.49	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	18	ASN	CA-C-N	5.31	126.48	119.84
1	I	18	ASN	C-N-CA	5.31	126.48	119.84
1	D	957	PHE	CA-CB-CG	-5.31	108.49	113.80
1	J	18	ASN	CA-C-N	5.31	126.47	119.84
1	J	18	ASN	C-N-CA	5.31	126.47	119.84
1	G	18	ASN	CA-C-N	5.30	126.47	119.84
1	G	18	ASN	C-N-CA	5.30	126.47	119.84
1	H	287	ASP	CA-CB-CG	-5.30	107.30	112.60
1	G	78	LEU	N-CA-CB	5.30	115.89	109.74
1	C	287	ASP	CA-CB-CG	-5.30	107.30	112.60
1	K	18	ASN	CA-C-N	5.30	126.47	119.84
1	K	18	ASN	C-N-CA	5.30	126.47	119.84
1	B	18	ASN	CA-C-N	5.30	126.47	119.84
1	B	18	ASN	C-N-CA	5.30	126.47	119.84
1	P	448	ARG	CA-C-N	-5.30	113.80	122.54
1	P	448	ARG	C-N-CA	-5.30	113.80	122.54
1	C	448	ARG	CA-C-N	-5.30	113.80	122.54
1	C	448	ARG	C-N-CA	-5.30	113.80	122.54
1	M	287	ASP	CA-CB-CG	-5.29	107.31	112.60
1	K	448	ARG	CA-C-N	-5.29	113.81	122.54
1	K	448	ARG	C-N-CA	-5.29	113.81	122.54
1	D	144	ASP	CA-CB-CG	-5.29	107.31	112.60
1	C	18	ASN	CA-C-N	5.29	126.45	119.84
1	C	18	ASN	C-N-CA	5.29	126.45	119.84
1	E	287	ASP	CA-CB-CG	-5.29	107.31	112.60
1	J	448	ARG	CA-C-N	-5.29	113.81	122.54
1	J	448	ARG	C-N-CA	-5.29	113.81	122.54
1	D	18	ASN	CA-C-N	5.29	126.45	119.84
1	D	18	ASN	C-N-CA	5.29	126.45	119.84
1	D	287	ASP	CA-CB-CG	-5.29	107.31	112.60
1	M	144	ASP	CA-CB-CG	-5.29	107.31	112.60
1	L	448	ARG	CA-C-N	-5.29	113.82	122.54
1	L	448	ARG	C-N-CA	-5.29	113.82	122.54
1	A	448	ARG	CA-C-N	-5.28	113.82	122.54
1	A	448	ARG	C-N-CA	-5.28	113.82	122.54
1	I	64	PRO	CB-CA-C	-5.28	104.35	111.85
1	E	448	ARG	CA-C-N	-5.28	113.83	122.54
1	E	448	ARG	C-N-CA	-5.28	113.83	122.54
1	A	144	ASP	CA-CB-CG	-5.28	107.32	112.60
1	O	448	ARG	CA-C-N	-5.28	113.83	122.54
1	O	448	ARG	C-N-CA	-5.28	113.83	122.54
1	B	448	ARG	CA-C-N	-5.28	113.83	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	448	ARG	C-N-CA	-5.28	113.83	122.54
1	H	144	ASP	CA-CB-CG	-5.28	107.32	112.60
1	N	448	ARG	CA-C-N	-5.28	113.83	122.54
1	N	448	ARG	C-N-CA	-5.28	113.83	122.54
1	E	144	ASP	CA-CB-CG	-5.28	107.32	112.60
1	O	741	THR	CB-CA-C	-5.28	104.19	110.94
1	J	741	THR	CB-CA-C	-5.27	104.19	110.94
1	G	927	THR	O-C-N	5.27	126.98	121.02
1	K	144	ASP	CA-CB-CG	-5.27	107.33	112.60
1	E	741	THR	CB-CA-C	-5.27	104.20	110.94
1	H	448	ARG	CA-C-N	-5.27	113.84	122.54
1	H	448	ARG	C-N-CA	-5.27	113.84	122.54
1	P	144	ASP	CA-CB-CG	-5.27	107.33	112.60
1	C	64	PRO	CB-CA-C	-5.27	104.37	111.85
1	F	448	ARG	CA-C-N	-5.27	113.85	122.54
1	F	448	ARG	C-N-CA	-5.27	113.85	122.54
1	F	741	THR	CB-CA-C	-5.27	104.20	110.94
1	P	741	THR	CB-CA-C	-5.27	104.20	110.94
1	G	448	ARG	CA-C-N	-5.26	113.86	122.54
1	G	448	ARG	C-N-CA	-5.26	113.86	122.54
1	M	448	ARG	CA-C-N	-5.26	113.85	122.54
1	M	448	ARG	C-N-CA	-5.26	113.85	122.54
1	C	741	THR	CB-CA-C	-5.26	104.21	110.94
1	L	64	PRO	CB-CA-C	-5.26	104.38	111.85
1	N	927	THR	O-C-N	5.26	126.97	121.02
1	A	741	THR	CB-CA-C	-5.26	104.21	110.94
1	E	64	PRO	CB-CA-C	-5.26	104.39	111.85
1	F	64	PRO	CB-CA-C	-5.26	104.39	111.85
1	L	741	THR	CB-CA-C	-5.26	104.21	110.94
1	B	741	THR	CB-CA-C	-5.25	104.22	110.94
1	D	64	PRO	CB-CA-C	-5.25	104.39	111.85
1	D	448	ARG	CA-C-N	-5.25	113.87	122.54
1	D	448	ARG	C-N-CA	-5.25	113.87	122.54
1	F	144	ASP	CA-CB-CG	-5.25	107.35	112.60
1	G	741	THR	CB-CA-C	-5.25	104.22	110.94
1	I	448	ARG	CA-C-N	-5.25	113.87	122.54
1	I	448	ARG	C-N-CA	-5.25	113.87	122.54
1	L	144	ASP	CA-CB-CG	-5.25	107.35	112.60
1	N	64	PRO	CB-CA-C	-5.25	104.39	111.85
1	O	144	ASP	CA-CB-CG	-5.25	107.35	112.60
1	H	741	THR	CB-CA-C	-5.25	104.22	110.94
1	P	64	PRO	CB-CA-C	-5.25	104.39	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	367	MET	N-CA-C	5.25	118.56	110.42
1	B	64	PRO	CB-CA-C	-5.25	104.40	111.85
1	D	741	THR	CB-CA-C	-5.25	104.22	110.94
1	B	927	THR	O-C-N	5.25	126.95	121.02
1	C	144	ASP	CA-CB-CG	-5.25	107.35	112.60
1	G	64	PRO	CB-CA-C	-5.25	104.40	111.85
1	J	64	PRO	CB-CA-C	-5.25	104.40	111.85
1	N	144	ASP	CA-CB-CG	-5.25	107.35	112.60
1	M	64	PRO	CB-CA-C	-5.24	104.41	111.85
1	A	64	PRO	CB-CA-C	-5.24	104.41	111.85
1	L	375	ASP	CA-CB-CG	-5.24	107.36	112.60
1	N	741	THR	CB-CA-C	-5.24	104.23	110.94
1	C	375	ASP	CA-CB-CG	-5.24	107.36	112.60
1	I	741	THR	CB-CA-C	-5.24	104.24	110.94
1	M	559	TYR	CA-C-O	5.24	124.55	119.62
1	A	927	THR	O-C-N	5.24	126.94	121.02
1	C	975	LEU	CA-C-N	-5.24	113.12	122.07
1	C	975	LEU	C-N-CA	-5.24	113.12	122.07
1	E	360	HIS	CA-C-N	5.23	125.54	119.47
1	E	360	HIS	C-N-CA	5.23	125.54	119.47
1	E	975	LEU	CA-C-N	-5.23	113.12	122.07
1	E	975	LEU	C-N-CA	-5.23	113.12	122.07
1	H	375	ASP	CA-CB-CG	-5.23	107.37	112.60
1	P	559	TYR	CA-C-O	5.23	124.54	119.62
1	P	975	LEU	CA-C-N	-5.23	113.12	122.07
1	P	975	LEU	C-N-CA	-5.23	113.12	122.07
1	F	367	MET	N-CA-C	5.23	118.53	110.42
1	L	927	THR	O-C-N	5.23	126.93	121.02
1	O	64	PRO	CB-CA-C	-5.23	104.42	111.85
1	H	559	TYR	CA-C-O	5.23	124.53	119.62
1	I	927	THR	O-C-N	5.23	126.93	121.02
1	J	367	MET	N-CA-C	5.23	118.52	110.42
1	K	64	PRO	CB-CA-C	-5.23	104.43	111.85
1	H	975	LEU	CA-C-N	-5.23	113.13	122.07
1	H	975	LEU	C-N-CA	-5.23	113.13	122.07
1	M	688	PRO	CB-CA-C	-5.23	104.70	111.39
1	C	927	THR	O-C-N	5.22	126.92	121.02
1	G	688	PRO	CB-CA-C	-5.22	104.70	111.39
1	K	741	THR	CB-CA-C	-5.22	104.25	110.94
1	P	360	HIS	CA-C-N	5.22	125.53	119.47
1	P	360	HIS	C-N-CA	5.22	125.53	119.47
1	B	559	TYR	CA-C-O	5.22	124.53	119.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	367	MET	N-CA-C	5.22	118.51	110.42
1	G	375	ASP	CA-CB-CG	-5.22	107.38	112.60
1	K	688	PRO	CB-CA-C	-5.22	104.70	111.39
1	L	367	MET	N-CA-C	5.22	118.51	110.42
1	M	975	LEU	CA-C-N	-5.22	113.14	122.07
1	M	975	LEU	C-N-CA	-5.22	113.14	122.07
1	P	927	THR	O-C-N	5.22	126.92	121.02
1	J	144	ASP	CA-CB-CG	-5.22	107.38	112.60
1	N	367	MET	N-CA-C	5.22	118.51	110.42
1	F	375	ASP	CA-CB-CG	-5.22	107.38	112.60
1	K	975	LEU	CA-C-N	-5.22	113.14	122.07
1	K	975	LEU	C-N-CA	-5.22	113.14	122.07
1	H	64	PRO	CB-CA-C	-5.22	104.44	111.85
1	F	688	PRO	CB-CA-C	-5.22	104.71	111.39
1	B	975	LEU	CA-C-N	-5.21	113.15	122.07
1	B	975	LEU	C-N-CA	-5.21	113.15	122.07
1	I	375	ASP	CA-CB-CG	-5.21	107.39	112.60
1	M	367	MET	N-CA-C	5.21	118.50	110.42
1	J	688	PRO	CB-CA-C	-5.21	104.72	111.39
1	C	367	MET	N-CA-C	5.21	118.50	110.42
1	O	927	THR	O-C-N	5.21	126.91	121.02
1	I	367	MET	N-CA-C	5.21	118.50	110.42
1	O	975	LEU	CA-C-N	-5.21	113.16	122.07
1	O	975	LEU	C-N-CA	-5.21	113.16	122.07
1	D	927	THR	O-C-N	5.21	126.91	121.02
1	D	975	LEU	CA-C-N	-5.21	113.16	122.07
1	D	975	LEU	C-N-CA	-5.21	113.16	122.07
1	P	375	ASP	CA-CB-CG	-5.21	107.39	112.60
1	A	367	MET	N-CA-C	5.21	118.49	110.42
1	F	360	HIS	CA-C-N	5.21	125.51	119.47
1	F	360	HIS	C-N-CA	5.21	125.51	119.47
1	N	375	ASP	CA-CB-CG	-5.21	107.39	112.60
1	N	975	LEU	CA-C-N	-5.21	113.17	122.07
1	N	975	LEU	C-N-CA	-5.21	113.17	122.07
1	P	367	MET	N-CA-C	5.21	118.49	110.42
1	E	367	MET	N-CA-C	5.20	118.49	110.42
1	J	975	LEU	CA-C-N	-5.20	113.17	122.07
1	J	975	LEU	C-N-CA	-5.20	113.17	122.07
1	M	741	THR	CB-CA-C	-5.20	104.28	110.94
1	O	367	MET	N-CA-C	5.20	118.49	110.42
1	A	375	ASP	CA-CB-CG	-5.20	107.40	112.60
1	G	559	TYR	CA-C-O	5.20	124.51	119.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	559	TYR	CA-C-O	5.20	124.51	119.62
1	B	367	MET	N-CA-C	5.20	118.48	110.42
1	P	688	PRO	CB-CA-C	-5.20	104.73	111.39
1	D	688	PRO	CB-CA-C	-5.20	104.74	111.39
1	K	375	ASP	CA-CB-CG	-5.20	107.40	112.60
1	O	688	PRO	CB-CA-C	-5.20	104.74	111.39
1	E	375	ASP	CA-CB-CG	-5.20	107.40	112.60
1	B	688	PRO	CB-CA-C	-5.19	104.74	111.39
1	I	975	LEU	CA-C-N	-5.19	113.19	122.07
1	I	975	LEU	C-N-CA	-5.19	113.19	122.07
1	L	559	TYR	CA-C-O	5.19	124.50	119.62
1	A	975	LEU	CA-C-N	-5.19	113.19	122.07
1	A	975	LEU	C-N-CA	-5.19	113.19	122.07
1	C	688	PRO	CB-CA-C	-5.19	104.74	111.39
1	E	688	PRO	CB-CA-C	-5.19	104.74	111.39
1	K	360	HIS	CA-C-N	5.19	125.49	119.47
1	K	360	HIS	C-N-CA	5.19	125.49	119.47
1	M	360	HIS	CA-C-N	5.19	125.49	119.47
1	M	360	HIS	C-N-CA	5.19	125.49	119.47
1	D	375	ASP	CA-CB-CG	-5.19	107.41	112.60
1	J	559	TYR	CA-C-O	5.19	124.50	119.62
1	F	975	LEU	CA-C-N	-5.19	113.20	122.07
1	F	975	LEU	C-N-CA	-5.19	113.20	122.07
1	G	360	HIS	CA-C-N	5.19	125.49	119.47
1	G	360	HIS	C-N-CA	5.19	125.49	119.47
1	I	559	TYR	CA-C-O	5.19	124.50	119.62
1	L	688	PRO	CB-CA-C	-5.19	104.75	111.39
1	D	367	MET	N-CA-C	5.19	118.46	110.42
1	M	375	ASP	CA-CB-CG	-5.19	107.41	112.60
1	O	360	HIS	CA-C-N	5.19	125.49	119.47
1	O	360	HIS	C-N-CA	5.19	125.49	119.47
1	A	559	TYR	CA-C-O	5.19	124.50	119.62
1	A	688	PRO	CB-CA-C	-5.19	104.75	111.39
1	H	688	PRO	CB-CA-C	-5.19	104.75	111.39
1	M	927	THR	O-C-N	5.19	126.88	121.02
1	E	927	THR	O-C-N	5.18	126.88	121.02
1	N	688	PRO	CB-CA-C	-5.18	104.75	111.39
1	E	559	TYR	CA-C-O	5.18	124.49	119.62
1	O	559	TYR	CA-C-O	5.18	124.49	119.62
1	L	975	LEU	CA-C-N	-5.18	113.21	122.07
1	L	975	LEU	C-N-CA	-5.18	113.21	122.07
1	O	375	ASP	CA-CB-CG	-5.18	107.42	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	559	TYR	CA-C-O	5.18	124.49	119.62
1	F	927	THR	O-C-N	5.18	126.87	121.02
1	H	367	MET	N-CA-C	5.18	118.45	110.42
1	M	475	ILE	CB-CA-C	-5.18	105.34	111.97
1	G	975	LEU	CA-C-N	-5.18	113.22	122.07
1	G	975	LEU	C-N-CA	-5.18	113.22	122.07
1	H	360	HIS	CA-C-N	5.18	125.47	119.47
1	H	360	HIS	C-N-CA	5.18	125.47	119.47
1	I	475	ILE	CB-CA-C	-5.18	105.34	111.97
1	J	375	ASP	CA-CB-CG	-5.17	107.43	112.60
1	O	475	ILE	CB-CA-C	-5.17	105.35	111.97
1	C	475	ILE	CB-CA-C	-5.17	105.35	111.97
1	I	688	PRO	CB-CA-C	-5.17	104.77	111.39
1	D	360	HIS	CA-C-N	5.17	125.47	119.47
1	D	360	HIS	C-N-CA	5.17	125.47	119.47
1	K	927	THR	O-C-N	5.17	126.86	121.02
1	E	475	ILE	CB-CA-C	-5.17	105.35	111.97
1	F	475	ILE	CB-CA-C	-5.17	105.35	111.97
1	K	559	TYR	CA-C-O	5.17	124.48	119.62
1	B	375	ASP	CA-CB-CG	-5.17	107.43	112.60
1	H	927	THR	O-C-N	5.17	126.86	121.02
1	J	927	THR	O-C-N	5.17	126.86	121.02
1	G	475	ILE	CB-CA-C	-5.16	105.36	111.97
1	N	360	HIS	CA-C-N	5.16	125.46	119.47
1	N	360	HIS	C-N-CA	5.16	125.46	119.47
1	C	360	HIS	CA-C-N	5.16	125.46	119.47
1	C	360	HIS	C-N-CA	5.16	125.46	119.47
1	E	150	PHE	N-CA-C	5.16	116.37	108.52
1	B	360	HIS	CA-C-N	5.16	125.45	119.47
1	B	360	HIS	C-N-CA	5.16	125.45	119.47
1	L	360	HIS	CA-C-N	5.16	125.45	119.47
1	L	360	HIS	C-N-CA	5.16	125.45	119.47
1	H	475	ILE	CB-CA-C	-5.16	105.37	111.97
1	C	559	TYR	CA-C-O	5.15	124.47	119.62
1	J	475	ILE	CB-CA-C	-5.15	105.37	111.97
1	B	150	PHE	N-CA-C	5.15	116.35	108.52
1	H	150	PHE	N-CA-C	5.15	116.35	108.52
1	I	150	PHE	N-CA-C	5.15	116.35	108.52
1	N	475	ILE	CB-CA-C	-5.15	105.37	111.97
1	G	150	PHE	N-CA-C	5.15	116.35	108.52
1	I	360	HIS	CA-C-N	5.15	125.44	119.47
1	I	360	HIS	C-N-CA	5.15	125.44	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	360	HIS	CA-C-N	5.15	125.44	119.47
1	J	360	HIS	C-N-CA	5.15	125.44	119.47
1	K	475	ILE	CB-CA-C	-5.15	105.38	111.97
1	L	475	ILE	CB-CA-C	-5.14	105.39	111.97
1	D	559	TYR	CA-C-O	5.14	124.45	119.62
1	L	150	PHE	N-CA-C	5.14	116.33	108.52
1	L	868	VAL	N-CA-C	5.14	115.52	108.12
1	A	475	ILE	CB-CA-C	-5.14	105.39	111.97
1	B	475	ILE	CB-CA-C	-5.14	105.40	111.97
1	D	645	ARG	N-CA-C	5.14	118.06	110.46
1	J	645	ARG	N-CA-C	5.14	118.06	110.46
1	M	150	PHE	N-CA-C	5.13	116.33	108.52
1	A	823	LEU	N-CA-C	-5.13	107.15	113.41
1	H	101	THR	OG1-CB-CG2	5.13	119.56	109.30
1	C	645	ARG	N-CA-C	5.13	118.05	110.46
1	N	150	PHE	N-CA-C	5.13	116.32	108.52
1	H	645	ARG	N-CA-C	5.13	118.05	110.46
1	A	150	PHE	N-CA-C	5.13	116.31	108.52
1	F	645	ARG	N-CA-C	5.13	118.05	110.46
1	J	150	PHE	N-CA-C	5.13	116.31	108.52
1	K	150	PHE	N-CA-C	5.13	116.31	108.52
1	O	150	PHE	N-CA-C	5.13	116.31	108.52
1	P	645	ARG	N-CA-C	5.13	118.05	110.46
1	H	332	PHE	CA-CB-CG	-5.12	108.67	113.80
1	B	101	THR	OG1-CB-CG2	5.12	119.55	109.30
1	D	150	PHE	N-CA-C	5.12	116.31	108.52
1	F	150	PHE	N-CA-C	5.12	116.31	108.52
1	J	702	GLN	CA-C-N	5.12	124.57	119.24
1	J	702	GLN	C-N-CA	5.12	124.57	119.24
1	A	868	VAL	N-CA-C	5.12	115.49	108.12
1	E	645	ARG	N-CA-C	5.12	118.04	110.46
1	L	101	THR	OG1-CB-CG2	5.12	119.54	109.30
1	L	645	ARG	N-CA-C	5.12	118.04	110.46
1	N	823	LEU	N-CA-C	-5.12	107.16	113.41
1	P	101	THR	OG1-CB-CG2	5.12	119.55	109.30
1	P	475	ILE	CB-CA-C	-5.12	105.41	111.97
1	C	823	LEU	N-CA-C	-5.12	107.17	113.41
1	K	101	THR	OG1-CB-CG2	5.12	119.54	109.30
1	O	101	THR	OG1-CB-CG2	5.12	119.54	109.30
1	B	645	ARG	N-CA-C	5.12	118.03	110.46
1	J	823	LEU	N-CA-C	-5.12	107.17	113.41
1	A	101	THR	OG1-CB-CG2	5.12	119.53	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	101	THR	OG1-CB-CG2	5.12	119.53	109.30
1	D	475	ILE	CB-CA-C	-5.12	105.42	111.97
1	G	101	THR	OG1-CB-CG2	5.12	119.53	109.30
1	G	823	LEU	N-CA-C	-5.12	107.17	113.41
1	I	101	THR	OG1-CB-CG2	5.12	119.53	109.30
1	J	101	THR	OG1-CB-CG2	5.12	119.53	109.30
1	P	150	PHE	N-CA-C	5.12	116.29	108.52
1	O	645	ARG	N-CA-C	5.11	118.03	110.46
1	O	823	LEU	N-CA-C	-5.11	107.17	113.41
1	F	823	LEU	N-CA-C	-5.11	107.17	113.41
1	G	645	ARG	N-CA-C	5.11	118.03	110.46
1	M	645	ARG	N-CA-C	5.11	118.03	110.46
1	A	702	GLN	CA-C-N	5.11	124.56	119.24
1	A	702	GLN	C-N-CA	5.11	124.56	119.24
1	C	150	PHE	N-CA-C	5.11	116.29	108.52
1	M	868	VAL	N-CA-C	5.11	115.48	108.12
1	E	101	THR	OG1-CB-CG2	5.11	119.52	109.30
1	I	868	VAL	N-CA-C	5.11	115.48	108.12
1	I	332	PHE	CA-CB-CG	-5.11	108.69	113.80
1	I	645	ARG	N-CA-C	5.11	118.02	110.46
1	K	868	VAL	N-CA-C	5.11	115.47	108.12
1	F	868	VAL	N-CA-C	5.10	115.47	108.12
1	M	685	LEU	CA-C-N	5.10	124.86	119.76
1	M	685	LEU	C-N-CA	5.10	124.86	119.76
1	O	868	VAL	N-CA-C	5.10	115.47	108.12
1	A	360	HIS	CA-C-N	5.10	125.39	119.47
1	A	360	HIS	C-N-CA	5.10	125.39	119.47
1	C	101	THR	OG1-CB-CG2	5.10	119.50	109.30
1	J	685	LEU	CA-C-N	5.10	124.86	119.76
1	J	685	LEU	C-N-CA	5.10	124.86	119.76
1	K	645	ARG	N-CA-C	5.10	118.01	110.46
1	H	823	LEU	N-CA-C	-5.10	107.19	113.41
1	I	685	LEU	CA-C-N	5.10	124.86	119.76
1	I	685	LEU	C-N-CA	5.10	124.86	119.76
1	N	101	THR	OG1-CB-CG2	5.10	119.50	109.30
1	O	874	SER	CA-C-N	-5.10	114.50	122.65
1	O	874	SER	C-N-CA	-5.10	114.50	122.65
1	P	868	VAL	N-CA-C	5.10	115.46	108.12
1	D	429	ASP	CA-C-N	5.09	126.21	119.84
1	D	429	ASP	C-N-CA	5.09	126.21	119.84
1	O	332	PHE	CA-CB-CG	-5.09	108.71	113.80
1	F	101	THR	OG1-CB-CG2	5.09	119.48	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	874	SER	CA-C-N	-5.09	114.50	122.65
1	J	874	SER	C-N-CA	-5.09	114.50	122.65
1	D	868	VAL	N-CA-C	5.09	115.45	108.12
1	N	429	ASP	CA-C-N	5.09	126.20	119.84
1	N	429	ASP	C-N-CA	5.09	126.20	119.84
1	A	645	ARG	N-CA-C	5.09	117.99	110.46
1	E	874	SER	CA-C-N	-5.09	114.51	122.65
1	E	874	SER	C-N-CA	-5.09	114.51	122.65
1	O	429	ASP	CA-C-N	5.09	126.20	119.84
1	O	429	ASP	C-N-CA	5.09	126.20	119.84
1	J	332	PHE	CA-CB-CG	-5.09	108.71	113.80
1	K	823	LEU	N-CA-C	-5.09	107.20	113.41
1	K	874	SER	CA-C-N	-5.09	114.51	122.65
1	K	874	SER	C-N-CA	-5.09	114.51	122.65
1	M	101	THR	OG1-CB-CG2	5.09	119.47	109.30
1	M	332	PHE	CA-CB-CG	-5.09	108.71	113.80
1	H	702	GLN	CA-C-N	5.08	124.53	119.24
1	H	702	GLN	C-N-CA	5.08	124.53	119.24
1	N	645	ARG	N-CA-C	5.08	117.99	110.46
1	H	685	LEU	CA-C-N	5.08	124.84	119.76
1	H	685	LEU	C-N-CA	5.08	124.84	119.76
1	P	823	LEU	N-CA-C	-5.08	107.21	113.41
1	G	874	SER	CA-C-N	-5.08	114.52	122.65
1	G	874	SER	C-N-CA	-5.08	114.52	122.65
1	J	868	VAL	N-CA-C	5.08	115.44	108.12
1	A	874	SER	CA-C-N	-5.08	114.52	122.65
1	A	874	SER	C-N-CA	-5.08	114.52	122.65
1	K	702	GLN	CA-C-N	5.08	124.52	119.24
1	K	702	GLN	C-N-CA	5.08	124.52	119.24
1	B	823	LEU	N-CA-C	-5.08	107.21	113.41
1	C	702	GLN	CA-C-N	5.08	124.52	119.24
1	C	702	GLN	C-N-CA	5.08	124.52	119.24
1	L	823	LEU	N-CA-C	-5.08	107.21	113.41
1	G	868	VAL	N-CA-C	5.08	115.43	108.12
1	L	685	LEU	CA-C-N	5.08	124.83	119.76
1	L	685	LEU	C-N-CA	5.08	124.83	119.76
1	M	823	LEU	N-CA-C	-5.08	107.22	113.41
1	N	868	VAL	N-CA-C	5.08	115.43	108.12
1	O	613	PRO	CB-CA-C	-5.08	104.73	111.23
1	A	332	PHE	CA-CB-CG	-5.07	108.73	113.80
1	C	332	PHE	CA-CB-CG	-5.07	108.73	113.80
1	F	310	ARG	N-CA-CB	5.07	119.66	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	332	PHE	CA-CB-CG	-5.07	108.73	113.80
1	I	823	LEU	N-CA-C	-5.07	107.22	113.41
1	M	874	SER	CA-C-N	-5.07	114.53	122.65
1	M	874	SER	C-N-CA	-5.07	114.53	122.65
1	O	310	ARG	N-CA-CB	5.07	119.66	110.83
1	F	874	SER	CA-C-N	-5.07	114.53	122.65
1	F	874	SER	C-N-CA	-5.07	114.53	122.65
1	H	868	VAL	N-CA-C	5.07	115.42	108.12
1	K	429	ASP	CA-C-N	5.07	126.18	119.84
1	K	429	ASP	C-N-CA	5.07	126.18	119.84
1	C	868	VAL	N-CA-C	5.07	115.42	108.12
1	C	874	SER	CA-C-N	-5.07	114.54	122.65
1	C	874	SER	C-N-CA	-5.07	114.54	122.65
1	P	512	PHE	CA-CB-CG	-5.07	108.73	113.80
1	G	702	GLN	CA-C-N	5.07	124.51	119.24
1	G	702	GLN	C-N-CA	5.07	124.51	119.24
1	N	332	PHE	CA-CB-CG	-5.07	108.73	113.80
1	O	702	GLN	CA-C-N	5.07	124.51	119.24
1	O	702	GLN	C-N-CA	5.07	124.51	119.24
1	A	685	LEU	CA-C-N	5.07	124.83	119.76
1	A	685	LEU	C-N-CA	5.07	124.83	119.76
1	B	868	VAL	N-CA-C	5.07	115.42	108.12
1	E	823	LEU	N-CA-C	-5.07	107.23	113.41
1	H	874	SER	CA-C-N	-5.07	114.54	122.65
1	H	874	SER	C-N-CA	-5.07	114.54	122.65
1	L	332	PHE	CA-CB-CG	-5.07	108.73	113.80
1	L	874	SER	CA-C-N	-5.07	114.54	122.65
1	L	874	SER	C-N-CA	-5.07	114.54	122.65
1	P	874	SER	CA-C-N	-5.07	114.54	122.65
1	P	874	SER	C-N-CA	-5.07	114.54	122.65
1	E	868	VAL	N-CA-C	5.07	115.42	108.12
1	F	702	GLN	CA-C-N	5.07	124.51	119.24
1	F	702	GLN	C-N-CA	5.07	124.51	119.24
1	P	702	GLN	CA-C-N	5.07	124.51	119.24
1	P	702	GLN	C-N-CA	5.07	124.51	119.24
1	D	332	PHE	CA-CB-CG	-5.06	108.74	113.80
1	D	685	LEU	CA-C-N	5.06	124.82	119.76
1	D	685	LEU	C-N-CA	5.06	124.82	119.76
1	I	874	SER	CA-C-N	-5.06	114.55	122.65
1	I	874	SER	C-N-CA	-5.06	114.55	122.65
1	M	429	ASP	CA-C-N	5.06	126.17	119.84
1	M	429	ASP	C-N-CA	5.06	126.17	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	685	LEU	CA-C-N	5.06	124.82	119.76
1	O	685	LEU	C-N-CA	5.06	124.82	119.76
1	B	613	PRO	CB-CA-C	-5.06	104.75	111.23
1	D	702	GLN	CA-C-N	5.06	124.50	119.24
1	D	702	GLN	C-N-CA	5.06	124.50	119.24
1	I	310	ARG	N-CA-CB	5.06	119.64	110.83
1	L	310	ARG	N-CA-CB	5.06	119.64	110.83
1	A	429	ASP	CA-C-N	5.06	126.16	119.84
1	A	429	ASP	C-N-CA	5.06	126.16	119.84
1	D	823	LEU	N-CA-C	-5.06	107.24	113.41
1	G	310	ARG	N-CA-CB	5.06	119.63	110.83
1	I	702	GLN	CA-C-N	5.06	124.50	119.24
1	I	702	GLN	C-N-CA	5.06	124.50	119.24
1	M	310	ARG	N-CA-CB	5.06	119.63	110.83
1	B	332	PHE	CA-CB-CG	-5.06	108.74	113.80
1	B	874	SER	CA-C-N	-5.06	114.56	122.65
1	B	874	SER	C-N-CA	-5.06	114.56	122.65
1	H	429	ASP	CA-C-N	5.06	126.16	119.84
1	H	429	ASP	C-N-CA	5.06	126.16	119.84
1	H	512	PHE	CA-CB-CG	-5.06	108.74	113.80
1	J	429	ASP	CA-C-N	5.06	126.16	119.84
1	J	429	ASP	C-N-CA	5.06	126.16	119.84
1	J	512	PHE	CA-CB-CG	-5.06	108.74	113.80
1	L	702	GLN	CA-C-N	5.06	124.50	119.24
1	L	702	GLN	C-N-CA	5.06	124.50	119.24
1	N	310	ARG	N-CA-CB	5.06	119.63	110.83
1	B	702	GLN	CA-C-N	5.06	124.50	119.24
1	B	702	GLN	C-N-CA	5.06	124.50	119.24
1	D	512	PHE	CA-CB-CG	-5.06	108.74	113.80
1	B	685	LEU	CA-C-N	5.05	124.81	119.76
1	B	685	LEU	C-N-CA	5.05	124.81	119.76
1	D	874	SER	CA-C-N	-5.05	114.56	122.65
1	D	874	SER	C-N-CA	-5.05	114.56	122.65
1	E	332	PHE	CA-CB-CG	-5.05	108.75	113.80
1	P	332	PHE	CA-CB-CG	-5.05	108.75	113.80
1	E	685	LEU	CA-C-N	5.05	124.81	119.76
1	E	685	LEU	C-N-CA	5.05	124.81	119.76
1	B	1019	VAL	N-CA-C	5.05	115.39	108.12
1	L	429	ASP	CA-C-N	5.05	126.15	119.84
1	L	429	ASP	C-N-CA	5.05	126.15	119.84
1	P	310	ARG	N-CA-CB	5.05	119.62	110.83
1	A	613	PRO	CB-CA-C	-5.05	104.77	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	310	ARG	N-CA-CB	5.05	119.62	110.83
1	C	1019	VAL	N-CA-C	5.05	115.39	108.12
1	F	685	LEU	CA-C-N	5.05	124.81	119.76
1	F	685	LEU	C-N-CA	5.05	124.81	119.76
1	I	802	ASP	CA-C-N	5.05	126.15	119.84
1	I	802	ASP	C-N-CA	5.05	126.15	119.84
1	K	512	PHE	CA-CB-CG	-5.05	108.75	113.80
1	P	429	ASP	CA-C-N	5.05	126.15	119.84
1	P	429	ASP	C-N-CA	5.05	126.15	119.84
1	B	512	PHE	CA-CB-CG	-5.05	108.75	113.80
1	L	613	PRO	CB-CA-C	-5.05	104.77	111.23
1	J	310	ARG	N-CA-CB	5.05	119.61	110.83
1	M	702	GLN	CA-C-N	5.05	124.49	119.24
1	M	702	GLN	C-N-CA	5.05	124.49	119.24
1	N	702	GLN	CA-C-N	5.05	124.49	119.24
1	N	702	GLN	C-N-CA	5.05	124.49	119.24
1	O	512	PHE	CA-CB-CG	-5.05	108.75	113.80
1	P	685	LEU	CA-C-N	5.05	124.81	119.76
1	P	685	LEU	C-N-CA	5.05	124.81	119.76
1	A	512	PHE	CA-CB-CG	-5.04	108.75	113.80
1	C	512	PHE	CA-CB-CG	-5.04	108.75	113.80
1	B	429	ASP	CA-C-N	5.04	126.14	119.84
1	B	429	ASP	C-N-CA	5.04	126.14	119.84
1	E	429	ASP	CA-C-N	5.04	126.14	119.84
1	E	429	ASP	C-N-CA	5.04	126.14	119.84
1	F	1019	VAL	N-CA-C	5.04	115.38	108.12
1	H	310	ARG	N-CA-CB	5.04	119.61	110.83
1	I	613	PRO	CB-CA-C	-5.04	104.78	111.23
1	N	874	SER	CA-C-N	-5.04	114.58	122.65
1	N	874	SER	C-N-CA	-5.04	114.58	122.65
1	D	1019	VAL	N-CA-C	5.04	115.38	108.12
1	G	1019	VAL	N-CA-C	5.04	115.38	108.12
1	I	512	PHE	CA-CB-CG	-5.04	108.76	113.80
1	N	512	PHE	CA-CB-CG	-5.04	108.76	113.80
1	E	702	GLN	CA-C-N	5.04	124.48	119.24
1	E	702	GLN	C-N-CA	5.04	124.48	119.24
1	F	332	PHE	CA-CB-CG	-5.04	108.76	113.80
1	G	685	LEU	CA-C-N	5.04	124.80	119.76
1	G	685	LEU	C-N-CA	5.04	124.80	119.76
1	K	332	PHE	CA-CB-CG	-5.04	108.76	113.80
1	N	685	LEU	CA-C-N	5.04	124.80	119.76
1	N	685	LEU	C-N-CA	5.04	124.80	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	1019	VAL	N-CA-C	5.04	115.38	108.12
1	G	802	ASP	CA-C-N	5.04	126.14	119.84
1	G	802	ASP	C-N-CA	5.04	126.14	119.84
1	H	613	PRO	CB-CA-C	-5.04	104.79	111.23
1	J	1019	VAL	N-CA-C	5.04	115.37	108.12
1	L	13	ARG	N-CA-C	5.04	117.50	111.71
1	L	512	PHE	CA-CB-CG	-5.04	108.77	113.80
1	O	997	ASP	N-CA-CB	5.04	119.37	111.56
1	C	429	ASP	CA-C-N	5.03	126.13	119.84
1	C	429	ASP	C-N-CA	5.03	126.13	119.84
1	C	685	LEU	CA-C-N	5.03	124.79	119.76
1	C	685	LEU	C-N-CA	5.03	124.79	119.76
1	E	613	PRO	CB-CA-C	-5.03	104.79	111.23
1	F	429	ASP	CA-C-N	5.03	126.13	119.84
1	F	429	ASP	C-N-CA	5.03	126.13	119.84
1	K	685	LEU	CA-C-N	5.03	124.79	119.76
1	K	685	LEU	C-N-CA	5.03	124.79	119.76
1	N	1019	VAL	N-CA-C	5.03	115.36	108.12
1	F	613	PRO	CB-CA-C	-5.03	104.79	111.23
1	I	13	ARG	N-CA-C	5.03	117.49	111.71
1	A	1019	VAL	N-CA-C	5.03	115.36	108.12
1	I	429	ASP	CA-C-N	5.03	126.12	119.84
1	I	429	ASP	C-N-CA	5.03	126.12	119.84
1	O	802	ASP	CA-C-N	5.03	126.12	119.84
1	O	802	ASP	C-N-CA	5.03	126.12	119.84
1	A	13	ARG	N-CA-C	5.03	117.49	111.71
1	G	429	ASP	CA-C-N	5.03	126.12	119.84
1	G	429	ASP	C-N-CA	5.03	126.12	119.84
1	I	997	ASP	N-CA-CB	5.03	119.35	111.56
1	B	310	ARG	N-CA-CB	5.02	119.57	110.83
1	M	512	PHE	CA-CB-CG	-5.02	108.78	113.80
1	M	802	ASP	CA-C-N	5.02	126.12	119.84
1	M	802	ASP	C-N-CA	5.02	126.12	119.84
1	A	310	ARG	N-CA-CB	5.02	119.57	110.83
1	E	310	ARG	N-CA-CB	5.02	119.57	110.83
1	K	997	ASP	N-CA-CB	5.02	119.34	111.56
1	K	1019	VAL	N-CA-C	5.02	115.35	108.12
1	D	310	ARG	N-CA-CB	5.02	119.57	110.83
1	K	613	PRO	CB-CA-C	-5.02	104.80	111.23
1	G	997	ASP	N-CA-CB	5.02	119.34	111.56
1	J	613	PRO	CB-CA-C	-5.02	104.81	111.23
1	B	802	ASP	CA-C-N	5.02	126.11	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	802	ASP	C-N-CA	5.02	126.11	119.84
1	D	802	ASP	CA-C-N	5.02	126.11	119.84
1	D	802	ASP	C-N-CA	5.02	126.11	119.84
1	H	1019	VAL	N-CA-C	5.02	115.35	108.12
1	P	613	PRO	CB-CA-C	-5.02	104.81	111.23
1	F	997	ASP	N-CA-CB	5.02	119.33	111.56
1	K	310	ARG	N-CA-CB	5.01	119.56	110.83
1	B	13	ARG	N-CA-C	5.01	117.47	111.71
1	M	613	PRO	CB-CA-C	-5.01	104.81	111.23
1	G	13	ARG	N-CA-C	5.01	117.47	111.71
1	K	13	ARG	N-CA-C	5.01	117.47	111.71
1	M	1019	VAL	N-CA-C	5.01	115.33	108.12
1	P	997	ASP	N-CA-CB	5.01	119.32	111.56
1	C	802	ASP	CA-C-N	5.01	126.10	119.84
1	C	802	ASP	C-N-CA	5.01	126.10	119.84
1	L	1019	VAL	N-CA-C	5.01	115.33	108.12
1	N	13	ARG	N-CA-C	5.01	117.47	111.71
1	E	335	VAL	CB-CA-C	-5.01	103.65	110.96
1	G	613	PRO	CB-CA-C	-5.01	104.82	111.23
1	P	802	ASP	CA-C-N	5.01	126.10	119.84
1	P	802	ASP	C-N-CA	5.01	126.10	119.84
1	E	1019	VAL	N-CA-C	5.00	115.33	108.12
1	H	997	ASP	N-CA-CB	5.00	119.32	111.56
1	N	613	PRO	CB-CA-C	-5.00	104.82	111.23
1	N	997	ASP	N-CA-CB	5.00	119.32	111.56
1	C	13	ARG	N-CA-C	5.00	117.46	111.71
1	I	1019	VAL	N-CA-C	5.00	115.33	108.12
1	J	13	ARG	N-CA-C	5.00	117.46	111.71
1	C	613	PRO	CB-CA-C	-5.00	104.83	111.23
1	E	512	PHE	CA-CB-CG	-5.00	108.80	113.80
1	F	13	ARG	N-CA-C	5.00	117.46	111.71
1	H	13	ARG	N-CA-C	5.00	117.46	111.71
1	L	335	VAL	CB-CA-C	-5.00	103.66	110.96
1	L	997	ASP	N-CA-CB	5.00	119.31	111.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8219	0	7811	614	3
1	B	8219	0	7811	596	5
1	C	8219	0	7811	578	1
1	D	8219	0	7811	610	0
1	E	8219	0	7811	600	0
1	F	8219	0	7811	591	1
1	G	8219	0	7811	600	1
1	H	8219	0	7811	591	0
1	I	8219	0	7811	600	1
1	J	8219	0	7811	598	0
1	K	8219	0	7811	593	0
1	L	8219	0	7811	606	1
1	M	8219	0	7811	610	0
1	N	8219	0	7811	602	0
1	O	8219	0	7811	606	0
1	P	8219	0	7811	610	2
2	Q	23	0	20	0	0
2	R	23	0	20	0	0
2	S	23	0	20	0	0
2	T	23	0	20	0	0
2	U	23	0	20	0	0
2	V	23	0	20	0	0
2	W	23	0	20	0	0
2	X	23	0	20	0	0
2	Y	23	0	20	0	0
2	Z	23	0	20	0	0
2	a	23	0	20	0	0
2	b	23	0	20	0	0
2	c	23	0	20	0	0
2	d	23	0	20	0	0
2	e	23	0	20	0	0
2	f	23	0	20	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
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	A	160	0	0	6	0
5	B	163	0	0	6	0
5	C	162	0	0	6	0
5	D	163	0	0	6	0
5	E	162	0	0	6	0
5	F	162	0	0	6	0
5	G	162	0	0	6	0
5	H	162	0	0	6	0
5	I	162	0	0	6	1
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	134528	0	125296	9467	8

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (9467) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:427:THR:HA	1:I:436:MET:HE1	1.17	1.16
1:J:427:THR:HA	1:J:436:MET:HE1	1.17	1.16
1:N:427:THR:HA	1:N:436:MET:HE1	1.17	1.16
1:F:427:THR:HA	1:F:436:MET:HE1	1.17	1.16
1:C:427:THR:HA	1:C:436:MET:HE1	1.17	1.15
1:B:427:THR:HA	1:B:436:MET:HE1	1.17	1.15
1:L:427:THR:HA	1:L:436:MET:HE1	1.17	1.14
1:O:427:THR:HA	1:O:436:MET:HE1	1.17	1.13
1:G:427:THR:HA	1:G:436:MET:HE1	1.17	1.13
1:M:427:THR:HA	1:M:436:MET:HE1	1.17	1.12
1:D:427:THR:HA	1:D:436:MET:HE1	1.17	1.11
1:E:427:THR:HA	1:E:436:MET:HE1	1.17	1.10
1:I:436:MET:HE3	1:I:467:ASN:HD22	1.16	1.10
1:M:436:MET:HE3	1:M:467:ASN:HD22	1.16	1.09
1:F:436:MET:HE3	1:F:467:ASN:HD22	1.16	1.09
1:L:436:MET:HE3	1:L:467:ASN:HD22	1.16	1.08
1:N:436:MET:HE3	1:N:467:ASN:HD22	1.16	1.08
1:B:436:MET:HE3	1:B:467:ASN:HD22	1.16	1.08
1:K:427:THR:HA	1:K:436:MET:HE1	1.17	1.08
1:P:427:THR:HA	1:P:436:MET:HE1	1.17	1.08
1:A:427:THR:HA	1:A:436:MET:HE1	1.17	1.07
1:E:436:MET:HE3	1:E:467:ASN:HD22	1.16	1.07
1:J:43:ARG:HH11	1:J:43:ARG:HG2	1.20	1.07
1:H:427:THR:HA	1:H:436:MET:HE1	1.17	1.07
1:H:43:ARG:HG2	1:H:43:ARG:HH11	1.20	1.07
1:I:43:ARG:HG2	1:I:43:ARG:HH11	1.20	1.07
1:A:43:ARG:HG2	1:A:43:ARG:HH11	1.20	1.07
1:C:436:MET:HE3	1:C:467:ASN:HD22	1.16	1.06
1:D:436:MET:HE3	1:D:467:ASN:HD22	1.16	1.06
1:M:43:ARG:HG2	1:M:43:ARG:HH11	1.20	1.06
1:G:436:MET:HE3	1:G:467:ASN:HD22	1.16	1.06
1:O:436:MET:HE3	1:O:467:ASN:HD22	1.16	1.06
1:K:436:MET:HE3	1:K:467:ASN:HD22	1.16	1.05
1:B:43:ARG:HG2	1:B:43:ARG:HH11	1.20	1.05
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.35	1.05
1:J:436:MET:HE3	1:J:467:ASN:HD22	1.16	1.05
1:P:436:MET:HE3	1:P:467:ASN:HD22	1.16	1.04
1:A:436:MET:HE3	1:A:467:ASN:HD22	1.16	1.03
1:C:43:ARG:HG2	1:C:43:ARG:HH11	1.20	1.03
1:E:43:ARG:HG2	1:E:43:ARG:HH11	1.20	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:43:ARG:HG2	1:P:43:ARG:HH11	1.20	1.02
1:O:43:ARG:HG2	1:O:43:ARG:HH11	1.20	1.02
1:F:43:ARG:HG2	1:F:43:ARG:HH11	1.20	1.02
1:G:43:ARG:HG2	1:G:43:ARG:HH11	1.20	1.02
1:H:436:MET:HE3	1:H:467:ASN:HD22	1.16	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:HG2	1:K:43:ARG:HH11	1.20	1.01
1:M:777:LEU:HD11	1:M:889:ALA:HA	1.43	1.01
1:D:43:ARG:HG2	1:D:43:ARG:HH11	1.20	1.01
1:J:777:LEU:HD11	1:J:889:ALA:HA	1.43	1.01
1:E:777:LEU:HD11	1:E:889:ALA:HA	1.43	1.00
1:K:777:LEU:HD11	1:K:889:ALA:HA	1.43	1.00
1:C:777:LEU:HD11	1:C:889:ALA:HA	1.43	1.00
1:A:777:LEU:HD11	1:A:889:ALA:HA	1.43	0.99
1:G:777:LEU:HD11	1:G:889:ALA:HA	1.43	0.99
1:O:777:LEU:HD11	1:O:889:ALA:HA	1.43	0.99
1:H:777:LEU:HD11	1:H:889:ALA:HA	1.43	0.98
1:D:777:LEU:HD11	1:D:889:ALA:HA	1.43	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:L:740:LEU:HD12	1:L:741:THR:H	1.29	0.98
1:N:740:LEU:HD12	1:N:741:THR:H	1.29	0.98
1:F:740:LEU:HD12	1:F:741:THR:H	1.29	0.97
1:G:740:LEU:HD12	1:G:741:THR:H	1.29	0.97
1:I:777:LEU:HD11	1:I:889:ALA:HA	1.43	0.97
1:B:777:LEU:HD11	1:B:889:ALA:HA	1.43	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:F:777:LEU:HD11	1:F:889:ALA:HA	1.43	0.97
1:H:740:LEU:HD12	1:H:741:THR:H	1.29	0.96
1:P:740:LEU:HD12	1:P:741:THR:H	1.29	0.96
1:B:740:LEU:HD12	1:B:741:THR:H	1.29	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:D:740:LEU:HD12	1:D:741:THR:H	1.29	0.95
1:E:740:LEU:HD12	1:E:741:THR:H	1.29	0.95
1:M:740:LEU:HD12	1:M:741:THR:H	1.29	0.95
1:C:740:LEU:HD12	1:C:741:THR:H	1.29	0.95
1:A:740:LEU:HD12	1:A:741:THR:H	1.29	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:427:THR:HA	1:L:436:MET:CE	1.98	0.93
1:A:427:THR:HA	1:A:436:MET:CE	1.98	0.93
1:H:427:THR:HA	1:H:436:MET:CE	1.98	0.93
1:D:427:THR:HA	1:D:436:MET:CE	1.98	0.93
1:F:427:THR:HA	1:F:436:MET:CE	1.98	0.93
1:O:427:THR:HA	1:O:436:MET:CE	1.98	0.93
1:G:427:THR:HA	1:G:436:MET:CE	1.98	0.92
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:B:427:THR:HA	1:B:436:MET:CE	1.98	0.92
1:M:427:THR:HA	1:M:436:MET:CE	1.98	0.92
1:C:427:THR:HA	1:C:436:MET:CE	1.98	0.92
1:I:102:ASN:HD22	1:I:201:ASP:HB2	1.35	0.92
1:I:427:THR:HA	1:I:436:MET:CE	1.98	0.92
1:E:427:THR:HA	1:E:436:MET:CE	1.98	0.92
1:B:102:ASN:HD22	1:B:201:ASP:HB2	1.35	0.92
1:J:102:ASN:HD22	1:J:201:ASP:HB2	1.35	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:H:102:ASN:HD22	1:H:201:ASP:HB2	1.35	0.91
1:C:46:ARG:HG3	1:C:46:ARG:HH11	1.36	0.90
1:F:46:ARG:HG3	1:F:46:ARG:HH11	1.37	0.90
1:A:46:ARG:HH11	1:A:46:ARG:HG3	1.36	0.90
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:HG3	1:K:46:ARG:HH11	1.37	0.90
1:M:46:ARG:HH11	1:M:46:ARG:HG3	1.36	0.90
1:D:102:ASN:HD22	1:D:201:ASP:HB2	1.35	0.90
1:G:744:GLU:HB3	1:G:745:MET:HE3	1.54	0.90
1:J:744:GLU:HB3	1:J:745:MET:HE3	1.54	0.90
1:O:744:GLU:HB3	1:O:745:MET:HE3	1.54	0.90
1:J:668:VAL:HG13	1:J:669:PRO:HD2	1.54	0.90
1:A:102:ASN:HD22	1:A:201:ASP:HB2	1.35	0.90
1:F:102:ASN:HD22	1:F:201:ASP:HB2	1.35	0.90
1:M:668:VAL:HG13	1:M:669:PRO:HD2	1.54	0.90
1:E:18:ASN:ND2	1:E:21:VAL:HG23	1.87	0.90
1:F:668:VAL:HG13	1:F:669:PRO:HD2	1.54	0.90
1:K:18:ASN:ND2	1:K:21:VAL:HG23	1.87	0.90
1:C:18:ASN:ND2	1:C:21:VAL:HG23	1.87	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ASN:HD22	1:C:201:ASP:HB2	1.35	0.90
1:J:18:ASN:ND2	1:J:21:VAL:HG23	1.87	0.90
1:L:316:HIS:HA	1:L:323:ILE:HD13	1.55	0.90
1:N:18:ASN:ND2	1:N:21:VAL:HG23	1.87	0.90
1:B:744:GLU:HB3	1:B:745:MET:HE3	1.54	0.89
1:E:668:VAL:HG13	1:E:669:PRO:HD2	1.54	0.89
1:F:18:ASN:ND2	1:F:21:VAL:HG23	1.87	0.89
1:L:18:ASN:ND2	1:L:21:VAL:HG23	1.87	0.89
1:N:668:VAL:HG13	1:N:669:PRO:HD2	1.54	0.89
1:H:46:ARG:HG3	1:H:46:ARG:HH11	1.36	0.89
1:I:316:HIS:HA	1:I:323:ILE:HD13	1.55	0.89
1:M:18:ASN:ND2	1:M:21:VAL:HG23	1.87	0.89
1:G:102:ASN:HD22	1:G:201:ASP:HB2	1.35	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:A:744:GLU:HB3	1:A:745:MET:HE3	1.54	0.89
1:G:18:ASN:ND2	1:G:21:VAL:HG23	1.87	0.89
1:H:18:ASN:ND2	1:H:21:VAL:HG23	1.87	0.89
1:K:668:VAL:HG13	1:K:669:PRO:HD2	1.54	0.89
1:O:102:ASN:HD22	1:O:201:ASP:HB2	1.35	0.89
1:P:316:HIS:HA	1:P:323:ILE:HD13	1.54	0.89
1:A:57:GLU:HG2	1:A:83:THR:CG2	2.03	0.89
1:B:46:ARG:HH11	1:B:46:ARG:HG3	1.37	0.89
1:A:18:ASN:ND2	1:A:21:VAL:HG23	1.87	0.89
1:D:316:HIS:HA	1:D:323:ILE:HD13	1.54	0.89
1:F:316:HIS:HA	1:F:323:ILE:HD13	1.55	0.89
1:H:57:GLU:HG2	1:H:83:THR:CG2	2.03	0.89
1:O:316:HIS:HA	1:O:323:ILE:HD13	1.54	0.89
1:D:18:ASN:ND2	1:D:21:VAL:HG23	1.87	0.89
1:D:744:GLU:HB3	1:D:745:MET:HE3	1.54	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:B:18:ASN:ND2	1:B:21:VAL:HG23	1.87	0.89
1:I:57:GLU:HG2	1:I:83:THR:CG2	2.03	0.89
1:P:18:ASN:ND2	1:P:21:VAL:HG23	1.87	0.89
1:P:57:GLU:HG2	1:P:83:THR:CG2	2.03	0.89
1:E:46:ARG:HH11	1:E:46:ARG:HG3	1.37	0.89
1:G:316:HIS:HA	1:G:323:ILE:HD13	1.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:HIS:HA	1:B:323:ILE:HD13	1.55	0.88
1:E:57:GLU:HG2	1:E:83:THR:CG2	2.03	0.88
1:H:744:GLU:HB3	1:H:745:MET:HE3	1.54	0.88
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:C:744:GLU:HB3	1:C:745:MET:HE3	1.54	0.88
1:D:46:ARG:HH11	1:D:46:ARG:HG3	1.37	0.88
1:P:668:VAL:HG13	1:P:669:PRO:HD2	1.54	0.88
1:C:668:VAL:HG13	1:C:669:PRO:HD2	1.54	0.88
1:F:57:GLU:HG2	1:F:83:THR:CG2	2.03	0.88
1:F:744:GLU:HB3	1:F:745:MET:HE3	1.54	0.88
1:H:316:HIS:HA	1:H:323:ILE:HD13	1.55	0.88
1:I:18:ASN:ND2	1:I:21:VAL:HG23	1.87	0.88
1:N:744:GLU:HB3	1:N:745:MET:HE3	1.54	0.88
1:C:57:GLU:HG2	1:C:83:THR:CG2	2.03	0.88
1:D:668:VAL:HG13	1:D:669:PRO:HD2	1.54	0.88
1:F:434:PRO:HB3	1:G:434:PRO:HB3	1.53	0.88
1:G:46:ARG:HH11	1:G:46:ARG:HG3	1.37	0.88
1:G:57:GLU:HG2	1:G:83:THR:CG2	2.03	0.88
1:I:46:ARG:HH11	1:I:46:ARG:HG3	1.37	0.88
1:L:46:ARG:HH11	1:L:46:ARG:HG3	1.37	0.88
1:P:102:ASN:HD22	1:P:201:ASP:HB2	1.35	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:E:102:ASN:HD22	1:E:201:ASP:HB2	1.35	0.88
1:H:668:VAL:HG13	1:H:669:PRO:HD2	1.54	0.88
1:N:102:ASN:HD22	1:N:201:ASP:HB2	1.35	0.88
1:A:668:VAL:HG13	1:A:669:PRO:HD2	1.54	0.88
1:L:57:GLU:HG2	1:L:83:THR:CG2	2.03	0.88
1:L:744:GLU:HB3	1:L:745:MET:HE3	1.54	0.88
1:M:744:GLU:HB3	1:M:745:MET:HE3	1.54	0.88
1:O:46:ARG:HH11	1:O:46:ARG:HG3	1.36	0.88
1:P:744:GLU:HB3	1:P:745:MET:HE3	1.54	0.88
1:P:46:ARG:HH11	1:P:46:ARG:HG3	1.37	0.88
1:A:316:HIS:HA	1:A:323:ILE:HD13	1.55	0.87
1:B:57:GLU:HG2	1:B:83:THR:CG2	2.03	0.87
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.10	0.87
1:N:46:ARG:HG3	1:N:46:ARG:HH11	1.37	0.87
1:B:668:VAL:HG13	1:B:669:PRO:HD2	1.54	0.87
1:H:360:HIS:CE1	1:H:362:LEU:HB2	2.10	0.87
1:J:7:LEU:HD13	1:J:74:LEU:HD11	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:7:LEU:HD13	1:O:74:LEU:HD11	1.57	0.87
1:P:360:HIS:CE1	1:P:362:LEU:HB2	2.10	0.87
1:B:437:SER:HB2	5:B:2263:HOH:O	1.72	0.87
1:D:57:GLU:HG2	1:D:83:THR:CG2	2.03	0.87
1:G:7:LEU:HD13	1:G:74:LEU:HD11	1.57	0.87
1:I:744:GLU:HB3	1:I:745:MET:HE3	1.54	0.87
1:O:57:GLU:HG2	1:O:83:THR:CG2	2.03	0.87
1:B:7:LEU:HD13	1:B:74:LEU:HD11	1.57	0.87
1:E:316:HIS:HA	1:E:323:ILE:HD13	1.55	0.87
1:F:7:LEU:HD13	1:F:74:LEU:HD11	1.57	0.87
1:I:7:LEU:HD13	1:I:74:LEU:HD11	1.57	0.87
1:K:360:HIS:CE1	1:K:362:LEU:HB2	2.10	0.87
1:L:360:HIS:CE1	1:L:362:LEU:HB2	2.10	0.87
1:N:7:LEU:HD13	1:N:74:LEU:HD11	1.57	0.87
1:M:360:HIS:CE1	1:M:362:LEU:HB2	2.10	0.87
1:C:7:LEU:HD13	1:C:74:LEU:HD11	1.57	0.87
1:C:316:HIS:HA	1:C:323:ILE:HD13	1.55	0.87
1:E:744:GLU:HB3	1:E:745:MET:HE3	1.54	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:A:360:HIS:CE1	1:A:362:LEU:HB2	2.10	0.86
1:J:856:TYR:HD2	1:J:864:MET:HE2	1.40	0.86
1:K:7:LEU:HD13	1:K:74:LEU:HD11	1.57	0.86
1:O:360:HIS:CE1	1:O:362:LEU:HB2	2.10	0.86
1:E:360:HIS:CE1	1:E:362:LEU:HB2	2.10	0.86
1:G:360:HIS:CE1	1:G:362:LEU:HB2	2.10	0.86
1:I:856:TYR:HD2	1:I:864:MET:HE2	1.41	0.86
1:E:856:TYR:HD2	1:E:864:MET:HE2	1.40	0.86
1:J:360:HIS:CE1	1:J:362:LEU:HB2	2.10	0.86
1:D:360:HIS:CE1	1:D:362:LEU:HB2	2.10	0.86
1:D:781:ARG:HG3	1:D:781:ARG:HH11	1.41	0.86
1:M:856:TYR:HD2	1:M:864:MET:HE2	1.40	0.86
1:N:360:HIS:CE1	1:N:362:LEU:HB2	2.10	0.86
1:B:781:ARG:HH11	1:B:781:ARG:HG3	1.41	0.86
1:L:781:ARG:HG3	1:L:781:ARG:HH11	1.41	0.86
1:D:7:LEU:HD13	1:D:74:LEU:HD11	1.57	0.86
1:D:856:TYR:HD2	1:D:864:MET:HE2	1.40	0.86
1:F:360:HIS:CE1	1:F:362:LEU:HB2	2.10	0.86
1:G:668:VAL:HG13	1:G:669:PRO:HD2	1.54	0.86
1:H:7:LEU:HD13	1:H:74:LEU:HD11	1.57	0.86
1:O:668:VAL:HG13	1:O:669:PRO:HD2	1.54	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:HIS:CE1	1:C:362:LEU:HB2	2.10	0.86
1:J:781:ARG:HH11	1:J:781:ARG:HG3	1.41	0.86
1:K:744:GLU:HB3	1:K:745:MET:HE3	1.54	0.86
1:P:7:LEU:HD13	1:P:74:LEU:HD11	1.57	0.86
1:P:856:TYR:HD2	1:P:864:MET:HE2	1.40	0.85
1:K:781:ARG:HH11	1:K:781:ARG:HG3	1.41	0.85
1:A:781:ARG:HH11	1:A:781:ARG:HG3	1.41	0.85
1:C:856:TYR:HD2	1:C:864:MET:HE2	1.40	0.85
1:E:434:PRO:HB3	1:H:434:PRO:HB3	1.59	0.85
1:G:781:ARG:HG3	1:G:781:ARG:HH11	1.41	0.85
1:K:856:TYR:HD2	1:K:864:MET:HE2	1.40	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:A:856:TYR:HD2	1:A:864:MET:HE2	1.40	0.85
1:E:781:ARG:HH11	1:E:781:ARG:HG3	1.41	0.85
1:L:7:LEU:HD13	1:L:74:LEU:HD11	1.57	0.85
1:P:249:GLU:HG2	1:P:251:ARG:NH1	1.92	0.85
1:F:856:TYR:HD2	1:F:864:MET:HE2	1.40	0.85
1:L:949:HIS:CD2	1:L:1020:TRP:HE1	1.95	0.85
1:N:856:TYR:HD2	1:N:864:MET:HE2	1.40	0.85
1:N:949:HIS:CD2	1:N:1020:TRP:HE1	1.95	0.85
1:K:249:GLU:HG2	1:K:251:ARG:NH1	1.92	0.85
1:A:360:HIS:ND1	1:A:361:PRO:HD2	1.93	0.84
1:H:249:GLU:HG2	1:H:251:ARG:NH1	1.92	0.84
1:I:249:GLU:HG2	1:I:251:ARG:NH1	1.92	0.84
1:M:949:HIS:CD2	1:M:1020:TRP:HE1	1.95	0.84
1:C:781:ARG:HH11	1:C:781:ARG:HG3	1.41	0.84
1:I:949:HIS:CD2	1:I:1020:TRP:HE1	1.95	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:E:360:HIS:ND1	1:E:361:PRO:HD2	1.92	0.84
1:F:360:HIS:ND1	1:F:361:PRO:HD2	1.93	0.84
1:O:949:HIS:CD2	1:O:1020:TRP:HE1	1.95	0.84
1:G:360:HIS:ND1	1:G:361:PRO:HD2	1.93	0.84
1:H:360:HIS:ND1	1:H:361:PRO:HD2	1.93	0.84
1:A:7:LEU:HD13	1:A:74:LEU:HD11	1.57	0.84
1:A:249:GLU:HG2	1:A:251:ARG:NH1	1.92	0.84
1:B:360:HIS:ND1	1:B:361:PRO:HD2	1.93	0.84
1:B:949:HIS:CD2	1:B:1020:TRP:HE1	1.95	0.84
1:E:249:GLU:HG2	1:E:251:ARG:NH1	1.92	0.84
1:J:360:HIS:ND1	1:J:361:PRO:HD2	1.93	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:249:GLU:HG2	1:M:251:ARG:NH1	1.92	0.84
1:A:419:GLY:HA2	1:D:282:ARG:NH1	1.92	0.84
1:B:856:TYR:HD2	1:B:864:MET:HE2	1.40	0.84
1:D:894:ARG:NH2	1:D:921:PRO:HD3	1.93	0.84
1:K:894:ARG:NH2	1:K:921:PRO:HD3	1.93	0.84
1:M:360:HIS:ND1	1:M:361:PRO:HD2	1.92	0.84
1:E:7:LEU:HD13	1:E:74:LEU:HD11	1.57	0.84
1:F:949:HIS:CD2	1:F:1020:TRP:HE1	1.95	0.84
1:J:249:GLU:HG2	1:J:251:ARG:NH1	1.92	0.84
1:L:856:TYR:HD2	1:L:864:MET:HE2	1.40	0.84
1:N:360:HIS:ND1	1:N:361:PRO:HD2	1.93	0.84
1:P:360:HIS:ND1	1:P:361:PRO:HD2	1.93	0.84
1:I:360:HIS:ND1	1:I:361:PRO:HD2	1.93	0.84
1:L:360:HIS:ND1	1:L:361:PRO:HD2	1.92	0.84
1:O:249:GLU:HG2	1:O:251:ARG:NH1	1.92	0.84
1:C:249:GLU:HG2	1:C:251:ARG:NH1	1.92	0.83
1:C:437:SER:HB2	5:C:2258:HOH:O	1.76	0.83
1:F:249:GLU:HG2	1:F:251:ARG:NH1	1.92	0.83
1:G:856:TYR:HD2	1:G:864:MET:HE2	1.40	0.83
1:H:781:ARG:HH11	1:H:781:ARG:HG3	1.41	0.83
1:H:894:ARG:NH2	1:H:921:PRO:HD3	1.93	0.83
1:J:434:PRO:HB3	1:K:434:PRO:HB3	1.57	0.83
1:J:894:ARG:NH2	1:J:921:PRO:HD3	1.93	0.83
1:O:856:TYR:HD2	1:O:864:MET:HE2	1.40	0.83
1:P:894:ARG:NH2	1:P:921:PRO:HD3	1.93	0.83
1:B:894:ARG:NH2	1:B:921:PRO:HD3	1.93	0.83
1:F:781:ARG:HH11	1:F:781:ARG:HG3	1.41	0.83
1:F:894:ARG:NH2	1:F:921:PRO:HD3	1.93	0.83
1:H:856:TYR:HD2	1:H:864:MET:HE2	1.40	0.83
1:J:949:HIS:CD2	1:J:1020:TRP:HE1	1.95	0.83
1:M:7:LEU:HD13	1:M:74:LEU:HD11	1.57	0.83
1:A:894:ARG:NH2	1:A:921:PRO:HD3	1.93	0.83
1:E:894:ARG:NH2	1:E:921:PRO:HD3	1.93	0.83
1:E:949:HIS:CD2	1:E:1020:TRP:HE1	1.95	0.83
1:P:949:HIS:CD2	1:P:1020:TRP:HE1	1.95	0.83
1:D:949:HIS:CD2	1:D:1020:TRP:HE1	1.95	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:M:781:ARG:HH11	1:M:781:ARG:HG3	1.41	0.83
1:C:360:HIS:ND1	1:C:361:PRO:HD2	1.93	0.83
1:D:249:GLU:HG2	1:D:251:ARG:NH1	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:949:HIS:CD2	1:G: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:A:949:HIS:CD2	1:A:1020:TRP:HE1	1.95	0.83
1:D:360:HIS:ND1	1:D:361:PRO:HD2	1.93	0.83
1:C:949:HIS:CD2	1:C:1020:TRP:HE1	1.95	0.83
1:A:746:ASP:HA	1:A:760:ARG:HG3	1.61	0.83
1:F:777:LEU:CD1	1:F:889:ALA:HA	2.09	0.83
1:L:777:LEU:CD1	1:L:889:ALA:HA	2.09	0.83
1:N:777:LEU:CD1	1:N:889:ALA:HA	2.09	0.83
1:P:777:LEU:CD1	1:P:889:ALA:HA	2.09	0.83
1:G:890:GLN:HG3	1:G:891:VAL:N	1.94	0.83
1:I:890:GLN:HG3	1:I:891:VAL:N	1.94	0.83
1:L:949:HIS:HD2	1:L:1020:TRP:HE1	1.27	0.83
1:O:360:HIS:ND1	1:O:361:PRO:HD2	1.93	0.83
1:C:777:LEU:CD1	1:C:889:ALA:HA	2.09	0.82
1:A:890:GLN:HG3	1:A:891:VAL:N	1.94	0.82
1:D:777:LEU:CD1	1:D:889:ALA:HA	2.09	0.82
1:H:53:SER:C	1:H:54:LEU:HD23	2.04	0.82
1:K:436:MET:CE	1:K:467:ASN:HD22	1.93	0.82
1:M:425:ARG:HH22	1:P:287:ASP:CG	1.87	0.82
1:N:249:GLU:HG2	1:N:251:ARG:NH1	1.92	0.82
1:C:894:ARG:NH2	1:C:921:PRO:HD3	1.93	0.82
1:D:53:SER:C	1:D:54:LEU:HD23	2.04	0.82
1:G:240:LEU:HD12	1:G:241:GLU:N	1.95	0.82
1:H:777:LEU:CD1	1:H:889:ALA:HA	2.09	0.82
1:N:894:ARG:NH2	1:N:921:PRO:HD3	1.93	0.82
1:E:53:SER:C	1:E:54:LEU:HD23	2.05	0.82
1:L:746:ASP:HA	1:L:760:ARG:HG3	1.61	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:O:894:ARG:NH2	1:O:921:PRO:HD3	1.93	0.82
1:G:249:GLU:HG2	1:G:251:ARG:NH1	1.92	0.82
1:I:777:LEU:CD1	1:I:889:ALA:HA	2.09	0.82
1:H:949:HIS:CD2	1:H:1020:TRP:HE1	1.95	0.82
1:I:894:ARG:NH2	1:I:921:PRO:HD3	1.93	0.82
1:J:53:SER:C	1:J:54:LEU:HD23	2.04	0.82
1:K:63:PHE:HB3	1:K:64:PRO:HD2	1.62	0.82
1:L:436:MET:CE	1:L:467:ASN:HD22	1.93	0.82
1:B:53:SER:C	1:B:54:LEU:HD23	2.04	0.82
1:G:777:LEU:CD1	1:G:889:ALA:HA	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:240:LEU:HD12	1:N:241:GLU:N	1.95	0.82
1:P:781:ARG:HH11	1:P:781:ARG:HG3	1.41	0.82
1:A:777:LEU:CD1	1:A:889:ALA:HA	2.09	0.82
1:B:249:GLU:HG2	1:B:251:ARG:NH1	1.92	0.82
1:F:240:LEU:HD12	1:F:241:GLU:N	1.95	0.82
1:H:63:PHE:HB3	1:H:64:PRO:HD2	1.62	0.82
1:H:436:MET:CE	1:H:467:ASN:HD22	1.93	0.82
1:H:746:ASP:HA	1:H:760:ARG:HG3	1.61	0.82
1:M:240:LEU:HD12	1:M:241:GLU:N	1.95	0.82
1:O:777:LEU:CD1	1:O:889:ALA:HA	2.09	0.82
1:P:240:LEU:HD12	1:P:241:GLU:N	1.95	0.82
1:A:53:SER:C	1:A:54:LEU:HD23	2.04	0.82
1:A:240:LEU:HD12	1:A:241:GLU:N	1.95	0.82
1:A:436:MET:CE	1:A:467:ASN:HD22	1.93	0.82
1:B:63:PHE:HB3	1:B:64:PRO:HD2	1.62	0.82
1:C:53:SER:C	1:C:54:LEU:HD23	2.05	0.82
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.61	0.82
1:F:890:GLN:HG3	1:F:891:VAL:N	1.94	0.82
1:G:949:HIS:HD2	1:G:1020:TRP:HE1	1.28	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:J:436:MET:CE	1:J:467:ASN:HD22	1.93	0.82
1:K:53:SER:C	1:K:54:LEU:HD23	2.04	0.82
1:O:63:PHE:HB3	1:O:64:PRO:HD2	1.62	0.82
1:P:436:MET:CE	1:P:467:ASN:HD22	1.93	0.82
1:B:240:LEU:HD12	1:B:241:GLU:N	1.95	0.82
1:F:227:VAL:HG13	1:F:240:LEU:HD11	1.62	0.82
1:G:63:PHE:HB3	1:G:64:PRO:HD2	1.62	0.82
1:H:316:HIS:HA	1:H:323:ILE:CD1	2.10	0.82
1:I:53:SER:C	1:I:54:LEU:HD23	2.04	0.82
1:J:890:GLN:HG3	1:J:891:VAL:N	1.94	0.82
1:N:227:VAL:HG13	1:N:240:LEU:HD11	1.62	0.82
1:P:63:PHE:HB3	1:P:64:PRO:HD2	1.62	0.82
1:P:316:HIS:HA	1:P:323:ILE:CD1	2.10	0.82
1:G:894:ARG:NH2	1:G:921:PRO:HD3	1.93	0.81
1:K:65:ALA:HB1	1:K:66:PRO:HD2	1.62	0.81
1:K:746:ASP:HA	1:K:760:ARG:HG3	1.61	0.81
1:L:53:SER:C	1:L:54:LEU:HD23	2.04	0.81
1:L:227:VAL:HG13	1:L:240:LEU:HD11	1.62	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:746:ASP:HA	1:P:760:ARG:HG3	1.61	0.81
1:C:255:ARG:HH11	1:C:255:ARG:HG2	1.45	0.81
1:D:255:ARG:HG2	1:D:255:ARG:HH11	1.45	0.81
1:E:255:ARG:HG2	1:E:255:ARG:HH11	1.45	0.81
1:E:316:HIS:HA	1:E:323:ILE:CD1	2.10	0.81
1:G:746:ASP:HA	1:G:760:ARG:HG3	1.61	0.81
1:H:240:LEU:HD12	1:H:241:GLU:N	1.95	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:K:777:LEU:CD1	1:K:889:ALA:HA	2.09	0.81
1:L:255:ARG:HG2	1:L:255:ARG:HH11	1.45	0.81
1:A:63:PHE:HB3	1:A:64:PRO:HD2	1.62	0.81
1:A:316:HIS:HA	1:A:323:ILE:CD1	2.10	0.81
1:C:63:PHE:HB3	1:C:64:PRO:HD2	1.62	0.81
1:E:777:LEU:CD1	1:E:889:ALA:HA	2.09	0.81
1:F:53:SER:C	1:F:54:LEU:HD23	2.04	0.81
1:F:65:ALA:HB1	1:F:66:PRO:HD2	1.62	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: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:M:53:SER:C	1:M:54:LEU:HD23	2.04	0.81
1:M:777:LEU:CD1	1:M:889:ALA:HA	2.09	0.81
1:O:316:HIS:HA	1:O:323:ILE:CD1	2.10	0.81
1:O:746:ASP:HA	1:O:760:ARG:HG3	1.61	0.81
1:B:227:VAL:HG13	1:B:240:LEU:HD11	1.62	0.81
1:B:777:LEU:CD1	1:B:889:ALA:HA	2.09	0.81
1:C:65:ALA:HB1	1:C:66:PRO:HD2	1.63	0.81
1:D:227:VAL:HG13	1:D:240:LEU:HD11	1.62	0.81
1:G:316:HIS:HA	1:G:323:ILE:CD1	2.10	0.81
1:H:890:GLN:HG3	1:H:891:VAL:N	1.94	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:A:128:ASN:ND2	1:A:180:GLY:HA2	1.96	0.81
1:C:240:LEU:HD12	1:C:241:GLU:N	1.95	0.81
1:F:128:ASN:ND2	1:F:180:GLY:HA2	1.96	0.81
1:G:65:ALA:HB1	1:G:66:PRO:HD2	1.62	0.81
1:L:65:ALA:HB1	1:L:66:PRO:HD2	1.62	0.81
1:L:890:GLN:HG3	1:L:891:VAL:N	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:240:LEU:HD12	1:D:241:GLU:N	1.95	0.81
1:D:436:MET:CE	1:D:467:ASN:HD22	1.93	0.81
1:E:436:MET:CE	1:E:467:ASN:HD22	1.93	0.81
1:G:53:SER:C	1:G:54:LEU:HD23	2.04	0.81
1:H:128:ASN:ND2	1:H:180:GLY:HA2	1.96	0.81
1:I:63:PHE:HB3	1:I:64:PRO:HD2	1.62	0.81
1:M:128:ASN:ND2	1:M:180:GLY:HA2	1.96	0.81
1:N:53:SER:C	1:N:54:LEU:HD23	2.04	0.81
1:O:53:SER:C	1:O:54:LEU:HD23	2.04	0.81
1:O:65:ALA:HB1	1:O:66:PRO:HD2	1.62	0.81
1:O:128:ASN:ND2	1:O:180:GLY:HA2	1.96	0.81
1:P:53:SER:C	1:P:54:LEU:HD23	2.04	0.81
1:B:890:GLN:HG3	1:B:891:VAL:N	1.94	0.81
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.62	0.81
1:N:128:ASN:ND2	1:N:180:GLY:HA2	1.96	0.81
1:B:746:ASP:HA	1:B:760:ARG:HG3	1.61	0.81
1:G:128:ASN:ND2	1:G:180:GLY:HA2	1.96	0.81
1:C:227:VAL:HG13	1:C:240:LEU:HD11	1.62	0.81
1:D:316:HIS:HA	1:D:323:ILE:CD1	2.10	0.81
1:D:890:GLN:HG3	1:D:891:VAL:N	1.94	0.81
1:F:255:ARG:HG2	1:F:255:ARG:HH11	1.45	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:316:HIS:HA	1:L:323:ILE:CD1	2.10	0.81
1:L:822:LEU:HD12	1:L:824:GLN:H	1.46	0.81
1:N:316:HIS:HA	1:N:323:ILE:CD1	2.10	0.81
1:C:890:GLN:HG3	1:C:891:VAL:N	1.94	0.81
1:O:890:GLN:HG3	1:O:891:VAL:N	1.94	0.81
1:D:746:ASP:HA	1:D:760:ARG:HG3	1.61	0.80
1:J:822:LEU:HD12	1:J:824:GLN:H	1.46	0.80
1:M:65:ALA:HB1	1:M:66:PRO:HD2	1.62	0.80
1:M:746:ASP:HA	1:M:760:ARG:HG3	1.61	0.80
1:N:255:ARG:HG2	1:N:255:ARG:HH11	1.45	0.80
1:B:316:HIS:HA	1:B:323:ILE:CD1	2.10	0.80
1:C:949:HIS:HD2	1:C:1020:TRP:HE1	1.27	0.80
1:I:255:ARG:HG2	1:I:255:ARG:HH11	1.45	0.80
1:I:316:HIS:HA	1:I:323:ILE:CD1	2.10	0.80
1:I:436:MET:CE	1:I:467:ASN:HD22	1.93	0.80
1:M:890:GLN:HG3	1:M:891:VAL:N	1.94	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:PHE:HB3	1:E:64:PRO:HD2	1.62	0.80
1:F:746:ASP:HA	1:F:760:ARG:HG3	1.61	0.80
1:P:227:VAL:HG13	1:P:240:LEU:HD11	1.62	0.80
1:B:65:ALA:HB1	1:B:66:PRO:HD2	1.63	0.80
1:C:316:HIS:HA	1:C:323:ILE:CD1	2.10	0.80
1:E:65:ALA:HB1	1:E:66:PRO:HD2	1.62	0.80
1:E:746:ASP:HA	1:E:760:ARG:HG3	1.61	0.80
1:G:227:VAL:HG13	1:G:240:LEU:HD11	1.62	0.80
1:L:128:ASN:ND2	1:L:180:GLY:HA2	1.96	0.80
1:N:63:PHE:HB3	1:N:64:PRO:HD2	1.62	0.80
1:A:227:VAL:HG13	1:A:240:LEU:HD11	1.62	0.80
1:F:63:PHE:HB3	1:F:64:PRO:HD2	1.62	0.80
1:N:746:ASP:HA	1:N:760:ARG:HG3	1.61	0.80
1:B:255:ARG:HG2	1:B:255:ARG:HH11	1.45	0.80
1:D:7:LEU:CD1	1:D:74:LEU:HD11	2.12	0.80
1:D:822:LEU:HD12	1:D:824:GLN:H	1.46	0.80
1:E:7:LEU:CD1	1:E:74:LEU:HD11	2.12	0.80
1:E:240:LEU:HD12	1:E:241:GLU:N	1.95	0.80
1:H:255:ARG:HG2	1:H:255:ARG:HH11	1.45	0.80
1:G:822:LEU:HD12	1:G:824:GLN:H	1.46	0.80
1:H:949:HIS:HD2	1:H:1020:TRP:HE1	1.27	0.80
1:I:128:ASN:ND2	1:I:180:GLY:HA2	1.96	0.80
1:K:255:ARG:HH11	1:K:255:ARG:HG2	1.45	0.80
1:O:227:VAL:HG13	1:O:240:LEU:HD11	1.62	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:P:890:GLN:HG3	1:P:891:VAL:N	1.94	0.80
1:A:949:HIS:HD2	1:A:1020:TRP:HE1	1.27	0.80
1:B:128:ASN:ND2	1:B:180:GLY:HA2	1.96	0.80
1:C:114:VAL:HG13	1:C:191:TRP:HB2	1.64	0.80
1:H:227:VAL:HG13	1:H:240:LEU:HD11	1.62	0.80
1:H:822:LEU:HD12	1:H:824:GLN:H	1.46	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:C:822:LEU:HD12	1:C:824:GLN:H	1.46	0.80
1:H:65:ALA:HB1	1:H:66:PRO:HD2	1.62	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:M:7:LEU:CD1	1:M:74:LEU:HD11	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:436:MET:CE	1:O:467:ASN:HD22	1.93	0.80
1:P:255:ARG:HG2	1:P:255:ARG:HH11	1.45	0.80
1:A:7:LEU:CD1	1:A:74:LEU:HD11	2.12	0.80
1:G:436:MET:CE	1:G:467:ASN:HD22	1.93	0.80
1:P:65:ALA:HB1	1:P:66:PRO:HD2	1.62	0.80
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.45	0.79
1:E:166:ARG:HD3	5:E:2120:HOH:O	1.83	0.79
1:E:292:ARG:C	1:E:293:LEU:HD23	2.08	0.79
1:I:114:VAL:HG13	1:I:191:TRP:HB2	1.64	0.79
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:O:255:ARG:HG2	1:O:255:ARG:HH11	1.45	0.79
1:B:949:HIS:HD2	1:B:1020:TRP:HE1	1.28	0.79
1:D:128:ASN:ND2	1:D:180:GLY:HA2	1.96	0.79
1:E:128:ASN:ND2	1:E:180:GLY:HA2	1.96	0.79
1:F:7:LEU:CD1	1:F:74:LEU:HD11	2.12	0.79
1:G:255:ARG:HG2	1:G:255:ARG:HH11	1.45	0.79
1:L:166:ARG:HD3	5:L:2120:HOH:O	1.83	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:N:292:ARG:C	1:N:293:LEU:HD23	2.08	0.79
1:C:436:MET:CE	1:C:467:ASN:HD22	1.93	0.79
1:D:949:HIS:HD2	1:D:1020:TRP:HE1	1.27	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:N:7:LEU:CD1	1:N:74:LEU:HD11	2.12	0.79
1:A:65:ALA:HB1	1:A:66:PRO:HD2	1.63	0.79
1:C:7:LEU:CD1	1:C:74:LEU:HD11	2.12	0.79
1:C:128:ASN:ND2	1:C:180:GLY:HA2	1.96	0.79
1:C:436:MET:HE3	1:C:467:ASN:ND2	1.97	0.79
1:D:65:ALA:HB1	1:D:66:PRO:HD2	1.62	0.79
1:E:890:GLN:HG3	1:E:891:VAL:N	1.94	0.79
1:F:114:VAL:HG13	1:F: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:2123:HOH:O	1.83	0.79
1:O:166:ARG:HD3	5:O:2120:HOH:O	1.83	0.79
1:P:114:VAL:HG13	1:P:191:TRP:HB2	1.64	0.79
1:F:292:ARG:C	1:F:293:LEU:HD23	2.08	0.79
1:I:7:LEU:CD1	1:I:74:LEU:HD11	2.12	0.79
1:J:255:ARG:HG2	1:J:255:ARG:HH11	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:166:ARG:HD3	5:K:2120:HOH:O	1.83	0.79
1:L:292:ARG:C	1:L:293:LEU:HD23	2.08	0.79
1:M:822:LEU:HD12	1:M:824:GLN:H	1.46	0.79
1:A:114:VAL:HG13	1:A:191:TRP:HB2	1.64	0.79
1:C:166:ARG:HD3	5:C:2120:HOH:O	1.83	0.79
1:D:292:ARG:C	1:D:293:LEU:HD23	2.08	0.79
1:E:436:MET:HE3	1:E:467:ASN:ND2	1.97	0.79
1:E:745:MET:HE2	1:E:745:MET:HA	1.65	0.79
1:F:316:HIS:HA	1:F:323:ILE:CD1	2.10	0.79
1:K:436:MET:HE3	1:K:467:ASN:ND2	1.97	0.79
1:L:682:LEU:HD22	1:L:683:PRO:HD2	1.65	0.79
1:B:436:MET:CE	1:B:467:ASN:HD22	1.93	0.79
1:B:822:LEU:HD12	1:B:824:GLN:H	1.46	0.79
1:D:436:MET:HE3	1:D:467:ASN:ND2	1.97	0.79
1:D:822:LEU:HD12	1:D:823:LEU:N	1.98	0.79
1:F:662:PRO:C	1:F:663:LEU:HD23	2.08	0.79
1:G:102:ASN:ND2	1:G:201:ASP:HB2	1.98	0.79
1:G:292:ARG:C	1:G:293:LEU:HD23	2.08	0.79
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:B:682:LEU:HD22	1:B:683:PRO:HD2	1.65	0.79
1:D:166:ARG:HD3	5:D:2126:HOH:O	1.83	0.79
1:E:227:VAL:HG13	1:E:240:LEU:HD11	1.62	0.79
1:E:822:LEU:HD12	1:E:824:GLN:H	1.46	0.79
1:F:166:ARG:HD3	5:F:2120:HOH:O	1.83	0.79
1:G:7:LEU:CD1	1:G:74:LEU:HD11	2.12	0.79
1:J:63:PHE:HB3	1:J:64:PRO:HD2	1.62	0.79
1:L:7:LEU:CD1	1:L:74:LEU:HD11	2.12	0.79
1:L:114:VAL:HG13	1:L:191:TRP:HB2	1.64	0.79
1:M:292:ARG:C	1:M:293:LEU:HD23	2.08	0.79
1:M:745:MET:HE2	1:M:745:MET:HA	1.65	0.79
1:O:7:LEU:CD1	1:O:74:LEU:HD11	2.12	0.79
1:O:292:ARG:C	1:O:293:LEU:HD23	2.08	0.79
1:O:436:MET:HE3	1:O:467:ASN:ND2	1.97	0.79
1:P:7:LEU:CD1	1:P:74:LEU:HD11	2.12	0.79
1:E:822:LEU:HD12	1:E:823:LEU:N	1.98	0.79
1:F:436:MET:CE	1:F:467:ASN:HD22	1.93	0.79
1:F:682:LEU:HD22	1:F:683:PRO:HD2	1.65	0.79
1:H:7:LEU:CD1	1:H:74:LEU:HD11	2.12	0.79
1:I:682:LEU:HD22	1:I:683:PRO:HD2	1.65	0.79
1:M:662:PRO:C	1:M:663:LEU:HD23	2.08	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:436:MET:CE	1:N:467:ASN:HD22	1.93	0.79
1:P:292:ARG:C	1:P:293:LEU:HD23	2.08	0.79
1:B:662:PRO:C	1:B:663:LEU:HD23	2.08	0.79
1:F:651:LEU:HD12	1:F:652:LEU:H	1.48	0.79
1:H:292:ARG:C	1:H:293:LEU:HD23	2.08	0.79
1:L:436:MET:HE3	1:L:467:ASN:ND2	1.97	0.79
1:O:682:LEU:HD22	1:O:683:PRO:HD2	1.65	0.79
1:P:682:LEU:HD22	1:P:683:PRO:HD2	1.65	0.79
1:E:949:HIS:HD2	1:E:1020:TRP:HE1	1.27	0.78
1:G:662:PRO:C	1:G:663:LEU:HD23	2.08	0.78
1:H:114:VAL:HG13	1:H:191:TRP:HB2	1.64	0.78
1:I:292:ARG:C	1:I:293:LEU:HD23	2.08	0.78
1:J:102:ASN:ND2	1:J:201:ASP:HB2	1.98	0.78
1:J:292:ARG:C	1:J:293:LEU:HD23	2.08	0.78
1:J:651:LEU:HD12	1:J:652:LEU:H	1.48	0.78
1:L:662:PRO:C	1:L:663:LEU:HD23	2.08	0.78
1:N:102:ASN:ND2	1:N:201:ASP:HB2	1.98	0.78
1:N:682:LEU:HD22	1:N:683:PRO:HD2	1.65	0.78
1:N:745:MET:HE2	1:N:745:MET:HA	1.65	0.78
1:A:292:ARG:C	1:A:293:LEU:HD23	2.08	0.78
1:A:662:PRO:C	1:A:663:LEU:HD23	2.08	0.78
1:A:822:LEU:HD12	1:A:823:LEU:N	1.98	0.78
1:A:822:LEU:HD12	1:A:824:GLN:H	1.46	0.78
1:B:102:ASN:ND2	1:B:201:ASP:HB2	1.98	0.78
1:B:210:ARG:NH1	1:B:395:HIS:N	2.32	0.78
1:C:651:LEU:HD12	1:C:652:LEU:H	1.48	0.78
1:C:662:PRO:C	1:C:663:LEU:HD23	2.08	0.78
1:C:822:LEU:HD12	1:C:823:LEU:N	1.98	0.78
1:D:662:PRO:C	1:D:663:LEU:HD23	2.08	0.78
1:D:745:MET:HA	1:D:745:MET:HE2	1.65	0.78
1:F:745:MET:HE2	1:F:745:MET:HA	1.65	0.78
1:G:682:LEU:HD22	1:G:683:PRO:HD2	1.65	0.78
1:H:651:LEU:HD12	1:H:652:LEU:H	1.48	0.78
1:I:436:MET:HE3	1:I:467:ASN:ND2	1.97	0.78
1:A:418:HIS:O	1:D:282:ARG:HD3	1.82	0.78
1:A:499:ILE:HB	1:A:533:LEU:HB2	1.66	0.78
1:B:114:VAL:HG13	1:B:191:TRP:HB2	1.64	0.78
1:C:745:MET:HE2	1:C:745:MET:HA	1.65	0.78
1:F:437:SER:HB2	5:F:2258:HOH:O	1.82	0.78
1:G:166:ARG:HD3	5:G:2120:HOH:O	1.83	0.78
1:G:822:LEU:HD12	1:G:823:LEU:N	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:114:VAL:HG13	1:K:191:TRP:HB2	1.64	0.78
1:M:682:LEU:HD22	1:M:683:PRO:HD2	1.65	0.78
1:O:822:LEU:HD12	1:O:823:LEU:N	1.98	0.78
1:C:499:ILE:HB	1:C:533:LEU:HB2	1.66	0.78
1:F:822:LEU:HD12	1:F:824:GLN:H	1.46	0.78
1:H:822:LEU:HD12	1:H:823:LEU:N	1.98	0.78
1:J:166:ARG:HD3	5:J:2120:HOH:O	1.83	0.78
1:J:210:ARG:NH1	1:J:395:HIS:N	2.32	0.78
1:K:43:ARG:HG2	1:K:43:ARG:NH1	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:A:166:ARG:HD3	5:A:2120:HOH:O	1.83	0.78
1:B:7:LEU:CD1	1:B:74:LEU:HD11	2.12	0.78
1:B:166:ARG:HD3	5:B:2123:HOH:O	1.83	0.78
1:C:292:ARG:C	1:C:293:LEU:HD23	2.08	0.78
1:F:210:ARG:NH1	1:F:395:HIS:N	2.32	0.78
1:H:745:MET:HE2	1:H:745:MET:HA	1.65	0.78
1:K:949:HIS:HD2	1:K:1020:TRP:HE1	1.27	0.78
1:O:651:LEU:HD12	1:O:652:LEU:H	1.48	0.78
1:D:682:LEU:HD22	1:D:683:PRO:HD2	1.65	0.78
1:E:662:PRO:C	1:E:663:LEU:HD23	2.08	0.78
1:F:822:LEU:HD12	1:F:823:LEU:N	1.98	0.78
1:G:651:LEU:HD12	1:G:652:LEU:H	1.48	0.78
1:H:499:ILE:HB	1:H:533:LEU:HB2	1.66	0.78
1:I:210:ARG:NH1	1:I:395:HIS:N	2.32	0.78
1:K:662:PRO:C	1:K:663:LEU:HD23	2.08	0.78
1:M:114:VAL:HG13	1:M:191:TRP:HB2	1.64	0.78
1:M:499:ILE:HB	1:M:533:LEU:HB2	1.66	0.78
1:M:949:HIS:HD2	1:M:1020:TRP:HE1	1.28	0.78
1:N:210:ARG:NH1	1:N:395:HIS:N	2.32	0.78
1:N:822:LEU:HD12	1:N:824:GLN:H	1.46	0.78
1:P:210:ARG:NH1	1:P:395:HIS:N	2.32	0.78
1:A:210:ARG:NH1	1:A:395:HIS:N	2.32	0.78
1:B:822:LEU:HD12	1:B:823:LEU:N	1.98	0.78
1:C:210:ARG:NH1	1:C:395:HIS:N	2.32	0.78
1:E:499:ILE:HB	1:E:533:LEU:HB2	1.66	0.78
1:G:210:ARG:NH1	1:G:395:HIS:N	2.32	0.78
1:H:210:ARG:NH1	1:H:395:HIS:N	2.32	0.78
1:I:166:ARG:HD3	5:I:2120:HOH:O	1.83	0.78
1:I:822:LEU:HD12	1:I:823:LEU:N	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:822:LEU:HD12	1:I:824:GLN:H	1.46	0.78
1:K:682:LEU:HD22	1:K:683:PRO:HD2	1.65	0.78
1:L:102:ASN:ND2	1:L:201:ASP:HB2	1.98	0.78
1:M:434:PRO:HB3	1:P:434:PRO:HB3	1.65	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:O:210:ARG:NH1	1:O:395:HIS:N	2.32	0.78
1:O:662:PRO:C	1:O:663:LEU:HD23	2.08	0.78
1:P:166:ARG:HD3	5:P:2125:HOH:O	1.83	0.78
1:P:499:ILE:HB	1:P:533:LEU:HB2	1.66	0.78
1:D:499:ILE:HB	1:D:533:LEU:HB2	1.66	0.78
1:E:651:LEU:HD12	1:E:652:LEU:H	1.48	0.78
1:H:662:PRO:C	1:H:663:LEU:HD23	2.08	0.78
1:H:682:LEU:HD22	1:H:683:PRO:HD2	1.65	0.78
1:J:662:PRO:C	1:J:663:LEU:HD23	2.08	0.78
1:J:682:LEU:HD22	1:J:683:PRO:HD2	1.65	0.78
1:J:822:LEU:HD12	1:J:823:LEU:N	1.98	0.78
1:M:436:MET:HE3	1:M:467:ASN:ND2	1.97	0.78
1:I:662:PRO:C	1:I:663:LEU:HD23	2.08	0.78
1:L:499:ILE:HB	1:L:533:LEU:HB2	1.66	0.78
1:N:662:PRO:C	1:N:663:LEU:HD23	2.08	0.78
1:P:745:MET:HE2	1:P:745:MET:HA	1.65	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:E:682:LEU:HD22	1:E:683:PRO:HD2	1.65	0.77
1:H:166:ARG:HD3	5:H:2120:HOH:O	1.83	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:L:822:LEU:HD12	1:L:823:LEU:N	1.98	0.77
1:N:949:HIS:HD2	1:N:1020:TRP:HE1	1.27	0.77
1:A:651:LEU:HD12	1:A:652:LEU:H	1.48	0.77
1:B:651:LEU:HD12	1:B:652:LEU:H	1.48	0.77
1:D:651:LEU:HD12	1:D:652:LEU:H	1.48	0.77
1:E:114:VAL:HG13	1:E:191:TRP:HB2	1.64	0.77
1:F:436:MET:HE3	1:F:467:ASN:ND2	1.97	0.77
1:G:114:VAL:HG13	1:G:191:TRP:HB2	1.64	0.77
1:H:102:ASN:ND2	1:H:201:ASP:HB2	1.98	0.77
1:K:360:HIS:CG	1:K:361:PRO:HD2	2.20	0.77
1:L:43:ARG:HG2	1:L:43:ARG:NH1	1.94	0.77
1:M:166:ARG:HD3	5:M:2120:HOH:O	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:436:MET:HE3	1:N:467:ASN:ND2	1.97	0.77
1:O:745:MET:HA	1:O:745:MET:HE2	1.65	0.77
1:P:360:HIS:CG	1:P:361:PRO:HD2	2.20	0.77
1:D:114:VAL:HG13	1:D:191:TRP:HB2	1.64	0.77
1:D:210:ARG:NH1	1:D:395:HIS:N	2.32	0.77
1:D:360:HIS:CG	1:D:361:PRO:HD2	2.20	0.77
1:G:745:MET:HA	1:G:745:MET:HE2	1.65	0.77
1:C:102:ASN:ND2	1:C:201:ASP:HB2	1.98	0.77
1:E:102:ASN:ND2	1:E:201:ASP:HB2	1.98	0.77
1:F:189:LEU:HD23	1:F:189:LEU:N	2.00	0.77
1:J:745:MET:HE2	1:J:745:MET:HA	1.65	0.77
1:K:292:ARG:C	1:K:293:LEU:HD23	2.08	0.77
1:N:189:LEU:HD23	1:N:189:LEU:N	2.00	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:B:189:LEU:N	1:B:189:LEU:HD23	2.00	0.77
1:B:745:MET:HE2	1:B:745:MET:HA	1.65	0.77
1:D:189:LEU:N	1:D:189:LEU:HD23	2.00	0.77
1:F:949:HIS:HD2	1:F:1020:TRP:HE1	1.27	0.77
1:G:499:ILE:HB	1:G:533:LEU:HB2	1.66	0.77
1:J:436:MET:HE3	1:J:467:ASN:ND2	1.97	0.77
1:L:189:LEU:N	1:L:189:LEU:HD23	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:P:662:PRO:C	1:P:663:LEU:HD23	2.08	0.77
1:C:395:HIS:CG	1:C:396:PRO:HD2	2.20	0.77
1:E:395:HIS:CG	1:E:396:PRO:HD2	2.20	0.77
1:M:210:ARG:NH1	1:M:395:HIS:N	2.32	0.77
1:A:745:MET:HE2	1:A:745:MET:HA	1.65	0.77
1:B:292:ARG:C	1:B:293:LEU:HD23	2.08	0.77
1:B:395:HIS:CG	1:B:396:PRO:HD2	2.20	0.77
1:C:189:LEU:N	1:C:189:LEU:HD23	2.00	0.77
1:D:102:ASN:ND2	1:D:201:ASP:HB2	1.98	0.77
1:F:360:HIS:CG	1:F:361:PRO:HD2	2.20	0.77
1:G:189:LEU:N	1:G:189:LEU:HD23	2.00	0.77
1:I:360:HIS:CG	1:I:361:PRO:HD2	2.20	0.77
1:K:260:LEU:O	1:K:267:VAL:HG23	1.85	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
1:P:651:LEU:HD12	1:P:652:LEU:H	1.48	0.77
1:P:949:HIS:HD2	1:P:1020:TRP:HE1	1.28	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:MET:HE3	1:B:467:ASN:ND2	1.97	0.77
1:C:682:LEU:HD22	1:C:683:PRO:HD2	1.65	0.77
1:H:395:HIS:CG	1:H:396:PRO:HD2	2.20	0.77
1:I:260:LEU:O	1:I:267:VAL:HG23	1.85	0.77
1:J:189:LEU:N	1:J:189:LEU:HD23	2.00	0.77
1:J:360:HIS:CG	1:J:361:PRO:HD2	2.20	0.77
1:K:102:ASN:ND2	1:K:201:ASP:HB2	1.98	0.77
1:K:745:MET:HE2	1:K:745:MET:HA	1.65	0.77
1:L:395:HIS:CG	1:L:396:PRO:HD2	2.20	0.77
1:P:189:LEU:N	1:P:189:LEU:HD23	2.00	0.77
1:A:102:ASN:ND2	1:A:201:ASP:HB2	1.98	0.77
1:B:360:HIS:CG	1:B:361:PRO:HD2	2.20	0.77
1:C:188:VAL:C	1:C:189:LEU:HD23	2.10	0.77
1:E:210:ARG:NH1	1:E:395:HIS:N	2.32	0.77
1:F:102:ASN:ND2	1:F:201:ASP:HB2	1.98	0.77
1:L:745:MET:HA	1:L:745:MET:HE2	1.65	0.77
1:M:188:VAL:C	1:M:189:LEU:HD23	2.10	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:B:260:LEU:O	1:B:267:VAL:HG23	1.85	0.77
1:B:654:TRP:CE2	1:B:666:GLY:HA3	2.20	0.77
1:E:188:VAL:C	1:E:189:LEU:HD23	2.10	0.77
1:I:395:HIS:CG	1:I:396:PRO:HD2	2.20	0.77
1:I:745:MET:HE2	1:I:745:MET:HA	1.65	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:L:360:HIS:CG	1:L:361:PRO:HD2	2.20	0.77
1:L:654:TRP:CE2	1:L:666:GLY:HA3	2.20	0.77
1:N:499:ILE:HB	1:N:533:LEU:HB2	1.66	0.77
1:C:260:LEU:O	1:C:267:VAL:HG23	1.85	0.76
1:C:360:HIS:CG	1:C:361:PRO:HD2	2.20	0.76
1:C:654:TRP:CE2	1:C:666:GLY:HA3	2.20	0.76
1:K:188:VAL:C	1:K:189:LEU:HD23	2.10	0.76
1:M:423:MET:HB2	1:P:282:ARG:HG3	1.65	0.76
1:O:395:HIS:CG	1:O:396:PRO:HD2	2.20	0.76
1:A:682:LEU:HD22	1:A:683:PRO:HD2	1.65	0.76
1:C:251:ARG:HB3	1:C:253:TYR:CE2	2.21	0.76
1:D:23:GLN:O	1:D:24:LEU:HD13	1.86	0.76
1:G:395:HIS:CG	1:G:396:PRO:HD2	2.20	0.76
1:H:189:LEU:N	1:H:189:LEU:HD23	2.00	0.76
1:H:436:MET:HE3	1:H:467:ASN:ND2	1.97	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:260:LEU:O	1:J:267:VAL:HG23	1.85	0.76
1:K:654:TRP:CE2	1:K:666:GLY:HA3	2.20	0.76
1:M:189:LEU:HD23	1:M:189:LEU:N	2.00	0.76
1:C:23:GLN:O	1:C:24:LEU:HD13	1.86	0.76
1:D:395:HIS:CG	1:D:396:PRO:HD2	2.20	0.76
1:G:436:MET:HE3	1:G:467:ASN:ND2	1.97	0.76
1:I:188:VAL:C	1:I:189:LEU:HD23	2.10	0.76
1:L:23:GLN:O	1:L:24:LEU:HD13	1.86	0.76
1:M:102:ASN:ND2	1:M:201:ASP:HB2	1.98	0.76
1:A:654:TRP:CE2	1:A:666:GLY:HA3	2.20	0.76
1:B:251:ARG:HB3	1:B:253:TYR:CE2	2.21	0.76
1:B:499:ILE:HB	1:B:533:LEU:HB2	1.66	0.76
1:D:188:VAL:C	1:D:189:LEU:HD23	2.10	0.76
1:D:251:ARG:HB3	1:D:253:TYR:CE2	2.21	0.76
1:E:360:HIS:CG	1:E:361:PRO:HD2	2.20	0.76
1:F:499:ILE:HB	1:F:533:LEU:HB2	1.66	0.76
1:J:188:VAL:C	1:J:189:LEU:HD23	2.10	0.76
1:L:188:VAL:C	1:L:189:LEU:HD23	2.10	0.76
1:P:436:MET:HE3	1:P:467:ASN:ND2	1.97	0.76
1:A:360:HIS:CG	1:A:361:PRO:HD2	2.20	0.76
1:B:23:GLN:O	1:B:24:LEU:HD13	1.86	0.76
1:E:654:TRP:CE2	1:E:666:GLY:HA3	2.21	0.76
1:F:395:HIS:CG	1:F:396:PRO:HD2	2.20	0.76
1:F:654:TRP:CE2	1:F:666:GLY:HA3	2.20	0.76
1:I:189:LEU:HD23	1:I:189:LEU:N	2.00	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:A:395:HIS:CG	1:A:396:PRO:HD2	2.20	0.76
1:E:23:GLN:O	1:E:24:LEU:HD13	1.86	0.76
1:G:23:GLN:O	1:G:24:LEU:HD13	1.86	0.76
1:G:360:HIS:CG	1:G:361:PRO:HD2	2.20	0.76
1:I:651:LEU:HD12	1:I:652:LEU:H	1.48	0.76
1:J:23:GLN:O	1:J:24:LEU:HD13	1.86	0.76
1:J:654:TRP:CE2	1:J:666:GLY:HA3	2.20	0.76
1:L:260:LEU:O	1:L:267:VAL:HG23	1.85	0.76
1:M:654:TRP:CE2	1:M:666:GLY:HA3	2.20	0.76
1:O:654:TRP:CE2	1:O:666:GLY:HA3	2.21	0.76
1:A:188:VAL:C	1:A:189:LEU:HD23	2.10	0.76
1:E:251:ARG:HB3	1:E:253:TYR:CE2	2.21	0.76
1:F:251:ARG:HB3	1:F:253:TYR:CE2	2.21	0.76
1:G:188:VAL:C	1:G:189:LEU:HD23	2.10	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:188:VAL:C	1:H:189:LEU:HD23	2.10	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:A:251:ARG:HB3	1:A:253:TYR:CE2	2.21	0.76
1:I:654:TRP:CE2	1:I:666:GLY:HA3	2.20	0.76
1:O:188:VAL:C	1:O:189:LEU:HD23	2.10	0.76
1:D:595:THR:HG23	1:D:596:PRO:HA	1.68	0.76
1:G:230:ARG:HH11	1:G:230:ARG:HG3	1.51	0.76
1:H:260:LEU:O	1:H:267:VAL:HG23	1.85	0.76
1:I:499:ILE:HB	1:I:533:LEU:HB2	1.66	0.76
1:I:595:THR:HG23	1:I:596:PRO:HA	1.68	0.76
1:M:360:HIS:CG	1:M:361:PRO:HD2	2.20	0.76
1:O:189:LEU:HD23	1:O:189:LEU:N	2.00	0.76
1:O:230:ARG:HH11	1:O:230:ARG:HG3	1.51	0.76
1:P:23:GLN:O	1:P:24:LEU:HD13	1.86	0.76
1:P:395:HIS:CG	1:P:396:PRO:HD2	2.20	0.76
1:A:189:LEU:HD23	1:A:189:LEU:N	2.00	0.76
1:G:595:THR:HG23	1:G:596:PRO:HA	1.68	0.76
1:H:360:HIS:CG	1:H:361:PRO:HD2	2.20	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:O:360:HIS:CG	1:O:361:PRO:HD2	2.20	0.76
1:O:595:THR:HG23	1:O:596:PRO:HA	1.68	0.76
1:P:230:ARG:HH11	1:P:230:ARG:HG3	1.51	0.76
1:P:251:ARG:HB3	1:P:253:TYR:CE2	2.21	0.76
1:C:696:LEU:HD12	1:C:697:THR:N	2.01	0.75
1:G:696:LEU:HD12	1:G:697:THR:N	2.01	0.75
1:J:595:THR:HG23	1:J:596:PRO:HA	1.68	0.75
1:L:230:ARG:HH11	1:L:230:ARG:HG3	1.51	0.75
1:M:23:GLN:O	1:M:24:LEU:HD13	1.86	0.75
1:M:251:ARG:HB3	1:M:253:TYR:CE2	2.21	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:A:436:MET:HE3	1:A:467:ASN:ND2	1.97	0.75
1:A:696:LEU:HD12	1:A:697:THR:H	1.51	0.75
1:D:696:LEU:HD12	1:D:697:THR:H	1.52	0.75
1:F:260:LEU:O	1:F:267:VAL:HG23	1.85	0.75
1:G:251:ARG:HB3	1:G:253:TYR:CE2	2.21	0.75
1:H:230:ARG:HH11	1:H:230:ARG:HG3	1.51	0.75
1:J:251:ARG:HB3	1:J:253:TYR:CE2	2.21	0.75
1:K:653[B]:HIS:CD2	1:K:667:GLU:HG3	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:230:ARG:HH11	1:M:230:ARG:HG3	1.51	0.75
1:M:653[B]:HIS:CD2	1:M:667:GLU:HG3	2.22	0.75
1:N:260:LEU:O	1:N:267:VAL:HG23	1.85	0.75
1:P:188:VAL:C	1:P:189:LEU:HD23	2.10	0.75
1:B:696:LEU:HD12	1:B:697:THR:N	2.02	0.75
1:B:696:LEU:HD12	1:B:697:THR:H	1.51	0.75
1:F:188:VAL:C	1:F:189:LEU:HD23	2.10	0.75
1:G:654:TRP:CE2	1:G:666:GLY:HA3	2.20	0.75
1:G:696:LEU:HD12	1:G:697:THR:H	1.51	0.75
1:H:23:GLN:O	1:H:24:LEU:HD13	1.86	0.75
1:I:696:LEU:HD12	1:I:697:THR:H	1.51	0.75
1:M:696:LEU:HD12	1:M:697:THR:N	2.01	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:P:43:ARG:HG2	1:P:43:ARG:NH1	1.94	0.75
1:P:654:TRP:CE2	1:P:666:GLY:HA3	2.20	0.75
1:F:23:GLN:O	1:F:24:LEU:HD13	1.86	0.75
1:G:260:LEU:O	1:G:267:VAL:HG23	1.85	0.75
1:H:654:TRP:CE2	1:H:666:GLY:HA3	2.20	0.75
1:I:251:ARG:HB3	1:I:253:TYR:CE2	2.21	0.75
1:I:653[B]:HIS:CD2	1:I:667:GLU:HG3	2.22	0.75
1:J:230:ARG:HH11	1:J:230:ARG:HG3	1.51	0.75
1:L:251:ARG:HB3	1:L:253:TYR:CE2	2.21	0.75
1:M:395:HIS:CG	1:M:396:PRO:HD2	2.20	0.75
1:N:188:VAL:C	1:N:189:LEU:HD23	2.10	0.75
1:A:23:GLN:O	1:A:24:LEU:HD13	1.86	0.75
1:B:653[B]:HIS:CD2	1:B:667:GLU:HG3	2.22	0.75
1:C:230:ARG:HG3	1:C:230:ARG:HH11	1.51	0.75
1:C:696:LEU:HD12	1:C:697:THR:H	1.52	0.75
1:D:653[B]:HIS:CD2	1:D:667:GLU:HG3	2.22	0.75
1:E:189:LEU:HD23	1:E:189:LEU:N	2.00	0.75
1:I:434:PRO:HB3	1:L:434:PRO:HB3	1.66	0.75
1:C:595:THR:HG23	1:C:596:PRO:HA	1.68	0.75
1:E:260:LEU:O	1:E:267:VAL:HG23	1.85	0.75
1:H:696:LEU:HD12	1:H:697:THR:N	2.01	0.75
1:M:260:LEU:O	1:M:267:VAL:HG23	1.85	0.75
1:B:188:VAL:C	1:B:189:LEU:HD23	2.11	0.75
1:F:230:ARG:HG3	1:F:230:ARG:HH11	1.51	0.75
1:J:653[B]:HIS:CD2	1:J:667:GLU:HG3	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:696:LEU:HD12	1:K:697:THR:H	1.51	0.75
1:L:653[B]:HIS:CD2	1:L:667:GLU:HG3	2.22	0.75
1:O:653[B]:HIS:CD2	1:O:667:GLU:HG3	2.22	0.75
1:C:654:TRP:NE1	1:C:666:GLY:HA3	2.02	0.75
1:D:654:TRP:CE2	1:D:666:GLY:HA3	2.21	0.75
1:G:653[B]:HIS:CD2	1:G:667:GLU:HG3	2.22	0.75
1:I:696:LEU:HD12	1:I:697:THR:N	2.01	0.75
1:K:23:GLN:O	1:K:24:LEU:HD13	1.86	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:P:696:LEU:HD12	1:P:697:THR:N	2.02	0.75
1:A:230:ARG:HH11	1:A:230:ARG:HG3	1.51	0.75
1:D:128:ASN:HD21	1:D:180:GLY:HA2	1.52	0.75
1:D:260:LEU:O	1:D:267:VAL:HG23	1.85	0.75
1:F:46:ARG:HG3	1:F:46:ARG:NH1	2.02	0.75
1:K:437:SER:HB2	5:K:2258:HOH:O	1.87	0.75
1:A:128:ASN:HD21	1:A:180:GLY:HA2	1.52	0.74
1:A:260:LEU:O	1:A:267:VAL:HG23	1.85	0.74
1:B:595:THR:HG23	1:B:596:PRO:HA	1.68	0.74
1:C:46:ARG:HG3	1:C:46:ARG:NH1	2.02	0.74
1:D:230:ARG:HH11	1:D:230:ARG:HG3	1.51	0.74
1:E:595:THR:HG23	1:E:596:PRO:HA	1.68	0.74
1:E:653[B]:HIS:CD2	1:E:667:GLU:HG3	2.22	0.74
1:E:696:LEU:HD12	1:E:697:THR:N	2.01	0.74
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:A:423:MET:HB2	1:D:282:ARG:HG3	1.68	0.74
1:D:654:TRP:NE1	1:D:666:GLY:HA3	2.02	0.74
1:E:654:TRP:NE1	1:E:666:GLY:HA3	2.02	0.74
1:H:653[B]:HIS:CD2	1:H:667:GLU:HG3	2.22	0.74
1:M:128:ASN:HD21	1:M:180:GLY:HA2	1.52	0.74
1:N:23:GLN:O	1:N:24:LEU:HD13	1.86	0.74
1:N:696:LEU:HD12	1:N:697:THR:N	2.01	0.74
1:P:128:ASN:HD21	1:P:180:GLY:HA2	1.52	0.74
1:A:696:LEU:HD12	1:A:697:THR:N	2.02	0.74
1:E:696:LEU:HD12	1:E:697:THR:H	1.52	0.74
1:F:653[B]:HIS:CD2	1:F:667:GLU:HG3	2.22	0.74
1:H:251:ARG:HB3	1:H:253:TYR:CE2	2.21	0.74
1:H:654:TRP:NE1	1:H:666:GLY:HA3	2.02	0.74
1:K:230:ARG:HG3	1:K:230:ARG:HH11	1.51	0.74
1:M:418:HIS:O	1:P:282:ARG:HD3	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:595:THR:HG23	1:N:596:PRO:HA	1.68	0.74
1:N:654:TRP:NE1	1:N:666:GLY:HA3	2.02	0.74
1:O:23:GLN:O	1:O:24:LEU:HD13	1.86	0.74
1:B:230:ARG:HH11	1:B:230:ARG:HG3	1.51	0.74
1:B:856:TYR:CD2	1:B:864:MET:HE2	2.23	0.74
1:E:128:ASN:HD21	1:E:180:GLY:HA2	1.52	0.74
1:F:654:TRP:NE1	1:F:666:GLY:HA3	2.02	0.74
1:G:856:TYR:CD2	1:G:864:MET:HE2	2.23	0.74
1:H:696:LEU:HD12	1:H:697:THR:H	1.51	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:43:ARG:HG2	1:N:43:ARG:NH1	1.94	0.74
1:N:434:PRO:HB3	1:O:434:PRO:HB3	1.68	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:A:653[B]:HIS:CD2	1:A:667:GLU:HG3	2.22	0.74
1:C:653[B]:HIS:CD2	1:C:667:GLU:HG3	2.22	0.74
1:F:595:THR:HG23	1:F:596:PRO:HA	1.68	0.74
1:H:128:ASN:HD21	1:H:180:GLY:HA2	1.52	0.74
1:I:23:GLN:O	1:I:24:LEU:HD13	1.86	0.74
1:L:696:LEU:HD12	1:L:697:THR:H	1.51	0.74
1:P:654:TRP:NE1	1:P:666:GLY:HA3	2.02	0.74
1:A:856:TYR:CD2	1:A:864:MET:HE2	2.23	0.74
1:D:696:LEU:HD12	1:D:697:THR:N	2.01	0.74
1:E:230:ARG:HH11	1:E:230:ARG:HG3	1.51	0.74
1:I:336:ARG:HH11	1:I:336:ARG:HG2	1.52	0.74
1:M:336:ARG:HG2	1:M:336:ARG:HH11	1.52	0.74
1:P:822:LEU:HD12	1:P:824:GLN:N	2.03	0.74
1:A:595:THR:HG23	1:A:596:PRO:HA	1.68	0.74
1:A:701:VAL:O	1:A:703:PRO:HD3	1.88	0.74
1:F:696:LEU:HD12	1:F:697:THR:N	2.01	0.74
1:H:46:ARG:HG3	1:H:46:ARG:NH1	2.02	0.74
1:J:43:ARG:HG2	1:J:43:ARG:NH1	1.94	0.74
1:J:856:TYR:CD2	1:J:864:MET:HE2	2.23	0.74
1:M:595:THR:HG23	1:M:596:PRO:HA	1.68	0.74
1:M:696:LEU:HD12	1:M:697:THR:H	1.51	0.74
1:D:822:LEU:HD12	1:D:824:GLN:N	2.03	0.74
1:H:595:THR:HG23	1:H:596:PRO:HA	1.68	0.74
1:H:822:LEU:HD12	1:H:824:GLN:N	2.03	0.74
1:I:856:TYR:CD2	1:I:864:MET:HE2	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:230:ARG:HG3	1:N:230:ARG:HH11	1.51	0.74
1:O:251:ARG:HB3	1:O:253:TYR:CE2	2.21	0.74
1:C:701:VAL:O	1:C:703:PRO:HD3	1.88	0.74
1:D:336:ARG:HG2	1:D:336:ARG:HH11	1.52	0.74
1:D:701:VAL:O	1:D:703:PRO:HD3	1.88	0.74
1:E:46:ARG:HG3	1:E:46:ARG:NH1	2.02	0.74
1:J:128:ASN:HD21	1:J:180:GLY:HA2	1.52	0.74
1:K:696:LEU:HD12	1:K:697:THR:N	2.02	0.74
1:N:336:ARG:HG2	1:N:336:ARG:HH11	1.52	0.74
1:P:701:VAL:O	1:P:703:PRO:HD3	1.88	0.74
1:A:654:TRP:NE1	1:A:666:GLY:HA3	2.02	0.74
1:E:336:ARG:HG2	1:E:336:ARG:HH11	1.52	0.74
1:E:822:LEU:HD12	1:E:824:GLN:N	2.03	0.74
1:F:856:TYR:CD2	1:F:864:MET:HE2	2.23	0.74
1:H:856:TYR:CD2	1:H:864:MET:HE2	2.23	0.74
1:I:701:VAL:O	1:I:703:PRO:HD3	1.88	0.74
1:J:701:VAL:O	1:J:703:PRO:HD3	1.88	0.74
1:K:427:THR:CA	1:K:436:MET:HE1	2.10	0.74
1:M:822:LEU:HD12	1:M:824:GLN:N	2.03	0.74
1:M:856:TYR:CD2	1:M:864:MET:HE2	2.23	0.74
1:O:701:VAL:O	1:O:703:PRO:HD3	1.88	0.74
1:G:654:TRP:NE1	1:G:666:GLY:HA3	2.02	0.73
1:K:46:ARG:HG3	1:K:46:ARG:NH1	2.02	0.73
1:M:419:GLY:HA2	1:P:282:ARG:NH1	2.02	0.73
1:F:701:VAL:O	1:F:703:PRO:HD3	1.88	0.73
1:N:701:VAL:O	1:N:703:PRO:HD3	1.88	0.73
1:O:654:TRP:NE1	1:O:666:GLY:HA3	2.02	0.73
1:A:336:ARG:HH11	1:A:336:ARG:HG2	1.52	0.73
1:B:701:VAL:O	1:B:703:PRO:HD3	1.88	0.73
1:E:856:TYR:CD2	1:E:864:MET:HE2	2.23	0.73
1:B:654:TRP:NE1	1:B:666:GLY:HA3	2.02	0.73
1:F:128:ASN:HD21	1:F:180:GLY:HA2	1.52	0.73
1:I:230:ARG:HH11	1:I:230:ARG:HG3	1.51	0.73
1:I:423:MET:HB2	1:L:282:ARG:HG3	1.70	0.73
1:J:336:ARG:HG2	1:J:336:ARG:HH11	1.52	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:M:46:ARG:HG3	1:M:46:ARG:NH1	2.02	0.73
1:A:822:LEU:HD12	1:A:824:GLN:N	2.03	0.73
1:B:128:ASN:HD21	1:B:180:GLY:HA2	1.52	0.73
1:G:437:SER:HB2	5:G:2258:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:701:VAL:O	1:H:703:PRO:HD3	1.88	0.73
1:O:128:ASN:HD21	1:O:180:GLY:HA2	1.52	0.73
1:P:856:TYR:CD2	1:P:864:MET:HE2	2.23	0.73
1:A:43:ARG:HG2	1:A:43:ARG:NH1	1.94	0.73
1:E:701:VAL:O	1:E:703:PRO:HD3	1.88	0.73
1:I:822:LEU:HD12	1:I:824:GLN:N	2.03	0.73
1:K:701:VAL:O	1:K:703:PRO:HD3	1.88	0.73
1:K:822:LEU:HD12	1:K:824:GLN:N	2.03	0.73
1:N:437:SER:HB2	5:N:2263:HOH:O	1.88	0.73
1:E:748:CME:C	1:E:749:ILE:HD13	2.19	0.73
1:G:128:ASN:HD21	1:G:180:GLY:HA2	1.52	0.73
1:G:822:LEU:HD12	1:G:824:GLN:N	2.03	0.73
1:I:128:ASN:HD21	1:I:180:GLY:HA2	1.52	0.73
1:N:128:ASN:HD21	1:N:180:GLY:HA2	1.52	0.73
1:P:696:LEU:HD12	1:P:697:THR:H	1.52	0.73
1:B:336:ARG:HG2	1:B:336:ARG:HH11	1.52	0.73
1:C:128:ASN:HD21	1:C:180:GLY:HA2	1.52	0.73
1:G:336:ARG:HG2	1:G:336:ARG:HH11	1.52	0.73
1:H:748:CME:C	1:H:749:ILE:HD13	2.19	0.73
1:O:427:THR:CA	1:O:436:MET:HE1	2.10	0.73
1:O:822:LEU:HD12	1:O:824:GLN:N	2.03	0.73
1:C:748:CME:C	1:C:749:ILE:HD13	2.19	0.73
1:D:748:CME:C	1:D:749:ILE:HD13	2.19	0.73
1:F:822:LEU:HD12	1:F:824:GLN:N	2.03	0.73
1:K:128:ASN:HD21	1:K:180:GLY:HA2	1.52	0.73
1:N:856:TYR:CD2	1:N:864:MET:HE2	2.23	0.73
1:P:748:CME:C	1:P:749:ILE:HD13	2.19	0.73
1:B:49:GLN:NE2	1:B:49:GLN:H	1.87	0.73
1:B:651:LEU:HD12	1:B:652:LEU:N	2.04	0.73
1:B:822:LEU:HD12	1:B:824:GLN:N	2.03	0.73
1:G:701:VAL:O	1:G:703:PRO:HD3	1.88	0.73
1:N:822:LEU:HD12	1:N:824:GLN:N	2.03	0.73
1:O:46:ARG:HG3	1:O:46:ARG:NH1	2.02	0.73
1:C:336:ARG:HG2	1:C:336:ARG:HH11	1.52	0.72
1:E:49:GLN:NE2	1:E:49:GLN:H	1.87	0.72
1:F:696:LEU:HD12	1:F:697:THR:H	1.51	0.72
1:G:49:GLN:NE2	1:G:49:GLN:H	1.87	0.72
1:H:43:ARG:HG2	1:H:43:ARG:NH1	1.94	0.72
1:I:43:ARG:HG2	1:I:43:ARG:NH1	1.94	0.72
1:J:748:CME:C	1:J:749:ILE:HD13	2.19	0.72
1:K:49:GLN:NE2	1:K:49:GLN:H	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:128:ASN:HD21	1:L:180:GLY:HA2	1.52	0.72
1:L:856:TYR:CD2	1:L:864:MET:HE2	2.23	0.72
1:I:651:LEU:HD12	1:I:652:LEU:N	2.04	0.72
1:K:856:TYR:CD2	1:K:864:MET:HE2	2.23	0.72
1:M:748:CME:C	1:M:749:ILE:HD13	2.19	0.72
1:O:748:CME:C	1:O:749:ILE:HD13	2.19	0.72
1:C:49:GLN:H	1:C:49:GLN:NE2	1.87	0.72
1:A:748:CME:C	1:A:749:ILE:HD13	2.19	0.72
1:B:748:CME:C	1:B:749:ILE:HD13	2.19	0.72
1:C:822:LEU:HD12	1:C:824:GLN:N	2.03	0.72
1:C:856:TYR:CD2	1:C:864:MET:HE2	2.23	0.72
1:D:856:TYR:CD2	1:D:864:MET:HE2	2.23	0.72
1:G:651:LEU:HD12	1:G:652:LEU:N	2.04	0.72
1:J:49:GLN:NE2	1:J:49:GLN:H	1.87	0.72
1:K:748:CME:C	1:K:749:ILE:HD13	2.19	0.72
1:L:336:ARG:HG2	1:L:336:ARG:HH11	1.52	0.72
1:O:49:GLN:NE2	1:O:49:GLN:H	1.87	0.72
1:B:43:ARG:HG2	1:B:43:ARG:NH1	1.94	0.72
1:M:49:GLN:NE2	1:M:49:GLN:H	1.87	0.72
1:M:651:LEU:HD12	1:M:652:LEU:N	2.05	0.72
1:A:49:GLN:NE2	1:A:49:GLN:H	1.87	0.72
1:A:419:GLY:HA2	1:D:282:ARG:HH11	1.52	0.72
1:F:49:GLN:NE2	1:F:49:GLN:H	1.87	0.72
1:J:822:LEU:HD12	1:J:824:GLN:N	2.03	0.72
1:L:748:CME:C	1:L:749:ILE:HD13	2.19	0.72
1:M:701:VAL:O	1:M:703:PRO:HD3	1.88	0.72
1:O:856:TYR:CD2	1:O:864:MET:HE2	2.23	0.72
1:C:651:LEU:HD12	1:C:652:LEU:N	2.04	0.72
1:F:748:CME:C	1:F:749:ILE:HD13	2.19	0.72
1:K:77:ASP:C	1:K:78:LEU:HD23	2.15	0.72
1:M:11:LEU:N	1:M:11:LEU:HD23	2.05	0.72
1:N:748:CME:C	1:N:749:ILE:HD13	2.19	0.72
1:E:651:LEU:HD12	1:E:652:LEU:N	2.04	0.72
1:H:11:LEU:HD23	1:H:11:LEU:N	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:L:822:LEU:HD12	1:L:824:GLN:N	2.03	0.72
1:O:651:LEU:HD12	1:O:652:LEU:N	2.04	0.72
1:A:11:LEU:N	1:A:11:LEU:HD23	2.05	0.72
1:M:77:ASP:C	1:M:78:LEU:HD23	2.15	0.72
1:N:49:GLN:NE2	1:N:49:GLN:H	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:49:GLN:NE2	1:P:49:GLN:H	1.87	0.72
1:A:77:ASP:C	1:A:78:LEU:HD23	2.15	0.72
1:B:681:GLU:HA	1:B:681:GLU:OE2	1.90	0.72
1:D:49:GLN:NE2	1:D:49:GLN:H	1.87	0.72
1:G:748:CME:C	1:G:749:ILE:HD13	2.19	0.72
1:H:77:ASP:C	1:H:78:LEU:HD23	2.15	0.72
1:J:77:ASP:C	1:J:78:LEU:HD23	2.15	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:N:11:LEU:N	1:N:11:LEU:HD23	2.05	0.72
1:F:336:ARG:HG2	1:F:336:ARG:HH11	1.52	0.71
1:K:11:LEU:HD23	1:K:11:LEU:N	2.05	0.71
1:L:49:GLN:NE2	1:L:49:GLN:H	1.87	0.71
1:E:77:ASP:C	1:E:78:LEU:HD23	2.15	0.71
1:G:77:ASP:C	1:G:78:LEU:HD23	2.15	0.71
1:L:77:ASP:C	1:L:78:LEU:HD23	2.15	0.71
1:D:681:GLU:OE2	1:D:681:GLU:HA	1.90	0.71
1:E:681:GLU:HA	1:E:681:GLU:OE2	1.90	0.71
1:F:77:ASP:C	1:F:78:LEU:HD23	2.15	0.71
1:H:49:GLN:NE2	1:H:49:GLN:H	1.87	0.71
1:H:240:LEU:HD12	1:H:241:GLU:H	1.56	0.71
1:H:336:ARG:HG2	1:H:336:ARG:HH11	1.52	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:N:77:ASP:C	1:N:78:LEU:HD23	2.15	0.71
1:N:651:LEU:HD12	1:N:652:LEU:N	2.04	0.71
1:O:77:ASP:C	1:O:78:LEU:HD23	2.15	0.71
1:C:77:ASP:C	1:C:78:LEU:HD23	2.15	0.71
1:I:77:ASP:C	1:I:78:LEU:HD23	2.15	0.71
1:P:240:LEU:HD12	1:P:241:GLU:H	1.56	0.71
1:D:427:THR:CA	1:D:436:MET:HE1	2.10	0.71
1:E:230:ARG:HG3	1:E:230:ARG:NH1	2.06	0.71
1:I:278:ILE:H	1:I:278:ILE:HD12	1.56	0.71
1:J:46:ARG:HG3	1:J:46:ARG:NH1	2.02	0.71
1:L:427:THR:CA	1:L:436:MET:HE1	2.10	0.71
1:M:230:ARG:HG3	1:M:230:ARG:NH1	2.06	0.71
1:P:651:LEU:HD12	1:P:652:LEU:N	2.04	0.71
1:B:46:ARG:HG3	1:B:46:ARG:NH1	2.02	0.71
1:B:77:ASP:C	1:B:78:LEU:HD23	2.15	0.71
1:B:230:ARG:HG3	1:B:230:ARG:NH1	2.05	0.71
1:C:622:HIS:O	1:C:625:GLN:HG2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:LEU:N	1:D:11:LEU:HD23	2.05	0.71
1:F:651:LEU:HD12	1:F:652:LEU:N	2.04	0.71
1:I:427:THR:CA	1:I:436:MET:HE1	2.10	0.71
1:L:230:ARG:HG3	1:L:230:ARG:NH1	2.06	0.71
1:P:336:ARG:HG2	1:P:336:ARG:HH11	1.52	0.71
1:A:240:LEU:HD12	1:A:241:GLU:H	1.56	0.71
1:A:425:ARG:HH22	1:D:287:ASP:CG	1.99	0.71
1:A:427:THR:CA	1:A:436:MET:HE1	2.10	0.71
1:G:11:LEU:N	1:G:11:LEU:HD23	2.05	0.71
1:G:43:ARG:HG2	1:G:43:ARG:NH1	1.94	0.71
1:H:651:LEU:HD12	1:H:652:LEU:N	2.04	0.71
1:I:49:GLN:NE2	1:I:49:GLN:H	1.87	0.71
1:L:681:GLU:OE2	1:L:681:GLU:HA	1.90	0.71
1:N:282:ARG:NH1	1:O:419:GLY:HA2	2.05	0.71
1:P:77:ASP:C	1:P:78:LEU:HD23	2.15	0.71
1:D:622:HIS:O	1:D:625:GLN:HG2	1.91	0.71
1:H:437:SER:HB2	5:H:2258:HOH:O	1.89	0.71
1:O:43:ARG:HG2	1:O:43:ARG:NH1	1.94	0.71
1:B:11:LEU:N	1:B:11:LEU:HD23	2.05	0.71
1:E:622:HIS:O	1:E:625:GLN:HG2	1.91	0.71
1:F:622:HIS:O	1:F:625:GLN:HG2	1.91	0.71
1:I:46:ARG:HG3	1:I:46:ARG:NH1	2.02	0.71
1:K:278:ILE:H	1:K:278:ILE:HD12	1.56	0.71
1:K:681:GLU:HA	1:K:681:GLU:OE2	1.90	0.71
1:O:11:LEU:N	1:O:11:LEU:HD23	2.05	0.71
1:O:336:ARG:HG2	1:O:336:ARG:HH11	1.52	0.71
1:P:278:ILE:HD12	1:P:278:ILE:H	1.56	0.71
1:P:681:GLU:HA	1:P:681:GLU:OE2	1.90	0.71
1:D:240:LEU:HD12	1:D:241:GLU:H	1.56	0.71
1:H:681:GLU:HA	1:H:681:GLU:OE2	1.90	0.71
1:D:77:ASP:C	1:D:78:LEU:HD23	2.15	0.70
1:D:920:LEU:HB3	1:D:921:PRO:HD2	1.73	0.70
1:E:920:LEU:HB3	1:E:921:PRO:HD2	1.73	0.70
1:I:11:LEU:N	1:I:11:LEU:HD23	2.05	0.70
1:J:437:SER:HB2	5:J:2258:HOH:O	1.90	0.70
1:P:230:ARG:HG3	1:P:230:ARG:NH1	2.05	0.70
1:A:651:LEU:HD12	1:A:652:LEU:N	2.04	0.70
1:F:11:LEU:N	1:F:11:LEU:HD23	2.05	0.70
1:G:46:ARG:HG3	1:G:46:ARG:NH1	2.02	0.70
1:K:622:HIS:O	1:K:625:GLN:HG2	1.91	0.70
1:C:43:ARG:HG2	1:C:43:ARG:NH1	1.94	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:LEU:N	1:E:11:LEU:HD23	2.05	0.70
1:G:622:HIS:O	1:G:625:GLN:HG2	1.91	0.70
1:G:681:GLU:HA	1:G:681:GLU:OE2	1.91	0.70
1:H:622:HIS:O	1:H:625:GLN:HG2	1.91	0.70
1:L:920:LEU:HB3	1:L:921:PRO:HD2	1.73	0.70
1:M:681:GLU:HA	1:M:681:GLU:OE2	1.90	0.70
1:N:622:HIS:O	1:N:625:GLN:HG2	1.91	0.70
1:N:740:LEU:HD12	1:N:741:THR:N	2.06	0.70
1:O:278:ILE:H	1:O:278:ILE:HD12	1.56	0.70
1:O:920:LEU:HB3	1:O:921:PRO:HD2	1.73	0.70
1:A:278:ILE:H	1:A:278:ILE:HD12	1.56	0.70
1:B:278:ILE:H	1:B:278:ILE:HD12	1.56	0.70
1:E:240:LEU:HD12	1:E:241:GLU:H	1.56	0.70
1:F:740:LEU:HD12	1:F:741:THR:N	2.06	0.70
1:G:920:LEU:HB3	1:G:921:PRO:HD2	1.73	0.70
1:I:740:LEU:HD12	1:I:741:THR:N	2.06	0.70
1:C:681:GLU:HA	1:C:681:GLU:OE2	1.90	0.70
1:D:740:LEU:HD12	1:D:741:THR:N	2.06	0.70
1:L:11:LEU:N	1:L:11:LEU:HD23	2.05	0.70
1:M:920:LEU:HB3	1:M:921:PRO:HD2	1.73	0.70
1:P:46:ARG:HG3	1:P:46:ARG:NH1	2.02	0.70
1:P:622:HIS:O	1:P:625:GLN:HG2	1.91	0.70
1:D:230:ARG:HG3	1:D:230:ARG:NH1	2.05	0.70
1:F:1017:GLN:HB3	5:F:2260:HOH:O	1.92	0.70
1:H:278:ILE:HD12	1:H:278:ILE:H	1.56	0.70
1:I:681:GLU:HA	1:I:681:GLU:OE2	1.90	0.70
1:J:11:LEU:N	1:J:11:LEU:HD23	2.05	0.70
1:P:11:LEU:HD23	1:P:11:LEU:N	2.05	0.70
1:A:920:LEU:HB3	1:A:921:PRO:HD2	1.73	0.70
1:C:427:THR:CA	1:C:436:MET:HE1	2.10	0.70
1:I:240:LEU:HD12	1:I:241:GLU:H	1.56	0.70
1:J:278:ILE:H	1:J:278:ILE:HD12	1.56	0.70
1:K:240:LEU:HD12	1:K:241:GLU:H	1.56	0.70
1:K:1017:GLN:HB3	5:K:2260:HOH:O	1.92	0.70
1:M:622:HIS:O	1:M:625:GLN:HG2	1.91	0.70
1:N:278:ILE:H	1:N:278:ILE:HD12	1.56	0.70
1:O:622:HIS:O	1:O:625:GLN:HG2	1.91	0.70
1:P:1017:GLN:HB3	5:P:2261:HOH:O	1.92	0.70
1:A:425:ARG:NH2	1:D:287:ASP:OD2	2.24	0.70
1:A:681:GLU:HA	1:A:681:GLU:OE2	1.90	0.70
1:C:230:ARG:HG3	1:C:230:ARG:NH1	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:651:LEU:HD12	1:D:652:LEU:N	2.05	0.70
1:G:740:LEU:HD12	1:G:741:THR:N	2.06	0.70
1:H:230:ARG:HG3	1:H:230:ARG:NH1	2.05	0.70
1:L:278:ILE:H	1:L:278:ILE:HD12	1.56	0.70
1:N:230:ARG:HG3	1:N:230:ARG:NH1	2.06	0.70
1:O:230:ARG:HG3	1:O:230:ARG:NH1	2.05	0.70
1:B:240:LEU:HD12	1:B:241:GLU:H	1.56	0.70
1:B:577:LYS:O	1:B:584:PRO:HA	1.92	0.70
1:E:437:SER:HB2	5:E:2258:HOH:O	1.91	0.70
1:E:577:LYS:O	1:E:584:PRO:HA	1.92	0.70
1:E:1017:GLN:HB3	5:E:2260:HOH:O	1.92	0.70
1:F:278:ILE:H	1:F:278:ILE:HD12	1.56	0.70
1:G:230:ARG:HG3	1:G:230:ARG:NH1	2.06	0.70
1:G:278:ILE:H	1:G:278:ILE:HD12	1.56	0.70
1:I:577:LYS:O	1:I:584:PRO:HA	1.92	0.70
1:J:78:LEU:HB3	1:J:79:PRO:HD2	1.74	0.70
1:J:622:HIS:O	1:J:625:GLN:HG2	1.91	0.70
1:A:46:ARG:HG3	1:A:46:ARG:NH1	2.02	0.70
1:I:622:HIS:O	1:I:625:GLN:HG2	1.91	0.70
1:L:240:LEU:HD12	1:L:241:GLU:H	1.56	0.70
1:L:622:HIS:O	1:L:625:GLN:HG2	1.91	0.70
1:M:577:LYS:O	1:M:584:PRO:HA	1.92	0.70
1:O:681:GLU:OE2	1:O:681:GLU:HA	1.90	0.70
1:P:78:LEU:HB3	1:P:79:PRO:HD2	1.74	0.70
1:D:78:LEU:HB3	1:D:79:PRO:HD2	1.74	0.69
1:H:293:LEU:HD23	1:H:293:LEU:N	2.07	0.69
1:I:78:LEU:HB3	1:I:79:PRO:HD2	1.74	0.69
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:A:740:LEU:HD12	1:A:741:THR:N	2.06	0.69
1:C:11:LEU:HD23	1:C:11:LEU:N	2.05	0.69
1:I:1017:GLN:HB3	5:I:2260:HOH:O	1.92	0.69
1:K:293:LEU:HD23	1:K:293:LEU:N	2.07	0.69
1:L:1017:GLN:HB3	5:L:2260:HOH:O	1.92	0.69
1:M:1017:GLN:HB3	5:M:2259:HOH:O	1.92	0.69
1:P:920:LEU:HB3	1:P:921:PRO:HD2	1.73	0.69
1:A:577:LYS:O	1:A:584:PRO:HA	1.92	0.69
1:A:622:HIS:O	1:A:625:GLN:HG2	1.91	0.69
1:B:622:HIS:O	1:B:625:GLN:HG2	1.91	0.69
1:D:1017:GLN:HB3	5:D:2261:HOH:O	1.92	0.69
1:F:427:THR:CA	1:F:436:MET:HE1	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:LEU:HB3	1:H:79:PRO:HD2	1.74	0.69
1:K:920:LEU:HB3	1:K:921:PRO:HD2	1.73	0.69
1:C:78:LEU:HB3	1:C:79:PRO:HD2	1.74	0.69
1:C:278:ILE:H	1:C:278:ILE:HD12	1.56	0.69
1:E:658:LEU:O	1:E:661:LYS:HD3	1.93	0.69
1:F:577:LYS:O	1:F:584:PRO:HA	1.92	0.69
1:F:920:LEU:HB3	1:F:921:PRO:HD2	1.73	0.69
1:G:240:LEU:HD12	1:G:241:GLU:H	1.55	0.69
1:K:78:LEU:HB3	1:K:79:PRO:HD2	1.74	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:B:920:LEU:HB3	1:B:921:PRO:HD2	1.73	0.69
1:D:278:ILE:H	1:D:278:ILE:HD12	1.56	0.69
1:D:577:LYS:O	1:D:584:PRO:HA	1.92	0.69
1:M:43:ARG:HG2	1:M:43:ARG:NH1	1.94	0.69
1:O:240:LEU:HD12	1:O:241:GLU:H	1.56	0.69
1:O:740:LEU:HD12	1:O:741:THR:N	2.06	0.69
1:C:658:LEU:O	1:C:661:LYS:HD3	1.93	0.69
1:C:861:SER:OG	1:C:863:GLN:HG3	1.93	0.69
1:D:658:LEU:O	1:D:661:LYS:HD3	1.93	0.69
1:E:740:LEU:HD12	1:E:741:THR:N	2.06	0.69
1:F:240:LEU:HD12	1:F:241:GLU:H	1.56	0.69
1:H:577:LYS:O	1:H:584:PRO:HA	1.92	0.69
1:K:36:TRP:C	1:K:37:ARG:HD3	2.18	0.69
1:M:658:LEU:O	1:M:661:LYS:HD3	1.93	0.69
1:C:577:LYS:O	1:C:584:PRO:HA	1.92	0.69
1:E:861:SER:OG	1:E:863:GLN:HG3	1.93	0.69
1:G:78:LEU:HB3	1:G:79:PRO:HD2	1.74	0.69
1:I:861:SER:OG	1:I:863:GLN:HG3	1.93	0.69
1:M:293:LEU:HD23	1:M:293:LEU:N	2.07	0.69
1:M:861:SER:OG	1:M:863:GLN:HG3	1.93	0.69
1:P:577:LYS:O	1:P:584:PRO:HA	1.92	0.69
1:A:36:TRP:C	1:A:37:ARG:HD3	2.18	0.69
1:C:240:LEU:HD12	1:C:241:GLU:H	1.56	0.69
1:E:278:ILE:HD12	1:E:278:ILE:H	1.56	0.69
1:F:230:ARG:HG3	1:F:230:ARG:NH1	2.06	0.69
1:F:861:SER:OG	1:F:863:GLN:HG3	1.93	0.69
1:G:861:SER:OG	1:G:863:GLN:HG3	1.93	0.69
1:H:920:LEU:HB3	1:H:921:PRO:HD2	1.73	0.69
1:I:230:ARG:HG3	1:I:230:ARG:NH1	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:658:LEU:O	1:I:661:LYS:HD3	1.93	0.69
1:J:577:LYS:O	1:J:584:PRO:HA	1.92	0.69
1:J:681:GLU:HA	1:J:681:GLU:OE2	1.90	0.69
1:K:658:LEU:O	1:K:661:LYS:HD3	1.93	0.69
1:L:78:LEU:HB3	1:L:79:PRO:HD2	1.74	0.69
1:M:36:TRP:C	1:M:37:ARG:HD3	2.18	0.69
1:N:240:LEU:HD12	1:N:241:GLU:H	1.56	0.69
1:N:427:THR:CA	1:N:436:MET:HE1	2.10	0.69
1:O:36:TRP:C	1:O:37:ARG:HD3	2.18	0.69
1:O:78:LEU:HB3	1:O:79:PRO:HD2	1.74	0.69
1:O:861:SER:OG	1:O:863:GLN:HG3	1.93	0.69
1:B:129:VAL:HG23	1:B:182:ASN:ND2	2.08	0.69
1:B:861:SER:OG	1:B:863:GLN:HG3	1.93	0.69
1:D:673:ALA:HB1	1:D:674:PRO:HD2	1.75	0.69
1:E:282:ARG:HG3	1:H:423:MET:HB2	1.73	0.69
1:F:129:VAL:HG23	1:F:182:ASN:ND2	2.08	0.69
1:F:658:LEU:O	1:F:661:LYS:HD3	1.93	0.69
1:H:36:TRP:C	1:H:37:ARG:HD3	2.18	0.69
1:H:861:SER:OG	1:H:863:GLN:HG3	1.93	0.69
1:I:673:ALA:HB1	1:I:674:PRO:HD2	1.75	0.69
1:J:920:LEU:HB3	1:J:921:PRO:HD2	1.73	0.69
1:M:129:VAL:HG23	1:M:182:ASN:ND2	2.08	0.69
1:N:129:VAL:HG23	1:N:182:ASN:ND2	2.08	0.69
1:O:577:LYS:O	1:O:584:PRO:HA	1.92	0.69
1:O:1017:GLN:HB3	5:O:2259:HOH:O	1.92	0.69
1:A:129:VAL:HG23	1:A:182:ASN:ND2	2.08	0.69
1:C:920:LEU:HB3	1:C:921:PRO:HD2	1.73	0.69
1:C:1017:GLN:HB3	5:C:2260:HOH:O	1.92	0.69
1:E:78:LEU:HB3	1:E:79:PRO:HD2	1.74	0.69
1:G:577:LYS:O	1:G:584:PRO:HA	1.92	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: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:36:TRP:C	1:P:37:ARG:HD3	2.18	0.69
1:P:861:SER:OG	1:P:863:GLN:HG3	1.93	0.69
1:B:36:TRP:C	1:B:37:ARG:HD3	2.18	0.68
1:D:322:LEU:HD11	1:D:324:GLU:O	1.94	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:M:240:LEU:HD12	1:M:241:GLU:H	1.55	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:129:VAL:HG23	1:C:182:ASN:ND2	2.08	0.68
1:C:740:LEU:HD12	1:C:741:THR:N	2.06	0.68
1:F:673:ALA:HB1	1:F:674:PRO:HD2	1.75	0.68
1:G:1017:GLN:HB3	5:G:2260:HOH:O	1.92	0.68
1:I:920:LEU:HB3	1:I:921:PRO:HD2	1.73	0.68
1:J:36:TRP:C	1:J:37:ARG:HD3	2.18	0.68
1:J:230:ARG:HG3	1:J:230:ARG:NH1	2.06	0.68
1:J:322:LEU:HD11	1:J:324:GLU:O	1.94	0.68
1:K:673:ALA:HB1	1:K:674:PRO:HD2	1.75	0.68
1:N:423:MET:HB2	1:O:282:ARG:HG3	1.73	0.68
1:N:673:ALA:HB1	1:N:674:PRO:HD2	1.75	0.68
1:N:1017:GLN:HB3	5:N:2259:HOH:O	1.92	0.68
1:B:1017:GLN:HB3	5:B:2259:HOH:O	1.92	0.68
1:C:36:TRP:C	1:C:37:ARG:HD3	2.18	0.68
1:D:861:SER:OG	1:D:863:GLN:HG3	1.93	0.68
1:E:427:THR:CA	1:E:436:MET:HE1	2.10	0.68
1:E:673:ALA:HB1	1:E:674:PRO:HD2	1.75	0.68
1:I:36:TRP:C	1:I:37:ARG:HD3	2.18	0.68
1:J:1017:GLN:HB3	5:J:2260:HOH:O	1.92	0.68
1:L:658:LEU:O	1:L:661:LYS:HD3	1.93	0.68
1:P:322:LEU:HD11	1:P:324:GLU:O	1.94	0.68
1:P:658:LEU:O	1:P:661:LYS:HD3	1.93	0.68
1:A:658:LEU:O	1:A:661:LYS:HD3	1.93	0.68
1:A:861:SER:OG	1:A:863:GLN:HG3	1.93	0.68
1:A:673:ALA:HB1	1:A:674:PRO:HD2	1.75	0.68
1:B:78:LEU:HB3	1:B:79:PRO:HD2	1.74	0.68
1:B:322:LEU:HD11	1:B:324:GLU:O	1.94	0.68
1:E:293:LEU:HD23	1:E:293:LEU:N	2.07	0.68
1:F:36:TRP:C	1:F:37:ARG:HD3	2.18	0.68
1:G:129:VAL:HG23	1:G:182:ASN:ND2	2.08	0.68
1:H:740:LEU:HD12	1:H:741:THR:N	2.06	0.68
1:H:1017:GLN:HB3	5:H:2260:HOH:O	1.92	0.68
1:I:293:LEU:HD23	1:I:293:LEU:N	2.07	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:O:129:VAL:HG23	1:O:182:ASN:ND2	2.08	0.68
1:A:282:ARG:HG3	1:D:423:MET:HB2	1.74	0.68
1:A:322:LEU:HD11	1:A:324:GLU:O	1.94	0.68
1:C:293:LEU:HD23	1:C:293:LEU:N	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:TRP:C	1:D:37:ARG:HD3	2.18	0.68
1:E:36:TRP:C	1:E:37:ARG:HD3	2.18	0.68
1:G:322:LEU:HD11	1:G:324:GLU:O	1.94	0.68
1:K:230:ARG:HG3	1:K:230:ARG:NH1	2.06	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:917:ARG:HH22	1:O:943:GLU:CD	2.02	0.68
1:A:230:ARG:HG3	1:A:230:ARG:NH1	2.06	0.68
1:B:658:LEU:O	1:B:661:LYS:HD3	1.93	0.68
1:D:1021:CME:HB3	1:D:1021:CME:CZ	2.21	0.68
1:E:322:LEU:HD11	1:E: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
1:O:322:LEU:HD11	1:O:324:GLU:O	1.94	0.68
1:A:293:LEU:HD23	1:A:293:LEU:N	2.07	0.68
1:A:917:ARG:HH22	1:A:943:GLU:CD	2.02	0.68
1:A:1017:GLN:HB3	5:A:2258:HOH:O	1.92	0.68
1:B:293:LEU:HD23	1:B:293:LEU:N	2.07	0.68
1:B:673:ALA:HB1	1:B:674:PRO:HD2	1.75	0.68
1:F:681:GLU:HA	1:F:681:GLU:OE2	1.90	0.68
1:J:293:LEU:HD23	1:J:293:LEU:N	2.07	0.68
1:J:579:ASP:CG	1:J:583:ASN:HB2	2.19	0.68
1:K:322:LEU:HD11	1:K:324:GLU:O	1.94	0.68
1:L:36:TRP:C	1:L:37:ARG:HD3	2.18	0.68
1:L:293:LEU:HD23	1:L:293:LEU:N	2.07	0.68
1:N:46:ARG:HG3	1:N:46:ARG:NH1	2.02	0.68
1:C:579:ASP:CG	1:C:583:ASN:HB2	2.19	0.68
1:E:423:MET:HB2	1:H:282:ARG:HG3	1.76	0.68
1:F:78:LEU:HB3	1:F:79:PRO:HD2	1.74	0.68
1:F:210:ARG:HH12	1:F:395:HIS:N	1.92	0.68
1:F:579:ASP:CG	1:F:583:ASN:HB2	2.19	0.68
1:I:322:LEU:HD11	1:I:324:GLU:O	1.93	0.68
1:L:917:ARG:HH22	1:L:943:GLU:CD	2.02	0.68
1:N:36:TRP:C	1:N:37:ARG:HD3	2.18	0.68
1:N:78:LEU:HB3	1:N:79:PRO:HD2	1.74	0.68
1:N:579:ASP:CG	1:N:583:ASN:HB2	2.19	0.68
1:A:579:ASP:CG	1:A:583:ASN:HB2	2.19	0.68
1:D:579:ASP:CG	1:D:583:ASN:HB2	2.19	0.68
1:F:322:LEU:HD11	1:F:324:GLU:O	1.94	0.68
1:G:658:LEU:O	1:G:661:LYS:HD3	1.93	0.68
1:H:658:LEU:O	1:H:661:LYS:HD3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:917:ARG:HH22	1:I:943:GLU:CD	2.02	0.68
1:M:673:ALA:HB1	1:M:674:PRO:HD2	1.75	0.68
1:M:917:ARG:HH22	1:M:943:GLU:CD	2.02	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:A:78:LEU:HB3	1:A:79:PRO:HD2	1.74	0.67
1:A:217:LYS:HG2	1:A:218:PRO:HD2	1.76	0.67
1:B:278:ILE:HD12	1:B:278:ILE:N	2.10	0.67
1:E:129:VAL:HG23	1:E:182:ASN:ND2	2.08	0.67
1:K:579:ASP:CG	1:K:583:ASN:HB2	2.19	0.67
1:K:917:ARG:HH22	1:K:943:GLU:CD	2.02	0.67
1:N:322:LEU:HD11	1:N:324:GLU:O	1.94	0.67
1:P:740:LEU:HD12	1:P:741:THR:N	2.06	0.67
1:A:278:ILE:HD12	1:A:278:ILE:N	2.10	0.67
1:B:740:LEU:HD12	1:B:741:THR:N	2.06	0.67
1:C:278:ILE:HD12	1:C:278:ILE:N	2.10	0.67
1:C:336:ARG:HG2	1:C:336:ARG:NH1	2.09	0.67
1:C:917:ARG:HH22	1:C:943:GLU:CD	2.02	0.67
1:F:278:ILE:HD12	1:F:278:ILE:N	2.10	0.67
1:G:36:TRP:C	1:G:37:ARG:HD3	2.18	0.67
1:H:129:VAL:HG23	1:H:182:ASN:ND2	2.08	0.67
1:H:217:LYS:HG2	1:H:218:PRO:HD2	1.76	0.67
1:J:427:THR:CA	1:J:436:MET:HE1	2.10	0.67
1:K:129:VAL:HG23	1:K:182:ASN:ND2	2.08	0.67
1:N:278:ILE:HD12	1:N:278:ILE:N	2.10	0.67
1:O:293:LEU:HD23	1:O:293:LEU:N	2.07	0.67
1:P:36:TRP:CE2	1:P:42:ALA:HA	2.30	0.67
1:B:579:ASP:CG	1:B:583:ASN:HB2	2.19	0.67
1:E:217:LYS:HG2	1:E:218:PRO:HD2	1.76	0.67
1:E:336:ARG:HG2	1:E:336:ARG:NH1	2.09	0.67
1:G:278:ILE:HD12	1:G:278:ILE:N	2.10	0.67
1:G:917:ARG:HH22	1:G:943:GLU:CD	2.02	0.67
1:H:917:ARG:HH22	1:H:943:GLU:CD	2.02	0.67
1:J:336:ARG:HG2	1:J:336:ARG:NH1	2.09	0.67
1:K:740:LEU:HD12	1:K:741:THR:N	2.06	0.67
1:L:129:VAL:HG23	1:L:182:ASN:ND2	2.08	0.67
1:O:278:ILE:HD12	1:O:278:ILE:N	2.10	0.67
1:P:129:VAL:HG23	1:P:182:ASN:ND2	2.08	0.67
1:D:278:ILE:HD12	1:D:278:ILE:N	2.10	0.67
1:E:749:ILE:HD13	1:E:749:ILE:N	2.10	0.67
1:E:917:ARG:HH22	1:E:943:GLU:CD	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:673:ALA:HB1	1:G:674:PRO:HD2	1.75	0.67
1:H:749:ILE:HD13	1:H:749:ILE:N	2.10	0.67
1:I:129:VAL:HG23	1:I:182:ASN:ND2	2.08	0.67
1:P:749:ILE:HD13	1:P:749:ILE:N	2.10	0.67
1:C:36:TRP:CE2	1:C:42:ALA:HA	2.30	0.67
1:D:917:ARG:HH22	1:D:943:GLU:CD	2.02	0.67
1:H:579:ASP:CG	1:H:583:ASN:HB2	2.19	0.67
1:M:427:THR:CA	1:M:436:MET:HE1	2.10	0.67
1:O:673:ALA:HB1	1:O:674:PRO:HD2	1.75	0.67
1:P:217:LYS:HG2	1:P:218:PRO:HD2	1.77	0.67
1:P:437:SER:HB2	5:P:2102:HOH:O	1.94	0.67
1:D:749:ILE:HD13	1:D:749:ILE:N	2.10	0.67
1:I:36:TRP:CE2	1:I:42:ALA:HA	2.30	0.67
1:I:579:ASP:CG	1:I:583:ASN:HB2	2.19	0.67
1:I:1021:CME:HB3	1:I:1021:CME:CZ	2.21	0.67
1:J:278:ILE:HD12	1:J:278:ILE:N	2.10	0.67
1:J:740:LEU:HD12	1:J:741:THR:N	2.06	0.67
1:K:42:ALA:O	1:K:310:ARG:NH1	2.28	0.67
1:M:24:LEU:HB2	1:M:161:TYR:HB3	1.77	0.67
1:M:42:ALA:O	1:M:310:ARG:NH1	2.28	0.67
1:M:217:LYS:HG2	1:M:218:PRO:HD2	1.76	0.67
1:N:293:LEU:HD23	1:N:293:LEU:N	2.07	0.67
1:O:336:ARG:HG2	1:O:336:ARG:NH1	2.09	0.67
1:P:24:LEU:HB2	1:P:161:TYR:HB3	1.77	0.67
1:P:673:ALA:HB1	1:P:674:PRO:HD2	1.75	0.67
1:D:36:TRP:CE2	1:D:42:ALA:HA	2.30	0.67
1:D:129:VAL:HG23	1:D:182:ASN:ND2	2.08	0.67
1:E:24:LEU:HB2	1:E:161:TYR:HB3	1.77	0.67
1:G:336:ARG:HG2	1:G:336:ARG:NH1	2.09	0.67
1:H:42:ALA:O	1:H:310:ARG:NH1	2.28	0.67
1:H:322:LEU:HD11	1:H:324:GLU:O	1.93	0.67
1:J:658:LEU:O	1:J:661:LYS:HD3	1.93	0.67
1:K:210:ARG:HH12	1:K:395:HIS:N	1.92	0.67
1:L:278:ILE:HD12	1:L:278:ILE:N	2.10	0.67
1:L:322:LEU:HD11	1:L:324:GLU:O	1.94	0.67
1:N:42:ALA:O	1:N:310:ARG:NH1	2.28	0.67
1:P:917:ARG:HH22	1:P:943:GLU:CD	2.02	0.67
1:A:749:ILE:HD13	1:A:749:ILE:N	2.10	0.67
1:D:217:LYS:HG2	1:D:218:PRO:HD2	1.76	0.67
1:E:42:ALA:O	1:E:310:ARG:NH1	2.28	0.67
1:F:1021:CME:HB3	1:F:1021:CME:CZ	2.21	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:377:LEU:HD22	1:G:708:TRP:HA	1.77	0.67
1:H:24:LEU:HB2	1:H:161:TYR:HB3	1.77	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:N:749:ILE:HD13	1:N:749:ILE:N	2.10	0.67
1:N:917:ARG:HH22	1:N:943:GLU:CD	2.02	0.67
1:O:377:LEU:HD22	1:O:708:TRP:HA	1.77	0.67
1:A:24:LEU:HB2	1:A:161:TYR:HB3	1.77	0.67
1:A:210:ARG:HH12	1:A:395:HIS:N	1.92	0.67
1:C:322:LEU:HD11	1:C:324:GLU:O	1.94	0.67
1:E:43:ARG:HG2	1:E:43:ARG:NH1	1.94	0.67
1:E:1021:CME:HB3	1:E:1021:CME:CZ	2.21	0.67
1:F:36:TRP:CE2	1:F:42:ALA:HA	2.30	0.67
1:I:278:ILE:HD12	1:I:278:ILE:N	2.10	0.67
1:J:917:ARG:HH22	1:J:943:GLU:CD	2.02	0.67
1:L:36:TRP:CE2	1:L:42:ALA:HA	2.30	0.67
1:L:336:ARG:HG2	1:L:336:ARG:NH1	2.09	0.67
1:M:210:ARG:HH12	1:M:395:HIS:N	1.92	0.67
1:N:36:TRP:CE2	1:N:42:ALA:HA	2.30	0.67
1:A:36:TRP:CE2	1:A:42:ALA:HA	2.30	0.67
1:B:36:TRP:CE2	1:B:42:ALA:HA	2.30	0.67
1:B:210:ARG:HH12	1:B:395:HIS:N	1.92	0.67
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.77	0.67
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.77	0.67
1:E:36:TRP:CE2	1:E:42:ALA:HA	2.30	0.67
1:F:117:GLU:OE1	1:F:117:GLU:N	2.27	0.67
1:F:293:LEU:HD23	1:F:293:LEU:N	2.07	0.67
1:H:377:LEU:HD22	1:H:708:TRP:HA	1.77	0.67
1:I:24:LEU:HB2	1:I:161:TYR:HB3	1.77	0.67
1:I:59:ARG:NH2	1:I:81:ALA:O	2.28	0.67
1:I:217:LYS:HG2	1:I:218:PRO:HD2	1.76	0.67
1:K:749:ILE:HD13	1:K:749:ILE:N	2.10	0.67
1:L:740:LEU:HD12	1:L:741:THR:N	2.06	0.67
1:L:861:SER:OG	1:L:863:GLN:HG3	1.93	0.67
1:P:377:LEU:HD22	1:P:708:TRP:HA	1.77	0.67
1:B:287:ASP:OD2	1:C:425:ARG:NH2	2.28	0.66
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.75	0.66
1:C:749:ILE:HD13	1:C:749:ILE:N	2.10	0.66
1:E:278:ILE:HD12	1:E:278:ILE:N	2.10	0.66
1:F:42:ALA:O	1:F:310:ARG:NH1	2.28	0.66
1:F:43:ARG:HG2	1:F:43:ARG:NH1	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:120:THR:HG21	1:G:187:MET:HE3	1.78	0.66
1:G:579:ASP:CG	1:G:583:ASN:HB2	2.19	0.66
1:H:433:LEU:HB3	1:H:434:PRO:HD3	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:L:24:LEU:HB2	1:L:161:TYR:HB3	1.77	0.66
1:M:579:ASP:CG	1:M:583:ASN:HB2	2.19	0.66
1:M:939:CYS:HA	1:M:956:GLN:HB3	1.78	0.66
1:N:120:THR:HG21	1:N:187:MET:HE3	1.78	0.66
1:O:120:THR:HG21	1:O:187:MET:HE3	1.78	0.66
1:O:579:ASP:CG	1:O:583:ASN:HB2	2.19	0.66
1:P:579:ASP:CG	1:P:583:ASN:HB2	2.19	0.66
1:A:42:ALA:O	1:A:310:ARG:NH1	2.28	0.66
1:A:59:ARG:NH2	1:A:81:ALA:O	2.28	0.66
1:B:917:ARG:HH22	1:B:943:GLU:CD	2.02	0.66
1:D:24:LEU:HB2	1:D:161:TYR:HB3	1.77	0.66
1:F:120:THR:HG21	1:F:187:MET:HE3	1.78	0.66
1:F:682:LEU:CD2	1:F:683:PRO:HD2	2.26	0.66
1:G:36:TRP:CE2	1:G:42:ALA:HA	2.30	0.66
1:H:673:ALA:HB1	1:H:674:PRO:HD2	1.75	0.66
1:J:42:ALA:O	1:J:310:ARG:NH1	2.28	0.66
1:K:377:LEU:HD22	1:K:708:TRP:HA	1.77	0.66
1:L:217:LYS:HG2	1:L:218:PRO:HD2	1.76	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:P:117:GLU:OE1	1:P:117:GLU:N	2.27	0.66
1:P:278:ILE:HD12	1:P:278:ILE:N	2.10	0.66
1:C:939:CYS:HA	1:C:956:GLN:HB3	1.77	0.66
1:D:917:ARG:NH2	1:D:943:GLU:OE1	2.29	0.66
1:E:210:ARG:HH12	1:E:395:HIS:N	1.92	0.66
1:E:433:LEU:HB3	1:E:434:PRO:HD3	1.77	0.66
1:E:939:CYS:HA	1:E:956:GLN:HB3	1.78	0.66
1:F:377:LEU:HD22	1:F:708:TRP:HA	1.77	0.66
1:H:36:TRP:CE2	1:H:42:ALA:HA	2.30	0.66
1:H:278:ILE:HD12	1:H:278:ILE:N	2.10	0.66
1:J:36:TRP:CE2	1:J:42:ALA:HA	2.30	0.66
1:L:579:ASP:CG	1:L:583:ASN:HB2	2.19	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
1:P:114:VAL:HG13	1:P:115:PRO:HD2	1.78	0.66
1:C:42:ALA:O	1:C:310:ARG:NH1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:579:ASP:CG	1:E:583:ASN:HB2	2.19	0.66
1:H:59:ARG:NH2	1:H:81:ALA:O	2.28	0.66
1:I:120:THR:HG21	1:I:187:MET:HE3	1.78	0.66
1:J:433:LEU:HB3	1:J:434:PRO:HD3	1.77	0.66
1:K:30:HIS:HB2	1:K:31:PRO:HD2	1.78	0.66
1:K:454:ILE:HG13	1:K:455:ILE:HG13	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:P:433:LEU:HB3	1:P:434:PRO:HD3	1.77	0.66
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.77	0.66
1:A:682:LEU:CD2	1:A:683:PRO:HD2	2.26	0.66
1:B:217:LYS:HG2	1:B:218:PRO:HD2	1.76	0.66
1:C:114:VAL:HG13	1:C:115:PRO:HD2	1.78	0.66
1:E:30:HIS:HB2	1:E:31:PRO:HD2	1.78	0.66
1:G:749:ILE:HD13	1:G:749:ILE:N	2.10	0.66
1:H:114:VAL:HG13	1:H:115:PRO:HD2	1.78	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:K:682:LEU:CD2	1:K:683:PRO:HD2	2.26	0.66
1:L:46:ARG:HG3	1:L:46:ARG:NH1	2.02	0.66
1:L:59:ARG:NH2	1:L:81:ALA:O	2.28	0.66
1:M:278:ILE:HD12	1:M:278:ILE:N	2.10	0.66
1:N:24:LEU:HB2	1:N:161:TYR:HB3	1.77	0.66
1:N:114:VAL:HG13	1:N:115:PRO:HD2	1.78	0.66
1:P:42:ALA:O	1:P:310:ARG:NH1	2.28	0.66
1:A:120:THR:HG21	1:A:187:MET:HE3	1.78	0.66
1:B:42:ALA:O	1:B:310:ARG:NH1	2.28	0.66
1:C:30:HIS:HB2	1:C:31:PRO:HD2	1.78	0.66
1:C:59:ARG:NH2	1:C:81:ALA:O	2.28	0.66
1:F:24:LEU:HB2	1:F:161:TYR:HB3	1.77	0.66
1:F:114:VAL:HG13	1:F:115:PRO:HD2	1.78	0.66
1:F:336:ARG:HG2	1:F:336:ARG:NH1	2.09	0.66
1:F:749:ILE:HD13	1:F:749:ILE:N	2.10	0.66
1:G:293:LEU:HD23	1:G:293:LEU:N	2.07	0.66
1:H:682:LEU:CD2	1:H:683:PRO:HD2	2.26	0.66
1:H:917:ARG:NH2	1:H:943:GLU:OE1	2.29	0.66
1:I:114:VAL:HG13	1:I:115:PRO:HD2	1.78	0.66
1:I:117:GLU:OE1	1:I:117:GLU:N	2.27	0.66
1:I:917:ARG:NH2	1:I:943:GLU:OE1	2.29	0.66
1:J:30:HIS:HB2	1:J:31:PRO:HD2	1.78	0.66
1:J:114:VAL:HG13	1:J:115:PRO:HD2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:917:ARG:NH2	1:O:943:GLU:OE1	2.29	0.66
1:P:682:LEU:CD2	1:P:683:PRO:HD2	2.26	0.66
1:B:749:ILE:HD13	1:B:749:ILE:N	2.10	0.66
1:C:210:ARG:HH12	1:C:395:HIS:N	1.92	0.66
1:C:682:LEU:CD2	1:C:683:PRO:HD2	2.26	0.66
1:G:24:LEU:HB2	1:G:161:TYR:HB3	1.77	0.66
1:G:210:ARG:HH12	1:G:395:HIS:N	1.92	0.66
1:I:42:ALA:O	1:I:310:ARG:NH1	2.28	0.66
1:J:3:ILE:HG13	1:J:4:THR:N	2.09	0.66
1:J:59:ARG:NH2	1:J:81:ALA:O	2.28	0.66
1:J:917:ARG:NH2	1:J:943:GLU:OE1	2.29	0.66
1:J:939:CYS:HA	1:J:956:GLN:HB3	1.77	0.66
1:K:114:VAL:HG13	1:K:115:PRO:HD2	1.78	0.66
1:L:30:HIS:HB2	1:L:31:PRO:HD2	1.78	0.66
1:M:433:LEU:HB3	1:M:434:PRO:HD3	1.77	0.66
1:N:282:ARG:HD3	1:O:418:HIS:O	1.96	0.66
1:N:360:HIS:HE1	1:N:362:LEU:HB2	1.61	0.66
1:P:917:ARG:NH2	1:P:943:GLU:OE1	2.29	0.66
1:B:120:THR:HG21	1:B:187:MET:HE3	1.78	0.66
1:B:336:ARG:HG2	1:B:336:ARG:NH1	2.09	0.66
1:B:454:ILE:HG13	1:B:455:ILE:HG13	1.78	0.66
1:C:917:ARG:NH2	1:C:943:GLU:OE1	2.29	0.66
1:D:59:ARG:NH2	1:D:81:ALA:O	2.28	0.66
1:E:377:LEU:HD22	1:E:708:TRP:HA	1.77	0.66
1:I:749:ILE:HD13	1:I:749:ILE:N	2.10	0.66
1:K:36:TRP:CE2	1:K:42:ALA:HA	2.30	0.66
1:K:59:ARG:NH2	1:K:81:ALA:O	2.28	0.66
1:L:454:ILE:HG13	1:L:455:ILE:HG13	1.78	0.66
1:M:336:ARG:HG2	1:M:336:ARG:NH1	2.09	0.66
1:M:454:ILE:HG13	1:M:455:ILE:HG13	1.78	0.66
1:O:24:LEU:HB2	1:O:161:TYR:HB3	1.77	0.66
1:P:59:ARG:NH2	1:P:81:ALA:O	2.29	0.66
1:B:24:LEU:HB2	1:B:161:TYR:HB3	1.77	0.66
1:C:217:LYS:HG2	1:C:218:PRO:HD2	1.76	0.66
1:D:42:ALA:O	1:D:310:ARG:NH1	2.28	0.66
1:F:59:ARG:NH2	1:F:81:ALA:O	2.28	0.66
1:J:114:VAL:CG1	1:J:191:TRP:HB2	2.26	0.66
1:K:433:LEU:HB3	1:K:434:PRO:HD3	1.77	0.66
1:L:210:ARG:HH12	1:L:395:HIS:N	1.92	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:1021:CME:CZ	1:M:1021:CME:HB3	2.21	0.66
1:O:360:HIS:HE1	1:O:362:LEU:HB2	1.61	0.66
1:O:682:LEU:CD2	1:O:683:PRO:HD2	2.26	0.66
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.77	0.66
1:B:682:LEU:CD2	1:B:683:PRO:HD2	2.26	0.66
1:C:120:THR:HG21	1:C:187:MET:HE3	1.78	0.66
1:D:682:LEU:CD2	1:D:683:PRO:HD2	2.26	0.66
1:E:246:MET:HG2	1:E:274:PHE:CE2	2.31	0.66
1:E:454:ILE:HG13	1:E:455:ILE:HG13	1.78	0.66
1:F:217:LYS:HG2	1:F:218:PRO:HD2	1.76	0.66
1:G:360:HIS:HE1	1:G:362:LEU:HB2	1.61	0.66
1:H:120:THR:HG21	1:H:187:MET:HE3	1.78	0.66
1:I:360:HIS:HE1	1:I:362:LEU:HB2	1.61	0.66
1:I:939:CYS:HA	1:I:956:GLN:HB3	1.78	0.66
1:J:423:MET:HB2	1:K:282:ARG:HG3	1.77	0.66
1:J:1021:CME:CZ	1:J:1021:CME:HB3	2.21	0.66
1:K:217:LYS:HG2	1:K:218:PRO:HD2	1.76	0.66
1:K:336:ARG:HG2	1:K:336:ARG:NH1	2.09	0.66
1:L:682:LEU:CD2	1:L:683:PRO:HD2	2.26	0.66
1:M:120:THR:HG21	1:M:187:MET:HE3	1.78	0.66
1:N:217:LYS:HG2	1:N:218:PRO:HD2	1.76	0.66
1:O:114:VAL:HG13	1:O:115:PRO:HD2	1.78	0.66
1:P:246:MET:HG2	1:P:274:PHE:CE2	2.31	0.66
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.77	0.65
1:E:59:ARG:NH2	1:E:81:ALA:O	2.29	0.65
1:G:114:VAL:HG13	1:G:115:PRO:HD2	1.78	0.65
1:G:246:MET:HG2	1:G:274:PHE:CE2	2.31	0.65
1:G:682:LEU:CD2	1:G:683:PRO:HD2	2.26	0.65
1:H:246:MET:HG2	1:H:274:PHE:CE2	2.31	0.65
1:I:246:MET:HG2	1:I:274:PHE:CE2	2.31	0.65
1:I:377:LEU:HD22	1:I:708:TRP:HA	1.77	0.65
1:M:753:ASN:N	1:M:753:ASN:OD1	2.30	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:N:336:ARG:HG2	1:N:336:ARG:NH1	2.09	0.65
1:O:246:MET:HG2	1:O:274:PHE:CE2	2.31	0.65
1:P:120:THR:HG21	1:P:187:MET:HE3	1.78	0.65
1:A:336:ARG:HG2	1:A:336:ARG:NH1	2.09	0.65
1:A:454:ILE:HG13	1:A:455:ILE:HG13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.77	0.65
1:F:246:MET:HG2	1:F:274:PHE:CE2	2.31	0.65
1:F:917:ARG:HH22	1:F:943:GLU:CD	2.02	0.65
1:H:117:GLU:OE1	1:H:117:GLU:N	2.27	0.65
1:H:210:ARG:HH12	1:H:395:HIS:N	1.92	0.65
1:I:433:LEU:HB3	1:I:434:PRO:HD3	1.77	0.65
1:J:217:LYS:HG2	1:J:218:PRO:HD2	1.76	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:L:917:ARG:NH2	1:L:943:GLU:OE1	2.29	0.65
1:L:939:CYS:HA	1:L:956:GLN:HB3	1.78	0.65
1:B:246:MET:HG2	1:B:274:PHE:CE2	2.31	0.65
1:B:703:PRO:O	1:B:711:ALA:HB1	1.97	0.65
1:D:114:VAL:CG1	1:D:191:TRP:HB2	2.26	0.65
1:G:59:ARG:NH2	1:G:81:ALA:O	2.29	0.65
1:G:917:ARG:NH2	1:G:943:GLU:OE1	2.29	0.65
1:H:114:VAL:CG1	1:H:191:TRP:HB2	2.26	0.65
1:H:703:PRO:O	1:H:711:ALA:HB1	1.97	0.65
1:K:24:LEU:HB2	1:K:161:TYR:HB3	1.77	0.65
1:P:114:VAL:CG1	1:P:191:TRP:HB2	2.26	0.65
1:A:753:ASN:OD1	1:A:753:ASN:N	2.30	0.65
1:B:427:THR:CA	1:B:436:MET:HE1	2.10	0.65
1:C:232:ASN:ND2	1:C:234:ASP:OD1	2.30	0.65
1:D:117:GLU:OE1	1:D:117:GLU:N	2.27	0.65
1:D:336:ARG:HG2	1:D:336:ARG:NH1	2.09	0.65
1:D:703:PRO:O	1:D:711:ALA:HB1	1.97	0.65
1:E:237:ARG:CB	1:E:237:ARG:HH11	2.10	0.65
1:F:454:ILE:HG13	1:F:455:ILE:HG13	1.78	0.65
1:F:917:ARG:NH2	1:F:943:GLU:OE1	2.29	0.65
1:G:427:THR:CA	1:G:436:MET:HE1	2.10	0.65
1:I:703:PRO:O	1:I:711:ALA:HB1	1.97	0.65
1:J:237:ARG:CB	1:J:237:ARG:HH11	2.10	0.65
1:K:246:MET:HG2	1:K:274:PHE:CE2	2.31	0.65
1:L:3:ILE:HG13	1:L:4:THR:N	2.09	0.65
1:N:232:ASN:ND2	1:N:234:ASP:OD1	2.30	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
1:O:42:ALA:O	1:O:310:ARG:NH1	2.28	0.65
1:O:59:ARG:NH2	1:O:81:ALA:O	2.29	0.65
1:A:114:VAL:CG1	1:A:191:TRP:HB2	2.26	0.65
1:B:114:VAL:HG13	1:B:115:PRO:HD2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:ILE:HG13	1:C:455:ILE:HG13	1.78	0.65
1:E:120:THR:HG21	1:E:187:MET:HE3	1.77	0.65
1:E:917:ARG:NH2	1:E:943:GLU:OE1	2.29	0.65
1:F:939:CYS:HA	1:F:956:GLN:HB3	1.77	0.65
1:G:433:LEU:HB3	1:G: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: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:P:30:HIS:HB2	1:P:31:PRO:HD2	1.78	0.65
1:P:360:HIS:HE1	1:P:362:LEU:HB2	1.61	0.65
1:A:800:ARG:NH1	1:A:800:ARG:HB3	2.12	0.65
1:B:800:ARG:HB3	1:B:800:ARG:NH1	2.12	0.65
1:B:917:ARG:NH2	1:B:943:GLU:OE1	2.29	0.65
1:C:114:VAL:CG1	1:C:191:TRP:HB2	2.26	0.65
1:C:237:ARG:CB	1:C:237:ARG:HH11	2.10	0.65
1:E:682:LEU:CD2	1:E:683:PRO:HD2	2.26	0.65
1:F:282:ARG:HG3	1:G:423:MET:HB2	1.79	0.65
1:G:3:ILE:HG13	1:G:4:THR:N	2.09	0.65
1:G:42:ALA:O	1:G:310:ARG:NH1	2.28	0.65
1:J:749:ILE:HD13	1:J:749:ILE:N	2.10	0.65
1:K:939:CYS:HA	1:K:956:GLN:HB3	1.77	0.65
1:L:237:ARG:CB	1:L:237:ARG:HH11	2.10	0.65
1:N:30:HIS:HB2	1:N:31:PRO:HD2	1.78	0.65
1:N:800:ARG:NH1	1:N:800:ARG:HB3	2.12	0.65
1:P:347:LYS:HB3	1:P:348:PRO:HD2	1.79	0.65
1:A:114:VAL:HG13	1:A:115:PRO:HD2	1.78	0.65
1:B:59:ARG:NH2	1:B:81:ALA:O	2.29	0.65
1:B:939:CYS:HA	1:B:956:GLN:HB3	1.78	0.65
1:C:246:MET:HG2	1:C:274:PHE:CE2	2.31	0.65
1:D:30:HIS:HB2	1:D:31:PRO:HD2	1.78	0.65
1:D:237:ARG:CB	1:D:237:ARG:HH11	2.10	0.65
1:D:246:MET:HG2	1:D:274:PHE:CE2	2.31	0.65
1:D:293:LEU:HD23	1:D:293:LEU:N	2.07	0.65
1:D:454:ILE:HG13	1:D:455:ILE:HG13	1.78	0.65
1:G:114:VAL:CG1	1:G:191:TRP:HB2	2.26	0.65
1:G:217:LYS:HG2	1:G:218:PRO:HD2	1.77	0.65
1:G:800:ARG:HB3	1:G:800:ARG:NH1	2.12	0.65
1:H:347:LYS:HB3	1:H:348:PRO:HD2	1.79	0.65
1:H:454:ILE:HG13	1:H:455:ILE:HG13	1.78	0.65
1:I:114:VAL:CG1	1:I:191:TRP:HB2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:360:HIS:HE1	1:M:362:LEU:HB2	1.61	0.65
1:M:682:LEU:CD2	1:M:683:PRO:HD2	2.26	0.65
1:O:3:ILE:HG13	1:O:4:THR:N	2.09	0.65
1:A:246:MET:HG2	1:A:274:PHE:CE2	2.31	0.65
1:A:703:PRO:O	1:A:711:ALA:HB1	1.97	0.65
1:A:917:ARG:NH2	1:A:943:GLU:OE1	2.29	0.65
1:B:30:HIS:HB2	1:B:31:PRO:HD2	1.78	0.65
1:D:114:VAL:HG13	1:D:115:PRO:HD2	1.78	0.65
1:D:232:ASN:ND2	1:D:234:ASP:OD1	2.30	0.65
1:E:114:VAL:HG13	1:E:115:PRO:HD2	1.78	0.65
1:E:114:VAL:CG1	1:E:191:TRP:HB2	2.26	0.65
1:E:232:ASN:ND2	1:E:234:ASP:OD1	2.30	0.65
1:F:30:HIS:HB2	1:F:31:PRO:HD2	1.78	0.65
1:I:336:ARG:HG2	1:I:336:ARG:NH1	2.09	0.65
1:J:120:THR:HG21	1:J:187:MET:HE3	1.78	0.65
1:J:800:ARG:HB3	1:J:800:ARG:NH1	2.12	0.65
1:K:347:LYS:HB3	1:K:348:PRO:HD2	1.79	0.65
1:K:703:PRO:O	1:K:711:ALA:HB1	1.97	0.65
1:L:703:PRO:O	1:L:711:ALA:HB1	1.97	0.65
1:O:703:PRO:O	1:O:711:ALA:HB1	1.97	0.65
1:O:749:ILE:HD13	1:O:749:ILE:N	2.10	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:A:237:ARG:CB	1:A:237:ARG:HH11	2.10	0.65
1:D:533:LEU:C	1:D:533:LEU:HD12	2.22	0.65
1:F:360:HIS:HE1	1:F:362:LEU:HB2	1.61	0.65
1:F:433:LEU:HB3	1:F:434:PRO:HD3	1.77	0.65
1:G:30:HIS:HB2	1:G:31:PRO:HD2	1.78	0.65
1:G:939:CYS:HA	1:G:956:GLN:HB3	1.77	0.65
1:H:30:HIS:HB2	1:H:31:PRO:HD2	1.78	0.65
1:H:232:ASN:ND2	1:H:234:ASP:OD1	2.30	0.65
1:I:682:LEU:CD2	1:I:683:PRO:HD2	2.26	0.65
1:I:800:ARG:NH1	1:I:800:ARG:HB3	2.12	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:L:433:LEU:HB3	1:L:434:PRO:HD3	1.77	0.65
1:M:114:VAL:CG1	1:M:191:TRP:HB2	2.26	0.65
1:N:533:LEU:C	1:N:533:LEU:HD12	2.22	0.65
1:O:114:VAL:CG1	1:O:191:TRP:HB2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:HIS:HE1	1:B:362:LEU:HB2	1.61	0.65
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.77	0.65
1:D:120:THR:HG21	1:D:187:MET:HE3	1.77	0.65
1:F:800:ARG:NH1	1:F:800:ARG:HB3	2.12	0.65
1:G:703:PRO:O	1:G:711:ALA:HB1	1.97	0.65
1:H:360:HIS:HE1	1:H:362:LEU:HB2	1.61	0.65
1:I:30:HIS:HB2	1:I:31:PRO:HD2	1.78	0.65
1:I:210:ARG:HH12	1:I:395:HIS:N	1.92	0.65
1:J:217:LYS:HE3	1:J:324:GLU:OE1	1.98	0.65
1:J:454:ILE:HG13	1:J:455:ILE:HG13	1.78	0.65
1:J:703:PRO:O	1:J:711:ALA:HB1	1.97	0.65
1:L:246:MET:HG2	1:L:274:PHE:CE2	2.31	0.65
1:M:114:VAL:HG13	1:M:115:PRO:HD2	1.78	0.65
1:N:237:ARG:CB	1:N:237:ARG:HH11	2.10	0.65
1:O:30:HIS:HB2	1:O:31:PRO:HD2	1.78	0.65
1:O:210:ARG:HH12	1:O:395:HIS:N	1.92	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:P:703:PRO:O	1:P:711:ALA:HB1	1.97	0.65
1:B:114:VAL:CG1	1:B:191:TRP:HB2	2.26	0.64
1:B:237:ARG:CB	1:B:237:ARG:HH11	2.10	0.64
1:C:24:LEU:HB2	1:C:161:TYR:HB3	1.77	0.64
1:C:753:ASN:N	1:C:753:ASN:OD1	2.30	0.64
1:D:217:LYS:HE3	1:D:324:GLU:OE1	1.98	0.64
1:D:939:CYS:HA	1:D:956:GLN:HB3	1.78	0.64
1:E:759:ASN:OD1	1:E:761:GLN:N	2.30	0.64
1:F:114:VAL:CG1	1:F:191:TRP:HB2	2.26	0.64
1:F:533:LEU:C	1:F:533:LEU:HD12	2.22	0.64
1:G:759:ASN:OD1	1:G:761:GLN:N	2.30	0.64
1:H:800:ARG:HB3	1:H:800:ARG:NH1	2.12	0.64
1:K:753:ASN:N	1:K:753:ASN:OD1	2.30	0.64
1:K:917:ARG:NH2	1:K:943:GLU:OE1	2.29	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:L:377:LEU:HD22	1:L:708:TRP:HA	1.77	0.64
1:L:533:LEU:C	1:L:533:LEU:HD12	2.22	0.64
1:L:759:ASN:OD1	1:L:761:GLN:N	2.30	0.64
1:M:759:ASN:OD1	1:M:761:GLN:N	2.30	0.64
1:N:114:VAL:CG1	1:N:191:TRP:HB2	2.26	0.64
1:P:939:CYS:HA	1:P:956:GLN:HB3	1.77	0.64
1:B:347:LYS:HB3	1:B:348:PRO:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:ARG:CB	1:F:237:ARG:HH11	2.10	0.64
1:F:753:ASN:OD1	1:F:753:ASN:N	2.30	0.64
1:J:533:LEU:C	1:J:533:LEU:HD12	2.22	0.64
1:K:114:VAL:CG1	1:K:191:TRP:HB2	2.26	0.64
1:K:120:THR:HG21	1:K:187:MET:HE3	1.78	0.64
1:K:533:LEU:C	1:K:533:LEU:HD12	2.22	0.64
1:L:120:THR:HG21	1:L:187:MET:HE3	1.77	0.64
1:M:419:GLY:HA2	1:P:282:ARG:HH11	1.63	0.64
1:M:800:ARG:HB3	1:M:800:ARG:NH1	2.12	0.64
1:O:759:ASN:OD1	1:O:761:GLN:N	2.30	0.64
1:A:759:ASN:OD1	1:A:761:GLN:N	2.30	0.64
1:C:800:ARG:NH1	1:C:800:ARG:HB3	2.12	0.64
1:D:800:ARG:HB3	1:D:800:ARG:NH1	2.12	0.64
1:F:759:ASN:OD1	1:F:761:GLN:N	2.30	0.64
1:G:533:LEU:C	1:G:533:LEU:HD12	2.22	0.64
1:I:347:LYS:HB3	1:I:348:PRO:HD2	1.79	0.64
1:I:533:LEU:HD12	1:I:533:LEU:C	2.22	0.64
1:K:800:ARG:NH1	1:K:800:ARG:HB3	2.12	0.64
1:N:433:LEU:HB3	1:N:434:PRO:HD3	1.78	0.64
1:N:1021:CME:HB3	1:N:1021:CME:CZ	2.21	0.64
1:O:800:ARG:HB3	1:O:800:ARG:NH1	2.12	0.64
1:P:533:LEU:C	1:P:533:LEU:HD12	2.22	0.64
1:P:800:ARG:HB3	1:P:800:ARG:NH1	2.12	0.64
1:A:655:MET:HE2	1:A:656:VAL:N	2.13	0.64
1:B:3:ILE:HG13	1:B:4:THR:N	2.09	0.64
1:C:533:LEU:C	1:C:533:LEU:HD12	2.22	0.64
1:C:759:ASN:OD1	1:C:761:GLN:N	2.30	0.64
1:D:210:ARG:HH12	1:D:395:HIS:N	1.92	0.64
1:F:703:PRO:O	1:F:711:ALA:HB1	1.97	0.64
1:G:237:ARG:CB	1:G:237:ARG:HH11	2.10	0.64
1:G:454:ILE:HG13	1:G:455:ILE:HG13	1.78	0.64
1:H:533:LEU:C	1:H:533:LEU:HD12	2.22	0.64
1:I:237:ARG:CB	1:I:237:ARG:HH11	2.10	0.64
1:K:217:LYS:HE3	1:K:324:GLU:OE1	1.98	0.64
1:L:800:ARG:NH1	1:L:800:ARG:HB3	2.12	0.64
1:M:237:ARG:CB	1:M:237:ARG:HH11	2.10	0.64
1:M:246:MET:HG2	1:M:274:PHE:CE2	2.31	0.64
1:N:759:ASN:OD1	1:N:761:GLN:N	2.30	0.64
1:O:454:ILE:HG13	1:O:455:ILE:HG13	1.78	0.64
1:O:533:LEU:C	1:O:533:LEU:HD12	2.22	0.64
1:B:533:LEU:C	1:B:533:LEU:HD12	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:377:LEU:CD2	1:F:708:TRP:HA	2.28	0.64
1:H:237:ARG:CB	1:H:237:ARG:HH11	2.10	0.64
1:H:939:CYS:HA	1:H:956:GLN:HB3	1.78	0.64
1:J:232:ASN:ND2	1:J:234:ASP:OD1	2.30	0.64
1:M:437:SER:HB2	5:M:2257:HOH:O	1.98	0.64
1:N:117:GLU:OE1	1:N:117:GLU:N	2.27	0.64
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:O:237:ARG:HH11	1:O:237:ARG:CB	2.10	0.64
1:O:753:ASN:OD1	1:O:753:ASN:N	2.30	0.64
1:B:217:LYS:HE3	1:B:324:GLU:OE1	1.98	0.64
1:D:655:MET:HE2	1:D:656:VAL:N	2.13	0.64
1:K:759:ASN:OD1	1:K:761:GLN:N	2.30	0.64
1:M:3:ILE:HG13	1:M:4:THR:N	2.09	0.64
1:M:217:LYS:HE3	1:M:324:GLU:OE1	1.98	0.64
1:N:655:MET:HE2	1:N:656:VAL:N	2.13	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:A:232:ASN:ND2	1:A:234:ASP:OD1	2.30	0.64
1:A:347:LYS:HB3	1:A:348:PRO:HD2	1.79	0.64
1:G:377:LEU:CD2	1:G:708:TRP:HA	2.28	0.64
1:G:655:MET:HE2	1:G:656:VAL:N	2.13	0.64
1:H:3:ILE:HG13	1:H:4:THR:N	2.09	0.64
1:I:232:ASN:ND2	1:I:234:ASP:OD1	2.30	0.64
1:I:437:SER:HB2	5:I:2258:HOH:O	1.97	0.64
1:J:655:MET:HE2	1:J:656:VAL:N	2.13	0.64
1:K:377:LEU:CD2	1:K:708:TRP:HA	2.28	0.64
1:L:117:GLU:OE1	1:L:117:GLU:N	2.27	0.64
1:M:740:LEU:HD12	1:M:741:THR:N	2.06	0.64
1:O:655:MET:HE2	1:O:656:VAL:N	2.13	0.64
1:P:427:THR:CA	1:P:436:MET:HE1	2.10	0.64
1:A:360:HIS:HE1	1:A:362:LEU:HB2	1.61	0.64
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.28	0.64
1:C:347:LYS:HB3	1:C:348:PRO:HD2	1.79	0.64
1:C:703:PRO:O	1:C:711:ALA:HB1	1.97	0.64
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.77	0.64
1:E:217:LYS:HE3	1:E:324:GLU:OE1	1.98	0.64
1:E:377:LEU:CD2	1:E:708:TRP:HA	2.28	0.64
1:E:701:VAL:HG12	1:E:702:GLN:N	2.13	0.64
1:I:377:LEU:CD2	1:I:708:TRP:HA	2.28	0.64
1:J:347:LYS:HB3	1:J:348:PRO:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:377:LEU:CD2	1:L:708:TRP:HA	2.28	0.64
1:M:377:LEU:CD2	1:M:708:TRP:HA	2.28	0.64
1:M:533:LEU:C	1:M:533:LEU:HD12	2.22	0.64
1:O:377:LEU:CD2	1:O:708:TRP:HA	2.28	0.64
1:P:237:ARG:CB	1:P:237:ARG:HH11	2.10	0.64
1:A:894:ARG:HD3	1:A:919:ASP:OD2	1.98	0.64
1:B:117:GLU:OE1	1:B:117:GLU:N	2.27	0.64
1:B:894:ARG:HD3	1:B:919:ASP:OD2	1.98	0.64
1:D:894:ARG:HD3	1:D:919:ASP:OD2	1.98	0.64
1:E:800:ARG:HB3	1:E:800:ARG:NH1	2.12	0.64
1:G:117:GLU:OE1	1:G:117:GLU:N	2.27	0.64
1:H:427:THR:CA	1:H:436:MET:HE1	2.10	0.64
1:I:753:ASN:OD1	1:I:753:ASN:N	2.30	0.64
1:J:701:VAL:HG12	1:J:702:GLN:N	2.13	0.64
1:L:655:MET:HE2	1:L:656:VAL: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:P:753:ASN:N	1:P:753:ASN:OD1	2.30	0.64
1:A:30:HIS:HB2	1:A:31:PRO:HD2	1.78	0.64
1:A:939:CYS:HA	1:A:956:GLN:HB3	1.77	0.64
1:C:217:LYS:HE3	1:C:324:GLU:OE1	1.98	0.64
1:E:703:PRO:O	1:E:711:ALA:HB1	1.97	0.64
1:G:217:LYS:HE3	1:G:324:GLU:OE1	1.98	0.64
1:H:655:MET:HE2	1:H:656:VAL:N	2.13	0.64
1:I:655:MET:HE2	1:I:656:VAL:N	2.13	0.64
1:J:894:ARG:HD3	1:J:919:ASP:OD2	1.98	0.64
1:K:655:MET:HE2	1:K:656:VAL:N	2.13	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:P:128:ASN:HA	1:P:180:GLY:O	1.98	0.64
1:P:217:LYS:HE3	1:P:324:GLU:OE1	1.98	0.64
1:P:655:MET:HE2	1:P:656:VAL:N	2.13	0.64
1:C:894:ARG:NH1	1:C:919:ASP:OD2	2.30	0.63
1:D:377:LEU:CD2	1:D:708:TRP:HA	2.28	0.63
1:E:655:MET:HE2	1:E:656:VAL:N	2.13	0.63
1:H:377:LEU:CD2	1:H:708:TRP:HA	2.28	0.63
1:H:753:ASN:N	1:H:753:ASN:OD1	2.30	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:M:703:PRO:O	1:M:711:ALA:HB1	1.97	0.63
1:P:336:ARG:HG2	1:P:336:ARG:NH1	2.09	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:VAL:HG12	1:A:702:GLN:N	2.13	0.63
1:D:43:ARG:HG2	1:D:43:ARG:NH1	1.94	0.63
1:D:701:VAL:HG12	1:D:702:GLN:N	2.13	0.63
1:F:217:LYS:HE3	1:F:324:GLU:OE1	1.98	0.63
1:F:568:TRP:HE1	1:F:604:ASN:HD22	1.47	0.63
1:G:347:LYS:HB3	1:G:348:PRO:HD2	1.79	0.63
1:H:217:LYS:HE3	1:H:324:GLU:OE1	1.98	0.63
1:J:377:LEU:CD2	1:J:708:TRP:HA	2.28	0.63
1:K:894:ARG:HD3	1:K:919:ASP:OD2	1.98	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:P:894:ARG:NH1	1:P:919:ASP:OD2	2.30	0.63
1:A:533:LEU:HD12	1:A:533:LEU:C	2.22	0.63
1:B:655:MET:HE2	1:B:656:VAL:N	2.13	0.63
1:G:894:ARG:HD3	1:G:919:ASP:OD2	1.98	0.63
1:H:128:ASN:HA	1:H:180:GLY:O	1.98	0.63
1:H:894:ARG:HD3	1:H:919:ASP:OD2	1.98	0.63
1:I:759:ASN:OD1	1:I:761:GLN:N	2.30	0.63
1:K:232:ASN:ND2	1:K:234:ASP:OD1	2.30	0.63
1:M:347:LYS:HB3	1:M:348:PRO:HD2	1.79	0.63
1:N:128:ASN:HA	1:N:180:GLY:O	1.99	0.63
1:N:568:TRP:HE1	1:N:604:ASN:HD22	1.47	0.63
1:O:347:LYS:HB3	1:O:348:PRO:HD2	1.79	0.63
1:A:128:ASN:HA	1:A:180:GLY:O	1.98	0.63
1:M:902:PRO:O	1:M:938:ARG:NH1	2.31	0.63
1:N:902:PRO:O	1:N:938:ARG:NH1	2.31	0.63
1:P:894:ARG:HD3	1:P:919:ASP:OD2	1.98	0.63
1:P:902:PRO:O	1:P:938:ARG:NH1	2.31	0.63
1:A:568:TRP:HE1	1:A:604:ASN:HD22	1.47	0.63
1:B:282:ARG:HG3	1:C:423:MET:HB2	1.80	0.63
1:C:128:ASN:HA	1:C:180:GLY:O	1.98	0.63
1:C:580:GLU:H	1:C:580:GLU:CD	2.07	0.63
1:D:902:PRO:O	1:D:938:ARG:NH1	2.32	0.63
1:F:423:MET:HB2	1:G:282:ARG:HG3	1.80	0.63
1:I:217:LYS:HE3	1:I:324:GLU:OE1	1.98	0.63
1:K:128:ASN:HA	1:K:180:GLY:O	1.98	0.63
1:M:655:MET:HE2	1:M:656:VAL:N	2.13	0.63
1:N:217:LYS:HE3	1:N:324:GLU:OE1	1.98	0.63
1:B:395:HIS:ND1	1:B:396:PRO:HD2	2.14	0.63
1:E:128:ASN:HA	1:E:180:GLY:O	1.99	0.63
1:E:533:LEU:C	1:E:533:LEU:HD12	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:894:ARG:HD3	1:E:919:ASP:OD2	1.98	0.63
1:E:902:PRO:O	1:E:938:ARG:NH1	2.32	0.63
1:F:655:MET:HE2	1:F:656:VAL:N	2.13	0.63
1:I:701:VAL:HG12	1:I:702:GLN:N	2.13	0.63
1:I:894:ARG:HD3	1:I:919:ASP:OD2	1.98	0.63
1:J:37:ARG:HH11	1:J:37:ARG:HG3	1.64	0.63
1:J:759:ASN:OD1	1:J:761:GLN:N	2.30	0.63
1:K:30:HIS:ND1	1:K:31:PRO:O	2.26	0.63
1:L:128:ASN:HA	1:L:180:GLY:O	1.98	0.63
1:M:894:ARG:NH1	1:M:919:ASP:OD2	2.30	0.63
1:B:568:TRP:HE1	1:B:604:ASN:HD22	1.47	0.63
1:C:377:LEU:CD2	1:C:708:TRP:HA	2.28	0.63
1:D:395:HIS:ND1	1:D:396:PRO:HD2	2.14	0.63
1:F:255:ARG:HG2	1:F:255:ARG:NH1	2.14	0.63
1:F:580:GLU:CD	1:F:580:GLU:H	2.07	0.63
1:G:128:ASN:HA	1:G:180:GLY:O	1.98	0.63
1:H:902:PRO:O	1:H:938:ARG:NH1	2.32	0.63
1:I:128:ASN:HA	1:I:180:GLY:O	1.98	0.63
1:I:599:ARG:HB2	1:I:600:GLN:OE1	1.99	0.63
1:J:18:ASN:HD22	1:J:21:VAL:HG23	1.64	0.63
1:J:395:HIS:ND1	1:J:396:PRO:HD2	2.14	0.63
1:K:117:GLU:OE1	1:K:117:GLU:N	2.27	0.63
1:K:395:HIS:ND1	1:K:396:PRO:HD2	2.14	0.63
1:K:599:ARG:HB2	1:K:600:GLN:OE1	1.99	0.63
1:L:945:ASN:OD1	1:L:950:GLN:NE2	2.30	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:B:128:ASN:HA	1:B:180:GLY:O	1.98	0.63
1:C:894:ARG:HD3	1:C:919:ASP:OD2	1.98	0.63
1:D:580:GLU:CD	1:D:580:GLU:H	2.07	0.63
1:E:395:HIS:ND1	1:E:396:PRO:HD2	2.14	0.63
1:E:580:GLU:H	1:E:580:GLU:CD	2.07	0.63
1:F:232:ASN:ND2	1:F:234:ASP:OD1	2.30	0.63
1:F:395:HIS:ND1	1:F:396:PRO:HD2	2.14	0.63
1:G:232:ASN:ND2	1:G:234:ASP:OD1	2.30	0.63
1:G:395:HIS:ND1	1:G:396:PRO:HD2	2.14	0.63
1:H:599:ARG:HB2	1:H:600:GLN:OE1	1.99	0.63
1:J:255:ARG:HG2	1:J:255:ARG:NH1	2.14	0.63
1:J:902:PRO:O	1:J:938:ARG:NH1	2.32	0.63
1:L:701:VAL:HG12	1:L:702:GLN:N	2.13	0.63
1:N:580:GLU:CD	1:N:580:GLU:H	2.07	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:395:HIS:ND1	1:O:396:PRO:HD2	2.14	0.63
1:O:847:LYS:HG3	1:O:848:THR:N	2.14	0.63
1:A:395:HIS:ND1	1:A:396:PRO:HD2	2.14	0.63
1:A:902:PRO:O	1:A:938:ARG:NH1	2.31	0.63
1:B:599:ARG:HB2	1:B:600:GLN:OE1	1.99	0.63
1:C:117:GLU:OE1	1:C:117:GLU:N	2.27	0.63
1:C:255:ARG:HG2	1:C:255:ARG:NH1	2.14	0.63
1:F:847:LYS:HG3	1:F:848:THR:N	2.14	0.63
1:J:117:GLU:OE1	1:J:117:GLU:N	2.27	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:M:599:ARG:HB2	1:M:600:GLN:OE1	1.99	0.63
1:M:847:LYS:HG3	1:M:848:THR:N	2.14	0.63
1:A:377:LEU:CD2	1:A:708:TRP:HA	2.28	0.62
1:C:655:MET:HE2	1:C:656:VAL:N	2.13	0.62
1:D:753:ASN:OD1	1:D:753:ASN:N	2.30	0.62
1:D:759:ASN:OD1	1:D:761:GLN:N	2.30	0.62
1:E:894:ARG:NH1	1:E:919:ASP:OD2	2.30	0.62
1:F:37:ARG:HG3	1:F:37:ARG:HH11	1.64	0.62
1:F:347:LYS:HB3	1:F:348:PRO:HD2	1.79	0.62
1:G:599:ARG:HB2	1:G:600:GLN:OE1	1.99	0.62
1:J:894:ARG:NH1	1:J:919:ASP:OD2	2.30	0.62
1:K:580:GLU:H	1:K:580:GLU:CD	2.07	0.62
1:L:37:ARG:HH11	1:L:37:ARG:HG3	1.64	0.62
1:L:753:ASN:OD1	1:L:753:ASN:N	2.30	0.62
1:L:894:ARG:HD3	1:L:919:ASP:OD2	1.98	0.62
1:M:128:ASN:HA	1:M:180:GLY:O	1.98	0.62
1:M:395:HIS:ND1	1:M:396:PRO:HD2	2.14	0.62
1:M:894:ARG:HD3	1:M:919:ASP:OD2	1.98	0.62
1:N:347:LYS:HB3	1:N:348:PRO:HD2	1.79	0.62
1:N:847:LYS:HG3	1:N:848:THR:N	2.14	0.62
1:O:190:ARG:HD3	1:O:191:TRP:CZ2	2.34	0.62
1:P:701:VAL:HG12	1:P:702:GLN:N	2.13	0.62
1:P:759:ASN:OD1	1:P:761:GLN:N	2.30	0.62
1:A:217:LYS:HE3	1:A:324:GLU:OE1	1.98	0.62
1:B:255:ARG:HG2	1:B:255:ARG:NH1	2.14	0.62
1:C:3:ILE:HG13	1:C:4:THR:N	2.09	0.62
1:C:37:ARG:HH11	1:C:37:ARG:HG3	1.64	0.62
1:C:847:LYS:HG3	1:C:848:THR:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:894:ARG:NH1	1:L:919:ASP:OD2	2.30	0.62
1:M:37:ARG:HH11	1:M:37:ARG:HG3	1.64	0.62
1:M:580:GLU:H	1:M:580:GLU:CD	2.07	0.62
1:O:894:ARG:HD3	1:O:919:ASP:OD2	1.98	0.62
1:A:117:GLU:OE1	1:A:117:GLU:N	2.27	0.62
1:B:190:ARG:HD3	1:B:191:TRP:CZ2	2.35	0.62
1:B:759:ASN:OD1	1:B:761:GLN:N	2.30	0.62
1:C:568:TRP:HE1	1:C:604:ASN:HD22	1.47	0.62
1:C:1021:CME:CZ	1:C:1021:CME:HB3	2.21	0.62
1:D:128:ASN:HA	1:D:180:GLY:O	1.99	0.62
1:D:347:LYS:HB3	1:D:348:PRO:HD2	1.79	0.62
1:E:347:LYS:HB3	1:E:348:PRO:HD2	1.79	0.62
1:F:902:PRO:O	1:F:938:ARG:NH1	2.31	0.62
1:G:37:ARG:HH11	1:G:37:ARG:HG3	1.64	0.62
1:G:190:ARG:HD3	1:G:191:TRP:CZ2	2.35	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: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:190:ARG:HD3	1:M:191:TRP:CZ2	2.34	0.62
1:M:742:THR:HG22	1:M:743:SER:N	2.14	0.62
1:N:395:HIS:ND1	1:N:396:PRO:HD2	2.14	0.62
1:A:3:ILE:HG13	1:A:4:THR:N	2.09	0.62
1:B:701:VAL:HG12	1:B:702:GLN:N	2.13	0.62
1:B:847:LYS:HG3	1:B:848:THR:N	2.14	0.62
1:C:902:PRO:O	1:C:938:ARG:NH1	2.31	0.62
1:D:46:ARG:HG3	1:D:46:ARG:NH1	2.02	0.62
1:D:190:ARG:HD3	1:D:191:TRP:CZ2	2.35	0.62
1:D:742:THR:HG22	1:D:743:SER:N	2.14	0.62
1:D:745:MET:HE2	1:D:745:MET:CA	2.30	0.62
1:F:599:ARG:HB2	1:F:600:GLN:OE1	1.99	0.62
1:F:742:THR:HG22	1:F:743:SER:N	2.14	0.62
1:H:336:ARG:HG2	1:H:336:ARG:NH1	2.09	0.62
1:H:395:HIS:ND1	1:H:396:PRO:HD2	2.14	0.62
1:I:255:ARG:HG2	1:I:255:ARG:NH1	2.14	0.62
1:J:742:THR:HG22	1:J:743:SER:N	2.14	0.62
1:L:902:PRO:O	1:L:938:ARG:NH1	2.31	0.62
1:N:287:ASP:OD2	1:O:425:ARG:NH2	2.31	0.62
1:O:37:ARG:HH11	1:O:37:ARG:HG3	1.64	0.62
1:P:395:HIS:ND1	1:P:396:PRO:HD2	2.14	0.62
1:P:599:ARG:HB2	1:P:600:GLN:OE1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:894:ARG:NH1	1:B:919:ASP:OD2	2.30	0.62
1:E:190:ARG:HD3	1:E:191:TRP:CZ2	2.35	0.62
1:F:894:ARG:HD3	1:F:919:ASP:OD2	1.98	0.62
1:F:894:ARG:NH1	1:F:919:ASP:OD2	2.30	0.62
1:H:127:PHE:HE2	1:H:184:LEU:HG	1.65	0.62
1:H:701:VAL:HG12	1:H:702:GLN:N	2.13	0.62
1:I:18:ASN:HD22	1:I:21:VAL:HG23	1.64	0.62
1:J:847:LYS:HG3	1:J:848:THR:N	2.14	0.62
1:K:745:MET:HE2	1:K:745:MET:CA	2.30	0.62
1:L:360:HIS:HE1	1:L:362:LEU:HB2	1.61	0.62
1:L:568:TRP:HE1	1:L:604:ASN:HD22	1.47	0.62
1:N:3:ILE:HG13	1:N:4:THR:N	2.09	0.62
1:P:37:ARG:HH11	1:P:37:ARG:HG3	1.64	0.62
1:A:599:ARG:HB2	1:A:600:GLN:OE1	1.99	0.62
1:D:568:TRP:HE1	1:D:604:ASN:HD22	1.47	0.62
1:E:742:THR:HG22	1:E:743:SER:N	2.14	0.62
1:F:127:PHE:HE2	1:F:184:LEU:HG	1.65	0.62
1:H:568:TRP:HE1	1:H:604:ASN:HD22	1.47	0.62
1:H:759:ASN:OD1	1:H:761:GLN:N	2.30	0.62
1:I:190:ARG:HD3	1:I:191:TRP:CZ2	2.35	0.62
1:I:568:TRP:HE1	1:I:604:ASN:HD22	1.47	0.62
1:I:742:THR:HG22	1:I:743:SER:N	2.14	0.62
1:J:190:ARG:HD3	1:J:191:TRP:CZ2	2.35	0.62
1:J:599:ARG:HB2	1:J:600:GLN:OE1	1.99	0.62
1:J:753:ASN:N	1:J:753:ASN:OD1	2.30	0.62
1:M:919:ASP:O	1:M:920:LEU:HD23	2.00	0.62
1:N:701:VAL:HG12	1:N:702:GLN:N	2.13	0.62
1:P:580:GLU:H	1:P:580:GLU:CD	2.07	0.62
1:A:742:THR:HG22	1:A:743:SER:N	2.14	0.62
1:B:580:GLU:H	1:B:580:GLU:CD	2.07	0.62
1:B:902:PRO:O	1:B:938:ARG:NH1	2.31	0.62
1:C:742:THR:HG22	1:C:743:SER:N	2.14	0.62
1:E:847:LYS:HG3	1:E:848:THR:N	2.14	0.62
1:F:701:VAL:HG12	1:F:702:GLN:N	2.13	0.62
1:I:945:ASN:OD1	1:I:950:GLN:NE2	2.30	0.62
1:J:580:GLU:H	1:J:580:GLU:CD	2.07	0.62
1:L:395:HIS:ND1	1:L:396:PRO:HD2	2.14	0.62
1:N:190:ARG:HD3	1:N:191:TRP:CZ2	2.35	0.62
1:N:599:ARG:HB2	1:N:600:GLN:OE1	1.99	0.62
1:N:742:THR:HG22	1:N:743:SER:N	2.14	0.62
1:P:190:ARG:HD3	1:P:191:TRP:CZ2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:919:ASP:O	1:A:920:LEU:HD23	2.00	0.62
1:C:190:ARG:HD3	1:C:191:TRP:CZ2	2.35	0.62
1:C:599:ARG:HB2	1:C:600:GLN:OE1	1.99	0.62
1:C:701:VAL:HG12	1:C:702:GLN:N	2.13	0.62
1:D:3:ILE:HG13	1:D:4:THR:N	2.09	0.62
1:E:599:ARG:HB2	1:E:600:GLN:OE1	1.99	0.62
1:E:835:LEU:C	1:E:836:ILE:HD13	2.25	0.62
1:F:128:ASN:HA	1:F:180:GLY:O	1.98	0.62
1:H:37:ARG:HH11	1:H:37:ARG:HG3	1.64	0.62
1:K:190:ARG:HD3	1:K:191:TRP:CZ2	2.35	0.62
1:K:255:ARG:HG2	1:K:255:ARG:NH1	2.14	0.62
1:K:835:LEU:C	1:K:836:ILE:HD13	2.25	0.62
1:L:190:ARG:HD3	1:L:191:TRP:CZ2	2.34	0.62
1:L:580:GLU:CD	1:L:580:GLU:H	2.07	0.62
1:M:127:PHE:HE2	1:M:184:LEU:HG	1.65	0.62
1:P:568:TRP:HE1	1:P:604:ASN:HD22	1.47	0.62
1:A:419:GLY:CA	1:D:282:ARG:HH11	2.11	0.62
1:C:127:PHE:HE2	1:C:184:LEU:HG	1.65	0.62
1:C:745:MET:HE2	1:C:745:MET:CA	2.30	0.62
1:C:835:LEU:C	1:C:836:ILE:HD13	2.25	0.62
1:D:599:ARG:HB2	1:D:600:GLN:OE1	1.99	0.62
1:E:117:GLU:OE1	1:E:117:GLU:N	2.27	0.62
1:E:745:MET:HE2	1:E:745:MET:CA	2.30	0.62
1:G:742:THR:HG22	1:G:743:SER:N	2.14	0.62
1:G:902:PRO:O	1:G:938:ARG:NH1	2.31	0.62
1:H:194:GLY:O	1:H:198:GLU:HG3	2.00	0.62
1:H:847:LYS:HG3	1:H:848:THR:N	2.14	0.62
1:J:835:LEU:C	1:J:836:ILE:HD13	2.25	0.62
1:K:919:ASP:O	1:K:920:LEU:HD23	2.00	0.62
1:M:194:GLY:O	1:M:198:GLU:HG3	2.00	0.62
1:P:578:TYR:HA	1:P:583:ASN:O	2.00	0.62
1:A:127:PHE:HE2	1:A:184:LEU:HG	1.65	0.62
1:A:847:LYS:HG3	1:A:848:THR:N	2.14	0.62
1:D:835:LEU:C	1:D:836:ILE:HD13	2.25	0.62
1:E:578:TYR:HA	1:E:583:ASN:O	2.00	0.62
1:F:3:ILE:HG13	1:F:4:THR:N	2.09	0.62
1:F:919:ASP:O	1:F:920:LEU:HD23	2.00	0.62
1:G:255:ARG:HG2	1:G:255:ARG:NH1	2.14	0.62
1:G:580:GLU:H	1:G:580:GLU:CD	2.07	0.62
1:G:701:VAL:HG12	1:G:702:GLN:N	2.13	0.62
1:G:847:LYS:HG3	1:G:848:THR:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:580:GLU:H	1:H:580:GLU:CD	2.07	0.62
1:H:1020:TRP:HD1	1:H:1021:CME:N	1.98	0.62
1:I:580:GLU:CD	1:I:580:GLU:H	2.07	0.62
1:I:902:PRO:O	1:I:938:ARG:NH1	2.32	0.62
1:J:360:HIS:HE1	1:J:362:LEU:HB2	1.61	0.62
1:N:753:ASN:OD1	1:N:753:ASN:N	2.30	0.62
1:O:4:THR:HA	1:O:9:VAL:HG11	1.82	0.62
1:O:568:TRP:HE1	1:O:604:ASN:HD22	1.47	0.62
1:O:580:GLU:CD	1:O:580:GLU:H	2.07	0.62
1:P:178:ARG:NH1	1:P:181:GLU:O	2.33	0.62
1:A:18:ASN:HD22	1:A:21:VAL:HG23	1.64	0.61
1:A:580:GLU:CD	1:A:580:GLU:H	2.07	0.61
1:B:835:LEU:C	1:B:836:ILE:HD13	2.25	0.61
1:E:127:PHE:HE2	1:E:184:LEU:HG	1.65	0.61
1:F:18:ASN:HD22	1:F:21:VAL:HG23	1.64	0.61
1:G:4:THR:HA	1:G:9:VAL:HG11	1.82	0.61
1:G:568:TRP:HE1	1:G:604:ASN:HD22	1.47	0.61
1:L:745:MET:HE2	1:L:745:MET:CA	2.30	0.61
1:M:745:MET:HE2	1:M:745:MET:CA	2.30	0.61
1:N:18:ASN:HD22	1:N:21:VAL:HG23	1.64	0.61
1:O:599:ARG:HB2	1:O:600:GLN:OE1	1.99	0.61
1:P:4:THR:HA	1:P:9:VAL:HG11	1.82	0.61
1:P:742:THR:HG22	1:P:743:SER:N	2.14	0.61
1:B:194:GLY:O	1:B:198:GLU:HG3	2.00	0.61
1:B:742:THR:HG22	1:B:743:SER:N	2.14	0.61
1:C:578:TYR:HA	1:C:583:ASN:O	2.00	0.61
1:D:127:PHE:HE2	1:D:184:LEU:HG	1.65	0.61
1:D:323:ILE:HD12	1:D:323:ILE:N	2.16	0.61
1:D:578:TYR:HA	1:D:583:ASN:O	2.00	0.61
1:D:945:ASN:OD1	1:D:950:GLN:NE2	2.30	0.61
1:F:190:ARG:HD3	1:F:191:TRP:CZ2	2.35	0.61
1:I:194:GLY:O	1:I:198:GLU:HG3	2.00	0.61
1:I:578:TYR:HA	1:I:583:ASN:O	2.00	0.61
1:K:651:LEU:HD13	1:K:669:PRO:HA	1.82	0.61
1:A:194:GLY:O	1:A:198:GLU:HG3	2.00	0.61
1:D:18:ASN:HD22	1:D:21:VAL:HG23	1.64	0.61
1:G:127:PHE:HE2	1:G:184:LEU:HG	1.65	0.61
1:G:1020:TRP:HD1	1:G:1021:CME:N	1.98	0.61
1:H:190:ARG:HD3	1:H:191:TRP:CZ2	2.35	0.61
1:H:919:ASP:O	1:H:920:LEU:HD23	2.00	0.61
1:I:745:MET:HE2	1:I:745:MET:CA	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1020:TRP:HD1	1:I:1021:CME:N	1.99	0.61
1:J:127:PHE:HE2	1:J:184:LEU:HG	1.65	0.61
1:J:568:TRP:HE1	1:J:604:ASN:HD22	1.47	0.61
1:K:786:ARG:HH11	1:K:990:HIS:CE1	2.18	0.61
1:L:30:HIS:ND1	1:L:31:PRO:O	2.26	0.61
1:M:786:ARG:HH11	1:M:990:HIS:CE1	2.18	0.61
1:M:1020:TRP:HD1	1:M:1021:CME:N	1.99	0.61
1:N:578:TYR:HA	1:N:583:ASN:O	2.00	0.61
1:N:745:MET:HE2	1:N:745:MET:CA	2.30	0.61
1:O:701:VAL:HG12	1:O:702:GLN:N	2.13	0.61
1:O:745:MET:HE2	1:O:745:MET:CA	2.30	0.61
1:A:689:GLU:HA	1:A:689:GLU:OE2	2.01	0.61
1:B:37:ARG:HH11	1:B:37:ARG:HG3	1.64	0.61
1:B:1021:CME:CZ	1:B:1021:CME:HB3	2.21	0.61
1:D:651:LEU:HD13	1:D:669:PRO:HA	1.82	0.61
1:D:689:GLU:HA	1:D:689:GLU:OE2	2.01	0.61
1:D:919:ASP:O	1:D:920:LEU:HD23	2.00	0.61
1:E:224:ASP:OD2	1:E:225:PHE:N	2.34	0.61
1:E:323:ILE:HD12	1:E:323:ILE:N	2.16	0.61
1:E:1020:TRP:HD1	1:E:1021:CME:N	1.99	0.61
1:G:782:ASP:HA	1:G:884:LEU:HD23	1.83	0.61
1:I:127:PHE:HE2	1:I:184:LEU:HG	1.65	0.61
1:J:651:LEU:HD13	1:J:669:PRO:HA	1.83	0.61
1:K:847:LYS:HG3	1:K:848:THR:N	2.14	0.61
1:O:127:PHE:HE2	1:O:184:LEU:HG	1.65	0.61
1:O:742:THR:HG22	1:O:743:SER:N	2.14	0.61
1:O:782:ASP:HA	1:O:884:LEU:HD23	1.83	0.61
1:O:945:ASN:OD1	1:O:950:GLN:NE2	2.30	0.61
1:A:37:ARG:HG3	1:A:37:ARG:HH11	1.64	0.61
1:A:224:ASP:OD2	1:A:225:PHE:N	2.34	0.61
1:A:255:ARG:HG2	1:A:255:ARG:NH1	2.14	0.61
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.65	0.61
1:B:232:ASN:ND2	1:B:234:ASP:OD1	2.30	0.61
1:B:782:ASP:HA	1:B:884:LEU:HD23	1.83	0.61
1:C:18:ASN:HD22	1:C:21:VAL:HG23	1.64	0.61
1:C:919:ASP:O	1:C:920:LEU:HD23	2.00	0.61
1:E:568:TRP:HE1	1:E:604:ASN:HD22	1.47	0.61
1:F:224:ASP:OD2	1:F:225:PHE:N	2.34	0.61
1:G:578:TYR:HA	1:G:583:ASN:O	2.00	0.61
1:H:4:THR:HA	1:H:9:VAL:HG11	1.82	0.61
1:K:568:TRP:HE1	1:K:604:ASN:HD22	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:919:ASP:O	1:N:920:LEU:HD23	2.00	0.61
1:O:360:HIS:CE1	1:O:361:PRO:HD2	2.36	0.61
1:O:437:SER:HB2	5:O:2257:HOH:O	2.01	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:A:835:LEU:C	1:A:836:ILE:HD13	2.25	0.61
1:A:1021:CME:CZ	1:A:1021:CME:HB3	2.21	0.61
1:B:224:ASP:OD2	1:B:225:PHE:N	2.34	0.61
1:B:689:GLU:HA	1:B:689:GLU:OE2	2.01	0.61
1:B:1020:TRP:HD1	1:B:1021:CME:N	1.99	0.61
1:C:360:HIS:CE1	1:C:361:PRO:HD2	2.36	0.61
1:C:395:HIS:ND1	1:C:396:PRO:HD2	2.14	0.61
1:C:651:LEU:HD13	1:C:669:PRO:HA	1.82	0.61
1:D:847:LYS:HG3	1:D:848:THR:N	2.14	0.61
1:F:194:GLY:O	1:F:198:GLU:HG3	2.00	0.61
1:F:689:GLU:HA	1:F:689:GLU:OE2	2.01	0.61
1:H:30:HIS:ND1	1:H:31:PRO:O	2.27	0.61
1:H:323:ILE:HD12	1:H:323:ILE:N	2.16	0.61
1:H:742:THR:HG22	1:H:743:SER:N	2.14	0.61
1:I:847:LYS:HG3	1:I:848:THR:N	2.14	0.61
1:I:919:ASP:O	1:I:920:LEU:HD23	2.00	0.61
1:J:919:ASP:O	1:J:920:LEU:HD23	2.00	0.61
1:L:323:ILE:N	1:L:323:ILE:HD12	2.16	0.61
1:L:578:TYR:HA	1:L:583:ASN:O	2.00	0.61
1:M:323:ILE:HD12	1:M:323:ILE:N	2.16	0.61
1:M:568:TRP:HE1	1:M:604:ASN:HD22	1.47	0.61
1:N:37:ARG:HG3	1:N:37:ARG:HH11	1.64	0.61
1:P:323:ILE:HD12	1:P:323:ILE:N	2.16	0.61
1:A:190:ARG:HD3	1:A:191:TRP:CZ2	2.35	0.61
1:B:4:THR:HA	1:B:9:VAL:HG11	1.82	0.61
1:B:786:ARG:HH11	1:B:990:HIS:CE1	2.18	0.61
1:D:37:ARG:HH11	1:D:37:ARG:HG3	1.64	0.61
1:E:782:ASP:HA	1:E:884:LEU:HD23	1.83	0.61
1:E:786:ARG:HH11	1:E:990:HIS:CE1	2.18	0.61
1:G:689:GLU:HA	1:G:689:GLU:OE2	2.01	0.61
1:G:919:ASP:O	1:G:920:LEU:HD23	2.00	0.61
1:G:1021:CME:HB3	1:G:1021:CME:CZ	2.21	0.61
1:K:4:THR:HA	1:K:9:VAL:HG11	1.82	0.61
1:K:578:TYR:HA	1:K:583:ASN:O	2.00	0.61
1:L:847:LYS:HG3	1:L:848:THR:N	2.14	0.61
1:N:224:ASP:OD2	1:N:225:PHE:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:323:ILE:N	1:N:323:ILE:HD12	2.16	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:B:919:ASP:O	1:B:920:LEU:HD23	2.00	0.61
1:C:224:ASP:OD2	1:C:225:PHE:N	2.34	0.61
1:D:786:ARG:HH11	1:D:990:HIS:CE1	2.18	0.61
1:E:4:THR:HA	1:E:9:VAL:HG11	1.82	0.61
1:E:194:GLY:O	1:E:198:GLU:HG3	2.00	0.61
1:H:662:PRO:O	1:H:663:LEU:HD23	2.01	0.61
1:H:689:GLU:HA	1:H:689:GLU:OE2	2.01	0.61
1:H:835:LEU:C	1:H:836:ILE:HD13	2.25	0.61
1:I:4:THR:HA	1:I:9:VAL:HG11	1.82	0.61
1:I:37:ARG:HG3	1:I:37:ARG:HH11	1.64	0.61
1:I:323:ILE:N	1:I:323:ILE:HD12	2.16	0.61
1:I:689:GLU:HA	1:I:689:GLU:OE2	2.01	0.61
1:J:1020:TRP:HD1	1:J:1021:CME:N	1.99	0.61
1:L:224:ASP:OD2	1:L:225:PHE:N	2.34	0.61
1:L:599:ARG:HB2	1:L:600:GLN:OE1	1.99	0.61
1:M:4:THR:HA	1:M:9:VAL:HG11	1.82	0.61
1:P:835:LEU:C	1:P:836:ILE:HD13	2.25	0.61
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.83	0.61
1:A:894:ARG:NH1	1:A:919:ASP:OD2	2.30	0.61
1:B:945:ASN:OD1	1:B:950:GLN:NE2	2.30	0.61
1:C:194:GLY:O	1:C:198:GLU:HG3	2.00	0.61
1:C:689:GLU:OE2	1:C:689:GLU:HA	2.01	0.61
1:D:224:ASP:OD2	1:D:225:PHE:N	2.34	0.61
1:D:287:ASP:OD1	1:D:287:ASP:N	2.29	0.61
1:E:37:ARG:HH11	1:E:37:ARG:HG3	1.64	0.61
1:E:651:LEU:HD13	1:E:669:PRO:HA	1.82	0.61
1:F:360:HIS:CE1	1:F:361:PRO:HD2	2.36	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:K:194:GLY:O	1:K:198:GLU:HG3	2.00	0.61
1:K:323:ILE:N	1:K:323:ILE:HD12	2.16	0.61
1:M:117:GLU:OE1	1:M:117:GLU:N	2.27	0.61
1:M:651:LEU:HD13	1:M:669:PRO:HA	1.82	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:O:1020:TRP:HD1	1:O:1021:CME:N	1.98	0.61
1:P:18:ASN:HD22	1:P:21:VAL:HG23	1.64	0.61
1:P:786:ARG:HH11	1:P:990:HIS:CE1	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:LEU:HD13	1:A:669:PRO:HA	1.83	0.61
1:C:1020:TRP:HD1	1:C:1021:CME:N	1.99	0.61
1:F:287:ASP:OD2	1:G:425:ARG:NH2	2.34	0.61
1:F:323:ILE:N	1:F:323:ILE:HD12	2.16	0.61
1:F:786:ARG:HH11	1:F:990:HIS:CE1	2.18	0.61
1:G:224:ASP:OD2	1:G:225:PHE:N	2.34	0.61
1:H:360:HIS:CE1	1:H:361:PRO:HD2	2.36	0.61
1:H:894:ARG:NH1	1:H:919:ASP:OD2	2.30	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
1:M:782:ASP:HA	1:M:884:LEU:HD23	1.83	0.61
1:N:125:LEU:HG	1:N:126:THR:N	2.16	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:P:54:LEU:HD23	1:P:54:LEU:N	2.15	0.61
1:P:127:PHE:HE2	1:P:184:LEU:HG	1.65	0.61
1:P:662:PRO:O	1:P:663:LEU:HD23	2.01	0.61
1:P:919:ASP:O	1:P:920:LEU:HD23	2.00	0.61
1:A:782:ASP:HA	1:A:884:LEU:HD23	1.83	0.60
1:A:786:ARG:HH11	1:A:990:HIS:CE1	2.18	0.60
1:A:1020:TRP:HD1	1:A:1021:CME:N	1.99	0.60
1:E:360:HIS:CE1	1:E:361:PRO:HD2	2.36	0.60
1:E:919:ASP:O	1:E:920:LEU:HD23	2.00	0.60
1:F:745:MET:HE2	1:F:745:MET:CA	2.30	0.60
1:G:54:LEU:HD23	1:G:54:LEU:N	2.15	0.60
1:G:651:LEU:HD13	1:G:669:PRO:HA	1.83	0.60
1:G:786:ARG:HH11	1:G:990:HIS:CE1	2.18	0.60
1:G:835:LEU:C	1:G:836:ILE:HD13	2.25	0.60
1:H:782:ASP:HA	1:H:884:LEU:HD23	1.83	0.60
1:H:786:ARG:HH11	1:H:990:HIS:CE1	2.18	0.60
1:H:1021:CME:CZ	1:H:1021:CME:HB3	2.21	0.60
1:I:662:PRO:O	1:I:663:LEU:HD23	2.01	0.60
1:I:835:LEU:C	1:I:836:ILE:HD13	2.25	0.60
1:J:689:GLU:HA	1:J:689:GLU:OE2	2.01	0.60
1:J:945:ASN:OD1	1:J:950:GLN:NE2	2.30	0.60
1:L:18:ASN:HD22	1:L:21:VAL:HG23	1.64	0.60
1:L:178:ARG:NH1	1:L:181:GLU:O	2.33	0.60
1:L:919:ASP:O	1:L:920:LEU:HD23	2.00	0.60
1:O:224:ASP:OD2	1:O:225:PHE:N	2.34	0.60
1:O:786:ARG:HH11	1:O:990:HIS:CE1	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1021:CME:HB3	1:O:1021:CME:CZ	2.21	0.60
1:A:745:MET:HE2	1:A:745:MET:CA	2.30	0.60
1:C:4:THR:HA	1:C:9:VAL:HG11	1.82	0.60
1:C:323:ILE:N	1:C:323:ILE:HD12	2.16	0.60
1:D:782:ASP:HA	1:D:884:LEU:HD23	1.83	0.60
1:E:3:ILE:HG13	1:E:4:THR:N	2.09	0.60
1:E:662:PRO:O	1:E:663:LEU:HD23	2.01	0.60
1:F:782:ASP:HA	1:F:884:LEU:HD23	1.83	0.60
1:F:1020:TRP:HD1	1:F:1021:CME:N	1.99	0.60
1:J:224:ASP:OD2	1:J:225:PHE:N	2.34	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:K:662:PRO:O	1:K:663:LEU:HD23	2.01	0.60
1:L:194:GLY:O	1:L:198:GLU:HG3	2.00	0.60
1:N:127:PHE:HE2	1:N:184:LEU:HG	1.65	0.60
1:N:287:ASP:CG	1:O:425:ARG:HH22	2.09	0.60
1:N:782:ASP:HA	1:N:884:LEU:HD23	1.83	0.60
1:N:894:ARG:NH1	1:N:919:ASP:OD2	2.30	0.60
1:O:651:LEU:HD13	1:O:669:PRO:HA	1.83	0.60
1:P:249:GLU:HG2	1:P:251:ARG:HH12	1.67	0.60
1:P:360:HIS:CE1	1:P:361:PRO:HD2	2.36	0.60
1:A:178:ARG:NH1	1:A:181:GLU:O	2.33	0.60
1:A:323:ILE:N	1:A:323:ILE:HD12	2.16	0.60
1:A:662:PRO:O	1:A:663:LEU:HD23	2.01	0.60
1:C:786:ARG:HH11	1:C:990:HIS:CE1	2.18	0.60
1:E:7:LEU:N	1:E:71:GLU:OE2	2.35	0.60
1:E:689:GLU:HA	1:E:689:GLU:OE2	2.01	0.60
1:F:578:TYR:HA	1:F:583:ASN:O	2.00	0.60
1:G:894:ARG:NH1	1:G:919:ASP:OD2	2.30	0.60
1:J:323:ILE:HD12	1:J:323:ILE:N	2.16	0.60
1:K:689:GLU:OE2	1:K:689:GLU:HA	2.01	0.60
1:L:127:PHE:HE2	1:L:184:LEU:HG	1.65	0.60
1:L:782:ASP:HA	1:L:884:LEU:HD23	1.83	0.60
1:L:1021:CME:HB3	1:L:1021:CME:HZ3	1.84	0.60
1:M:835:LEU:C	1:M:836:ILE:HD13	2.25	0.60
1:N:651:LEU:HD13	1:N:669:PRO:HA	1.83	0.60
1:O:835:LEU:C	1:O:836:ILE:HD13	2.25	0.60
1:P:782:ASP:HA	1:P:884:LEU:HD23	1.83	0.60
1:A:4:THR:HA	1:A:9:VAL:HG11	1.82	0.60
1:A:945:ASN:OD1	1:A:950:GLN:NE2	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:651:LEU:HD13	1:F:669:PRO:HA	1.82	0.60
1:G:125:LEU:HG	1:G:126:THR:N	2.16	0.60
1:G:1021:CME:HB3	1:G:1021:CME:HZ3	1.84	0.60
1:H:224:ASP:OD2	1:H:225:PHE:N	2.34	0.60
1:H:249:GLU:HG2	1:H:251:ARG:HH12	1.67	0.60
1:H:578:TYR:HA	1:H:583:ASN:O	2.00	0.60
1:I:786:ARG:HH11	1:I:990:HIS:CE1	2.18	0.60
1:J:130:ASP:OD1	1:J:132:SER:N	2.29	0.60
1:K:3:ILE:HG13	1:K:4:THR:N	2.09	0.60
1:K:1011:ALA:HB3	1:K:1014:TYR:CZ	2.37	0.60
1:M:1021:CME:HB3	1:M:1021:CME:HZ3	1.84	0.60
1:N:662:PRO:O	1:N:663:LEU:HD23	2.01	0.60
1:P:194:GLY:O	1:P:198:GLU:HG3	2.00	0.60
1:A:578:TYR:HA	1:A:583:ASN:O	2.00	0.60
1:B:18:ASN:HD22	1:B:21:VAL:HG23	1.64	0.60
1:B:745:MET:HE2	1:B:745:MET:CA	2.30	0.60
1:B:1011:ALA:HB3	1:B:1014:TYR:CZ	2.37	0.60
1:B:1021:CME:HB3	1:B:1021:CME:HZ3	1.84	0.60
1:C:782:ASP:HA	1:C:884:LEU:HD23	1.83	0.60
1:D:255:ARG:HG2	1:D:255:ARG:NH1	2.14	0.60
1:E:360:HIS:HE1	1:E:362:LEU:HB2	1.61	0.60
1:E:1021:CME:HB3	1:E:1021:CME:HZ3	1.84	0.60
1:I:249:GLU:HG2	1:I:251:ARG:HH12	1.67	0.60
1:I:360:HIS:CE1	1:I:361:PRO:HD2	2.36	0.60
1:J:4:THR:HA	1:J:9:VAL:HG11	1.82	0.60
1:J:578:TYR:HA	1:J:583:ASN:O	2.00	0.60
1:J:1011:ALA:HB3	1:J:1014:TYR:CZ	2.37	0.60
1:K:125:LEU:HG	1:K:126:THR:N	2.16	0.60
1:K:224:ASP:OD2	1:K:225:PHE:N	2.34	0.60
1:L:7:LEU:N	1:L:71:GLU:OE2	2.35	0.60
1:L:14:ARG:HA	1:L:16:TRP:CZ3	2.37	0.60
1:M:224:ASP:OD2	1:M:225:PHE:N	2.34	0.60
1:O:125:LEU:HG	1:O:126:THR:N	2.16	0.60
1:P:7:LEU:N	1:P:71:GLU:OE2	2.35	0.60
1:P:224:ASP:OD2	1:P:225:PHE:N	2.34	0.60
1:B:873:ALA:O	1:B:876:THR:HG22	2.02	0.60
1:C:14:ARG:HA	1:C:16:TRP:CZ3	2.37	0.60
1:C:360:HIS:HE1	1:C:362:LEU:HB2	1.61	0.60
1:C:1021:CME:HB3	1:C:1021:CME:HZ3	1.84	0.60
1:E:460:ASN:ND2	1:E:461:GLU:HG3	2.17	0.60
1:H:1021:CME:HB3	1:H:1021:CME:HZ3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:651:LEU:HD13	1:I:669:PRO:HA	1.82	0.60
1:I:1021:CME:HB3	1:I:1021:CME:HZ3	1.84	0.60
1:J:360:HIS:CE1	1:J:361:PRO:HD2	2.36	0.60
1:L:651:LEU:HD13	1:L:669:PRO:HA	1.83	0.60
1:L:1020:TRP:HD1	1:L:1021:CME:N	1.99	0.60
1:M:125:LEU:HG	1:M:126:THR:N	2.16	0.60
1:N:689:GLU:HA	1:N:689:GLU:OE2	2.01	0.60
1:O:662:PRO:O	1:O:663:LEU:HD23	2.01	0.60
1:P:1011:ALA:HB3	1:P:1014:TYR:CZ	2.37	0.60
1:A:360:HIS:CE1	1:A:361:PRO:HD2	2.36	0.60
1:D:1020:TRP:HD1	1:D:1021:CME:N	1.99	0.60
1:F:4:THR:HA	1:F:9:VAL:HG11	1.82	0.60
1:F:7:LEU:N	1:F:71:GLU:OE2	2.35	0.60
1:G:7:LEU:N	1:G:71:GLU:OE2	2.35	0.60
1:G:360:HIS:CE1	1:G:361:PRO:HD2	2.36	0.60
1:H:7:LEU:N	1:H:71:GLU:OE2	2.35	0.60
1:I:3:ILE:HG13	1:I:4:THR:N	2.09	0.60
1:I:460:ASN:ND2	1:I:461:GLU:HG3	2.17	0.60
1:J:36:TRP:O	1:J:37:ARG:HD3	2.02	0.60
1:J:782:ASP:HA	1:J:884:LEU:HD23	1.83	0.60
1:K:1020:TRP:HD1	1:K:1021:CME:N	1.99	0.60
1:L:460:ASN:ND2	1:L:461:GLU:HG3	2.17	0.60
1:M:578:TYR:HA	1:M:583:ASN:O	2.00	0.60
1:M:662:PRO:O	1:M:663:LEU:HD23	2.01	0.60
1:M:1011:ALA:HB3	1:M:1014:TYR:CZ	2.37	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:A:282:ARG:NH1	1:D:419:GLY:O	2.35	0.60
1:D:125:LEU:HG	1:D:126:THR:N	2.16	0.60
1:D:360:HIS:HE1	1:D:362:LEU:HB2	1.61	0.60
1:D:460:ASN:ND2	1:D:461:GLU:HG3	2.17	0.60
1:E:502:MET:HB2	1:E:537:GLU:HB2	1.84	0.60
1:F:14:ARG:HA	1:F:16:TRP:CZ3	2.37	0.60
1:F:502:MET:HB2	1:F:537:GLU:HB2	1.84	0.60
1:G:194:GLY:O	1:G:198:GLU:HG3	2.00	0.60
1:L:36:TRP:O	1:L:37:ARG:HD3	2.02	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:M:689:GLU:HA	1:M:689:GLU:OE2	2.01	0.60
1:N:4:THR:HA	1:N:9:VAL:HG11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:7:LEU:N	1:N:71:GLU:OE2	2.35	0.60
1:N:786:ARG:HH11	1:N:990:HIS:CE1	2.18	0.60
1:N:1020:TRP:HD1	1:N:1021:CME:N	1.99	0.60
1:O:194:GLY:O	1:O:198:GLU:HG3	2.00	0.60
1:O:323:ILE:HD12	1:O:323:ILE:N	2.16	0.60
1:O:460:ASN:ND2	1:O:461:GLU:HG3	2.17	0.60
1:P:651:LEU:HD13	1:P:669:PRO:HA	1.82	0.60
1:A:1011:ALA:HB3	1:A:1014:TYR:CZ	2.37	0.60
1:B:14:ARG:HA	1:B:16:TRP:CZ3	2.37	0.60
1:B:323:ILE:HD12	1:B:323:ILE:N	2.16	0.60
1:B:360:HIS:CE1	1:B:361:PRO:HD2	2.36	0.60
1:C:7:LEU:N	1:C:71:GLU:OE2	2.35	0.60
1:D:849:LEU:HD23	1:D:849:LEU:N	2.17	0.60
1:E:753:ASN:N	1:E:753:ASN:OD1	2.30	0.60
1:F:1021:CME:HB3	1:F:1021:CME:HZ3	1.84	0.60
1:G:745:MET:HE2	1:G:745:MET:CA	2.30	0.60
1:H:125:LEU:HG	1:H:126:THR:N	2.16	0.60
1:H:178:ARG:NH1	1:H:181:GLU:O	2.33	0.60
1:H:460:ASN:ND2	1:H:461:GLU:HG3	2.17	0.60
1:J:7:LEU:N	1:J:71:GLU:OE2	2.35	0.60
1:K:178:ARG:NH1	1:K:181:GLU:O	2.33	0.60
1:K:360:HIS:CE1	1:K:361:PRO:HD2	2.36	0.60
1:L:662:PRO:O	1:L:663:LEU:HD23	2.01	0.60
1:M:36:TRP:O	1:M:37:ARG:HD3	2.02	0.60
1:M:502:MET:HB2	1:M:537:GLU:HB2	1.84	0.60
1:N:14:ARG:HA	1:N:16:TRP:CZ3	2.37	0.60
1:N:502:MET:HB2	1:N:537:GLU:HB2	1.84	0.60
1:N:835:LEU:C	1:N:836:ILE:HD13	2.25	0.60
1:O:36:TRP:O	1:O:37:ARG:HD3	2.02	0.60
1:P:261:TRP:CH2	1:P:266:GLN:HB2	2.37	0.60
1:A:36:TRP:O	1:A:37:ARG:HD3	2.02	0.60
1:B:651:LEU:HD13	1:B:669:PRO:HA	1.82	0.60
1:B:753:ASN:N	1:B:753:ASN:OD1	2.30	0.60
1:C:54:LEU:HD23	1:C:54:LEU:N	2.15	0.60
1:C:460:ASN:ND2	1:C:461:GLU:HG3	2.17	0.60
1:D:4:THR:HA	1:D:9:VAL:HG11	1.82	0.60
1:D:14:ARG:HA	1:D:16:TRP:CZ3	2.37	0.60
1:D:194:GLY:O	1:D:198:GLU:HG3	2.00	0.60
1:D:1021:CME:HB3	1:D:1021:CME:HZ3	1.84	0.60
1:E:14:ARG:HA	1:E:16:TRP:CZ3	2.37	0.60
1:F:835:LEU:C	1:F:836:ILE:HD13	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:873:ALA:O	1:F:876:THR:HG22	2.02	0.60
1:F:1011:ALA:HB3	1:F:1014:TYR:CZ	2.37	0.60
1:H:772:ASP:OD1	1:H:772:ASP:N	2.30	0.60
1:I:261:TRP:CH2	1:I:266:GLN:HB2	2.37	0.60
1:I:782:ASP:HA	1:I:884:LEU:HD23	1.83	0.60
1:K:36:TRP:O	1:K:37:ARG:HD3	2.02	0.60
1:K:782:ASP:HA	1:K:884:LEU:HD23	1.83	0.60
1:L:37:ARG:NH2	1:L:218:PRO:HD3	2.17	0.60
1:L:689:GLU:HA	1:L:689:GLU:OE2	2.01	0.60
1:L:835:LEU:C	1:L:836:ILE:HD13	2.25	0.60
1:N:261:TRP:CH2	1:N:266:GLN:HB2	2.37	0.60
1:N:360:HIS:CE1	1:N:361:PRO:HD2	2.36	0.60
1:N:873:ALA:O	1:N:876:THR:HG22	2.02	0.60
1:P:14:ARG:HA	1:P:16:TRP:CZ3	2.37	0.60
1:P:945:ASN:OD1	1:P:950:GLN:NE2	2.30	0.60
1:P:1021:CME:HB3	1:P:1021:CME:CZ	2.21	0.60
1:A:7:LEU:N	1:A:71:GLU:OE2	2.35	0.59
1:A:125:LEU:HG	1:A:126:THR:N	2.16	0.59
1:A:1021:CME:HB3	1:A:1021:CME:HZ3	1.83	0.59
1:B:30:HIS:ND1	1:B:31:PRO:O	2.26	0.59
1:B:578:TYR:HA	1:B:583:ASN:O	2.00	0.59
1:C:23:GLN:OE1	1:C:26:ARG:HB3	2.02	0.59
1:D:261:TRP:CH2	1:D:266:GLN:HB2	2.37	0.59
1:D:662:PRO:O	1:D:663:LEU:HD23	2.01	0.59
1:E:261:TRP:CH2	1:E:266:GLN:HB2	2.37	0.59
1:E:1011:ALA:HB3	1:E:1014:TYR:CZ	2.37	0.59
1:G:37:ARG:NH2	1:G:218:PRO:HD3	2.17	0.59
1:I:125:LEU:HG	1:I:126:THR:N	2.16	0.59
1:I:502:MET:HB2	1:I:537:GLU:HB2	1.84	0.59
1:J:125:LEU:HG	1:J:126:THR:N	2.16	0.59
1:J:745:MET:HE2	1:J:745:MET:CA	2.30	0.59
1:J:873:ALA:O	1:J:876:THR:HG22	2.02	0.59
1:K:579:ASP:OD1	1:K:583:ASN:HB2	2.03	0.59
1:M:460:ASN:ND2	1:M:461:GLU:HG3	2.17	0.59
1:M:579:ASP:OD1	1:M:583:ASN:HB2	2.02	0.59
1:O:18:ASN:HD22	1:O:21:VAL:HG23	1.64	0.59
1:O:37:ARG:NH2	1:O:218:PRO:HD3	2.17	0.59
1:B:125:LEU:HG	1:B:126:THR:N	2.16	0.59
1:C:36:TRP:O	1:C:37:ARG:HD3	2.02	0.59
1:D:30:HIS:ND1	1:D:31:PRO:O	2.27	0.59
1:D:360:HIS:CE1	1:D:361:PRO:HD2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:ASN:HD22	1:E:21:VAL:HG23	1.64	0.59
1:F:178:ARG:NH1	1:F:181:GLU:O	2.33	0.59
1:F:261:TRP:CH2	1:F:266:GLN:HB2	2.37	0.59
1:F:460:ASN:ND2	1:F:461:GLU:HG3	2.17	0.59
1:F:849:LEU:N	1:F:849:LEU:HD23	2.17	0.59
1:G:873:ALA:O	1:G:876:THR:HG22	2.02	0.59
1:H:745:MET:HE2	1:H:745:MET:CA	2.30	0.59
1:I:23:GLN:OE1	1:I:26:ARG:HB3	2.02	0.59
1:I:849:LEU:N	1:I:849:LEU:HD23	2.17	0.59
1:J:23:GLN:OE1	1:J:26:ARG:HB3	2.03	0.59
1:J:57:GLU:HG2	1:J:83:THR:HG23	1.85	0.59
1:J:261:TRP:CH2	1:J:266:GLN:HB2	2.37	0.59
1:K:873:ALA:O	1:K:876:THR:HG22	2.02	0.59
1:M:7:LEU:N	1:M:71:GLU:OE2	2.35	0.59
1:M:30:HIS:HB2	1:M:31:PRO:CD	2.33	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:A:57:GLU:HG2	1:A:83:THR:HG23	1.85	0.59
1:B:23:GLN:OE1	1:B:26:ARG:HB3	2.02	0.59
1:B:30:HIS:HB2	1:B:31:PRO:CD	2.33	0.59
1:C:579:ASP:OD1	1:C:583:ASN:HB2	2.03	0.59
1:D:502:MET:HB2	1:D:537:GLU:HB2	1.84	0.59
1:E:36:TRP:O	1:E:37:ARG:HD3	2.02	0.59
1:E:125:LEU:HG	1:E:126:THR:N	2.16	0.59
1:E:873:ALA:O	1:E:876:THR:HG22	2.02	0.59
1:G:18:ASN:HD22	1:G:21:VAL:HG23	1.64	0.59
1:G:23:GLN:OE1	1:G:26:ARG:HB3	2.02	0.59
1:G:662:PRO:O	1:G:663:LEU:HD23	2.01	0.59
1:G:753:ASN:N	1:G:753:ASN:OD1	2.30	0.59
1:G:1021:CME:OH	1:G:1023:LYS:HG2	2.03	0.59
1:H:30:HIS:HB2	1:H:31:PRO:CD	2.32	0.59
1:H:261:TRP:CH2	1:H:266:GLN:HB2	2.37	0.59
1:H:502:MET:HB2	1:H:537:GLU:HB2	1.84	0.59
1:H:579:ASP:OD1	1:H:583:ASN:HB2	2.02	0.59
1:H:651:LEU:HD13	1:H:669:PRO:HA	1.82	0.59
1:H:1011:ALA:HB3	1:H:1014:TYR:CZ	2.37	0.59
1:I:1011:ALA:HB3	1:I:1014:TYR:CZ	2.37	0.59
1:I:1021:CME:OH	1:I:1023:LYS:HG2	2.03	0.59
1:J:14:ARG:HA	1:J:16:TRP:CZ3	2.37	0.59
1:J:460:ASN:ND2	1:J:461:GLU:HG3	2.17	0.59
1:J:502:MET:HB2	1:J:537:GLU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:579:ASP:OD1	1:J:583:ASN:HB2	2.03	0.59
1:K:261:TRP:CH2	1:K:266:GLN:HB2	2.37	0.59
1:K:1021:CME:HB3	1:K:1021:CME:HZ3	1.84	0.59
1:L:822:LEU:CD1	1:L:824:GLN:H	2.16	0.59
1:M:14:ARG:HA	1:M:16:TRP:CZ3	2.37	0.59
1:M:23:GLN:OE1	1:M:26:ARG:HB3	2.02	0.59
1:M:822:LEU:CD1	1:M:824:GLN:H	2.16	0.59
1:M:1021:CME:OH	1:M:1023:LYS:HG2	2.03	0.59
1:O:57:GLU:HG2	1:O:83:THR:HG23	1.85	0.59
1:P:689:GLU:HA	1:P:689:GLU:OE2	2.01	0.59
1:P:745:MET:HE2	1:P:745:MET:CA	2.30	0.59
1:B:37:ARG:NH2	1:B:218:PRO:HD3	2.17	0.59
1:C:502:MET:HB2	1:C:537:GLU:HB2	1.84	0.59
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.37	0.59
1:D:30:HIS:HB2	1:D:31:PRO:CD	2.32	0.59
1:D:873:ALA:O	1:D:876:THR:HG22	2.02	0.59
1:D:894:ARG:NH1	1:D:919:ASP:OD2	2.30	0.59
1:G:323:ILE:HD12	1:G:323:ILE:N	2.16	0.59
1:G:460:ASN:ND2	1:G:461:GLU:HG3	2.17	0.59
1:G:579:ASP:OD1	1:G:583:ASN:HB2	2.03	0.59
1:I:14:ARG:HA	1:I:16:TRP:CZ3	2.37	0.59
1:J:1021:CME:OH	1:J:1023:LYS:HG2	2.03	0.59
1:L:1011:ALA:HB3	1:L:1014:TYR:CZ	2.37	0.59
1:M:18:ASN:HD22	1:M:21:VAL:HG23	1.64	0.59
1:N:460:ASN:ND2	1:N:461:GLU:HG3	2.17	0.59
1:O:23:GLN:OE1	1:O:26:ARG:HB3	2.02	0.59
1:O:178:ARG:NH1	1:O:181:GLU:O	2.33	0.59
1:O:689:GLU:HA	1:O:689:GLU:OE2	2.01	0.59
1:P:873:ALA:O	1:P:876:THR:HG22	2.02	0.59
1:A:249:GLU:HG2	1:A:251:ARG:HH12	1.67	0.59
1:B:822:LEU:CD1	1:B:824:GLN:H	2.16	0.59
1:D:37:ARG:NH2	1:D:218:PRO:HD3	2.17	0.59
1:D:272:ALA:HB1	1:D:273:PRO:HD2	1.85	0.59
1:E:579:ASP:OD1	1:E:583:ASN:HB2	2.03	0.59
1:G:36:TRP:O	1:G:37:ARG:HD3	2.02	0.59
1:H:1021:CME:OH	1:H:1023:LYS:HG2	2.03	0.59
1:L:30:HIS:HB2	1:L:31:PRO:CD	2.33	0.59
1:M:57:GLU:HG2	1:M:83:THR:HG23	1.85	0.59
1:M:178:ARG:NH1	1:M:181:GLU:O	2.33	0.59
1:M:873:ALA:O	1:M:876:THR:HG22	2.02	0.59
1:N:849:LEU:N	1:N:849:LEU:HD23	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:14:ARG:HA	1:O:16:TRP:CZ3	2.37	0.59
1:A:30:HIS:HB2	1:A:31:PRO:CD	2.33	0.59
1:B:579:ASP:OD1	1:B:583:ASN:HB2	2.03	0.59
1:B:849:LEU:N	1:B:849:LEU:HD23	2.17	0.59
1:F:822:LEU:CD1	1:F:824:GLN:H	2.16	0.59
1:G:14:ARG:HA	1:G:16:TRP:CZ3	2.37	0.59
1:H:57:GLU:HG2	1:H:83:THR:HG23	1.84	0.59
1:I:30:HIS:HB2	1:I:31:PRO:CD	2.32	0.59
1:K:7:LEU:N	1:K:71:GLU:OE2	2.35	0.59
1:K:14:ARG:HA	1:K:16:TRP:CZ3	2.37	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:L:272:ALA:HB1	1:L:273:PRO:HD2	1.85	0.59
1:L:849:LEU:HD23	1:L:849:LEU:N	2.17	0.59
1:N:249:GLU:HG2	1:N:251:ARG:HH12	1.67	0.59
1:O:873:ALA:O	1:O:876:THR:HG22	2.02	0.59
1:A:261:TRP:CZ3	1:A:266:GLN:HB2	2.38	0.59
1:B:261:TRP:CH2	1:B:266:GLN:HB2	2.37	0.59
1:B:1021:CME:OH	1:B:1023:LYS:HG2	2.03	0.59
1:D:7:LEU:N	1:D:71:GLU:OE2	2.35	0.59
1:D:1021:CME:OH	1:D:1023:LYS:HG2	2.03	0.59
1:E:178:ARG:NH1	1:E:181:GLU:O	2.33	0.59
1:E:255:ARG:HG2	1:E:255:ARG:NH1	2.14	0.59
1:G:178:ARG:NH1	1:G:181:GLU:O	2.33	0.59
1:G:849:LEU:HD23	1:G:849:LEU:N	2.17	0.59
1:H:873:ALA:O	1:H:876:THR:HG22	2.02	0.59
1:I:7:LEU:N	1:I:71:GLU:OE2	2.35	0.59
1:I:178:ARG:NH1	1:I:181:GLU:O	2.33	0.59
1:I:493:THR:HG23	5:I:2113:HOH:O	2.03	0.59
1:I:873:ALA:O	1:I:876:THR:HG22	2.02	0.59
1:J:37:ARG:NH2	1:J:218:PRO:HD3	2.17	0.59
1:J:272:ALA:HB1	1:J:273:PRO:HD2	1.85	0.59
1:L:437:SER:HB2	5:L:2258:HOH:O	2.01	0.59
1:N:178:ARG:NH1	1:N:181:GLU:O	2.33	0.59
1:O:261:TRP:CH2	1:O:266:GLN:HB2	2.37	0.59
1:O:1011:ALA:HB3	1:O:1014:TYR:CZ	2.37	0.59
1:P:502:MET:HB2	1:P:537:GLU:HB2	1.84	0.59
1:A:460:ASN:ND2	1:A:461:GLU:HG3	2.17	0.59
1:A:502:MET:HB2	1:A:537:GLU:HB2	1.84	0.59
1:B:36:TRP:O	1:B:37:ARG:HD3	2.02	0.59
1:B:261:TRP:CZ3	1:B:266:GLN:HB2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:763:GLY:HA3	1:C:822:LEU:CD2	2.33	0.59
1:D:36:TRP:O	1:D:37:ARG:HD3	2.02	0.59
1:E:37:ARG:NH2	1:E:218:PRO:HD3	2.17	0.59
1:F:125:LEU:HG	1:F:126:THR:N	2.16	0.59
1:F:662:PRO:O	1:F:663:LEU:HD23	2.01	0.59
1:G:30:HIS:HB2	1:G:31:PRO:CD	2.33	0.59
1:H:730:LEU:HB3	1:H:731:PRO:HD2	1.85	0.59
1:I:54:LEU:HD23	1:I:54:LEU:N	2.15	0.59
1:I:763:GLY:HA3	1:I:822:LEU:CD2	2.33	0.59
1:J:30:HIS:HB2	1:J:31:PRO:CD	2.33	0.59
1:J:906:TYR:HB3	1:J:907:PRO:HD2	1.85	0.59
1:K:849:LEU:N	1:K:849:LEU:HD23	2.17	0.59
1:M:255:ARG:HG2	1:M:255:ARG:NH1	2.14	0.59
1:M:261:TRP:CH2	1:M:266:GLN:HB2	2.37	0.59
1:N:30:HIS:HB2	1:N:31:PRO:CD	2.33	0.59
1:N:763:GLY:HA3	1:N:822:LEU:CD2	2.33	0.59
1:O:30:HIS:HB2	1:O:31:PRO:CD	2.33	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:P:125:LEU:HG	1:P:126:THR:N	2.16	0.59
1:P:261:TRP:CZ3	1:P:266:GLN:HB2	2.38	0.59
1:P:473:ARG:O	1:P:473:ARG:HD3	2.03	0.59
1:P:1021:CME:OH	1:P:1023:LYS:HG2	2.03	0.59
1:A:30:HIS:ND1	1:A:31:PRO:O	2.26	0.59
1:A:849:LEU:N	1:A:849:LEU:HD23	2.17	0.59
1:B:249:GLU:HG2	1:B:251:ARG:HH12	1.67	0.59
1:B:460:ASN:ND2	1:B:461:GLU:HG3	2.17	0.59
1:B:662:PRO:O	1:B:663:LEU:HD23	2.01	0.59
1:C:822:LEU:CD1	1:C:824:GLN:H	2.16	0.59
1:C:873:ALA:O	1:C:876:THR:HG22	2.02	0.59
1:D:493:THR:HG23	5:D:2119:HOH:O	2.03	0.59
1:E:23:GLN:OE1	1:E:26:ARG:HB3	2.02	0.59
1:E:772:ASP:OD1	1:E:772:ASP:N	2.30	0.59
1:F:30:HIS:HB2	1:F:31:PRO:CD	2.33	0.59
1:F:166:ARG:HG3	1:F:392:TYR:HB2	1.85	0.59
1:F:763:GLY:HA3	1:F:822:LEU:CD2	2.33	0.59
1:H:14:ARG:HA	1:H:16:TRP:CZ3	2.37	0.59
1:H:261:TRP:CZ3	1:H:266:GLN:HB2	2.38	0.59
1:L:166:ARG:HG3	1:L:392:TYR:HB2	1.85	0.59
1:L:502:MET:HB2	1:L:537:GLU:HB2	1.84	0.59
1:M:473:ARG:O	1:M:473:ARG:HD3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:493:THR:HG23	5:M:2113:HOH:O	2.03	0.59
1:N:166:ARG:HG3	1:N:392:TYR:HB2	1.85	0.59
1:N:473:ARG:O	1:N:473:ARG:HD3	2.03	0.59
1:O:54:LEU:HD23	1:O:54:LEU:N	2.15	0.59
1:O:473:ARG:O	1:O:473:ARG:HD3	2.03	0.59
1:P:493:THR:HG23	5:P:2118:HOH:O	2.03	0.59
1:P:730:LEU:HB3	1:P:731:PRO:HD2	1.85	0.59
1:P:906:TYR:HB3	1:P:907:PRO:HD2	1.85	0.59
1:A:493:THR:HG23	5:A:2113:HOH:O	2.03	0.59
1:A:778:THR:HB	1:A:887:GLN:HB3	1.85	0.59
1:C:57:GLU:HG2	1:C:83:THR:HG23	1.85	0.59
1:C:178:ARG:NH1	1:C:181:GLU:O	2.33	0.59
1:C:261:TRP:CZ3	1:C:266:GLN:HB2	2.38	0.59
1:C:473:ARG:O	1:C:473:ARG:HD3	2.03	0.59
1:C:1021:CME:OH	1:C:1023:LYS:HG2	2.03	0.59
1:D:54:LEU:HD23	1:D:54:LEU:N	2.15	0.59
1:D:249:GLU:HG2	1:D:251:ARG:HH12	1.67	0.59
1:E:54:LEU:HD23	1:E:54:LEU:N	2.15	0.59
1:E:291:LEU:HD12	1:E:291:LEU:N	2.18	0.59
1:F:272:ALA:HB1	1:F:273:PRO:HD2	1.85	0.59
1:F:493:THR:HG23	5:F:2113:HOH:O	2.03	0.59
1:G:57:GLU:HG2	1:G:83:THR:HG23	1.85	0.59
1:G:730:LEU:HB3	1:G:731:PRO:HD2	1.85	0.59
1:G:1011:ALA:HB3	1:G:1014:TYR:CZ	2.37	0.59
1:H:37:ARG:NH2	1:H:218:PRO:HD3	2.17	0.59
1:H:493:THR:HG23	5:H:2113:HOH:O	2.03	0.59
1:H:763:GLY:HA3	1:H:822:LEU:CD2	2.33	0.59
1:H:906:TYR:HB3	1:H:907:PRO:HD2	1.85	0.59
1:H:945:ASN:OD1	1:H:950:GLN:NE2	2.30	0.59
1:I:287:ASP:OD2	1:L:425:ARG:NH2	2.36	0.59
1:I:473:ARG:O	1:I:473:ARG:HD3	2.03	0.59
1:K:473:ARG:O	1:K:473:ARG:HD3	2.03	0.59
1:K:493:THR:HG23	5:K:2113:HOH:O	2.03	0.59
1:K:763:GLY:HA3	1:K:822:LEU:CD2	2.33	0.59
1:K:945:ASN:OD1	1:K:950:GLN:NE2	2.30	0.59
1:L:57:GLU:HG2	1:L:83:THR:HG23	1.84	0.59
1:L:261:TRP:CH2	1:L:266:GLN:HB2	2.37	0.59
1:L:873:ALA:O	1:L:876:THR:HG22	2.02	0.59
1:M:945:ASN:OD1	1:M:950:GLN:NE2	2.30	0.59
1:N:261:TRP:CZ3	1:N:266:GLN:HB2	2.38	0.59
1:N:272:ALA:HB1	1:N:273:PRO:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1011:ALA:HB3	1:N:1014:TYR:CZ	2.37	0.59
1:O:730:LEU:HB3	1:O:731:PRO:HD2	1.85	0.59
1:P:763:GLY:HA3	1:P:822:LEU:CD2	2.33	0.59
1:B:7:LEU:N	1:B:71:GLU:OE2	2.35	0.58
1:B:54:LEU:HD23	1:B:54:LEU:N	2.15	0.58
1:C:125:LEU:HG	1:C:126:THR:N	2.16	0.58
1:C:261:TRP:CH2	1:C:266:GLN:HB2	2.37	0.58
1:D:23:GLN:OE1	1:D:26:ARG:HB3	2.02	0.58
1:D:1011:ALA:HB3	1:D:1014:TYR:CZ	2.37	0.58
1:E:763:GLY:HA3	1:E:822:LEU:CD2	2.33	0.58
1:F:23:GLN:OE1	1:F:26:ARG:HB3	2.02	0.58
1:F:429:ASP:OD1	1:F:430:PRO:HD2	2.03	0.58
1:F:1021:CME:OH	1:F:1023:LYS:HG2	2.02	0.58
1:H:36:TRP:O	1:H:37:ARG:HD3	2.02	0.58
1:H:473:ARG:O	1:H:473:ARG:HD3	2.03	0.58
1:K:254:LEU:C	1:K:255:ARG:HG2	2.28	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:M:291:LEU:N	1:M:291:LEU:HD12	2.18	0.58
1:N:23:GLN:OE1	1:N:26:ARG:HB3	2.02	0.58
1:P:291:LEU:HD12	1:P:291:LEU:N	2.18	0.58
1:P:460:ASN:ND2	1:P:461:GLU:HG3	2.17	0.58
1:A:37:ARG:NH2	1:A:218:PRO:HD3	2.17	0.58
1:B:272:ALA:HB1	1:B:273:PRO:HD2	1.85	0.58
1:B:433:LEU:C	1:B:433:LEU:HD12	2.28	0.58
1:C:433:LEU:C	1:C:433:LEU:HD12	2.28	0.58
1:C:645:ARG:HH22	1:C:650:GLU:CD	2.12	0.58
1:D:261:TRP:CZ3	1:D:266:GLN:HB2	2.38	0.58
1:D:763:GLY:HA3	1:D:822:LEU:CD2	2.33	0.58
1:E:730:LEU:HB3	1:E:731:PRO:HD2	1.85	0.58
1:E:849:LEU:N	1:E:849:LEU:HD23	2.17	0.58
1:E:1021:CME:OH	1:E:1023:LYS:HG2	2.03	0.58
1:F:37:ARG:NH2	1:F:218:PRO:HD3	2.17	0.58
1:F:54:LEU:HD23	1:F:54:LEU:N	2.15	0.58
1:F:473:ARG:O	1:F:473:ARG:HD3	2.03	0.58
1:F:945:ASN:OD1	1:F:950:GLN:NE2	2.30	0.58
1:G:166:ARG:HG3	1:G:392:TYR:HB2	1.85	0.58
1:G:502:MET:HB2	1:G:537:GLU:HB2	1.84	0.58
1:H:18:ASN:HD22	1:H:21:VAL:HG23	1.64	0.58
1:H:254:LEU:C	1:H:255:ARG:HG2	2.28	0.58
1:H:429:ASP:OD1	1:H:430:PRO:HD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:7:LEU:HD13	1:I:74:LEU:CD1	2.32	0.58
1:I:166:ARG:HG3	1:I:392:TYR:HB2	1.85	0.58
1:I:645:ARG:NH2	1:I:650:GLU:OE1	2.37	0.58
1:J:54:LEU:HD23	1:J:54:LEU:N	2.15	0.58
1:K:433:LEU:C	1:K:433:LEU:HD12	2.28	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:M:54:LEU:HD23	1:M:54:LEU:N	2.15	0.58
1:M:772:ASP:OD1	1:M:772:ASP:N	2.30	0.58
1:N:493:THR:HG23	5:N:2116:HOH:O	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:O:502:MET:HB2	1:O:537:GLU:HB2	1.84	0.58
1:O:579:ASP:OD1	1:O:583:ASN:HB2	2.03	0.58
1:P:37:ARG:NH2	1:P:218:PRO:HD3	2.17	0.58
1:P:579:ASP:OD1	1:P:583:ASN:HB2	2.03	0.58
1:A:54:LEU:HD23	1:A:54:LEU:N	2.15	0.58
1:A:425:ARG:NH2	1:D:287:ASP:CG	2.60	0.58
1:A:873:ALA:O	1:A:876:THR:HG22	2.02	0.58
1:B:166:ARG:HG3	1:B:392:TYR:HB2	1.85	0.58
1:B:291:LEU:N	1:B:291:LEU:HD12	2.18	0.58
1:B:493:THR:HG23	5:B:2116:HOH:O	2.03	0.58
1:C:30:HIS:HB2	1:C:31:PRO:CD	2.32	0.58
1:C:730:LEU:HB3	1:C:731:PRO:HD2	1.85	0.58
1:D:645:ARG:HH22	1:D:650:GLU:CD	2.12	0.58
1:D:730:LEU:HB3	1:D:731:PRO:HD2	1.85	0.58
1:E:272:ALA:HB1	1:E:273:PRO:HD2	1.85	0.58
1:E:433:LEU:C	1:E:433:LEU:HD12	2.28	0.58
1:E:473:ARG:O	1:E:473:ARG:HD3	2.03	0.58
1:E:645:ARG:NH2	1:E:650:GLU:OE1	2.37	0.58
1:F:291:LEU:HD12	1:F:291:LEU:N	2.18	0.58
1:G:822:LEU:CD1	1:G:824:GLN:H	2.16	0.58
1:H:54:LEU:HD23	1:H:54:LEU:N	2.15	0.58
1:H:291:LEU:HD12	1:H:291:LEU:N	2.18	0.58
1:I:36:TRP:O	1:I:37:ARG:HD3	2.02	0.58
1:J:493:THR:HG23	5:J:2113:HOH:O	2.03	0.58
1:J:763:GLY:HA3	1:J:822:LEU:CD2	2.33	0.58
1:K:7:LEU:HD13	1:K:74:LEU:CD1	2.32	0.58
1:K:18:ASN:HD22	1:K:21:VAL:HG23	1.64	0.58
1:K:37:ARG:NH2	1:K:218:PRO:HD3	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:54:LEU:HD23	1:K:54:LEU:N	2.15	0.58
1:K:906:TYR:HB3	1:K:907:PRO:HD2	1.85	0.58
1:L:473:ARG:O	1:L:473:ARG:HD3	2.03	0.58
1:M:37:ARG:NH2	1:M:218:PRO:HD3	2.17	0.58
1:M:429:ASP:OD1	1:M:430:PRO:HD2	2.03	0.58
1:M:730:LEU:HB3	1:M:731:PRO:HD2	1.85	0.58
1:N:37:ARG:NH2	1:N:218:PRO:HD3	2.17	0.58
1:N:291:LEU:HD12	1:N:291:LEU:N	2.18	0.58
1:O:291:LEU:N	1:O:291:LEU:HD12	2.18	0.58
1:P:30:HIS:HB2	1:P:31:PRO:CD	2.33	0.58
1:P:57:GLU:HG2	1:P:83:THR:HG23	1.85	0.58
1:A:291:LEU:HD12	1:A:291:LEU:N	2.18	0.58
1:A:579:ASP:OD1	1:A:583:ASN:HB2	2.03	0.58
1:A:906:TYR:HB3	1:A:907:PRO:HD2	1.85	0.58
1:A:1021:CME:OH	1:A:1023:LYS:HG2	2.03	0.58
1:B:502:MET:HB2	1:B:537:GLU:HB2	1.84	0.58
1:B:645:ARG:HH22	1:B:650:GLU:CD	2.12	0.58
1:C:37:ARG:NH2	1:C:218:PRO:HD3	2.17	0.58
1:C:291:LEU:HD12	1:C:291:LEU:N	2.18	0.58
1:C:429:ASP:OD1	1:C:430:PRO:HD2	2.03	0.58
1:C:662:PRO:O	1:C:663:LEU:HD23	2.01	0.58
1:C:849:LEU:N	1:C:849:LEU:HD23	2.17	0.58
1:D:473:ARG:O	1:D:473:ARG:HD3	2.03	0.58
1:D:579:ASP:OD1	1:D:583:ASN:HB2	2.03	0.58
1:E:261:TRP:CZ3	1:E:266:GLN:HB2	2.38	0.58
1:E:493:THR:HG23	5:E:2113:HOH:O	2.03	0.58
1:F:36:TRP:O	1:F:37:ARG:HD3	2.02	0.58
1:F:906:TYR:HB3	1:F:907:PRO:HD2	1.85	0.58
1:G:261:TRP:CH2	1:G:266:GLN:HB2	2.37	0.58
1:G:473:ARG:O	1:G:473:ARG:HD3	2.03	0.58
1:I:282:ARG:NH1	1:L:419:GLY:HA2	2.18	0.58
1:I:433:LEU:HD12	1:I:433:LEU:C	2.28	0.58
1:J:433:LEU:C	1:J:433:LEU:HD12	2.28	0.58
1:K:894:ARG:NH1	1:K:919:ASP:OD2	2.30	0.58
1:L:291:LEU:N	1:L:291:LEU:HD12	2.18	0.58
1:L:433:LEU:C	1:L:433:LEU:HD12	2.28	0.58
1:L:763:GLY:HA3	1:L:822:LEU:CD2	2.33	0.58
1:M:261:TRP:CZ3	1:M:266:GLN:HB2	2.38	0.58
1:N:730:LEU:HB3	1:N:731:PRO:HD2	1.85	0.58
1:N:906:TYR:HB3	1:N:907:PRO:HD2	1.85	0.58
1:N:1021:CME:OH	1:N:1023:LYS:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:23:GLN:OE1	1:P:26:ARG:HB3	2.02	0.58
1:P:254:LEU:C	1:P:255:ARG:HG2	2.28	0.58
1:P:433:LEU:C	1:P:433:LEU:HD12	2.28	0.58
1:P:645:ARG:NH2	1:P:650:GLU:OE1	2.37	0.58
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.85	0.58
1:B:423:MET:HB2	1:C:282:ARG:HG3	1.85	0.58
1:C:945:ASN:OD1	1:C:950:GLN:NE2	2.30	0.58
1:D:429:ASP:OD1	1:D:430:PRO:HD2	2.03	0.58
1:D:645:ARG:NH2	1:D:650:GLU:OE1	2.37	0.58
1:D:668:VAL:CG1	1:D:669:PRO:HD2	2.31	0.58
1:D:778:THR:HB	1:D:887:GLN:HB3	1.85	0.58
1:F:579:ASP:OD1	1:F:583:ASN:HB2	2.02	0.58
1:G:249:GLU:HG2	1:G:251:ARG:HH12	1.67	0.58
1:G:254:LEU:C	1:G:255:ARG:HG2	2.28	0.58
1:G:261:TRP:CZ3	1:G:266:GLN:HB2	2.38	0.58
1:G:291:LEU:N	1:G:291:LEU:HD12	2.18	0.58
1:G:429:ASP:OD1	1:G:430:PRO:HD2	2.03	0.58
1:I:254:LEU:C	1:I:255:ARG:HG2	2.28	0.58
1:I:291:LEU:HD12	1:I:291:LEU:N	2.18	0.58
1:K:730:LEU:HB3	1:K:731:PRO:HD2	1.85	0.58
1:L:645:ARG:HH22	1:L:650:GLU:CD	2.12	0.58
1:M:130:ASP:OD1	1:M:132:SER:N	2.29	0.58
1:M:166:ARG:HG3	1:M:392:TYR:HB2	1.85	0.58
1:O:272:ALA:HB1	1:O:273:PRO:HD2	1.85	0.58
1:P:36:TRP:O	1:P:37:ARG:HD3	2.02	0.58
1:A:14:ARG:HA	1:A:16:TRP:CZ3	2.37	0.58
1:A:23:GLN:OE1	1:A:26:ARG:HB3	2.02	0.58
1:A:254:LEU:C	1:A:255:ARG:HG2	2.28	0.58
1:B:763:GLY:HA3	1:B:822:LEU:CD2	2.33	0.58
1:C:272:ALA:HB1	1:C:273:PRO:HD2	1.85	0.58
1:D:910:LEU:C	1:D:910:LEU:HD12	2.29	0.58
1:E:166:ARG:HG3	1:E:392:TYR:HB2	1.85	0.58
1:F:433:LEU:C	1:F:433:LEU:HD12	2.28	0.58
1:F:645:ARG:HH22	1:F:650:GLU:CD	2.12	0.58
1:H:23:GLN:OE1	1:H:26:ARG:HB3	2.02	0.58
1:J:249:GLU:HG2	1:J:251:ARG:HH12	1.67	0.58
1:K:23:GLN:OE1	1:K:26:ARG:HB3	2.02	0.58
1:K:57:GLU:HG2	1:K:83:THR:HG23	1.84	0.58
1:K:645:ARG:HH22	1:K:650:GLU:CD	2.12	0.58
1:L:23:GLN:OE1	1:L:26:ARG:HB3	2.02	0.58
1:L:254:LEU:C	1:L:255:ARG:HG2	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:849:LEU:N	1:M:849:LEU:HD23	2.17	0.58
1:N:36:TRP:O	1:N:37:ARG:HD3	2.02	0.58
1:N:645:ARG:NH2	1:N:650:GLU:OE1	2.37	0.58
1:O:645:ARG:HH22	1:O:650:GLU:CD	2.12	0.58
1:O:822:LEU:CD1	1:O:824:GLN:H	2.15	0.58
1:P:849:LEU:N	1:P:849:LEU:HD23	2.17	0.58
1:E:906:TYR:HB3	1:E:907:PRO:HD2	1.85	0.58
1:E:910:LEU:C	1:E:910:LEU:HD12	2.29	0.58
1:F:645:ARG:NH2	1:F:650:GLU:OE1	2.37	0.58
1:G:272:ALA:HB1	1:G:273:PRO:HD2	1.85	0.58
1:G:645:ARG:HH22	1:G:650:GLU:CD	2.12	0.58
1:G:763:GLY:HA3	1:G:822:LEU:CD2	2.33	0.58
1:H:645:ARG:HH22	1:H:650:GLU:CD	2.12	0.58
1:I:272:ALA:HB1	1:I:273:PRO:HD2	1.85	0.58
1:J:822:LEU:CD1	1:J:824:GLN:H	2.16	0.58
1:J:1021:CME:HB3	1:J:1021:CME:HZ3	1.84	0.58
1:K:291:LEU:HD12	1:K:291:LEU:N	2.18	0.58
1:K:502:MET:HB2	1:K:537:GLU:HB2	1.84	0.58
1:K:580:GLU:HG2	1:K:581:ASN:OD1	2.04	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:M:272:ALA:HB1	1:M:273:PRO:HD2	1.85	0.58
1:N:433:LEU:C	1:N:433:LEU:HD12	2.28	0.58
1:N:668:VAL:CG1	1:N:669:PRO:HD2	2.31	0.58
1:O:910:LEU:C	1:O:910:LEU:HD12	2.29	0.58
1:O:1021:CME:OH	1:O:1023:LYS:HG2	2.03	0.58
1:A:730:LEU:HB3	1:A:731:PRO:HD2	1.85	0.58
1:B:316:HIS:HD2	1:B:317:THR:O	1.87	0.58
1:C:7:LEU:HD13	1:C:74:LEU:CD1	2.32	0.58
1:C:778:THR:HB	1:C:887:GLN:HB3	1.85	0.58
1:C:910:LEU:C	1:C:910:LEU:HD12	2.29	0.58
1:E:429:ASP:OD1	1:E:430:PRO:HD2	2.03	0.58
1:F:730:LEU:HB3	1:F:731:PRO:HD2	1.85	0.58
1:H:433:LEU:C	1:H:433:LEU:HD12	2.28	0.58
1:H:778:THR:HB	1:H:887:GLN:HB3	1.85	0.58
1:I:261:TRP:CZ3	1:I:266:GLN:HB2	2.38	0.58
1:I:668:VAL:CG1	1:I:669:PRO:HD2	2.31	0.58
1:J:261:TRP:CZ3	1:J:266:GLN:HB2	2.38	0.58
1:J:291:LEU:N	1:J:291:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:645:ARG:NH2	1:L:650:GLU:OE1	2.37	0.58
1:L:1021:CME:OH	1:L:1023:LYS:HG2	2.03	0.58
1:M:645:ARG:NH2	1:M:650:GLU:OE1	2.37	0.58
1:N:57:GLU:HG2	1:N:83:THR:HG23	1.84	0.58
1:O:645:ARG:NH2	1:O:650:GLU:OE1	2.37	0.58
1:P:645:ARG:HH22	1:P:650:GLU:CD	2.12	0.58
1:P:740:LEU:CD1	1:P:741:THR:H	2.12	0.58
1:A:153:TRP:CD1	1:A:158:TRP:HA	2.39	0.58
1:A:763:GLY:HA3	1:A:822:LEU:CD2	2.33	0.58
1:B:254:LEU:C	1:B:255:ARG:HG2	2.28	0.58
1:B:910:LEU:C	1:B:910:LEU:HD12	2.29	0.58
1:C:130:ASP:OD1	1:C:132:SER:N	2.29	0.58
1:C:906:TYR:HB3	1:C:907:PRO:HD2	1.85	0.58
1:E:30:HIS:HB2	1:E:31:PRO:CD	2.33	0.58
1:E:316:HIS:HD2	1:E:317:THR:O	1.87	0.58
1:E:945:ASN:OD1	1:E:950:GLN:NE2	2.30	0.58
1:H:153:TRP:CD1	1:H:158:TRP:HA	2.39	0.58
1:H:849:LEU:N	1:H:849:LEU:HD23	2.17	0.58
1:H:910:LEU:C	1:H:910:LEU:HD12	2.29	0.58
1:I:153:TRP:CD1	1:I:158:TRP:HA	2.39	0.58
1:I:429:ASP:OD1	1:I:430:PRO:HD2	2.03	0.58
1:K:153:TRP:CD1	1:K:158:TRP:HA	2.39	0.58
1:L:493:THR:HG23	5:L:2113:HOH:O	2.03	0.58
1:M:30:HIS:ND1	1:M:31:PRO:O	2.26	0.58
1:M:580:GLU:HG2	1:M:581:ASN:OD1	2.04	0.58
1:N:778:THR:HB	1:N:887:GLN:HB3	1.85	0.58
1:P:910:LEU:C	1:P:910:LEU:HD12	2.29	0.58
1:A:261:TRP:CH2	1:A:266:GLN:HB2	2.37	0.58
1:A:429:ASP:OD1	1:A:430:PRO:HD2	2.03	0.58
1:A:473:ARG:O	1:A:473:ARG:HD3	2.03	0.58
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.04	0.58
1:B:473:ARG:O	1:B:473:ARG:HD3	2.03	0.58
1:B:645:ARG:NH2	1:B:650:GLU:OE1	2.37	0.58
1:D:166:ARG:HG3	1:D:392:TYR:HB2	1.85	0.58
1:D:906:TYR:HB3	1:D:907:PRO:HD2	1.85	0.58
1:F:7:LEU:HD13	1:F:74:LEU:CD1	2.32	0.58
1:F:166:ARG:HG3	1:F:392:TYR:CB	2.34	0.58
1:F:261:TRP:CZ3	1:F:266:GLN:HB2	2.38	0.58
1:G:316:HIS:HD2	1:G:317:THR:O	1.87	0.58
1:H:355:ASN:OD1	1:H:388:ARG:HD3	2.04	0.58
1:H:645:ARG:NH2	1:H:650:GLU:OE1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:740:LEU:CD1	1:H:741:THR:H	2.12	0.58
1:I:166:ARG:HG3	1:I:392:TYR:CB	2.34	0.58
1:I:579:ASP:OD1	1:I:583:ASN:HB2	2.03	0.58
1:J:429:ASP:OD1	1:J:430:PRO:HD2	2.03	0.58
1:J:473:ARG:O	1:J:473:ARG:HD3	2.03	0.58
1:J:645:ARG:HH22	1:J:650:GLU:CD	2.12	0.58
1:J:778:THR:HB	1:J:887:GLN:HB3	1.85	0.58
1:K:473:ARG:HD3	1:K:473:ARG:C	2.29	0.58
1:K:1021:CME:OH	1:K:1023:LYS:HG2	2.03	0.58
1:L:730:LEU:HB3	1:L:731:PRO:HD2	1.85	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:N:54:LEU:HD23	1:N:54:LEU:N	2.15	0.58
1:N:254:LEU:C	1:N:255:ARG:HG2	2.28	0.58
1:N:580:GLU:HG2	1:N:581:ASN:OD1	2.04	0.58
1:A:645:ARG:NH2	1:A:650:GLU:OE1	2.37	0.57
1:B:166:ARG:HG3	1:B:392:TYR:CB	2.34	0.57
1:B:429:ASP:OD1	1:B:430:PRO:HD2	2.03	0.57
1:D:153:TRP:CD1	1:D:158:TRP:HA	2.39	0.57
1:E:30:HIS:ND1	1:E:31:PRO:O	2.27	0.57
1:E:778:THR:HB	1:E:887:GLN:HB3	1.85	0.57
1:F:254:LEU:C	1:F:255:ARG:HG2	2.28	0.57
1:H:166:ARG:HG3	1:H:392:TYR:CB	2.34	0.57
1:I:580:GLU:HG2	1:I:581:ASN:OD1	2.04	0.57
1:L:153:TRP:CD1	1:L:158:TRP:HA	2.39	0.57
1:M:316:HIS:HD2	1:M:317:THR:O	1.87	0.57
1:N:166:ARG:HG3	1:N:392:TYR:CB	2.34	0.57
1:N:355:ASN:OD1	1:N:388:ARG:HD3	2.04	0.57
1:O:7:LEU:HD13	1:O:74:LEU:CD1	2.32	0.57
1:O:493:THR:HG23	5:O:2113:HOH:O	2.03	0.57
1:P:153:TRP:CD1	1:P:158:TRP:HA	2.39	0.57
1:P:429:ASP:OD1	1:P:430:PRO:HD2	2.03	0.57
1:A:130:ASP:OD1	1:A:132:SER:N	2.29	0.57
1:A:272:ALA:HB1	1:A:273:PRO:HD2	1.85	0.57
1:A:433:LEU:HD12	1:A:433:LEU:C	2.28	0.57
1:A:910:LEU:C	1:A:910:LEU:HD12	2.29	0.57
1:B:730:LEU:HB3	1:B:731:PRO:HD2	1.85	0.57
1:B:906:TYR:HB3	1:B:907:PRO:HD2	1.85	0.57
1:C:166:ARG:HG3	1:C:392:TYR:HB2	1.85	0.57
1:C:254:LEU:C	1:C:255:ARG:HG2	2.28	0.57
1:C:493:THR:HG23	5:C:2113:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:ARG:HG3	1:D:392:TYR:CB	2.34	0.57
1:D:433:LEU:C	1:D:433:LEU:HD12	2.28	0.57
1:E:254:LEU:C	1:E:255:ARG:HG2	2.28	0.57
1:E:580:GLU:HG2	1:E:581:ASN:OD1	2.04	0.57
1:F:778:THR:HB	1:F:887:GLN:HB3	1.85	0.57
1:G:130:ASP:OD1	1:G:132:SER:N	2.29	0.57
1:G:166:ARG:HG3	1:G:392:TYR:CB	2.34	0.57
1:G:645:ARG:NH2	1:G:650:GLU:OE1	2.37	0.57
1:H:316:HIS:HD2	1:H:317:THR:O	1.87	0.57
1:I:37:ARG:NH2	1:I:218:PRO:HD3	2.17	0.57
1:J:355:ASN:OD1	1:J:388:ARG:HD3	2.04	0.57
1:J:849:LEU:N	1:J:849:LEU:HD23	2.17	0.57
1:L:910:LEU:C	1:L:910:LEU:HD12	2.29	0.57
1:M:355:ASN:OD1	1:M:388:ARG:HD3	2.04	0.57
1:N:316:HIS:HD2	1:N:317:THR:O	1.87	0.57
1:N:645:ARG:HH22	1:N:650:GLU:CD	2.12	0.57
1:O:130:ASP:OD1	1:O:132:SER:N	2.30	0.57
1:O:166:ARG:HG3	1:O:392:TYR:CB	2.34	0.57
1:P:473:ARG:HD3	1:P:473:ARG:C	2.29	0.57
1:A:316:HIS:HD2	1:A:317:THR:O	1.87	0.57
1:B:153:TRP:CD1	1:B:158:TRP:HA	2.39	0.57
1:C:355:ASN:OD1	1:C:388:ARG:HD3	2.04	0.57
1:C:645:ARG:NH2	1:C:650:GLU:OE1	2.37	0.57
1:D:291:LEU:N	1:D:291:LEU:HD12	2.18	0.57
1:D:316:HIS:HD2	1:D:317:THR:O	1.87	0.57
1:E:153:TRP:CD1	1:E:158:TRP:HA	2.39	0.57
1:F:701:VAL:HG22	1:F:714:ILE:HD12	1.87	0.57
1:G:84:VAL:HG12	1:G:85:VAL:N	2.20	0.57
1:G:668:VAL:CG1	1:G:669:PRO:HD2	2.31	0.57
1:G:778:THR:HB	1:G:887:GLN:HB3	1.85	0.57
1:J:166:ARG:HG3	1:J:392:TYR:CB	2.34	0.57
1:J:910:LEU:C	1:J:910:LEU:HD12	2.29	0.57
1:K:360:HIS:HE1	1:K:362:LEU:HB2	1.61	0.57
1:K:429:ASP:OD1	1:K:430:PRO:HD2	2.03	0.57
1:K:714:ILE:HD13	1:K:714:ILE:N	2.20	0.57
1:L:255:ARG:HG2	1:L:255:ARG:NH1	2.14	0.57
1:M:153:TRP:CD1	1:M:158:TRP:HA	2.39	0.57
1:M:668:VAL:CG1	1:M:669:PRO:HD2	2.31	0.57
1:M:906:TYR:HB3	1:M:907:PRO:HD2	1.85	0.57
1:N:429:ASP:OD1	1:N:430:PRO:HD2	2.03	0.57
1:N:701:VAL:HG22	1:N:714:ILE:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:429:ASP:OD1	1:O:430:PRO:HD2	2.03	0.57
1:P:7:LEU:HD13	1:P:74:LEU:CD1	2.32	0.57
1:A:3:ILE:HG23	1:A:4:THR:H	1.70	0.57
1:A:645:ARG:HH22	1:A:650:GLU:CD	2.12	0.57
1:B:57:GLU:HG2	1:B:83:THR:HG23	1.85	0.57
1:B:178:ARG:NH1	1:B:181:GLU:O	2.33	0.57
1:C:30:HIS:ND1	1:C:31:PRO:O	2.26	0.57
1:D:254:LEU:C	1:D:255:ARG:HG2	2.28	0.57
1:E:822:LEU:CD1	1:E:824:GLN:H	2.15	0.57
1:F:910:LEU:HD12	1:F:910:LEU:C	2.29	0.57
1:G:153:TRP:CD1	1:G:158:TRP:HA	2.39	0.57
1:H:822:LEU:CD1	1:H:824:GLN:H	2.16	0.57
1:I:906:TYR:HB3	1:I:907:PRO:HD2	1.85	0.57
1:J:7:LEU:HD13	1:J:74:LEU:CD1	2.32	0.57
1:J:153:TRP:CD1	1:J:158:TRP:HA	2.39	0.57
1:J:254:LEU:C	1:J:255:ARG:HG2	2.28	0.57
1:J:473:ARG:HD3	1:J:473:ARG:C	2.29	0.57
1:J:580:GLU:HG2	1:J:581:ASN:OD1	2.04	0.57
1:K:166:ARG:HG3	1:K:392:TYR:CB	2.34	0.57
1:K:910:LEU:C	1:K:910:LEU:HD12	2.29	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:O:316:HIS:CA	1:O:323:ILE:HD13	2.32	0.57
1:O:778:THR:HB	1:O:887:GLN:HB3	1.85	0.57
1:P:166:ARG:HG3	1:P:392:TYR:CB	2.34	0.57
1:P:272:ALA:HB1	1:P:273:PRO:HD2	1.85	0.57
1:A:418:HIS:O	1:D:282:ARG:CD	2.53	0.57
1:A:580:GLU:HG2	1:A:581:ASN:OD1	2.04	0.57
1:A:822:LEU:CD1	1:A:824:GLN:H	2.16	0.57
1:B:580:GLU:HG2	1:B:581:ASN:OD1	2.04	0.57
1:C:580:GLU:HG2	1:C:581:ASN:OD1	2.04	0.57
1:D:473:ARG:HD3	1:D:473:ARG:C	2.30	0.57
1:E:57:GLU:HG2	1:E:83:THR:HG23	1.85	0.57
1:E:249:GLU:HG2	1:E:251:ARG:HH12	1.67	0.57
1:F:57:GLU:HG2	1:F:83:THR:HG23	1.85	0.57
1:F:772:ASP:OD1	1:F:772:ASP:N	2.30	0.57
1:G:3:ILE:HG23	1:G:4:THR:H	1.70	0.57
1:G:910:LEU:C	1:G:910:LEU:HD12	2.29	0.57
1:G:945:ASN:OD1	1:G:950:GLN:NE2	2.30	0.57
1:H:7:LEU:HD13	1:H:74:LEU:CD1	2.32	0.57
1:H:403:ASP:OD1	1:H:451:PRO:HD2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:316:HIS:HD2	1:I:317:THR:O	1.87	0.57
1:I:425:ARG:NH2	1:L:287:ASP:OD2	2.36	0.57
1:J:166:ARG:HG3	1:J:392:TYR:HB2	1.85	0.57
1:J:316:HIS:HD2	1:J:317:THR:O	1.87	0.57
1:J:730:LEU:HB3	1:J:731:PRO:HD2	1.85	0.57
1:L:429:ASP:OD1	1:L:430:PRO:HD2	2.03	0.57
1:L:701:VAL:HG22	1:L:714:ILE:HD12	1.87	0.57
1:L:714:ILE:HD13	1:L:714:ILE:N	2.20	0.57
1:M:403:ASP:OD1	1:M:451:PRO:HD2	2.05	0.57
1:M:645:ARG:HH22	1:M:650:GLU:CD	2.12	0.57
1:M:910:LEU:C	1:M:910:LEU:HD12	2.29	0.57
1:O:153:TRP:CD1	1:O:158:TRP:HA	2.39	0.57
1:O:763:GLY:HA3	1:O:822:LEU:CD2	2.33	0.57
1:P:166:ARG:HG3	1:P:392:TYR:HB2	1.85	0.57
1:P:403:ASP:OD1	1:P:451:PRO:HD2	2.05	0.57
1:P:778:THR:HB	1:P:887:GLN:HB3	1.85	0.57
1:A:355:ASN:OD1	1:A:388:ARG:HD3	2.04	0.57
1:B:316:HIS:CA	1:B:323:ILE:HD13	2.32	0.57
1:C:166:ARG:HG3	1:C:392:TYR:CB	2.34	0.57
1:D:84:VAL:HG12	1:D:85:VAL:N	2.20	0.57
1:D:714:ILE:N	1:D:714:ILE:HD13	2.20	0.57
1:E:473:ARG:HD3	1:E:473:ARG:C	2.29	0.57
1:E:740:LEU:CD1	1:E:741:THR:H	2.12	0.57
1:F:580:GLU:HG2	1:F:581:ASN:OD1	2.04	0.57
1:H:781:ARG:HG3	1:H:781:ARG:NH1	2.17	0.57
1:J:403:ASP:OD1	1:J:451:PRO:HD2	2.05	0.57
1:K:403:ASP:OD1	1:K:451:PRO:HD2	2.05	0.57
1:L:166:ARG:HG3	1:L:392:TYR:CB	2.34	0.57
1:N:910:LEU:HD12	1:N:910:LEU:C	2.29	0.57
1:O:3:ILE:HG23	1:O:4:THR:H	1.69	0.57
1:A:282:ARG:HH11	1:D:419:GLY:C	2.12	0.57
1:B:403:ASP:OD1	1:B:451:PRO:HD2	2.05	0.57
1:D:781:ARG:HG3	1:D:781:ARG:NH1	2.17	0.57
1:F:316:HIS:CA	1:F:323:ILE:HD13	2.32	0.57
1:G:493:THR:HG23	5:G:2113:HOH:O	2.03	0.57
1:I:894:ARG:NH1	1:I:919:ASP:OD2	2.30	0.57
1:K:166:ARG:HG3	1:K:392:TYR:HB2	1.85	0.57
1:L:316:HIS:CA	1:L:323:ILE:HD13	2.32	0.57
1:M:166:ARG:HG3	1:M:392:TYR:CB	2.34	0.57
1:M:433:LEU:C	1:M:433:LEU:HD12	2.28	0.57
1:M:778:THR:HB	1:M:887:GLN:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:153:TRP:CD1	1:N:158:TRP:HA	2.39	0.57
1:O:316:HIS:HD2	1:O:317:THR:O	1.87	0.57
1:O:355:ASN:OD1	1:O:388:ARG:HD3	2.04	0.57
1:P:781:ARG:HG3	1:P:781:ARG:NH1	2.17	0.57
1:A:166:ARG:HG3	1:A:392:TYR:CB	2.34	0.57
1:B:84:VAL:HG12	1:B:85:VAL:N	2.20	0.57
1:C:66:PRO:HB3	1:C:187:MET:CE	2.35	0.57
1:C:71:GLU:HB2	5:C:2262:HOH:O	2.05	0.57
1:C:153:TRP:CD1	1:C:158:TRP:HA	2.39	0.57
1:D:580:GLU:HG2	1:D:581:ASN:OD1	2.04	0.57
1:E:355:ASN:OD1	1:E:388:ARG:HD3	2.04	0.57
1:E:645:ARG:HH22	1:E:650:GLU:CD	2.12	0.57
1:E:701:VAL:HG22	1:E:714:ILE:HD12	1.87	0.57
1:F:153:TRP:CD1	1:F:158:TRP:HA	2.39	0.57
1:G:355:ASN:OD1	1:G:388:ARG:HD3	2.04	0.57
1:G:767:GLN:HG3	1:G:768:MET:N	2.20	0.57
1:H:166:ARG:HG3	1:H:392:TYR:HB2	1.85	0.57
1:I:3:ILE:HG23	1:I:4:THR:H	1.70	0.57
1:I:473:ARG:HD3	1:I:473:ARG:C	2.29	0.57
1:I:778:THR:HB	1:I:887:GLN:HB3	1.85	0.57
1:K:355:ASN:OD1	1:K:388:ARG:HD3	2.04	0.57
1:L:1021:CME:HB3	1:L:1021:CME:CZ	2.21	0.57
1:M:763:GLY:HA3	1:M:822:LEU:CD2	2.33	0.57
1:O:254:LEU:C	1:O:255:ARG:HG2	2.28	0.57
1:O:906:TYR:HB3	1:O:907:PRO:HD2	1.85	0.57
1:A:403:ASP:OD1	1:A:451:PRO:HD2	2.05	0.57
1:B:701:VAL:HG22	1:B:714:ILE:HD12	1.87	0.57
1:C:316:HIS:HD2	1:C:317:THR:O	1.87	0.57
1:C:473:ARG:HD3	1:C:473:ARG:C	2.29	0.57
1:C:701:VAL:HG22	1:C:714:ILE:HD12	1.87	0.57
1:D:3:ILE:HG23	1:D:4:THR:H	1.70	0.57
1:E:3:ILE:HG23	1:E:4:THR:H	1.70	0.57
1:E:66:PRO:HB3	1:E:187:MET:CE	2.35	0.57
1:G:580:GLU:HG2	1:G:581:ASN:OD1	2.04	0.57
1:G:906:TYR:HB3	1:G:907:PRO:HD2	1.85	0.57
1:H:272:ALA:HB1	1:H:273:PRO:HD2	1.85	0.57
1:I:910:LEU:C	1:I:910:LEU:HD12	2.29	0.57
1:J:3:ILE:HG23	1:J:4:THR:H	1.69	0.57
1:J:66:PRO:HB3	1:J:187:MET:CE	2.35	0.57
1:K:272:ALA:HB1	1:K:273:PRO:HD2	1.85	0.57
1:K:781:ARG:HG3	1:K:781:ARG:NH1	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:130:ASP:OD1	1:L:132:SER:N	2.29	0.57
1:L:249:GLU:HG2	1:L:251:ARG:HH12	1.67	0.57
1:M:3:ILE:HG23	1:M:4:THR:H	1.70	0.57
1:O:71:GLU:HB2	5:O:2261:HOH:O	2.05	0.57
1:O:403:ASP:OD1	1:O:451:PRO:HD2	2.05	0.57
1:P:66:PRO:HB3	1:P:187:MET:CE	2.35	0.57
1:P:316:HIS:HD2	1:P:317:THR:O	1.87	0.57
1:P:580:GLU:HG2	1:P:581:ASN:OD1	2.04	0.57
1:B:66:PRO:HB3	1:B:187:MET:CE	2.35	0.57
1:D:403:ASP:OD1	1:D:451:PRO:HD2	2.05	0.57
1:F:30:HIS:ND1	1:F:31:PRO:O	2.26	0.57
1:F:66:PRO:HB3	1:F:187:MET:CE	2.35	0.57
1:F:654:TRP:CE3	1:F:655:MET:HA	2.40	0.57
1:G:701:VAL:HG22	1:G:714:ILE:HD12	1.87	0.57
1:H:473:ARG:HD3	1:H:473:ARG:C	2.29	0.57
1:I:66:PRO:HB3	1:I:187:MET:CE	2.35	0.57
1:I:316:HIS:CA	1:I:323:ILE:HD13	2.32	0.57
1:K:66:PRO:HB3	1:K:187:MET:CE	2.35	0.57
1:M:84:VAL:HG12	1:M:85:VAL:N	2.20	0.57
1:M:701:VAL:HG22	1:M:714:ILE:HD12	1.87	0.57
1:N:66:PRO:HB3	1:N:187:MET:CE	2.35	0.57
1:N:287:ASP:OD1	1:N:287:ASP:N	2.29	0.57
1:N:316:HIS:CA	1:N:323:ILE:HD13	2.33	0.57
1:O:580:GLU:HG2	1:O:581:ASN:OD1	2.04	0.57
1:P:822:LEU:CD1	1:P:824:GLN:H	2.16	0.57
1:A:654:TRP:CE3	1:A:655:MET:HA	2.40	0.56
1:B:654:TRP:CE3	1:B:655:MET:HA	2.40	0.56
1:C:3:ILE:HG23	1:C:4:THR:H	1.70	0.56
1:C:84:VAL:HG12	1:C:85:VAL:N	2.20	0.56
1:C:654:TRP:CE3	1:C:655:MET:HA	2.40	0.56
1:C:714:ILE:HD13	1:C:714:ILE:N	2.20	0.56
1:E:668:VAL:CG1	1:E:669:PRO:HD2	2.31	0.56
1:F:84:VAL:HG12	1:F:85:VAL:N	2.20	0.56
1:F:403:ASP:OD1	1:F:451:PRO:HD2	2.05	0.56
1:F:714:ILE:HD13	1:F:714:ILE:N	2.20	0.56
1:G:71:GLU:HB2	5:G:2262:HOH:O	2.05	0.56
1:G:403:ASP:OD1	1:G:451:PRO:HD2	2.05	0.56
1:H:66:PRO:HB3	1:H:187:MET:CE	2.35	0.56
1:J:30:HIS:ND1	1:J:31:PRO:O	2.26	0.56
1:J:767:GLN:HG3	1:J:768:MET:N	2.20	0.56
1:K:3:ILE:HG23	1:K:4:THR:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:84:VAL:HG12	1:K:85:VAL:N	2.20	0.56
1:L:654:TRP:CE3	1:L:655:MET:HA	2.40	0.56
1:M:254:LEU:C	1:M:255:ARG:HG2	2.28	0.56
1:M:473:ARG:HD3	1:M:473:ARG:C	2.29	0.56
1:O:66:PRO:HB3	1:O:187:MET:CE	2.35	0.56
1:O:701:VAL:HG22	1:O:714:ILE:HD12	1.87	0.56
1:P:355:ASN:OD1	1:P:388:ARG:HD3	2.04	0.56
1:A:71:GLU:HB2	5:A:2260:HOH:O	2.05	0.56
1:B:71:GLU:HB2	5:B:2261:HOH:O	2.05	0.56
1:E:78:LEU:HD23	1:E:78:LEU:N	2.21	0.56
1:G:66:PRO:HB3	1:G:187:MET:CE	2.35	0.56
1:H:580:GLU:HG2	1:H:581:ASN:OD1	2.04	0.56
1:I:355:ASN:OD1	1:I:388:ARG:HD3	2.04	0.56
1:I:645:ARG:HH22	1:I:650:GLU:CD	2.12	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:822:LEU:CD1	1:K:824:GLN:H	2.15	0.56
1:L:3:ILE:HG23	1:L:4:THR:H	1.69	0.56
1:N:654:TRP:CE3	1:N:655:MET:HA	2.40	0.56
1:P:714:ILE:HD13	1:P:714:ILE:N	2.20	0.56
1:A:140:ARG:HB2	1:A:171:PHE:O	2.06	0.56
1:A:767:GLN:HG3	1:A:768:MET:N	2.20	0.56
1:B:767:GLN:HG3	1:B:768:MET:N	2.20	0.56
1:B:778:THR:HB	1:B:887:GLN:HB3	1.85	0.56
1:B:800:ARG:HB3	1:B:800:ARG:CZ	2.36	0.56
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.04	0.56
1:E:166:ARG:HG3	1:E:392:TYR:CB	2.34	0.56
1:E:767:GLN:HA	1:E:776:LEU:HD12	1.88	0.56
1:F:71:GLU:HB2	5:F:2262:HOH:O	2.05	0.56
1:F:140:ARG:HB2	1:F:171:PHE:O	2.06	0.56
1:F:355:ASN:OD1	1:F:388:ARG:HD3	2.04	0.56
1:F:668:VAL:CG1	1:F:669:PRO:HD2	2.31	0.56
1:F:894:ARG:HH22	1:F:921:PRO:HD3	1.71	0.56
1:G:433:LEU:C	1:G:433:LEU:HD12	2.28	0.56
1:G:767:GLN:HA	1:G:776:LEU:HD12	1.88	0.56
1:G:800:ARG:HB3	1:G:800:ARG:CZ	2.36	0.56
1:H:3:ILE:HG23	1:H:4:THR:H	1.69	0.56
1:H:140:ARG:HB2	1:H:171:PHE:O	2.06	0.56
1:H:654:TRP:CE3	1:H:655:MET:HA	2.40	0.56
1:H:714:ILE:HD13	1:H:714:ILE:N	2.20	0.56
1:I:140:ARG:HB2	1:I:171:PHE:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:767:GLN:HG3	1:I:768:MET:N	2.20	0.56
1:J:654:TRP:CE3	1:J:655:MET:HA	2.40	0.56
1:K:740:LEU:CD1	1:K:741:THR:H	2.12	0.56
1:L:84:VAL:HG12	1:L:85:VAL:N	2.20	0.56
1:L:767:GLN:HG3	1:L:768:MET:N	2.20	0.56
1:L:906:TYR:HB3	1:L:907:PRO:HD2	1.85	0.56
1:M:249:GLU:HG2	1:M:251:ARG:HH12	1.67	0.56
1:M:767:GLN:HA	1:M:776:LEU:HD12	1.88	0.56
1:N:140:ARG:HB2	1:N:171:PHE:O	2.06	0.56
1:N:255:ARG:HG2	1:N:255:ARG:NH1	2.14	0.56
1:O:287:ASP:OD1	1:O:287:ASP:N	2.29	0.56
1:O:433:LEU:C	1:O:433:LEU:HD12	2.28	0.56
1:O:724:GLU:O	1:P:847:LYS:NZ	2.27	0.56
1:O:767:GLN:HA	1:O:776:LEU:HD12	1.88	0.56
1:O:800:ARG:HB3	1:O:800:ARG:CZ	2.36	0.56
1:P:140:ARG:HB2	1:P:171:PHE:O	2.06	0.56
1:P:894:ARG:HH22	1:P:921:PRO:HD3	1.71	0.56
1:B:3:ILE:HG23	1:B:4:THR:H	1.70	0.56
1:C:403:ASP:OD1	1:C:451:PRO:HD2	2.05	0.56
1:D:140:ARG:HB2	1:D:171:PHE:O	2.06	0.56
1:D:178:ARG:NH1	1:D:181:GLU:O	2.33	0.56
1:D:701:VAL:HG22	1:D:714:ILE:HD12	1.87	0.56
1:D:800:ARG:HB3	1:D:800:ARG:CZ	2.36	0.56
1:E:71:GLU:HB2	5:E:2262:HOH:O	2.05	0.56
1:F:786:ARG:HH11	1:F:990:HIS:HE1	1.54	0.56
1:G:894:ARG:HH22	1:G:921:PRO:HD3	1.71	0.56
1:H:701:VAL:HG22	1:H:714:ILE:HD12	1.87	0.56
1:H:894:ARG:HH22	1:H:921:PRO:HD3	1.71	0.56
1:I:654:TRP:CE3	1:I:655:MET:HA	2.40	0.56
1:J:714:ILE:HD13	1:J:714:ILE:N	2.20	0.56
1:J:800:ARG:HB3	1:J:800:ARG:CZ	2.36	0.56
1:N:71:GLU:HB2	5:N:2261:HOH:O	2.05	0.56
1:N:786:ARG:HH11	1:N:990:HIS:HE1	1.54	0.56
1:P:668:VAL:CG1	1:P:669:PRO:HD2	2.31	0.56
1:A:334:GLU:OE1	1:A:336:ARG:NH1	2.39	0.56
1:B:130:ASP:OD1	1:B:132:SER:N	2.29	0.56
1:B:473:ARG:HD3	1:B:473:ARG:C	2.29	0.56
1:B:714:ILE:HD13	1:B:714:ILE:N	2.20	0.56
1:C:786:ARG:HH11	1:C:990:HIS:HE1	1.54	0.56
1:F:334:GLU:OE1	1:F:336:ARG:NH1	2.39	0.56
1:G:654:TRP:CE3	1:G:655:MET:HA	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:130:ASP:OD1	1:H:132:SER:N	2.29	0.56
1:I:287:ASP:CG	1:L:425:ARG:HH22	2.13	0.56
1:I:800:ARG:HB3	1:I:800:ARG:CZ	2.36	0.56
1:K:654:TRP:CE3	1:K:655:MET:HA	2.40	0.56
1:M:66:PRO:HB3	1:M:187:MET:CE	2.35	0.56
1:M:71:GLU:HB2	5:M:2261:HOH:O	2.05	0.56
1:M:740:LEU:CD1	1:M:741:THR:H	2.12	0.56
1:M:894:ARG:HH22	1:M:921:PRO:HD3	1.71	0.56
1:N:3:ILE:HG23	1:N:4:THR:H	1.69	0.56
1:O:84:VAL:HG12	1:O:85:VAL:N	2.20	0.56
1:O:654:TRP:CE3	1:O:655:MET:HA	2.40	0.56
1:O:786:ARG:HH11	1:O:990:HIS:HE1	1.54	0.56
1:O:894:ARG:HH22	1:O:921:PRO:HD3	1.71	0.56
1:P:701:VAL:HG22	1:P:714:ILE:HD12	1.87	0.56
1:A:66:PRO:HB3	1:A:187:MET:CE	2.35	0.56
1:A:473:ARG:HD3	1:A:473:ARG:C	2.29	0.56
1:A:701:VAL:HG22	1:A:714:ILE:HD12	1.87	0.56
1:B:334:GLU:OE1	1:B:336:ARG:NH1	2.39	0.56
1:D:7:LEU:HD13	1:D:74:LEU:CD1	2.32	0.56
1:E:84:VAL:HG12	1:E:85:VAL:N	2.20	0.56
1:E:334:GLU:OE1	1:E:336:ARG:NH1	2.39	0.56
1:G:786:ARG:HH11	1:G:990:HIS:HE1	1.54	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:K:71:GLU:HB2	5:K:2262:HOH:O	2.05	0.56
1:K:894:ARG:HH22	1:K:921:PRO:HD3	1.71	0.56
1:M:166:ARG:HG2	1:M:414:ASN:ND2	2.21	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:N:473:ARG:HD3	1:N:473:ARG:C	2.29	0.56
1:N:822:LEU:CD1	1:N:824:GLN:H	2.16	0.56
1:P:654:TRP:CE3	1:P:655:MET:HA	2.40	0.56
1:A:975:LEU:N	1:A:975:LEU:HD23	2.21	0.56
1:B:140:ARG:HB2	1:B:171:PHE:O	2.06	0.56
1:B:767:GLN:HA	1:B:776:LEU:HD12	1.88	0.56
1:C:975:LEU:N	1:C:975:LEU:HD23	2.21	0.56
1:D:66:PRO:HB3	1:D:187:MET:CE	2.35	0.56
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.39	0.56
1:D:767:GLN:HG3	1:D:768:MET:N	2.20	0.56
1:F:767:GLN:HA	1:F:776:LEU:HD12	1.88	0.56
1:H:71:GLU:HB2	5:H:2262:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:71:GLU:HB2	5:I:2262:HOH:O	2.05	0.56
1:I:701:VAL:HG22	1:I:714:ILE:HD12	1.87	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:K:166:ARG:HG2	1:K:414:ASN:ND2	2.21	0.56
1:K:316:HIS:HD2	1:K:317:THR:O	1.87	0.56
1:L:316:HIS:HD2	1:L:317:THR:O	1.87	0.56
1:M:334:GLU:OE1	1:M:336:ARG:NH1	2.39	0.56
1:M:654:TRP:CE3	1:M:655:MET:HA	2.40	0.56
1:N:767:GLN:HA	1:N:776:LEU:HD12	1.88	0.56
1:P:3:ILE:HG23	1:P:4:THR:H	1.69	0.56
1:A:800:ARG:HB3	1:A:800:ARG:CZ	2.36	0.56
1:B:166:ARG:HG2	1:B:414:ASN:ND2	2.21	0.56
1:F:316:HIS:HD2	1:F:317:THR:O	1.87	0.56
1:H:744:GLU:C	1:H:745:MET:HE2	2.31	0.56
1:I:166:ARG:HG2	1:I:414:ASN:ND2	2.21	0.56
1:I:714:ILE:HD13	1:I:714:ILE:N	2.20	0.56
1:I:767:GLN:HA	1:I:776:LEU:HD12	1.88	0.56
1:J:166:ARG:HG2	1:J:414:ASN:ND2	2.21	0.56
1:J:781:ARG:HG3	1:J:781:ARG:NH1	2.17	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:A:419:GLY:CA	1:D:282:ARG:NH1	2.65	0.56
1:C:166:ARG:HG2	1:C:414:ASN:ND2	2.21	0.56
1:D:57:GLU:HG2	1:D:83:THR:HG23	1.85	0.56
1:D:740:LEU:CD1	1:D:741:THR:H	2.12	0.56
1:D:744:GLU:C	1:D:745:MET:HE2	2.31	0.56
1:E:403:ASP:OD1	1:E:451:PRO:HD2	2.05	0.56
1:E:714:ILE:HD13	1:E:714:ILE:N	2.20	0.56
1:E:767:GLN:HG3	1:E:768:MET:N	2.20	0.56
1:H:334:GLU:OE1	1:H:336:ARG:NH1	2.39	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:K:334:GLU:OE1	1:K:336:ARG:NH1	2.39	0.56
1:L:767:GLN:HA	1:L:776:LEU:HD12	1.88	0.56
1:L:800:ARG:HB3	1:L:800:ARG:CZ	2.36	0.56
1:N:800:ARG:HB3	1:N:800:ARG:CZ	2.36	0.56
1:O:473:ARG:HD3	1:O:473:ARG:C	2.29	0.56
1:P:71:GLU:HB2	5:P:2263:HOH:O	2.05	0.56
1:D:822:LEU:CD1	1:D:824:GLN:H	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:654:TRP:CE3	1:E:655:MET:HA	2.40	0.56
1:F:473:ARG:HD3	1:F:473:ARG:C	2.29	0.56
1:F:800:ARG:HB3	1:F:800:ARG:CZ	2.36	0.56
1:G:140:ARG:HB2	1:G:171:PHE:O	2.06	0.56
1:G:473:ARG:HD3	1:G:473:ARG:C	2.29	0.56
1:I:744:GLU:C	1:I:745:MET:HE2	2.31	0.56
1:J:701:VAL:HG22	1:J:714:ILE:HD12	1.87	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:L:140:ARG:HB2	1:L:171:PHE:O	2.06	0.56
1:L:894:ARG:HH22	1:L:921:PRO:HD3	1.71	0.56
1:M:140:ARG:HB2	1:M:171:PHE:O	2.06	0.56
1:M:767:GLN:HG3	1:M:768:MET:N	2.20	0.56
1:M:786:ARG:HH11	1:M:990:HIS:HE1	1.54	0.56
1:O:334:GLU:OE1	1:O:336:ARG:NH1	2.39	0.56
1:O:767:GLN:HG3	1:O:768:MET:N	2.20	0.56
1:A:84:VAL:HG12	1:A:85:VAL:N	2.20	0.55
1:A:744:GLU:C	1:A:745:MET:HE2	2.31	0.55
1:C:744:GLU:C	1:C:745:MET:HE2	2.31	0.55
1:D:166:ARG:HG2	1:D:414:ASN:ND2	2.21	0.55
1:D:767:GLN:HA	1:D:776:LEU:HD12	1.88	0.55
1:E:140:ARG:HB2	1:E:171:PHE:O	2.06	0.55
1:E:166:ARG:HG2	1:E:414:ASN:ND2	2.21	0.55
1:E:786:ARG:HH11	1:E:990:HIS:HE1	1.54	0.55
1:F:166:ARG:HG2	1:F:414:ASN:ND2	2.21	0.55
1:H:767:GLN:HA	1:H:776:LEU:HD12	1.88	0.55
1:I:84:VAL:HG12	1:I:85:VAL:N	2.20	0.55
1:K:800:ARG:HB3	1:K:800:ARG:CZ	2.36	0.55
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:HB3	1:M:800:ARG:CZ	2.36	0.55
1:N:84:VAL:HG12	1:N:85:VAL:N	2.20	0.55
1:N:989:PHE:CE1	1:N:1014:TYR:HB3	2.42	0.55
1:P:767:GLN:HA	1:P:776:LEU:HD12	1.88	0.55
1:A:714:ILE:HD13	1:A:714:ILE:N	2.20	0.55
1:C:334:GLU:OE1	1:C:336:ARG:NH1	2.39	0.55
1:D:989:PHE:CE1	1:D:1014:TYR:HB3	2.42	0.55
1:G:166:ARG:HG2	1:G:414:ASN:ND2	2.21	0.55
1:H:84:VAL:HG12	1:H:85:VAL:N	2.20	0.55
1:K:767:GLN:HG3	1:K:768:MET:N	2.20	0.55
1:L:403:ASP:OD1	1:L:451:PRO:HD2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:714:ILE:HD13	1:N:714:ILE:N	2.20	0.55
1:O:166:ARG:HG2	1:O:414:ASN:ND2	2.21	0.55
1:P:316:HIS:CA	1:P:323:ILE:HD13	2.32	0.55
1:C:767:GLN:HG3	1:C:768:MET:N	2.20	0.55
1:E:5:ASP:OD2	1:E:157:ARG:HA	2.07	0.55
1:F:50:GLN:O	1:F:215:LEU:HA	2.07	0.55
1:F:975:LEU:N	1:F:975:LEU:HD23	2.21	0.55
1:G:30:HIS:ND1	1:G:31:PRO:O	2.26	0.55
1:G:744:GLU:C	1:G:745:MET:HE2	2.31	0.55
1:H:767:GLN:HG3	1:H:768:MET:N	2.20	0.55
1:H:786:ARG:HH11	1:H:990:HIS:HE1	1.54	0.55
1:H:975:LEU:N	1:H:975:LEU:HD23	2.21	0.55
1:I:975:LEU:N	1:I:975:LEU:HD23	2.21	0.55
1:J:71:GLU:HB2	5:J:2262:HOH:O	2.05	0.55
1:K:249:GLU:HG2	1:K:251:ARG:HH12	1.67	0.55
1:K:701:VAL:HG22	1:K:714:ILE:HD12	1.87	0.55
1:K:989:PHE:CE1	1:K:1014:TYR:HB3	2.42	0.55
1:M:78:LEU:HD23	1:M:78:LEU:N	2.21	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:O:744:GLU:C	1:O:745:MET:HE2	2.31	0.55
1:P:767:GLN:HG3	1:P:768:MET:N	2.20	0.55
1:P:772:ASP:OD1	1:P:772:ASP:N	2.30	0.55
1:P:786:ARG:HH11	1:P:990:HIS:HE1	1.54	0.55
1:A:668:VAL:CG1	1:A:669:PRO:HD2	2.31	0.55
1:B:78:LEU:HD23	1:B:78:LEU:N	2.21	0.55
1:C:894:ARG:HH22	1:C:921:PRO:HD3	1.71	0.55
1:D:71:GLU:HB2	5:D:2263:HOH:O	2.05	0.55
1:E:7:LEU:HD13	1:E:74:LEU:CD1	2.32	0.55
1:E:781:ARG:HG3	1:E:781:ARG:NH1	2.17	0.55
1:F:3:ILE:HG23	1:F:4:THR:H	1.70	0.55
1:G:334:GLU:OE1	1:G:336:ARG:NH1	2.39	0.55
1:L:66:PRO:HB3	1:L:187:MET:CE	2.35	0.55
1:L:71:GLU:HB2	5:L:2262:HOH:O	2.05	0.55
1:L:473:ARG:HD3	1:L:473:ARG:C	2.29	0.55
1:M:282:ARG:HB2	1:P:422:PRO:HA	1.87	0.55
1:M:781:ARG:HG3	1:M:781:ARG:NH1	2.17	0.55
1:N:166:ARG:HG2	1:N:414:ASN:ND2	2.21	0.55
1:N:767:GLN:HG3	1:N:768:MET:N	2.20	0.55
1:O:975:LEU:N	1:O:975:LEU:HD23	2.21	0.55
1:B:744:GLU:C	1:B:745:MET:HE2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:ARG:HH11	1:B:990:HIS:HE1	1.54	0.55
1:D:50:GLN:O	1:D:215:LEU:HA	2.07	0.55
1:E:989:PHE:CE1	1:E:1014:TYR:HB3	2.42	0.55
1:H:50:GLN:O	1:H:215:LEU:HA	2.07	0.55
1:J:140:ARG:HB2	1:J:171:PHE:O	2.06	0.55
1:K:975:LEU:N	1:K:975:LEU:HD23	2.21	0.55
1:N:78:LEU:HD23	1:N:78:LEU:N	2.21	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:P:800:ARG:HB3	1:P:800:ARG:CZ	2.36	0.55
1:A:166:ARG:HG2	1:A:414:ASN:ND2	2.21	0.55
1:C:258:VAL:HA	1:C:312:VAL:O	2.07	0.55
1:C:800:ARG:HB3	1:C:800:ARG:CZ	2.36	0.55
1:D:5:ASP:OD2	1:D:157:ARG:HA	2.07	0.55
1:D:786:ARG:HH11	1:D:990:HIS:HE1	1.54	0.55
1:F:258:VAL:HA	1:F:312:VAL:O	2.07	0.55
1:G:5:ASP:OD2	1:G:157:ARG:HA	2.07	0.55
1:G:316:HIS:CA	1:G:323:ILE:HD13	2.32	0.55
1:G:714:ILE:HD13	1:G:714:ILE:N	2.20	0.55
1:H:258:VAL:HA	1:H:312:VAL:O	2.07	0.55
1:H:316:HIS:CA	1:H:323:ILE:HD13	2.32	0.55
1:H:668:VAL:CG1	1:H:669:PRO:HD2	2.31	0.55
1:H:800:ARG:HB3	1:H:800:ARG:CZ	2.36	0.55
1:I:57:GLU:HG2	1:I:83:THR:HG23	1.84	0.55
1:I:282:ARG:HD3	1:L:418:HIS:O	2.06	0.55
1:K:786:ARG:HH11	1:K:990:HIS:HE1	1.54	0.55
1:L:668:VAL:CG1	1:L:669:PRO:HD2	2.31	0.55
1:M:7:LEU:HD13	1:M:74:LEU:CD1	2.32	0.55
1:O:30:HIS:ND1	1:O:31:PRO:O	2.26	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:P:334:GLU:OE1	1:P:336:ARG:NH1	2.39	0.55
1:A:50:GLN:O	1:A:215:LEU:HA	2.07	0.55
1:A:258:VAL:HA	1:A:312:VAL:O	2.07	0.55
1:A:786:ARG:HH11	1:A:990:HIS:HE1	1.54	0.55
1:B:975:LEU:HD23	1:B:975:LEU:N	2.21	0.55
1:C:140:ARG:HB2	1:C:171:PHE:O	2.06	0.55
1:E:800:ARG:HB3	1:E:800:ARG:CZ	2.36	0.55
1:G:50:GLN:O	1:G:215:LEU:HA	2.07	0.55
1:G:989:PHE:CE1	1:G: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	Interatomic distance (Å)	Clash overlap (Å)
1:J:5:ASP:OD2	1:J:157:ARG:HA	2.07	0.55
1:J:744:GLU:C	1:J:745:MET:HE2	2.31	0.55
1:M:5:ASP:OD2	1:M:157:ARG:HA	2.07	0.55
1:M:989:PHE:CE1	1:M:1014:TYR:HB3	2.42	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:P:50:GLN:O	1:P:215:LEU:HA	2.07	0.55
1:A:7:LEU:HD13	1:A:74:LEU:CD1	2.32	0.55
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.42	0.55
1:A:989:PHE:CE1	1:A:1014:TYR:HB3	2.42	0.55
1:C:767:GLN:HA	1:C:776:LEU:HD12	1.88	0.55
1:D:975:LEU:N	1:D:975:LEU:HD23	2.21	0.55
1:E:37:ARG:HH11	1:E:37:ARG:CG	2.20	0.55
1:G:258:VAL:HA	1:G:312:VAL:O	2.07	0.55
1:I:37:ARG:HH11	1:I:37:ARG:CG	2.20	0.55
1:J:50:GLN:O	1:J:215:LEU:HA	2.07	0.55
1:J:989:PHE:CE1	1:J:1014:TYR:HB3	2.42	0.55
1:K:744:GLU:C	1:K:745:MET:HE2	2.31	0.55
1:L:744:GLU:C	1:L:745:MET:HE2	2.31	0.55
1:M:37:ARG:HH11	1:M:37:ARG:CG	2.20	0.55
1:M:975:LEU:HD23	1:M:975:LEU:N	2.21	0.55
1:O:989:PHE:CE1	1:O:1014:TYR:HB3	2.42	0.55
1:A:767:GLN:HA	1:A:776:LEU:HD12	1.88	0.55
1:C:78:LEU:HD23	1:C:78:LEU:N	2.21	0.55
1:D:437:SER:HB2	5:D:2103:HOH:O	2.07	0.55
1:E:258:VAL:HA	1:E:312:VAL:O	2.07	0.55
1:E:744:GLU:C	1:E:745:MET:HE2	2.31	0.55
1:E:975:LEU:HD23	1:E:975:LEU:N	2.21	0.55
1:F:5:ASP:OD2	1:F:157:ARG:HA	2.07	0.55
1:F:39:SER:OG	1:F:40:GLU:N	2.40	0.55
1:F:767:GLN:HG3	1:F:768:MET:N	2.20	0.55
1:F:989:PHE:CE1	1:F:1014:TYR:HB3	2.42	0.55
1:G:37:ARG:HH11	1:G:37:ARG:CG	2.20	0.55
1:J:178:ARG:NH1	1:J:181:GLU:O	2.33	0.55
1:K:130:ASP:OD1	1:K:132:SER:N	2.30	0.55
1:L:50:GLN:O	1:L:215:LEU:HA	2.07	0.55
1:L:989:PHE:CE1	1:L:1014:TYR:HB3	2.42	0.55
1:M:744:GLU:C	1:M:745:MET:HE2	2.31	0.55
1:P:595:THR:HG23	1:P:596:PRO:CA	2.37	0.55
1:P:744:GLU:C	1:P:745:MET:HE2	2.31	0.55
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:GLN:O	1:B:682:LEU:HB2	2.07	0.55
1:D:258:VAL:HA	1:D:312:VAL:O	2.07	0.55
1:E:425:ARG:NH2	1:H:287:ASP:OD2	2.40	0.55
1:F:744:GLU:C	1:F:745:MET:HE2	2.31	0.55
1:H:595:THR:HG23	1:H:596:PRO:CA	2.37	0.55
1:H:989:PHE:CE1	1:H:1014:TYR:HB3	2.42	0.55
1:I:258:VAL:HA	1:I:312:VAL:O	2.07	0.55
1:J:258:VAL:HA	1:J:312:VAL:O	2.07	0.55
1:L:37:ARG:HH11	1:L:37:ARG:CG	2.20	0.55
1:M:258:VAL:HA	1:M:312:VAL:O	2.07	0.55
1:N:39:SER:OG	1:N:40:GLU:N	2.40	0.55
1:N:403:ASP:OD2	1:N:450:HIS:ND1	2.34	0.55
1:O:740:LEU:CD1	1:O:741:THR:H	2.12	0.55
1:P:5:ASP:OD2	1:P:157:ARG:HA	2.07	0.55
1:P:166:ARG:HG2	1:P:414:ASN:ND2	2.21	0.55
1:P:975:LEU:HD23	1:P:975:LEU:N	2.21	0.55
1:C:50:GLN:O	1:C:215:LEU:HA	2.07	0.54
1:C:668:VAL:CG1	1:C:669:PRO:HD2	2.31	0.54
1:E:634:GLN:O	1:E:682:LEU:HB2	2.07	0.54
1:G:127:PHE:CE2	1:G:184:LEU:HG	2.42	0.54
1:G:634:GLN:O	1:G:682:LEU:HB2	2.07	0.54
1:I:50:GLN:O	1:I:215:LEU:HA	2.07	0.54
1:J:37:ARG:HH11	1:J:37:ARG:CG	2.20	0.54
1:L:287:ASP:OD1	1:L:287:ASP:N	2.29	0.54
1:L:975:LEU:N	1:L:975:LEU:HD23	2.21	0.54
1:M:50:GLN:O	1:M:215:LEU:HA	2.07	0.54
1:N:5:ASP:OD2	1:N:157:ARG:HA	2.07	0.54
1:N:744:GLU:C	1:N:745:MET:HE2	2.31	0.54
1:O:37:ARG:HH11	1:O:37:ARG:CG	2.20	0.54
1:P:39:SER:OG	1:P:40:GLU:N	2.40	0.54
1:P:78:LEU:HD23	1:P:78:LEU:N	2.21	0.54
1:B:37:ARG:HH11	1:B:37:ARG:CG	2.20	0.54
1:B:50:GLN:O	1:B:215:LEU:HA	2.07	0.54
1:B:742:THR:HG22	1:B:743:SER:H	1.73	0.54
1:D:39:SER:OG	1:D:40:GLU:N	2.40	0.54
1:D:634:GLN:O	1:D:682:LEU:HB2	2.07	0.54
1:F:130:ASP:OD1	1:F:132:SER:N	2.29	0.54
1:H:39:SER:OG	1:H:40:GLU:N	2.40	0.54
1:K:5:ASP:OD2	1:K:157:ARG:HA	2.07	0.54
1:L:78:LEU:HD23	1:L:78:LEU:N	2.21	0.54
1:M:282:ARG:HG3	1:P:423:MET:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:37:ARG:HH11	1:P:37:ARG:CG	2.20	0.54
1:P:952:ARG:O	1:P:1018:LEU:HD23	2.08	0.54
1:A:78:LEU:HD23	1:A:78:LEU:N	2.21	0.54
1:B:595:THR:HG23	1:B:596:PRO:CA	2.38	0.54
1:B:989:PHE:CE1	1:B:1014:TYR:HB3	2.42	0.54
1:C:5:ASP:OD2	1:C:157:ARG:HA	2.07	0.54
1:D:654:TRP:CE3	1:D:655:MET:HA	2.40	0.54
1:F:742:THR:HG22	1:F:743:SER:H	1.73	0.54
1:G:742:THR:HG22	1:G:743:SER:H	1.73	0.54
1:H:127:PHE:CE2	1:H:184:LEU:HG	2.42	0.54
1:H:166:ARG:HG2	1:H:414:ASN:ND2	2.21	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:N:130:ASP:OD1	1:N:132:SER:N	2.29	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:A:808:GLU:OE1	1:A:808:GLU:HA	2.08	0.54
1:A:952:ARG:O	1:A:1018:LEU:HD23	2.08	0.54
1:B:287:ASP:CG	1:C:425:ARG:HH22	2.16	0.54
1:C:742:THR:HG22	1:C:743:SER:H	1.73	0.54
1:C:952:ARG:O	1:C:1018:LEU:HD23	2.08	0.54
1:D:952:ARG:O	1:D:1018:LEU:HD23	2.08	0.54
1:E:952:ARG:O	1:E:1018:LEU:HD23	2.08	0.54
1:F:952:ARG:O	1:F:1018:LEU:HD23	2.08	0.54
1:I:127:PHE:CE2	1:I:184:LEU:HG	2.42	0.54
1:I:822:LEU:CD1	1:I:824:GLN:H	2.16	0.54
1:J:668:VAL:CG1	1:J:669:PRO:HD2	2.31	0.54
1:K:634:GLN:O	1:K:682:LEU:HB2	2.07	0.54
1:L:5:ASP:OD2	1:L:157:ARG:HA	2.07	0.54
1:P:989:PHE:CE1	1:P:1014:TYR:HB3	2.42	0.54
1:A:742:THR:HG22	1:A:743:SER:H	1.72	0.54
1:B:737:ILE:HB	1:B:738:PRO:HD2	1.90	0.54
1:D:37:ARG:HH11	1:D:37:ARG:CG	2.20	0.54
1:E:50:GLN:O	1:E:215:LEU:HA	2.07	0.54
1:L:952:ARG:O	1:L:1018:LEU:HD23	2.08	0.54
1:P:127:PHE:CE2	1:P:184:LEU:HG	2.42	0.54
1:C:316:HIS:CA	1:C:323:ILE:HD13	2.33	0.54
1:C:989:PHE:CE1	1:C:1014:TYR:HB3	2.42	0.54
1:D:127:PHE:CE2	1:D:184:LEU:HG	2.42	0.54
1:G:876:THR:OG1	1:G:877:PRO:HD2	2.08	0.54
1:H:808:GLU:OE1	1:H:808:GLU:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:5:ASP:OD2	1:I:157:ARG:HA	2.07	0.54
1:I:894:ARG:HH22	1:I:921:PRO:HD3	1.71	0.54
1:J:952:ARG:O	1:J:1018:LEU:HD23	2.08	0.54
1:K:920:LEU:HB3	1:K:921:PRO:CD	2.38	0.54
1:L:258:VAL:HA	1:L:312:VAL:O	2.07	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:N:50:GLN:O	1:N:215:LEU:HA	2.07	0.54
1:N:515:VAL:HG21	1:O:281:GLU:HG3	1.90	0.54
1:N:894:ARG:HH22	1:N:921:PRO:HD3	1.71	0.54
1:O:876:THR:OG1	1:O:877:PRO:HD2	2.08	0.54
1:B:5:ASP:OD2	1:B:157:ARG:HA	2.07	0.54
1:B:258:VAL:HA	1:B:312:VAL:O	2.07	0.54
1:C:634:GLN:O	1:C:682:LEU:HB2	2.07	0.54
1:E:876:THR:OG1	1:E:877:PRO:HD2	2.08	0.54
1:F:737:ILE:HB	1:F:738:PRO:HD2	1.90	0.54
1:G:595:THR:HG23	1:G:596:PRO:CA	2.38	0.54
1:G:952:ARG:O	1:G:1018:LEU:HD23	2.08	0.54
1:G:975:LEU:N	1:G:975:LEU:HD23	2.21	0.54
1:I:737:ILE:HB	1:I:738:PRO:HD2	1.90	0.54
1:K:869:ASP:OD2	1:K:1015:HIS:ND1	2.33	0.54
1:L:920:LEU:HB3	1:L:921:PRO:CD	2.38	0.54
1:N:737:ILE:HB	1:N:738:PRO:HD2	1.90	0.54
1:P:278:ILE:H	1:P:278:ILE:CD1	2.21	0.54
1:P:737:ILE:HB	1:P:738:PRO:HD2	1.90	0.54
1:C:37:ARG:HH11	1:C:37:ARG:CG	2.20	0.54
1:C:876:THR:OG1	1:C:877:PRO:HD2	2.08	0.54
1:E:202:MET:HE3	1:E:357:HIS:CE1	2.43	0.54
1:F:634:GLN:O	1:F:682:LEU:HB2	2.07	0.54
1:F:781:ARG:HG3	1:F:781:ARG:NH1	2.17	0.54
1:I:673:ALA:O	1:I:674:PRO:C	2.51	0.54
1:I:876:THR:OG1	1:I:877:PRO:HD2	2.08	0.54
1:J:130:ASP:OD1	1:J:131:GLU:N	2.41	0.54
1:K:952:ARG:O	1:K:1018:LEU:HD23	2.08	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
1:N:202:MET:HE3	1:N:357:HIS:CE1	2.43	0.54
1:O:130:ASP:OD1	1:O:131:GLU:N	2.41	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:P:808:GLU:OE1	1:P:808:GLU:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:MET:HE3	1:A:357:HIS:CE1	2.43	0.54
1:A:634:GLN:O	1:A:682:LEU:HB2	2.08	0.54
1:B:39:SER:OG	1:B:40:GLU:N	2.40	0.54
1:B:920:LEU:HB3	1:B:921:PRO:CD	2.38	0.54
1:G:39:SER:OG	1:G:40:GLU:N	2.40	0.54
1:J:786:ARG:HH11	1:J:990:HIS:HE1	1.54	0.54
1:K:37:ARG:HH11	1:K:37:ARG:CG	2.20	0.54
1:M:595:THR:HG23	1:M:596:PRO:CA	2.37	0.54
1:N:634:GLN:O	1:N:682:LEU:HB2	2.07	0.54
1:N:975:LEU:N	1:N:975:LEU:HD23	2.21	0.54
1:O:39:SER:OG	1:O:40:GLU:N	2.40	0.54
1:O:952:ARG:O	1:O:1018:LEU:HD23	2.08	0.54
1:P:130:ASP:OD1	1:P:131:GLU:N	2.41	0.54
1:A:595:THR:HG23	1:A:596:PRO:CA	2.37	0.54
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.42	0.54
1:E:130:ASP:OD1	1:E:132:SER:N	2.30	0.54
1:F:127:PHE:CE2	1:F:184:LEU:HG	2.42	0.54
1:G:673:ALA:O	1:G:674:PRO:C	2.51	0.54
1:H:255:ARG:HG2	1:H:255:ARG:NH1	2.14	0.54
1:I:742:THR:HG22	1:I:743:SER:H	1.73	0.54
1:J:39:SER:OG	1:J:40:GLU:N	2.40	0.54
1:J:673:ALA:O	1:J:674:PRO:C	2.51	0.54
1:K:258:VAL:HA	1:K:312:VAL:O	2.07	0.54
1:K:742:THR:HG22	1:K:743:SER:H	1.73	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:N:876:THR:OG1	1:N:877:PRO:HD2	2.08	0.54
1:O:202:MET:HE3	1:O:357:HIS:CE1	2.43	0.54
1:O:673:ALA:O	1:O:674:PRO:C	2.51	0.54
1:O:737:ILE:HB	1:O:738:PRO:HD2	1.90	0.54
1:A:649:ASN:OD1	1:A:703:PRO:HD2	2.09	0.53
1:B:202:MET:HE3	1:B:357:HIS:CE1	2.43	0.53
1:B:952:ARG:O	1:B:1018:LEU:HD23	2.08	0.53
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.08	0.53
1:E:894:ARG:HH22	1:E:921:PRO:HD3	1.71	0.53
1:G:808:GLU:HA	1:G:808:GLU:OE1	2.08	0.53
1:H:78:LEU:HD23	1:H:78:LEU:N	2.21	0.53
1:H:737:ILE:HB	1:H:738:PRO:HD2	1.90	0.53
1:H:952:ARG:O	1:H:1018:LEU:HD23	2.08	0.53
1:I:202:MET:HE3	1:I:357:HIS:CE1	2.43	0.53
1:I:344:LEU:HD23	1:I:344:LEU:C	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:246:MET:HE3	1:J:247:CYS:CA	2.39	0.53
1:K:14:ARG:HG2	1:K:16:TRP:CZ2	2.43	0.53
1:L:202:MET:HE3	1:L:357:HIS:CE1	2.43	0.53
1:L:246:MET:HE3	1:L:247:CYS:CA	2.39	0.53
1:L:631:LEU:HD12	1:L:632:SER:N	2.24	0.53
1:M:130:ASP:OD1	1:M:131:GLU:N	2.41	0.53
1:M:423:MET:HE2	1:P:282:ARG:HG2	1.89	0.53
1:B:7:LEU:HD13	1:B:74:LEU:CD1	2.32	0.53
1:C:249:GLU:HG2	1:C:251:ARG:HH12	1.67	0.53
1:C:808:GLU:OE1	1:C:808:GLU:HA	2.08	0.53
1:D:649:ASN:OD1	1:D:703:PRO:HD2	2.09	0.53
1:E:127:PHE:CE2	1:E:184:LEU:HG	2.42	0.53
1:F:141:ILE:HG12	1:F:142:ILE:N	2.24	0.53
1:G:737:ILE:HB	1:G:738:PRO:HD2	1.90	0.53
1:H:634:GLN:O	1:H:682:LEU:HB2	2.07	0.53
1:I:952:ARG:O	1:I:1018:LEU:HD23	2.08	0.53
1:J:631:LEU:HD12	1:J:632:SER:N	2.24	0.53
1:J:876:THR:OG1	1:J:877:PRO:HD2	2.08	0.53
1:K:127:PHE:CE2	1:K:184:LEU:HG	2.42	0.53
1:K:673:ALA:O	1:K:674:PRO:C	2.51	0.53
1:K:808:GLU:OE1	1:K:808:GLU:HA	2.08	0.53
1:K:876:THR:OG1	1:K:877:PRO:HD2	2.08	0.53
1:M:236:SER:OG	1:M:237:ARG:HD3	2.09	0.53
1:N:37:ARG:HH11	1:N:37:ARG:CG	2.20	0.53
1:N:130:ASP:OD1	1:N:131:GLU:N	2.41	0.53
1:O:141:ILE:HG12	1:O:142:ILE:N	2.24	0.53
1:P:920:LEU:HB3	1:P:921:PRO:CD	2.38	0.53
1:A:39:SER:OG	1:A:40:GLU:N	2.40	0.53
1:A:130:ASP:OD1	1:A:131:GLU:N	2.41	0.53
1:B:631:LEU:HD12	1:B:632:SER:N	2.24	0.53
1:E:130:ASP:OD1	1:E:131:GLU:N	2.41	0.53
1:E:141:ILE:HG12	1:E:142:ILE:N	2.24	0.53
1:E:236:SER:OG	1:E:237:ARG:HD3	2.09	0.53
1:E:638:VAL:O	1:E:677:LYS:HA	2.09	0.53
1:F:808:GLU:OE1	1:F:808:GLU:HA	2.08	0.53
1:H:130:ASP:OD1	1:H:131:GLU:N	2.41	0.53
1:I:14:ARG:HG2	1:I:16:TRP:CZ2	2.43	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:J:737:ILE:HB	1:J:738:PRO:HD2	1.90	0.53
1:J:742:THR:HG22	1:J:743:SER:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:737:ILE:HB	1:K:738:PRO:HD2	1.90	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:N:638:VAL:O	1:N:677:LYS:HA	2.09	0.53
1:O:344:LEU:HD23	1:O:344:LEU:C	2.34	0.53
1:A:631:LEU:HD12	1:A:632:SER:N	2.24	0.53
1:B:638:VAL:O	1:B:677:LYS:HA	2.09	0.53
1:B:649:ASN:OD1	1:B:703:PRO:HD2	2.09	0.53
1:C:130:ASP:OD1	1:C:131:GLU:N	2.41	0.53
1:E:246:MET:HE3	1:E:247:CYS:CA	2.39	0.53
1:E:287:ASP:OD2	1:H:425:ARG:NH2	2.42	0.53
1:F:14:ARG:HG2	1:F:16:TRP:CZ2	2.44	0.53
1:F:202:MET:HE3	1:F:357:HIS:CE1	2.43	0.53
1:F:631:LEU:HD12	1:F:632:SER:N	2.24	0.53
1:G:7:LEU:HD13	1:G:74:LEU:CD1	2.32	0.53
1:G:78:LEU:HD23	1:G:78:LEU:N	2.21	0.53
1:G:130:ASP:OD1	1:G:131:GLU:N	2.41	0.53
1:G:638:VAL:O	1:G:677:LYS:HA	2.09	0.53
1:H:37:ARG:HH11	1:H:37:ARG:CG	2.20	0.53
1:H:344:LEU:HD23	1:H:344:LEU:C	2.34	0.53
1:H:631:LEU:HD12	1:H:632:SER:N	2.24	0.53
1:H:649:ASN:OD1	1:H:703:PRO:HD2	2.09	0.53
1:H:974:HIS:NE2	1:H:975:LEU:HD21	2.24	0.53
1:L:130:ASP:OD1	1:L:131:GLU:N	2.41	0.53
1:M:808:GLU:OE1	1:M:808:GLU:HA	2.08	0.53
1:N:14:ARG:HG2	1:N:16:TRP:CZ2	2.43	0.53
1:O:127:PHE:CE2	1:O:184:LEU:HG	2.42	0.53
1:P:130:ASP:OD1	1:P:132:SER:N	2.30	0.53
1:P:141:ILE:HG12	1:P:142:ILE:N	2.24	0.53
1:P:344:LEU:C	1:P:344:LEU:HD23	2.34	0.53
1:A:5:ASP:OD2	1:A:157:ARG:HA	2.07	0.53
1:A:246:MET:HE3	1:A:247:CYS:CA	2.39	0.53
1:A:344:LEU:HD23	1:A:344:LEU:C	2.34	0.53
1:B:473:ARG:HD2	1:C:469:ASP:HB3	1.90	0.53
1:B:673:ALA:O	1:B:674:PRO:C	2.51	0.53
1:C:246:MET:HE3	1:C:247:CYS:CA	2.39	0.53
1:C:595:THR:HG23	1:C:596:PRO:CA	2.37	0.53
1:D:246:MET:HE3	1:D:247:CYS:CA	2.39	0.53
1:E:344:LEU:C	1:E:344:LEU:HD23	2.33	0.53
1:E:737:ILE:HB	1:E:738:PRO:HD2	1.90	0.53
1:F:236:SER:OG	1:F:237:ARG:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:ASP:OD2	1:H:157:ARG:HA	2.07	0.53
1:I:651:LEU:CD1	1:I:669:PRO:HA	2.39	0.53
1:J:127:PHE:CE2	1:J:184:LEU:HG	2.42	0.53
1:J:202:MET:HE3	1:J:357:HIS:CE1	2.43	0.53
1:J:920:LEU:HB3	1:J:921:PRO:CD	2.38	0.53
1:K:202:MET:HE3	1:K:357:HIS:CE1	2.43	0.53
1:L:7:LEU:HD13	1:L:74:LEU:CD1	2.32	0.53
1:L:14:ARG:HG2	1:L:16:TRP:CZ2	2.44	0.53
1:L:649:ASN:OD1	1:L:703:PRO:HD2	2.09	0.53
1:M:246:MET:HE3	1:M:247:CYS:CA	2.39	0.53
1:M:282:ARG:HB3	1:P:421:VAL:HG22	1.91	0.53
1:M:673:ALA:O	1:M:674:PRO:C	2.51	0.53
1:N:278:ILE:H	1:N:278:ILE:CD1	2.21	0.53
1:N:808:GLU:OE1	1:N:808:GLU:HA	2.08	0.53
1:O:236:SER:OG	1:O:237:ARG:HD3	2.09	0.53
1:P:236:SER:OG	1:P:237:ARG:HD3	2.09	0.53
1:A:638:VAL:O	1:A:677:LYS:HA	2.09	0.53
1:C:14:ARG:HG2	1:C:16:TRP:CZ2	2.43	0.53
1:C:673:ALA:O	1:C:674:PRO:C	2.51	0.53
1:F:344:LEU:HD23	1:F:344:LEU:C	2.33	0.53
1:G:202:MET:HE3	1:G:357:HIS:CE1	2.43	0.53
1:G:631:LEU:HD12	1:G:632:SER:N	2.24	0.53
1:I:78:LEU:HD23	1:I:78:LEU:N	2.21	0.53
1:K:316:HIS:CA	1:K:323:ILE:HD13	2.32	0.53
1:K:649:ASN:OD1	1:K:703:PRO:HD2	2.09	0.53
1:L:742:THR:HG22	1:L:743:SER:H	1.73	0.53
1:M:344:LEU:C	1:M:344:LEU:HD23	2.34	0.53
1:N:344:LEU:HD23	1:N:344:LEU:C	2.33	0.53
1:O:78:LEU:HD23	1:O:78:LEU:N	2.21	0.53
1:O:631:LEU:HD12	1:O:632:SER:N	2.24	0.53
1:P:649:ASN:OD1	1:P:703:PRO:HD2	2.09	0.53
1:P:974:HIS:NE2	1:P:975:LEU:HD21	2.24	0.53
1:B:876:THR:OG1	1:B:877:PRO:HD2	2.08	0.53
1:C:634:GLN:HE22	1:C:685:LEU:H	1.57	0.53
1:C:638:VAL:O	1:C:677:LYS:HA	2.09	0.53
1:D:631:LEU:HD12	1:D:632:SER:N	2.24	0.53
1:D:737:ILE:HB	1:D:738:PRO:HD2	1.90	0.53
1:D:920:LEU:HB3	1:D:921:PRO:CD	2.38	0.53
1:F:249:GLU:HG2	1:F:251:ARG:HH12	1.67	0.53
1:F:876:THR:OG1	1:F:877:PRO:HD2	2.08	0.53
1:G:649:ASN:OD1	1:G:703:PRO:HD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:835:LEU:O	1:G:836:ILE:HD13	2.09	0.53
1:I:39:SER:OG	1:I:40:GLU:N	2.40	0.53
1:I:425:ARG:HH22	1:L:287:ASP:CG	2.15	0.53
1:I:638:VAL:O	1:I:677:LYS:HA	2.09	0.53
1:I:974:HIS:NE2	1:I:975:LEU:HD21	2.24	0.53
1:J:287:ASP:OD2	1:K:425:ARG:NH2	2.41	0.53
1:J:316:HIS:CA	1:J:323:ILE:HD13	2.32	0.53
1:K:73:TRP:CE2	1:K:122:CYS:HB3	2.44	0.53
1:L:141:ILE:HG12	1:L:142:ILE:N	2.24	0.53
1:L:236:SER:OG	1:L:237:ARG:HD3	2.09	0.53
1:L:634:GLN:O	1:L:682:LEU:HB2	2.07	0.53
1:L:651:LEU:CD1	1:L:669:PRO:HA	2.39	0.53
1:M:14:ARG:HG2	1:M:16:TRP:CZ2	2.43	0.53
1:M:73:TRP:CE2	1:M:122:CYS:HB3	2.44	0.53
1:M:651:LEU:CD1	1:M:669:PRO:HA	2.39	0.53
1:N:631:LEU:HD12	1:N:632:SER:N	2.24	0.53
1:N:649:ASN:OD1	1:N:703:PRO:HD2	2.09	0.53
1:N:651:LEU:CD1	1:N:669:PRO:HA	2.39	0.53
1:A:634:GLN:HE22	1:A:685:LEU:H	1.57	0.53
1:A:737:ILE:HB	1:A:738:PRO:HD2	1.90	0.53
1:A:974:HIS:NE2	1:A:975:LEU:HD21	2.24	0.53
1:B:130:ASP:OD1	1:B:131:GLU:N	2.41	0.53
1:B:668:VAL:CG1	1:B:669:PRO:HD2	2.31	0.53
1:B:808:GLU:OE1	1:B:808:GLU:HA	2.08	0.53
1:D:974:HIS:NE2	1:D:975:LEU:HD21	2.24	0.53
1:E:631:LEU:HD12	1:E:632:SER:N	2.24	0.53
1:H:742:THR:HG22	1:H:743:SER:H	1.73	0.53
1:I:73:TRP:CE2	1:I:122:CYS:HB3	2.44	0.53
1:I:141:ILE:HG12	1:I:142:ILE:N	2.24	0.53
1:J:73:TRP:CE2	1:J:122:CYS:HB3	2.44	0.53
1:J:808:GLU:OE1	1:J:808:GLU:HA	2.08	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:K:130:ASP:OD1	1:K:131:GLU:N	2.41	0.53
1:K:246:MET:HE3	1:K:247:CYS:CA	2.39	0.53
1:K:287:ASP:OD1	1:K:287:ASP:N	2.29	0.53
1:L:403:ASP:OD2	1:L:450:HIS:ND1	2.34	0.53
1:L:974:HIS:NE2	1:L:975:LEU:HD21	2.24	0.53
1:M:127:PHE:CE2	1:M:184:LEU:HG	2.42	0.53
1:M:202:MET:HE3	1:M:357:HIS:CE1	2.43	0.53
1:M:974:HIS:NE2	1:M:975:LEU:HD21	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:867:THR:O	1:N:867:THR:HG22	2.09	0.53
1:N:952:ARG:O	1:N:1018:LEU:HD23	2.08	0.53
1:O:808:GLU:HA	1:O:808:GLU:OE1	2.08	0.53
1:P:255:ARG:HG2	1:P:255:ARG:NH1	2.14	0.53
1:B:344:LEU:C	1:B:344:LEU:HD23	2.33	0.53
1:B:974:HIS:NE2	1:B:975:LEU:HD21	2.24	0.53
1:C:236:SER:OG	1:C:237:ARG:HD3	2.09	0.53
1:C:737:ILE:HB	1:C:738:PRO:HD2	1.90	0.53
1:D:638:VAL:O	1:D:677:LYS:HA	2.09	0.53
1:E:649:ASN:OD1	1:E:703:PRO:HD2	2.09	0.53
1:E:835:LEU:O	1:E:836:ILE:HD13	2.09	0.53
1:G:344:LEU:HD23	1:G:344:LEU:C	2.34	0.53
1:G:403:ASP:OD2	1:G:450:HIS:ND1	2.34	0.53
1:H:73:TRP:CE2	1:H:122:CYS:HB3	2.44	0.53
1:H:202:MET:HE3	1:H:357:HIS:CE1	2.43	0.53
1:H:651:LEU:CD1	1:H:669:PRO:HA	2.39	0.53
1:J:14:ARG:HG2	1:J:16:TRP:CZ2	2.43	0.53
1:J:78:LEU:HD23	1:J:78:LEU:N	2.21	0.53
1:J:236:SER:OG	1:J:237:ARG:HD3	2.09	0.53
1:K:651:LEU:CD1	1:K:669:PRO:HA	2.39	0.53
1:L:638:VAL:O	1:L:677:LYS:HA	2.09	0.53
1:L:740:LEU:CD1	1:L:741:THR:H	2.12	0.53
1:L:835:LEU:O	1:L:836:ILE:HD13	2.09	0.53
1:M:141:ILE:HG12	1:M:142:ILE:N	2.24	0.53
1:O:246:MET:HE3	1:O:247:CYS:CA	2.39	0.53
1:O:403:ASP:OD2	1:O:450:HIS:ND1	2.34	0.53
1:O:649:ASN:OD1	1:O:703:PRO:HD2	2.09	0.53
1:O:742:THR:HG22	1:O:743:SER:H	1.73	0.53
1:P:69:VAL:HG13	1:P:70:PRO:HD2	1.91	0.53
1:P:673:ALA:O	1:P:674:PRO:C	2.51	0.53
1:P:876:THR:OG1	1:P:877:PRO:HD2	2.08	0.53
1:A:673:ALA:O	1:A:674:PRO:C	2.51	0.53
1:B:14:ARG:HG2	1:B:16:TRP:CZ2	2.43	0.53
1:B:246:MET:HE3	1:B:247:CYS:CA	2.39	0.53
1:B:651:LEU:CD1	1:B:669:PRO:HA	2.39	0.53
1:C:579:ASP:N	1:C:583:ASN:O	2.40	0.53
1:C:835:LEU:O	1:C:836:ILE:HD13	2.09	0.53
1:D:211:ASP:OD1	1:D:211:ASP:N	2.42	0.53
1:D:278:ILE:H	1:D:278:ILE:CD1	2.21	0.53
1:D:344:LEU:HD23	1:D:344:LEU:C	2.34	0.53
1:D:781:ARG:HH11	1:D:781:ARG:CG	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:TRP:CE2	1:E:122:CYS:HB3	2.44	0.53
1:E:808:GLU:OE1	1:E:808:GLU:HA	2.08	0.53
1:F:73:TRP:CE2	1:F:122:CYS:HB3	2.44	0.53
1:F:638:VAL:O	1:F:677:LYS:HA	2.09	0.53
1:G:73:TRP:CE2	1:G:122:CYS:HB3	2.44	0.53
1:G:141:ILE:HG12	1:G:142:ILE:N	2.24	0.53
1:G:236:SER:OG	1:G:237:ARG:HD3	2.09	0.53
1:G:246:MET:HE3	1:G:247:CYS:CA	2.39	0.53
1:G:920:LEU:HB3	1:G:921:PRO:CD	2.38	0.53
1:I:246:MET:HE3	1:I:247:CYS:CA	2.39	0.53
1:I:579:ASP:N	1:I:583:ASN:O	2.40	0.53
1:I:819:GLU:HA	1:I:819:GLU:OE2	2.09	0.53
1:J:344:LEU:C	1:J:344:LEU:HD23	2.34	0.53
1:K:39:SER:OG	1:K:40:GLU:N	2.40	0.53
1:K:78:LEU:HD23	1:K:78:LEU:N	2.21	0.53
1:K:344:LEU:HD23	1:K:344:LEU:C	2.34	0.53
1:K:631:LEU:HD12	1:K:632:SER:N	2.24	0.53
1:L:808:GLU:OE1	1:L:808:GLU:HA	2.08	0.53
1:M:278:ILE:H	1:M:278:ILE:CD1	2.21	0.53
1:M:631:LEU:HD12	1:M:632:SER:N	2.24	0.53
1:M:987:ASP:OD2	1:M:990:HIS:HD2	1.92	0.53
1:O:278:ILE:H	1:O:278:ILE:CD1	2.21	0.53
1:P:202:MET:HE3	1:P:357:HIS:CE1	2.43	0.53
1:B:819:GLU:OE2	1:B:819:GLU:HA	2.09	0.52
1:C:202:MET:HE3	1:C:357:HIS:CE1	2.43	0.52
1:C:344:LEU:HD23	1:C:344:LEU:C	2.34	0.52
1:C:740:LEU:CD1	1:C:741:THR:H	2.12	0.52
1:D:69:VAL:HG13	1:D:70:PRO:HD2	1.91	0.52
1:D:130:ASP:OD1	1:D:131:GLU:N	2.41	0.52
1:F:130:ASP:OD1	1:F:131:GLU:N	2.41	0.52
1:F:287:ASP:CG	1:G:425:ARG:HH22	2.17	0.52
1:F:974:HIS:NE2	1:F:975:LEU:HD21	2.24	0.52
1:G:14:ARG:HG2	1:G:16:TRP:CZ2	2.44	0.52
1:H:69:VAL:HG13	1:H:70:PRO:HD2	1.91	0.52
1:H:420:MET:HA	1:H:420:MET:HE3	1.91	0.52
1:H:638:VAL:O	1:H:677:LYS:HA	2.09	0.52
1:H:920:LEU:HB3	1:H:921:PRO:CD	2.38	0.52
1:I:130:ASP:OD1	1:I:131:GLU:N	2.41	0.52
1:I:236:SER:OG	1:I:237:ARG:HD3	2.09	0.52
1:I:808:GLU:OE1	1:I:808:GLU:HA	2.08	0.52
1:J:420:MET:HE3	1:J:420:MET:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:425:ARG:NH2	1:K:287:ASP:OD2	2.42	0.52
1:J:595:THR:HG23	1:J:596:PRO:CA	2.37	0.52
1:K:69:VAL:HG13	1:K:70:PRO:HD2	1.91	0.52
1:K:638:VAL:O	1:K:677:LYS:HA	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: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: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:O:595:THR:HG23	1:O:596:PRO:CA	2.38	0.52
1:P:420:MET:HA	1:P:420:MET:HE3	1.92	0.52
1:P:651:LEU:CD1	1:P:669:PRO:HA	2.39	0.52
1:A:14:ARG:HG2	1:A:16:TRP:CZ2	2.44	0.52
1:A:597:ASN:HD22	1:A:599:ARG:H	1.57	0.52
1:A:867:THR:O	1:A:867:THR:HG22	2.09	0.52
1:B:420:MET:HA	1:B:420:MET:HE3	1.91	0.52
1:C:73:TRP:CE2	1:C:122:CYS:HB3	2.44	0.52
1:C:403:ASP:OD2	1:C:450:HIS:ND1	2.34	0.52
1:D:78:LEU:HD23	1:D:78:LEU:N	2.21	0.52
1:D:742:THR:HG22	1:D:743:SER:H	1.73	0.52
1:H:673:ALA:O	1:H:674:PRO:C	2.51	0.52
1:I:69:VAL:HG13	1:I:70:PRO:HD2	1.91	0.52
1:I:282:ARG:HH11	1:L:419:GLY:HA2	1.74	0.52
1:I:631:LEU:HD12	1:I:632:SER:N	2.24	0.52
1:J:141:ILE:HG12	1:J:142:ILE:N	2.24	0.52
1:J:819:GLU:OE2	1:J:819:GLU:HA	2.09	0.52
1:K:634:GLN:HE22	1:K:685:LEU:H	1.57	0.52
1:L:344:LEU:HD23	1:L:344:LEU:C	2.34	0.52
1:L:673:ALA:O	1:L:674:PRO:C	2.51	0.52
1:L:819:GLU:HA	1:L:819:GLU:OE2	2.09	0.52
1:M:638:VAL:O	1:M:677:LYS:HA	2.09	0.52
1:N:246:MET:HE3	1:N:247:CYS:CA	2.39	0.52
1:O:68:ALA:O	1:O:70:PRO:HD3	2.10	0.52
1:P:742:THR:HG22	1:P:743:SER:H	1.73	0.52
1:A:37:ARG:HH11	1:A:37:ARG:CG	2.20	0.52
1:A:419:GLY:C	1:D:282:ARG:HH11	2.17	0.52
1:A:653[A]:HIS:HD2	1:A:666:GLY:O	1.93	0.52
1:A:835:LEU:O	1:A:836:ILE:HD13	2.09	0.52
1:D:420:MET:HA	1:D:420:MET:HE3	1.91	0.52
1:D:867:THR:O	1:D:867:THR:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:SER:OG	1:E:40:GLU:N	2.40	0.52
1:E:316:HIS:CA	1:E:323:ILE:HD13	2.32	0.52
1:E:974:HIS:NE2	1:E:975:LEU:HD21	2.24	0.52
1:F:649:ASN:OD1	1:F:703:PRO:HD2	2.09	0.52
1:F:987:ASP:OD2	1:F:990:HIS:HD2	1.93	0.52
1:G:651:LEU:CD1	1:G:669:PRO:HA	2.39	0.52
1:G:974:HIS:NE2	1:G:975:LEU:HD21	2.24	0.52
1:I:597:ASN:HD22	1:I:599:ARG:H	1.57	0.52
1:J:894:ARG:HH22	1:J:921:PRO:HD3	1.71	0.52
1:L:39:SER:OG	1:L:40:GLU:N	2.40	0.52
1:L:68:ALA:O	1:L:70:PRO:HD3	2.10	0.52
1:M:742:THR:HG22	1:M:743:SER:H	1.73	0.52
1:N:73:TRP:CE2	1:N:122:CYS:HB3	2.44	0.52
1:O:638:VAL:O	1:O:677:LYS:HA	2.09	0.52
1:P:68:ALA:O	1:P:70:PRO:HD3	2.10	0.52
1:P:819:GLU:HA	1:P:819:GLU:OE2	2.09	0.52
1:A:278:ILE:H	1:A:278:ILE:CD1	2.21	0.52
1:A:420:MET:HA	1:A:420:MET:HE3	1.91	0.52
1:A:987:ASP:OD2	1:A:990:HIS:HD2	1.92	0.52
1:B:236:SER:OG	1:B:237:ARG:HD3	2.09	0.52
1:C:141:ILE:HG12	1:C:142:ILE:N	2.24	0.52
1:C:649:ASN:OD1	1:C:703:PRO:HD2	2.09	0.52
1:D:202:MET:HE3	1:D:357:HIS:CE1	2.43	0.52
1:D:316:HIS:CA	1:D:323:ILE:HD13	2.32	0.52
1:D:673:ALA:O	1:D:674:PRO:C	2.51	0.52
1:D:894:ARG:HH22	1:D:921:PRO:HD3	1.71	0.52
1:E:6:SER:O	1:E:9:VAL:HG12	2.10	0.52
1:F:69:VAL:HG13	1:F:70:PRO:HD2	1.91	0.52
1:F:597:ASN:HD22	1:F:599:ARG:H	1.57	0.52
1:F:740:LEU:CD1	1:F:741:THR:H	2.12	0.52
1:G:6:SER:O	1:G:9:VAL:HG12	2.10	0.52
1:H:14:ARG:HG2	1:H:16:TRP:CZ2	2.44	0.52
1:H:634:GLN:HE22	1:H:685:LEU:H	1.57	0.52
1:H:653[A]:HIS:HD2	1:H:666:GLY:O	1.93	0.52
1:J:638:VAL:O	1:J:677:LYS:HA	2.09	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:K:987:ASP:OD2	1:K:990:HIS:HD2	1.93	0.52
1:L:420:MET:HA	1:L:420:MET:HE3	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:236:SER:OG	1:N:237:ARG:HD3	2.09	0.52
1:P:634:GLN:HE22	1:P:685:LEU:H	1.57	0.52
1:A:6:SER:O	1:A:9:VAL:HG12	2.10	0.52
1:A:894:ARG:HH22	1:A:921:PRO:HD3	1.71	0.52
1:C:974:HIS:NE2	1:C:975:LEU:HD21	2.24	0.52
1:D:236:SER:OG	1:D:237:ARG:HD3	2.09	0.52
1:D:835:LEU:O	1:D:836:ILE:HD13	2.09	0.52
1:E:651:LEU:CD1	1:E:669:PRO:HA	2.39	0.52
1:F:473:ARG:HD2	1:G:469:ASP:HB3	1.91	0.52
1:G:781:ARG:HG3	1:G:781:ARG:NH1	2.17	0.52
1:G:819:GLU:HA	1:G:819:GLU:OE2	2.09	0.52
1:H:876:THR:OG1	1:H:877:PRO:HD2	2.08	0.52
1:J:403:ASP:OD2	1:J:450:HIS:ND1	2.34	0.52
1:J:651:LEU:CD1	1:J:669:PRO:HA	2.39	0.52
1:L:73:TRP:CE2	1:L:122:CYS:HB3	2.44	0.52
1:L:127:PHE:CE2	1:L:184:LEU:HG	2.42	0.52
1:M:39:SER:OG	1:M:40:GLU:N	2.40	0.52
1:M:724:GLU:O	1:N:847:LYS:NZ	2.23	0.52
1:N:69:VAL:HG13	1:N:70:PRO:HD2	1.91	0.52
1:N:595:THR:HG23	1:N:596:PRO:CA	2.37	0.52
1:O:69:VAL:HG13	1:O:70:PRO:HD2	1.91	0.52
1:P:73:TRP:CE2	1:P:122:CYS:HB3	2.44	0.52
1:P:653[A]:HIS:HD2	1:P:666:GLY:O	1.93	0.52
1:P:987:ASP:OD2	1:P:990:HIS:HD2	1.93	0.52
1:A:236:SER:OG	1:A:237:ARG:HD3	2.09	0.52
1:A:876:THR:OG1	1:A:877:PRO:HD2	2.08	0.52
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.44	0.52
1:B:987:ASP:OD2	1:B:990:HIS:HD2	1.93	0.52
1:D:772:ASP:OD1	1:D:772:ASP:N	2.30	0.52
1:E:9:VAL:O	1:E:12:GLN:HB3	2.10	0.52
1:E:14:ARG:HG2	1:E:16:TRP:CZ2	2.43	0.52
1:E:68:ALA:O	1:E:70:PRO:HD3	2.10	0.52
1:F:6:SER:O	1:F:9:VAL:HG12	2.10	0.52
1:F:651:LEU:CD1	1:F:669:PRO:HA	2.39	0.52
1:G:69:VAL:HG13	1:G:70:PRO:HD2	1.91	0.52
1:H:141:ILE:HG12	1:H:142:ILE:N	2.24	0.52
1:H:246:MET:HE3	1:H:247:CYS:CA	2.39	0.52
1:I:278:ILE:H	1:I:278:ILE:CD1	2.21	0.52
1:I:433:LEU:N	1:I:434:PRO:CD	2.73	0.52
1:I:634:GLN:HE22	1:I:685:LEU:H	1.57	0.52
1:J:6:SER:O	1:J:9:VAL:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:433:LEU:N	1:J:434:PRO:CD	2.73	0.52
1:K:6:SER:O	1:K:9:VAL:HG12	2.10	0.52
1:K:433:LEU:N	1:K:434:PRO:CD	2.73	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: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:N:653[A]:HIS:HD2	1:N:666:GLY:O	1.93	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:P:246:MET:HE3	1:P:247:CYS:CA	2.39	0.52
1:A:282:ARG:NH1	1:D:419:GLY:HA2	2.25	0.52
1:B:53:SER:O	1:B:54:LEU:HD23	2.10	0.52
1:B:835:LEU:O	1:B:836:ILE:HD13	2.09	0.52
1:B:894:ARG:HH22	1:B:921:PRO:HD3	1.71	0.52
1:C:9:VAL:O	1:C:12:GLN:HB3	2.10	0.52
1:C:39:SER:OG	1:C:40:GLU:N	2.40	0.52
1:C:420:MET:HA	1:C:420:MET:HE3	1.92	0.52
1:D:130:ASP:OD1	1:D:132:SER:N	2.29	0.52
1:E:742:THR:HG22	1:E:743:SER:H	1.73	0.52
1:F:246:MET:HE3	1:F:247:CYS:CA	2.39	0.52
1:G:597:ASN:HD22	1:G:599:ARG:H	1.57	0.52
1:H:403:ASP:OD2	1:H:450:HIS:ND1	2.34	0.52
1:I:6:SER:O	1:I:9:VAL:HG12	2.10	0.52
1:J:68:ALA:O	1:J:70:PRO:HD3	2.10	0.52
1:J:512:PHE:HE1	1:J:517:LYS:HG3	1.75	0.52
1:K:9:VAL:O	1:K:12:GLN:HB3	2.10	0.52
1:K:30:HIS:CE1	1:K:33:PHE:CD1	2.98	0.52
1:K:595:THR:HG23	1:K:596:PRO:CA	2.37	0.52
1:K:974:HIS:NE2	1:K:975:LEU:HD21	2.24	0.52
1:L:6:SER:O	1:L:9:VAL:HG12	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
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:N:740:LEU:CD1	1:N:741:THR:H	2.12	0.52
1:N:835:LEU:O	1:N:836:ILE:HD13	2.09	0.52
1:O:974:HIS:NE2	1:O:975:LEU:HD21	2.24	0.52
1:P:9:VAL:O	1:P:12:GLN:HB3	2.10	0.52
1:P:14:ARG:HG2	1:P:16:TRP:CZ2	2.43	0.52
1:P:638:VAL:O	1:P:677:LYS:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:835:LEU:O	1:P:836:ILE:HD13	2.09	0.52
1:B:6:SER:O	1:B:9:VAL:HG12	2.10	0.52
1:B:141:ILE:HG12	1:B:142:ILE:N	2.24	0.52
1:B:610:ASP:O	1:B:611:ARG:HB2	2.10	0.52
1:C:68:ALA:O	1:C:70:PRO:HD3	2.10	0.52
1:C:610:ASP:O	1:C:611:ARG:HB2	2.10	0.52
1:C:631:LEU:HD12	1:C:632:SER:N	2.24	0.52
1:D:597:ASN:HD22	1:D:599:ARG:H	1.57	0.52
1:D:651:LEU:CD1	1:D:669:PRO:HA	2.39	0.52
1:D:653[A]:HIS:HD2	1:D:666:GLY:O	1.93	0.52
1:D:808:GLU:OE1	1:D:808:GLU:HA	2.08	0.52
1:D:819:GLU:HA	1:D:819:GLU:OE2	2.09	0.52
1:E:867:THR:O	1:E:867:THR:HG22	2.09	0.52
1:E:869:ASP:OD2	1:E:1015:HIS:ND1	2.33	0.52
1:E:987:ASP:OD2	1:E:990:HIS:HD2	1.93	0.52
1:F:211:ASP:OD1	1:F:211:ASP:N	2.42	0.52
1:F:595:THR:HG23	1:F:596:PRO:CA	2.38	0.52
1:F:835:LEU:O	1:F:836:ILE:HD13	2.09	0.52
1:G:68:ALA:O	1:G:70:PRO:HD3	2.10	0.52
1:G:869:ASP:OD2	1:G:1015:HIS:ND1	2.33	0.52
1:I:30:HIS:CE1	1:I:33:PHE:CD1	2.98	0.52
1:I:65:ALA:HB1	1:I:66:PRO:CD	2.39	0.52
1:I:68:ALA:O	1:I:70:PRO:HD3	2.10	0.52
1:I:649:ASN:OD1	1:I:703:PRO:HD2	2.09	0.52
1:I:653[A]:HIS:HD2	1:I:666:GLY:O	1.93	0.52
1:I:987:ASP:OD2	1:I:990:HIS:HD2	1.93	0.52
1:J:278:ILE:H	1:J:278:ILE:CD1	2.21	0.52
1:K:819:GLU:HA	1:K:819:GLU:OE2	2.09	0.52
1:L:278:ILE:H	1:L:278:ILE:CD1	2.21	0.52
1:L:433:LEU:N	1:L:434:PRO:CD	2.73	0.52
1:N:610:ASP:O	1:N:611:ARG:HB2	2.10	0.52
1:P:403:ASP:OD2	1:P:450:HIS:ND1	2.34	0.52
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.44	0.52
1:A:512:PHE:HE1	1:A:517:LYS:HG3	1.75	0.52
1:B:9:VAL:O	1:B:12:GLN:HB3	2.10	0.52
1:B:433:LEU:N	1:B:434:PRO:CD	2.73	0.52
1:C:278:ILE:H	1:C:278:ILE:CD1	2.21	0.52
1:C:920:LEU:HB3	1:C:921:PRO:CD	2.38	0.52
1:D:6:SER:O	1:D:9:VAL:HG12	2.10	0.52
1:D:14:ARG:HG2	1:D:16:TRP:CZ2	2.43	0.52
1:D:141:ILE:HG12	1:D:142:ILE:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:VAL:HG13	1:E:70:PRO:HD2	1.91	0.52
1:E:278:ILE:H	1:E:278:ILE:CD1	2.21	0.52
1:E:653[A]:HIS:HD2	1:E:666:GLY:O	1.93	0.52
1:F:37:ARG:HH11	1:F:37:ARG:CG	2.20	0.52
1:F:237:ARG:HH11	1:F:237:ARG:CG	2.23	0.52
1:F:920:LEU:HB3	1:F:921:PRO:CD	2.38	0.52
1:G:9:VAL:O	1:G:12:GLN:HB3	2.10	0.52
1:G:278:ILE:H	1:G:278:ILE:CD1	2.21	0.52
1:G:740:LEU:CD1	1:G:741:THR:H	2.12	0.52
1:H:512:PHE:HE1	1:H:517:LYS:HG3	1.75	0.52
1:H:987:ASP:OD2	1:H:990:HIS:HD2	1.93	0.52
1:I:867:THR:O	1:I:867:THR:HG22	2.09	0.52
1:J:781:ARG:HH11	1:J:781:ARG:CG	2.19	0.52
1:K:597:ASN:HD22	1:K:599:ARG:H	1.57	0.52
1:M:819:GLU:OE2	1:M:819:GLU:HA	2.10	0.52
1:M:870:VAL:HG12	1:M:871:GLU:N	2.25	0.52
1:N:6:SER:O	1:N:9:VAL:HG12	2.10	0.52
1:N:53:SER:O	1:N:54:LEU:HD23	2.10	0.52
1:N:141:ILE:HG12	1:N:142:ILE:N	2.24	0.52
1:N:781:ARG:HG3	1:N:781:ARG:NH1	2.17	0.52
1:O:597:ASN:HD22	1:O:599:ARG:H	1.57	0.52
1:P:500:CYS:HA	1:P:534:ILE:O	2.10	0.52
1:P:631:LEU:HD12	1:P:632:SER:N	2.24	0.52
1:A:68:ALA:O	1:A:70:PRO:HD3	2.10	0.52
1:A:141:ILE:HG12	1:A:142:ILE:N	2.24	0.52
1:A:433:LEU:N	1:A:434:PRO:CD	2.73	0.52
1:A:651:LEU:CD1	1:A:669:PRO:HA	2.39	0.52
1:B:287:ASP:OD1	1:B:287:ASP:N	2.29	0.52
1:B:500:CYS:HA	1:B:534:ILE:O	2.10	0.52
1:C:211:ASP:OD1	1:C:211:ASP:N	2.42	0.52
1:C:653[A]:HIS:HD2	1:C:666:GLY:O	1.93	0.52
1:D:595:THR:HG23	1:D:596:PRO:CA	2.38	0.52
1:E:211:ASP:N	1:E:211:ASP:OD1	2.42	0.52
1:E:287:ASP:OD1	1:E:287:ASP:N	2.29	0.52
1:E:634:GLN:HE22	1:E:685:LEU:H	1.57	0.52
1:E:870:VAL:HG12	1:E:871:GLU:N	2.25	0.52
1:F:68:ALA:O	1:F:70:PRO:HD3	2.10	0.52
1:F:708:TRP:CE3	1:F:709:SER:HB3	2.45	0.52
1:G:832:ASP:OD1	1:G:832:ASP:N	2.43	0.52
1:H:30:HIS:CE1	1:H:33:PHE:CD1	2.98	0.52
1:H:236:SER:OG	1:H:237:ARG:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:835:LEU:O	1:H:836:ILE:HD13	2.09	0.52
1:I:53:SER:O	1:I:54:LEU:HD23	2.10	0.52
1:K:141:ILE:HG12	1:K:142:ILE:N	2.24	0.52
1:K:867:THR:O	1:K:867:THR:HG22	2.09	0.52
1:L:53:SER:O	1:L:54:LEU:HD23	2.10	0.52
1:N:673:ALA:O	1:N:674:PRO:C	2.51	0.52
1:O:9:VAL:O	1:O:12:GLN:HB3	2.10	0.52
1:O:651:LEU:CD1	1:O:669:PRO:HA	2.39	0.52
1:O:819:GLU:HA	1:O:819:GLU:OE2	2.09	0.52
1:O:835:LEU:O	1:O:836:ILE:HD13	2.09	0.52
1:P:512:PHE:HE1	1:P:517:LYS:HG3	1.75	0.52
1:A:30:HIS:CE1	1:A:33:PHE:CD1	2.98	0.51
1:A:500:CYS:HA	1:A:534:ILE:O	2.10	0.51
1:A:920:LEU:HB3	1:A:921:PRO:CD	2.38	0.51
1:B:832:ASP:OD1	1:B:832:ASP:N	2.43	0.51
1:C:237:ARG:HH11	1:C:237:ARG:CG	2.23	0.51
1:C:708:TRP:CE3	1:C:709:SER:HB3	2.45	0.51
1:C:819:GLU:HA	1:C:819:GLU:OE2	2.09	0.51
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.23	0.51
1:D:634:GLN:HE22	1:D:685:LEU:H	1.57	0.51
1:D:987:ASP:OD2	1:D:990:HIS:HD2	1.93	0.51
1:E:819:GLU:OE2	1:E:819:GLU:HA	2.10	0.51
1:F:30:HIS:CE1	1:F:33:PHE:CD1	2.98	0.51
1:F:512:PHE:HE1	1:F:517:LYS:HG3	1.75	0.51
1:F:819:GLU:HA	1:F:819:GLU:OE2	2.09	0.51
1:G:30:HIS:CE1	1:G:33:PHE:CD1	2.98	0.51
1:G:176:PHE:N	1:G:176:PHE:CD1	2.78	0.51
1:G:568:TRP:HE1	1:G:604:ASN:ND2	2.08	0.51
1:I:9:VAL:O	1:I:12:GLN:HB3	2.10	0.51
1:I:500:CYS:HA	1:I:534:ILE:O	2.11	0.51
1:J:30:HIS:CE1	1:J:33:PHE:CD1	2.98	0.51
1:J:237:ARG:HH11	1:J:237:ARG:CG	2.23	0.51
1:J:500:CYS:HA	1:J:534:ILE:O	2.11	0.51
1:K:512:PHE:HE1	1:K:517:LYS:HG3	1.75	0.51
1:K:668:VAL:CG1	1:K:669:PRO:HD2	2.31	0.51
1:K:708:TRP:CE3	1:K:709:SER:HB3	2.45	0.51
1:K:835:LEU:O	1:K:836:ILE:HD13	2.09	0.51
1:K:870:VAL:HG12	1:K:871:GLU:N	2.25	0.51
1:L:237:ARG:HH11	1:L:237:ARG:CG	2.24	0.51
1:N:65:ALA:HB1	1:N:66:PRO:CD	2.39	0.51
1:N:176:PHE:N	1:N:176:PHE:CD1	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:237:ARG:HH11	1:N:237:ARG:CG	2.23	0.51
1:N:634:GLN:HE22	1:N:685:LEU:H	1.57	0.51
1:N:708:TRP:CE3	1:N:709:SER:HB3	2.45	0.51
1:N:781:ARG:HH11	1:N:781:ARG:CG	2.19	0.51
1:P:30:HIS:CE1	1:P:33:PHE:CD1	2.98	0.51
1:P:870:VAL:HG12	1:P:871:GLU:N	2.25	0.51
1:A:579:ASP:N	1:A:583:ASN:O	2.40	0.51
1:B:278:ILE:H	1:B:278:ILE:CD1	2.21	0.51
1:C:176:PHE:N	1:C:176:PHE:CD1	2.79	0.51
1:C:651:LEU:CD1	1:C:669:PRO:HA	2.39	0.51
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.44	0.51
1:D:512:PHE:HE1	1:D:517:LYS:HG3	1.75	0.51
1:F:634:GLN:HE22	1:F:685:LEU:H	1.57	0.51
1:F:673:ALA:O	1:F:674:PRO:C	2.51	0.51
1:G:610:ASP:O	1:G:611:ARG:HB2	2.10	0.51
1:H:68:ALA:O	1:H:70:PRO:HD3	2.10	0.51
1:H:597:ASN:HD22	1:H:599:ARG:H	1.57	0.51
1:H:867:THR:O	1:H:867:THR:HG22	2.09	0.51
1:J:9:VAL:O	1:J:12:GLN:HB3	2.10	0.51
1:J:634:GLN:HE22	1:J:685:LEU:H	1.57	0.51
1:J:649:ASN:OD1	1:J:703:PRO:HD2	2.09	0.51
1:K:568:TRP:HE1	1:K:604:ASN:ND2	2.08	0.51
1:K:781:ARG:HH11	1:K:781:ARG:CG	2.19	0.51
1:M:176:PHE:N	1:M:176:PHE:CD1	2.78	0.51
1:N:30:HIS:CE1	1:N:33:PHE:CD1	2.98	0.51
1:N:433:LEU:N	1:N:434:PRO:CD	2.73	0.51
1:N:500:CYS:HA	1:N:534:ILE:O	2.11	0.51
1:N:920:LEU:HB3	1:N:921:PRO:CD	2.38	0.51
1:O:30:HIS:CE1	1:O:33:PHE:CD1	2.98	0.51
1:O:73:TRP:CE2	1:O:122:CYS:HB3	2.44	0.51
1:O:568:TRP:HE1	1:O:604:ASN:ND2	2.09	0.51
1:A:9:VAL:O	1:A:12:GLN:HB3	2.10	0.51
1:A:176:PHE:N	1:A:176:PHE:CD1	2.79	0.51
1:A:237:ARG:HH11	1:A:237:ARG:CG	2.23	0.51
1:A:434:PRO:HA	1:A:437:SER:OG	2.11	0.51
1:A:819:GLU:HA	1:A:819:GLU:OE2	2.09	0.51
1:B:653[A]:HIS:HD2	1:B:666:GLY:O	1.93	0.51
1:C:69:VAL:HG13	1:C:70:PRO:HD2	1.91	0.51
1:D:568:TRP:HE1	1:D:604:ASN:ND2	2.08	0.51
1:E:176:PHE:N	1:E:176:PHE:CD1	2.79	0.51
1:E:420:MET:HA	1:E:420:MET:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:610:ASP:O	1:E:611:ARG:HB2	2.10	0.51
1:F:420:MET:HA	1:F:420:MET:HE3	1.91	0.51
1:G:433:LEU:N	1:G:434:PRO:CD	2.73	0.51
1:G:987:ASP:OD2	1:G:990:HIS:HD2	1.92	0.51
1:H:6:SER:O	1:H:9:VAL:HG12	2.10	0.51
1:H:870:VAL:HG12	1:H:871:GLU:N	2.26	0.51
1:I:663:LEU:HD23	1:I:663:LEU:N	2.24	0.51
1:J:597:ASN:HD22	1:J:599:ARG:H	1.57	0.51
1:K:236:SER:OG	1:K:237:ARG:HD3	2.09	0.51
1:L:500:CYS:HA	1:L:534:ILE:O	2.10	0.51
1:M:69:VAL:HG13	1:M:70:PRO:HD2	1.91	0.51
1:M:500:CYS:HA	1:M:534:ILE:O	2.10	0.51
1:M:920:LEU:HB3	1:M:921:PRO:CD	2.38	0.51
1:N:420:MET:HA	1:N:420:MET:HE3	1.92	0.51
1:N:512:PHE:HE1	1:N:517:LYS:HG3	1.75	0.51
1:O:433:LEU:N	1:O:434:PRO:CD	2.73	0.51
1:O:867:THR:HG22	1:O:867:THR:O	2.09	0.51
1:O:987:ASP:OD2	1:O:990:HIS:HD2	1.93	0.51
1:P:53:SER:O	1:P:54:LEU:HD23	2.10	0.51
1:A:822:LEU:HD11	1:A:824:GLN:O	2.11	0.51
1:B:568:TRP:HE1	1:B:604:ASN:ND2	2.08	0.51
1:B:634:GLN:HE22	1:B:685:LEU:H	1.57	0.51
1:C:6:SER:O	1:C:9:VAL:HG12	2.10	0.51
1:D:9:VAL:O	1:D:12:GLN:HB3	2.10	0.51
1:D:30:HIS:CE1	1:D:33:PHE:CD1	2.98	0.51
1:D:663:LEU:HD23	1:D:663:LEU:N	2.24	0.51
1:E:237:ARG:HH11	1:E:237:ARG:CG	2.23	0.51
1:E:433:LEU:N	1:E:434:PRO:CD	2.73	0.51
1:F:433:LEU:N	1:F:434:PRO:CD	2.73	0.51
1:H:9:VAL:O	1:H:12:GLN:HB3	2.10	0.51
1:H:500:CYS:HA	1:H:534:ILE:O	2.11	0.51
1:I:512:PHE:HE1	1:I:517:LYS:HG3	1.75	0.51
1:I:832:ASP:OD1	1:I:832:ASP:N	2.43	0.51
1:J:53:SER:O	1:J:54:LEU:HD23	2.10	0.51
1:J:176:PHE:CD1	1:J:176:PHE:N	2.79	0.51
1:K:68:ALA:O	1:K:70:PRO:HD3	2.10	0.51
1:L:211:ASP:OD1	1:L:211:ASP:N	2.42	0.51
1:M:822:LEU:HD11	1:M:824:GLN:O	2.11	0.51
1:O:53:SER:O	1:O:54:LEU:HD23	2.10	0.51
1:O:237:ARG:HH11	1:O:237:ARG:CG	2.23	0.51
1:O:781:ARG:HG3	1:O:781:ARG:NH1	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:6:SER:O	1:P:9:VAL:HG12	2.10	0.51
1:B:30:HIS:CE1	1:B:33:PHE:CD1	2.98	0.51
1:B:68:ALA:O	1:B:70:PRO:HD3	2.10	0.51
1:B:867:THR:HG22	1:B:867:THR:O	2.09	0.51
1:C:30:HIS:CE1	1:C:33:PHE:CD1	2.98	0.51
1:C:500:CYS:HA	1:C:534:ILE:O	2.10	0.51
1:C:869:ASP:OD2	1:C:1015:HIS:ND1	2.33	0.51
1:D:433:LEU:N	1:D:434:PRO:CD	2.73	0.51
1:E:579:ASP:N	1:E:583:ASN:O	2.40	0.51
1:E:673:ALA:O	1:E:674:PRO:C	2.51	0.51
1:E:708:TRP:CE3	1:E:709:SER:HB3	2.45	0.51
1:F:568:TRP:HE1	1:F:604:ASN:ND2	2.08	0.51
1:G:53:SER:O	1:G:54:LEU:HD23	2.10	0.51
1:G:420:MET:HE3	1:G:420:MET:HA	1.91	0.51
1:G:708:TRP:CE3	1:G:709:SER:HB3	2.45	0.51
1:H:434:PRO:HA	1:H:437:SER:OG	2.11	0.51
1:I:419:GLY:HA2	1:L:282:ARG:NH1	2.25	0.51
1:I:420:MET:HA	1:I:420:MET:HE3	1.92	0.51
1:I:708:TRP:CE3	1:I:709:SER:HB3	2.45	0.51
1:I:781:ARG:HH11	1:I:781:ARG:CG	2.19	0.51
1:J:987:ASP:OD2	1:J:990:HIS:HD2	1.92	0.51
1:K:822:LEU:HD11	1:K:824:GLN:O	2.11	0.51
1:L:512:PHE:HE1	1:L:517:LYS:HG3	1.75	0.51
1:L:568:TRP:HE1	1:L:604:ASN:ND2	2.08	0.51
1:L:653[A]:HIS:HD2	1:L:666:GLY:O	1.93	0.51
1:L:867:THR:O	1:L:867:THR:HG22	2.09	0.51
1:M:420:MET:HA	1:M:420:MET:HE3	1.91	0.51
1:O:420:MET:HA	1:O:420:MET:HE3	1.91	0.51
1:O:653[A]:HIS:HD2	1:O:666:GLY:O	1.93	0.51
1:O:708:TRP:CE3	1:O:709:SER:HB3	2.45	0.51
1:O:822:LEU:HD11	1:O:824:GLN:O	2.11	0.51
1:A:287:ASP:OD1	1:A:287:ASP:N	2.29	0.51
1:B:69:VAL:HG13	1:B:70:PRO:HD2	1.91	0.51
1:B:176:PHE:CD1	1:B:176:PHE:N	2.78	0.51
1:C:433:LEU:N	1:C:434:PRO:CD	2.73	0.51
1:C:987:ASP:OD2	1:C:990:HIS:HD2	1.92	0.51
1:D:579:ASP:N	1:D:583:ASN:O	2.40	0.51
1:E:30:HIS:CE1	1:E:33:PHE:CD1	2.98	0.51
1:G:500:CYS:HA	1:G:534:ILE:O	2.10	0.51
1:G:867:THR:HG22	1:G:867:THR:O	2.09	0.51
1:H:819:GLU:HA	1:H:819:GLU:OE2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:568:TRP:HE1	1:J:604:ASN:ND2	2.08	0.51
1:J:579:ASP:OD2	1:J:583:ASN:HB2	2.11	0.51
1:J:870:VAL:HG12	1:J:871:GLU:N	2.25	0.51
1:K:610:ASP:O	1:K:611:ARG:HB2	2.10	0.51
1:L:634:GLN:HE22	1:L:685:LEU:H	1.57	0.51
1:L:708:TRP:CE3	1:L:709:SER:HB3	2.45	0.51
1:L:822:LEU:HD11	1:L:824:GLN:O	2.11	0.51
1:M:127:PHE:N	1:M:127:PHE:CD2	2.79	0.51
1:M:211:ASP:N	1:M:211:ASP:OD1	2.42	0.51
1:N:579:ASP:OD2	1:N:583:ASN:HB2	2.11	0.51
1:O:500:CYS:HA	1:O:534:ILE:O	2.10	0.51
1:O:512:PHE:HE1	1:O:517:LYS:HG3	1.75	0.51
1:P:211:ASP:OD1	1:P:211:ASP:N	2.42	0.51
1:P:597:ASN:HD22	1:P:599:ARG:H	1.57	0.51
1:A:53:SER:O	1:A:54:LEU:HD23	2.10	0.51
1:A:69:VAL:HG13	1:A:70:PRO:HD2	1.91	0.51
1:A:869:ASP:OD2	1:A:1015:HIS:ND1	2.33	0.51
1:B:237:ARG:HH11	1:B:237:ARG:CG	2.24	0.51
1:E:512:PHE:HE1	1:E:517:LYS:HG3	1.75	0.51
1:E:595:THR:HG23	1:E:596:PRO:CA	2.37	0.51
1:E:822:LEU:HD11	1:E:824:GLN:O	2.11	0.51
1:E:974:HIS:C	1:E:975:LEU:HD23	2.36	0.51
1:F:434:PRO:HA	1:F:437:SER:OG	2.11	0.51
1:F:500:CYS:HA	1:F:534:ILE:O	2.10	0.51
1:F:870:VAL:HG12	1:F:871:GLU:N	2.25	0.51
1:G:653[A]:HIS:HD2	1:G:666:GLY:O	1.93	0.51
1:H:53:SER:O	1:H:54:LEU:HD23	2.10	0.51
1:H:278:ILE:H	1:H:278:ILE:CD1	2.21	0.51
1:H:822:LEU:HD11	1:H:824:GLN:O	2.11	0.51
1:H:832:ASP:OD1	1:H:832:ASP:N	2.43	0.51
1:I:176:PHE:N	1:I:176:PHE:CD1	2.79	0.51
1:J:127:PHE:CD2	1:J:127:PHE:N	2.79	0.51
1:J:610:ASP:O	1:J:611:ARG:HB2	2.10	0.51
1:K:176:PHE:N	1:K:176:PHE:CD1	2.78	0.51
1:K:420:MET:HA	1:K:420:MET:HE3	1.91	0.51
1:M:568:TRP:HE1	1:M:604:ASN:ND2	2.09	0.51
1:M:708:TRP:CE3	1:M:709:SER:HB3	2.45	0.51
1:N:68:ALA:O	1:N:70:PRO:HD3	2.10	0.51
1:N:663:LEU:HD23	1:N:663:LEU:N	2.24	0.51
1:O:434:PRO:HA	1:O:437:SER:OG	2.11	0.51
1:P:433:LEU:N	1:P:434:PRO:CD	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:ARG:HH11	1:A:781:ARG:CG	2.19	0.51
1:B:974:HIS:C	1:B:975:LEU:HD23	2.36	0.51
1:C:597:ASN:HD22	1:C:599:ARG:H	1.57	0.51
1:E:833:ALA:HB1	1:E:858:ILE:O	2.11	0.51
1:E:920:LEU:HB3	1:E:921:PRO:CD	2.38	0.51
1:F:9:VAL:O	1:F:12:GLN:HB3	2.10	0.51
1:F:579:ASP:OD2	1:F:583:ASN:HB2	2.11	0.51
1:F:610:ASP:O	1:F:611:ARG:HB2	2.10	0.51
1:G:237:ARG:HH11	1:G:237:ARG:CG	2.23	0.51
1:G:512:PHE:HE1	1:G:517:LYS:HG3	1.75	0.51
1:G:974:HIS:C	1:G:975:LEU:HD23	2.36	0.51
1:K:53:SER:O	1:K:54:LEU:HD23	2.10	0.51
1:K:278:ILE:H	1:K:278:ILE:CD1	2.21	0.51
1:L:176:PHE:N	1:L:176:PHE:CD1	2.79	0.51
1:L:579:ASP:OD2	1:L:583:ASN:HB2	2.11	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:HH11	1:M:237:ARG:CG	2.23	0.51
1:M:512:PHE:HE1	1:M:517:LYS:HG3	1.75	0.51
1:N:282:ARG:HH11	1:O:419:GLY:CA	2.23	0.51
1:N:870:VAL:HG12	1:N:871:GLU:N	2.25	0.51
1:O:974:HIS:C	1:O:975:LEU:HD23	2.36	0.51
1:A:870:VAL:HG12	1:A:871:GLU:N	2.25	0.51
1:B:592:PHE:N	1:B:592:PHE:CD1	2.79	0.51
1:E:178:ARG:HH11	1:E:178:ARG:HB2	1.76	0.51
1:F:653[A]:HIS:HD2	1:F:666:GLY:O	1.93	0.51
1:G:592:PHE:N	1:G:592:PHE:CD1	2.79	0.51
1:H:579:ASP:N	1:H:583:ASN:O	2.40	0.51
1:I:822:LEU:HD11	1:I:824:GLN:O	2.11	0.51
1:I:833:ALA:HB1	1:I:858:ILE:O	2.11	0.51
1:J:708:TRP:CE3	1:J:709:SER:HB3	2.45	0.51
1:M:30:HIS:CE1	1:M:33:PHE:CD1	2.98	0.51
1:M:433:LEU:N	1:M:434:PRO:CD	2.73	0.51
1:N:434:PRO:HA	1:N:437:SER:OG	2.11	0.51
1:O:6:SER:O	1:O:9:VAL:HG12	2.10	0.51
1:O:176:PHE:N	1:O:176:PHE:CD1	2.78	0.51
1:P:579:ASP:OD2	1:P:583:ASN:HB2	2.11	0.51
1:P:832:ASP:OD1	1:P:832:ASP:N	2.43	0.51
1:P:961:ARG:NH2	1:P:979:GLU:O	2.37	0.51
1:P:974:HIS:C	1:P:975:LEU:HD23	2.36	0.51
1:B:708:TRP:CE3	1:B:709:SER:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:579:ASP:OD2	1:C:583:ASN:HB2	2.11	0.51
1:D:68:ALA:O	1:D:70:PRO:HD3	2.10	0.51
1:D:176:PHE:N	1:D:176:PHE:CD1	2.79	0.51
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.46	0.51
1:E:568:TRP:HE1	1:E:604:ASN:ND2	2.09	0.51
1:E:579:ASP:OD2	1:E:583:ASN:HB2	2.11	0.51
1:F:127:PHE:N	1:F:127:PHE:CD2	2.79	0.51
1:G:433:LEU:N	1:G:434:PRO:HD2	2.26	0.51
1:H:433:LEU:N	1:H:434:PRO:CD	2.73	0.51
1:I:130:ASP:OD1	1:I:132:SER:N	2.30	0.51
1:I:835:LEU:O	1:I:836:ILE:HD13	2.09	0.51
1:J:822:LEU:HD11	1:J:824:GLN:O	2.11	0.51
1:J:867:THR:HG22	1:J:867:THR:O	2.09	0.51
1:K:73:TRP:CZ2	1:K:185:ALA:HB1	2.46	0.51
1:K:178:ARG:HH11	1:K:178:ARG:HB2	1.76	0.51
1:L:9:VAL:O	1:L:12:GLN:HB3	2.10	0.51
1:L:581:ASN:OD1	1:L:581:ASN:N	2.44	0.51
1:L:833:ALA:HB1	1:L:858:ILE:O	2.11	0.51
1:M:833:ALA:HB1	1:M:858:ILE:O	2.11	0.51
1:N:579:ASP:N	1:N:583:ASN:O	2.40	0.51
1:P:131:GLU:HG3	1:P:132:SER:N	2.26	0.51
1:P:822:LEU:HD11	1:P:824:GLN:O	2.11	0.51
1:A:833:ALA:HB1	1:A:858:ILE:O	2.11	0.50
1:A:974:HIS:C	1:A:975:LEU:HD23	2.36	0.50
1:B:49:GLN:H	1:B:49:GLN:HE21	1.59	0.50
1:B:434:PRO:HA	1:B:437:SER:OG	2.11	0.50
1:B:781:ARG:HG3	1:B:781:ARG:NH1	2.17	0.50
1:B:869:ASP:OD2	1:B:1015:HIS:ND1	2.33	0.50
1:C:434:PRO:HA	1:C:437:SER:OG	2.11	0.50
1:C:512:PHE:HE1	1:C:517:LYS:HG3	1.75	0.50
1:C:822:LEU:HD12	1:C:822:LEU:C	2.37	0.50
1:D:610:ASP:O	1:D:611:ARG:HB2	2.10	0.50
1:E:131:GLU:HG3	1:E:132:SER:N	2.26	0.50
1:F:53:SER:O	1:F:54:LEU:HD23	2.10	0.50
1:F:73:TRP:CZ2	1:F:185:ALA:HB1	2.47	0.50
1:F:78:LEU:HD23	1:F:78:LEU:N	2.21	0.50
1:G:210:ARG:HH12	1:G:394:ASN:C	2.20	0.50
1:G:434:PRO:HA	1:G:437:SER:OG	2.11	0.50
1:H:178:ARG:HH11	1:H:178:ARG:HB2	1.76	0.50
1:H:211:ASP:OD1	1:H:211:ASP:N	2.42	0.50
1:H:237:ARG:HH11	1:H:237:ARG:HB3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:595:THR:HG23	1:I:596:PRO:CA	2.37	0.50
1:J:69:VAL:HG13	1:J:70:PRO:HD2	1.91	0.50
1:J:178:ARG:HB2	1:J:178:ARG:HH11	1.76	0.50
1:K:579:ASP:OD2	1:K:583:ASN:HB2	2.11	0.50
1:K:974:HIS:C	1:K:975:LEU:HD23	2.36	0.50
1:M:178:ARG:HH11	1:M:178:ARG:HB2	1.77	0.50
1:N:73:TRP:CZ2	1:N:185:ALA:HB1	2.47	0.50
1:N:127:PHE:N	1:N:127:PHE:CD2	2.79	0.50
1:P:708:TRP:CE3	1:P:709:SER:HB3	2.45	0.50
1:A:433:LEU:N	1:A:434:PRO:HD2	2.26	0.50
1:A:610:ASP:O	1:A:611:ARG:HB2	2.10	0.50
1:B:210:ARG:HH12	1:B:394:ASN:C	2.19	0.50
1:C:49:GLN:H	1:C:49:GLN:HE21	1.59	0.50
1:D:833:ALA:HB1	1:D:858:ILE:O	2.11	0.50
1:E:434:PRO:HA	1:E:437:SER:OG	2.11	0.50
1:E:500:CYS:HA	1:E:534:ILE:O	2.11	0.50
1:E:597:ASN:HD22	1:E:599:ARG:H	1.57	0.50
1:F:65:ALA:HB1	1:F:66:PRO:CD	2.39	0.50
1:F:581:ASN:OD1	1:F:581:ASN:N	2.44	0.50
1:F:867:THR:O	1:F:867:THR:HG22	2.09	0.50
1:F:974:HIS:C	1:F:975:LEU:HD23	2.36	0.50
1:G:23:GLN:HB3	1:G:26:ARG:NH2	2.27	0.50
1:H:579:ASP:OD2	1:H:583:ASN:HB2	2.11	0.50
1:H:708:TRP:CE3	1:H:709:SER:HB3	2.45	0.50
1:I:73:TRP:CZ2	1:I:185:ALA:HB1	2.47	0.50
1:I:127:PHE:CD2	1:I:127:PHE:N	2.79	0.50
1:L:30:HIS:CE1	1:L:33:PHE:CD1	2.98	0.50
1:L:73:TRP:CZ2	1:L:185:ALA:HB1	2.47	0.50
1:L:433:LEU:N	1:L:434:PRO:HD2	2.26	0.50
1:L:870:VAL:HG12	1:L:871:GLU:N	2.25	0.50
1:M:423:MET:HE2	1:P:282:ARG:CG	2.40	0.50
1:M:579:ASP:OD2	1:M:583:ASN:HB2	2.11	0.50
1:N:210:ARG:HH12	1:N:394:ASN:C	2.20	0.50
1:N:869:ASP:OD2	1:N:1015:HIS:ND1	2.33	0.50
1:O:49:GLN:H	1:O:49:GLN:HE21	1.59	0.50
1:O:178:ARG:HB2	1:O:178:ARG:HH11	1.76	0.50
1:O:610:ASP:O	1:O:611:ARG:HB2	2.10	0.50
1:P:592:PHE:N	1:P:592:PHE:CD1	2.79	0.50
1:P:867:THR:O	1:P:867:THR:HG22	2.09	0.50
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.77	0.50
1:A:592:PHE:N	1:A:592:PHE:CD1	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ASP:OD2	1:B:450:HIS:ND1	2.34	0.50
1:B:433:LEU:N	1:B:434:PRO:HD2	2.26	0.50
1:B:512:PHE:HE1	1:B:517:LYS:HG3	1.75	0.50
1:C:822:LEU:HD11	1:C:824:GLN:O	2.11	0.50
1:F:210:ARG:HH12	1:F:394:ASN:C	2.20	0.50
1:H:176:PHE:N	1:H:176:PHE:CD1	2.79	0.50
1:H:433:LEU:N	1:H:434:PRO:HD2	2.26	0.50
1:H:568:TRP:HE1	1:H:604:ASN:ND2	2.08	0.50
1:I:433:LEU:N	1:I:434:PRO:HD2	2.26	0.50
1:I:568:TRP:HE1	1:I:604:ASN:ND2	2.09	0.50
1:I:660:GLY:O	1:I:662:PRO:HD3	2.12	0.50
1:J:581:ASN:OD1	1:J:581:ASN:N	2.44	0.50
1:K:36:TRP:CD2	1:K:42:ALA:HA	2.47	0.50
1:K:49:GLN:H	1:K:49:GLN:HE21	1.59	0.50
1:K:65:ALA:HB1	1:K:66:PRO:CD	2.38	0.50
1:M:36:TRP:CD2	1:M:42:ALA:HA	2.47	0.50
1:M:53:SER:O	1:M:54:LEU:HD23	2.10	0.50
1:N:974:HIS:C	1:N:975:LEU:HD23	2.36	0.50
1:O:822:LEU:HD12	1:O:822:LEU:C	2.36	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:P:570:TRP:CD1	1:P:571:VAL:HG22	2.47	0.50
1:A:49:GLN:H	1:A:49:GLN:HE21	1.59	0.50
1:A:178:ARG:HB2	1:A:178:ARG:HH11	1.76	0.50
1:A:282:ARG:NH1	1:D:419:GLY:C	2.69	0.50
1:A:419:GLY:C	1:D:282:ARG:NH1	2.69	0.50
1:A:579:ASP:OD2	1:A:583:ASN:HB2	2.11	0.50
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.45	0.50
1:B:36:TRP:CD2	1:B:42:ALA:HA	2.47	0.50
1:B:211:ASP:OD1	1:B:211:ASP:N	2.42	0.50
1:B:597:ASN:HD22	1:B:599:ARG:H	1.57	0.50
1:B:870:VAL:HG12	1:B:871:GLU:N	2.25	0.50
1:C:131:GLU:HG3	1:C:132:SER:N	2.26	0.50
1:C:433:LEU:N	1:C:434:PRO:HD2	2.26	0.50
1:D:127:PHE:CD2	1:D:127:PHE:N	2.79	0.50
1:D:434:PRO:HA	1:D:437:SER:OG	2.11	0.50
1:D:974:HIS:C	1:D:975:LEU:HD23	2.36	0.50
1:E:127:PHE:N	1:E:127:PHE:CD2	2.79	0.50
1:E:570:TRP:CD1	1:E:571:VAL:HG22	2.47	0.50
1:F:403:ASP:OD2	1:F:450:HIS:ND1	2.34	0.50
1:G:49:GLN:H	1:G:49:GLN:HE21	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:660:GLY:O	1:G:662:PRO:HD3	2.12	0.50
1:G:822:LEU:HD11	1:G:824:GLN:O	2.11	0.50
1:G:870:VAL:HG12	1:G:871:GLU:N	2.25	0.50
1:H:974:HIS:C	1:H:975:LEU:HD23	2.36	0.50
1:I:403:ASP:OD2	1:I:450:HIS:ND1	2.34	0.50
1:I:434:PRO:HA	1:I:437:SER:OG	2.11	0.50
1:I:579:ASP:OD2	1:I:583:ASN:HB2	2.11	0.50
1:I:920:LEU:HB3	1:I:921:PRO:CD	2.38	0.50
1:J:73:TRP:CZ2	1:J:185:ALA:HB1	2.46	0.50
1:J:822:LEU:HD12	1:J:822:LEU:C	2.37	0.50
1:K:127:PHE:N	1:K:127:PHE:CD2	2.79	0.50
1:K:131:GLU:HG3	1:K:132:SER:N	2.26	0.50
1:K:433:LEU:N	1:K:434:PRO:HD2	2.26	0.50
1:K:833:ALA:HB1	1:K:858:ILE:O	2.11	0.50
1:L:131:GLU:HG3	1:L:132:SER:N	2.26	0.50
1:M:974:HIS:C	1:M:975:LEU:HD23	2.36	0.50
1:N:36:TRP:CD2	1:N:42:ALA:HA	2.47	0.50
1:N:131:GLU:HG3	1:N:132:SER:N	2.26	0.50
1:N:833:ALA:HB1	1:N:858:ILE:O	2.11	0.50
1:O:660:GLY:O	1:O:662:PRO:HD3	2.12	0.50
1:O:833:ALA:HB1	1:O:858:ILE:O	2.11	0.50
1:O:920:LEU:HB3	1:O:921:PRO:CD	2.38	0.50
1:P:237:ARG:HH11	1:P:237:ARG:CG	2.23	0.50
1:P:869:ASP:OD2	1:P:1015:HIS:ND1	2.33	0.50
1:A:211:ASP:OD1	1:A:211:ASP:N	2.42	0.50
1:A:403:ASP:OD2	1:A:450:HIS:ND1	2.34	0.50
1:A:581:ASN:OD1	1:A:581:ASN:N	2.44	0.50
1:B:73:TRP:CZ2	1:B:185:ALA:HB1	2.47	0.50
1:B:127:PHE:CD2	1:B:127:PHE:N	2.79	0.50
1:B:660:GLY:O	1:B:662:PRO:HD3	2.12	0.50
1:C:36:TRP:CD2	1:C:42:ALA:HA	2.47	0.50
1:C:832:ASP:OD1	1:C:832:ASP:N	2.43	0.50
1:C:974:HIS:C	1:C:975:LEU:HD23	2.36	0.50
1:D:73:TRP:CZ2	1:D:185:ALA:HB1	2.47	0.50
1:D:178:ARG:HB2	1:D:178:ARG:HH11	1.76	0.50
1:D:403:ASP:OD2	1:D:450:HIS:ND1	2.34	0.50
1:D:433:LEU:N	1:D:434:PRO:HD2	2.26	0.50
1:E:53:SER:O	1:E:54:LEU:HD23	2.10	0.50
1:E:660:GLY:O	1:E:662:PRO:HD3	2.12	0.50
1:F:36:TRP:CD2	1:F:42:ALA:HA	2.47	0.50
1:F:131:GLU:HG3	1:F:132:SER:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:ILE:H	1:F:278:ILE:CD1	2.21	0.50
1:F:570:TRP:CD1	1:F:571:VAL:HG22	2.47	0.50
1:F:822:LEU:HD11	1:F:824:GLN:O	2.11	0.50
1:F:833:ALA:HB1	1:F:858:ILE:O	2.11	0.50
1:G:635:THR:HG23	1:G:681:GLU:OE2	2.12	0.50
1:G:822:LEU:HD12	1:G:822:LEU:C	2.37	0.50
1:G:833:ALA:HB1	1:G:858:ILE:O	2.11	0.50
1:H:559:TYR:HB2	1:H:562:LEU:HD12	1.94	0.50
1:H:592:PHE:N	1:H:592:PHE:CD1	2.79	0.50
1:H:660:GLY:O	1:H:662:PRO:HD3	2.12	0.50
1:H:833:ALA:HB1	1:H:858:ILE:O	2.11	0.50
1:H:869:ASP:OD2	1:H:1015:HIS:ND1	2.33	0.50
1:I:635:THR:HG23	1:I:681:GLU:OE2	2.12	0.50
1:J:36:TRP:CD2	1:J:42:ALA:HA	2.47	0.50
1:J:433:LEU:N	1:J:434:PRO:HD2	2.26	0.50
1:K:500:CYS:HA	1:K:534:ILE:O	2.11	0.50
1:K:592:PHE:CD1	1:K:592:PHE:N	2.79	0.50
1:K:660:GLY:O	1:K:662:PRO:HD3	2.12	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:L:635:THR:HG23	1:L:681:GLU:OE2	2.12	0.50
1:L:767:GLN:CG	1:L:768:MET:N	2.75	0.50
1:M:433:LEU:N	1:M:434:PRO:HD2	2.26	0.50
1:M:570:TRP:CD1	1:M:571:VAL:HG22	2.47	0.50
1:M:767:GLN:CG	1:M:768:MET:N	2.75	0.50
1:N:570:TRP:CD1	1:N:571:VAL:HG22	2.47	0.50
1:O:23:GLN:HB3	1:O:26:ARG:NH2	2.27	0.50
1:O:579:ASP:OD2	1:O:583:ASN:HB2	2.11	0.50
1:O:870:VAL:HG12	1:O:871:GLU:N	2.25	0.50
1:P:568:TRP:HE1	1:P:604:ASN:ND2	2.08	0.50
1:P:660:GLY:O	1:P:662:PRO:HD3	2.12	0.50
1:A:568:TRP:HE1	1:A:604:ASN:ND2	2.08	0.50
1:A:832:ASP:OD1	1:A:832:ASP:N	2.43	0.50
1:D:23:GLN:HB3	1:D:26:ARG:NH2	2.27	0.50
1:D:570:TRP:CD1	1:D:571:VAL:HG22	2.47	0.50
1:D:579:ASP:OD2	1:D:583:ASN:HB2	2.11	0.50
1:E:36:TRP:CD2	1:E:42:ALA:HA	2.47	0.50
1:F:23:GLN:HB3	1:F:26:ARG:NH2	2.27	0.50
1:F:31:PRO:CB	1:F:32:PRO:HD2	2.42	0.50
1:G:73:TRP:CZ2	1:G:185:ALA:HB1	2.47	0.50
1:H:237:ARG:HH11	1:H:237:ARG:CG	2.23	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:210:ARG:HH12	1:I:394:ASN:C	2.19	0.50
1:I:870:VAL:HG12	1:I:871:GLU:N	2.25	0.50
1:J:434:PRO:HA	1:J:437:SER:OG	2.11	0.50
1:J:833:ALA:HB1	1:J:858:ILE:O	2.11	0.50
1:L:178:ARG:HB2	1:L:178:ARG:HH11	1.76	0.50
1:M:23:GLN:HB3	1:M:26:ARG:NH2	2.27	0.50
1:M:832:ASP:OD1	1:M:832:ASP:N	2.43	0.50
1:N:473:ARG:HD2	1:O:469:ASP:HB3	1.94	0.50
1:N:660:GLY:O	1:N:662:PRO:HD3	2.12	0.50
1:O:36:TRP:CD2	1:O:42:ALA:HA	2.47	0.50
1:O:635:THR:HG23	1:O:681:GLU:OE2	2.12	0.50
1:A:316:HIS:CA	1:A:323:ILE:HD13	2.32	0.50
1:A:567:VAL:HG12	1:A:568:TRP:N	2.27	0.50
1:A:660:GLY:O	1:A:662:PRO:HD3	2.12	0.50
1:C:73:TRP:CZ2	1:C:185:ALA:HB1	2.47	0.50
1:C:592:PHE:CD1	1:C:592:PHE:N	2.79	0.50
1:C:870:VAL:HG12	1:C:871:GLU:N	2.25	0.50
1:E:433:LEU:N	1:E:434:PRO:HD2	2.26	0.50
1:E:635:THR:HG23	1:E:681:GLU:OE2	2.12	0.50
1:F:176:PHE:N	1:F:176:PHE:CD1	2.79	0.50
1:F:869:ASP:OD2	1:F:1015:HIS:ND1	2.33	0.50
1:G:36:TRP:CD2	1:G:42:ALA:HA	2.47	0.50
1:H:567:VAL:HG12	1:H:568:TRP:N	2.27	0.50
1:I:31:PRO:CB	1:I:32:PRO:HD2	2.42	0.50
1:J:832:ASP:OD1	1:J:832:ASP:N	2.43	0.50
1:K:237:ARG:HH11	1:K:237:ARG:CG	2.23	0.50
1:K:237:ARG:HH11	1:K:237:ARG:HB3	1.77	0.50
1:L:31:PRO:CB	1:L:32:PRO:HD2	2.42	0.50
1:M:465:GLY:O	1:M:468:HIS:HB2	2.12	0.50
1:M:822:LEU:HD12	1:M:822:LEU:C	2.37	0.50
1:N:31:PRO:CB	1:N:32:PRO:HD2	2.42	0.50
1:O:73:TRP:CZ2	1:O:185:ALA:HB1	2.47	0.50
1:O:127:PHE:CD2	1:O:127:PHE:N	2.79	0.50
1:O:592:PHE:N	1:O:592:PHE:CD1	2.79	0.50
1:P:559:TYR:HB2	1:P:562:LEU:HD12	1.94	0.50
1:P:635:THR:HG23	1:P:681:GLU:OE2	2.12	0.50
1:A:465:GLY:O	1:A:468:HIS:HB2	2.12	0.50
1:B:559:TYR:HB2	1:B:562:LEU:HD12	1.94	0.50
1:B:579:ASP:OD2	1:B:583:ASN:HB2	2.11	0.50
1:B:635:THR:HG23	1:B:681:GLU:OE2	2.12	0.50
1:B:833:ALA:HB1	1:B:858:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ARG:HH12	1:C:394:ASN:C	2.20	0.50
1:C:237:ARG:HH11	1:C:237:ARG:HB3	1.77	0.50
1:C:559:TYR:HB2	1:C:562:LEU:HD12	1.94	0.50
1:C:568:TRP:HE1	1:C:604:ASN:ND2	2.08	0.50
1:C:635:THR:HG23	1:C:681:GLU:OE2	2.12	0.50
1:D:500:CYS:HA	1:D:534:ILE:O	2.10	0.50
1:E:23:GLN:HB3	1:E:26:ARG:NH2	2.27	0.50
1:E:31:PRO:CB	1:E:32:PRO:HD2	2.42	0.50
1:E:465:GLY:O	1:E:468:HIS:HB2	2.12	0.50
1:G:127:PHE:CD2	1:G:127:PHE:N	2.79	0.50
1:H:610:ASP:O	1:H:611:ARG:HB2	2.10	0.50
1:H:767:GLN:CG	1:H:768:MET:N	2.75	0.50
1:I:23:GLN:HB3	1:I:26:ARG:NH2	2.27	0.50
1:I:237:ARG:HH11	1:I:237:ARG:CG	2.23	0.50
1:J:559:TYR:HB2	1:J:562:LEU:HD12	1.94	0.50
1:J:974:HIS:C	1:J:975:LEU:HD23	2.36	0.50
1:K:434:PRO:HA	1:K:437:SER:OG	2.11	0.50
1:K:465:GLY:O	1:K:468:HIS:HB2	2.12	0.50
1:K:832:ASP:OD1	1:K:832:ASP:N	2.43	0.50
1:L:36:TRP:CD2	1:L:42:ALA:HA	2.47	0.50
1:L:579:ASP:N	1:L:583:ASN:O	2.40	0.50
1:M:210:ARG:HH12	1:M:394:ASN:C	2.19	0.50
1:N:23:GLN:HB3	1:N:26:ARG:NH2	2.27	0.50
1:N:237:ARG:HH11	1:N:237:ARG:HB3	1.77	0.50
1:N:592:PHE:N	1:N:592:PHE:CD1	2.79	0.50
1:N:822:LEU:HD11	1:N:824:GLN:O	2.11	0.50
1:O:433:LEU:N	1:O:434:PRO:HD2	2.26	0.50
1:O:634:GLN:HE22	1:O:685:LEU:H	1.57	0.50
1:P:767:GLN:CG	1:P:768:MET:N	2.75	0.50
1:A:437:SER:HB2	5:A:2256:HOH:O	2.12	0.50
1:B:7:LEU:O	1:B:8:ALA:C	2.55	0.50
1:B:23:GLN:HB3	1:B:26:ARG:NH2	2.27	0.50
1:B:31:PRO:CB	1:B:32:PRO:HD2	2.42	0.50
1:B:465:GLY:O	1:B:468:HIS:HB2	2.12	0.50
1:B:961:ARG:NH2	1:B:979:GLU:O	2.38	0.50
1:C:178:ARG:HH11	1:C:178:ARG:HB2	1.76	0.50
1:C:581:ASN:OD1	1:C:581:ASN:N	2.44	0.50
1:C:660:GLY:O	1:C:662:PRO:HD3	2.12	0.50
1:C:781:ARG:HG3	1:C:781:ARG:NH1	2.17	0.50
1:D:31:PRO:CB	1:D:32:PRO:HD2	2.42	0.50
1:D:592:PHE:N	1:D:592:PHE:CD1	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:822:LEU:HD11	1:D:824:GLN:O	2.11	0.50
1:D:870:VAL:HG12	1:D:871:GLU:N	2.25	0.50
1:E:210:ARG:HH12	1:E:394:ASN:C	2.19	0.50
1:F:822:LEU:HD12	1:F:822:LEU:C	2.37	0.50
1:G:634:GLN:HE22	1:G:685:LEU:H	1.57	0.50
1:H:49:GLN:H	1:H:49:GLN:HE21	1.59	0.50
1:H:635:THR:HG23	1:H:681:GLU:OE2	2.12	0.50
1:H:1020:TRP:CD1	1:H:1021:CME:N	2.80	0.50
1:I:610:ASP:O	1:I:611:ARG:HB2	2.10	0.50
1:I:974:HIS:C	1:I:975:LEU:HD23	2.36	0.50
1:K:570:TRP:CD1	1:K:571:VAL:HG22	2.47	0.50
1:K:579:ASP:N	1:K:583:ASN:O	2.40	0.50
1:N:7:LEU:O	1:N:8:ALA:C	2.55	0.50
1:N:465:GLY:O	1:N:468:HIS:HB2	2.12	0.50
1:N:822:LEU:HD12	1:N:822:LEU:C	2.37	0.50
1:O:210:ARG:HH12	1:O:394:ASN:C	2.19	0.50
1:P:73:TRP:CZ2	1:P:185:ALA:HB1	2.47	0.50
1:P:748:CME:SD	1:P:755:ARG:HG2	2.52	0.50
1:B:570:TRP:CD1	1:B:571:VAL:HG22	2.47	0.49
1:C:53:SER:O	1:C:54:LEU:HD23	2.10	0.49
1:C:767:GLN:CG	1:C:768:MET:N	2.75	0.49
1:C:833:ALA:HB1	1:C:858:ILE:O	2.11	0.49
1:D:748:CME:SD	1:D:755:ARG:HG2	2.52	0.49
1:F:178:ARG:HB2	1:F:178:ARG:HH11	1.76	0.49
1:F:592:PHE:N	1:F:592:PHE:CD1	2.79	0.49
1:G:581:ASN:OD1	1:G:581:ASN:N	2.44	0.49
1:G:748:CME:SD	1:G:755:ARG:HG2	2.52	0.49
1:H:23:GLN:HB3	1:H:26:ARG:NH2	2.27	0.49
1:J:660:GLY:O	1:J:662:PRO:HD3	2.12	0.49
1:L:822:LEU:HD12	1:L:822:LEU:C	2.37	0.49
1:L:974:HIS:C	1:L:975:LEU:HD23	2.36	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:O:961:ARG:NH2	1:O:979:GLU:O	2.37	0.49
1:O:1020:TRP:CD1	1:O:1021:CME:N	2.80	0.49
1:P:49:GLN:H	1:P:49:GLN:HE21	1.59	0.49
1:A:740:LEU:CD1	1:A:741:THR:H	2.12	0.49
1:C:567:VAL:HG12	1:C:568:TRP:N	2.27	0.49
1:C:867:THR:O	1:C:867:THR:HG22	2.09	0.49
1:D:36:TRP:CD2	1:D:42:ALA:HA	2.47	0.49
1:D:53:SER:O	1:D:54:LEU:HD23	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:748:CME:SD	1:E:755:ARG:HG2	2.52	0.49
1:E:767:GLN:CG	1:E:768:MET:N	2.75	0.49
1:F:287:ASP:OD1	1:F:287:ASP:N	2.29	0.49
1:F:579:ASP:N	1:F:583:ASN:O	2.40	0.49
1:F:660:GLY:O	1:F:662:PRO:HD3	2.12	0.49
1:F:767:GLN:CG	1:F:768:MET:N	2.75	0.49
1:G:579:ASP:OD2	1:G:583:ASN:HB2	2.11	0.49
1:G:767:GLN:CG	1:G:768:MET:N	2.75	0.49
1:H:73:TRP:CZ2	1:H:185:ALA:HB1	2.47	0.49
1:H:210:ARG:HH12	1:H:394:ASN:C	2.20	0.49
1:H:465:GLY:O	1:H:468:HIS:HB2	2.12	0.49
1:H:570:TRP:CD1	1:H:571:VAL:HG22	2.47	0.49
1:H:663:LEU:HD23	1:H:663:LEU:N	2.24	0.49
1:L:570:TRP:CD1	1:L:571:VAL:HG22	2.47	0.49
1:L:660:GLY:O	1:L:662:PRO:HD3	2.12	0.49
1:M:65:ALA:HB1	1:M:66:PRO:CD	2.38	0.49
1:M:282:ARG:NH1	1:P:419:GLY:O	2.45	0.49
1:M:567:VAL:HG12	1:M:568:TRP:N	2.27	0.49
1:P:23:GLN:HB3	1:P:26:ARG:NH2	2.27	0.49
1:P:210:ARG:HH12	1:P:394:ASN:C	2.20	0.49
1:A:36:TRP:CD2	1:A:42:ALA:HA	2.47	0.49
1:A:767:GLN:CG	1:A:768:MET:N	2.75	0.49
1:B:822:LEU:HD11	1:B:824:GLN:O	2.11	0.49
1:C:23:GLN:HB3	1:C:26:ARG:NH2	2.27	0.49
1:D:49:GLN:H	1:D:49:GLN:HE21	1.59	0.49
1:E:237:ARG:HH11	1:E:237:ARG:HB3	1.76	0.49
1:F:748:CME:SD	1:F:755:ARG:HG2	2.52	0.49
1:G:240:LEU:HD12	1:G:240:LEU:C	2.36	0.49
1:H:131:GLU:HG3	1:H:132:SER:N	2.26	0.49
1:H:748:CME:SD	1:H:755:ARG:HG2	2.52	0.49
1:I:567:VAL:HG12	1:I:568:TRP:N	2.27	0.49
1:J:210:ARG:HH12	1:J:394:ASN:C	2.20	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:178:ARG:HB2	1:N:178:ARG:HH11	1.76	0.49
1:N:567:VAL:HG12	1:N:568:TRP:N	2.27	0.49
1:N:581:ASN:OD1	1:N:581:ASN:N	2.44	0.49
1:N:767:GLN:CG	1:N:768:MET:N	2.75	0.49
1:O:240:LEU:HD12	1:O:240:LEU:C	2.36	0.49
1:P:833:ALA:HB1	1:P:858:ILE:O	2.11	0.49
1:A:73:TRP:CZ2	1:A:185:ALA:HB1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:TRP:CD1	1:A:571:VAL:HG22	2.47	0.49
1:B:131:GLU:HG3	1:B:132:SER:N	2.26	0.49
1:B:608:PHE:O	1:B:611:ARG:N	2.41	0.49
1:B:748:CME:SD	1:B:755:ARG:HG2	2.52	0.49
1:C:894:ARG:NH1	1:C:920:LEU:HA	2.28	0.49
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.77	0.49
1:D:465:GLY:O	1:D:468:HIS:HB2	2.12	0.49
1:F:433:LEU:N	1:F:434:PRO:HD2	2.26	0.49
1:G:559:TYR:HB2	1:G:562:LEU:HD12	1.94	0.49
1:I:36:TRP:CD2	1:I:42:ALA:HA	2.47	0.49
1:I:570:TRP:CD1	1:I:571:VAL:HG22	2.47	0.49
1:I:767:GLN:CG	1:I:768:MET:N	2.75	0.49
1:J:23:GLN:HB3	1:J:26:ARG:NH2	2.27	0.49
1:J:49:GLN:H	1:J:49:GLN:HE21	1.59	0.49
1:J:592:PHE:N	1:J:592:PHE:CD1	2.79	0.49
1:J:740:LEU:CD1	1:J:741:THR:H	2.12	0.49
1:M:592:PHE:N	1:M:592:PHE:CD1	2.79	0.49
1:O:65:ALA:HB1	1:O:66:PRO:CD	2.38	0.49
1:P:178:ARG:HH11	1:P:178:ARG:HB2	1.76	0.49
1:P:610:ASP:O	1:P:611:ARG:HB2	2.10	0.49
1:P:822:LEU:HD12	1:P:822:LEU:C	2.37	0.49
1:A:23:GLN:HB3	1:A:26:ARG:NH2	2.27	0.49
1:A:559:TYR:HB2	1:A:562:LEU:HD12	1.94	0.49
1:A:635:THR:HG23	1:A:681:GLU:OE2	2.12	0.49
1:B:515:VAL:HG21	1:C:281:GLU:HG3	1.95	0.49
1:B:581:ASN:OD1	1:B:581:ASN:N	2.44	0.49
1:B:767:GLN:CG	1:B:768:MET:N	2.75	0.49
1:C:748:CME:SD	1:C:755:ARG:HG2	2.53	0.49
1:D:767:GLN:CG	1:D:768:MET:N	2.75	0.49
1:D:832:ASP:OD1	1:D:832:ASP:N	2.43	0.49
1:E:73:TRP:CZ2	1:E:185:ALA:HB1	2.47	0.49
1:E:1020:TRP:CD1	1:E:1021:CME:N	2.80	0.49
1:F:7:LEU:O	1:F:8:ALA:C	2.55	0.49
1:F:567:VAL:HG12	1:F:568:TRP:N	2.27	0.49
1:G:570:TRP:CD1	1:G:571:VAL:HG22	2.47	0.49
1:H:49:GLN:H	1:H:49:GLN:CD	2.20	0.49
1:I:581:ASN:OD1	1:I:581:ASN:N	2.44	0.49
1:I:961:ARG:NH2	1:I:979:GLU:O	2.37	0.49
1:J:211:ASP:OD1	1:J:211:ASP:N	2.42	0.49
1:J:663:LEU:HD23	1:J:663:LEU:N	2.24	0.49
1:J:767:GLN:CG	1:J:768:MET:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:824:GLN:HG3	1:J:825:CYS:N	2.28	0.49
1:K:581:ASN:OD1	1:K:581:ASN:N	2.44	0.49
1:L:210:ARG:HH12	1:L:394:ASN:C	2.20	0.49
1:M:434:PRO:HA	1:M:437:SER:OG	2.11	0.49
1:N:559:TYR:HB2	1:N:562:LEU:HD12	1.94	0.49
1:N:635:THR:HG23	1:N:681:GLU:OE2	2.12	0.49
1:N:961:ARG:NH2	1:N:979:GLU:O	2.38	0.49
1:O:49:GLN:H	1:O:49:GLN:CD	2.20	0.49
1:O:559:TYR:HB2	1:O:562:LEU:HD12	1.94	0.49
1:O:581:ASN:OD1	1:O:581:ASN:N	2.44	0.49
1:P:127:PHE:N	1:P:127:PHE:CD2	2.79	0.49
1:B:567:VAL:HG12	1:B:568:TRP:N	2.27	0.49
1:B:822:LEU:HD12	1:B:822:LEU:C	2.37	0.49
1:D:635:THR:HG23	1:D:681:GLU:OE2	2.12	0.49
1:D:660:GLY:O	1:D:662:PRO:HD3	2.12	0.49
1:E:131:GLU:O	1:E:134:LEU:N	2.46	0.49
1:E:567:VAL:HG12	1:E:568:TRP:N	2.27	0.49
1:F:559:TYR:HB2	1:F:562:LEU:HD12	1.94	0.49
1:F:635:THR:HG23	1:F:681:GLU:OE2	2.12	0.49
1:F:894:ARG:NH1	1:F:920:LEU:HA	2.28	0.49
1:G:65:ALA:HB1	1:G:66:PRO:CD	2.39	0.49
1:G:211:ASP:N	1:G:211:ASP:OD1	2.42	0.49
1:H:36:TRP:CD2	1:H:42:ALA:HA	2.47	0.49
1:H:131:GLU:O	1:H:134:LEU:N	2.46	0.49
1:H:581:ASN:OD1	1:H:581:ASN:N	2.44	0.49
1:I:131:GLU:HG3	1:I:132:SER:N	2.26	0.49
1:I:894:ARG:NH1	1:I:920:LEU:HA	2.28	0.49
1:J:317:THR:HG23	1:J:323:ILE:HD11	1.95	0.49
1:J:465:GLY:O	1:J:468:HIS:HB2	2.12	0.49
1:K:131:GLU:O	1:K:134:LEU:N	2.46	0.49
1:L:127:PHE:CD2	1:L:127:PHE:N	2.79	0.49
1:L:317:THR:HG23	1:L:323:ILE:HD11	1.95	0.49
1:L:961:ARG:NH2	1:L:979:GLU:O	2.37	0.49
1:M:748:CME:SD	1:M:755:ARG:HG2	2.52	0.49
1:N:894:ARG:NH1	1:N:920:LEU:HA	2.28	0.49
1:O:832:ASP:OD1	1:O:832:ASP:N	2.43	0.49
1:P:663:LEU:HD23	1:P:663:LEU:N	2.24	0.49
1:P:928:PRO:HB2	1:P:973:ARG:HH11	1.78	0.49
1:A:131:GLU:HG3	1:A:132:SER:N	2.26	0.49
1:C:570:TRP:CD1	1:C:571:VAL:HG22	2.47	0.49
1:G:894:ARG:NH1	1:G:920:LEU:HA	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:928:PRO:HB2	1:H:973:ARG:HH11	1.78	0.49
1:I:131:GLU:O	1:I:134:LEU:N	2.46	0.49
1:J:131:GLU:O	1:J:134:LEU:N	2.46	0.49
1:K:23:GLN:HB3	1:K:26:ARG:NH2	2.27	0.49
1:K:31:PRO:CB	1:K:32:PRO:HD2	2.42	0.49
1:K:210:ARG:HH12	1:K:394:ASN:C	2.19	0.49
1:K:230:ARG:HH11	1:K:230:ARG:CG	2.24	0.49
1:K:559:TYR:HB2	1:K:562:LEU:HD12	1.94	0.49
1:L:592:PHE:N	1:L:592:PHE:CD1	2.79	0.49
1:L:894:ARG:NH1	1:L:920:LEU:HA	2.28	0.49
1:M:317:THR:HG23	1:M:323:ILE:HD11	1.95	0.49
1:M:894:ARG:NH1	1:M:920:LEU:HA	2.28	0.49
1:N:287:ASP:CG	1:O:425:ARG:NH2	2.71	0.49
1:O:211:ASP:N	1:O:211:ASP:OD1	2.42	0.49
1:O:570:TRP:CD1	1:O:571:VAL:HG22	2.47	0.49
1:O:894:ARG:NH1	1:O:920:LEU:HA	2.28	0.49
1:P:131:GLU:O	1:P:134:LEU:N	2.46	0.49
1:P:176:PHE:N	1:P:176:PHE:CD1	2.79	0.49
1:P:781:ARG:HH11	1:P:781:ARG:CG	2.19	0.49
1:A:49:GLN:H	1:A:49:GLN:CD	2.20	0.49
1:A:1020:TRP:CD1	1:A:1021:CME:N	2.80	0.49
1:C:131:GLU:O	1:C:134:LEU:N	2.46	0.49
1:D:567:VAL:HG12	1:D:568:TRP:N	2.27	0.49
1:D:581:ASN:OD1	1:D:581:ASN:N	2.44	0.49
1:E:49:GLN:H	1:E:49:GLN:HE21	1.59	0.49
1:F:367:MET:HB3	1:F:372:MET:HE3	1.95	0.49
1:H:31:PRO:CB	1:H:32:PRO:HD2	2.42	0.49
1:J:230:ARG:HH11	1:J:230:ARG:CG	2.24	0.49
1:J:315:LEU:O	1:J:322:LEU:HD12	2.13	0.49
1:J:570:TRP:CD1	1:J:571:VAL:HG22	2.47	0.49
1:K:260:LEU:HA	1:K:260:LEU:HD12	1.61	0.49
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:L:367:MET:HB3	1:L:372:MET:HE3	1.95	0.49
1:M:31:PRO:CB	1:M:32:PRO:HD2	2.42	0.49
1:M:635:THR:HG23	1:M:681:GLU:OE2	2.12	0.49
1:N:367:MET:HB3	1:N:372:MET:HE3	1.95	0.49
1:N:568:TRP:HE1	1:N:604:ASN:ND2	2.09	0.49
1:N:928:PRO:HB2	1:N:973:ARG:HH11	1.78	0.49
1:P:31:PRO:CB	1:P:32:PRO:HD2	2.42	0.49
1:P:65:ALA:HB1	1:P:66:PRO:CD	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:465:GLY:O	1:P:468:HIS:HB2	2.12	0.49
1:P:581:ASN:OD1	1:P:581:ASN:N	2.44	0.49
1:A:663:LEU:HD23	1:A:663:LEU:N	2.24	0.49
1:A:746:ASP:HA	1:A:760:ARG:CG	2.39	0.49
1:B:79:PRO:HG2	1:B:80:GLU:OE2	2.13	0.49
1:B:740:LEU:CD1	1:B:741:THR:H	2.12	0.49
1:D:131:GLU:HG3	1:D:132:SER:N	2.26	0.49
1:E:425:ARG:HH22	1:H:287:ASP:CG	2.21	0.49
1:F:131:GLU:O	1:F:134:LEU:N	2.46	0.49
1:F:317:THR:HG23	1:F:323:ILE:HD11	1.95	0.49
1:G:742:THR:CG2	1:G:743:SER:N	2.76	0.49
1:H:79:PRO:HG2	1:H:80:GLU:OE2	2.13	0.49
1:I:49:GLN:H	1:I:49:GLN:CD	2.20	0.49
1:J:631:LEU:HD12	1:J:632:SER:H	1.78	0.49
1:L:237:ARG:HH11	1:L:237:ARG:HB3	1.77	0.49
1:M:7:LEU:O	1:M:8:ALA:C	2.55	0.49
1:M:73:TRP:CZ2	1:M:185:ALA:HB1	2.47	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:N:317:THR:HG23	1:N:323:ILE:HD11	1.95	0.49
1:N:824:GLN:HG3	1:N:825:CYS:N	2.28	0.49
1:N:1020:TRP:CD1	1:N:1021:CME:N	2.80	0.49
1:A:65:ALA:HB1	1:A:66:PRO:CD	2.39	0.49
1:A:210:ARG:HH12	1:A:394:ASN:C	2.19	0.49
1:B:131:GLU:O	1:B:134:LEU:N	2.46	0.49
1:B:469:ASP:HB3	1:C:473:ARG:HD2	1.93	0.49
1:C:127:PHE:N	1:C:127:PHE:CD2	2.79	0.49
1:C:433:LEU:HD12	1:C:433:LEU:O	2.13	0.49
1:D:131:GLU:O	1:D:134:LEU:N	2.46	0.49
1:D:315:LEU:O	1:D:322:LEU:HD12	2.13	0.49
1:E:86:VAL:HG13	1:E:87:PRO:HA	1.95	0.49
1:E:317:THR:HG23	1:E:323:ILE:HD11	1.95	0.49
1:E:469:ASP:HB3	1:H:473:ARG:HD2	1.95	0.49
1:G:178:ARG:HB2	1:G:178:ARG:HH11	1.76	0.49
1:G:824:GLN:HG3	1:G:825:CYS:N	2.28	0.49
1:H:433:LEU:HD12	1:H:433:LEU:O	2.13	0.49
1:I:748:CME:SD	1:I:755:ARG:HG2	2.52	0.49
1:J:31:PRO:CB	1:J:32:PRO:HD2	2.42	0.49
1:J:928:PRO:HB2	1:J:973:ARG:HH11	1.78	0.49
1:J:1020:TRP:CD1	1:J:1021:CME:N	2.80	0.49
1:K:317:THR:HG23	1:K:323:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:403:ASP:OD2	1:K:450:HIS:ND1	2.34	0.49
1:K:567:VAL:HG12	1:K:568:TRP:N	2.27	0.49
1:L:465:GLY:O	1:L:468:HIS:HB2	2.12	0.49
1:L:567:VAL:HG12	1:L:568:TRP:N	2.27	0.49
1:M:131:GLU:HG3	1:M:132:SER:N	2.26	0.49
1:M:367:MET:HB3	1:M:372:MET:HE3	1.95	0.49
1:M:660:GLY:O	1:M:662:PRO:HD3	2.12	0.49
1:M:867:THR:O	1:M:867:THR:HG22	2.09	0.49
1:A:31:PRO:CB	1:A:32:PRO:HD2	2.42	0.48
1:A:131:GLU:O	1:A:134:LEU:N	2.46	0.48
1:A:748:CME:SD	1:A:755:ARG:HG2	2.52	0.48
1:A:802:ASP:OD1	1:A:803:PRO:HD2	2.13	0.48
1:C:7:LEU:O	1:C:8:ALA:C	2.55	0.48
1:C:287:ASP:OD1	1:C:287:ASP:N	2.29	0.48
1:C:465:GLY:O	1:C:468:HIS:HB2	2.12	0.48
1:C:1020:TRP:CD1	1:C:1021:CME:N	2.80	0.48
1:D:742:THR:CG2	1:D:743:SER:N	2.76	0.48
1:E:367:MET:HB3	1:E:372:MET:HE3	1.95	0.48
1:E:559:TYR:HB2	1:E:562:LEU:HD12	1.94	0.48
1:E:592:PHE:N	1:E:592:PHE:CD1	2.79	0.48
1:F:57:GLU:HG2	1:F:83:THR:HG21	1.94	0.48
1:F:465:GLY:O	1:F:468:HIS:HB2	2.12	0.48
1:F:1020:TRP:CD1	1:F:1021:CME:N	2.80	0.48
1:G:567:VAL:HG12	1:G:568:TRP:N	2.27	0.48
1:H:7:LEU:O	1:H:8:ALA:C	2.55	0.48
1:H:65:ALA:HB1	1:H:66:PRO:CD	2.39	0.48
1:H:612:THR:HB	1:H:613:PRO:HD2	1.95	0.48
1:I:167:LEU:HB3	1:I:168:PRO:HD2	1.95	0.48
1:I:178:ARG:HB2	1:I:178:ARG:HH11	1.76	0.48
1:I:465:GLY:O	1:I:468:HIS:HB2	2.12	0.48
1:J:131:GLU:HG3	1:J:132:SER:N	2.26	0.48
1:J:748:CME:SD	1:J:755:ARG:HG2	2.52	0.48
1:J:961:ARG:NH2	1:J:979:GLU:O	2.37	0.48
1:K:631:LEU:HD12	1:K:632:SER:H	1.78	0.48
1:K:767:GLN:CG	1:K:768:MET:N	2.75	0.48
1:K:772:ASP:OD1	1:K:772:ASP:N	2.30	0.48
1:L:746:ASP:HA	1:L:760:ARG:CG	2.39	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:M:86:VAL:HG13	1:M:87:PRO:HA	1.95	0.48
1:N:433:LEU:N	1:N:434:PRO:HD2	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:P:237:ARG:HH11	1:P:237:ARG:HB3	1.77	0.48
1:P:315:LEU:O	1:P:322:LEU:HD12	2.13	0.48
1:P:567:VAL:HG12	1:P:568:TRP:N	2.27	0.48
1:P:631:LEU:HD12	1:P:632:SER:H	1.78	0.48
1:B:612:THR:HB	1:B:613:PRO:HD2	1.95	0.48
1:C:31:PRO:CB	1:C:32:PRO:HD2	2.42	0.48
1:C:824:GLN:O	1:C:838:THR:HA	2.14	0.48
1:D:802:ASP:OD1	1:D:803:PRO:HD2	2.14	0.48
1:D:824:GLN:O	1:D:838:THR:HA	2.14	0.48
1:D:928:PRO:HB2	1:D:973:ARG:HH11	1.78	0.48
1:E:167:LEU:HB3	1:E:168:PRO:HD2	1.95	0.48
1:F:507:ASP:C	1:F:519:SER:HB2	2.39	0.48
1:F:631:LEU:HD12	1:F:632:SER:H	1.78	0.48
1:F:742:THR:CG2	1:F:743:SER:N	2.76	0.48
1:H:167:LEU:HB3	1:H:168:PRO:HD2	1.95	0.48
1:I:79:PRO:HG2	1:I:80:GLU:OE2	2.13	0.48
1:I:418:HIS:O	1:L:282:ARG:HD3	2.12	0.48
1:I:822:LEU:HD12	1:I:822:LEU:C	2.37	0.48
1:J:567:VAL:HG12	1:J:568:TRP:N	2.27	0.48
1:K:73:TRP:CH2	1:K:185:ALA:HB1	2.49	0.48
1:K:635:THR:HG23	1:K:681:GLU:OE2	2.12	0.48
1:L:86:VAL:HG13	1:L:87:PRO:HA	1.96	0.48
1:L:748:CME:SD	1:L:755:ARG:HG2	2.52	0.48
1:L:824:GLN:O	1:L:838:THR:HA	2.14	0.48
1:M:167:LEU:HB3	1:M:168:PRO:HD2	1.95	0.48
1:M:433:LEU:HD12	1:M:433:LEU:O	2.13	0.48
1:O:237:ARG:HH11	1:O:237:ARG:HB3	1.77	0.48
1:O:567:VAL:HG12	1:O:568:TRP:N	2.27	0.48
1:O:631:LEU:HD12	1:O:632:SER:H	1.78	0.48
1:O:748:CME:SD	1:O:755:ARG:HG2	2.53	0.48
1:P:36:TRP:CD2	1:P:42:ALA:HA	2.46	0.48
1:P:442:ARG:HA	1:P:445:GLN:HG3	1.95	0.48
1:P:742:THR:CG2	1:P:743:SER:N	2.76	0.48
1:P:824:GLN:HG3	1:P:825:CYS:N	2.28	0.48
1:A:433:LEU:HD12	1:A:433:LEU:O	2.13	0.48
1:A:824:GLN:O	1:A:838:THR:HA	2.13	0.48
1:A:928:PRO:HB2	1:A:973:ARG:HH11	1.78	0.48
1:B:57:GLU:HG2	1:B:83:THR:HG21	1.93	0.48
1:C:317:THR:HG23	1:C:323:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:928:PRO:HB2	1:C:973:ARG:HH11	1.78	0.48
1:D:79:PRO:HG2	1:D:80:GLU:OE2	2.13	0.48
1:D:210:ARG:HH12	1:D:394:ASN:C	2.20	0.48
1:E:928:PRO:HB2	1:E:973:ARG:HH11	1.78	0.48
1:G:237:ARG:HH11	1:G:237:ARG:HB3	1.77	0.48
1:G:433:LEU:HD12	1:G:433:LEU:O	2.13	0.48
1:H:127:PHE:N	1:H:127:PHE:CD2	2.79	0.48
1:H:824:GLN:O	1:H:838:THR:HA	2.14	0.48
1:I:442:ARG:HA	1:I:445:GLN:HG3	1.95	0.48
1:J:189:LEU:N	1:J:189:LEU:CD2	2.75	0.48
1:J:742:THR:CG2	1:J:743:SER:N	2.76	0.48
1:J:894:ARG:NH1	1:J:920:LEU:HA	2.28	0.48
1:K:211:ASP:OD1	1:K:211:ASP:N	2.42	0.48
1:L:131:GLU:O	1:L:134:LEU:N	2.46	0.48
1:L:507:ASP:C	1:L:519:SER:HB2	2.39	0.48
1:L:559:TYR:HB2	1:L:562:LEU:HD12	1.94	0.48
1:M:131:GLU:O	1:M:134:LEU:N	2.46	0.48
1:M:559:TYR:HB2	1:M:562:LEU:HD12	1.94	0.48
1:M:802:ASP:OD1	1:M:803:PRO:HD2	2.13	0.48
1:M:928:PRO:HB2	1:M:973:ARG:HH11	1.78	0.48
1:N:79:PRO:HG2	1:N:80:GLU:OE2	2.13	0.48
1:N:748:CME:SD	1:N:755:ARG:HG2	2.52	0.48
1:A:127:PHE:CD2	1:A:127:PHE:N	2.79	0.48
1:A:507:ASP:C	1:A:519:SER:HB2	2.39	0.48
1:A:652:LEU:HB3	1:A:668:VAL:O	2.14	0.48
1:B:742:THR:CG2	1:B:743:SER:N	2.76	0.48
1:B:746:ASP:HA	1:B:760:ARG:CG	2.39	0.48
1:C:253:TYR:CD2	1:C:253:TYR:N	2.82	0.48
1:C:631:LEU:HD12	1:C:632:SER:H	1.78	0.48
1:D:57:GLU:HG2	1:D:83:THR:HG21	1.93	0.48
1:D:73:TRP:CH2	1:D:185:ALA:HB1	2.49	0.48
1:D:559:TYR:HB2	1:D:562:LEU:HD12	1.94	0.48
1:D:742:THR:CG2	1:D:743:SER:H	2.27	0.48
1:E:652:LEU:HB3	1:E:668:VAL:O	2.14	0.48
1:F:167:LEU:HB3	1:F:168:PRO:HD2	1.95	0.48
1:F:237:ARG:HH11	1:F:237:ARG:HB3	1.77	0.48
1:F:442:ARG:HA	1:F:445:GLN:HG3	1.96	0.48
1:G:31:PRO:CB	1:G:32:PRO:HD2	2.42	0.48
1:G:612:THR:HB	1:G:613:PRO:HD2	1.96	0.48
1:G:631:LEU:HD12	1:G:632:SER:H	1.79	0.48
1:G:802:ASP:OD1	1:G:803:PRO:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:507:ASP:C	1:H:519:SER:HB2	2.39	0.48
1:I:240:LEU:HD12	1:I:240:LEU:C	2.36	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:J:367:MET:HB3	1:J:372:MET:HE3	1.95	0.48
1:K:507:ASP:C	1:K:519:SER:HB2	2.39	0.48
1:K:802:ASP:OD1	1:K:803:PRO:HD2	2.13	0.48
1:L:663:LEU:HD23	1:L:663:LEU:N	2.24	0.48
1:L:742:THR:CG2	1:L:743:SER:N	2.76	0.48
1:M:612:THR:HB	1:M:613:PRO:HD2	1.95	0.48
1:M:824:GLN:HG3	1:M:825:CYS:N	2.28	0.48
1:N:167:LEU:HB3	1:N:168:PRO:HD2	1.96	0.48
1:N:433:LEU:HD12	1:N:433:LEU:O	2.13	0.48
1:N:442:ARG:HA	1:N:445:GLN:HG3	1.96	0.48
1:N:631:LEU:HD12	1:N:632:SER:H	1.79	0.48
1:O:433:LEU:HD12	1:O:433:LEU:O	2.13	0.48
1:O:465:GLY:O	1:O:468:HIS:HB2	2.12	0.48
1:O:612:THR:HB	1:O:613:PRO:HD2	1.96	0.48
1:O:685:LEU:HA	1:O:686:PRO:HD3	1.70	0.48
1:O:824:GLN:O	1:O:838:THR:HA	2.14	0.48
1:P:79:PRO:HG2	1:P:80:GLU:OE2	2.13	0.48
1:P:612:THR:HB	1:P:613:PRO:HD2	1.95	0.48
1:P:778:THR:HG22	1:P:887:GLN:H	1.79	0.48
1:A:367:MET:HB3	1:A:372:MET:HE3	1.95	0.48
1:B:367:MET:HB3	1:B:372:MET:HE3	1.95	0.48
1:B:802:ASP:OD1	1:B:803:PRO:HD2	2.13	0.48
1:B:928:PRO:HB2	1:B:973:ARG:HH11	1.78	0.48
1:D:347:LYS:CB	1:D:348:PRO:HD2	2.43	0.48
1:E:73:TRP:CH2	1:E:185:ALA:HB1	2.49	0.48
1:E:315:LEU:O	1:E:322:LEU:HD12	2.13	0.48
1:E:433:LEU:HD12	1:E:433:LEU:O	2.13	0.48
1:F:433:LEU:HD12	1:F:433:LEU:O	2.13	0.48
1:G:465:GLY:O	1:G:468:HIS:HB2	2.12	0.48
1:H:442:ARG:HA	1:H:445:GLN:HG3	1.95	0.48
1:H:894:ARG:NH1	1:H:920:LEU:HA	2.28	0.48
1:I:781:ARG:HG3	1:I:781:ARG:NH1	2.17	0.48
1:I:928:PRO:HB2	1:I:973:ARG:HH11	1.78	0.48
1:J:237:ARG:HH11	1:J:237:ARG:HB3	1.77	0.48
1:J:433:LEU:HD12	1:J:433:LEU:O	2.13	0.48
1:J:507:ASP:C	1:J:519:SER:HB2	2.39	0.48
1:K:928:PRO:HB2	1:K:973:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:49:GLN:H	1:L:49:GLN:CD	2.20	0.48
1:L:442:ARG:HA	1:L:445:GLN:HG3	1.95	0.48
1:M:79:PRO:HG2	1:M:80:GLU:OE2	2.13	0.48
1:M:652:LEU:HB3	1:M:668:VAL:O	2.14	0.48
1:M:742:THR:CG2	1:M:743:SER:H	2.27	0.48
1:M:961:ARG:NH2	1:M:979:GLU:O	2.37	0.48
1:N:86:VAL:HG13	1:N:87:PRO:HA	1.95	0.48
1:O:31:PRO:CB	1:O:32:PRO:HD2	2.42	0.48
1:P:507:ASP:C	1:P:519:SER:HB2	2.39	0.48
1:A:73:TRP:CH2	1:A:185:ALA:HB1	2.49	0.48
1:A:612:THR:HB	1:A:613:PRO:HD2	1.96	0.48
1:B:65:ALA:HB1	1:B:66:PRO:CD	2.39	0.48
1:B:442:ARG:HA	1:B:445:GLN:HG3	1.95	0.48
1:C:86:VAL:HG13	1:C:87:PRO:HA	1.96	0.48
1:C:367:MET:HB3	1:C:372:MET:HE3	1.95	0.48
1:C:507:ASP:C	1:C:519:SER:HB2	2.39	0.48
1:D:147:ASN:HA	1:D:148:SER:HA	1.55	0.48
1:E:612:THR:HB	1:E:613:PRO:HD2	1.96	0.48
1:F:86:VAL:HG13	1:F:87:PRO:HA	1.95	0.48
1:F:824:GLN:O	1:F:838:THR:HA	2.13	0.48
1:G:287:ASP:OD1	1:G:287:ASP:N	2.29	0.48
1:G:317:THR:HG23	1:G:323:ILE:HD11	1.95	0.48
1:G:442:ARG:HA	1:G:445:GLN:HG3	1.96	0.48
1:G:778:THR:HG22	1:G:887:GLN:H	1.79	0.48
1:H:126:THR:HA	1:H:182:ASN:O	2.14	0.48
1:H:781:ARG:HH11	1:H:781:ARG:CG	2.19	0.48
1:I:73:TRP:CH2	1:I:185:ALA:HB1	2.49	0.48
1:I:317:THR:HG23	1:I:323:ILE:HD11	1.95	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: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:K:652:LEU:HB3	1:K:668:VAL:O	2.14	0.48
1:K:824:GLN:O	1:K:838:THR:HA	2.13	0.48
1:M:230:ARG:HH11	1:M:230:ARG:CG	2.24	0.48
1:M:778:THR:HG22	1:M:887:GLN:H	1.79	0.48
1:O:126:THR:HA	1:O:182:ASN:O	2.14	0.48
1:O:652:LEU:HB3	1:O:668:VAL:O	2.14	0.48
1:O:802:ASP:OD1	1:O:803:PRO:HD2	2.13	0.48
1:P:63:PHE:CB	1:P:64:PRO:HD2	2.32	0.48
1:P:579:ASP:N	1:P:583:ASN:O	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:824:GLN:O	1:P:838:THR:HA	2.14	0.48
1:A:167:LEU:HB3	1:A:168:PRO:HD2	1.96	0.48
1:B:178:ARG:HB2	1:B:178:ARG:HH11	1.77	0.48
1:B:507:ASP:C	1:B:519:SER:HB2	2.39	0.48
1:C:679:LEU:HA	1:C:679:LEU:HD23	1.26	0.48
1:C:802:ASP:OD1	1:C:803:PRO:HD2	2.14	0.48
1:D:253:TYR:CD2	1:D:253:TYR:N	2.82	0.48
1:D:433:LEU:HD12	1:D:433:LEU:O	2.13	0.48
1:D:961:ARG:NH2	1:D:979:GLU:O	2.37	0.48
1:E:49:GLN:H	1:E:49:GLN:CD	2.20	0.48
1:E:742:THR:CG2	1:E:743:SER:H	2.27	0.48
1:F:79:PRO:HG2	1:F:80:GLU:OE2	2.13	0.48
1:F:282:ARG:NH1	1:G:419:GLY:HA2	2.28	0.48
1:G:253:TYR:CD2	1:G:253:TYR:N	2.82	0.48
1:G:507:ASP:C	1:G:519:SER:HB2	2.38	0.48
1:G:928:PRO:HB2	1:G:973:ARG:HH11	1.78	0.48
1:H:652:LEU:HB3	1:H:668:VAL:O	2.14	0.48
1:I:211:ASP:OD1	1:I:211:ASP:N	2.42	0.48
1:J:79:PRO:HG2	1:J:80:GLU:OE2	2.13	0.48
1:K:1020:TRP:CD1	1:K:1021:CME:N	2.80	0.48
1:L:30:HIS:ND1	1:L:33:PHE:CE1	2.82	0.48
1:L:167:LEU:HB3	1:L:168:PRO:HD2	1.96	0.48
1:M:73:TRP:CH2	1:M:185:ALA:HB1	2.49	0.48
1:N:49:GLN:H	1:N:49:GLN:CD	2.20	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:N:742:THR:CG2	1:N:743:SER:N	2.76	0.48
1:O:131:GLU:O	1:O:134:LEU:N	2.46	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:N	2.76	0.48
1:P:49:GLN:H	1:P:49:GLN:CD	2.20	0.48
1:P:73:TRP:CH2	1:P:185:ALA:HB1	2.49	0.48
1:A:126:THR:HA	1:A:182:ASN:O	2.14	0.48
1:A:315:LEU:O	1:A:322:LEU:HD12	2.13	0.48
1:A:742:THR:CG2	1:A:743:SER:H	2.27	0.48
1:B:778:THR:HG22	1:B:887:GLN:H	1.79	0.48
1:C:30:HIS:ND1	1:C:33:PHE:CE1	2.82	0.48
1:C:79:PRO:HG2	1:C:80:GLU:OE2	2.13	0.48
1:C:608:PHE:O	1:C:611:ARG:N	2.41	0.48
1:C:824:GLN:HG3	1:C:825:CYS:N	2.28	0.48
1:D:86:VAL:HG13	1:D:87:PRO:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:507:ASP:C	1:D:519:SER:HB2	2.39	0.48
1:D:631:LEU:HD12	1:D:632:SER:H	1.78	0.48
1:D:875:ASP:N	1:D:875:ASP:OD2	2.47	0.48
1:E:663:LEU:HD23	1:E:663:LEU:N	2.24	0.48
1:E:778:THR:HG22	1:E:887:GLN:H	1.79	0.48
1:E:802:ASP:OD1	1:E:803:PRO:HD2	2.13	0.48
1:E:824:GLN:HG3	1:E:825:CYS:N	2.28	0.48
1:E:832:ASP:OD1	1:E:832:ASP:N	2.43	0.48
1:E:894:ARG:NH1	1:E:920:LEU:HA	2.28	0.48
1:F:315:LEU:O	1:F:322:LEU:HD12	2.13	0.48
1:F:824:GLN:HG3	1:F:825:CYS:N	2.28	0.48
1:G:131:GLU:O	1:G:134:LEU:N	2.46	0.48
1:G:230:ARG:HH11	1:G:230:ARG:CG	2.24	0.48
1:H:66:PRO:HD2	1:H:67:GLU:OE2	2.14	0.48
1:H:315:LEU:O	1:H:322:LEU:HD12	2.13	0.48
1:H:367:MET:HB3	1:H:372:MET:HE3	1.95	0.48
1:H:822:LEU:HD12	1:H:822:LEU:C	2.37	0.48
1:I:237:ARG:HH11	1:I:237:ARG:HB3	1.77	0.48
1:I:631:LEU:HD12	1:I:632:SER:H	1.78	0.48
1:I:824:GLN:O	1:I:838:THR:HA	2.14	0.48
1:J:253:TYR:CD2	1:J:253:TYR:N	2.82	0.48
1:J:778:THR:HG22	1:J:887:GLN:H	1.79	0.48
1:K:79:PRO:HG2	1:K:80:GLU:OE2	2.13	0.48
1:L:271:THR:HG22	1:L:272:ALA:N	2.29	0.48
1:L:315:LEU:O	1:L:322:LEU:HD12	2.13	0.48
1:L:742:THR:CG2	1:L:743:SER:H	2.27	0.48
1:L:772:ASP:OD1	1:L:772:ASP:N	2.30	0.48
1:L:869:ASP:OD2	1:L:1015:HIS:ND1	2.33	0.48
1:M:824:GLN:O	1:M:838:THR:HA	2.14	0.48
1:N:66:PRO:HD2	1:N:67:GLU:OE2	2.14	0.48
1:N:73:TRP:CH2	1:N:185:ALA:HB1	2.48	0.48
1:N:824:GLN:O	1:N:838:THR:HA	2.14	0.48
1:O:73:TRP:CH2	1:O:185:ALA:HB1	2.49	0.48
1:O:742:THR:CG2	1:O:743:SER:H	2.27	0.48
1:O:928:PRO:HB2	1:O:973:ARG:HH11	1.78	0.48
1:P:599:ARG:HB2	1:P:600:GLN:H	1.40	0.48
1:P:894:ARG:NH1	1:P:920:LEU:HA	2.28	0.48
1:A:79:PRO:HG2	1:A:80:GLU:OE2	2.13	0.48
1:A:894:ARG:NH1	1:A:920:LEU:HA	2.28	0.48
1:B:271:THR:HG22	1:B:272:ALA:N	2.29	0.48
1:B:315:LEU:O	1:B:322:LEU:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:THR:HG23	1:B:323:ILE:HD11	1.95	0.48
1:C:73:TRP:CH2	1:C:185:ALA:HB1	2.49	0.48
1:C:442:ARG:HA	1:C:445:GLN:HG3	1.95	0.48
1:C:742:THR:CG2	1:C:743:SER:H	2.27	0.48
1:D:612:THR:HB	1:D:613:PRO:HD2	1.95	0.48
1:D:1018:LEU:HD23	1:D:1018:LEU:HA	1.51	0.48
1:E:30:HIS:ND1	1:E:33:PHE:CE1	2.82	0.48
1:E:126:THR:HA	1:E:182:ASN:O	2.14	0.48
1:E:608:PHE:O	1:E:611:ARG:N	2.41	0.48
1:E:742:THR:CG2	1:E:743:SER:N	2.76	0.48
1:F:73:TRP:CH2	1:F:185:ALA:HB1	2.49	0.48
1:G:79:PRO:HG2	1:G:80:GLU:OE2	2.13	0.48
1:H:129:VAL:CG2	1:H:182:ASN:ND2	2.77	0.48
1:H:531:ARG:O	1:H:561:ARG:NH1	2.46	0.48
1:H:742:THR:CG2	1:H:743:SER:N	2.76	0.48
1:H:824:GLN:HG3	1:H:825:CYS:N	2.28	0.48
1:I:315:LEU:O	1:I:322:LEU:HD12	2.13	0.48
1:I:742:THR:CG2	1:I:743:SER:N	2.76	0.48
1:I:778:THR:HG22	1:I:887:GLN:H	1.79	0.48
1:J:73:TRP:CH2	1:J:185:ALA:HB1	2.49	0.48
1:J:118:ASN:HA	1:J:119:PRO:HD2	1.60	0.48
1:J:167:LEU:HB3	1:J:168:PRO:HD2	1.95	0.48
1:K:66:PRO:HD2	1:K:67:GLU:OE2	2.14	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:M:1020:TRP:CD1	1:M:1021:CME:N	2.80	0.48
1:N:126:THR:HA	1:N:182:ASN:O	2.14	0.48
1:N:315:LEU:O	1:N:322:LEU:HD12	2.13	0.48
1:N:802:ASP:OD1	1:N:803:PRO:HD2	2.13	0.48
1:O:315:LEU:O	1:O:322:LEU:HD12	2.13	0.48
1:O:317:THR:HG23	1:O:323:ILE:HD11	1.95	0.48
1:O:507:ASP:C	1:O:519:SER:HB2	2.39	0.48
1:O:824:GLN:HG3	1:O:825:CYS:N	2.28	0.48
1:P:24:LEU:HD12	1:P:24:LEU:HA	1.62	0.48
1:P:86:VAL:HG13	1:P:87:PRO:HA	1.96	0.48
1:P:433:LEU:HD12	1:P:433:LEU:O	2.13	0.48
1:P:655:MET:HE3	1:P:655:MET:HB2	1.60	0.48
1:A:7:LEU:O	1:A:8:ALA:C	2.55	0.48
1:A:66:PRO:HD2	1:A:67:GLU:OE2	2.14	0.48
1:A:948:PRO:O	1:A:1022:GLN:HA	2.14	0.48
1:B:652:LEU:HB3	1:B:668:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:824:GLN:O	1:B:838:THR:HA	2.13	0.48
1:B:894:ARG:NH1	1:B:920:LEU:HA	2.28	0.48
1:D:373:VAL:O	1:D:374:GLN:C	2.56	0.48
1:D:531:ARG:O	1:D:561:ARG:NH1	2.46	0.48
1:E:7:LEU:O	1:E:8:ALA:C	2.55	0.48
1:E:24:LEU:HD12	1:E:24:LEU:HA	1.62	0.48
1:E:824:GLN:O	1:E:838:THR:HA	2.13	0.48
1:F:66:PRO:HD2	1:F:67:GLU:OE2	2.14	0.48
1:F:129:VAL:CG2	1:F:182:ASN:ND2	2.77	0.48
1:G:11:LEU:N	1:G:11:LEU:CD2	2.76	0.48
1:G:131:GLU:HG3	1:G:132:SER:N	2.26	0.48
1:G:315:LEU:O	1:G:322:LEU:HD12	2.13	0.48
1:G:367:MET:HB3	1:G:372:MET:HE3	1.95	0.48
1:G:579:ASP:N	1:G:583:ASN:O	2.40	0.48
1:G:948:PRO:O	1:G:1022:GLN:HA	2.14	0.48
1:H:63:PHE:CB	1:H:64:PRO:HD2	2.32	0.48
1:H:86:VAL:HG13	1:H:87:PRO:HA	1.95	0.48
1:I:126:THR:HA	1:I:182:ASN:O	2.14	0.48
1:I:507:ASP:C	1:I:519:SER:HB2	2.38	0.48
1:J:612:THR:HB	1:J:613:PRO:HD2	1.96	0.48
1:J:631:LEU:HD12	1:J:635:THR:O	2.14	0.48
1:K:30:HIS:ND1	1:K:33:PHE:CE1	2.82	0.48
1:K:240:LEU:HD12	1:K:240:LEU:C	2.36	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:H	2.27	0.48
1:L:66:PRO:HD2	1:L:67:GLU:OE2	2.14	0.48
1:L:73:TRP:CH2	1:L:185:ALA:HB1	2.49	0.48
1:L:79:PRO:HG2	1:L:80:GLU:OE2	2.13	0.48
1:L:781:ARG:HG3	1:L:781:ARG:NH1	2.17	0.48
1:M:129:VAL:CG2	1:M:182:ASN:ND2	2.77	0.48
1:O:131:GLU:HG3	1:O:132:SER:N	2.26	0.48
1:P:253:TYR:CD2	1:P:253:TYR:N	2.82	0.48
1:P:317:THR:HG23	1:P:323:ILE:HD11	1.95	0.48
1:A:271:THR:HG22	1:A:272:ALA:N	2.29	0.47
1:A:778:THR:HG22	1:A:887:GLN:H	1.79	0.47
1:B:167:LEU:HB3	1:B:168:PRO:HD2	1.96	0.47
1:C:78:LEU:CB	1:C:79:PRO:HD2	2.44	0.47
1:D:30:HIS:ND1	1:D:33:PHE:CE1	2.82	0.47
1:D:126:THR:HA	1:D:182:ASN:O	2.14	0.47
1:D:631:LEU:HD12	1:D:635:THR:O	2.14	0.47
1:E:79:PRO:HG2	1:E:80:GLU:OE2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:HIS:ND1	1:F:33:PHE:CE1	2.82	0.47
1:F:612:THR:HB	1:F:613:PRO:HD2	1.95	0.47
1:F:742:THR:CG2	1:F:743:SER:H	2.27	0.47
1:F:948:PRO:O	1:F:1022:GLN:HA	2.14	0.47
1:G:30:HIS:ND1	1:G:33:PHE:CE1	2.82	0.47
1:G:746:ASP:HA	1:G:760:ARG:CG	2.39	0.47
1:H:84:VAL:CG1	1:H:85:VAL:N	2.77	0.47
1:H:93:HIS:HB3	1:H:95:TYR:CE1	2.49	0.47
1:H:610:ASP:OD2	1:H:612:THR:HG23	2.14	0.47
1:I:84:VAL:CG1	1:I:85:VAL:N	2.77	0.47
1:I:253:TYR:CD2	1:I:253:TYR:N	2.82	0.47
1:I:802:ASP:OD1	1:I:803:PRO:HD2	2.13	0.47
1:I:948:PRO:O	1:I:1022:GLN:HA	2.14	0.47
1:J:409:VAL:HG12	1:J:410:VAL:N	2.29	0.47
1:K:742:THR:CG2	1:K:743:SER:N	2.76	0.47
1:L:126:THR:HA	1:L:182:ASN:O	2.14	0.47
1:L:652:LEU:HB3	1:L:668:VAL:O	2.14	0.47
1:M:742:THR:CG2	1:M:743:SER:N	2.76	0.47
1:M:878:HIS:HA	1:M:879:PRO:HD3	1.66	0.47
1:N:948:PRO:O	1:N:1022:GLN:HA	2.14	0.47
1:O:856:TYR:CD2	1:O:864:MET:CE	2.97	0.47
1:P:652:LEU:HB3	1:P:668:VAL:O	2.14	0.47
1:A:631:LEU:HD12	1:A:635:THR:O	2.14	0.47
1:C:88:SER:HA	1:C:366:VAL:HG21	1.97	0.47
1:C:167:LEU:HB3	1:C:168:PRO:HD2	1.95	0.47
1:C:315:LEU:O	1:C:322:LEU:HD12	2.13	0.47
1:C:948:PRO:O	1:C:1022:GLN:HA	2.14	0.47
1:D:610:ASP:OD2	1:D:612:THR:HG23	2.15	0.47
1:D:894:ARG:NH1	1:D:920:LEU:HA	2.28	0.47
1:F:778:THR:HG22	1:F:887:GLN:H	1.79	0.47
1:F:802:ASP:OD1	1:F:803:PRO:HD2	2.13	0.47
1:F:928:PRO:HB2	1:F:973:ARG:HH11	1.78	0.47
1:G:652:LEU:HB3	1:G:668:VAL:O	2.14	0.47
1:I:652:LEU:HB3	1:I:668:VAL:O	2.14	0.47
1:J:287:ASP:CG	1:K:425:ARG:HH22	2.22	0.47
1:J:652:LEU:HB3	1:J:668:VAL:O	2.14	0.47
1:J:824:GLN:O	1:J:838:THR:HA	2.14	0.47
1:K:315:LEU:O	1:K:322:LEU:HD12	2.13	0.47
1:K:433:LEU:HD12	1:K:433:LEU:O	2.13	0.47
1:K:824:GLN:HG3	1:K:825:CYS:N	2.28	0.47
1:L:24:LEU:HD12	1:L:24:LEU:HA	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:507:ASP:C	1:M:519:SER:HB2	2.39	0.47
1:N:30:HIS:ND1	1:N:33:PHE:CE1	2.82	0.47
1:N:84:VAL:CG1	1:N:85:VAL:N	2.78	0.47
1:N:253:TYR:CD2	1:N:253:TYR:N	2.82	0.47
1:N:742:THR:CG2	1:N:743:SER:H	2.27	0.47
1:N:832:ASP:OD1	1:N:832:ASP:N	2.43	0.47
1:O:11:LEU:N	1:O:11:LEU:CD2	2.76	0.47
1:O:30:HIS:ND1	1:O:33:PHE:CE1	2.82	0.47
1:O:367:MET:HB3	1:O:372:MET:HE3	1.95	0.47
1:O:395:HIS:HA	1:O:396:PRO:HD3	1.48	0.47
1:O:948:PRO:O	1:O:1022:GLN:HA	2.14	0.47
1:P:367:MET:HB3	1:P:372:MET:HE3	1.95	0.47
1:A:88:SER:HA	1:A:366:VAL:HG21	1.97	0.47
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.97	0.47
1:A:742:THR:CG2	1:A:743:SER:N	2.76	0.47
1:B:63:PHE:CB	1:B:64:PRO:HD2	2.32	0.47
1:B:246:MET:HE3	1:B:246:MET:C	2.40	0.47
1:B:377:LEU:HD22	1:B:708:TRP:CA	2.44	0.47
1:B:742:THR:CG2	1:B:743:SER:H	2.27	0.47
1:C:240:LEU:HD12	1:C:240:LEU:C	2.36	0.47
1:C:655:MET:HE3	1:C:655:MET:HB2	1.60	0.47
1:C:742:THR:CG2	1:C:743:SER:N	2.76	0.47
1:D:367:MET:HB3	1:D:372:MET:HE3	1.95	0.47
1:D:869:ASP:OD2	1:D:1015:HIS:ND1	2.33	0.47
1:E:1018:LEU:HD23	1:E:1018:LEU:HA	1.51	0.47
1:F:93:HIS:HB3	1:F:95:TYR:CE1	2.49	0.47
1:F:253:TYR:CD2	1:F:253:TYR:N	2.82	0.47
1:F:353:GLY:C	1:F:566:PHE:HA	2.40	0.47
1:F:373:VAL:O	1:F:374:GLN:C	2.57	0.47
1:G:73:TRP:CH2	1:G:185:ALA:HB1	2.49	0.47
1:G:1020:TRP:CD1	1:G:1021:CME:N	2.80	0.47
1:H:73:TRP:CH2	1:H:185:ALA:HB1	2.49	0.47
1:H:802:ASP:OD1	1:H:803:PRO:HD2	2.13	0.47
1:I:824:GLN:HG3	1:I:825:CYS:N	2.28	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:K:253:TYR:CD2	1:K:253:TYR:N	2.82	0.47
1:K:367:MET:HB3	1:K:372:MET:HE3	1.95	0.47
1:K:631:LEU:HD12	1:K:635:THR:O	2.14	0.47
1:L:702:GLN:O	1:L:712:GLY:N	2.45	0.47
1:M:30:HIS:ND1	1:M:33:PHE:CE1	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:126:THR:HA	1:M:182:ASN:O	2.14	0.47
1:M:730:LEU:HA	1:M:731:PRO:HD3	1.74	0.47
1:M:856:TYR:CD2	1:M:864:MET:CE	2.97	0.47
1:N:93:HIS:HB3	1:N:95:TYR:CE1	2.50	0.47
1:N:778:THR:HG22	1:N:887:GLN:H	1.79	0.47
1:O:610:ASP:OD2	1:O:612:THR:HG23	2.15	0.47
1:P:66:PRO:HD2	1:P:67:GLU:OE2	2.14	0.47
1:A:84:VAL:CG1	1:A:85:VAL:N	2.78	0.47
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.95	0.47
1:A:610:ASP:OD2	1:A:612:THR:HG23	2.15	0.47
1:A:824:GLN:HG3	1:A:825:CYS:N	2.28	0.47
1:B:93:HIS:HB3	1:B:95:TYR:CE1	2.50	0.47
1:B:237:ARG:HH11	1:B:237:ARG:HB3	1.77	0.47
1:B:274:PHE:HB3	1:B:286:ALA:O	2.15	0.47
1:B:409:VAL:HG12	1:B:410:VAL:N	2.29	0.47
1:B:433:LEU:HD12	1:B:433:LEU:O	2.13	0.47
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.97	0.47
1:C:746:ASP:HA	1:C:760:ARG:CG	2.39	0.47
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.97	0.47
1:D:271:THR:HG22	1:D:272:ALA:N	2.29	0.47
1:D:442:ARG:HA	1:D:445:GLN:HG3	1.96	0.47
1:D:652:LEU:HB3	1:D:668:VAL:O	2.14	0.47
1:E:73:TRP:CZ2	1:E:122:CYS:HB3	2.50	0.47
1:E:142:ILE:HG12	1:E:170:GLU:HG2	1.97	0.47
1:E:271:THR:HG22	1:E:272:ALA:N	2.29	0.47
1:E:507:ASP:C	1:E:519:SER:HB2	2.39	0.47
1:F:579:ASP:OD1	1:F:583:ASN:N	2.43	0.47
1:F:740:LEU:HD13	1:F:749:ILE:CD1	2.45	0.47
1:H:317:THR:HG23	1:H:323:ILE:HD11	1.95	0.47
1:H:631:LEU:HD12	1:H:632:SER:H	1.79	0.47
1:H:1018:LEU:HD23	1:H:1018:LEU:HA	1.51	0.47
1:I:30:HIS:ND1	1:I:33:PHE:CE1	2.82	0.47
1:I:353:GLY:C	1:I:566:PHE:HA	2.40	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:K:86:VAL:HG13	1:K:87:PRO:HA	1.95	0.47
1:K:167:LEU:HB3	1:K:168:PRO:HD2	1.95	0.47
1:K:655:MET:HB2	1:K:655:MET:HE3	1.60	0.47
1:K:661:LYS:HA	1:K:662:PRO:HD3	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:347:LYS:CB	1:L:348:PRO:HD2	2.43	0.47
1:L:353:GLY:C	1:L:566:PHE:HA	2.40	0.47
1:L:612:THR:HB	1:L:613:PRO:HD2	1.96	0.47
1:M:49:GLN:H	1:M:49:GLN:CD	2.20	0.47
1:M:353:GLY:C	1:M:566:PHE:HA	2.40	0.47
1:N:240:LEU:HD12	1:N:240:LEU:C	2.36	0.47
1:N:353:GLY:C	1:N:566:PHE:HA	2.40	0.47
1:O:631:LEU:HD12	1:O:635:THR:O	2.14	0.47
1:O:663:LEU:HD23	1:O:663:LEU:N	2.24	0.47
1:P:409:VAL:HG12	1:P:410:VAL:N	2.29	0.47
1:A:73:TRP:CZ2	1:A:122:CYS:HB3	2.50	0.47
1:A:93:HIS:HB3	1:A:95:TYR:CE1	2.49	0.47
1:A:282:ARG:HB3	1:D:421:VAL:HG22	1.95	0.47
1:A:682:LEU:HA	1:A:682:LEU:HD23	1.66	0.47
1:B:66:PRO:HD2	1:B:67:GLU:OE2	2.14	0.47
1:B:86:VAL:HG13	1:B:87:PRO:HA	1.96	0.47
1:B:702:GLN:O	1:B:712:GLY:N	2.45	0.47
1:C:73:TRP:CZ2	1:C:122:CYS:HB3	2.50	0.47
1:C:740:LEU:HD13	1:C:749:ILE:CD1	2.45	0.47
1:D:49:GLN:H	1:D:49:GLN:CD	2.20	0.47
1:D:73:TRP:CZ2	1:D:122:CYS:HB3	2.50	0.47
1:D:167:LEU:HB3	1:D:168:PRO:HD2	1.96	0.47
1:D:317:THR:HG23	1:D:323:ILE:HD11	1.95	0.47
1:D:353:GLY:C	1:D:566:PHE:HA	2.40	0.47
1:E:147:ASN:HA	1:E:148:SER:HA	1.54	0.47
1:F:469:ASP:HB3	1:G:473:ARG:HD2	1.97	0.47
1:G:86:VAL:HG13	1:G:87:PRO:HA	1.95	0.47
1:G:651:LEU:HD13	1:G:651:LEU:HA	1.51	0.47
1:H:138:GLN:N	1:H:217:LYS:O	2.36	0.47
1:H:142:ILE:HG12	1:H:170:GLU:HG2	1.96	0.47
1:I:142:ILE:HG12	1:I:170:GLU:HG2	1.97	0.47
1:I:246:MET:HE3	1:I:246:MET:C	2.40	0.47
1:I:367:MET:HB3	1:I:372:MET:HE3	1.95	0.47
1:I:631:LEU:HD12	1:I:635:THR:O	2.14	0.47
1:I:856:TYR:CD2	1:I:864:MET:CE	2.97	0.47
1:J:93:HIS:HB3	1:J:95:TYR:CE1	2.50	0.47
1:J:373:VAL:O	1:J:374:GLN:C	2.57	0.47
1:J:579:ASP:OD1	1:J:583:ASN:N	2.43	0.47
1:J:948:PRO:O	1:J:1022:GLN:HA	2.14	0.47
1:K:129:VAL:CG2	1:K:182:ASN:ND2	2.77	0.47
1:L:610:ASP:OD2	1:L:612:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:73:TRP:CZ2	1:M:122:CYS:HB3	2.50	0.47
1:M:88:SER:HA	1:M:366:VAL:HG21	1.97	0.47
1:M:142:ILE:HG12	1:M:170:GLU:HG2	1.97	0.47
1:M:274:PHE:HB3	1:M:286:ALA:O	2.15	0.47
1:N:142:ILE:HG12	1:N:170:GLU:HG2	1.97	0.47
1:O:781:ARG:HH11	1:O:781:ARG:CG	2.19	0.47
1:A:24:LEU:HD12	1:A:24:LEU:HA	1.62	0.47
1:A:317:THR:HG23	1:A:323:ILE:HD11	1.95	0.47
1:A:631:LEU:HD12	1:A:632:SER:H	1.78	0.47
1:B:30:HIS:ND1	1:B:33:PHE:CE1	2.82	0.47
1:B:353:GLY:C	1:B:566:PHE:HA	2.40	0.47
1:C:84:VAL:CG1	1:C:85:VAL:N	2.77	0.47
1:C:778:THR:HG22	1:C:887:GLN:H	1.79	0.47
1:D:66:PRO:HD2	1:D:67:GLU:OE2	2.14	0.47
1:E:260:LEU:HD12	1:E:260:LEU:HA	1.61	0.47
1:E:274:PHE:HB3	1:E:286:ALA:O	2.15	0.47
1:E:610:ASP:OD2	1:E:612:THR:HG23	2.15	0.47
1:E:682:LEU:HA	1:E:682:LEU:HD23	1.67	0.47
1:F:126:THR:HA	1:F:182:ASN:O	2.14	0.47
1:F:832:ASP:OD1	1:F:832:ASP:N	2.43	0.47
1:G:57:GLU:HG2	1:G:83:THR:HG21	1.94	0.47
1:G:126:THR:HA	1:G:182:ASN:O	2.14	0.47
1:G:167:LEU:HB3	1:G:168:PRO:HD2	1.95	0.47
1:G:353:GLY:C	1:G:566:PHE:HA	2.40	0.47
1:H:30:HIS:ND1	1:H:33:PHE:CE1	2.82	0.47
1:H:353:GLY:C	1:H:566:PHE:HA	2.40	0.47
1:H:746:ASP:HA	1:H:760:ARG:CG	2.39	0.47
1:H:948:PRO:O	1:H:1022:GLN:HA	2.14	0.47
1:I:93:HIS:HB3	1:I:95:TYR:CE1	2.49	0.47
1:I:274:PHE:HB3	1:I:286:ALA:O	2.15	0.47
1:I:377:LEU:HD22	1:I:708:TRP:CA	2.44	0.47
1:I:433:LEU:HD12	1:I:433:LEU:O	2.13	0.47
1:I:694:LEU:HD12	1:I:694:LEU:HA	1.69	0.47
1:J:30:HIS:ND1	1:J:33:PHE:CE1	2.82	0.47
1:J:469:ASP:HB3	1:K:473:ARG:HD2	1.95	0.47
1:J:742:THR:CG2	1:J:743:SER:H	2.27	0.47
1:K:7:LEU:O	1:K:8:ALA:C	2.55	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:N:507:ASP:C	1:N:519:SER:HB2	2.39	0.47
1:O:88:SER:HA	1:O:366:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:167:LEU:HB3	1:O:168:PRO:HD2	1.95	0.47
1:O:253:TYR:CD2	1:O:253:TYR:N	2.82	0.47
1:P:142:ILE:HG12	1:P:170:GLU:HG2	1.97	0.47
1:P:246:MET:HE3	1:P:246:MET:C	2.40	0.47
1:P:353:GLY:C	1:P:566:PHE:HA	2.40	0.47
1:P:531:ARG:O	1:P:561:ARG:NH1	2.46	0.47
1:P:802:ASP:OD1	1:P:803:PRO:HD2	2.14	0.47
1:P:856:TYR:CD2	1:P:864:MET:CE	2.97	0.47
1:A:409:VAL:HG12	1:A:410:VAL:N	2.29	0.47
1:A:651:LEU:HD13	1:A:651:LEU:HA	1.51	0.47
1:B:73:TRP:CZ2	1:B:122:CYS:HB3	2.50	0.47
1:B:126:THR:HA	1:B:182:ASN:O	2.14	0.47
1:B:610:ASP:OD2	1:B:612:THR:HG23	2.15	0.47
1:B:878:HIS:HA	1:B:879:PRO:HD3	1.66	0.47
1:B:930:VAL:HA	1:B:973:ARG:HD3	1.97	0.47
1:B:948:PRO:O	1:B:1022:GLN:HA	2.15	0.47
1:C:93:HIS:HB3	1:C:95:TYR:CE1	2.49	0.47
1:C:126:THR:HA	1:C:182:ASN:O	2.14	0.47
1:C:368:ASP:O	1:C:369:GLU:C	2.58	0.47
1:C:445:GLN:HE21	1:C:445:GLN:HB3	1.54	0.47
1:C:702:GLN:O	1:C:712:GLY:N	2.45	0.47
1:C:856:TYR:CD2	1:C:864:MET:CE	2.97	0.47
1:D:646:HIS:O	1:D:648:ASP:N	2.47	0.47
1:E:77:ASP:O	1:E:78:LEU:HD23	2.15	0.47
1:E:88:SER:HA	1:E:366:VAL:HG21	1.97	0.47
1:E:409:VAL:HG12	1:E:410:VAL:N	2.29	0.47
1:E:631:LEU:HD12	1:E:635:THR:O	2.14	0.47
1:E:948:PRO:O	1:E:1022:GLN:HA	2.14	0.47
1:F:142:ILE:HG12	1:F:170:GLU:HG2	1.97	0.47
1:F:246:MET:HE3	1:F:246:MET:C	2.40	0.47
1:F:749:ILE:N	1:F:749:ILE:CD1	2.78	0.47
1:G:66:PRO:HD2	1:G:67:GLU:OE2	2.14	0.47
1:G:73:TRP:CZ2	1:G:122:CYS:HB3	2.50	0.47
1:G:88:SER:HA	1:G:366:VAL:HG21	1.97	0.47
1:G:246:MET:HE3	1:G:246:MET:C	2.40	0.47
1:G:260:LEU:HD12	1:G:260:LEU:HA	1.61	0.47
1:G:271:THR:HG22	1:G:272:ALA:N	2.29	0.47
1:G:377:LEU:HD22	1:G:708:TRP:CA	2.44	0.47
1:G:610:ASP:OD2	1:G:612:THR:HG23	2.15	0.47
1:G:824:GLN:O	1:G:838:THR:HA	2.13	0.47
1:G:1021:CME:HB3	1:G:1021:CME:HE2	1.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:271:THR:HG22	1:H:272:ALA:N	2.29	0.47
1:H:391:HIS:ND1	1:H:412:GLU:OE1	2.44	0.47
1:H:742:THR:CG2	1:H:743:SER:H	2.27	0.47
1:H:778:THR:HG22	1:H:887:GLN:H	1.79	0.47
1:I:271:THR:HG22	1:I:272:ALA:N	2.29	0.47
1:I:473:ARG:HD2	1:L:469:ASP:HB3	1.96	0.47
1:J:86:VAL:HG13	1:J:87:PRO:HA	1.96	0.47
1:J:246:MET:HE3	1:J:246:MET:C	2.40	0.47
1:J:377:LEU:HD22	1:J:708:TRP:CA	2.44	0.47
1:K:88:SER:HA	1:K:366:VAL:HG21	1.97	0.47
1:K:608:PHE:O	1:K:611:ARG:N	2.41	0.47
1:K:778:THR:HG22	1:K:887:GLN:H	1.79	0.47
1:L:84:VAL:CG1	1:L:85:VAL:N	2.77	0.47
1:L:246:MET:HE3	1:L:246:MET:C	2.40	0.47
1:L:631:LEU:HD12	1:L:632:SER:H	1.78	0.47
1:L:740:LEU:HD13	1:L:749:ILE:CD1	2.45	0.47
1:L:778:THR:HG22	1:L:887:GLN:H	1.79	0.47
1:L:832:ASP:OD1	1:L:832:ASP:N	2.43	0.47
1:M:77:ASP:O	1:M:78:LEU:HD23	2.15	0.47
1:M:84:VAL:CG1	1:M:85:VAL:N	2.78	0.47
1:M:409:VAL:HG12	1:M:410:VAL:N	2.29	0.47
1:M:646:HIS:O	1:M:648:ASP:N	2.47	0.47
1:M:663:LEU:HD23	1:M:663:LEU:N	2.24	0.47
1:N:246:MET:HE3	1:N:246:MET:C	2.40	0.47
1:N:274:PHE:HB3	1:N:286:ALA:O	2.15	0.47
1:N:395:HIS:HA	1:N:396:PRO:HD3	1.48	0.47
1:N:409:VAL:HG12	1:N:410:VAL:N	2.29	0.47
1:N:579:ASP:OD1	1:N:583:ASN:N	2.43	0.47
1:O:66:PRO:HD2	1:O:67:GLU:OE2	2.14	0.47
1:O:73:TRP:CZ2	1:O:122:CYS:HB3	2.50	0.47
1:O:86:VAL:HG13	1:O:87:PRO:HA	1.96	0.47
1:O:246:MET:HE3	1:O:246:MET:C	2.40	0.47
1:O:260:LEU:HD12	1:O:260:LEU:HA	1.61	0.47
1:O:377:LEU:HD22	1:O:708:TRP:CA	2.44	0.47
1:O:778:THR:HG22	1:O:887:GLN:H	1.79	0.47
1:O:1021:CME:HB3	1:O:1021:CME:HE2	1.41	0.47
1:P:30:HIS:ND1	1:P:33:PHE:CE1	2.82	0.47
1:P:73:TRP:CZ2	1:P:122:CYS:HB3	2.50	0.47
1:P:84:VAL:CG1	1:P:85:VAL:N	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:230:ARG:HH11	1:P:230:ARG:CG	2.24	0.47
1:P:740:LEU:HD13	1:P:749:ILE:CD1	2.45	0.47
1:P:746:ASP:HA	1:P:760:ARG:CG	2.39	0.47
1:A:260:LEU:C	1:A:267:VAL:HG23	2.40	0.47
1:A:822:LEU:HD12	1:A:822:LEU:C	2.37	0.47
1:B:73:TRP:CH2	1:B:185:ALA:HB1	2.49	0.47
1:B:77:ASP:O	1:B:78:LEU:HD23	2.15	0.47
1:B:1020:TRP:CD1	1:B:1021:CME:N	2.80	0.47
1:C:579:ASP:OD1	1:C:583:ASN:N	2.43	0.47
1:C:631:LEU:HD12	1:C:635:THR:O	2.14	0.47
1:C:930:VAL:HA	1:C:973:ARG:HD3	1.97	0.47
1:E:93:HIS:HB3	1:E:95:TYR:CE1	2.49	0.47
1:E:278:ILE:N	1:E:278:ILE:CD1	2.78	0.47
1:E:353:GLY:C	1:E:566:PHE:HA	2.40	0.47
1:E:599:ARG:HB2	1:E:600:GLN:H	1.40	0.47
1:E:631:LEU:HD12	1:E:632:SER:H	1.78	0.47
1:E:646:HIS:O	1:E:648:ASP:N	2.48	0.47
1:E:749:ILE:N	1:E:749:ILE:CD1	2.78	0.47
1:F:368:ASP:O	1:F:369:GLU:C	2.58	0.47
1:F:409:VAL:HG12	1:F:410:VAL:N	2.29	0.47
1:F:610:ASP:OD2	1:F:612:THR:HG23	2.14	0.47
1:F:663:LEU:HD23	1:F:663:LEU:N	2.24	0.47
1:G:608:PHE:O	1:G:611:ARG:N	2.41	0.47
1:G:654:TRP:O	1:G:655:MET:HB3	2.15	0.47
1:H:73:TRP:CZ2	1:H:122:CYS:HB3	2.50	0.47
1:H:278:ILE:N	1:H:278:ILE:CD1	2.78	0.47
1:H:368:ASP:O	1:H:369:GLU:C	2.58	0.47
1:H:378:LEU:HA	1:H:378:LEU:HD23	1.53	0.47
1:I:7:LEU:O	1:I:8:ALA:C	2.55	0.47
1:I:347:LYS:CB	1:I:348:PRO:HD2	2.43	0.47
1:I:612:THR:HB	1:I:613:PRO:HD2	1.96	0.47
1:J:49:GLN:H	1:J:49:GLN:CD	2.20	0.47
1:J:66:PRO:HD2	1:J:67:GLU:OE2	2.14	0.47
1:J:740:LEU:HD13	1:J:749:ILE:CD1	2.45	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:K:77:ASP:O	1:K:78:LEU:HD23	2.15	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:K:948:PRO:O	1:K:1022:GLN:HA	2.14	0.47
1:L:93:HIS:HB3	1:L:95:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:142:ILE:HG12	1:L:170:GLU:HG2	1.97	0.47
1:M:253:TYR:CD2	1:M:253:TYR:N	2.82	0.47
1:M:271:THR:HG22	1:M:272:ALA:N	2.29	0.47
1:M:631:LEU:HD12	1:M:635:THR:O	2.14	0.47
1:N:73:TRP:CZ2	1:N:122:CYS:HB3	2.50	0.47
1:N:129:VAL:CG2	1:N:182:ASN:ND2	2.77	0.47
1:N:740:LEU:HD13	1:N:749:ILE:CD1	2.45	0.47
1:O:79:PRO:HG2	1:O:80:GLU:OE2	2.13	0.47
1:O:271:THR:HG22	1:O:272:ALA:N	2.29	0.47
1:O:274:PHE:HB3	1:O:286:ALA:O	2.15	0.47
1:O:353:GLY:C	1:O:566:PHE:HA	2.40	0.47
1:P:274:PHE:HB3	1:P:286:ALA:O	2.15	0.47
1:P:278:ILE:N	1:P:278:ILE:CD1	2.78	0.47
1:A:599:ARG:HB2	1:A:600:GLN:H	1.40	0.47
1:B:84:VAL:CG1	1:B:85:VAL:N	2.78	0.47
1:B:129:VAL:CG2	1:B:182:ASN:ND2	2.77	0.47
1:B:210:ARG:NH1	1:B:395:HIS:CA	2.78	0.47
1:B:631:LEU:HD12	1:B:632:SER:H	1.79	0.47
1:C:66:PRO:HD2	1:C:67:GLU:OE2	2.14	0.47
1:C:246:MET:HE3	1:C:246:MET:C	2.40	0.47
1:C:942:ARG:HA	1:C:953:GLY:O	2.15	0.47
1:D:77:ASP:O	1:D:78:LEU:HD23	2.15	0.47
1:D:274:PHE:HB3	1:D:286:ALA:O	2.15	0.47
1:D:377:LEU:HD22	1:D:708:TRP:CA	2.44	0.47
1:D:948:PRO:O	1:D:1022:GLN:HA	2.15	0.47
1:E:240:LEU:HD12	1:E:240:LEU:C	2.36	0.47
1:E:253:TYR:CD2	1:E:253:TYR:N	2.82	0.47
1:E:368:ASP:O	1:E:369:GLU:C	2.58	0.47
1:E:658:LEU:O	1:E:659:ASP:C	2.58	0.47
1:E:942:ARG:HA	1:E:953:GLY:O	2.15	0.47
1:F:62:TRP:C	1:F:63:PHE:CD1	2.93	0.47
1:F:73:TRP:CZ2	1:F:122:CYS:HB3	2.50	0.47
1:F:631:LEU:HD12	1:F:635:THR:O	2.14	0.47
1:F:942:ARG:HA	1:F:953:GLY:O	2.15	0.47
1:G:93:HIS:HB3	1:G:95:TYR:CE1	2.49	0.47
1:G:274:PHE:HB3	1:G:286:ALA:O	2.15	0.47
1:G:942:ARG:HA	1:G:953:GLY:O	2.15	0.47
1:H:88:SER:HA	1:H:366:VAL:HG21	1.97	0.47
1:H:246:MET:HE3	1:H:246:MET:C	2.40	0.47
1:H:740:LEU:HD13	1:H:749:ILE:CD1	2.45	0.47
1:I:62:TRP:C	1:I:63:PHE:CD1	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:66:PRO:HD2	1:I:67:GLU:OE2	2.14	0.47
1:I:78:LEU:CB	1:I:79:PRO:HD2	2.44	0.47
1:I:610:ASP:OD2	1:I:612:THR:HG23	2.15	0.47
1:I:740:LEU:HD13	1:I:749:ILE:CD1	2.45	0.47
1:J:73:TRP:CZ2	1:J:122:CYS:HB3	2.50	0.47
1:J:126:THR:HA	1:J:182:ASN:O	2.14	0.47
1:J:531:ARG:O	1:J:561:ARG:NH1	2.46	0.47
1:J:829:THR:C	1:J:830:LEU:HD12	2.40	0.47
1:K:62:TRP:C	1:K:63:PHE:CD1	2.93	0.47
1:K:210:ARG:NH1	1:K:395:HIS:CA	2.78	0.47
1:K:646:HIS:O	1:K:648:ASP:N	2.47	0.47
1:K:679:LEU:HA	1:K:679:LEU:HD23	1.26	0.47
1:K:930:VAL:HA	1:K:973:ARG:HD3	1.97	0.47
1:L:73:TRP:CZ2	1:L:122:CYS:HB3	2.50	0.47
1:L:210:ARG:NH1	1:L:395:HIS:CA	2.78	0.47
1:L:433:LEU:HD12	1:L:433:LEU:O	2.13	0.47
1:L:749:ILE:N	1:L:749:ILE:CD1	2.78	0.47
1:L:948:PRO:O	1:L:1022:GLN:HA	2.14	0.47
1:M:210:ARG:NH1	1:M:395:HIS:CA	2.78	0.47
1:M:740:LEU:HD13	1:M:749:ILE:CD1	2.45	0.47
1:M:829:THR:C	1:M:830:LEU:HD12	2.40	0.47
1:M:942:ARG:HA	1:M:953:GLY:O	2.15	0.47
1:N:942:ARG:HA	1:N:953:GLY:O	2.15	0.47
1:O:77:ASP:O	1:O:78:LEU:HD23	2.15	0.47
1:O:579:ASP:N	1:O:583:ASN:O	2.40	0.47
1:O:654:TRP:O	1:O:655:MET:HB3	2.15	0.47
1:O:740:LEU:HD13	1:O:749:ILE:CD1	2.45	0.47
1:O:829:THR:C	1:O:830:LEU:HD12	2.40	0.47
1:O:942:ARG:HA	1:O:953:GLY:O	2.15	0.47
1:P:7:LEU:O	1:P:8:ALA:C	2.55	0.47
1:P:631:LEU:HD12	1:P:635:THR:O	2.14	0.47
1:A:246:MET:HE3	1:A:246:MET:C	2.40	0.47
1:A:274:PHE:HB3	1:A:286:ALA:O	2.15	0.47
1:A:442:ARG:HA	1:A:445:GLN:HG3	1.95	0.47
1:B:253:TYR:CD2	1:B:253:TYR:N	2.82	0.47
1:B:278:ILE:N	1:B:278:ILE:CD1	2.78	0.47
1:B:654:TRP:O	1:B:655:MET:HB3	2.15	0.47
1:B:658:LEU:O	1:B:659:ASP:C	2.58	0.47
1:C:260:LEU:HA	1:C:260:LEU:HD12	1.61	0.47
1:D:569:ASP:O	1:D:605:GLY:HA2	2.16	0.47
1:D:740:LEU:HD13	1:D:749:ILE:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:VAL:CG1	1:E:85:VAL:N	2.78	0.47
1:E:138:GLN:N	1:E:217:LYS:O	2.36	0.47
1:E:403:ASP:OD2	1:E:450:HIS:ND1	2.34	0.47
1:E:730:LEU:HA	1:E:731:PRO:HD3	1.74	0.47
1:F:84:VAL:CG1	1:F:85:VAL:N	2.78	0.47
1:F:652:LEU:HB3	1:F:668:VAL:O	2.14	0.47
1:F:654:TRP:O	1:F:655:MET:HB3	2.15	0.47
1:F:655:MET:HB2	1:F:655:MET:HE3	1.60	0.47
1:G:742:THR:CG2	1:G:743:SER:H	2.27	0.47
1:H:274:PHE:HB3	1:H:286:ALA:O	2.15	0.47
1:H:409:VAL:HG12	1:H:410:VAL:N	2.29	0.47
1:I:86:VAL:HG13	1:I:87:PRO:HA	1.95	0.47
1:I:118:ASN:HA	1:I:119:PRO:HD2	1.60	0.47
1:I:260:LEU:C	1:I:267:VAL:HG23	2.40	0.47
1:I:742:THR:CG2	1:I:743:SER:H	2.27	0.47
1:J:57:GLU:HG2	1:J:83:THR:HG21	1.93	0.47
1:K:829:THR:C	1:K:830:LEU:HD12	2.40	0.47
1:L:65:ALA:HB1	1:L:66:PRO:CD	2.39	0.47
1:L:88:SER:HA	1:L:366:VAL:HG21	1.97	0.47
1:L:395:HIS:HA	1:L:396:PRO:HD3	1.48	0.47
1:L:875:ASP:OD2	1:L:875:ASP:N	2.47	0.47
1:L:930:VAL:HA	1:L:973:ARG:HD3	1.97	0.47
1:L:942:ARG:HA	1:L:953:GLY:O	2.15	0.47
1:M:581:ASN:OD1	1:M:581:ASN:N	2.44	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:O:93:HIS:HB3	1:O:95:TYR:CE1	2.50	0.47
1:O:210:ARG:NH1	1:O:395:HIS:CA	2.78	0.47
1:P:62:TRP:C	1:P:63:PHE:CD1	2.93	0.47
1:A:30:HIS:ND1	1:A:33:PHE:CE1	2.82	0.46
1:A:829:THR:C	1:A:830:LEU:HD12	2.40	0.46
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.97	0.46
1:B:824:GLN:HG3	1:B:825:CYS:N	2.28	0.46
1:C:316:HIS:HB2	1:C:321:THR:O	2.16	0.46
1:C:610:ASP:OD2	1:C:612:THR:HG23	2.15	0.46
1:D:829:THR:C	1:D:830:LEU:HD12	2.40	0.46
1:E:66:PRO:HD2	1:E:67:GLU:OE2	2.14	0.46
1:E:740:LEU:HD13	1:E:749:ILE:CD1	2.45	0.46
1:E:822:LEU:HD12	1:E:822:LEU:C	2.37	0.46
1:F:63:PHE:CB	1:F:64:PRO:HD2	2.32	0.46
1:F:930:VAL:HA	1:F:973:ARG:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:702:GLN:O	1:G:712:GLY:N	2.45	0.46
1:G:830:LEU:N	1:G:830:LEU:CD1	2.78	0.46
1:H:210:ARG:NH1	1:H:395:HIS:CA	2.78	0.46
1:H:702:GLN:O	1:H:712:GLY:N	2.45	0.46
1:H:829:THR:C	1:H:830:LEU:HD12	2.40	0.46
1:I:129:VAL:CG2	1:I:182:ASN:ND2	2.77	0.46
1:I:316:HIS:HB2	1:I:321:THR:O	2.15	0.46
1:I:409:VAL:HG12	1:I:410:VAL:N	2.29	0.46
1:I:702:GLN:O	1:I:712:GLY:N	2.45	0.46
1:I:829:THR:C	1:I:830:LEU:HD12	2.40	0.46
1:J:84:VAL:CG1	1:J:85:VAL:N	2.77	0.46
1:J:210:ARG:NH1	1:J:395:HIS:CA	2.78	0.46
1:J:274:PHE:HB3	1:J:286:ALA:O	2.15	0.46
1:K:49:GLN:H	1:K:49:GLN:CD	2.20	0.46
1:K:93:HIS:HB3	1:K:95:TYR:CE1	2.50	0.46
1:K:126:THR:HA	1:K:182:ASN:O	2.14	0.46
1:K:246:MET:HE3	1:K:246:MET:C	2.40	0.46
1:K:271:THR:HG22	1:K:272:ALA:N	2.29	0.46
1:K:569:ASP:O	1:K:605:GLY:HA2	2.15	0.46
1:K:654:TRP:O	1:K:655:MET:HB3	2.15	0.46
1:K:740:LEU:HD13	1:K:749:ILE:CD1	2.45	0.46
1:L:7:LEU:O	1:L:8:ALA:C	2.55	0.46
1:L:646:HIS:O	1:L:648:ASP:N	2.47	0.46
1:L:654:TRP:O	1:L:655:MET:HB3	2.15	0.46
1:L:682:LEU:HD23	1:L:682:LEU:HA	1.67	0.46
1:L:740:LEU:HD13	1:L:749:ILE:HD12	1.97	0.46
1:M:442:ARG:HA	1:M:445:GLN:HG3	1.96	0.46
1:M:569:ASP:O	1:M:605:GLY:HA2	2.16	0.46
1:M:610:ASP:OD2	1:M:612:THR:HG23	2.15	0.46
1:M:654:TRP:O	1:M:655:MET:HB3	2.15	0.46
1:M:749:ILE:N	1:M:749:ILE:CD1	2.78	0.46
1:N:652:LEU:HB3	1:N:668:VAL:O	2.14	0.46
1:P:316:HIS:HB2	1:P:321:THR:O	2.15	0.46
1:P:610:ASP:OD2	1:P:612:THR:HG23	2.15	0.46
1:P:942:ARG:HA	1:P:953:GLY:O	2.15	0.46
1:A:353:GLY:C	1:A:566:PHE:HA	2.40	0.46
1:B:347:LYS:CB	1:B:348:PRO:HD2	2.43	0.46
1:B:740:LEU:HD13	1:B:749:ILE:CD1	2.45	0.46
1:C:353:GLY:C	1:C:566:PHE:HA	2.40	0.46
1:C:409:VAL:HG12	1:C:410:VAL:N	2.29	0.46
1:C:652:LEU:HB3	1:C:668:VAL:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:HIS:HB3	1:D:95:TYR:CE1	2.49	0.46
1:D:246:MET:HE3	1:D:246:MET:C	2.40	0.46
1:D:658:LEU:O	1:D:659:ASP:C	2.58	0.46
1:E:581:ASN:OD1	1:E:581:ASN:N	2.44	0.46
1:F:88:SER:HA	1:F:366:VAL:HG21	1.97	0.46
1:F:274:PHE:HB3	1:F:286:ALA:O	2.15	0.46
1:F:569:ASP:O	1:F:605:GLY:HA2	2.15	0.46
1:F:599:ARG:HB2	1:F:600:GLN:H	1.40	0.46
1:G:316:HIS:HB2	1:G:321:THR:O	2.15	0.46
1:G:576:ILE:CG2	1:G:577:LYS:N	2.78	0.46
1:G:875:ASP:OD2	1:G:875:ASP:N	2.47	0.46
1:H:13:ARG:O	1:H:14:ARG:HB2	2.16	0.46
1:H:100:TYR:HB2	1:H:203:TRP:CE3	2.51	0.46
1:H:260:LEU:C	1:H:267:VAL:HG23	2.40	0.46
1:H:856:TYR:CD2	1:H:864:MET:CE	2.97	0.46
1:I:579:ASP:OD1	1:I:583:ASN:N	2.43	0.46
1:I:608:PHE:O	1:I:611:ARG:N	2.41	0.46
1:I:875:ASP:N	1:I:875:ASP:OD2	2.47	0.46
1:J:62:TRP:C	1:J:63:PHE:CD1	2.93	0.46
1:J:147:ASN:HA	1:J:148:SER:HA	1.54	0.46
1:J:569:ASP:O	1:J:605:GLY:HA2	2.15	0.46
1:J:740:LEU:HD13	1:J:749:ILE:HD12	1.97	0.46
1:J:830:LEU:CD1	1:J:830:LEU:N	2.78	0.46
1:K:73:TRP:CZ2	1:K:122:CYS:HB3	2.50	0.46
1:K:147:ASN:HA	1:K:148:SER:HA	1.55	0.46
1:K:353:GLY:C	1:K:566:PHE:HA	2.40	0.46
1:K:702:GLN:O	1:K:712:GLY:N	2.45	0.46
1:K:856:TYR:CD2	1:K:864:MET:CE	2.97	0.46
1:K:878:HIS:HA	1:K:879:PRO:HD3	1.66	0.46
1:L:62:TRP:C	1:L:63:PHE:CD1	2.93	0.46
1:L:378:LEU:HD23	1:L:378:LEU:HA	1.53	0.46
1:L:486:TYR:CZ	1:L:488:GLY:HA3	2.51	0.46
1:L:569:ASP:O	1:L:605:GLY:HA2	2.15	0.46
1:L:631:LEU:HD12	1:L:635:THR:O	2.14	0.46
1:L:829:THR:C	1:L:830:LEU:HD12	2.40	0.46
1:M:93:HIS:HB3	1:M:95:TYR:CE1	2.50	0.46
1:M:316:HIS:HB2	1:M:321:THR:O	2.15	0.46
1:N:88:SER:HA	1:N:366:VAL:HG21	1.97	0.46
1:N:271:THR:HG22	1:N:272:ALA:N	2.29	0.46
1:N:830:LEU:N	1:N:830:LEU:CD1	2.78	0.46
1:O:63:PHE:CB	1:O:64:PRO:HD2	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:84:VAL:CG1	1:O:85:VAL:N	2.77	0.46
1:O:100:TYR:HB2	1:O:203:TRP:CE3	2.51	0.46
1:O:316:HIS:HB2	1:O:321:THR:O	2.16	0.46
1:O:445:GLN:HE21	1:O:445:GLN:HB3	1.54	0.46
1:O:830:LEU:N	1:O:830:LEU:CD1	2.78	0.46
1:P:126:THR:HA	1:P:182:ASN:O	2.14	0.46
1:A:63:PHE:CB	1:A:64:PRO:HD2	2.32	0.46
1:A:740:LEU:HD13	1:A:749:ILE:CD1	2.45	0.46
1:B:316:HIS:HB2	1:B:321:THR:O	2.16	0.46
1:B:875:ASP:OD2	1:B:875:ASP:N	2.47	0.46
1:C:654:TRP:O	1:C:655:MET:HB3	2.15	0.46
1:D:409:VAL:HG12	1:D:410:VAL:N	2.29	0.46
1:D:778:THR:HG22	1:D:887:GLN:H	1.79	0.46
1:D:824:GLN:HG3	1:D:825:CYS:N	2.28	0.46
1:D:942:ARG:HA	1:D:953:GLY:O	2.15	0.46
1:E:111:PRO:HA	1:E:112:PRO:HA	1.58	0.46
1:F:100:TYR:HB2	1:F:203:TRP:CE3	2.51	0.46
1:F:210:ARG:NH1	1:F:395:HIS:CA	2.78	0.46
1:F:260:LEU:HD12	1:F:260:LEU:HA	1.61	0.46
1:F:830:LEU:N	1:F:830:LEU:CD1	2.78	0.46
1:G:37:ARG:CG	1:G:37:ARG:NH1	2.79	0.46
1:G:63:PHE:CB	1:G:64:PRO:HD2	2.32	0.46
1:G:77:ASP:O	1:G:78:LEU:HD23	2.15	0.46
1:G:142:ILE:HG12	1:G:170:GLU:HG2	1.97	0.46
1:G:210:ARG:NH1	1:G:395:HIS:CA	2.78	0.46
1:G:278:ILE:N	1:G:278:ILE:CD1	2.78	0.46
1:G:409:VAL:HG12	1:G:410:VAL:N	2.29	0.46
1:G:930:VAL:HA	1:G:973:ARG:HD3	1.97	0.46
1:H:253:TYR:CD2	1:H:253:TYR:N	2.82	0.46
1:H:316:HIS:HB2	1:H:321:THR:O	2.16	0.46
1:H:646:HIS:O	1:H:648:ASP:N	2.47	0.46
1:I:230:ARG:HH11	1:I:230:ARG:CG	2.24	0.46
1:I:746:ASP:HA	1:I:760:ARG:CG	2.39	0.46
1:I:930:VAL:HA	1:I:973:ARG:HD3	1.97	0.46
1:J:129:VAL:CG2	1:J:182:ASN:ND2	2.77	0.46
1:J:368:ASP:O	1:J:369:GLU:C	2.58	0.46
1:J:425:ARG:HH22	1:K:287:ASP:CG	2.23	0.46
1:K:84:VAL:CG1	1:K:85:VAL:N	2.78	0.46
1:K:278:ILE:N	1:K:278:ILE:CD1	2.78	0.46
1:K:740:LEU:HD13	1:K:749:ILE:HD12	1.97	0.46
1:L:274:PHE:HB3	1:L:286:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:100:TYR:HB2	1:M:203:TRP:CE3	2.51	0.46
1:N:210:ARG:NH1	1:N:395:HIS:CA	2.78	0.46
1:N:631:LEU:HD12	1:N:635:THR:O	2.14	0.46
1:N:655:MET:HB2	1:N:655:MET:HE3	1.60	0.46
1:O:930:VAL:HA	1:O:973:ARG:HD3	1.97	0.46
1:P:13:ARG:O	1:P:14:ARG:HB2	2.16	0.46
1:P:829:THR:C	1:P:830:LEU:HD12	2.40	0.46
1:A:13:ARG:O	1:A:14:ARG:HB2	2.16	0.46
1:A:646:HIS:O	1:A:648:ASP:N	2.47	0.46
1:A:942:ARG:HA	1:A:953:GLY:O	2.15	0.46
1:B:740:LEU:HD13	1:B:749:ILE:HD12	1.97	0.46
1:D:100:TYR:HB2	1:D:203:TRP:CE3	2.51	0.46
1:D:316:HIS:HB2	1:D:321:THR:O	2.16	0.46
1:E:378:LEU:HD23	1:E:378:LEU:HA	1.53	0.46
1:E:391:HIS:ND1	1:E:412:GLU:OE1	2.44	0.46
1:F:49:GLN:H	1:F:49:GLN:CD	2.20	0.46
1:F:316:HIS:HB2	1:F:321:THR:O	2.15	0.46
1:F:658:LEU:O	1:F:659:ASP:C	2.58	0.46
1:H:631:LEU:HD12	1:H:635:THR:O	2.14	0.46
1:H:658:LEU:O	1:H:659:ASP:C	2.58	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:J:260:LEU:C	1:J:267:VAL:HG23	2.40	0.46
1:J:930:VAL:HA	1:J:973:ARG:HD3	1.97	0.46
1:K:316:HIS:HB2	1:K:321:THR:O	2.16	0.46
1:K:743:SER:O	1:K:760:ARG:NH1	2.49	0.46
1:L:655:MET:HE3	1:L:655:MET:HB2	1.60	0.46
1:M:631:LEU:HD12	1:M:632:SER:H	1.78	0.46
1:N:608:PHE:O	1:N:611:ARG:N	2.41	0.46
1:N:781:ARG:O	1:N:884:LEU:HA	2.16	0.46
1:O:37:ARG:CG	1:O:37:ARG:NH1	2.79	0.46
1:O:142:ILE:HG12	1:O:170:GLU:HG2	1.97	0.46
1:O:147:ASN:HA	1:O:148:SER:HA	1.54	0.46
1:O:339:ASN:O	1:P:527:PRO:HB3	2.15	0.46
1:O:409:VAL:HG12	1:O:410:VAL:N	2.29	0.46
1:O:429:ASP:HA	1:O:430:PRO:HD3	1.51	0.46
1:P:88:SER:HA	1:P:366:VAL:HG21	1.97	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:P:391:HIS:ND1	1:P:412:GLU:OE1	2.44	0.46
1:P:740:LEU:HD13	1:P:749:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:942:ARG:HA	1:B:953:GLY:O	2.15	0.46
1:C:274:PHE:HB3	1:C:286:ALA:O	2.15	0.46
1:C:377:LEU:HD22	1:C:708:TRP:CA	2.44	0.46
1:C:875:ASP:OD2	1:C:875:ASP:N	2.47	0.46
1:D:67:GLU:H	1:D:67:GLU:HG2	1.30	0.46
1:D:579:ASP:OD1	1:D:583:ASN:N	2.43	0.46
1:E:100:TYR:HB2	1:E:203:TRP:CE3	2.51	0.46
1:E:781:ARG:O	1:E:884:LEU:HA	2.16	0.46
1:E:829:THR:C	1:E:830:LEU:HD12	2.40	0.46
1:F:726:LEU:HA	1:F:726:LEU:HD23	1.65	0.46
1:G:260:LEU:C	1:G:267:VAL:HG23	2.40	0.46
1:G:740:LEU:HD13	1:G:749:ILE:CD1	2.45	0.46
1:H:62:TRP:C	1:H:63:PHE:CD1	2.93	0.46
1:H:599:ARG:HB2	1:H:600:GLN:H	1.41	0.46
1:H:781:ARG:O	1:H:884:LEU:HA	2.16	0.46
1:I:77:ASP:O	1:I:78:LEU:HD23	2.15	0.46
1:I:569:ASP:O	1:I:605:GLY:HA2	2.15	0.46
1:I:658:LEU:O	1:I:659:ASP:C	2.58	0.46
1:J:260:LEU:HA	1:J:260:LEU:HD12	1.61	0.46
1:J:353:GLY:C	1:J:566:PHE:HA	2.40	0.46
1:J:512:PHE:CE1	1:J:517:LYS:HG3	2.51	0.46
1:J:670:LEU:HA	1:J:670:LEU:HD23	1.67	0.46
1:K:99:ILE:HG23	1:K:594:ASP:HB2	1.98	0.46
1:K:377:LEU:HD22	1:K:708:TRP:CA	2.44	0.46
1:K:395:HIS:HA	1:K:396:PRO:HD3	1.48	0.46
1:K:400:THR:O	1:K:404:ARG:HD2	2.16	0.46
1:K:486:TYR:CZ	1:K:488:GLY:HA3	2.51	0.46
1:L:400:THR:O	1:L:404:ARG:HD2	2.16	0.46
1:L:743:SER:O	1:L:760:ARG:NH1	2.49	0.46
1:M:900:LEU:HA	1:M:900:LEU:HD23	1.75	0.46
1:M:930:VAL:HA	1:M:973:ARG:HD3	1.97	0.46
1:N:78:LEU:CB	1:N:79:PRO:HD2	2.44	0.46
1:N:316:HIS:HB2	1:N:321:THR:O	2.16	0.46
1:N:368:ASP:O	1:N:369:GLU:C	2.58	0.46
1:N:569:ASP:O	1:N: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:P:37:ARG:CG	1:P:37:ARG:NH1	2.79	0.46
1:P:702:GLN:O	1:P:712:GLY:N	2.45	0.46
1:P:781:ARG:O	1:P:884:LEU:HA	2.16	0.46
1:P:930:VAL:HA	1:P:973:ARG:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:TRP:C	1:A:63:PHE:CD1	2.93	0.46
1:B:576:ILE:CG2	1:B:577:LYS:N	2.78	0.46
1:B:830:LEU:CD1	1:B:830:LEU:N	2.78	0.46
1:C:62:TRP:C	1:C:63:PHE:CD1	2.93	0.46
1:C:99:ILE:HG23	1:C:594:ASP:HB2	1.98	0.46
1:C:129:VAL:CG2	1:C:182:ASN:ND2	2.77	0.46
1:C:400:THR:O	1:C:404:ARG:HD2	2.16	0.46
1:C:486:TYR:CZ	1:C:488:GLY:HA3	2.51	0.46
1:C:743:SER:O	1:C:760:ARG:NH1	2.49	0.46
1:D:486:TYR:CZ	1:D:488:GLY:HA3	2.51	0.46
1:E:419:GLY:HA2	1:H:282:ARG:NH1	2.30	0.46
1:E:442:ARG:HA	1:E:445:GLN:HG3	1.95	0.46
1:E:702:GLN:HA	1:E:703:PRO:HD2	1.84	0.46
1:F:282:ARG:HD3	1:G:418:HIS:O	2.15	0.46
1:G:486:TYR:CZ	1:G:488:GLY:HA3	2.51	0.46
1:G:658:LEU:O	1:G:659:ASP:C	2.58	0.46
1:G:743:SER:O	1:G:760:ARG:NH1	2.49	0.46
1:G:829:THR:C	1:G:830:LEU:HD12	2.40	0.46
1:H:37:ARG:CG	1:H:37:ARG:NH1	2.79	0.46
1:H:99:ILE:HG23	1:H:594:ASP:HB2	1.98	0.46
1:H:246:MET:HE3	1:H:247:CYS:C	2.41	0.46
1:H:661:LYS:HA	1:H:662:PRO:HD3	1.63	0.46
1:H:740:LEU:HD13	1:H:749:ILE:HD12	1.97	0.46
1:H:930:VAL:HA	1:H:973:ARG:HD3	1.97	0.46
1:I:147:ASN:HA	1:I:148:SER:HA	1.55	0.46
1:I:612:THR:HA	1:I:613:PRO:HD3	1.68	0.46
1:I:646:HIS:O	1:I:648:ASP:N	2.47	0.46
1:J:99:ILE:HG23	1:J:594:ASP:HB2	1.98	0.46
1:J:316:HIS:HB2	1:J:321:THR:O	2.16	0.46
1:J:400:THR:O	1:J:404:ARG:HD2	2.16	0.46
1:J:486:TYR:CZ	1:J:488:GLY:HA3	2.51	0.46
1:J:772:ASP:OD1	1:J:772:ASP:N	2.30	0.46
1:K:274:PHE:HB3	1:K:286:ALA:O	2.15	0.46
1:K:610:ASP:OD2	1:K:612:THR:HG23	2.15	0.46
1:K:781:ARG:O	1:K:884:LEU:HA	2.16	0.46
1:L:37:ARG:CG	1:L:37:ARG:NH1	2.79	0.46
1:L:118:ASN:HA	1:L:119:PRO:HD2	1.60	0.46
1:L:409:VAL:HG12	1:L:410:VAL:N	2.29	0.46
1:L:856:TYR:CD2	1:L:864:MET:CE	2.97	0.46
1:M:368:ASP:O	1:M:369:GLU:C	2.58	0.46
1:N:486:TYR:CZ	1:N:488:GLY:HA3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:7:LEU:O	1:O:8:ALA:C	2.55	0.46
1:O:569:ASP:O	1:O:605:GLY:HA2	2.15	0.46
1:P:743:SER:O	1:P:760:ARG:NH1	2.49	0.46
1:P:948:PRO:O	1:P:1022:GLN:HA	2.14	0.46
1:A:99:ILE:HG23	1:A:594:ASP:HB2	1.98	0.46
1:A:129:VAL:CG2	1:A:182:ASN:ND2	2.77	0.46
1:A:1021:CME:HB3	1:A:1021:CME:HE2	1.41	0.46
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.62	0.46
1:C:612:THR:HB	1:C:613:PRO:HD2	1.96	0.46
1:C:829:THR:C	1:C:830:LEU:HD12	2.40	0.46
1:D:62:TRP:C	1:D:63:PHE:CD1	2.93	0.46
1:D:78:LEU:HB3	1:D:79:PRO:CD	2.45	0.46
1:D:260:LEU:C	1:D:267:VAL:HG23	2.40	0.46
1:D:612:THR:HA	1:D:613:PRO:HD3	1.68	0.46
1:D:856:TYR:CD2	1:D:864:MET:CE	2.97	0.46
1:E:347:LYS:CB	1:E:348:PRO:HD2	2.43	0.46
1:E:486:TYR:CZ	1:E:488:GLY:HA3	2.51	0.46
1:E:569:ASP:O	1:E:605:GLY:HA2	2.15	0.46
1:E:740:LEU:HD13	1:E:749:ILE:HD12	1.97	0.46
1:E:875:ASP:OD2	1:E:875:ASP:N	2.47	0.46
1:E:878:HIS:HA	1:E:879:PRO:HD3	1.66	0.46
1:F:49:GLN:H	1:F:49:GLN:HE21	1.59	0.46
1:F:77:ASP:O	1:F:78:LEU:HD23	2.15	0.46
1:F:486:TYR:CZ	1:F:488:GLY:HA3	2.51	0.46
1:G:99:ILE:HG23	1:G:594:ASP:HB2	1.98	0.46
1:G:445:GLN:HE21	1:G:445:GLN:HB3	1.55	0.46
1:G:645:ARG:NH2	1:G:650:GLU:CD	2.74	0.46
1:H:24:LEU:HD12	1:H:24:LEU:HA	1.62	0.46
1:H:400:THR:O	1:H:404:ARG:HD2	2.16	0.46
1:I:13:ARG:O	1:I:14:ARG:HB2	2.16	0.46
1:I:88:SER:HA	1:I:366:VAL:HG21	1.97	0.46
1:I:1020:TRP:CD1	1:I:1021:CME:N	2.80	0.46
1:J:576:ILE:CG2	1:J:577:LYS:N	2.78	0.46
1:J:646:HIS:O	1:J:648:ASP:N	2.47	0.46
1:J:658:LEU:O	1:J:659:ASP:C	2.58	0.46
1:K:260:LEU:C	1:K:267:VAL:HG23	2.40	0.46
1:K:830:LEU:N	1:K:830:LEU:CD1	2.78	0.46
1:K:875:ASP:OD2	1:K:875:ASP:N	2.47	0.46
1:L:49:GLN:H	1:L:49:GLN:HE21	1.59	0.46
1:L:260:LEU:C	1:L:267:VAL:HG23	2.40	0.46
1:L:830:LEU:N	1:L:830:LEU:CD1	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:260:LEU:HA	1:M:260:LEU:HD12	1.61	0.46
1:M:781:ARG:O	1:M:884:LEU:HA	2.16	0.46
1:N:77:ASP:O	1:N:78:LEU:HD23	2.15	0.46
1:N:211:ASP:OD1	1:N:211:ASP:N	2.42	0.46
1:N:230:ARG:HH11	1:N:230:ARG:CG	2.24	0.46
1:O:99:ILE:HG23	1:O:594:ASP:HB2	1.98	0.46
1:O:645:ARG:NH2	1:O:650:GLU:CD	2.74	0.46
1:P:99:ILE:HG23	1:P:594:ASP:HB2	1.98	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:P:742:THR:CG2	1:P:743:SER:H	2.27	0.46
1:A:37:ARG:CG	1:A:37:ARG:NH1	2.79	0.46
1:A:100:TYR:HB2	1:A:203:TRP:CE3	2.51	0.46
1:A:210:ARG:NH1	1:A:395:HIS:CA	2.78	0.46
1:A:253:TYR:CD2	1:A:253:TYR:N	2.82	0.46
1:A:344:LEU:N	1:A:347:LYS:O	2.36	0.46
1:A:400:THR:O	1:A:404:ARG:HD2	2.16	0.46
1:A:486:TYR:CE2	1:A:488:GLY:HA3	2.51	0.46
1:A:486:TYR:CZ	1:A:488:GLY:HA3	2.51	0.46
1:A:654:TRP:O	1:A:655:MET:HB3	2.15	0.46
1:A:745:MET:HE2	1:A:745:MET:N	2.31	0.46
1:B:368:ASP:O	1:B:369:GLU:C	2.58	0.46
1:B:400:THR:O	1:B:404:ARG:HD2	2.16	0.46
1:B:583:ASN:HA	1:B:584:PRO:HD3	1.80	0.46
1:C:77:ASP:O	1:C:78:LEU:HD23	2.15	0.46
1:C:367:MET:HB3	1:C:367:MET:HE3	1.72	0.46
1:C:645:ARG:NH2	1:C:650:GLU:CD	2.74	0.46
1:D:84:VAL:CG1	1:D:85:VAL:N	2.78	0.46
1:D:708:TRP:CD1	1:D:708:TRP:N	2.84	0.46
1:E:287:ASP:CG	1:H:425:ARG:HH22	2.23	0.46
1:E:409:VAL:CG1	1:E:410:VAL:N	2.79	0.46
1:E:724:GLU:OE1	1:F:874:SER:HB3	2.16	0.46
1:E:746:ASP:HA	1:E:760:ARG:CG	2.39	0.46
1:E:894:ARG:HH12	1:E:920:LEU:HA	1.81	0.46
1:F:271:THR:HG22	1:F:272:ALA:N	2.29	0.46
1:F:400:THR:O	1:F:404:ARG:HD2	2.16	0.46
1:F:512:PHE:CE1	1:F:517:LYS:HG3	2.51	0.46
1:F:745:MET:HE2	1:F:745:MET:N	2.31	0.46
1:G:13:ARG:O	1:G:14:ARG:HB2	2.16	0.46
1:G:84:VAL:CG1	1:G:85:VAL:N	2.78	0.46
1:G:631:LEU:HD12	1:G:635:THR:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:287:ASP:OD1	1:H:287:ASP:N	2.29	0.46
1:H:745:MET:HE2	1:H:745:MET:N	2.31	0.46
1:I:246:MET:HE3	1:I:247:CYS:C	2.41	0.46
1:I:576:ILE:CG2	1:I:577:LYS:N	2.78	0.46
1:I:749:ILE:N	1:I:749:ILE:CD1	2.78	0.46
1:J:66:PRO:HB3	1:J:187:MET:HE2	1.98	0.46
1:J:486:TYR:CE2	1:J:488:GLY:HA3	2.51	0.46
1:K:663:LEU:HD23	1:K:663:LEU:N	2.24	0.46
1:L:70:PRO:O	1:L:73:TRP:N	2.45	0.46
1:L:78:LEU:HB3	1:L:79:PRO:CD	2.45	0.46
1:L:99:ILE:HG23	1:L:594:ASP:HB2	1.98	0.46
1:L:251:ARG:CB	1:L:253:TYR:CE2	2.98	0.46
1:L:409:VAL:CG1	1:L:410:VAL:N	2.79	0.46
1:L:486:TYR:CE2	1:L:488:GLY:HA3	2.51	0.46
1:L:583:ASN:HA	1:L:584:PRO:HD3	1.80	0.46
1:L:645:ARG:NH2	1:L:650:GLU:CD	2.74	0.46
1:M:62:TRP:C	1:M:63:PHE:CD1	2.93	0.46
1:M:66:PRO:HD2	1:M:67:GLU:OE2	2.14	0.46
1:M:246:MET:HE3	1:M:246:MET:C	2.40	0.46
1:M:246:MET:HE3	1:M:247:CYS:C	2.41	0.46
1:M:403:ASP:OD2	1:M:450:HIS:ND1	2.34	0.46
1:M:486:TYR:CZ	1:M:488:GLY:HA3	2.51	0.46
1:N:49:GLN:H	1:N:49:GLN:HE21	1.59	0.46
1:N:62:TRP:C	1:N:63:PHE:CD1	2.93	0.46
1:N:100:TYR:HB2	1:N:203:TRP:CE3	2.51	0.46
1:N:400:THR:O	1:N:404:ARG:HD2	2.16	0.46
1:N:486:TYR:CE2	1:N:488:GLY:HA3	2.51	0.46
1:N:749:ILE:N	1:N:749:ILE:CD1	2.78	0.46
1:N:894:ARG:HH12	1:N:920:LEU:HA	1.81	0.46
1:O:62:TRP:C	1:O:63:PHE:CD1	2.93	0.46
1:O:272:ALA:HA	1:O:273:PRO:HD3	1.76	0.46
1:O:486:TYR:CZ	1:O:488:GLY:HA3	2.51	0.46
1:O:743:SER:O	1:O:760:ARG:NH1	2.49	0.46
1:P:486:TYR:CZ	1:P:488:GLY:HA3	2.51	0.46
1:P:708:TRP:CD1	1:P:708:TRP:N	2.84	0.46
1:P:830:LEU:N	1:P:830:LEU:CD1	2.78	0.46
1:A:279:ILE:HD11	1:D:424:ASN:OD1	2.16	0.46
1:A:569:ASP:O	1:A:605:GLY:HA2	2.16	0.46
1:A:724:GLU:OE1	1:B:874:SER:HB3	2.16	0.46
1:B:62:TRP:C	1:B:63:PHE:CD1	2.93	0.46
1:B:646:HIS:O	1:B:648:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:829:THR:C	1:B:830:LEU:HD12	2.40	0.46
1:C:57:GLU:HG2	1:C:83:THR:HG21	1.93	0.46
1:C:210:ARG:NH1	1:C:395:HIS:CA	2.78	0.46
1:C:246:MET:HE3	1:C:247:CYS:C	2.41	0.46
1:C:682:LEU:HD23	1:C:682:LEU:HA	1.67	0.46
1:D:730:LEU:HA	1:D:731:PRO:HD3	1.74	0.46
1:D:1020:TRP:CD1	1:D:1021:CME:N	2.80	0.46
1:E:210:ARG:NH1	1:E:395:HIS:CA	2.78	0.46
1:E:246:MET:HE3	1:E:246:MET:C	2.40	0.46
1:E:255:ARG:NH1	1:E:255:ARG:CG	2.79	0.46
1:E:373:VAL:O	1:E:374:GLN:C	2.57	0.46
1:E:479:ASP:HA	1:E:480:PRO:HD2	1.61	0.46
1:E:745:MET:HE2	1:E:745:MET:N	2.31	0.46
1:E:930:VAL:HA	1:E:973:ARG:HD3	1.97	0.46
1:F:740:LEU:HD13	1:F:749:ILE:HD12	1.97	0.46
1:G:7:LEU:O	1:G:8:ALA:C	2.55	0.46
1:G:726:LEU:HD23	1:G:726:LEU:HA	1.65	0.46
1:H:512:PHE:CE1	1:H:517:LYS:HG3	2.51	0.46
1:I:210:ARG:HH11	1:I:395:HIS:HB2	1.81	0.46
1:J:743:SER:OG	1:J: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:H	1:K:67:GLU:HG2	1.30	0.46
1:K:254:LEU:HA	1:K:254:LEU:HD23	1.62	0.46
1:K:368:ASP:O	1:K:369:GLU:C	2.58	0.46
1:K:658:LEU:O	1:K:659:ASP:C	2.58	0.46
1:K:743:SER:OG	1:K:744:GLU:N	2.49	0.46
1:L:576:ILE:CG2	1:L:577:LYS:N	2.78	0.46
1:L:745:MET:HE2	1:L:745:MET:N	2.31	0.46
1:M:486:TYR:CE2	1:M:488:GLY:HA3	2.51	0.46
1:M:645:ARG:NH2	1:M:650:GLU:CD	2.74	0.46
1:M:708:TRP:CD1	1:M:708:TRP:N	2.84	0.46
1:M:830:LEU:N	1:M:830:LEU:CD1	2.78	0.46
1:N:11:LEU:N	1:N:11:LEU:CD2	2.76	0.46
1:N:512:PHE:CE1	1:N:517:LYS:HG3	2.51	0.46
1:N:745:MET:HE2	1:N:745:MET:N	2.31	0.46
1:O:278:ILE:N	1:O:278:ILE:CD1	2.78	0.46
1:O:512:PHE:CE1	1:O:517:LYS:HG3	2.51	0.46
1:P:78:LEU:CB	1:P:79:PRO:HD2	2.44	0.46
1:P:646:HIS:O	1:P:648:ASP:N	2.47	0.46
1:A:781:ARG:O	1:A:884:LEU:HA	2.16	0.46
1:A:856:TYR:CD2	1:A:864:MET:CE	2.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:VAL:HA	1:A:973:ARG:HD3	1.97	0.46
1:B:79:PRO:HD2	1:B:80:GLU:OE2	2.17	0.46
1:B:486:TYR:CE2	1:B:488:GLY:HA3	2.51	0.46
1:B:486:TYR:CZ	1:B:488:GLY:HA3	2.51	0.46
1:B:631:LEU:HD12	1:B:635:THR:O	2.14	0.46
1:B:708:TRP:CD1	1:B:708:TRP:N	2.84	0.46
1:C:210:ARG:HH11	1:C:395:HIS:HB2	1.81	0.46
1:C:612:THR:HA	1:C:613:PRO:HD3	1.68	0.46
1:C:646:HIS:O	1:C:648:ASP:N	2.48	0.46
1:C:830:LEU:N	1:C:830:LEU:CD1	2.78	0.46
1:D:88:SER:HA	1:D:366:VAL:HG21	1.97	0.46
1:D:246:MET:HE3	1:D:247:CYS:C	2.41	0.46
1:D:654:TRP:O	1:D:655:MET:HB3	2.15	0.46
1:D:745:MET:HE2	1:D:745:MET:N	2.31	0.46
1:D:781:ARG:NH1	1:D:781:ARG:CG	2.79	0.46
1:D:822:LEU:HD12	1:D:822:LEU:C	2.37	0.46
1:E:37:ARG:CG	1:E:37:ARG:NH1	2.79	0.46
1:E:400:THR:O	1:E:404:ARG:HD2	2.16	0.46
1:E:807:VAL:CG1	1:E:808:GLU:N	2.79	0.46
1:F:78:LEU:HB3	1:F:79:PRO:CD	2.45	0.46
1:F:479:ASP:HA	1:F:480:PRO:HD2	1.61	0.46
1:F:743:SER:OG	1:F:744:GLU:N	2.49	0.46
1:G:62:TRP:C	1:G:63:PHE:CD1	2.93	0.46
1:G:100:TYR:HB2	1:G:203:TRP:CE3	2.51	0.46
1:G:894:ARG:HH12	1:G:920:LEU:HA	1.81	0.46
1:H:66:PRO:HB3	1:H:187:MET:HE2	1.98	0.46
1:H:77:ASP:O	1:H:78:LEU:HD23	2.15	0.46
1:I:654:TRP:O	1:I:655:MET:HB3	2.15	0.46
1:I:740:LEU:HD13	1:I:749:ILE:HD12	1.97	0.46
1:I:781:ARG:O	1:I:884:LEU:HA	2.16	0.46
1:J:254:LEU:HD23	1:J:254:LEU:HA	1.62	0.46
1:J:743:SER:O	1:J:760:ARG:NH1	2.49	0.46
1:J:900:LEU:HD23	1:J:900:LEU:HA	1.75	0.46
1:K:708:TRP:CD1	1:K:708:TRP:N	2.84	0.46
1:K:942:ARG:HA	1:K:953:GLY:O	2.15	0.46
1:L:781:ARG:O	1:L:884:LEU:HA	2.16	0.46
1:M:111:PRO:HA	1:M:112:PRO:HA	1.57	0.46
1:M:473:ARG:HD2	1:P:469:ASP:HB3	1.96	0.46
1:N:99:ILE:HG23	1:N:594:ASP:HB2	1.98	0.46
1:N:255:ARG:NH1	1:N:255:ARG:CG	2.79	0.46
1:N:391:HIS:ND1	1:N:412:GLU:OE1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:726:LEU:HA	1:N:726:LEU:HD23	1.65	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
1:O:78:LEU:HB3	1:O:79:PRO:CD	2.45	0.46
1:O:246:MET:HE3	1:O:247:CYS:C	2.41	0.46
1:O:740:LEU:HD13	1:O:749:ILE:HD12	1.97	0.46
1:O:894:ARG:HH12	1:O:920:LEU:HA	1.81	0.46
1:P:745:MET:HE2	1:P:745:MET:N	2.31	0.46
1:P:1020:TRP:CD1	1:P:1021:CME:N	2.80	0.46
1:A:246:MET:HE3	1:A:247:CYS:C	2.41	0.45
1:A:740:LEU:HD13	1:A:749:ILE:HD12	1.97	0.45
1:B:78:LEU:HB3	1:B:79:PRO:CD	2.45	0.45
1:C:658:LEU:O	1:C:659:ASP:C	2.58	0.45
1:C:894:ARG:HH12	1:C:920:LEU:HA	1.81	0.45
1:D:240:LEU:HD12	1:D:240:LEU:C	2.36	0.45
1:D:486:TYR:CE2	1:D:488:GLY:HA3	2.51	0.45
1:F:99:ILE:HG23	1:F:594:ASP:HB2	1.98	0.45
1:F:486:TYR:CE2	1:F:488:GLY:HA3	2.51	0.45
1:G:79:PRO:HD2	1:G:80:GLU:OE2	2.17	0.45
1:G:227:VAL:CG1	1:G:240:LEU:HD11	2.42	0.45
1:G:246:MET:HE3	1:G:247:CYS:C	2.41	0.45
1:H:395:HIS:HA	1:H:396:PRO:HD3	1.48	0.45
1:H:403:ASP:CG	1:H:451:PRO:HD2	2.42	0.45
1:I:37:ARG:CG	1:I:37:ARG:NH1	2.79	0.45
1:I:73:TRP:CZ2	1:I:122:CYS:HB3	2.50	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:J:7:LEU:O	1:J:8:ALA:C	2.55	0.45
1:K:70:PRO:O	1:K:73:TRP:N	2.45	0.45
1:K:403:ASP:CG	1:K:451:PRO:HD2	2.41	0.45
1:K:746:ASP:HA	1:K:760:ARG:CG	2.39	0.45
1:M:260:LEU:C	1:M:267:VAL:HG23	2.40	0.45
1:M:445:GLN:HE21	1:M:445:GLN:HB3	1.54	0.45
1:M:740:LEU:HD13	1:M:749:ILE:HD12	1.97	0.45
1:M:743:SER:OG	1:M:744:GLU:N	2.49	0.45
1:N:654:TRP:O	1:N:655:MET:HB3	2.15	0.45
1:N:807:VAL:CG1	1:N:808:GLU:N	2.80	0.45
1:O:726:LEU:HD23	1:O:726:LEU:HA	1.65	0.45
1:P:77:ASP:O	1:P:78:LEU:HD23	2.15	0.45
1:P:100:TYR:HB2	1:P:203:TRP:CE3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:400:THR:O	1:P:404:ARG:HD2	2.16	0.45
1:P:403:ASP:CG	1:P:451:PRO:HD2	2.41	0.45
1:A:377:LEU:HD22	1:A:708:TRP:CA	2.44	0.45
1:B:13:ARG:O	1:B:14:ARG:HB2	2.16	0.45
1:B:88:SER:HA	1:B:366:VAL:HG21	1.97	0.45
1:B:445:GLN:HE21	1:B:445:GLN:HB3	1.54	0.45
1:B:515:VAL:HG21	1:C:281:GLU:CD	2.41	0.45
1:B:807:VAL:CG1	1:B:808:GLU:N	2.80	0.45
1:C:743:SER:OG	1:C:744:GLU:N	2.49	0.45
1:D:743:SER:OG	1:D:744:GLU:N	2.49	0.45
1:D:746:ASP:HA	1:D:760:ARG:CG	2.39	0.45
1:D:894:ARG:HH12	1:D:920:LEU:HA	1.81	0.45
1:E:62:TRP:C	1:E:63:PHE:CD1	2.93	0.45
1:F:260:LEU:C	1:F:267:VAL:HG23	2.40	0.45
1:G:740:LEU:HD13	1:G:749:ILE:HD12	1.97	0.45
1:G:822:LEU:HD12	1:G:823:LEU:H	1.80	0.45
1:H:409:VAL:CG1	1:H:410:VAL:N	2.79	0.45
1:H:569:ASP:O	1:H:605:GLY:HA2	2.15	0.45
1:H:743:SER:OG	1:H:744:GLU:N	2.49	0.45
1:H:830:LEU:N	1:H:830:LEU:CD1	2.78	0.45
1:H:942:ARG:HA	1:H:953:GLY:O	2.15	0.45
1:I:79:PRO:HD2	1:I:80:GLU:OE2	2.17	0.45
1:I:210:ARG:NH1	1:I:395:HIS:CA	2.78	0.45
1:I:368:ASP:O	1:I:369:GLU:C	2.58	0.45
1:I:869:ASP:CG	1:I:1015:HIS:HD1	2.24	0.45
1:J:173:LEU:HA	1:J:173:LEU:HD23	1.69	0.45
1:J:271:THR:HG22	1:J:272:ALA:N	2.29	0.45
1:J:403:ASP:CG	1:J:451:PRO:HD2	2.41	0.45
1:J:682:LEU:HD23	1:J:682:LEU:HA	1.67	0.45
1:J:749:ILE:N	1:J:749:ILE:CD1	2.78	0.45
1:J:781:ARG:O	1:J:884:LEU:HA	2.16	0.45
1:J:856:TYR:CD2	1:J:864:MET:CE	2.97	0.45
1:K:409:VAL:CG1	1:K:410:VAL:N	2.79	0.45
1:L:246:MET:HE3	1:L:247:CYS:C	2.41	0.45
1:L:670:LEU:HA	1:L:670:LEU:HD23	1.67	0.45
1:L:894:ARG:HH12	1:L:920:LEU:HA	1.81	0.45
1:N:78:LEU:HB3	1:N:79:PRO:CD	2.45	0.45
1:N:829:THR:C	1:N:830:LEU:HD12	2.40	0.45
1:N:875:ASP:N	1:N:875:ASP:OD2	2.47	0.45
1:O:66:PRO:HB3	1:O:187:MET:HE2	1.98	0.45
1:O:391:HIS:ND1	1:O:412:GLU:OE1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:486:TYR:CE2	1:O:488:GLY:HA3	2.51	0.45
1:P:210:ARG:NH1	1:P:395:HIS:CA	2.78	0.45
1:P:409:VAL:CG1	1:P:410:VAL:N	2.79	0.45
1:P:685:LEU:HA	1:P:686:PRO:HD3	1.70	0.45
1:P:894:ARG:HH12	1:P:920:LEU:HA	1.81	0.45
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.62	0.45
1:A:282:ARG:HD3	1:D:418:HIS:O	2.15	0.45
1:A:409:VAL:CG1	1:A:410:VAL:N	2.79	0.45
1:A:429:ASP:HA	1:A:430:PRO:HD3	1.51	0.45
1:B:66:PRO:HB3	1:B:187:MET:HE2	1.99	0.45
1:B:260:LEU:HD12	1:B:260:LEU:HA	1.61	0.45
1:B:743:SER:O	1:B:760:ARG:NH1	2.49	0.45
1:B:745:MET:HE2	1:B:745:MET:N	2.31	0.45
1:C:271:THR:HG22	1:C:272:ALA:N	2.29	0.45
1:D:7:LEU:O	1:D:8:ALA:C	2.55	0.45
1:D:37:ARG:CG	1:D:37:ARG:NH1	2.79	0.45
1:D:576:ILE:CG2	1:D:577:LYS:N	2.78	0.45
1:D:743:SER:O	1:D:760:ARG:NH1	2.49	0.45
1:D:830:LEU:N	1:D:830:LEU:CD1	2.78	0.45
1:D:900:LEU:HD23	1:D:900:LEU:HA	1.75	0.45
1:D:930:VAL:HA	1:D:973:ARG:HD3	1.97	0.45
1:E:254:LEU:HA	1:E:254:LEU:HD23	1.62	0.45
1:E:531:ARG:O	1:E:561:ARG:NH1	2.46	0.45
1:E:825:CYS:HA	1:E:837:THR:O	2.17	0.45
1:F:79:PRO:HD2	1:F:80:GLU:OE2	2.17	0.45
1:F:377:LEU:HD22	1:F:708:TRP:CA	2.44	0.45
1:F:743:SER:O	1:F:760:ARG:NH1	2.49	0.45
1:F:781:ARG:O	1:F:884:LEU:HA	2.16	0.45
1:G:66:PRO:HB3	1:G:187:MET:HE2	1.98	0.45
1:G:486:TYR:CE2	1:G:488:GLY:HA3	2.51	0.45
1:G:569:ASP:O	1:G:605:GLY:HA2	2.15	0.45
1:G:781:ARG:O	1:G:884:LEU:HA	2.16	0.45
1:G:825:CYS:HA	1:G:837:THR:O	2.17	0.45
1:G:856:TYR:CD2	1:G:864:MET:CE	2.97	0.45
1:H:344:LEU:N	1:H:347:LYS:O	2.36	0.45
1:I:4:THR:CA	1:I:9:VAL:HG11	2.47	0.45
1:I:63:PHE:CB	1:I:64:PRO:HD2	2.32	0.45
1:I:645:ARG:NH2	1:I:650:GLU:CD	2.74	0.45
1:I:830:LEU:N	1:I:830:LEU:CD1	2.78	0.45
1:J:37:ARG:CG	1:J:37:ARG:NH1	2.79	0.45
1:J:579:ASP:N	1:J:583:ASN:O	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:599:ARG:HB2	1:J:600:GLN:H	1.41	0.45
1:K:512:PHE:CE1	1:K:517:LYS:HG3	2.51	0.45
1:K:807:VAL:CG1	1:K:808:GLU:N	2.80	0.45
1:K:894:ARG:HH12	1:K:920:LEU:HA	1.81	0.45
1:L:13:ARG:O	1:L:14:ARG:HB2	2.15	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:L:316:HIS:HB2	1:L:321:THR:O	2.16	0.45
1:L:363:HIS:CD2	1:L:363:HIS:N	2.81	0.45
1:L:824:GLN:HG3	1:L:825:CYS:N	2.28	0.45
1:M:373:VAL:O	1:M:374:GLN:C	2.57	0.45
1:M:745:MET:HE2	1:M:745:MET:N	2.31	0.45
1:M:746:ASP:HA	1:M:760:ARG:CG	2.39	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:N:347:LYS:HA	1:N:348:PRO:HD3	1.77	0.45
1:O:400:THR:O	1:O:404:ARG:HD2	2.16	0.45
1:O:745:MET:HE2	1:O:745:MET:N	2.31	0.45
1:O:781:ARG:O	1:O:884:LEU:HA	2.16	0.45
1:P:46:ARG:NH1	1:P:46:ARG:CG	2.78	0.45
1:P:608:PHE:O	1:P:611:ARG:N	2.41	0.45
1:P:825:CYS:HA	1:P:837:THR:O	2.17	0.45
1:A:12:GLN:OE1	1:A:12:GLN:HA	2.17	0.45
1:A:423:MET:HE2	1:D:282:ARG:HG2	1.98	0.45
1:B:37:ARG:CG	1:B:37:ARG:NH1	2.79	0.45
1:B:246:MET:HE3	1:B:247:CYS:C	2.41	0.45
1:B:579:ASP:N	1:B:583:ASN:O	2.40	0.45
1:C:79:PRO:HD2	1:C:80:GLU:OE2	2.16	0.45
1:C:569:ASP:O	1:C:605:GLY:HA2	2.15	0.45
1:C:781:ARG:O	1:C:884:LEU:HA	2.16	0.45
1:D:210:ARG:NH1	1:D:395:HIS:CA	2.78	0.45
1:D:227:VAL:CG1	1:D:240:LEU:HD11	2.42	0.45
1:D:368:ASP:O	1:D:369:GLU:C	2.58	0.45
1:D:655:MET:HE3	1:D:655:MET:HB2	1.60	0.45
1:E:129:VAL:CG2	1:E:182:ASN:ND2	2.77	0.45
1:E:316:HIS:HB2	1:E:321:THR:O	2.15	0.45
1:E:418:HIS:O	1:H:282:ARG:HD3	2.17	0.45
1:E:486:TYR:CE2	1:E:488:GLY:HA3	2.51	0.45
1:E:654:TRP:O	1:E:655:MET:HB3	2.15	0.45
1:E:830:LEU:N	1:E:830:LEU:CD1	2.78	0.45
1:F:210:ARG:HH11	1:F:395:HIS:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:343:LEU:HD23	1:G:348:PRO:HA	1.99	0.45
1:G:403:ASP:CG	1:G:451:PRO:HD2	2.41	0.45
1:G:702:GLN:HA	1:G:703:PRO:HD2	1.84	0.45
1:G:745:MET:HE2	1:G:745:MET:N	2.31	0.45
1:G:961:ARG:NH2	1:G:979:GLU:O	2.37	0.45
1:H:807:VAL:CG1	1:H:808:GLU:N	2.80	0.45
1:I:46:ARG:NH1	1:I:46:ARG:CG	2.78	0.45
1:I:260:LEU:HD12	1:I:260:LEU:HA	1.61	0.45
1:I:403:ASP:CG	1:I:451:PRO:HD2	2.41	0.45
1:I:486:TYR:CE2	1:I:488:GLY:HA3	2.51	0.45
1:J:409:VAL:CG1	1:J:410:VAL:N	2.79	0.45
1:J:654:TRP:O	1:J:655:MET:HB3	2.15	0.45
1:K:100:TYR:HB2	1:K:203:TRP:CE3	2.51	0.45
1:K:210:ARG:HH11	1:K:395:HIS:HB2	1.81	0.45
1:L:230:ARG:HH11	1:L:230:ARG:CG	2.24	0.45
1:L:387:VAL:CG2	1:L:388:ARG:N	2.80	0.45
1:M:13:ARG:O	1:M:14:ARG:HB2	2.16	0.45
1:M:49:GLN:H	1:M:49:GLN:HE21	1.59	0.45
1:M:210:ARG:HH11	1:M:395:HIS:HB2	1.81	0.45
1:M:875:ASP:N	1:M:875:ASP:OD2	2.47	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:O:368:ASP:O	1:O:369:GLU:C	2.58	0.45
1:O:702:GLN:HA	1:O:703:PRO:HD2	1.84	0.45
1:P:569:ASP:O	1:P:605:GLY:HA2	2.15	0.45
1:A:316:HIS:HB2	1:A:321:THR:O	2.16	0.45
1:A:512:PHE:CE1	1:A:517:LYS:HG3	2.51	0.45
1:A:825:CYS:HA	1:A:837:THR:O	2.17	0.45
1:A:830:LEU:N	1:A:830:LEU:CD1	2.78	0.45
1:B:569:ASP:O	1:B:605:GLY:HA2	2.15	0.45
1:B:637:GLU:HA	1:B:679:LEU:CD2	2.47	0.45
1:C:12:GLN:OE1	1:C:12:GLN:HA	2.17	0.45
1:C:13:ARG:O	1:C:14:ARG:HB2	2.16	0.45
1:C:100:TYR:HB2	1:C:203:TRP:CE3	2.51	0.45
1:C:403:ASP:CG	1:C:451:PRO:HD2	2.41	0.45
1:C:409:VAL:CG1	1:C:410:VAL:N	2.79	0.45
1:C:486:TYR:CE2	1:C:488:GLY:HA3	2.51	0.45
1:D:6:SER:O	1:D:7:LEU:C	2.60	0.45
1:D:781:ARG:O	1:D:884:LEU:HA	2.16	0.45
1:E:13:ARG:O	1:E:14:ARG:HB2	2.16	0.45
1:E:246:MET:HE3	1:E:247:CYS:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:LEU:C	1:E:267:VAL:HG23	2.40	0.45
1:E:377:LEU:HD22	1:E:708:TRP:CA	2.44	0.45
1:E:743:SER:O	1:E:760:ARG:NH1	2.49	0.45
1:E:856:TYR:CD2	1:E:864:MET:CE	2.97	0.45
1:F:694:LEU:HD12	1:F:694:LEU:HA	1.69	0.45
1:F:829:THR:C	1:F:830:LEU:HD12	2.40	0.45
1:G:210:ARG:HH11	1:G:395:HIS:HB2	1.82	0.45
1:G:400:THR:O	1:G:404:ARG:HD2	2.16	0.45
1:H:4:THR:CA	1:H:9:VAL:HG11	2.47	0.45
1:H:894:ARG:HH12	1:H:920:LEU:HA	1.81	0.45
1:I:373:VAL:O	1:I:374:GLN:C	2.57	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:807:VAL:CG1	1:I:808:GLU:N	2.80	0.45
1:J:246:MET:HE3	1:J:247:CYS:C	2.41	0.45
1:J:347:LYS:CB	1:J:348:PRO:HD2	2.43	0.45
1:J:651:LEU:HD13	1:J:651:LEU:HA	1.51	0.45
1:J:807:VAL:CG1	1:J:808:GLU:N	2.79	0.45
1:K:46:ARG:NH1	1:K:46:ARG:CG	2.78	0.45
1:K:745:MET:HE2	1:K:745:MET:N	2.31	0.45
1:L:377:LEU:HD22	1:L:708:TRP:CA	2.44	0.45
1:M:66:PRO:HB3	1:M:187:MET:HE2	1.98	0.45
1:M:79:PRO:HD2	1:M:80:GLU:OE2	2.16	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:M:743:SER:O	1:M:760:ARG:NH1	2.49	0.45
1:O:210:ARG:HH11	1:O:395:HIS:HB2	1.82	0.45
1:O:255:ARG:NH1	1:O:255:ARG:CG	2.79	0.45
1:P:202:MET:HE3	1:P:357:HIS:ND1	2.32	0.45
1:P:246:MET:HE3	1:P:247:CYS:C	2.41	0.45
1:P:807:VAL:CG1	1:P:808:GLU:N	2.80	0.45
1:A:387:VAL:CG2	1:A:388:ARG:N	2.80	0.45
1:A:645:ARG:NH2	1:A:650:GLU:CD	2.74	0.45
1:B:99:ILE:HG23	1:B:594:ASP:HB2	1.98	0.45
1:B:100:TYR:HB2	1:B:203:TRP:CE3	2.51	0.45
1:B:251:ARG:CB	1:B:253:TYR:CE2	2.98	0.45
1:B:260:LEU:C	1:B:267:VAL:HG23	2.40	0.45
1:B:403:ASP:CG	1:B:451:PRO:HD2	2.41	0.45
1:B:425:ARG:NH2	1:C:287:ASP:OD2	2.50	0.45
1:B:670:LEU:HD23	1:B:670:LEU:HA	1.67	0.45
1:B:825:CYS:HA	1:B:837:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:663:LEU:HD23	1:C:663:LEU:N	2.24	0.45
1:C:807:VAL:CG1	1:C:808:GLU:N	2.79	0.45
1:D:807:VAL:CG1	1:D:808:GLU:N	2.79	0.45
1:E:11:LEU:N	1:E:11:LEU:CD2	2.76	0.45
1:E:66:PRO:HB3	1:E:187:MET:HE2	1.98	0.45
1:E:637:GLU:HA	1:E:679:LEU:CD2	2.47	0.45
1:E:661:LYS:HA	1:E:662:PRO:HD3	1.63	0.45
1:F:645:ARG:NH2	1:F:650:GLU:CD	2.74	0.45
1:F:825:CYS:HA	1:F:837:THR:O	2.17	0.45
1:G:67:GLU:H	1:G:67:GLU:HG2	1.31	0.45
1:G:255:ARG:NH1	1:G:255:ARG:CG	2.79	0.45
1:G:512:PHE:CE1	1:G:517:LYS:HG3	2.51	0.45
1:H:78:LEU:HB3	1:H:79:PRO:CD	2.45	0.45
1:H:79:PRO:HD2	1:H:80:GLU:OE2	2.16	0.45
1:H:202:MET:HE3	1:H:357:HIS:ND1	2.32	0.45
1:H:486:TYR:CZ	1:H:488:GLY:HA3	2.51	0.45
1:H:645:ARG:NH2	1:H:650:GLU:CD	2.74	0.45
1:H:743:SER:O	1:H:760:ARG:NH1	2.49	0.45
1:I:12:GLN:OE1	1:I:12:GLN:HA	2.17	0.45
1:I:409:VAL:CG1	1:I:410:VAL:N	2.79	0.45
1:I:743:SER:O	1:I:760:ARG:NH1	2.49	0.45
1:J:343:LEU:HD23	1:J:348:PRO:HA	1.99	0.45
1:J:655:MET:HE3	1:J:655:MET:HB2	1.60	0.45
1:J:708:TRP:CD1	1:J:708:TRP:N	2.84	0.45
1:K:757:GLN:O	1:K:757:GLN:HG2	2.12	0.45
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:L:343:LEU:HD23	1:L:348:PRO:HA	1.99	0.45
1:L:637:GLU:HA	1:L:679:LEU:CD2	2.47	0.45
1:L:668:VAL:HG13	1:L:669:PRO:CD	2.38	0.45
1:M:99:ILE:HG23	1:M:594:ASP:HB2	1.98	0.45
1:M:118:ASN:HA	1:M:119:PRO:HD2	1.60	0.45
1:M:202:MET:HE3	1:M:357:HIS:ND1	2.32	0.45
1:M:400:THR:O	1:M:404:ARG:HD2	2.16	0.45
1:N:57:GLU:HG2	1:N:83:THR:HG21	1.93	0.45
1:N:531:ARG:O	1:N:561:ARG:NH1	2.46	0.45
1:O:403:ASP:CG	1:O:451:PRO:HD2	2.41	0.45
1:P:363:HIS:CD2	1:P:363:HIS:N	2.81	0.45
1:P:645:ARG:NH2	1:P:650:GLU:CD	2.74	0.45
1:A:66:PRO:HB3	1:A:187:MET:HE2	1.98	0.45
1:A:77:ASP:O	1:A:78:LEU:HD23	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:ARG:NH2	1:B:650:GLU:CD	2.74	0.45
1:C:708:TRP:CD1	1:C:708:TRP:N	2.84	0.45
1:C:730:LEU:HA	1:C:731:PRO:HD3	1.74	0.45
1:C:745:MET:HE2	1:C:745:MET:N	2.31	0.45
1:D:13:ARG:O	1:D:14:ARG:HB2	2.16	0.45
1:D:254:LEU:HA	1:D:254:LEU:HD23	1.62	0.45
1:D:825:CYS:HA	1:D:837:THR:O	2.17	0.45
1:D:927:THR:HA	1:D:928:PRO:HD3	1.62	0.45
1:E:202:MET:HE3	1:E:357:HIS:ND1	2.32	0.45
1:E:343:LEU:HD23	1:E:348:PRO:HA	1.99	0.45
1:E:512:PHE:CE1	1:E:517:LYS:HG3	2.51	0.45
1:F:66:PRO:HB3	1:F:187:MET:HE2	1.98	0.45
1:F:646:HIS:O	1:F:648:ASP:N	2.47	0.45
1:G:129:VAL:CG2	1:G:182:ASN:ND2	2.77	0.45
1:G:202:MET:HE3	1:G:357:HIS:ND1	2.32	0.45
1:H:12:GLN:OE1	1:H:12:GLN:HA	2.17	0.45
1:H:429:ASP:HA	1:H:430:PRO:HD3	1.51	0.45
1:I:512:PHE:CE1	1:I:517:LYS:HG3	2.51	0.45
1:J:637:GLU:HA	1:J:679:LEU:CD2	2.47	0.45
1:K:246:MET:HE3	1:K:247:CYS:C	2.41	0.45
1:K:822:LEU:HD12	1:K:822:LEU:C	2.37	0.45
1:L:12:GLN:OE1	1:L:12:GLN:HA	2.17	0.45
1:L:757:GLN:O	1:L:757:GLN:HG2	2.12	0.45
1:M:12:GLN:OE1	1:M:12:GLN:HA	2.17	0.45
1:M:377:LEU:HD22	1:M:708:TRP:CA	2.44	0.45
1:N:13:ARG:O	1:N:14:ARG:HB2	2.16	0.45
1:N:147:ASN:HA	1:N:148:SER:HA	1.55	0.45
1:N:202:MET:HE3	1:N:357:HIS:ND1	2.32	0.45
1:N:246:MET:HE3	1:N:247:CYS:C	2.41	0.45
1:N:377:LEU:HD22	1:N:708:TRP:CA	2.44	0.45
1:N:409:VAL:CG1	1:N:410:VAL:N	2.79	0.45
1:N:479:ASP:HA	1:N:480:PRO:HD2	1.61	0.45
1:O:637:GLU:HA	1:O:679:LEU:CD2	2.47	0.45
1:P:254:LEU:HA	1:P:254:LEU:HD23	1.62	0.45
1:P:368:ASP:O	1:P:369:GLU:C	2.58	0.45
1:P:743:SER:OG	1:P:744:GLU:N	2.49	0.45
1:A:363:HIS:CD2	1:A:363:HIS:N	2.81	0.45
1:A:403:ASP:CG	1:A:451:PRO:HD2	2.41	0.45
1:B:67:GLU:H	1:B:67:GLU:HG2	1.30	0.45
1:B:210:ARG:HH11	1:B:395:HIS:HB2	1.81	0.45
1:C:387:VAL:CG2	1:C:388:ARG:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:740:LEU:HD13	1:C:749:ILE:HD12	1.97	0.45
1:D:65:ALA:HB1	1:D:66:PRO:CD	2.38	0.45
1:D:99:ILE:HG23	1:D:594:ASP:HB2	1.98	0.45
1:D:343:LEU:HD23	1:D:348:PRO:HA	1.99	0.45
1:D:400:THR:O	1:D:404:ARG:HD2	2.16	0.45
1:D:740:LEU:HD13	1:D:749:ILE:HD12	1.97	0.45
1:D:878:HIS:HA	1:D:879:PRO:HD3	1.66	0.45
1:E:655:MET:HE2	1:E:656:VAL:C	2.42	0.45
1:E:745:MET:HA	1:E:745:MET:CE	2.43	0.45
1:F:202:MET:HE3	1:F:357:HIS:ND1	2.32	0.45
1:G:363:HIS:N	1:G:363:HIS:CD2	2.81	0.45
1:G:368:ASP:O	1:G:369:GLU:C	2.58	0.45
1:G:387:VAL:CG2	1:G:388:ARG:N	2.80	0.45
1:G:708:TRP:CD1	1:G:708:TRP:N	2.84	0.45
1:G:1018:LEU:HD23	1:G:1018:LEU:HA	1.51	0.45
1:H:486:TYR:CE2	1:H:488:GLY:HA3	2.51	0.45
1:H:654:TRP:O	1:H:655:MET:HB3	2.15	0.45
1:H:670:LEU:HA	1:H:670:LEU:HD23	1.67	0.45
1:H:708:TRP:CD1	1:H:708:TRP:N	2.84	0.45
1:I:24:LEU:HD12	1:I:24:LEU:HA	1.62	0.45
1:I:745:MET:HE2	1:I:745:MET:N	2.31	0.45
1:J:210:ARG:HH11	1:J:395:HIS:HB2	1.81	0.45
1:K:13:ARG:O	1:K:14:ARG:HB2	2.16	0.45
1:K:66:PRO:HB3	1:K:187:MET:HE2	1.98	0.45
1:K:645:ARG:NH2	1:K:650:GLU:CD	2.74	0.45
1:L:67:GLU:H	1:L:67:GLU:HG2	1.31	0.45
1:L:272:ALA:HB1	1:L:273:PRO:CD	2.47	0.45
1:M:173:LEU:HD23	1:M:173:LEU:HA	1.69	0.45
1:M:343:LEU:HD23	1:M:348:PRO:HA	1.99	0.45
1:M:637:GLU:HA	1:M:679:LEU:CD2	2.47	0.45
1:M:869:ASP:CG	1:M:1015:HIS:HD1	2.24	0.45
1:O:4:THR:CA	1:O:9:VAL:HG11	2.47	0.45
1:O:129:VAL:CG2	1:O:182:ASN:ND2	2.77	0.45
1:O:702:GLN:O	1:O:712:GLY:N	2.45	0.45
1:O:708:TRP:CD1	1:O:708:TRP:N	2.84	0.45
1:P:79:PRO:HD2	1:P:80:GLU:OE2	2.17	0.45
1:P:429:ASP:HA	1:P:430:PRO:HD3	1.51	0.45
1:P:702:GLN:HA	1:P:703:PRO:HD2	1.84	0.45
1:A:6:SER:O	1:A:7:LEU:C	2.60	0.45
1:A:131:GLU:O	1:A:132:SER:C	2.60	0.45
1:A:234:ASP:O	1:A:235:PHE:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:VAL:CG1	1:A:808:GLU:N	2.79	0.45
1:B:4:THR:CA	1:B:9:VAL:HG11	2.47	0.45
1:B:70:PRO:O	1:B:73:TRP:N	2.45	0.45
1:B:202:MET:HE3	1:B:357:HIS:ND1	2.32	0.45
1:B:234:ASP:O	1:B:235:PHE:HB2	2.17	0.45
1:B:479:ASP:HA	1:B:480:PRO:HD2	1.61	0.45
1:C:343:LEU:HD23	1:C:348:PRO:HA	1.99	0.45
1:D:645:ARG:NH2	1:D:650:GLU:CD	2.74	0.45
1:E:99:ILE:HG23	1:E:594:ASP:HB2	1.98	0.45
1:E:210:ARG:HH11	1:E:395:HIS:HB2	1.82	0.45
1:E:234:ASP:O	1:E:235:PHE:HB2	2.17	0.45
1:E:722:LEU:HD23	1:E:722:LEU:HA	1.75	0.45
1:E:743:SER:OG	1:E:744:GLU:N	2.49	0.45
1:F:246:MET:HE3	1:F:247:CYS:C	2.41	0.45
1:F:403:ASP:CG	1:F:451:PRO:HD2	2.41	0.45
1:F:878:HIS:HA	1:F:879:PRO:HD3	1.66	0.45
1:G:479:ASP:HA	1:G:480:PRO:HD2	1.61	0.45
1:G:637:GLU:HA	1:G:679:LEU:CD2	2.47	0.45
1:H:210:ARG:HH11	1:H:395:HIS:HB2	1.81	0.45
1:I:49:GLN:H	1:I:49:GLN:HE21	1.59	0.45
1:I:131:GLU:HA	1:I:134:LEU:HB2	1.99	0.45
1:I:395:HIS:HA	1:I:396:PRO:HD3	1.48	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:J:387:VAL:CG2	1:J:388:ARG:N	2.80	0.45
1:J:745:MET:HE2	1:J:745:MET:N	2.31	0.45
1:J:894:ARG:HH12	1:J:920:LEU:HA	1.81	0.45
1:K:12:GLN:OE1	1:K:12:GLN:HA	2.17	0.45
1:K:202:MET:HE3	1:K:357:HIS:ND1	2.32	0.45
1:K:272:ALA:HA	1:K:273:PRO:HD3	1.76	0.45
1:K:576:ILE:CG2	1:K:577:LYS:N	2.78	0.45
1:L:79:PRO:HD2	1:L:80:GLU:OE2	2.17	0.45
1:L:347:LYS:HA	1:L:348:PRO:HD3	1.77	0.45
1:L:655:MET:HE2	1:L:656:VAL:C	2.42	0.45
1:L:825:CYS:HA	1:L:837:THR:O	2.17	0.45
1:L:878:HIS:HA	1:L:879:PRO:HD3	1.66	0.45
1:M:251:ARG:CB	1:M:253:TYR:CE2	2.98	0.45
1:M:599:ARG:HB2	1:M:600:GLN:H	1.41	0.45
1:M:807:VAL:CG1	1:M:808:GLU:N	2.80	0.45
1:N:66:PRO:HB3	1:N:187:MET:HE2	1.98	0.45
1:N:79:PRO:HD2	1:N:80:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:646:HIS:O	1:N:648:ASP:N	2.47	0.45
1:O:272:ALA:HB1	1:O:273:PRO:CD	2.47	0.45
1:O:363:HIS:N	1:O:363:HIS:CD2	2.81	0.45
1:O:409:VAL:CG1	1:O:410:VAL:N	2.79	0.45
1:P:6:SER:O	1:P:7:LEU:C	2.60	0.45
1:P:12:GLN:OE1	1:P:12:GLN:HA	2.17	0.45
1:A:4:THR:CA	1:A:9:VAL:HG11	2.47	0.45
1:A:202:MET:HE3	1:A:357:HIS:ND1	2.32	0.45
1:A:251:ARG:CB	1:A:253:TYR:CE2	2.98	0.45
1:A:655:MET:HE2	1:A:656:VAL:C	2.42	0.45
1:A:781:ARG:CG	1:A:781:ARG:NH1	2.79	0.45
1:B:512:PHE:CE1	1:B:517:LYS:HG3	2.51	0.45
1:B:743:SER:OG	1:B:744:GLU:N	2.49	0.45
1:C:260:LEU:C	1:C:267:VAL:HG23	2.40	0.45
1:C:272:ALA:HB1	1:C:273:PRO:CD	2.47	0.45
1:C:655:MET:HE2	1:C:656:VAL:C	2.42	0.45
1:D:234:ASP:O	1:D:235:PHE:HB2	2.17	0.45
1:D:260:LEU:HD12	1:D:260:LEU:HA	1.61	0.45
1:D:272:ALA:HB1	1:D:273:PRO:CD	2.47	0.45
1:D:387:VAL:CG2	1:D:388:ARG:N	2.80	0.45
1:E:12:GLN:OE1	1:E:12:GLN:HA	2.17	0.45
1:E:65:ALA:HB1	1:E:66:PRO:CD	2.38	0.45
1:E:79:PRO:HD2	1:E:80:GLU:OE2	2.16	0.45
1:E:403:ASP:CG	1:E:451:PRO:HD2	2.42	0.45
1:F:823:LEU:HD23	1:F:823:LEU:HA	1.73	0.45
1:G:49:GLN:H	1:G:49:GLN:CD	2.20	0.45
1:G:645:ARG:NH2	1:G:650:GLU:OE2	2.48	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:740:LEU:CD1	1:I:741:THR:H	2.12	0.45
1:I:878:HIS:HA	1:I:879:PRO:HD3	1.66	0.45
1:J:583:ASN:HA	1:J:584:PRO:HD3	1.79	0.45
1:K:37:ARG:CG	1:K:37:ARG:NH1	2.79	0.45
1:L:272:ALA:HA	1:L:273:PRO:HD3	1.77	0.45
1:L:368:ASP:O	1:L:369:GLU:C	2.58	0.45
1:M:403:ASP:CG	1:M:451:PRO:HD2	2.41	0.45
1:N:234:ASP:O	1:N:235:PHE:HB2	2.17	0.45
1:N:272:ALA:HB1	1:N:273:PRO:CD	2.47	0.45
1:N:682:LEU:HA	1:N:682:LEU:HD23	1.67	0.45
1:N:702:GLN:O	1:N:712:GLY:N	2.45	0.45
1:O:202:MET:HE3	1:O:357:HIS:ND1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:227:VAL:CG1	1:P:240:LEU:HD11	2.42	0.45
1:P:654:TRP:O	1:P:655:MET:HB3	2.15	0.45
1:P:722:LEU:HD23	1:P:722:LEU:HA	1.75	0.45
1:P:822:LEU:HD12	1:P:823:LEU:H	1.81	0.45
1:P:900:LEU:HD23	1:P:900:LEU:HA	1.75	0.45
1:A:571:VAL:HG13	1:A:607:VAL:HG23	1.99	0.44
1:A:608:PHE:O	1:A:611:ARG:N	2.41	0.44
1:A:781:ARG:HG3	1:A:781:ARG:NH1	2.17	0.44
1:B:49:GLN:H	1:B:49:GLN:CD	2.20	0.44
1:B:73:TRP:O	1:B:183:ARG:NH1	2.48	0.44
1:B:663:LEU:HD23	1:B:663:LEU:N	2.24	0.44
1:B:822:LEU:HD12	1:B:823:LEU:H	1.80	0.44
1:D:571:VAL:HG13	1:D:607:VAL:HG23	1.99	0.44
1:D:608:PHE:O	1:D:611:ARG:N	2.41	0.44
1:D:637:GLU:HA	1:D:679:LEU:CD2	2.47	0.44
1:D:668:VAL:HG13	1:D:669:PRO:CD	2.38	0.44
1:E:576:ILE:CG2	1:E:577:LYS:N	2.78	0.44
1:E:757:GLN:O	1:E:757:GLN:HG2	2.12	0.44
1:F:894:ARG:HH12	1:F:920:LEU:HA	1.81	0.44
1:G:409:VAL:CG1	1:G:410:VAL:N	2.79	0.44
1:H:254:LEU:HA	1:H:254:LEU:HD23	1.62	0.44
1:H:387:VAL:CG2	1:H:388:ARG:N	2.80	0.44
1:H:571:VAL:HG13	1:H:607:VAL:HG23	1.99	0.44
1:H:722:LEU:HD23	1:H:722:LEU:HA	1.75	0.44
1:I:1018:LEU:HD23	1:I:1018:LEU:HA	1.51	0.44
1:I:1021:CME:HB3	1:I:1021:CME:HE2	1.41	0.44
1:J:4:THR:CA	1:J:9:VAL:HG11	2.47	0.44
1:J:395:HIS:HA	1:J:396:PRO:HD3	1.48	0.44
1:J:655:MET:HE2	1:J:656:VAL:C	2.42	0.44
1:K:343:LEU:HD23	1:K:348:PRO:HA	1.99	0.44
1:L:173:LEU:HD23	1:L:173:LEU:HA	1.69	0.44
1:L:708:TRP:CD1	1:L:708:TRP:N	2.84	0.44
1:M:78:LEU:HB3	1:M:79:PRO:CD	2.45	0.44
1:M:234:ASP:O	1:M:235:PHE:HB2	2.17	0.44
1:M:409:VAL:CG1	1:M:410:VAL:N	2.79	0.44
1:M:655:MET:HE2	1:M:656:VAL:C	2.42	0.44
1:N:260:LEU:C	1:N:267:VAL:HG23	2.40	0.44
1:N:403:ASP:CG	1:N:451:PRO:HD2	2.42	0.44
1:O:387:VAL:CG2	1:O:388:ARG:N	2.80	0.44
1:O:645:ARG:NH2	1:O:650:GLU:OE2	2.48	0.44
1:P:240:LEU:HD12	1:P:240:LEU:C	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:373:VAL:O	1:P:374:GLN:C	2.57	0.44
1:P:571:VAL:HG13	1:P:607:VAL:HG23	1.99	0.44
1:A:78:LEU:HB3	1:A:79:PRO:CD	2.45	0.44
1:A:343:LEU:HD23	1:A:348:PRO:HA	1.99	0.44
1:A:658:LEU:O	1:A:659:ASP:C	2.58	0.44
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.99	0.44
1:A:708:TRP:CD1	1:A:708:TRP:N	2.84	0.44
1:B:24:LEU:HD12	1:B:24:LEU:HA	1.62	0.44
1:B:34:ALA:HB3	1:B:36:TRP:CZ3	2.53	0.44
1:B:343:LEU:HD23	1:B:348:PRO:HA	1.99	0.44
1:B:647:SER:OG	1:B:672:VAL:N	2.35	0.44
1:B:685:LEU:HB3	1:B:686:PRO:HD2	1.99	0.44
1:B:722:LEU:HA	1:B:722:LEU:HD23	1.75	0.44
1:B:749:ILE:N	1:B:749:ILE:CD1	2.78	0.44
1:B:781:ARG:O	1:B:884:LEU:HA	2.16	0.44
1:C:512:PHE:CE1	1:C:517:LYS:HG3	2.51	0.44
1:D:12:GLN:OE1	1:D:12:GLN:HA	2.17	0.44
1:D:63:PHE:CB	1:D:64:PRO:HD2	2.32	0.44
1:D:131:GLU:HA	1:D:134:LEU:HB2	1.99	0.44
1:D:512:PHE:CE1	1:D:517:LYS:HG3	2.51	0.44
1:E:63:PHE:CB	1:E:64:PRO:HD2	2.32	0.44
1:E:251:ARG:CB	1:E:253:TYR:CE2	2.98	0.44
1:F:343:LEU:HD23	1:F:348:PRO:HA	1.99	0.44
1:F:344:LEU:N	1:F:347:LYS:O	2.36	0.44
1:G:78:LEU:HB3	1:G:79:PRO:CD	2.45	0.44
1:G:254:LEU:HA	1:G:254:LEU:HD23	1.62	0.44
1:G:679:LEU:HA	1:G:679:LEU:HD23	1.26	0.44
1:H:131:GLU:O	1:H:132:SER:C	2.60	0.44
1:I:99:ILE:HG23	1:I:594:ASP:HB2	1.98	0.44
1:I:287:ASP:OD1	1:I:287:ASP:N	2.29	0.44
1:I:743:SER:OG	1:I:744:GLU:N	2.49	0.44
1:J:13:ARG:O	1:J:14:ARG:HB2	2.16	0.44
1:J:685:LEU:HA	1:J:686:PRO:HD3	1.70	0.44
1:J:701:VAL:CG1	1:J:702:GLN:N	2.81	0.44
1:J:869:ASP:CG	1:J:1015:HIS:HD1	2.24	0.44
1:K:79:PRO:HD2	1:K:80:GLU:OE2	2.17	0.44
1:K:272:ALA:HB1	1:K:273:PRO:CD	2.47	0.44
1:K:387:VAL:CG2	1:K:388:ARG:N	2.80	0.44
1:K:571:VAL:HG13	1:K:607:VAL:HG23	1.99	0.44
1:K:701:VAL:HG12	1:K:702:GLN:H	1.83	0.44
1:L:4:THR:CA	1:L:9:VAL:HG11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:100:TYR:HB2	1:L:203:TRP:CE3	2.51	0.44
1:L:807:VAL:CG1	1:L:808:GLU:N	2.79	0.44
1:L:1018:LEU:HD23	1:L:1018:LEU:HA	1.51	0.44
1:M:34:ALA:HB3	1:M:36:TRP:CZ3	2.53	0.44
1:M:131:GLU:HA	1:M:134:LEU:HB2	2.00	0.44
1:M:254:LEU:HA	1:M:254:LEU:HD23	1.62	0.44
1:M:479:ASP:HA	1:M:480:PRO:HD2	1.61	0.44
1:M:894:ARG:HH12	1:M:920:LEU:HA	1.81	0.44
1:N:4:THR:CA	1:N:9:VAL:HG11	2.47	0.44
1:N:118:ASN:HA	1:N:119:PRO:HD2	1.60	0.44
1:N:230:ARG:NH2	1:N:241:GLU:OE2	2.51	0.44
1:N:260:LEU:HA	1:N:260:LEU:HD12	1.61	0.44
1:N:343:LEU:HD23	1:N:348:PRO:HA	1.99	0.44
1:N:746:ASP:HA	1:N:760:ARG:CG	2.39	0.44
1:N:757:GLN:O	1:N:757:GLN:HG2	2.12	0.44
1:O:807:VAL:CG1	1:O:808:GLU:N	2.79	0.44
1:A:73:TRP:O	1:A:183:ARG:NH1	2.48	0.44
1:A:210:ARG:HH11	1:A:395:HIS:HB2	1.81	0.44
1:A:260:LEU:HA	1:A:260:LEU:HD12	1.61	0.44
1:A:743:SER:OG	1:A:744:GLU:N	2.49	0.44
1:A:894:ARG:HH12	1:A:920:LEU:HA	1.81	0.44
1:C:576:ILE:CG2	1:C:577:LYS:N	2.78	0.44
1:C:637:GLU:HA	1:C:679:LEU:CD2	2.47	0.44
1:D:79:PRO:HD2	1:D:80:GLU:OE2	2.17	0.44
1:D:702:GLN:O	1:D:712:GLY:N	2.45	0.44
1:E:131:GLU:HA	1:E:134:LEU:HB2	2.00	0.44
1:E:387:VAL:CG2	1:E:388:ARG:N	2.80	0.44
1:E:702:GLN:O	1:E:712:GLY:N	2.45	0.44
1:F:12:GLN:OE1	1:F:12:GLN:HA	2.17	0.44
1:F:131:GLU:O	1:F:132:SER:C	2.60	0.44
1:F:255:ARG:NH1	1:F:255:ARG:CG	2.79	0.44
1:F:746:ASP:HA	1:F:760:ARG:CG	2.39	0.44
1:F:807:VAL:CG1	1:F:808:GLU:N	2.79	0.44
1:F:906:TYR:OH	1:F:934:GLU:OE2	2.30	0.44
1:G:4:THR:CA	1:G:9:VAL:HG11	2.47	0.44
1:G:12:GLN:HA	1:G:12:GLN:OE1	2.17	0.44
1:G:69:VAL:HA	1:G:70:PRO:HD2	1.77	0.44
1:G:807:VAL:CG1	1:G:808:GLU:N	2.80	0.44
1:H:3:ILE:O	1:H:6:SER:HB3	2.18	0.44
1:H:34:ALA:HB3	1:H:36:TRP:CZ3	2.53	0.44
1:H:377:LEU:HD22	1:H:708:TRP:CA	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:66:PRO:HB3	1:I:187:MET:HE2	1.98	0.44
1:I:772:ASP:OD1	1:I:772:ASP:N	2.30	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:J:240:LEU:HD12	1:J:240:LEU:C	2.36	0.44
1:K:378:LEU:HA	1:K:378:LEU:HD23	1.53	0.44
1:K:637:GLU:HA	1:K:679:LEU:CD2	2.47	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:L:685:LEU:HB3	1:L:686:PRO:HD2	1.99	0.44
1:L:743:SER:OG	1:L:744:GLU:N	2.49	0.44
1:N:12:GLN:OE1	1:N:12:GLN:HA	2.17	0.44
1:N:645:ARG:NH2	1:N:650:GLU:CD	2.74	0.44
1:N:670:LEU:HA	1:N:670:LEU:HD23	1.67	0.44
1:N:856:TYR:CD2	1:N:864:MET:CE	2.97	0.44
1:O:3:ILE:O	1:O:6:SER:HB3	2.18	0.44
1:O:6:SER:O	1:O:7:LEU:C	2.60	0.44
1:O:347:LYS:CB	1:O:348:PRO:HD2	2.43	0.44
1:O:825:CYS:HA	1:O:837:THR:O	2.17	0.44
1:O:875:ASP:OD2	1:O:875:ASP:N	2.47	0.44
1:P:260:LEU:C	1:P:267:VAL:HG23	2.40	0.44
1:P:486:TYR:CE2	1:P:488:GLY:HA3	2.51	0.44
1:P:645:ARG:NH2	1:P:650:GLU:OE2	2.48	0.44
1:P:730:LEU:HA	1:P:731:PRO:HD3	1.74	0.44
1:B:12:GLN:OE1	1:B:12:GLN:HA	2.17	0.44
1:B:463:GLY:O	1:B:486:TYR:OH	2.32	0.44
1:B:655:MET:HE2	1:B:656:VAL:C	2.42	0.44
1:D:403:ASP:CG	1:D:451:PRO:HD2	2.42	0.44
1:E:6:SER:O	1:E:7:LEU:C	2.60	0.44
1:E:164:ASP:OD2	1:E:167:LEU:HD12	2.18	0.44
1:E:173:LEU:HD23	1:E:173:LEU:HA	1.69	0.44
1:F:13:ARG:O	1:F:14:ARG:HB2	2.16	0.44
1:F:264:GLU:OE2	1:F:264:GLU:HA	2.17	0.44
1:F:701:VAL:CG1	1:F:702:GLN:N	2.81	0.44
1:G:24:LEU:HD12	1:G:24:LEU:HA	1.62	0.44
1:G:164:ASP:OD2	1:G:167:LEU:HD12	2.18	0.44
1:G:655:MET:HE2	1:G:656:VAL:C	2.42	0.44
1:G:743:SER:OG	1:G:744:GLU:N	2.49	0.44
1:H:164:ASP:OD2	1:H:167:LEU:HD12	2.18	0.44
1:H:655:MET:HE2	1:H:656:VAL:C	2.42	0.44
1:H:702:GLN:HA	1:H:703:PRO:HD2	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:78:LEU:HB3	1:I:79:PRO:CD	2.45	0.44
1:I:571:VAL:HG13	1:I:607:VAL:HG23	1.99	0.44
1:I:658:LEU:HD12	1:I:693:GLN:O	2.18	0.44
1:I:701:VAL:HG12	1:I:702:GLN:H	1.83	0.44
1:J:3:ILE:O	1:J:6:SER:HB3	2.18	0.44
1:K:131:GLU:HA	1:K:134:LEU:HB2	1.99	0.44
1:K:749:ILE:N	1:K:749:ILE:CD1	2.78	0.44
1:L:230:ARG:NH2	1:L:241:GLU:OE2	2.51	0.44
1:N:637:GLU:HA	1:N:679:LEU:CD2	2.47	0.44
1:N:743:SER:OG	1:N:744:GLU:N	2.49	0.44
1:N:825:CYS:HA	1:N:837:THR:O	2.17	0.44
1:N:878:HIS:HA	1:N:879:PRO:HD3	1.66	0.44
1:O:12:GLN:HA	1:O:12:GLN:OE1	2.17	0.44
1:O:576:ILE:CG2	1:O:577:LYS:N	2.78	0.44
1:O:788:PRO:O	1:O:933:SER:HB2	2.18	0.44
1:P:343:LEU:HD23	1:P:348:PRO:HA	1.99	0.44
1:P:378:LEU:HD23	1:P:378:LEU:HA	1.53	0.44
1:P:847:LYS:HZ3	1:P:875:ASP:CG	2.26	0.44
1:A:34:ALA:HB3	1:A:36:TRP:CZ3	2.53	0.44
1:A:79:PRO:HD2	1:A:80:GLU:OE2	2.17	0.44
1:A:368:ASP:O	1:A:369:GLU:C	2.58	0.44
1:A:658:LEU:HD12	1:A:693:GLN:O	2.18	0.44
1:A:743:SER:O	1:A:760:ARG:NH1	2.49	0.44
1:B:894:ARG:HH12	1:B:920:LEU:HA	1.81	0.44
1:C:66:PRO:HB3	1:C:187:MET:HE2	1.98	0.44
1:D:3:ILE:O	1:D:6:SER:HB3	2.18	0.44
1:D:111:PRO:HA	1:D:112:PRO:HA	1.57	0.44
1:D:210:ARG:HH11	1:D:395:HIS:HB2	1.82	0.44
1:E:189:LEU:N	1:E:189:LEU:CD2	2.75	0.44
1:F:34:ALA:HB3	1:F:36:TRP:CZ3	2.53	0.44
1:F:50:GLN:HB3	1:F:216:HIS:HB3	2.00	0.44
1:F:111:PRO:HA	1:F:112:PRO:HA	1.57	0.44
1:F:409:VAL:CG1	1:F:410:VAL:N	2.79	0.44
1:G:788:PRO:O	1:G:933:SER:HB2	2.18	0.44
1:H:43:ARG:NH1	1:H:44:THR:CG2	2.81	0.44
1:H:343:LEU:HD23	1:H:348:PRO:HA	1.99	0.44
1:H:749:ILE:N	1:H:749:ILE:CD1	2.78	0.44
1:I:343:LEU:HD23	1:I:348:PRO:HA	1.99	0.44
1:I:655:MET:HE2	1:I:656:VAL:C	2.42	0.44
1:J:419:GLY:HA2	1:K:282:ARG:NH1	2.33	0.44
1:K:230:ARG:NH2	1:K:241:GLU:OE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:486:TYR:CE2	1:K:488:GLY:HA3	2.51	0.44
1:K:655:MET:HE2	1:K:656:VAL:C	2.42	0.44
1:L:3:ILE:O	1:L:6:SER:HB3	2.18	0.44
1:L:34:ALA:HB3	1:L:36:TRP:CZ3	2.53	0.44
1:L:344:LEU:N	1:L:347:LYS:O	2.36	0.44
1:L:658:LEU:HD12	1:L:693:GLN:O	2.18	0.44
1:M:3:ILE:O	1:M:6:SER:HB3	2.18	0.44
1:M:701:VAL:CG1	1:M:702:GLN:N	2.81	0.44
1:N:131:GLU:O	1:N:132:SER:C	2.60	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:O:260:LEU:C	1:O:267:VAL:HG23	2.40	0.44
1:O:743:SER:OG	1:O:744:GLU:N	2.49	0.44
1:A:131:GLU:HA	1:A:134:LEU:HB2	2.00	0.44
1:A:647:SER:OG	1:A:672:VAL:N	2.35	0.44
1:C:673:ALA:O	1:C:676:GLY:N	2.47	0.44
1:C:757:GLN:O	1:C:757:GLN:HG2	2.12	0.44
1:C:825:CYS:HA	1:C:837:THR:O	2.17	0.44
1:E:70:PRO:O	1:E:73:TRP:N	2.45	0.44
1:F:234:ASP:O	1:F:235:PHE:HB2	2.17	0.44
1:F:637:GLU:HA	1:F:679:LEU:CD2	2.47	0.44
1:G:50:GLN:HB3	1:G:216:HIS:HB3	2.00	0.44
1:G:73:TRP:O	1:G:183:ARG:NH1	2.48	0.44
1:G:234:ASP:O	1:G:235:PHE:HB2	2.17	0.44
1:G:251:ARG:CB	1:G:253:TYR:CE2	2.98	0.44
1:H:272:ALA:HB1	1:H:273:PRO:CD	2.47	0.44
1:H:637:GLU:HA	1:H:679:LEU:CD2	2.47	0.44
1:H:658:LEU:HD12	1:H:693:GLN:O	2.18	0.44
1:H:682:LEU:HA	1:H:682:LEU:HD23	1.67	0.44
1:I:234:ASP:O	1:I:235:PHE:HB2	2.17	0.44
1:I:287:ASP:CG	1:L:425:ARG:NH2	2.76	0.44
1:I:730:LEU:HA	1:I:731:PRO:HD3	1.74	0.44
1:J:12:GLN:OE1	1:J:12:GLN:HA	2.17	0.44
1:J:234:ASP:O	1:J:235:PHE:HB2	2.17	0.44
1:J:825:CYS:HA	1:J:837:THR:O	2.17	0.44
1:J:894:ARG:NH1	1:J:920:LEU:CA	2.81	0.44
1:K:788:PRO:O	1:K:933:SER:HB2	2.18	0.44
1:L:43:ARG:NH1	1:L:44:THR:CG2	2.81	0.44
1:L:66:PRO:HB3	1:L:187:MET:HE2	1.98	0.44
1:L:781:ARG:NH1	1:L:781:ARG:CG	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:894:ARG:NH1	1:L:920:LEU:CA	2.81	0.44
1:M:4:THR:CA	1:M:9:VAL:HG11	2.47	0.44
1:M:429:ASP:HA	1:M:430:PRO:HD3	1.51	0.44
1:M:658:LEU:HD12	1:M:693:GLN:O	2.18	0.44
1:N:164:ASP:OD2	1:N:167:LEU:HD12	2.18	0.44
1:N:264:GLU:OE2	1:N:264:GLU:HA	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:251:ARG:CB	1:O:253:TYR:CE2	2.98	0.44
1:O:655:MET:HE2	1:O:656:VAL:C	2.42	0.44
1:P:164:ASP:OD2	1:P:167:LEU:HD12	2.18	0.44
1:P:272:ALA:HB1	1:P:273:PRO:CD	2.47	0.44
1:P:658:LEU:O	1:P:659:ASP:C	2.58	0.44
1:A:637:GLU:HA	1:A:679:LEU:CD2	2.47	0.44
1:A:749:ILE:N	1:A:749:ILE:CD1	2.78	0.44
1:A:972:HIS:HB3	5:A:2155:HOH:O	2.18	0.44
1:B:43:ARG:NH1	1:B:44:THR:CG2	2.81	0.44
1:B:164:ASP:OD2	1:B:167:LEU:HD12	2.18	0.44
1:B:409:VAL:CG1	1:B:410:VAL:N	2.79	0.44
1:C:49:GLN:H	1:C:49:GLN:CD	2.20	0.44
1:C:533:LEU:HD12	1:C:534:ILE:N	2.33	0.44
1:C:645:ARG:NH2	1:C:650:GLU:OE2	2.48	0.44
1:C:749:ILE:N	1:C:749:ILE:CD1	2.78	0.44
1:C:874:SER:HB3	1:D:724:GLU:OE1	2.18	0.44
1:C:961:ARG:NH2	1:C:979:GLU:O	2.38	0.44
1:D:66:PRO:HB3	1:D:187:MET:HE2	1.98	0.44
1:D:701:VAL:CG1	1:D:702:GLN:N	2.81	0.44
1:E:3:ILE:O	1:E:6:SER:HB3	2.18	0.44
1:E:272:ALA:HB1	1:E:273:PRO:CD	2.47	0.44
1:E:473:ARG:HD2	1:H:469:ASP:HB3	1.99	0.44
1:E:972:HIS:HB3	5:E:2155:HOH:O	2.18	0.44
1:F:360:HIS:HA	1:F:361:PRO:HD3	1.86	0.44
1:F:571:VAL:HG13	1:F:607:VAL:HG23	1.99	0.44
1:F:655:MET:HE2	1:F:656:VAL:C	2.42	0.44
1:F:856:TYR:CD2	1:F:864:MET:CE	2.97	0.44
1:H:685:LEU:HB3	1:H:686:PRO:HD2	1.99	0.44
1:I:131:GLU:O	1:I:132:SER:C	2.60	0.44
1:I:825:CYS:HA	1:I:837:THR:O	2.17	0.44
1:M:43:ARG:NH1	1:M:44:THR:CG2	2.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:419:GLY:CA	1:P:282:ARG:HH11	2.30	0.44
1:N:50:GLN:HB3	1:N:216:HIS:HB3	2.00	0.44
1:N:655:MET:HE2	1:N:656:VAL:C	2.42	0.44
1:N:788:PRO:O	1:N:933:SER:HB2	2.18	0.44
1:O:234:ASP:O	1:O:235:PHE:HB2	2.17	0.44
1:O:254:LEU:HA	1:O:254:LEU:HD23	1.62	0.44
1:O:730:LEU:HA	1:O:731:PRO:HD3	1.74	0.44
1:P:637:GLU:HA	1:P:679:LEU:CD2	2.47	0.44
1:P:869:ASP:CG	1:P:1015:HIS:HD1	2.24	0.44
1:A:164:ASP:OD2	1:A:167:LEU:HD12	2.18	0.44
1:A:429:ASP:OD1	1:A:431:ARG:HD3	2.18	0.44
1:A:559:TYR:HA	1:A:560:PRO:HD2	1.73	0.44
1:A:702:GLN:O	1:A:712:GLY:N	2.45	0.44
1:B:344:LEU:N	1:B:347:LYS:O	2.36	0.44
1:B:533:LEU:HD12	1:B:534:ILE:N	2.33	0.44
1:B:658:LEU:HD12	1:B:693:GLN:O	2.18	0.44
1:B:788:PRO:O	1:B:933:SER:HB2	2.18	0.44
1:B:900:LEU:HA	1:B:900:LEU:HD23	1.75	0.44
1:C:78:LEU:HB3	1:C:79:PRO:CD	2.45	0.44
1:C:391:HIS:ND1	1:C:412:GLU:OE1	2.44	0.44
1:D:129:VAL:CG2	1:D:182:ASN:ND2	2.77	0.44
1:D:164:ASP:OD2	1:D:167:LEU:HD12	2.18	0.44
1:E:57:GLU:HG2	1:E:83:THR:HG21	1.94	0.44
1:E:645:ARG:NH2	1:E:650:GLU:CD	2.74	0.44
1:F:43:ARG:NH1	1:F:44:THR:CG2	2.81	0.44
1:F:387:VAL:CG2	1:F:388:ARG:N	2.80	0.44
1:F:429:ASP:OD1	1:F:431:ARG:HD3	2.18	0.44
1:F:788:PRO:O	1:F:933:SER:HB2	2.18	0.44
1:G:43:ARG:NH1	1:G:44:THR:CG2	2.81	0.44
1:G:372:MET:HE1	1:G:395:HIS:HB3	2.00	0.44
1:G:533:LEU:HD12	1:G:534:ILE:N	2.33	0.44
1:G:583:ASN:HA	1:G:584:PRO:HD3	1.79	0.44
1:H:227:VAL:CG1	1:H:240:LEU:HD11	2.42	0.44
1:H:234:ASP:O	1:H:235:PHE:HB2	2.17	0.44
1:H:576:ILE:CG2	1:H:577:LYS:N	2.78	0.44
1:H:825:CYS:HA	1:H:837:THR:O	2.17	0.44
1:I:111:PRO:HA	1:I:112:PRO:HA	1.57	0.44
1:I:202:MET:HE3	1:I:357:HIS:ND1	2.32	0.44
1:I:894:ARG:HH12	1:I:920:LEU:HA	1.81	0.44
1:J:70:PRO:O	1:J:73:TRP:N	2.45	0.44
1:J:406:GLY:O	1:J:407:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:822:LEU:HD12	1:J:823:LEU:H	1.80	0.44
1:K:78:LEU:CB	1:K:79:PRO:HD2	2.44	0.44
1:K:111:PRO:HA	1:K:112:PRO:HA	1.57	0.44
1:K:406:GLY:O	1:K:407:LEU:HD23	2.18	0.44
1:K:673:ALA:O	1:K:676:GLY:N	2.47	0.44
1:K:894:ARG:NH1	1:K:920:LEU:CA	2.81	0.44
1:L:202:MET:HE3	1:L:357:HIS:ND1	2.32	0.44
1:L:403:ASP:CG	1:L:451:PRO:HD2	2.42	0.44
1:L:406:GLY:O	1:L:407:LEU:HD23	2.18	0.44
1:L:645:ARG:NH2	1:L:650:GLU:OE2	2.48	0.44
1:M:50:GLN:HB3	1:M:216:HIS:HB3	2.00	0.44
1:M:230:ARG:NH2	1:M:241:GLU:OE2	2.51	0.44
1:M:272:ALA:HB1	1:M:273:PRO:CD	2.47	0.44
1:M:387:VAL:CG2	1:M:388:ARG:N	2.80	0.44
1:N:34:ALA:HB3	1:N:36:TRP:CZ3	2.53	0.44
1:O:43:ARG:NH1	1:O:44:THR:CG2	2.81	0.44
1:O:131:GLU:O	1:O:132:SER:C	2.60	0.44
1:O:164:ASP:OD2	1:O:167:LEU:HD12	2.18	0.44
1:O:173:LEU:HD23	1:O:173:LEU:HA	1.69	0.44
1:O:406:GLY:O	1:O:407:LEU:HD23	2.18	0.44
1:O:429:ASP:OD1	1:O:431:ARG:HD3	2.18	0.44
1:O:571:VAL:HG13	1:O:607:VAL:HG23	1.99	0.44
1:P:66:PRO:HB3	1:P:187:MET:HE2	1.98	0.44
1:P:287:ASP:OD1	1:P:287:ASP:N	2.29	0.44
1:P:658:LEU:HD12	1:P:693:GLN:O	2.18	0.44
1:A:43:ARG:NH1	1:A:44:THR:CG2	2.81	0.44
1:A:463:GLY:O	1:A:486:TYR:OH	2.32	0.44
1:A:533:LEU:HD12	1:A:534:ILE:N	2.33	0.44
1:A:701:VAL:CG1	1:A:702:GLN:N	2.81	0.44
1:A:878:HIS:HA	1:A:879:PRO:HD3	1.66	0.44
1:B:1021:CME:HB3	1:B:1021:CME:HE2	1.41	0.44
1:C:6:SER:O	1:C:7:LEU:C	2.60	0.44
1:C:43:ARG:NH1	1:C:44:THR:CG2	2.81	0.44
1:C:202:MET:HE3	1:C:357:HIS:ND1	2.32	0.44
1:C:360:HIS:HA	1:C:361:PRO:HD3	1.86	0.44
1:D:202:MET:HE3	1:D:357:HIS:ND1	2.32	0.44
1:D:685:LEU:HB3	1:D:686:PRO:HD2	1.99	0.44
1:E:43:ARG:NH1	1:E:44:THR:CG2	2.81	0.44
1:E:788:PRO:O	1:E:933:SER:HB2	2.18	0.44
1:F:63:PHE:CD1	1:F:63:PHE:N	2.86	0.44
1:F:131:GLU:HA	1:F:134:LEU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:533:LEU:HD12	1:F:534:ILE:N	2.33	0.44
1:G:571:VAL:HG13	1:G:607:VAL:HG23	2.00	0.44
1:G:972:HIS:HB3	5:G:2155:HOH:O	2.18	0.44
1:H:240:LEU:HD12	1:H:240:LEU:C	2.36	0.44
1:H:373:VAL:O	1:H:374:GLN:C	2.57	0.44
1:H:869:ASP:CG	1:H:1015:HIS:HD1	2.24	0.44
1:I:387:VAL:CG2	1:I:388:ARG:N	2.80	0.44
1:I:708:TRP:CD1	1:I:708:TRP:N	2.84	0.44
1:I:894:ARG:NH1	1:I:920:LEU:CA	2.81	0.44
1:J:24:LEU:HD12	1:J:24:LEU:HA	1.62	0.44
1:J:63:PHE:CB	1:J:64:PRO:HD2	2.32	0.44
1:J:202:MET:HE3	1:J:357:HIS:ND1	2.32	0.44
1:J:372:MET:HE1	1:J:395:HIS:HB3	2.00	0.44
1:J:454:ILE:C	1:J:455:ILE:HG13	2.43	0.44
1:J:522:LYS:O	1:J:523:TRP:C	2.61	0.44
1:J:645:ARG:NH2	1:J:650:GLU:CD	2.74	0.44
1:J:781:ARG:NH1	1:J:781:ARG:CG	2.79	0.44
1:K:34:ALA:HB3	1:K:36:TRP:CZ3	2.53	0.44
1:K:658:LEU:HD12	1:K:693:GLN:O	2.18	0.44
1:K:870:VAL:CG1	1:K:871:GLU:N	2.81	0.44
1:L:234:ASP:O	1:L:235:PHE:HB2	2.17	0.44
1:L:788:PRO:O	1:L:933:SER:HB2	2.18	0.44
1:M:35:SER:O	1:M:50:GLN:HG3	2.18	0.44
1:M:372:MET:HE1	1:M:395:HIS:HB3	2.00	0.44
1:M:658:LEU:O	1:M:659:ASP:C	2.58	0.44
1:M:757:GLN:O	1:M:757:GLN:HG2	2.12	0.44
1:M:972:HIS:HB3	5:M:2155:HOH:O	2.18	0.44
1:N:35:SER:O	1:N:50:GLN:HG3	2.18	0.44
1:N:131:GLU:HA	1:N:134:LEU:HB2	1.99	0.44
1:N:254:LEU:HD23	1:N:254:LEU:HA	1.62	0.44
1:N:454:ILE:C	1:N:455:ILE:HG13	2.43	0.44
1:O:67:GLU:H	1:O:67:GLU:HG2	1.30	0.44
1:O:533:LEU:HD12	1:O:534:ILE:N	2.33	0.44
1:O:583:ASN:HA	1:O:584:PRO:HD3	1.79	0.44
1:O:701:VAL:CG1	1:O:702:GLN:N	2.81	0.44
1:O:894:ARG:NH1	1:O:920:LEU:CA	2.81	0.44
1:P:118:ASN:HA	1:P:119:PRO:HD2	1.60	0.44
1:P:272:ALA:HA	1:P:273:PRO:HD3	1.76	0.44
1:P:522:LYS:O	1:P:523:TRP:C	2.61	0.44
1:P:559:TYR:HA	1:P:560:PRO:HD2	1.73	0.44
1:P:870:VAL:CG1	1:P:871:GLU:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:894:ARG:NH1	1:P:920:LEU:CA	2.81	0.44
1:A:3:ILE:O	1:A:6:SER:HB3	2.18	0.43
1:A:57:GLU:HG2	1:A:83:THR:HG21	1.93	0.43
1:A:147:ASN:HA	1:A:148:SER:HA	1.55	0.43
1:C:234:ASP:O	1:C:235:PHE:HB2	2.17	0.43
1:C:378:LEU:HA	1:C:378:LEU:HD23	1.53	0.43
1:C:571:VAL:HG13	1:C:607:VAL:HG23	2.00	0.43
1:C:894:ARG:NH1	1:C:920:LEU:CA	2.81	0.43
1:D:409:VAL:CG1	1:D:410:VAL:N	2.79	0.43
1:E:34:ALA:HB3	1:E:36:TRP:CZ3	2.53	0.43
1:E:50:GLN:HB3	1:E:216:HIS:HB3	2.00	0.43
1:E:63:PHE:CD1	1:E:63:PHE:N	2.86	0.43
1:E:372:MET:HE1	1:E:395:HIS:HB3	2.00	0.43
1:E:406:GLY:O	1:E:407:LEU:HD23	2.18	0.43
1:F:164:ASP:OD2	1:F:167:LEU:HD12	2.18	0.43
1:F:670:LEU:HA	1:F:670:LEU:HD23	1.67	0.43
1:F:702:GLN:O	1:F:712:GLY:N	2.45	0.43
1:F:708:TRP:CD1	1:F:708:TRP:N	2.84	0.43
1:G:34:ALA:HB3	1:G:36:TRP:CZ3	2.53	0.43
1:G:63:PHE:CD1	1:G:63:PHE:N	2.86	0.43
1:G:347:LYS:CB	1:G:348:PRO:HD2	2.43	0.43
1:H:46:ARG:HB3	1:H:47:PRO:HD2	2.00	0.43
1:H:73:TRP:O	1:H:183:ARG:NH1	2.48	0.43
1:H:463:GLY:O	1:H:486:TYR:OH	2.32	0.43
1:I:685:LEU:HB3	1:I:686:PRO:HD2	1.99	0.43
1:J:34:ALA:HB3	1:J:36:TRP:CZ3	2.53	0.43
1:J:658:LEU:HD12	1:J:693:GLN:O	2.18	0.43
1:K:3:ILE:O	1:K:6:SER:HB3	2.18	0.43
1:K:164:ASP:OD2	1:K:167:LEU:HD12	2.18	0.43
1:K:234:ASP:O	1:K:235:PHE:HB2	2.17	0.43
1:L:50:GLN:HB3	1:L:216:HIS:HB3	2.00	0.43
1:L:149:ALA:O	1:L:150:PHE:HB3	2.18	0.43
1:L:260:LEU:HD12	1:L:260:LEU:HA	1.61	0.43
1:L:372:MET:HE1	1:L:395:HIS:HB3	2.00	0.43
1:L:533:LEU:HD12	1:L:534:ILE:N	2.33	0.43
1:L:661:LYS:HA	1:L:662:PRO:HD3	1.63	0.43
1:L:972:HIS:HB3	5:L:2155:HOH:O	2.18	0.43
1:M:670:LEU:HA	1:M:670:LEU:HD23	1.67	0.43
1:N:3:ILE:O	1:N:6:SER:HB3	2.18	0.43
1:N:44:THR:O	1:N:45:ASP:C	2.61	0.43
1:N:70:PRO:O	1:N:73:TRP:N	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:360:HIS:HA	1:N:361:PRO:HD3	1.86	0.43
1:N:571:VAL:HG13	1:N:607:VAL:HG23	2.00	0.43
1:O:372:MET:HE1	1:O:395:HIS:HB3	2.00	0.43
1:O:522:LYS:O	1:O:523:TRP:C	2.61	0.43
1:P:131:GLU:HA	1:P:134:LEU:HB2	2.00	0.43
1:P:200:GLN:OE1	1:P:200:GLN:N	2.44	0.43
1:P:210:ARG:HH11	1:P:395:HIS:HB2	1.82	0.43
1:P:260:LEU:HD12	1:P:260:LEU:HA	1.61	0.43
1:P:454:ILE:C	1:P:455:ILE:HG13	2.43	0.43
1:P:576:ILE:CG2	1:P:577:LYS:N	2.78	0.43
1:P:685:LEU:HB3	1:P:686:PRO:HD2	1.99	0.43
1:A:360:HIS:HA	1:A:361:PRO:HD3	1.86	0.43
1:A:757:GLN:O	1:A:757:GLN:HG2	2.12	0.43
1:A:788:PRO:O	1:A:933:SER:HB2	2.18	0.43
1:A:894:ARG:NH1	1:A:920:LEU:CA	2.81	0.43
1:B:35:SER:O	1:B:50:GLN:HG3	2.18	0.43
1:B:50:GLN:HB3	1:B:216:HIS:HB3	2.00	0.43
1:B:571:VAL:HG13	1:B:607:VAL:HG23	1.99	0.43
1:C:4:THR:CA	1:C:9:VAL:HG11	2.47	0.43
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.99	0.43
1:D:372:MET:HE1	1:D:395:HIS:HB3	2.00	0.43
1:D:406:GLY:O	1:D:407:LEU:HD23	2.18	0.43
1:D:429:ASP:OD1	1:D:431:ARG:HD3	2.18	0.43
1:D:533:LEU:HD12	1:D:534:ILE:N	2.33	0.43
1:D:894:ARG:NH1	1:D:920:LEU:CA	2.81	0.43
1:E:4:THR:CA	1:E:9:VAL:HG11	2.47	0.43
1:E:35:SER:O	1:E:50:GLN:HG3	2.18	0.43
1:E:149:ALA:O	1:E:150:PHE:HB3	2.18	0.43
1:E:658:LEU:HD12	1:E:693:GLN:O	2.18	0.43
1:E:894:ARG:NH1	1:E:920:LEU:CA	2.81	0.43
1:E:961:ARG:NH2	1:E:979:GLU:O	2.37	0.43
1:F:3:ILE:O	1:F:6:SER:HB3	2.18	0.43
1:F:718:GLN:HG3	1:F:719:GLN:N	2.34	0.43
1:F:961:ARG:NH2	1:F:979:GLU:O	2.37	0.43
1:G:230:ARG:NH2	1:G:241:GLU:OE2	2.50	0.43
1:H:35:SER:O	1:H:50:GLN:HG3	2.18	0.43
1:H:637:GLU:HA	1:H:679:LEU:HD23	2.01	0.43
1:H:647:SER:OG	1:H:672:VAL:N	2.35	0.43
1:H:894:ARG:NH1	1:H:920:LEU:CA	2.81	0.43
1:H:961:ARG:NH2	1:H:979:GLU:O	2.37	0.43
1:I:372:MET:HE1	1:I:395:HIS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:419:GLY:HA2	1:L:282:ARG:HH11	1.83	0.43
1:I:533:LEU:HD12	1:I:534:ILE:N	2.33	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:J:429:ASP:OD1	1:J:431:ARG:HD3	2.18	0.43
1:J:870:VAL:CG1	1:J:871:GLU:N	2.81	0.43
1:K:63:PHE:CD1	1:K:63:PHE:N	2.86	0.43
1:K:237:ARG:CG	1:K:237:ARG:NH1	2.82	0.43
1:K:533:LEU:HD12	1:K:534:ILE:N	2.33	0.43
1:L:63:PHE:CD1	1:L:63:PHE:N	2.86	0.43
1:L:512:PHE:CE1	1:L:517:LYS:HG3	2.51	0.43
1:M:131:GLU:O	1:M:132:SER:C	2.60	0.43
1:M:149:ALA:O	1:M:150:PHE:HB3	2.18	0.43
1:M:645:ARG:NH2	1:M:650:GLU:OE2	2.48	0.43
1:M:894:ARG:NH1	1:M:920:LEU:CA	2.81	0.43
1:N:63:PHE:CD1	1:N:63:PHE:N	2.86	0.43
1:N:378:LEU:HD23	1:N:378:LEU:HA	1.53	0.43
1:N:533:LEU:HD12	1:N:534:ILE:N	2.33	0.43
1:N:576:ILE:CG2	1:N:577:LYS:N	2.78	0.43
1:N:658:LEU:HD12	1:N:693:GLN:O	2.18	0.43
1:O:73:TRP:O	1:O:183:ARG:NH1	2.48	0.43
1:P:3:ILE:O	1:P:6:SER:HB3	2.18	0.43
1:P:46:ARG:HB3	1:P:47:PRO:HD2	2.00	0.43
1:P:63:PHE:CD1	1:P:63:PHE:N	2.86	0.43
1:P:347:LYS:CB	1:P:348:PRO:HD2	2.43	0.43
1:P:406:GLY:O	1:P:407:LEU:HD23	2.18	0.43
1:P:637:GLU:HA	1:P:679:LEU:HD23	2.01	0.43
1:A:583:ASN:HA	1:A:584:PRO:HD3	1.79	0.43
1:A:694:LEU:HD12	1:A:694:LEU:HA	1.69	0.43
1:B:44:THR:O	1:B:45:ASP:C	2.61	0.43
1:B:131:GLU:HA	1:B:134:LEU:HB2	1.99	0.43
1:B:429:ASP:OD1	1:B:431:ARG:HD3	2.18	0.43
1:C:149:ALA:O	1:C:150:PHE:HB3	2.18	0.43
1:C:164:ASP:OD2	1:C:167:LEU:HD12	2.18	0.43
1:C:372:MET:HE1	1:C:395:HIS:HB3	2.00	0.43
1:C:429:ASP:OD1	1:C:431:ARG:HD3	2.18	0.43
1:C:476:LYS:HD2	1:C:476:LYS:HA	1.81	0.43
1:C:778:THR:HB	1:C:887:GLN:CB	2.49	0.43
1:D:70:PRO:O	1:D:73:TRP:N	2.45	0.43
1:D:210:ARG:HH11	1:D:395:HIS:CA	2.32	0.43
1:D:972:HIS:HB3	5:D:2161:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:ARG:NH2	1:E:241:GLU:OE2	2.51	0.43
1:F:4:THR:CA	1:F:9:VAL:HG11	2.47	0.43
1:F:6:SER:O	1:F:7:LEU:C	2.60	0.43
1:F:230:ARG:NH2	1:F:241:GLU:OE2	2.51	0.43
1:F:237:ARG:CG	1:F:237:ARG:NH1	2.82	0.43
1:F:454:ILE:C	1:F:455:ILE:HG13	2.43	0.43
1:F:778:THR:HB	1:F:887:GLN:CB	2.48	0.43
1:F:972:HIS:HB3	5:F:2155:HOH:O	2.18	0.43
1:G:6:SER:O	1:G:7:LEU:C	2.60	0.43
1:G:406:GLY:O	1:G:407:LEU:HD23	2.18	0.43
1:G:663:LEU:HD23	1:G:663:LEU:N	2.24	0.43
1:G:722:LEU:HD23	1:G:722:LEU:HA	1.75	0.43
1:G:757:GLN:O	1:G:757:GLN:HG2	2.12	0.43
1:H:131:GLU:HA	1:H:134:LEU:HB2	2.00	0.43
1:H:375:ASP:O	1:H:379:MET:HG3	2.19	0.43
1:I:3:ILE:O	1:I:6:SER:HB3	2.18	0.43
1:I:34:ALA:HB3	1:I:36:TRP:CZ3	2.53	0.43
1:I:50:GLN:HB3	1:I:216:HIS:HB3	2.00	0.43
1:I:363:HIS:N	1:I:363:HIS:CD2	2.81	0.43
1:I:454:ILE:C	1:I:455:ILE:HG13	2.43	0.43
1:I:726:LEU:HA	1:I:726:LEU:HD23	1.66	0.43
1:K:4:THR:CA	1:K:9:VAL:HG11	2.47	0.43
1:K:35:SER:O	1:K:50:GLN:HG3	2.18	0.43
1:K:668:VAL:HG13	1:K:669:PRO:CD	2.38	0.43
1:K:694:LEU:HD12	1:K:694:LEU:HA	1.69	0.43
1:K:763:GLY:HA3	1:K:822:LEU:HD22	2.01	0.43
1:K:778:THR:HB	1:K:887:GLN:CB	2.48	0.43
1:K:961:ARG:NH2	1:K:979:GLU:O	2.37	0.43
1:L:44:THR:O	1:L:45:ASP:C	2.61	0.43
1:M:63:PHE:CD1	1:M:63:PHE:N	2.86	0.43
1:M:189:LEU:N	1:M:189:LEU:CD2	2.75	0.43
1:M:454:ILE:C	1:M:455:ILE:HG13	2.43	0.43
1:M:685:LEU:HB3	1:M:686:PRO:HD2	1.99	0.43
1:M:1018:LEU:HD23	1:M:1018:LEU:HA	1.51	0.43
1:N:237:ARG:CG	1:N:237:ARG:NH1	2.82	0.43
1:O:44:THR:O	1:O:45:ASP:C	2.61	0.43
1:O:230:ARG:NH2	1:O:241:GLU:OE2	2.51	0.43
1:O:1021:CME:HZ3	1:O:1022:GLN:O	2.19	0.43
1:A:35:SER:O	1:A:50:GLN:HG3	2.18	0.43
1:A:70:PRO:O	1:A:73:TRP:N	2.45	0.43
1:A:210:ARG:HH11	1:A:395:HIS:CA	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ARG:HH11	1:A:230:ARG:CG	2.24	0.43
1:A:230:ARG:NH2	1:A:241:GLU:OE2	2.50	0.43
1:A:272:ALA:HB1	1:A:273:PRO:CD	2.47	0.43
1:A:375:ASP:O	1:A:379:MET:HG3	2.19	0.43
1:B:131:GLU:O	1:B:132:SER:C	2.60	0.43
1:B:189:LEU:N	1:B:189:LEU:CD2	2.75	0.43
1:B:637:GLU:HA	1:B:679:LEU:HD23	2.01	0.43
1:B:972:HIS:HB3	5:B:2158:HOH:O	2.18	0.43
1:C:34:ALA:HB3	1:C:36:TRP:CZ3	2.53	0.43
1:C:63:PHE:CD1	1:C:63:PHE:N	2.86	0.43
1:C:237:ARG:CG	1:C:237:ARG:NH1	2.81	0.43
1:C:658:LEU:HD12	1:C:693:GLN:O	2.18	0.43
1:C:722:LEU:HD23	1:C:722:LEU:HA	1.75	0.43
1:C:788:PRO:O	1:C:933:SER:HB2	2.18	0.43
1:C:878:HIS:HA	1:C:879:PRO:HD3	1.66	0.43
1:D:788:PRO:O	1:D:933:SER:HB2	2.18	0.43
1:E:131:GLU:O	1:E:132:SER:C	2.60	0.43
1:E:559:TYR:HA	1:E:560:PRO:HD2	1.73	0.43
1:E:571:VAL:HG13	1:E:607:VAL:HG23	1.99	0.43
1:E:685:LEU:HB3	1:E:686:PRO:HD2	1.99	0.43
1:E:708:TRP:CD1	1:E:708:TRP:N	2.84	0.43
1:E:778:THR:HB	1:E:887:GLN:CB	2.48	0.43
1:F:110:ASN:O	1:F:113:PHE:HB2	2.19	0.43
1:F:658:LEU:HD12	1:F:693:GLN:O	2.18	0.43
1:F:894:ARG:NH1	1:F:920:LEU:CA	2.81	0.43
1:G:149:ALA:O	1:G:150:PHE:HB3	2.18	0.43
1:H:406:GLY:O	1:H:407:LEU:HD23	2.18	0.43
1:H:429:ASP:OD1	1:H:431:ARG:HD3	2.18	0.43
1:H:645:ARG:NH2	1:H:650:GLU:OE2	2.48	0.43
1:H:870:VAL:CG1	1:H:871:GLU:N	2.81	0.43
1:I:138:GLN:N	1:I:217:LYS:O	2.36	0.43
1:J:210:ARG:HH11	1:J:395:HIS:CA	2.32	0.43
1:J:637:GLU:HA	1:J:679:LEU:HD23	2.01	0.43
1:K:50:GLN:HB3	1:K:216:HIS:HB3	2.00	0.43
1:K:647:SER:OG	1:K:672:VAL:N	2.35	0.43
1:K:701:VAL:CG1	1:K:702:GLN:N	2.81	0.43
1:K:722:LEU:HD23	1:K:722:LEU:HA	1.75	0.43
1:L:131:GLU:O	1:L:132:SER:C	2.60	0.43
1:M:57:GLU:HG2	1:M:83:THR:HG21	1.93	0.43
1:M:164:ASP:OD2	1:M:167:LEU:HD12	2.18	0.43
1:M:347:LYS:CB	1:M:348:PRO:HD2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:533:LEU:HD12	1:M:534:ILE:N	2.33	0.43
1:M:870:VAL:CG1	1:M:871:GLU:N	2.81	0.43
1:N:37:ARG:CG	1:N:37:ARG:NH1	2.79	0.43
1:N:43:ARG:NH1	1:N:44:THR:CG2	2.81	0.43
1:N:149:ALA:O	1:N:150:PHE:HB3	2.18	0.43
1:N:422:PRO:HA	1:O:282:ARG:HB2	1.99	0.43
1:N:1021:CME:HB3	1:N:1021:CME:HE2	1.41	0.43
1:O:757:GLN:O	1:O:757:GLN:HG2	2.12	0.43
1:P:655:MET:HE2	1:P:656:VAL:C	2.42	0.43
1:P:788:PRO:O	1:P:933:SER:HB2	2.18	0.43
1:A:869:ASP:CG	1:A:1015:HIS:HD1	2.24	0.43
1:B:3:ILE:O	1:B:6:SER:HB3	2.18	0.43
1:B:111:PRO:HA	1:B:112:PRO:HA	1.57	0.43
1:B:210:ARG:HH11	1:B:395:HIS:CA	2.32	0.43
1:B:272:ALA:HB1	1:B:273:PRO:CD	2.47	0.43
1:B:373:VAL:O	1:B:374:GLN:C	2.57	0.43
1:B:387:VAL:CG2	1:B:388:ARG:N	2.80	0.43
1:B:406:GLY:O	1:B:407:LEU:HD23	2.18	0.43
1:B:701:VAL:CG1	1:B:702:GLN:N	2.81	0.43
1:C:3:ILE:O	1:C:6:SER:HB3	2.18	0.43
1:C:454:ILE:C	1:C:455:ILE:HG13	2.43	0.43
1:D:131:GLU:O	1:D:132:SER:C	2.60	0.43
1:D:378:LEU:HD23	1:D:378:LEU:HA	1.53	0.43
1:D:655:MET:HE2	1:D:656:VAL:C	2.42	0.43
1:D:658:LEU:HD12	1:D:693:GLN:O	2.18	0.43
1:E:807:VAL:HG13	1:E:808:GLU:N	2.34	0.43
1:E:1021:CME:HB3	1:E:1021:CME:HE2	1.41	0.43
1:F:46:ARG:HB3	1:F:47:PRO:HD2	2.00	0.43
1:F:378:LEU:HD23	1:F:378:LEU:HA	1.53	0.43
1:F:870:VAL:CG1	1:F:871:GLU:N	2.81	0.43
1:G:70:PRO:O	1:G:73:TRP:N	2.45	0.43
1:G:237:ARG:CG	1:G:237:ARG:NH1	2.82	0.43
1:G:454:ILE:C	1:G:455:ILE:HG13	2.43	0.43
1:G:637:GLU:HA	1:G:679:LEU:HD23	2.01	0.43
1:G:646:HIS:O	1:G:648:ASP:N	2.47	0.43
1:I:6:SER:O	1:I:7:LEU:C	2.60	0.43
1:I:336:ARG:HH11	1:I:336:ARG:CG	2.26	0.43
1:I:429:ASP:HA	1:I:430:PRO:HD3	1.51	0.43
1:J:149:ALA:O	1:J:150:PHE:HB3	2.18	0.43
1:J:533:LEU:HD12	1:J:534:ILE:N	2.33	0.43
1:J:788:PRO:O	1:J:933:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:870:VAL:CG1	1:L:871:GLU:N	2.81	0.43
1:M:287:ASP:OD1	1:M:287:ASP:N	2.29	0.43
1:N:46:ARG:HB3	1:N:47:PRO:HD2	2.00	0.43
1:N:173:LEU:HA	1:N:173:LEU:HD23	1.69	0.43
1:N:429:ASP:OD1	1:N:431:ARG:HD3	2.18	0.43
1:N:701:VAL:HG12	1:N:702:GLN:H	1.83	0.43
1:O:149:ALA:O	1:O:150:PHE:HB3	2.18	0.43
1:O:454:ILE:C	1:O:455:ILE:HG13	2.43	0.43
1:O:637:GLU:HA	1:O:679:LEU:HD23	2.01	0.43
1:P:375:ASP:O	1:P:379:MET:HG3	2.19	0.43
1:A:419:GLY:O	1:D:282:ARG:NH1	2.51	0.43
1:A:673:ALA:O	1:A:676:GLY:N	2.47	0.43
1:B:6:SER:O	1:B:7:LEU:C	2.60	0.43
1:B:347:LYS:HA	1:B:348:PRO:HD3	1.77	0.43
1:B:599:ARG:HB2	1:B:600:GLN:H	1.41	0.43
1:B:895:VAL:O	1:B:919:ASP:HA	2.19	0.43
1:C:50:GLN:HB3	1:C:216:HIS:HB3	2.00	0.43
1:C:375:ASP:O	1:C:379:MET:HG3	2.19	0.43
1:C:599:ARG:HB2	1:C:600:GLN:H	1.41	0.43
1:C:701:VAL:CG1	1:C:702:GLN:N	2.81	0.43
1:D:454:ILE:C	1:D:455:ILE:HG13	2.43	0.43
1:D:763:GLY:HA3	1:D:822:LEU:HD22	2.01	0.43
1:D:870:VAL:CG1	1:D:871:GLU:N	2.81	0.43
1:E:454:ILE:C	1:E:455:ILE:HG13	2.43	0.43
1:E:533:LEU:HD12	1:E:534:ILE:N	2.33	0.43
1:F:576:ILE:CG2	1:F:577:LYS:N	2.78	0.43
1:F:685:LEU:HA	1:F:686:PRO:HD3	1.70	0.43
1:F:701:VAL:HG12	1:F:702:GLN:H	1.83	0.43
1:F:702:GLN:HA	1:F:703:PRO:HD2	1.84	0.43
1:F:1021:CME:HZ3	1:F:1022:GLN:O	2.19	0.43
1:G:272:ALA:HB1	1:G:273:PRO:CD	2.47	0.43
1:G:373:VAL:O	1:G:374:GLN:C	2.57	0.43
1:G:658:LEU:HD12	1:G:693:GLN:O	2.18	0.43
1:H:251:ARG:CB	1:H:253:TYR:CE2	2.98	0.43
1:H:347:LYS:CB	1:H:348:PRO:HD2	2.43	0.43
1:I:70:PRO:O	1:I:73:TRP:N	2.45	0.43
1:I:870:VAL:CG1	1:I:871:GLU:N	2.81	0.43
1:I:895:VAL:O	1:I:919:ASP:HA	2.19	0.43
1:J:63:PHE:CD1	1:J:63:PHE:N	2.86	0.43
1:J:164:ASP:OD2	1:J:167:LEU:HD12	2.18	0.43
1:J:375:ASP:O	1:J:379:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:685:LEU:HB3	1:J:686:PRO:HD2	1.99	0.43
1:J:778:THR:HB	1:J:887:GLN:CB	2.48	0.43
1:J:823:LEU:HD23	1:J:823:LEU:HA	1.73	0.43
1:K:6:SER:O	1:K:7:LEU:C	2.60	0.43
1:K:46:ARG:HB3	1:K:47:PRO:HD2	2.00	0.43
1:K:429:ASP:OD1	1:K:431:ARG:HD3	2.18	0.43
1:L:6:SER:O	1:L:7:LEU:C	2.60	0.43
1:L:673:ALA:O	1:L:676:GLY:N	2.47	0.43
1:L:778:THR:HB	1:L:887:GLN:CB	2.49	0.43
1:L:823:LEU:HD23	1:L:823:LEU:HA	1.73	0.43
1:M:406:GLY:O	1:M:407:LEU:HD23	2.18	0.43
1:M:571:VAL:HG13	1:M:607:VAL:HG23	1.99	0.43
1:M:637:GLU:HA	1:M:679:LEU:HD23	2.01	0.43
1:N:708:TRP:CD1	1:N:708:TRP:N	2.84	0.43
1:N:807:VAL:HG13	1:N:808:GLU:N	2.34	0.43
1:O:63:PHE:CD1	1:O:63:PHE:N	2.86	0.43
1:O:559:TYR:HA	1:O:560:PRO:HD2	1.73	0.43
1:O:646:HIS:O	1:O:648:ASP:N	2.48	0.43
1:O:682:LEU:HD23	1:O:682:LEU:HA	1.67	0.43
1:P:372:MET:HE1	1:P:395:HIS:HB3	2.00	0.43
1:A:285:TYR:HB3	1:A:288:ARG:HG3	2.01	0.43
1:A:645:ARG:NH2	1:A:650:GLU:OE2	2.48	0.43
1:A:895:VAL:O	1:A:919:ASP:HA	2.19	0.43
1:A:933:SER:O	1:A:934:GLU:C	2.62	0.43
1:A:1021:CME:HZ3	1:A:1022:GLN:O	2.19	0.43
1:B:63:PHE:CD1	1:B:63:PHE:N	2.86	0.43
1:B:110:ASN:O	1:B:113:PHE:HB2	2.19	0.43
1:B:149:ALA:O	1:B:150:PHE:HB3	2.18	0.43
1:B:237:ARG:CG	1:B:237:ARG:NH1	2.82	0.43
1:B:395:HIS:HA	1:B:396:PRO:HD3	1.48	0.43
1:B:708:TRP:CZ3	1:B:709:SER:HB3	2.54	0.43
1:B:807:VAL:HG13	1:B:808:GLU:N	2.34	0.43
1:B:856:TYR:CD2	1:B:864:MET:CE	2.97	0.43
1:C:230:ARG:NH2	1:C:241:GLU:OE2	2.50	0.43
1:C:251:ARG:CB	1:C:253:TYR:CE2	2.98	0.43
1:C:406:GLY:O	1:C:407:LEU:HD23	2.18	0.43
1:C:870:VAL:CG1	1:C:871:GLU:N	2.81	0.43
1:C:1021:CME:HZ3	1:C:1022:GLN:O	2.19	0.43
1:D:63:PHE:CD1	1:D:63:PHE:N	2.86	0.43
1:D:363:HIS:CD2	1:D:363:HIS:N	2.81	0.43
1:D:479:ASP:HA	1:D:480:PRO:HD2	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1021:CME:HZ3	1:D:1022:GLN:O	2.19	0.43
1:E:118:ASN:HA	1:E:119:PRO:HD2	1.60	0.43
1:E:637:GLU:HA	1:E:679:LEU:HD23	2.01	0.43
1:F:35:SER:O	1:F:50:GLN:HG3	2.18	0.43
1:G:110:ASN:O	1:G:113:PHE:HB2	2.19	0.43
1:G:599:ARG:HB2	1:G:600:GLN:H	1.41	0.43
1:G:701:VAL:CG1	1:G:702:GLN:N	2.81	0.43
1:G:718:GLN:HG3	1:G:719:GLN:N	2.34	0.43
1:H:63:PHE:CD1	1:H:63:PHE:N	2.86	0.43
1:H:372:MET:HE1	1:H:395:HIS:HB3	2.00	0.43
1:H:651:LEU:HD12	1:H:668:VAL:O	2.19	0.43
1:H:822:LEU:HD12	1:H:823:LEU:H	1.80	0.43
1:I:63:PHE:CD1	1:I:63:PHE:N	2.86	0.43
1:J:110:ASN:O	1:J:113:PHE:HB2	2.19	0.43
1:J:308:LEU:HD23	1:J:308:LEU:HA	1.80	0.43
1:J:570:TRP:HD1	1:J:571:VAL:HG22	1.84	0.43
1:J:651:LEU:HD12	1:J:668:VAL:O	2.19	0.43
1:K:43:ARG:NH1	1:K:44:THR:CG2	2.81	0.43
1:K:255:ARG:NH1	1:K:255:ARG:CG	2.79	0.43
1:K:454:ILE:C	1:K:455:ILE:HG13	2.43	0.43
1:L:131:GLU:HA	1:L:134:LEU:HB2	2.00	0.43
1:L:210:ARG:HH11	1:L:395:HIS:CA	2.32	0.43
1:L:479:ASP:HA	1:L:480:PRO:HD2	1.61	0.43
1:L:895:VAL:O	1:L:919:ASP:HA	2.19	0.43
1:M:608:PHE:O	1:M:611:ARG:N	2.41	0.43
1:M:778:THR:HB	1:M:887:GLN:CB	2.48	0.43
1:N:651:LEU:HD12	1:N:668:VAL:O	2.19	0.43
1:N:778:THR:HB	1:N:887:GLN:CB	2.48	0.43
1:O:658:LEU:HD12	1:O:693:GLN:O	2.18	0.43
1:O:694:LEU:O	1:O:722:LEU:N	2.51	0.43
1:P:34:ALA:HB3	1:P:36:TRP:CZ3	2.53	0.43
1:P:43:ARG:NH1	1:P:44:THR:CG2	2.81	0.43
1:P:50:GLN:HB3	1:P:216:HIS:HB3	2.00	0.43
1:P:210:ARG:HH11	1:P:395:HIS:CA	2.32	0.43
1:P:387:VAL:CG2	1:P:388:ARG:N	2.80	0.43
1:P:463:GLY:O	1:P:486:TYR:OH	2.32	0.43
1:P:670:LEU:HA	1:P:670:LEU:HD23	1.67	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:A:637:GLU:HA	1:A:679:LEU:HD23	2.01	0.43
1:A:763:GLY:HA3	1:A:822:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:LEU:HD12	1:A:823:LEU:H	1.80	0.43
1:B:454:ILE:C	1:B:455:ILE:HG13	2.43	0.43
1:B:651:LEU:HD13	1:B:651:LEU:HA	1.51	0.43
1:B:894:ARG:NH1	1:B:920:LEU:CA	2.81	0.43
1:D:4:THR:CA	1:D:9:VAL:HG11	2.47	0.43
1:D:35:SER:O	1:D:50:GLN:HG3	2.18	0.43
1:D:138:GLN:N	1:D:217:LYS:O	2.36	0.43
1:D:237:ARG:CG	1:D:237:ARG:NH1	2.82	0.43
1:D:673:ALA:O	1:D:676:GLY:N	2.47	0.43
1:D:718:GLN:HG3	1:D:719:GLN:N	2.34	0.43
1:E:210:ARG:HH11	1:E:395:HIS:CA	2.32	0.43
1:E:429:ASP:OD1	1:E:431:ARG:HD3	2.18	0.43
1:E:694:LEU:O	1:E:722:LEU:N	2.51	0.43
1:E:701:VAL:CG1	1:E:702:GLN:N	2.81	0.43
1:F:44:THR:O	1:F:45:ASP:C	2.61	0.43
1:F:118:ASN:HA	1:F:119:PRO:HD2	1.60	0.43
1:F:369:GLU:O	1:F:373:VAL:HG23	2.19	0.43
1:F:406:GLY:O	1:F:407:LEU:HD23	2.18	0.43
1:F:637:GLU:HA	1:F:679:LEU:HD23	2.01	0.43
1:F:673:ALA:O	1:F:676:GLY:N	2.47	0.43
1:G:3:ILE:O	1:G:6:SER:HB3	2.18	0.43
1:G:46:ARG:HB3	1:G:47:PRO:HD2	2.00	0.43
1:G:111:PRO:HA	1:G:112:PRO:HA	1.57	0.43
1:G:285:TYR:HB3	1:G:288:ARG:HG3	2.01	0.43
1:G:429:ASP:OD1	1:G:431:ARG:HD3	2.18	0.43
1:G:568:TRP:CD2	1:G:569:ASP:HB3	2.54	0.43
1:G:682:LEU:HA	1:G:682:LEU:HD23	1.67	0.43
1:G:708:TRP:CZ3	1:G:709:SER:HB3	2.54	0.43
1:G:894:ARG:NH1	1:G:920:LEU:CA	2.81	0.43
1:H:210:ARG:HH11	1:H:395:HIS:CA	2.32	0.43
1:H:285:TYR:HB3	1:H:288:ARG:HG3	2.01	0.43
1:H:568:TRP:CD2	1:H:569:ASP:HB3	2.54	0.43
1:H:972:HIS:HB3	5:H:2155:HOH:O	2.18	0.43
1:I:708:TRP:CZ3	1:I:709:SER:HB3	2.54	0.43
1:I:718:GLN:HG3	1:I:719:GLN:N	2.34	0.43
1:I:778:THR:HB	1:I:887:GLN:CB	2.48	0.43
1:J:287:ASP:OD1	1:J:287:ASP:N	2.29	0.43
1:K:93:HIS:HB3	1:K:95:TYR:HE1	1.84	0.43
1:K:260:LEU:HD12	1:K:310:ARG:O	2.19	0.43
1:K:264:GLU:OE2	1:K:264:GLU:HA	2.17	0.43
1:K:375:ASP:O	1:K:379:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:637:GLU:HA	1:K:679:LEU:HD23	2.01	0.43
1:K:651:LEU:HD12	1:K:668:VAL:O	2.19	0.43
1:L:35:SER:O	1:L:50:GLN:HG3	2.18	0.43
1:L:579:ASP:OD1	1:L:583:ASN:N	2.43	0.43
1:L:933:SER:O	1:L:934:GLU:C	2.62	0.43
1:M:110:ASN:O	1:M:113:PHE:HB2	2.19	0.43
1:M:260:LEU:HD12	1:M:310:ARG:O	2.19	0.43
1:M:682:LEU:HA	1:M:682:LEU:HD23	1.67	0.43
1:M:694:LEU:HA	1:M:694:LEU:HD12	1.69	0.43
1:M:694:LEU:O	1:M:722:LEU:N	2.51	0.43
1:M:708:TRP:CZ3	1:M:709:SER:HB3	2.54	0.43
1:M:895:VAL:O	1:M:919:ASP:HA	2.19	0.43
1:N:375:ASP:O	1:N:379:MET:HG3	2.19	0.43
1:N:522:LYS:O	1:N:523:TRP:C	2.61	0.43
1:N:637:GLU:HA	1:N:679:LEU:HD23	2.01	0.43
1:N:933:SER:O	1:N:934:GLU:C	2.62	0.43
1:O:46:ARG:HB3	1:O:47:PRO:HD2	2.00	0.43
1:O:685:LEU:HB3	1:O:686:PRO:HD2	1.99	0.43
1:O:708:TRP:CZ3	1:O:709:SER:HB3	2.54	0.43
1:O:718:GLN:HG3	1:O:719:GLN:N	2.34	0.43
1:P:73:TRP:O	1:P:183:ARG:NH1	2.48	0.43
1:P:568:TRP:CD2	1:P:569:ASP:HB3	2.54	0.43
1:P:682:LEU:HA	1:P:682:LEU:HD23	1.67	0.43
1:P:1018:LEU:HD23	1:P:1018:LEU:HA	1.51	0.43
1:P:1021:CME:HZ3	1:P:1022:GLN:O	2.19	0.43
1:A:237:ARG:CG	1:A:237:ARG:NH1	2.82	0.43
1:A:347:LYS:CB	1:A:348:PRO:HD2	2.43	0.43
1:A:372:MET:HE1	1:A:395:HIS:HB3	2.00	0.43
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.54	0.43
1:A:900:LEU:HD23	1:A:900:LEU:HA	1.75	0.43
1:B:260:LEU:HD12	1:B:310:ARG:O	2.19	0.43
1:B:285:TYR:HB3	1:B:288:ARG:HG3	2.01	0.43
1:B:372:MET:HE1	1:B:395:HIS:HB3	2.00	0.43
1:B:476:LYS:HA	1:B:476:LYS:HD2	1.81	0.43
1:B:651:LEU:HD12	1:B:668:VAL:O	2.19	0.43
1:B:702:GLN:HA	1:B:703:PRO:HD2	1.84	0.43
1:C:131:GLU:HA	1:C:134:LEU:HB2	2.00	0.43
1:C:254:LEU:HD23	1:C:254:LEU:HA	1.62	0.43
1:C:972:HIS:HB3	5:C:2155:HOH:O	2.18	0.43
1:D:375:ASP:O	1:D:379:MET:HG3	2.19	0.43
1:D:391:HIS:ND1	1:D:412:GLU:OE1	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:694:LEU:HD12	1:D:694:LEU:HA	1.69	0.43
1:E:260:LEU:HD12	1:E:310:ARG:O	2.19	0.43
1:E:651:LEU:HD12	1:E:668:VAL:O	2.19	0.43
1:F:70:PRO:O	1:F:73:TRP:N	2.45	0.43
1:F:149:ALA:O	1:F:150:PHE:HB3	2.18	0.43
1:F:173:LEU:HA	1:F:173:LEU:HD23	1.69	0.43
1:F:657:ALA:HA	1:F:661:LYS:O	2.19	0.43
1:G:93:HIS:HB3	1:G:95:TYR:HE1	1.84	0.43
1:G:210:ARG:HH11	1:G:395:HIS:CA	2.32	0.43
1:G:781:ARG:NH1	1:G:781:ARG:CG	2.79	0.43
1:G:807:VAL:HG13	1:G:808:GLU:N	2.34	0.43
1:G:895:VAL:O	1:G:919:ASP:HA	2.19	0.43
1:H:50:GLN:HB3	1:H:216:HIS:HB3	2.00	0.43
1:H:694:LEU:O	1:H:722:LEU:N	2.51	0.43
1:I:93:HIS:HB3	1:I:95:TYR:HE1	1.84	0.43
1:I:251:ARG:CB	1:I:253:TYR:CE2	2.98	0.43
1:I:260:LEU:HD12	1:I:310:ARG:O	2.19	0.43
1:I:369:GLU:O	1:I:373:VAL:HG23	2.19	0.43
1:I:375:ASP:O	1:I:379:MET:HG3	2.19	0.43
1:J:568:TRP:CD2	1:J:569:ASP:HB3	2.54	0.43
1:J:920:LEU:CB	1:J:921:PRO:CD	2.97	0.43
1:J:972:HIS:HB3	5:J:2155:HOH:O	2.18	0.43
1:K:367:MET:HB3	1:K:367:MET:HE3	1.72	0.43
1:K:568:TRP:CD2	1:K:569:ASP:HB3	2.54	0.43
1:K:612:THR:HA	1:K:613:PRO:HD3	1.68	0.43
1:L:63:PHE:CB	1:L:64:PRO:HD2	2.32	0.43
1:L:237:ARG:CG	1:L:237:ARG:NH1	2.82	0.43
1:L:531:ARG:O	1:L:561:ARG:NH1	2.46	0.43
1:L:658:LEU:O	1:L:659:ASP:C	2.58	0.43
1:M:264:GLU:OE2	1:M:264:GLU:HA	2.17	0.43
1:M:429:ASP:OD1	1:M:431:ARG:HD3	2.18	0.43
1:M:576:ILE:CG2	1:M:577:LYS:N	2.78	0.43
1:M:655:MET:HB2	1:M:655:MET:HE3	1.60	0.43
1:M:726:LEU:HA	1:M:726:LEU:HD23	1.66	0.43
1:N:6:SER:O	1:N:7:LEU:C	2.60	0.43
1:N:282:ARG:HH11	1:O:419:GLY:C	2.26	0.43
1:N:406:GLY:O	1:N:407:LEU:HD23	2.18	0.43
1:N:708:TRP:CZ3	1:N:709:SER:HB3	2.54	0.43
1:N:778:THR:CG2	1:N:887:GLN:H	2.32	0.43
1:O:43:ARG:NH1	1:O:44:THR:HG23	2.34	0.43
1:O:210:ARG:HH11	1:O:395:HIS:CA	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:264:GLU:OE2	1:O:264:GLU:HA	2.17	0.43
1:O:285:TYR:HB3	1:O:288:ARG:HG3	2.01	0.43
1:O:421:VAL:O	1:O:425:ARG:NH1	2.46	0.43
1:O:781:ARG:NH1	1:O:781:ARG:CG	2.79	0.43
1:P:237:ARG:CG	1:P:237:ARG:NH1	2.82	0.43
1:P:285:TYR:HB3	1:P:288:ARG:HG3	2.01	0.43
1:P:445:GLN:HE21	1:P:445:GLN:HB3	1.54	0.43
1:A:46:ARG:HB3	1:A:47:PRO:HD2	2.00	0.43
1:A:260:LEU:HD12	1:A:310:ARG:O	2.19	0.43
1:A:579:ASP:OD1	1:A:583:ASN:N	2.43	0.43
1:A:708:TRP:CZ3	1:A:709:SER:HB3	2.54	0.43
1:B:323:ILE:CD1	1:B:323:ILE:N	2.82	0.43
1:B:657:ALA:HA	1:B:661:LYS:O	2.19	0.43
1:C:65:ALA:HB1	1:C:66:PRO:CD	2.39	0.43
1:C:110:ASN:O	1:C:113:PHE:HB2	2.19	0.43
1:C:260:LEU:HD12	1:C:310:ARG:O	2.19	0.43
1:C:369:GLU:O	1:C:373:VAL:HG23	2.19	0.43
1:C:373:VAL:O	1:C:374:GLN:C	2.57	0.43
1:C:995:GLY:O	1:C:996:ASP:C	2.62	0.43
1:D:78:LEU:CB	1:D:79:PRO:HD2	2.44	0.43
1:D:184:LEU:HD23	1:D:184:LEU:HA	1.83	0.43
1:D:395:HIS:HA	1:D:396:PRO:HD3	1.48	0.43
1:D:778:THR:HB	1:D:887:GLN:CB	2.49	0.43
1:D:933:SER:O	1:D:934:GLU:C	2.62	0.43
1:E:679:LEU:HD23	1:E:679:LEU:HA	1.26	0.43
1:F:708:TRP:CZ3	1:F:709:SER:HB3	2.54	0.43
1:G:43:ARG:NH1	1:G:44:THR:HG23	2.34	0.43
1:G:421:VAL:O	1:G:425:ARG:NH1	2.46	0.43
1:G:597:ASN:ND2	1:G:599:ARG:H	2.17	0.43
1:G:657:ALA:HA	1:G:661:LYS:O	2.19	0.43
1:G:685:LEU:HB3	1:G:686:PRO:HD2	2.00	0.43
1:H:533:LEU:HD12	1:H:534:ILE:N	2.33	0.43
1:H:546:LEU:HD12	1:H:546:LEU:HA	1.84	0.43
1:H:788:PRO:O	1:H:933:SER:HB2	2.18	0.43
1:I:568:TRP:CD2	1:I:569:ASP:HB3	2.54	0.43
1:I:701:VAL:CG1	1:I:702:GLN:N	2.81	0.43
1:I:788:PRO:O	1:I:933:SER:HB2	2.18	0.43
1:I:933:SER:O	1:I:934:GLU:C	2.62	0.43
1:J:473:ARG:HD2	1:K:469:ASP:HB3	1.99	0.43
1:J:1020:TRP:CD1	1:J:1020:TRP:C	2.97	0.43
1:L:110:ASN:O	1:L:113:PHE:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:454:ILE:C	1:L:455:ILE:HG13	2.43	0.43
1:L:571:VAL:HG13	1:L:607:VAL:HG23	1.99	0.43
1:L:1021:CME:HZ3	1:L:1022:GLN:O	2.19	0.43
1:M:395:HIS:HA	1:M:396:PRO:HD3	1.48	0.43
1:M:647:SER:OG	1:M:672:VAL:N	2.35	0.43
1:M:778:THR:CG2	1:M:887:GLN:H	2.32	0.43
1:M:788:PRO:O	1:M:933:SER:HB2	2.18	0.43
1:M:807:VAL:HG13	1:M:808:GLU:N	2.34	0.43
1:N:210:ARG:HH11	1:N:395:HIS:CA	2.32	0.43
1:N:260:LEU:HD12	1:N:310:ARG:O	2.19	0.43
1:N:657:ALA:HA	1:N:661:LYS:O	2.19	0.43
1:N:894:ARG:NH1	1:N:920:LEU:CA	2.81	0.43
1:N:1021:CME:HZ3	1:N:1022:GLN:O	2.19	0.43
1:O:110:ASN:O	1:O:113:PHE:HB2	2.19	0.43
1:O:138:GLN:N	1:O:217:LYS:O	2.36	0.43
1:O:344:LEU:N	1:O:347:LYS:O	2.36	0.43
1:O:597:ASN:ND2	1:O:599:ARG:H	2.17	0.43
1:O:870:VAL:CG1	1:O:871:GLU:N	2.81	0.43
1:P:44:THR:O	1:P:45:ASP:C	2.61	0.43
1:A:50:GLN:HB3	1:A:216:HIS:HB3	2.00	0.42
1:A:110:ASN:O	1:A:113:PHE:HB2	2.19	0.42
1:A:406:GLY:O	1:A:407:LEU:HD23	2.18	0.42
1:A:445:GLN:HE21	1:A:445:GLN:HB3	1.54	0.42
1:A:651:LEU:HD12	1:A:668:VAL:O	2.19	0.42
1:B:230:ARG:NH2	1:B:241:GLU:OE2	2.51	0.42
1:B:679:LEU:HD23	1:B:679:LEU:HA	1.26	0.42
1:B:870:VAL:CG1	1:B:871:GLU:N	2.81	0.42
1:C:93:HIS:HB3	1:C:95:TYR:HE1	1.84	0.42
1:C:657:ALA:HA	1:C:661:LYS:O	2.19	0.42
1:D:34:ALA:HB3	1:D:36:TRP:CE3	2.55	0.42
1:D:149:ALA:O	1:D:150:PHE:HB3	2.18	0.42
1:D:260:LEU:HD12	1:D:310:ARG:O	2.19	0.42
1:D:651:LEU:HD12	1:D:668:VAL:O	2.19	0.42
1:E:694:LEU:HD12	1:E:694:LEU:HA	1.69	0.42
1:E:708:TRP:CZ3	1:E:709:SER:HB3	2.54	0.42
1:E:778:THR:CG2	1:E:887:GLN:H	2.32	0.42
1:E:995:GLY:O	1:E:996:ASP:C	2.62	0.42
1:E:1020:TRP:CD1	1:E:1020:TRP:C	2.97	0.42
1:F:93:HIS:HB3	1:F:95:TYR:HE1	1.84	0.42
1:F:260:LEU:HD12	1:F:310:ARG:O	2.19	0.42
1:F:375:ASP:O	1:F:379:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:778:THR:CG2	1:F:887:GLN:H	2.32	0.42
1:H:445:GLN:HE21	1:H:445:GLN:HB3	1.54	0.42
1:H:657:ALA:HA	1:H:661:LYS:O	2.19	0.42
1:I:43:ARG:NH1	1:I:44:THR:HG23	2.34	0.42
1:I:164:ASP:OD2	1:I:167:LEU:HD12	2.18	0.42
1:I:210:ARG:NH1	1:I:394:ASN:C	2.77	0.42
1:I:237:ARG:CG	1:I:237:ARG:NH1	2.82	0.42
1:I:429:ASP:OD1	1:I:431:ARG:HD3	2.18	0.42
1:I:661:LYS:HA	1:I:662:PRO:HD3	1.63	0.42
1:I:807:VAL:HG13	1:I:808:GLU:N	2.34	0.42
1:I:1021:CME:HZ3	1:I:1022:GLN:O	2.19	0.42
1:J:34:ALA:HB3	1:J:36:TRP:CE3	2.54	0.42
1:J:272:ALA:HB1	1:J:273:PRO:CD	2.47	0.42
1:J:369:GLU:O	1:J:373:VAL:HG23	2.19	0.42
1:K:372:MET:HE1	1:K:395:HIS:HB3	2.00	0.42
1:K:895:VAL:O	1:K:919:ASP:HA	2.19	0.42
1:K:972:HIS:HB3	5:K:2155:HOH:O	2.18	0.42
1:L:164:ASP:OD2	1:L:167:LEU:HD12	2.18	0.42
1:L:254:LEU:HD23	1:L:254:LEU:HA	1.62	0.42
1:L:685:LEU:HA	1:L:686:PRO:HD3	1.70	0.42
1:L:869:ASP:CG	1:L:1015:HIS:HD1	2.24	0.42
1:L:900:LEU:HD23	1:L:900:LEU:HA	1.75	0.42
1:M:44:THR:O	1:M:45:ASP:C	2.61	0.42
1:M:651:LEU:HD12	1:M:668:VAL:O	2.19	0.42
1:M:995:GLY:O	1:M:996:ASP:C	2.62	0.42
1:N:110:ASN:O	1:N:113:PHE:HB2	2.19	0.42
1:N:369:GLU:O	1:N:373:VAL:HG23	2.19	0.42
1:N:847:LYS:HZ3	1:N:875:ASP:CG	2.26	0.42
1:O:93:HIS:HB3	1:O:95:TYR:HE1	1.84	0.42
1:O:230:ARG:HH11	1:O:230:ARG:CG	2.24	0.42
1:P:251:ARG:CB	1:P:253:TYR:CE2	2.98	0.42
1:P:369:GLU:O	1:P:373:VAL:HG23	2.19	0.42
1:P:533:LEU:HD12	1:P:534:ILE:N	2.33	0.42
1:A:85:VAL:HG12	1:A:86:VAL:N	2.35	0.42
1:A:369:GLU:O	1:A:373:VAL:HG23	2.19	0.42
1:A:454:ILE:C	1:A:455:ILE:HG13	2.43	0.42
1:A:576:ILE:CG2	1:A:577:LYS:N	2.78	0.42
1:A:800:ARG:CZ	1:A:800:ARG:CB	2.98	0.42
1:A:870:VAL:CG1	1:A:871:GLU:N	2.81	0.42
1:B:34:ALA:HB3	1:B:36:TRP:CE3	2.54	0.42
1:B:46:ARG:HB3	1:B:47:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:ASP:O	1:B:379:MET:HG3	2.19	0.42
1:B:597:ASN:ND2	1:B:599:ARG:H	2.17	0.42
1:B:1004:SER:HB2	1:B:1006:GLU:OE2	2.20	0.42
1:C:34:ALA:HB3	1:C:36:TRP:CE3	2.54	0.42
1:C:147:ASN:HB2	1:C:165:SER:HB3	2.02	0.42
1:D:43:ARG:NH1	1:D:44:THR:CG2	2.81	0.42
1:D:93:HIS:HB3	1:D:95:TYR:HE1	1.84	0.42
1:D:995:GLY:O	1:D:996:ASP:C	2.62	0.42
1:E:141:ILE:HD13	1:E:143:PHE:CE1	2.55	0.42
1:E:237:ARG:CG	1:E:237:ARG:NH1	2.81	0.42
1:E:264:GLU:OE2	1:E:264:GLU:HA	2.17	0.42
1:F:37:ARG:CG	1:F:37:ARG:NH1	2.79	0.42
1:F:445:GLN:HE21	1:F:445:GLN:HB3	1.55	0.42
1:F:685:LEU:HB3	1:F:686:PRO:HD2	1.99	0.42
1:G:44:THR:O	1:G:45:ASP:C	2.61	0.42
1:G:369:GLU:O	1:G:373:VAL:HG23	2.19	0.42
1:G:1004:SER:HB2	1:G:1006:GLU:OE2	2.20	0.42
1:G:1018:LEU:HD22	1:G:1019:VAL:N	2.35	0.42
1:G:1021:CME:HZ3	1:G:1022:GLN:O	2.19	0.42
1:H:85:VAL:HG12	1:H:86:VAL:N	2.34	0.42
1:H:708:TRP:CZ3	1:H:709:SER:HB3	2.54	0.42
1:H:730:LEU:HA	1:H:731:PRO:HD3	1.74	0.42
1:H:1021:CME:HZ3	1:H:1022:GLN:O	2.19	0.42
1:I:43:ARG:NH1	1:I:44:THR:CG2	2.81	0.42
1:I:85:VAL:HG12	1:I:86:VAL:N	2.34	0.42
1:I:264:GLU:OE2	1:I:264:GLU:HA	2.17	0.42
1:I:285:TYR:HB3	1:I:288:ARG:HG3	2.01	0.42
1:I:548:GLY:O	1:I:549:PHE:C	2.63	0.42
1:J:114:VAL:HG21	1:J:192:SER:N	2.35	0.42
1:J:778:THR:CG2	1:J:887:GLN:H	2.32	0.42
1:K:73:TRP:O	1:K:183:ARG:NH1	2.48	0.42
1:K:645:ARG:NH2	1:K:650:GLU:OE2	2.48	0.42
1:L:34:ALA:HB3	1:L:36:TRP:CE3	2.54	0.42
1:L:93:HIS:HB3	1:L:95:TYR:HE1	1.84	0.42
1:L:114:VAL:HG21	1:L:192:SER:N	2.35	0.42
1:L:260:LEU:HD12	1:L:310:ARG:O	2.19	0.42
1:L:429:ASP:OD1	1:L:431:ARG:HD3	2.18	0.42
1:L:651:LEU:HD12	1:L:668:VAL:O	2.19	0.42
1:L:718:GLN:HG3	1:L:719:GLN:N	2.34	0.42
1:L:745:MET:HA	1:L:745:MET:CE	2.44	0.42
1:M:141:ILE:HD13	1:M:143:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:745:MET:HA	1:M:745:MET:CE	2.43	0.42
1:N:658:LEU:O	1:N:659:ASP:C	2.58	0.42
1:N:685:LEU:HB3	1:N:686:PRO:HD2	1.99	0.42
1:O:657:ALA:HA	1:O:661:LYS:O	2.19	0.42
1:O:658:LEU:O	1:O:659:ASP:C	2.58	0.42
1:O:746:ASP:HA	1:O:760:ARG:CG	2.39	0.42
1:O:778:THR:HB	1:O:887:GLN:CB	2.49	0.42
1:O:800:ARG:CZ	1:O:800:ARG:CB	2.98	0.42
1:O:1004:SER:HB2	1:O:1006:GLU:OE2	2.19	0.42
1:P:43:ARG:NH1	1:P:44:THR:HG23	2.34	0.42
1:P:260:LEU:HD12	1:P:310:ARG:O	2.19	0.42
1:P:395:HIS:HA	1:P:396:PRO:HD3	1.48	0.42
1:P:927:THR:HA	1:P:928:PRO:HD3	1.62	0.42
1:P:972:HIS:HB3	5:P:2160:HOH:O	2.18	0.42
1:A:531:ARG:O	1:A:561:ARG:NH1	2.46	0.42
1:A:570:TRP:HD1	1:A:571:VAL:HG22	1.84	0.42
1:A:718:GLN:HG3	1:A:719:GLN:N	2.34	0.42
1:A:778:THR:HB	1:A:887:GLN:CB	2.48	0.42
1:A:875:ASP:N	1:A:875:ASP:OD2	2.47	0.42
1:B:43:ARG:NH1	1:B:44:THR:HG23	2.34	0.42
1:B:147:ASN:HB2	1:B:165:SER:HB3	2.02	0.42
1:B:579:ASP:OD1	1:B:583:ASN:N	2.43	0.42
1:B:718:GLN:HG3	1:B:719:GLN:N	2.34	0.42
1:B:757:GLN:O	1:B:757:GLN:HG2	2.12	0.42
1:B:869:ASP:CG	1:B:1015:HIS:HD1	2.24	0.42
1:C:531:ARG:O	1:C:561:ARG:NH1	2.46	0.42
1:C:718:GLN:HG3	1:C:719:GLN:N	2.33	0.42
1:C:778:THR:CG2	1:C:887:GLN:H	2.32	0.42
1:C:807:VAL:HG13	1:C:808:GLU:N	2.34	0.42
1:D:34:ALA:HB3	1:D:36:TRP:CZ3	2.53	0.42
1:D:210:ARG:NH1	1:D:394:ASN:C	2.77	0.42
1:D:257:THR:OG1	1:D:316:HIS:HE1	2.03	0.42
1:D:369:GLU:O	1:D:373:VAL:HG23	2.19	0.42
1:D:708:TRP:CZ3	1:D:709:SER:HB3	2.54	0.42
1:D:807:VAL:HG13	1:D:808:GLU:N	2.34	0.42
1:E:44:THR:O	1:E:45:ASP:C	2.61	0.42
1:E:46:ARG:HB3	1:E:47:PRO:HD2	2.00	0.42
1:E:110:ASN:O	1:E:113:PHE:HB2	2.19	0.42
1:E:375:ASP:O	1:E:379:MET:HG3	2.19	0.42
1:E:657:ALA:HA	1:E:661:LYS:O	2.19	0.42
1:E:763:GLY:HA3	1:E:822:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1018:LEU:HD22	1:E:1019:VAL:N	2.35	0.42
1:F:800:ARG:CZ	1:F:800:ARG:CB	2.98	0.42
1:F:895:VAL:O	1:F:919:ASP:HA	2.19	0.42
1:F:1018:LEU:HD22	1:F:1019:VAL:N	2.35	0.42
1:G:344:LEU:N	1:G:347:LYS:O	2.36	0.42
1:G:655:MET:HB2	1:G:655:MET:HE3	1.60	0.42
1:H:43:ARG:NH1	1:H:44:THR:HG23	2.34	0.42
1:H:347:LYS:HA	1:H:348:PRO:HD3	1.77	0.42
1:H:369:GLU:O	1:H:373:VAL:HG23	2.19	0.42
1:H:612:THR:HA	1:H:613:PRO:HD3	1.68	0.42
1:I:210:ARG:HH11	1:I:395:HIS:CA	2.32	0.42
1:I:406:GLY:O	1:I:407:LEU:HD23	2.18	0.42
1:I:637:GLU:HA	1:I:679:LEU:HD23	2.01	0.42
1:I:995:GLY:O	1:I:996:ASP:C	2.62	0.42
1:J:6:SER:O	1:J:7:LEU:C	2.60	0.42
1:J:43:ARG:NH1	1:J:44:THR:HG23	2.34	0.42
1:J:50:GLN:HB3	1:J:216:HIS:HB3	2.00	0.42
1:J:251:ARG:CB	1:J:253:TYR:CE2	2.98	0.42
1:J:272:ALA:HA	1:J:273:PRO:HD3	1.76	0.42
1:J:378:LEU:HD23	1:J:378:LEU:HA	1.53	0.42
1:J:708:TRP:CZ3	1:J:709:SER:HB3	2.54	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:K:131:GLU:O	1:K:132:SER:C	2.60	0.42
1:K:141:ILE:HD13	1:K:143:PHE:CE1	2.55	0.42
1:M:43:ARG:NH1	1:M:44:THR:HG23	2.34	0.42
1:M:597:ASN:ND2	1:M:599:ARG:H	2.17	0.42
1:M:657:ALA:HA	1:M:661:LYS:O	2.19	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:O:373:VAL:O	1:O:374:GLN:C	2.57	0.42
1:O:972:HIS:HB3	5:O:2155:HOH:O	2.18	0.42
1:P:778:THR:CG2	1:P:887:GLN:H	2.32	0.42
1:P:807:VAL:HG13	1:P:808:GLU:N	2.34	0.42
1:A:147:ASN:HB2	1:A:165:SER:HB3	2.02	0.42
1:B:173:LEU:HA	1:B:173:LEU:HD23	1.69	0.42
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.54	0.42
1:B:1021:CME:HZ3	1:B:1022:GLN:O	2.19	0.42
1:C:35:SER:O	1:C:50:GLN:HG3	2.18	0.42
1:C:46:ARG:HB3	1:C:47:PRO:HD2	2.00	0.42
1:C:570:TRP:HD1	1:C:571:VAL:HG22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:763:GLY:HA3	1:C:822:LEU:HD22	2.01	0.42
1:C:800:ARG:CZ	1:C:800:ARG:CB	2.98	0.42
1:D:44:THR:O	1:D:45:ASP:C	2.61	0.42
1:D:50:GLN:HB3	1:D:216:HIS:HB3	2.00	0.42
1:D:114:VAL:HG21	1:D:192:SER:N	2.35	0.42
1:D:347:LYS:HA	1:D:348:PRO:HD3	1.77	0.42
1:D:475:ILE:O	1:D:476:LYS:C	2.63	0.42
1:D:502:MET:HA	1:D:537:GLU:O	2.20	0.42
1:D:800:ARG:CZ	1:D:800:ARG:CB	2.98	0.42
1:E:34:ALA:HB3	1:E:36:TRP:CE3	2.54	0.42
1:E:579:ASP:OD1	1:E:583:ASN:N	2.43	0.42
1:E:933:SER:O	1:E:934:GLU:C	2.62	0.42
1:F:43:ARG:NH1	1:F:44:THR:HG23	2.34	0.42
1:F:230:ARG:HH11	1:F:230:ARG:CG	2.24	0.42
1:F:568:TRP:CD2	1:F:569:ASP:HB3	2.54	0.42
1:F:1004:SER:HB2	1:F:1006:GLU:OE2	2.20	0.42
1:G:85:VAL:HG12	1:G:86:VAL:N	2.34	0.42
1:G:138:GLN:N	1:G:217:LYS:O	2.36	0.42
1:G:189:LEU:N	1:G:189:LEU:CD2	2.75	0.42
1:H:272:ALA:HA	1:H:273:PRO:HD3	1.76	0.42
1:H:763:GLY:HA3	1:H:822:LEU:HD22	2.01	0.42
1:I:35:SER:O	1:I:50:GLN:HG3	2.18	0.42
1:I:230:ARG:NH2	1:I:241:GLU:OE2	2.51	0.42
1:I:651:LEU:HD12	1:I:668:VAL:O	2.19	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:J:657:ALA:HA	1:J:661:LYS:O	2.19	0.42
1:J:1004:SER:HB2	1:J:1006:GLU:OE2	2.19	0.42
1:K:43:ARG:NH1	1:K:44:THR:HG23	2.34	0.42
1:K:78:LEU:HB3	1:K:79:PRO:CD	2.45	0.42
1:K:110:ASN:O	1:K:113:PHE:HB2	2.19	0.42
1:K:149:ALA:O	1:K:150:PHE:HB3	2.18	0.42
1:K:1021:CME:HZ3	1:K:1022:GLN:O	2.19	0.42
1:L:46:ARG:NH1	1:L:46:ARG:CG	2.78	0.42
1:L:46:ARG:HB3	1:L:47:PRO:HD2	2.00	0.42
1:L:184:LEU:HD23	1:L:184:LEU:HA	1.83	0.42
1:L:285:TYR:HB3	1:L:288:ARG:HG3	2.01	0.42
1:L:391:HIS:ND1	1:L:412:GLU:OE1	2.44	0.42
1:L:568:TRP:CD2	1:L:569:ASP:HB3	2.54	0.42
1:L:708:TRP:CZ3	1:L:709:SER:HB3	2.54	0.42
1:L:1004:SER:HB2	1:L:1006:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:6:SER:O	1:M:7:LEU:C	2.60	0.42
1:M:46:ARG:HB3	1:M:47:PRO:HD2	2.00	0.42
1:M:210:ARG:HH11	1:M:395:HIS:CA	2.32	0.42
1:M:237:ARG:CG	1:M:237:ARG:NH1	2.82	0.42
1:M:679:LEU:HD23	1:M:679:LEU:HA	1.26	0.42
1:N:718:GLN:HG3	1:N:719:GLN:N	2.34	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
1:O:476:LYS:HD2	1:O:476:LYS:HA	1.81	0.42
1:O:655:MET:HB2	1:O:655:MET:HE3	1.60	0.42
1:O:807:VAL:HG13	1:O:808:GLU:N	2.34	0.42
1:O:895:VAL:O	1:O:919:ASP:HA	2.19	0.42
1:P:35:SER:O	1:P:50:GLN:HG3	2.18	0.42
1:P:110:ASN:O	1:P:113:PHE:HB2	2.19	0.42
1:P:429:ASP:OD1	1:P:431:ARG:HD3	2.18	0.42
1:P:657:ALA:HA	1:P:661:LYS:O	2.19	0.42
1:P:823:LEU:HA	1:P:823:LEU:HD23	1.73	0.42
1:A:63:PHE:CD1	1:A:63:PHE:N	2.86	0.42
1:A:141:ILE:HD13	1:A:143:PHE:CE1	2.55	0.42
1:A:257:THR:OG1	1:A:316:HIS:HE1	2.03	0.42
1:A:502:MET:HA	1:A:537:GLU:O	2.20	0.42
1:A:657:ALA:HA	1:A:661:LYS:O	2.19	0.42
1:A:745:MET:HA	1:A:745:MET:CE	2.44	0.42
1:A:1018:LEU:HD22	1:A:1019:VAL:N	2.35	0.42
1:B:141:ILE:HD13	1:B:143:PHE:CE1	2.55	0.42
1:B:559:TYR:HA	1:B:560:PRO:HD2	1.74	0.42
1:C:85:VAL:HG12	1:C:86:VAL:N	2.35	0.42
1:C:131:GLU:O	1:C:132:SER:C	2.60	0.42
1:C:210:ARG:HH11	1:C:395:HIS:CA	2.32	0.42
1:C:502:MET:HA	1:C:537:GLU:O	2.20	0.42
1:C:637:GLU:HA	1:C:679:LEU:HD23	2.01	0.42
1:C:651:LEU:HD12	1:C:668:VAL:O	2.19	0.42
1:C:1004:SER:HB2	1:C:1006:GLU:OE2	2.20	0.42
1:D:18:ASN:OD1	1:D:19:PRO:HD2	2.20	0.42
1:D:43:ARG:NH1	1:D:44:THR:HG23	2.34	0.42
1:D:46:ARG:HB3	1:D:47:PRO:HD2	2.00	0.42
1:D:85:VAL:HG12	1:D:86:VAL:N	2.34	0.42
1:D:570:TRP:HD1	1:D:571:VAL:HG22	1.84	0.42
1:E:18:ASN:OD1	1:E:19:PRO:HD2	2.20	0.42
1:E:43:ARG:NH1	1:E:44:THR:HG23	2.34	0.42
1:E:93:HIS:HB3	1:E:95:TYR:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:THR:OG1	1:E:316:HIS:HE1	2.03	0.42
1:E:421:VAL:O	1:E:425:ARG:NH1	2.46	0.42
1:E:502:MET:HA	1:E:537:GLU:O	2.20	0.42
1:E:597:ASN:ND2	1:E:599:ARG:H	2.17	0.42
1:F:18:ASN:OD1	1:F:19:PRO:HD2	2.20	0.42
1:F:138:GLN:N	1:F:217:LYS:O	2.36	0.42
1:F:682:LEU:HD23	1:F:682:LEU:HA	1.67	0.42
1:F:730:LEU:HA	1:F:731:PRO:HD3	1.74	0.42
1:F:781:ARG:NH1	1:F:781:ARG:CG	2.79	0.42
1:G:131:GLU:HA	1:G:134:LEU:HB2	2.00	0.42
1:G:200:GLN:OE1	1:G:200:GLN:N	2.44	0.42
1:G:347:LYS:HA	1:G:348:PRO:HD3	1.77	0.42
1:G:375:ASP:O	1:G:379:MET:HG3	2.19	0.42
1:G:548:GLY:O	1:G:549:PHE:C	2.63	0.42
1:H:454:ILE:C	1:H:455:ILE:HG13	2.43	0.42
1:H:778:THR:CG2	1:H:887:GLN:H	2.32	0.42
1:H:807:VAL:HG13	1:H:808:GLU:N	2.34	0.42
1:H:895:VAL:O	1:H:919:ASP:HA	2.19	0.42
1:I:49:GLN:C	1:I:51:LEU:H	2.28	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:I:347:LYS:HA	1:I:348:PRO:HD3	1.77	0.42
1:I:655:MET:HE3	1:I:655:MET:HB2	1.60	0.42
1:I:722:LEU:HD23	1:I:722:LEU:HA	1.75	0.42
1:J:35:SER:O	1:J:50:GLN:HG3	2.18	0.42
1:J:257:THR:OG1	1:J:316:HIS:HE1	2.03	0.42
1:J:1018:LEU:HD22	1:J:1019:VAL:N	2.35	0.42
1:K:708:TRP:CZ3	1:K:709:SER:HB3	2.54	0.42
1:K:778:THR:CG2	1:K:887:GLN:H	2.32	0.42
1:K:800:ARG:CZ	1:K:800:ARG:CB	2.98	0.42
1:K:1004:SER:HB2	1:K:1006:GLU:OE2	2.20	0.42
1:L:49:GLN:C	1:L:51:LEU:H	2.28	0.42
1:L:375:ASP:O	1:L:379:MET:HG3	2.19	0.42
1:L:475:ILE:O	1:L:476:LYS:C	2.63	0.42
1:L:597:ASN:ND2	1:L:599:ARG:H	2.17	0.42
1:L:612:THR:HA	1:L:613:PRO:HD3	1.68	0.42
1:L:694:LEU:HD12	1:L:694:LEU:HA	1.69	0.42
1:L:701:VAL:CG1	1:L:702:GLN:N	2.81	0.42
1:L:730:LEU:HA	1:L:731:PRO:HD3	1.74	0.42
1:L:1018:LEU:HD22	1:L:1019:VAL:N	2.35	0.42
1:M:469:ASP:HB3	1:P:473:ARG:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:522:LYS:O	1:M:523:TRP:C	2.61	0.42
1:N:548:GLY:O	1:N:549:PHE:C	2.62	0.42
1:N:701:VAL:CG1	1:N:702:GLN:N	2.81	0.42
1:N:781:ARG:NH1	1:N:781:ARG:CG	2.79	0.42
1:O:131:GLU:HA	1:O:134:LEU:HB2	1.99	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:P:149:ALA:O	1:P:150:PHE:HB3	2.18	0.42
1:P:377:LEU:HD23	1:P:377:LEU:HA	1.91	0.42
1:P:1004:SER:HB2	1:P:1006:GLU:OE2	2.20	0.42
1:P:1018:LEU:HD22	1:P:1019:VAL:N	2.34	0.42
1:A:18:ASN:OD1	1:A:19:PRO:HD2	2.20	0.42
1:A:34:ALA:HB3	1:A:36:TRP:CE3	2.54	0.42
1:A:1020:TRP:CD1	1:A:1020:TRP:C	2.97	0.42
1:B:369:GLU:O	1:B:373:VAL:HG23	2.19	0.42
1:B:701:VAL:HG12	1:B:702:GLN:H	1.83	0.42
1:C:822:LEU:HD13	1:C:822:LEU:HA	1.88	0.42
1:D:214:LEU:HD23	1:D:214:LEU:HA	1.84	0.42
1:D:657:ALA:HA	1:D:661:LYS:O	2.19	0.42
1:D:694:LEU:O	1:D:722:LEU:N	2.51	0.42
1:D:778:THR:CG2	1:D:887:GLN:H	2.32	0.42
1:D:895:VAL:O	1:D:919:ASP:HA	2.19	0.42
1:E:570:TRP:HD1	1:E:571:VAL:HG22	1.84	0.42
1:E:800:ARG:CZ	1:E:800:ARG:CB	2.98	0.42
1:E:895:VAL:O	1:E:919:ASP:HA	2.19	0.42
1:E:1021:CME:HZ3	1:E:1022:GLN:O	2.19	0.42
1:F:141:ILE:HD13	1:F:143:PHE:CE1	2.55	0.42
1:F:272:ALA:HB1	1:F:273:PRO:CD	2.47	0.42
1:F:583:ASN:HA	1:F:584:PRO:HD3	1.79	0.42
1:F:763:GLY:HA3	1:F:822:LEU:HD22	2.01	0.42
1:F:869:ASP:CG	1:F:1015:HIS:HD1	2.24	0.42
1:G:35:SER:O	1:G:50:GLN:HG3	2.18	0.42
1:H:18:ASN:OD1	1:H:19:PRO:HD2	2.20	0.42
1:H:141:ILE:HD13	1:H:143:PHE:CE1	2.55	0.42
1:H:256:VAL:O	1:H:271:THR:HA	2.20	0.42
1:H:778:THR:HB	1:H:887:GLN:CB	2.48	0.42
1:I:34:ALA:HB3	1:I:36:TRP:CE3	2.54	0.42
1:I:141:ILE:HD13	1:I:143:PHE:CE1	2.55	0.42
1:I:272:ALA:HB1	1:I:273:PRO:CD	2.47	0.42
1:I:469:ASP:HB3	1:L:473:ARG:HD2	2.01	0.42
1:J:44:THR:O	1:J:45:ASP:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:131:GLU:HA	1:J:134:LEU:HB2	2.00	0.42
1:J:746:ASP:HA	1:J:760:ARG:CG	2.39	0.42
1:K:49:GLN:C	1:K:51:LEU:H	2.28	0.42
1:K:210:ARG:HH11	1:K:395:HIS:CA	2.32	0.42
1:K:285:TYR:HB3	1:K:288:ARG:HG3	2.01	0.42
1:K:531:ARG:O	1:K:561:ARG:NH1	2.46	0.42
1:K:718:GLN:HG3	1:K:719:GLN:N	2.33	0.42
1:K:1020:TRP:CD1	1:K:1020:TRP:C	2.97	0.42
1:L:18:ASN:OD1	1:L:19:PRO:HD2	2.20	0.42
1:L:43:ARG:HH11	1:L:43:ARG:CG	2.10	0.42
1:L:369:GLU:O	1:L:373:VAL:HG23	2.19	0.42
1:L:445:GLN:HE21	1:L:445:GLN:HB3	1.54	0.42
1:M:18:ASN:OD1	1:M:19:PRO:HD2	2.20	0.42
1:M:568:TRP:CD2	1:M:569:ASP:HB3	2.54	0.42
1:M:823:LEU:HD23	1:M:823:LEU:HA	1.73	0.42
1:N:43:ARG:NH1	1:N:44:THR:HG23	2.34	0.42
1:N:141:ILE:HD13	1:N:143:PHE:CE1	2.55	0.42
1:N:372:MET:HE1	1:N:395:HIS:HB3	2.00	0.42
1:N:568:TRP:CD2	1:N:569:ASP:HB3	2.54	0.42
1:O:85:VAL:HG12	1:O:86:VAL:N	2.35	0.42
1:O:568:TRP:CD2	1:O:569:ASP:HB3	2.54	0.42
1:O:933:SER:O	1:O:934:GLU:C	2.62	0.42
1:O:1018:LEU:HD22	1:O:1019:VAL:N	2.35	0.42
1:P:230:ARG:NH2	1:P:241:GLU:OE2	2.50	0.42
1:P:234:ASP:O	1:P:235:PHE:HB2	2.17	0.42
1:P:651:LEU:HD12	1:P:668:VAL:O	2.19	0.42
1:A:149:ALA:O	1:A:150:PHE:HB3	2.18	0.42
1:A:256:VAL:O	1:A:271:THR:HA	2.20	0.42
1:B:264:GLU:OE2	1:B:264:GLU:HA	2.17	0.42
1:B:745:MET:HA	1:B:745:MET:CE	2.43	0.42
1:C:18:ASN:OD1	1:C:19:PRO:HD2	2.20	0.42
1:C:43:ARG:NH1	1:C:44:THR:HG23	2.34	0.42
1:C:141:ILE:HD13	1:C:143:PHE:CE1	2.55	0.42
1:C:895:VAL:O	1:C:919:ASP:HA	2.19	0.42
1:D:110:ASN:O	1:D:113:PHE:HB2	2.19	0.42
1:D:285:TYR:HB3	1:D:288:ARG:HG3	2.01	0.42
1:E:612:THR:HA	1:E:613:PRO:HD3	1.68	0.42
1:E:668:VAL:HG13	1:E:669:PRO:CD	2.38	0.42
1:F:102:ASN:ND2	1:F:201:ASP:CB	2.78	0.42
1:F:285:TYR:HB3	1:F:288:ARG:HG3	2.01	0.42
1:F:425:ARG:NH2	1:G:287:ASP:OD2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:931:PHE:CD2	1:F:931:PHE:C	2.98	0.42
1:G:34:ALA:HB3	1:G:36:TRP:CE3	2.54	0.42
1:G:184:LEU:HA	1:G:184:LEU:HD23	1.83	0.42
1:G:391:HIS:ND1	1:G:412:GLU:OE1	2.44	0.42
1:G:694:LEU:HA	1:G:694:LEU:HD12	1.69	0.42
1:H:149:ALA:O	1:H:150:PHE:HB3	2.18	0.42
1:H:230:ARG:NH2	1:H:241:GLU:OE2	2.51	0.42
1:H:502:MET:HA	1:H:537:GLU:O	2.20	0.42
1:H:597:ASN:ND2	1:H:599:ARG:H	2.17	0.42
1:H:685:LEU:HA	1:H:686:PRO:HD3	1.70	0.42
1:I:149:ALA:O	1:I:150:PHE:HB3	2.18	0.42
1:I:221:GLN:H	1:I:221:GLN:HG2	1.70	0.42
1:I:344:LEU:N	1:I:347:LYS:O	2.36	0.42
1:I:476:LYS:HA	1:I:476:LYS:HD2	1.81	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:J:85:VAL:HG12	1:J:86:VAL:N	2.34	0.42
1:J:90:TRP:HE1	1:J:96:ASP:CG	2.28	0.42
1:J:933:SER:O	1:J:934:GLU:C	2.62	0.42
1:J:1021:CME:HZ3	1:J:1022:GLN:O	2.19	0.42
1:K:18:ASN:OD1	1:K:19:PRO:HD2	2.20	0.42
1:K:147:ASN:HB2	1:K:165:SER:HB3	2.01	0.42
1:K:210:ARG:NH1	1:K:394:ASN:C	2.77	0.42
1:K:369:GLU:O	1:K:373:VAL:HG23	2.19	0.42
1:K:475:ILE:O	1:K:476:LYS:C	2.63	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:M:93:HIS:HB3	1:M:95:TYR:HE1	1.84	0.42
1:M:240:LEU:HD12	1:M:240:LEU:C	2.36	0.42
1:M:257:THR:OG1	1:M:316:HIS:HE1	2.03	0.42
1:M:931:PHE:CD2	1:M:931:PHE:C	2.98	0.42
1:N:90:TRP:HE1	1:N:96:ASP:CG	2.28	0.42
1:N:114:VAL:HG21	1:N:192:SER:N	2.35	0.42
1:N:285:TYR:HB3	1:N:288:ARG:HG3	2.01	0.42
1:N:694:LEU:HD12	1:N:694:LEU:HA	1.69	0.42
1:N:870:VAL:CG1	1:N:871:GLU:N	2.81	0.42
1:O:34:ALA:HB3	1:O:36:TRP:CE3	2.54	0.42
1:O:35:SER:O	1:O:50:GLN:HG3	2.18	0.42
1:O:189:LEU:N	1:O:189:LEU:CD2	2.75	0.42
1:P:93:HIS:HB3	1:P:95:TYR:HE1	1.84	0.42
1:P:708:TRP:CZ3	1:P:709:SER:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:HH11	1:D:419:GLY:HA2	1.84	0.42
1:A:391:HIS:ND1	1:A:412:GLU:OE1	2.44	0.42
1:A:423:MET:HB2	1:D:282:ARG:CG	2.44	0.42
1:A:722:LEU:HD23	1:A:722:LEU:HA	1.75	0.42
1:A:931:PHE:CD2	1:A:931:PHE:C	2.98	0.42
1:B:18:ASN:OD1	1:B:19:PRO:HD2	2.20	0.42
1:B:475:ILE:O	1:B:476:LYS:C	2.63	0.42
1:B:645:ARG:NH2	1:B:650:GLU:OE2	2.48	0.42
1:C:285:TYR:HB3	1:C:288:ARG:HG3	2.01	0.42
1:C:670:LEU:HA	1:C:670:LEU:HD23	1.67	0.42
1:C:701:VAL:HG12	1:C:702:GLN:H	1.82	0.42
1:C:708:TRP:CZ3	1:C:709:SER:HB3	2.54	0.42
1:D:90:TRP:HE1	1:D:96:ASP:CG	2.28	0.42
1:D:685:LEU:HA	1:D:686:PRO:HD3	1.70	0.42
1:E:256:VAL:O	1:E:271:THR:HA	2.20	0.42
1:E:522:LYS:O	1:E:523:TRP:C	2.61	0.42
1:E:548:GLY:O	1:E:549:PHE:C	2.62	0.42
1:E:781:ARG:HH11	1:E:781:ARG:CG	2.19	0.42
1:E:870:VAL:CG1	1:E:871:GLU:N	2.81	0.42
1:E:931:PHE:CD2	1:E:931:PHE:C	2.98	0.42
1:E:1004:SER:HB2	1:E:1006:GLU:OE2	2.20	0.42
1:F:90:TRP:HE1	1:F:96:ASP:CG	2.28	0.42
1:F:147:ASN:HB2	1:F:165:SER:HB3	2.02	0.42
1:F:372:MET:HE1	1:F:395:HIS:HB3	2.00	0.42
1:G:118:ASN:HA	1:G:119:PRO:HD2	1.60	0.42
1:G:256:VAL:O	1:G:271:THR:HA	2.20	0.42
1:G:257:THR:OG1	1:G:316:HIS:HE1	2.03	0.42
1:G:260:LEU:HD12	1:G:310:ARG:O	2.19	0.42
1:G:476:LYS:HD2	1:G:476:LYS:HA	1.81	0.42
1:G:579:ASP:OD1	1:G:583:ASN:N	2.43	0.42
1:H:110:ASN:O	1:H:113:PHE:HB2	2.19	0.42
1:H:230:ARG:HH11	1:H:230:ARG:CG	2.24	0.42
1:H:260:LEU:HD12	1:H:260:LEU:HA	1.61	0.42
1:H:701:VAL:CG1	1:H:702:GLN:N	2.81	0.42
1:H:800:ARG:CZ	1:H:800:ARG:CB	2.98	0.42
1:H:1004:SER:HB2	1:H:1006:GLU:OE2	2.20	0.42
1:I:44:THR:O	1:I:45:ASP:C	2.61	0.42
1:I:46:ARG:HB3	1:I:47:PRO:HD2	2.00	0.42
1:I:57:GLU:HG2	1:I:83:THR:HG21	1.93	0.42
1:I:645:ARG:NH2	1:I:650:GLU:OE2	2.48	0.42
1:I:931:PHE:CD2	1:I:931:PHE:C	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:972:HIS:HB3	5:I:2155:HOH:O	2.18	0.42
1:J:178:ARG:HH11	1:J:178:ARG:CB	2.33	0.42
1:J:256:VAL:O	1:J:271:THR:HA	2.20	0.42
1:J:418:HIS:O	1:K:282:ARG:HD3	2.20	0.42
1:J:763:GLY:HA3	1:J:822:LEU:HD22	2.01	0.42
1:J:800:ARG:CZ	1:J:800:ARG:CB	2.98	0.42
1:L:637:GLU:HA	1:L:679:LEU:HD23	2.01	0.42
1:M:281:GLU:HG3	1:P:515:VAL:HG21	2.02	0.42
1:M:375:ASP:O	1:M:379:MET:HG3	2.19	0.42
1:M:673:ALA:O	1:M:676:GLY:N	2.47	0.42
1:M:800:ARG:CZ	1:M:800:ARG:CB	2.98	0.42
1:M:1004:SER:HB2	1:M:1006:GLU:OE2	2.20	0.42
1:N:111:PRO:HA	1:N:112:PRO:HA	1.57	0.42
1:N:221:GLN:H	1:N:221:GLN:HG2	1.70	0.42
1:N:583:ASN:HA	1:N:584:PRO:HD3	1.79	0.42
1:N:869:ASP:CG	1:N:1015:HIS:HD1	2.24	0.42
1:N:931:PHE:CD2	1:N:931:PHE:C	2.98	0.42
1:N:972:HIS:HB3	5:N:2158:HOH:O	2.18	0.42
1:O:118:ASN:HA	1:O:119:PRO:HD2	1.60	0.42
1:O:141:ILE:HD13	1:O:143:PHE:CE1	2.55	0.42
1:O:931:PHE:CD2	1:O:931:PHE:C	2.98	0.42
1:P:70:PRO:O	1:P:73:TRP:N	2.45	0.42
1:P:78:LEU:HB3	1:P:79:PRO:CD	2.45	0.42
1:P:138:GLN:N	1:P:217:LYS:O	2.36	0.42
1:P:141:ILE:HD13	1:P:143:PHE:CE1	2.55	0.42
1:P:256:VAL:O	1:P:271:THR:HA	2.20	0.42
1:P:933:SER:O	1:P:934:GLU:C	2.62	0.42
1:A:114:VAL:HG21	1:A:192:SER:N	2.34	0.42
1:A:373:VAL:O	1:A:374:GLN:C	2.57	0.42
1:A:378:LEU:HD23	1:A:378:LEU:HA	1.53	0.42
1:A:546:LEU:HD12	1:A:546:LEU:HA	1.84	0.42
1:B:93:HIS:HB3	1:B:95:TYR:HE1	1.84	0.42
1:B:118:ASN:HA	1:B:119:PRO:HD2	1.60	0.42
1:B:178:ARG:HH11	1:B:178:ARG:CB	2.33	0.42
1:B:1018:LEU:HD22	1:B:1019:VAL:N	2.35	0.42
1:C:90:TRP:HE1	1:C:96:ASP:CG	2.28	0.42
1:C:264:GLU:OE2	1:C:264:GLU:HA	2.17	0.42
1:C:933:SER:O	1:C:934:GLU:C	2.62	0.42
1:D:476:LYS:HA	1:D:476:LYS:HD2	1.81	0.42
1:E:90:TRP:HE1	1:E:96:ASP:CG	2.28	0.42
1:E:282:ARG:NH1	1:H:419:GLY:HA2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:475:ILE:O	1:E:476:LYS:C	2.63	0.42
1:E:718:GLN:HG3	1:E:719:GLN:N	2.34	0.42
1:F:367:MET:HB3	1:F:367:MET:HE3	1.72	0.42
1:F:390:SER:HA	1:F:391:HIS:HA	1.91	0.42
1:G:316:HIS:HA	1:G:323:ILE:HD12	1.99	0.42
1:G:670:LEU:HD23	1:G:670:LEU:HA	1.67	0.42
1:H:114:VAL:HG21	1:H:192:SER:N	2.35	0.42
1:H:147:ASN:HB2	1:H:165:SER:HB3	2.02	0.42
1:H:200:GLN:OE1	1:H:200:GLN:N	2.44	0.42
1:H:237:ARG:CG	1:H:237:ARG:NH1	2.81	0.42
1:H:363:HIS:CD2	1:H:363:HIS:N	2.81	0.42
1:H:757:GLN:O	1:H:757:GLN:HG2	2.12	0.42
1:I:114:VAL:HG21	1:I:192:SER:N	2.35	0.42
1:I:360:HIS:ND1	1:I:362:LEU:HB2	2.35	0.42
1:I:1004:SER:HB2	1:I:1006:GLU:OE2	2.20	0.42
1:J:597:ASN:ND2	1:J:599:ARG:H	2.17	0.42
1:J:726:LEU:HD23	1:J:726:LEU:HA	1.65	0.42
1:K:214:LEU:HD23	1:K:214:LEU:HA	1.84	0.42
1:K:257:THR:OG1	1:K:316:HIS:HE1	2.03	0.42
1:K:931:PHE:CD2	1:K:931:PHE:C	2.98	0.42
1:L:264:GLU:OE2	1:L:264:GLU:HA	2.17	0.42
1:L:657:ALA:HA	1:L:661:LYS:O	2.19	0.42
1:L:807:VAL:HG13	1:L:808:GLU:N	2.34	0.42
1:M:90:TRP:HE1	1:M:96:ASP:CG	2.28	0.42
1:M:256:VAL:O	1:M:271:THR:HA	2.20	0.42
1:M:475:ILE:O	1:M:476:LYS:C	2.63	0.42
1:M:718:GLN:HG3	1:M:719:GLN:N	2.34	0.42
1:M:781:ARG:HH11	1:M:781:ARG:CG	2.19	0.42
1:N:147:ASN:HB2	1:N:165:SER:HB3	2.02	0.42
1:N:210:ARG:NH1	1:N:394:ASN:C	2.77	0.42
1:N:234:ASP:OD1	1:N:236:SER:HB3	2.20	0.42
1:N:256:VAL:O	1:N:271:THR:HA	2.20	0.42
1:N:772:ASP:OD1	1:N:772:ASP:N	2.30	0.42
1:N:895:VAL:O	1:N:919:ASP:HA	2.19	0.42
1:O:114:VAL:HG21	1:O:192:SER:N	2.34	0.42
1:O:184:LEU:HA	1:O:184:LEU:HD23	1.84	0.42
1:O:234:ASP:OD1	1:O:236:SER:HB3	2.20	0.42
1:O:256:VAL:O	1:O:271:THR:HA	2.20	0.42
1:O:579:ASP:OD1	1:O:583:ASN:N	2.43	0.42
1:P:147:ASN:HB2	1:P:165:SER:HB3	2.02	0.42
1:P:173:LEU:HD23	1:P:173:LEU:HA	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:VAL:HG12	1:A:70:PRO:N	2.35	0.42
1:A:612:THR:HA	1:A:613:PRO:HD3	1.68	0.42
1:A:807:VAL:HG13	1:A:808:GLU:N	2.34	0.42
1:A:961:ARG:NH2	1:A:979:GLU:O	2.37	0.42
1:B:531:ARG:O	1:B:561:ARG:NH1	2.46	0.42
1:C:114:VAL:HG21	1:C:192:SER:N	2.35	0.42
1:D:141:ILE:HD13	1:D:143:PHE:CE1	2.55	0.42
1:D:178:ARG:HH11	1:D:178:ARG:CB	2.33	0.42
1:D:230:ARG:HH11	1:D:230:ARG:CG	2.24	0.42
1:D:513:PRO:O	1:D:514:ALA:HB3	2.20	0.42
1:D:869:ASP:CG	1:D:1015:HIS:HD1	2.24	0.42
1:E:78:LEU:HB3	1:E:79:PRO:CD	2.45	0.42
1:E:114:VAL:HG21	1:E:192:SER:N	2.35	0.42
1:E:360:HIS:HA	1:E:361:PRO:HD3	1.86	0.42
1:F:10:VAL:C	1:F:12:GLN:H	2.28	0.42
1:F:210:ARG:NH1	1:F:394:ASN:C	2.77	0.42
1:F:210:ARG:HH11	1:F:395:HIS:CA	2.32	0.42
1:F:933:SER:O	1:F:934:GLU:C	2.62	0.42
1:G:178:ARG:HH11	1:G:178:ARG:CB	2.33	0.42
1:G:360:HIS:ND1	1:G:362:LEU:HB2	2.35	0.42
1:G:870:VAL:CG1	1:G:871:GLU:N	2.81	0.42
1:H:44:THR:O	1:H:45:ASP:C	2.61	0.42
1:H:257:THR:OG1	1:H:316:HIS:HE1	2.03	0.42
1:H:260:LEU:HD12	1:H:310:ARG:O	2.19	0.42
1:I:425:ARG:NH2	1:L:287:ASP:CG	2.78	0.42
1:I:502:MET:HA	1:I:537:GLU:O	2.20	0.42
1:J:93:HIS:HB3	1:J:95:TYR:HE1	1.84	0.42
1:J:285:TYR:HB3	1:J:288:ARG:HG3	2.01	0.42
1:K:256:VAL:O	1:K:271:THR:HA	2.20	0.42
1:K:657:ALA:HA	1:K:661:LYS:O	2.19	0.42
1:K:670:LEU:HD23	1:K:670:LEU:HA	1.67	0.42
1:L:43:ARG:NH1	1:L:44:THR:HG23	2.34	0.42
1:L:46:ARG:HB3	1:L:47:PRO:CD	2.50	0.42
1:L:141:ILE:HD13	1:L:143:PHE:CE1	2.55	0.42
1:L:257:THR:OG1	1:L:316:HIS:HE1	2.03	0.42
1:L:513:PRO:O	1:L:514:ALA:HB3	2.20	0.42
1:L:778:THR:CG2	1:L:887:GLN:H	2.32	0.42
1:M:37:ARG:CG	1:M:37:ARG:NH1	2.79	0.42
1:M:360:HIS:ND1	1:M:362:LEU:HB2	2.35	0.42
1:M:425:ARG:NH2	1:P:287:ASP:CG	2.57	0.42
1:N:69:VAL:HG12	1:N:70:PRO:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:763:GLY:HA3	1:N:822:LEU:HD22	2.01	0.42
1:N:906:TYR:HB3	1:N:907:PRO:CD	2.50	0.42
1:O:18:ASN:OD1	1:O:19:PRO:HD2	2.20	0.42
1:O:178:ARG:HH11	1:O:178:ARG:CB	2.33	0.42
1:O:210:ARG:NH1	1:O:394:ASN:C	2.77	0.42
1:O:260:LEU:HD12	1:O:310:ARG:O	2.19	0.42
1:O:360:HIS:ND1	1:O:362:LEU:HB2	2.35	0.42
1:P:4:THR:CA	1:P:9:VAL:HG11	2.47	0.42
1:P:85:VAL:HG12	1:P:86:VAL:N	2.34	0.42
1:P:476:LYS:HA	1:P:476:LYS:HD2	1.81	0.42
1:P:597:ASN:ND2	1:P:599:ARG:H	2.17	0.42
1:P:895:VAL:O	1:P:919:ASP:HA	2.19	0.42
1:A:43:ARG:NH1	1:A:44:THR:HG23	2.34	0.41
1:A:46:ARG:HB3	1:A:47:PRO:CD	2.50	0.41
1:A:93:HIS:HB3	1:A:95:TYR:HE1	1.84	0.41
1:A:282:ARG:HB2	1:D:422:PRO:HA	2.01	0.41
1:A:513:PRO:O	1:A:514:ALA:HB3	2.20	0.41
1:B:10:VAL:C	1:B:12:GLN:H	2.28	0.41
1:B:200:GLN:OE1	1:B:200:GLN:N	2.44	0.41
1:B:256:VAL:O	1:B:271:THR:HA	2.20	0.41
1:B:257:THR:HA	1:B:270:GLY:O	2.20	0.41
1:B:570:TRP:HD1	1:B:571:VAL:HG22	1.84	0.41
1:B:580:GLU:CD	1:B:580:GLU:N	2.78	0.41
1:B:655:MET:HB2	1:B:655:MET:HE3	1.60	0.41
1:B:778:THR:CG2	1:B:887:GLN:H	2.32	0.41
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.54	0.41
1:C:772:ASP:OD1	1:C:772:ASP:N	2.30	0.41
1:C:1018:LEU:HD22	1:C:1019:VAL:N	2.35	0.41
1:D:46:ARG:HB3	1:D:47:PRO:CD	2.50	0.41
1:D:49:GLN:C	1:D:51:LEU:H	2.28	0.41
1:D:230:ARG:NH2	1:D:241:GLU:OE2	2.51	0.41
1:D:251:ARG:CB	1:D:253:TYR:CE2	2.98	0.41
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.54	0.41
1:D:931:PHE:CD2	1:D:931:PHE:C	2.98	0.41
1:E:46:ARG:HB3	1:E:47:PRO:CD	2.50	0.41
1:E:285:TYR:HB3	1:E:288:ARG:HG3	2.01	0.41
1:E:369:GLU:O	1:E:373:VAL:HG23	2.19	0.41
1:E:542:MET:HE3	1:E:601:PHE:HA	2.02	0.41
1:E:568:TRP:CD2	1:E:569:ASP:HB3	2.54	0.41
1:F:257:THR:HA	1:F:270:GLY:O	2.20	0.41
1:F:542:MET:HE3	1:F:601:PHE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:807:VAL:HG13	1:F:808:GLU:N	2.34	0.41
1:G:18:ASN:OD1	1:G:19:PRO:HD2	2.20	0.41
1:G:147:ASN:HA	1:G:148:SER:HA	1.54	0.41
1:G:378:LEU:HD23	1:G:378:LEU:HA	1.53	0.41
1:G:513:PRO:O	1:G:514:ALA:HB3	2.20	0.41
1:G:651:LEU:HD12	1:G:668:VAL:O	2.19	0.41
1:H:43:ARG:HH11	1:H:43:ARG:CG	2.10	0.41
1:H:178:ARG:HH11	1:H:178:ARG:CB	2.33	0.41
1:H:896:ASN:HA	1:H:918:TRP:O	2.20	0.41
1:H:931:PHE:CD2	1:H:931:PHE:C	2.98	0.41
1:H:1020:TRP:CD1	1:H:1020:TRP:C	2.97	0.41
1:I:10:VAL:C	1:I:12:GLN:H	2.28	0.41
1:I:110:ASN:O	1:I:113:PHE:HB2	2.19	0.41
1:I:178:ARG:HH11	1:I:178:ARG:CB	2.33	0.41
1:I:257:THR:HA	1:I:270:GLY:O	2.20	0.41
1:I:570:TRP:HD1	1:I:571:VAL:HG22	1.84	0.41
1:I:651:LEU:HD13	1:I:651:LEU:HA	1.51	0.41
1:J:138:GLN:N	1:J:217:LYS:O	2.36	0.41
1:J:214:LEU:HD23	1:J:214:LEU:HA	1.84	0.41
1:J:336:ARG:HH11	1:J:336:ARG:CG	2.26	0.41
1:J:502:MET:HA	1:J:537:GLU:O	2.20	0.41
1:J:645:ARG:NH2	1:J:650:GLU:OE2	2.48	0.41
1:J:718:GLN:HG3	1:J:719:GLN:N	2.34	0.41
1:J:995:GLY:O	1:J:996:ASP:C	2.62	0.41
1:K:24:LEU:HD12	1:K:24:LEU:HA	1.62	0.41
1:K:350:LEU:HD12	1:K:350:LEU:HA	1.78	0.41
1:K:502:MET:HA	1:K:537:GLU:O	2.20	0.41
1:K:579:ASP:OD1	1:K:583:ASN:N	2.43	0.41
1:L:800:ARG:CZ	1:L:800:ARG:CB	2.98	0.41
1:L:900:LEU:HB2	1:L:939:CYS:O	2.20	0.41
1:M:114:VAL:HG21	1:M:192:SER:N	2.34	0.41
1:M:200:GLN:OE1	1:M:200:GLN:N	2.44	0.41
1:M:231:PHE:CD1	1:M:231:PHE:N	2.88	0.41
1:M:502:MET:HA	1:M:537:GLU:O	2.20	0.41
1:N:10:VAL:C	1:N:12:GLN:H	2.28	0.41
1:N:34:ALA:HB3	1:N:36:TRP:CE3	2.54	0.41
1:N:73:TRP:O	1:N:183:ARG:NH1	2.48	0.41
1:N:542:MET:HE3	1:N:601:PHE:HA	2.02	0.41
1:O:378:LEU:HD23	1:O:378:LEU:HA	1.53	0.41
1:O:673:ALA:O	1:O:676:GLY:N	2.47	0.41
1:O:1020:TRP:CD1	1:O:1020:TRP:C	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:34:ALA:HB3	1:P:36:TRP:CE3	2.54	0.41
1:P:90:TRP:HE1	1:P:96:ASP:CG	2.28	0.41
1:P:114:VAL:HG21	1:P:192:SER:N	2.34	0.41
1:P:178:ARG:HH11	1:P:178:ARG:CB	2.33	0.41
1:P:502:MET:HA	1:P:537:GLU:O	2.20	0.41
1:P:548:GLY:O	1:P:549:PHE:C	2.63	0.41
1:P:757:GLN:O	1:P:757:GLN:HG2	2.12	0.41
1:P:800:ARG:CZ	1:P:800:ARG:CB	2.98	0.41
1:A:66:PRO:CB	1:A:187:MET:HE1	2.50	0.41
1:A:568:TRP:CD1	1:A:568:TRP:C	2.99	0.41
1:A:906:TYR:HB3	1:A:907:PRO:CD	2.50	0.41
1:B:46:ARG:HB3	1:B:47:PRO:CD	2.50	0.41
1:B:90:TRP:HE1	1:B:96:ASP:CG	2.28	0.41
1:B:778:THR:HB	1:B:887:GLN:CB	2.48	0.41
1:C:46:ARG:HB3	1:C:47:PRO:CD	2.50	0.41
1:C:363:HIS:CD2	1:C:363:HIS:N	2.81	0.41
1:C:597:ASN:ND2	1:C:599:ARG:H	2.17	0.41
1:C:781:ARG:NH1	1:C:781:ARG:CG	2.79	0.41
1:D:231:PHE:CD1	1:D:231:PHE:N	2.88	0.41
1:D:323:ILE:CD1	1:D:323:ILE:N	2.82	0.41
1:D:637:GLU:HA	1:D:679:LEU:HD23	2.01	0.41
1:D:1018:LEU:HD22	1:D:1019:VAL:N	2.35	0.41
1:E:66:PRO:CB	1:E:187:MET:HE1	2.50	0.41
1:F:34:ALA:HB3	1:F:36:TRP:CE3	2.54	0.41
1:F:46:ARG:HB3	1:F:47:PRO:CD	2.50	0.41
1:F:531:ARG:O	1:F:561:ARG:NH1	2.46	0.41
1:F:570:TRP:HD1	1:F:571:VAL:HG22	1.84	0.41
1:G:46:ARG:HB3	1:G:47:PRO:CD	2.50	0.41
1:G:147:ASN:HB2	1:G:165:SER:HB3	2.02	0.41
1:G:668:VAL:HG13	1:G:669:PRO:CD	2.38	0.41
1:G:778:THR:HB	1:G:887:GLN:CB	2.49	0.41
1:G:869:ASP:CG	1:G:1015:HIS:HD1	2.24	0.41
1:H:34:ALA:HB3	1:H:36:TRP:CE3	2.54	0.41
1:H:360:HIS:HA	1:H:361:PRO:HD3	1.86	0.41
1:H:713:HIS:C	1:H:714:ILE:HD13	2.46	0.41
1:I:69:VAL:HG12	1:I:70:PRO:N	2.35	0.41
1:I:367:MET:HB3	1:I:367:MET:HE3	1.72	0.41
1:I:800:ARG:CZ	1:I:800:ARG:CB	2.98	0.41
1:I:900:LEU:HD23	1:I:900:LEU:HA	1.75	0.41
1:I:1018:LEU:HD22	1:I:1019:VAL:N	2.35	0.41
1:J:131:GLU:O	1:J:132:SER:C	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:237:ARG:CG	1:J:237:ARG:NH1	2.81	0.41
1:J:255:ARG:NH1	1:J:255:ARG:CG	2.79	0.41
1:J:260:LEU:HD12	1:J:310:ARG:O	2.19	0.41
1:J:363:HIS:N	1:J:363:HIS:CD2	2.81	0.41
1:K:46:ARG:HB3	1:K:47:PRO:CD	2.50	0.41
1:K:685:LEU:HA	1:K:686:PRO:HD3	1.70	0.41
1:K:995:GLY:O	1:K:996:ASP:C	2.62	0.41
1:L:617:LEU:HD12	1:L:617:LEU:HA	1.88	0.41
1:M:69:VAL:HA	1:M:70:PRO:HD2	1.77	0.41
1:M:234:ASP:OD1	1:M:236:SER:HB3	2.20	0.41
1:M:542:MET:HE3	1:M:601:PHE:HA	2.03	0.41
1:M:778:THR:HG22	1:M:778:THR:O	2.20	0.41
1:N:390:SER:HA	1:N:391:HIS:HA	1.91	0.41
1:N:475:ILE:O	1:N:476:LYS:C	2.63	0.41
1:N:730:LEU:HA	1:N:731:PRO:HD3	1.74	0.41
1:O:46:ARG:HB3	1:O:47:PRO:CD	2.50	0.41
1:O:147:ASN:HB2	1:O:165:SER:HB3	2.02	0.41
1:O:231:PHE:CD1	1:O:231:PHE:N	2.88	0.41
1:P:66:PRO:CB	1:P:187:MET:HE1	2.50	0.41
1:P:67:GLU:H	1:P:67:GLU:HG2	1.31	0.41
1:P:131:GLU:O	1:P:132:SER:C	2.60	0.41
1:P:210:ARG:NH1	1:P:394:ASN:C	2.77	0.41
1:P:713:HIS:C	1:P:714:ILE:HD13	2.46	0.41
1:P:896:ASN:HA	1:P:918:TRP:O	2.21	0.41
1:P:1020:TRP:CD1	1:P:1020:TRP:C	2.97	0.41
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.84	0.41
1:A:580:GLU:C	1:A:582:GLY:H	2.28	0.41
1:A:713:HIS:C	1:A:714:ILE:HD13	2.46	0.41
1:B:363:HIS:CD2	1:B:363:HIS:N	2.81	0.41
1:B:617:LEU:HD12	1:B:617:LEU:HA	1.88	0.41
1:B:800:ARG:CZ	1:B:800:ARG:CB	2.98	0.41
1:B:900:LEU:HB2	1:B:939:CYS:O	2.21	0.41
1:B:933:SER:O	1:B:934:GLU:C	2.62	0.41
1:B:1018:LEU:HD23	1:B:1018:LEU:HA	1.51	0.41
1:C:66:PRO:CB	1:C:187:MET:HE1	2.50	0.41
1:C:668:VAL:HG13	1:C:669:PRO:CD	2.38	0.41
1:D:257:THR:HA	1:D:270:GLY:O	2.20	0.41
1:D:542:MET:HE3	1:D:601:PHE:HA	2.02	0.41
1:D:749:ILE:N	1:D:749:ILE:CD1	2.78	0.41
1:D:778:THR:HG22	1:D:778:THR:O	2.20	0.41
1:E:227:VAL:CG1	1:E:240:LEU:HD11	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:363:HIS:CD2	1:E:363:HIS:N	2.81	0.41
1:E:655:MET:HE3	1:E:655:MET:HB2	1.60	0.41
1:E:726:LEU:HA	1:E:726:LEU:HD23	1.65	0.41
1:F:66:PRO:CB	1:F:187:MET:HE1	2.50	0.41
1:F:114:VAL:HG21	1:F:192:SER:N	2.35	0.41
1:F:282:ARG:HH11	1:G:419:GLY:HA2	1.83	0.41
1:F:347:LYS:CB	1:F:348:PRO:HD2	2.43	0.41
1:F:377:LEU:HD23	1:F:377:LEU:HA	1.91	0.41
1:F:597:ASN:ND2	1:F:599:ARG:H	2.17	0.41
1:F:651:LEU:HD12	1:F:668:VAL:O	2.19	0.41
1:G:49:GLN:NE2	1:G:49:GLN:N	2.64	0.41
1:G:141:ILE:HD13	1:G:143:PHE:CE1	2.55	0.41
1:G:568:TRP:CD1	1:G:568:TRP:C	2.99	0.41
1:G:713:HIS:C	1:G:714:ILE:HD13	2.46	0.41
1:G:800:ARG:CZ	1:G:800:ARG:CB	2.98	0.41
1:G:900:LEU:HD23	1:G:900:LEU:HA	1.75	0.41
1:H:69:VAL:HG12	1:H:70:PRO:N	2.35	0.41
1:H:90:TRP:HE1	1:H:96:ASP:CG	2.28	0.41
1:H:257:THR:HA	1:H:270:GLY:O	2.20	0.41
1:H:542:MET:HE3	1:H:601:PHE:HA	2.02	0.41
1:I:257:THR:OG1	1:I:316:HIS:HE1	2.03	0.41
1:I:763:GLY:HA3	1:I:822:LEU:HD22	2.01	0.41
1:I:778:THR:CG2	1:I:887:GLN:H	2.32	0.41
1:I:896:ASN:HA	1:I:918:TRP:O	2.21	0.41
1:K:85:VAL:HG12	1:K:86:VAL:N	2.34	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:K:597:ASN:ND2	1:K:599:ARG:H	2.17	0.41
1:K:694:LEU:O	1:K:722:LEU:N	2.51	0.41
1:L:234:ASP:OD1	1:L:236:SER:HB3	2.20	0.41
1:L:256:VAL:O	1:L:271:THR:HA	2.20	0.41
1:M:285:TYR:HB3	1:M:288:ARG:HG3	2.01	0.41
1:M:363:HIS:CD2	1:M:363:HIS:N	2.81	0.41
1:M:531:ARG:O	1:M:561:ARG:NH1	2.46	0.41
1:M:548:GLY:O	1:M:549:PHE:C	2.63	0.41
1:M:713:HIS:C	1:M:714:ILE:HD13	2.46	0.41
1:M:781:ARG:NH1	1:M:781:ARG:CG	2.79	0.41
1:M:933:SER:O	1:M:934:GLU:C	2.62	0.41
1:N:373:VAL:O	1:N:374:GLN:C	2.56	0.41
1:O:24:LEU:HD12	1:O:24:LEU:HA	1.62	0.41
1:O:237:ARG:CG	1:O:237:ARG:NH1	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:369:GLU:O	1:O:373:VAL:HG23	2.19	0.41
1:O:570:TRP:HD1	1:O:571:VAL:HG22	1.84	0.41
1:O:580:GLU:CD	1:O:580:GLU:N	2.78	0.41
1:O:617:LEU:HD12	1:O:617:LEU:HA	1.88	0.41
1:O:668:VAL:HG13	1:O:669:PRO:CD	2.38	0.41
1:O:822:LEU:HD12	1:O:823:LEU:H	1.80	0.41
1:O:869:ASP:CG	1:O:1015:HIS:HD1	2.24	0.41
1:O:901:GLY:HA3	1:O:902:PRO:HA	1.86	0.41
1:P:257:THR:HA	1:P:270:GLY:O	2.20	0.41
1:P:360:HIS:HA	1:P:361:PRO:HD3	1.86	0.41
1:P:542:MET:HE3	1:P:601:PHE:HA	2.02	0.41
1:P:900:LEU:HB2	1:P:939:CYS:O	2.21	0.41
1:A:257:THR:HA	1:A:270:GLY:O	2.20	0.41
1:A:542:MET:HE3	1:A:601:PHE:HA	2.02	0.41
1:A:696:LEU:CD1	1:A:697:THR:N	2.80	0.41
1:A:1004:SER:HB2	1:A:1006:GLU:OE2	2.20	0.41
1:B:10:VAL:C	1:B:12:GLN:N	2.79	0.41
1:B:184:LEU:HD23	1:B:184:LEU:HA	1.84	0.41
1:B:257:THR:OG1	1:B:316:HIS:HE1	2.03	0.41
1:B:421:VAL:O	1:B:425:ARG:NH1	2.46	0.41
1:B:781:ARG:NH1	1:B:781:ARG:CG	2.79	0.41
1:B:857:ARG:HG2	1:B:857:ARG:HH11	1.86	0.41
1:C:31:PRO:HA	1:C:32:PRO:HD3	1.88	0.41
1:C:138:GLN:N	1:C:217:LYS:O	2.36	0.41
1:C:214:LEU:HD23	1:C:214:LEU:HA	1.84	0.41
1:C:257:THR:OG1	1:C:316:HIS:HE1	2.03	0.41
1:C:323:ILE:CD1	1:C:323:ILE:N	2.82	0.41
1:C:522:LYS:O	1:C:523:TRP:C	2.61	0.41
1:C:542:MET:HE3	1:C:601:PHE:HA	2.02	0.41
1:C:595:THR:CG2	1:C:596:PRO:HA	2.46	0.41
1:C:931:PHE:CD2	1:C:931:PHE:C	2.98	0.41
1:D:69:VAL:HG12	1:D:70:PRO:N	2.35	0.41
1:D:264:GLU:OE2	1:D:264:GLU:HA	2.17	0.41
1:D:267:VAL:HG23	1:D:267:VAL:H	1.51	0.41
1:D:580:GLU:C	1:D:582:GLY:H	2.28	0.41
1:D:901:GLY:HA3	1:D:902:PRO:HA	1.86	0.41
1:F:69:VAL:HG12	1:F:70:PRO:N	2.35	0.41
1:F:580:GLU:CD	1:F:580:GLU:N	2.78	0.41
1:F:580:GLU:C	1:F:582:GLY:H	2.28	0.41
1:G:10:VAL:C	1:G:12:GLN:H	2.28	0.41
1:G:69:VAL:HG12	1:G:70:PRO:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:TRP:HE1	1:G:96:ASP:CG	2.28	0.41
1:G:114:VAL:HG21	1:G:192:SER:N	2.35	0.41
1:G:570:TRP:HD1	1:G:571:VAL:HG22	1.84	0.41
1:G:778:THR:CG2	1:G:887:GLN:H	2.32	0.41
1:G:900:LEU:HB2	1:G:939:CYS:O	2.21	0.41
1:H:6:SER:O	1:H:7:LEU:C	2.60	0.41
1:H:513:PRO:O	1:H:514:ALA:HB3	2.20	0.41
1:H:1018:LEU:HD22	1:H:1019:VAL:N	2.35	0.41
1:I:463:GLY:O	1:I:486:TYR:OH	2.32	0.41
1:I:583:ASN:HA	1:I:584:PRO:HD3	1.80	0.41
1:I:657:ALA:HA	1:I:661:LYS:O	2.19	0.41
1:J:323:ILE:CD1	1:J:323:ILE:N	2.82	0.41
1:J:391:HIS:ND1	1:J:412:GLU:OE1	2.44	0.41
1:J:580:GLU:CD	1:J:580:GLU:N	2.78	0.41
1:K:114:VAL:HG21	1:K:192:SER:N	2.34	0.41
1:K:251:ARG:CB	1:K:253:TYR:CE2	2.98	0.41
1:K:429:ASP:O	1:K:432:TRP:N	2.44	0.41
1:K:513:PRO:O	1:K:514:ALA:HB3	2.20	0.41
1:L:69:VAL:HG12	1:L:70:PRO:N	2.35	0.41
1:L:85:VAL:HG12	1:L:86:VAL:N	2.34	0.41
1:L:373:VAL:O	1:L:374:GLN:C	2.57	0.41
1:L:931:PHE:CD2	1:L:931:PHE:C	2.98	0.41
1:M:10:VAL:C	1:M:12:GLN:N	2.79	0.41
1:M:66:PRO:CB	1:M:187:MET:HE1	2.50	0.41
1:M:85:VAL:HG12	1:M:86:VAL:N	2.34	0.41
1:M:391:HIS:ND1	1:M:412:GLU:OE1	2.44	0.41
1:M:421:VAL:O	1:M:425:ARG:NH1	2.46	0.41
1:M:580:GLU:C	1:M:582:GLY:H	2.28	0.41
1:M:730:LEU:HD21	1:N:823:LEU:O	2.19	0.41
1:M:1021:CME:HZ3	1:M:1022:GLN:O	2.19	0.41
1:N:46:ARG:HB3	1:N:47:PRO:CD	2.50	0.41
1:N:66:PRO:CB	1:N:187:MET:HE1	2.51	0.41
1:O:49:GLN:NE2	1:O:49:GLN:N	2.64	0.41
1:O:57:GLU:HG2	1:O:83:THR:HG21	1.94	0.41
1:O:78:LEU:HA	1:O:79:PRO:HD3	1.94	0.41
1:O:568:TRP:CD1	1:O:568:TRP:C	2.99	0.41
1:O:651:LEU:HD12	1:O:668:VAL:O	2.19	0.41
1:O:763:GLY:HA3	1:O:822:LEU:HD22	2.01	0.41
1:O:874:SER:HB3	1:P:724:GLU:OE1	2.20	0.41
1:O:900:LEU:HB2	1:O:939:CYS:O	2.21	0.41
1:P:18:ASN:OD1	1:P:19:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:568:TRP:CD1	1:P:568:TRP:C	2.99	0.41
1:P:580:GLU:C	1:P:582:GLY:H	2.28	0.41
1:P:694:LEU:O	1:P:722:LEU:N	2.51	0.41
1:A:134:LEU:CD1	1:A:179:ALA:HA	2.51	0.41
1:A:424:ASN:OD1	1:D:279:ILE:HD11	2.21	0.41
1:A:548:GLY:O	1:A:549:PHE:C	2.63	0.41
1:A:670:LEU:HD23	1:A:670:LEU:HA	1.67	0.41
1:A:900:LEU:HB2	1:A:939:CYS:O	2.21	0.41
1:B:114:VAL:HG21	1:B:192:SER:N	2.34	0.41
1:B:429:ASP:OD1	1:B:431:ARG:N	2.51	0.41
1:C:255:ARG:NH1	1:C:255:ARG:CG	2.79	0.41
1:C:308:LEU:HA	1:C:308:LEU:HD23	1.79	0.41
1:C:344:LEU:N	1:C:347:LYS:O	2.36	0.41
1:C:580:GLU:CD	1:C:580:GLU:N	2.78	0.41
1:C:778:THR:HG22	1:C:778:THR:O	2.20	0.41
1:C:822:LEU:HD12	1:C:823:LEU:H	1.80	0.41
1:C:896:ASN:HA	1:C:918:TRP:O	2.21	0.41
1:D:66:PRO:CB	1:D:187:MET:HE1	2.50	0.41
1:D:255:ARG:NH1	1:D:255:ARG:CG	2.79	0.41
1:D:1004:SER:HB2	1:D:1006:GLU:OE2	2.19	0.41
1:E:69:VAL:HG12	1:E:70:PRO:N	2.35	0.41
1:E:85:VAL:HG12	1:E:86:VAL:N	2.34	0.41
1:E:231:PHE:CD1	1:E:231:PHE:N	2.88	0.41
1:E:673:ALA:O	1:E:676:GLY:N	2.47	0.41
1:E:869:ASP:CG	1:E:1015:HIS:HD1	2.24	0.41
1:E:896:ASN:HA	1:E:918:TRP:O	2.21	0.41
1:F:85:VAL:HG12	1:F:86:VAL:N	2.35	0.41
1:F:475:ILE:O	1:F:476:LYS:C	2.63	0.41
1:G:10:VAL:C	1:G:12:GLN:N	2.79	0.41
1:G:66:PRO:CB	1:G:187:MET:HE1	2.51	0.41
1:G:580:GLU:CD	1:G:580:GLU:N	2.78	0.41
1:G:931:PHE:CD2	1:G:931:PHE:C	2.98	0.41
1:G:1020:TRP:CD1	1:G:1020:TRP:C	2.97	0.41
1:H:49:GLN:C	1:H:51:LEU:H	2.28	0.41
1:H:173:LEU:HA	1:H:173:LEU:HD23	1.69	0.41
1:H:377:LEU:HD23	1:H:377:LEU:HA	1.90	0.41
1:H:429:ASP:O	1:H:432:TRP:N	2.44	0.41
1:H:568:TRP:CD1	1:H:568:TRP:C	2.99	0.41
1:H:718:GLN:HG3	1:H:719:GLN:N	2.33	0.41
1:H:740:LEU:CD1	1:H:741:THR:N	2.80	0.41
1:H:900:LEU:HB2	1:H:939:CYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:378:LEU:HD23	1:I:378:LEU:HA	1.53	0.41
1:I:522:LYS:O	1:I:523:TRP:C	2.61	0.41
1:I:679:LEU:HD23	1:I:679:LEU:HA	1.26	0.41
1:I:713:HIS:C	1:I:714:ILE:HD13	2.46	0.41
1:J:66:PRO:CB	1:J:187:MET:HE1	2.50	0.41
1:J:744:GLU:HB3	1:J:745:MET:CE	2.39	0.41
1:J:778:THR:HG22	1:J:778:THR:O	2.20	0.41
1:J:857:ARG:HG2	1:J:857:ARG:HH11	1.86	0.41
1:K:363:HIS:CD2	1:K:363:HIS:N	2.81	0.41
1:K:391:HIS:ND1	1:K:412:GLU:OE1	2.44	0.41
1:K:583:ASN:HA	1:K:584:PRO:HD3	1.79	0.41
1:K:696:LEU:CD1	1:K:697:THR:N	2.80	0.41
1:L:49:GLN:NE2	1:L:49:GLN:N	2.64	0.41
1:L:78:LEU:CB	1:L:79:PRO:CD	2.99	0.41
1:L:178:ARG:HH11	1:L:178:ARG:CB	2.33	0.41
1:M:369:GLU:O	1:M:373:VAL:HG23	2.19	0.41
1:M:463:GLY:O	1:M:486:TYR:OH	2.32	0.41
1:N:580:GLU:CD	1:N:580:GLU:N	2.78	0.41
1:N:580:GLU:C	1:N:582:GLY:H	2.28	0.41
1:N:597:ASN:ND2	1:N:599:ARG:H	2.17	0.41
1:O:608:PHE:O	1:O:611:ARG:N	2.41	0.41
1:P:69:VAL:HG12	1:P:70:PRO:N	2.35	0.41
1:P:234:ASP:OD1	1:P:236:SER:HB3	2.20	0.41
1:P:361:PRO:HB2	1:P:576:ILE:HD12	2.03	0.41
1:P:668:VAL:HG13	1:P:669:PRO:CD	2.38	0.41
1:P:922:LEU:HD12	1:P:922:LEU:HA	1.87	0.41
1:A:90:TRP:HE1	1:A:96:ASP:CG	2.28	0.41
1:A:702:GLN:HA	1:A:703:PRO:HD2	1.84	0.41
1:A:778:THR:CG2	1:A:887:GLN:H	2.32	0.41
1:A:896:ASN:HA	1:A:918:TRP:O	2.21	0.41
1:B:234:ASP:OD1	1:B:236:SER:HB3	2.20	0.41
1:B:240:LEU:HD12	1:B:240:LEU:C	2.36	0.41
1:B:502:MET:HA	1:B:537:GLU:O	2.20	0.41
1:B:713:HIS:C	1:B:714:ILE:HD13	2.46	0.41
1:B:772:ASP:OD1	1:B:772:ASP:N	2.30	0.41
1:B:835:LEU:HA	1:B:835:LEU:HD12	1.88	0.41
1:B:901:GLY:HA3	1:B:902:PRO:HA	1.86	0.41
1:C:210:ARG:NH1	1:C:394:ASN:C	2.77	0.41
1:D:429:ASP:O	1:D:432:TRP:N	2.44	0.41
1:D:896:ASN:HA	1:D:918:TRP:O	2.21	0.41
1:D:900:LEU:HB2	1:D:939:CYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:SER:O	1:E:36:TRP:C	2.62	0.41
1:E:78:LEU:CB	1:E:79:PRO:CD	2.99	0.41
1:E:134:LEU:CD1	1:E:179:ALA:HA	2.51	0.41
1:E:210:ARG:NH1	1:E:394:ASN:C	2.77	0.41
1:E:308:LEU:HA	1:E:308:LEU:HD23	1.80	0.41
1:F:184:LEU:HD23	1:F:184:LEU:HA	1.83	0.41
1:F:231:PHE:CD1	1:F:231:PHE:N	2.88	0.41
1:F:728:VAL:H	1:F:728:VAL:HG22	1.62	0.41
1:G:131:GLU:O	1:G:132:SER:C	2.60	0.41
1:G:257:THR:HA	1:G:270:GLY:O	2.20	0.41
1:G:361:PRO:HB2	1:G:576:ILE:HD12	2.03	0.41
1:G:522:LYS:O	1:G:523:TRP:C	2.61	0.41
1:G:857:ARG:HG2	1:G:857:ARG:HH11	1.86	0.41
1:G:933:SER:O	1:G:934:GLU:C	2.62	0.41
1:H:361:PRO:HB2	1:H:576:ILE:HD12	2.03	0.41
1:H:522:LYS:O	1:H:523:TRP:C	2.61	0.41
1:I:231:PHE:CD1	1:I:231:PHE:N	2.88	0.41
1:I:323:ILE:CD1	1:I:323:ILE:N	2.82	0.41
1:I:361:PRO:HB2	1:I:576:ILE:HD12	2.03	0.41
1:I:580:GLU:C	1:I:582:GLY:H	2.28	0.41
1:I:597:ASN:ND2	1:I:599:ARG:H	2.17	0.41
1:I:740:LEU:CD1	1:I:741:THR:N	2.80	0.41
1:I:906:TYR:HB3	1:I:907:PRO:CD	2.50	0.41
1:J:69:VAL:HG12	1:J:70:PRO:N	2.35	0.41
1:J:513:PRO:O	1:J:514:ALA:HB3	2.20	0.41
1:J:580:GLU:C	1:J:582:GLY:H	2.28	0.41
1:J:740:LEU:CD1	1:J:741:THR:N	2.80	0.41
1:J:922:LEU:HD12	1:J:922:LEU:HA	1.87	0.41
1:K:10:VAL:C	1:K:12:GLN:H	2.28	0.41
1:K:66:PRO:CB	1:K:187:MET:HE1	2.50	0.41
1:K:90:TRP:HE1	1:K:96:ASP:CG	2.28	0.41
1:K:713:HIS:C	1:K:714:ILE:HD13	2.46	0.41
1:K:933:SER:O	1:K:934:GLU:C	2.62	0.41
1:L:10:VAL:C	1:L:12:GLN:N	2.79	0.41
1:L:35:SER:O	1:L:36:TRP:C	2.62	0.41
1:L:134:LEU:CD1	1:L:179:ALA:HA	2.51	0.41
1:L:502:MET:HA	1:L:537:GLU:O	2.20	0.41
1:L:568:TRP:CD1	1:L:568:TRP:C	2.99	0.41
1:L:763:GLY:HA3	1:L:822:LEU:HD22	2.01	0.41
1:M:24:LEU:HD12	1:M:24:LEU:HA	1.62	0.41
1:M:34:ALA:HB3	1:M:36:TRP:CE3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:134:LEU:CD1	1:M:179:ALA:HA	2.51	0.41
1:M:347:LYS:HA	1:M:348:PRO:HD3	1.77	0.41
1:M:568:TRP:CD1	1:M:568:TRP:C	2.99	0.41
1:N:18:ASN:OD1	1:N:19:PRO:HD2	2.20	0.41
1:N:713:HIS:C	1:N:714:ILE:HD13	2.46	0.41
1:O:10:VAL:C	1:O:12:GLN:H	2.28	0.41
1:O:857:ARG:HG2	1:O:857:ARG:HH11	1.86	0.41
1:P:595:THR:CG2	1:P:596:PRO:HA	2.46	0.41
1:A:44:THR:O	1:A:45:ASP:C	2.61	0.41
1:A:730:LEU:HA	1:A:731:PRO:HD3	1.74	0.41
1:B:66:PRO:CB	1:B:187:MET:HE1	2.50	0.41
1:B:69:VAL:HG12	1:B:70:PRO:N	2.35	0.41
1:B:134:LEU:CD1	1:B:179:ALA:HA	2.51	0.41
1:B:210:ARG:NH1	1:B:394:ASN:C	2.77	0.41
1:B:231:PHE:CD1	1:B:231:PHE:N	2.88	0.41
1:B:308:LEU:HA	1:B:308:LEU:HD23	1.79	0.41
1:B:361:PRO:HB2	1:B:576:ILE:HD12	2.03	0.41
1:B:513:PRO:O	1:B:514:ALA:HB3	2.20	0.41
1:B:685:LEU:HA	1:B:686:PRO:HD3	1.70	0.41
1:C:44:THR:O	1:C:45:ASP:C	2.61	0.41
1:C:316:HIS:HA	1:C:323:ILE:HD12	1.99	0.41
1:D:134:LEU:CD1	1:D:179:ALA:HA	2.51	0.41
1:D:654:TRP:CE3	1:D:654:TRP:C	2.99	0.41
1:D:670:LEU:HD23	1:D:670:LEU:HA	1.67	0.41
1:E:178:ARG:HH11	1:E:178:ARG:CB	2.33	0.41
1:E:513:PRO:O	1:E:514:ALA:HB3	2.20	0.41
1:E:857:ARG:HG2	1:E:857:ARG:HH11	1.86	0.41
1:F:178:ARG:HH11	1:F:178:ARG:CB	2.33	0.41
1:F:502:MET:HA	1:F:537:GLU:O	2.20	0.41
1:F:713:HIS:C	1:F:714:ILE:HD13	2.46	0.41
1:F:875:ASP:N	1:F:875:ASP:OD2	2.47	0.41
1:G:51:LEU:HD12	1:G:51:LEU:HA	1.85	0.41
1:G:502:MET:HA	1:G:537:GLU:O	2.20	0.41
1:G:772:ASP:OD1	1:G:772:ASP:N	2.30	0.41
1:H:234:ASP:OD1	1:H:236:SER:HB3	2.20	0.41
1:H:631:LEU:HD12	1:H:631:LEU:HA	1.80	0.41
1:H:696:LEU:CD1	1:H:697:THR:N	2.80	0.41
1:I:46:ARG:HB3	1:I:47:PRO:CD	2.50	0.41
1:I:66:PRO:CB	1:I:187:MET:HE1	2.50	0.41
1:I:90:TRP:HE1	1:I:96:ASP:CG	2.28	0.41
1:I:822:LEU:HD12	1:I:823:LEU:H	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:900:LEU:HB2	1:I:939:CYS:O	2.20	0.41
1:J:475:ILE:O	1:J:476:LYS:C	2.63	0.41
1:J:559:TYR:HA	1:J:560:PRO:HD2	1.73	0.41
1:J:608:PHE:O	1:J:611:ARG:N	2.41	0.41
1:J:668:VAL:HG13	1:J:669:PRO:CD	2.38	0.41
1:J:807:VAL:HG13	1:J:808:GLU:N	2.34	0.41
1:K:49:GLN:NE2	1:K:49:GLN:N	2.64	0.41
1:L:147:ASN:HB2	1:L:165:SER:HB3	2.01	0.41
1:L:548:GLY:O	1:L:549:PHE:C	2.63	0.41
1:L:570:TRP:HD1	1:L:571:VAL:HG22	1.84	0.41
1:L:744:GLU:HB3	1:L:745:MET:CE	2.39	0.41
1:M:35:SER:O	1:M:36:TRP:C	2.62	0.41
1:M:78:LEU:CB	1:M:79:PRO:CD	2.99	0.41
1:M:227:VAL:CG1	1:M:240:LEU:HD11	2.42	0.41
1:M:900:LEU:HB2	1:M:939:CYS:O	2.21	0.41
1:N:85:VAL:HG12	1:N:86:VAL:N	2.34	0.41
1:N:93:HIS:HB3	1:N:95:TYR:HE1	1.84	0.41
1:N:251:ARG:CB	1:N:253:TYR:CE2	2.98	0.41
1:N:347:LYS:CB	1:N:348:PRO:HD2	2.43	0.41
1:N:647:SER:OG	1:N:672:VAL:N	2.35	0.41
1:N:896:ASN:HA	1:N:918:TRP:O	2.21	0.41
1:O:51:LEU:HD12	1:O:51:LEU:HA	1.84	0.41
1:O:66:PRO:CB	1:O:187:MET:HE1	2.50	0.41
1:O:361:PRO:HB2	1:O:576:ILE:HD12	2.03	0.41
1:O:502:MET:HA	1:O:537:GLU:O	2.20	0.41
1:P:35:SER:O	1:P:36:TRP:C	2.62	0.41
1:P:49:GLN:C	1:P:51:LEU:H	2.28	0.41
1:P:231:PHE:CD1	1:P:231:PHE:N	2.88	0.41
1:P:246:MET:HE3	1:P:247:CYS:N	2.36	0.41
1:P:612:THR:HA	1:P:613:PRO:HD3	1.68	0.41
1:P:654:TRP:CE3	1:P:654:TRP:C	2.99	0.41
1:A:246:MET:HE3	1:A:247:CYS:N	2.36	0.41
1:A:323:ILE:CD1	1:A:323:ILE:N	2.82	0.41
1:A:857:ARG:HH11	1:A:857:ARG:HG2	1.86	0.41
1:B:85:VAL:HG12	1:B:86:VAL:N	2.35	0.41
1:B:654:TRP:CE3	1:B:654:TRP:C	2.99	0.41
1:B:694:LEU:HD12	1:B:694:LEU:HA	1.69	0.41
1:C:178:ARG:HH11	1:C:178:ARG:CB	2.33	0.41
1:C:234:ASP:OD1	1:C:236:SER:HB3	2.20	0.41
1:C:360:HIS:ND1	1:C:362:LEU:HB2	2.35	0.41
1:C:475:ILE:O	1:C:476:LYS:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:GLY:O	1:D:486:TYR:OH	2.32	0.41
1:D:823:LEU:HD23	1:D:823:LEU:HA	1.73	0.41
1:D:906:TYR:HB3	1:D:907:PRO:CD	2.50	0.41
1:E:67:GLU:H	1:E:67:GLU:HG2	1.30	0.41
1:E:102:ASN:ND2	1:E:201:ASP:CB	2.78	0.41
1:E:407:LEU:HD23	1:E:407:LEU:HA	1.89	0.41
1:E:894:ARG:NH1	1:E:919:ASP:C	2.79	0.41
1:F:256:VAL:O	1:F:271:THR:HA	2.20	0.41
1:F:894:ARG:NH1	1:F:919:ASP:C	2.79	0.41
1:G:231:PHE:CD1	1:G:231:PHE:N	2.88	0.41
1:G:463:GLY:O	1:G:486:TYR:OH	2.32	0.41
1:G:673:ALA:O	1:G:676:GLY:N	2.47	0.41
1:G:894:ARG:NH1	1:G:919:ASP:C	2.79	0.41
1:H:134:LEU:CD1	1:H:179:ALA:HA	2.51	0.41
1:H:231:PHE:CD1	1:H:231:PHE:N	2.88	0.41
1:H:579:ASP:OD1	1:H:583:ASN:N	2.43	0.41
1:H:608:PHE:O	1:H:611:ARG:N	2.41	0.41
1:I:147:ASN:HB2	1:I:165:SER:HB3	2.02	0.41
1:I:256:VAL:O	1:I:271:THR:HA	2.20	0.41
1:J:46:ARG:HB3	1:J:47:PRO:CD	2.50	0.41
1:J:147:ASN:HB2	1:J:165:SER:HB3	2.02	0.41
1:J:246:MET:HE3	1:J:247:CYS:N	2.36	0.41
1:J:282:ARG:NH1	1:K:419:GLY:HA2	2.36	0.41
1:J:654:TRP:CE3	1:J:654:TRP:C	2.99	0.41
1:K:44:THR:O	1:K:45:ASP:C	2.61	0.41
1:K:65:ALA:CB	1:K:66:PRO:CD	2.99	0.41
1:K:344:LEU:N	1:K:347:LYS:O	2.36	0.41
1:K:429:ASP:OD2	1:K:431:ARG:NH1	2.54	0.41
1:K:654:TRP:CE3	1:K:654:TRP:C	2.99	0.41
1:K:869:ASP:CG	1:K:1015:HIS:HD1	2.24	0.41
1:L:90:TRP:HE1	1:L:96:ASP:CG	2.28	0.41
1:L:227:VAL:CG1	1:L:240:LEU:HD11	2.42	0.41
1:L:654:TRP:CE3	1:L:654:TRP:C	2.99	0.41
1:L:894:ARG:NH1	1:L:919:ASP:C	2.79	0.41
1:M:31:PRO:HA	1:M:32:PRO:HD3	1.88	0.41
1:M:230:ARG:NH2	1:M:241:GLU:CD	2.79	0.41
1:M:513:PRO:O	1:M:514:ALA:HB3	2.20	0.41
1:N:445:GLN:HE21	1:N:445:GLN:HB3	1.54	0.41
1:N:502:MET:HA	1:N:537:GLU:O	2.20	0.41
1:O:257:THR:HA	1:O:270:GLY:O	2.20	0.41
1:O:429:ASP:OD1	1:O:431:ARG:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:548:GLY:O	1:O:549:PHE:C	2.63	0.41
1:O:713:HIS:C	1:O:714:ILE:HD13	2.46	0.41
1:O:772:ASP:OD1	1:O:772:ASP:N	2.30	0.41
1:P:323:ILE:CD1	1:P:323:ILE:N	2.82	0.41
1:P:570:TRP:HD1	1:P:571:VAL:HG22	1.84	0.41
1:P:931:PHE:CD2	1:P:931:PHE:C	2.98	0.41
1:A:78:LEU:CB	1:A:79:PRO:CD	2.99	0.41
1:A:111:PRO:HA	1:A:112:PRO:HA	1.58	0.41
1:A:178:ARG:HH11	1:A:178:ARG:CB	2.33	0.41
1:A:479:ASP:HA	1:A:480:PRO:HD2	1.61	0.41
1:A:597:ASN:ND2	1:A:599:ARG:H	2.17	0.41
1:A:957:PHE:CD1	1:A:957:PHE:C	2.97	0.41
1:A:995:GLY:O	1:A:996:ASP:C	2.62	0.41
1:B:147:ASN:HA	1:B:148:SER:HA	1.54	0.41
1:B:542:MET:HE3	1:B:601:PHE:HA	2.03	0.41
1:B:763:GLY:HA3	1:B:822:LEU:HD22	2.01	0.41
1:B:894:ARG:NH1	1:B:919:ASP:C	2.79	0.41
1:B:931:PHE:CD2	1:B:931:PHE:C	2.98	0.41
1:B:1020:TRP:CD1	1:B:1020:TRP:C	2.97	0.41
1:C:10:VAL:C	1:C:12:GLN:H	2.28	0.41
1:C:70:PRO:O	1:C:73:TRP:N	2.45	0.41
1:C:173:LEU:HD23	1:C:173:LEU:HA	1.69	0.41
1:C:231:PHE:CD1	1:C:231:PHE:N	2.88	0.41
1:C:256:VAL:O	1:C:271:THR:HA	2.20	0.41
1:C:257:THR:HA	1:C:270:GLY:O	2.20	0.41
1:C:421:VAL:O	1:C:425:ARG:NH1	2.46	0.41
1:C:654:TRP:CE3	1:C:654:TRP:C	2.99	0.41
1:C:857:ARG:HG2	1:C:857:ARG:HH11	1.86	0.41
1:C:858:ILE:HG12	1:C:864:MET:HG3	2.03	0.41
1:D:49:GLN:CD	1:D:49:GLN:N	2.79	0.41
1:D:230:ARG:NH2	1:D:241:GLU:CD	2.79	0.41
1:D:256:VAL:O	1:D:271:THR:HA	2.20	0.41
1:D:362:LEU:HA	1:D:362:LEU:HD23	1.88	0.41
1:D:580:GLU:CD	1:D:580:GLU:N	2.78	0.41
1:D:682:LEU:HD23	1:D:682:LEU:HA	1.67	0.41
1:D:894:ARG:NH1	1:D:919:ASP:C	2.79	0.41
1:E:78:LEU:CB	1:E:79:PRO:HD2	2.44	0.41
1:E:230:ARG:NH2	1:E:241:GLU:CD	2.79	0.41
1:E:234:ASP:OD1	1:E:236:SER:HB3	2.20	0.41
1:E:246:MET:HE3	1:E:247:CYS:N	2.36	0.41
1:E:323:ILE:CD1	1:E:323:ILE:N	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:419:GLY:HA2	1:H:282:ARG:HH11	1.86	0.41
1:E:463:GLY:O	1:E:486:TYR:OH	2.32	0.41
1:E:482:ARG:HH11	1:E:482:ARG:HD2	1.71	0.41
1:E:568:TRP:CD1	1:E:568:TRP:C	2.99	0.41
1:E:823:LEU:HD23	1:E:823:LEU:HA	1.73	0.41
1:F:251:ARG:CB	1:F:253:TYR:CE2	2.98	0.41
1:F:361:PRO:HB2	1:F:576:ILE:HD12	2.03	0.41
1:F:407:LEU:HD23	1:F:407:LEU:HA	1.89	0.41
1:F:513:PRO:O	1:F:514:ALA:HB3	2.20	0.41
1:F:608:PHE:O	1:F:611:ARG:N	2.41	0.41
1:F:654:TRP:CE3	1:F:654:TRP:C	2.99	0.41
1:F:817:GLN:HE21	1:F:817:GLN:HB3	1.63	0.41
1:G:173:LEU:HA	1:G:173:LEU:HD23	1.69	0.41
1:G:230:ARG:NH2	1:G:241:GLU:CD	2.79	0.41
1:G:234:ASP:OD1	1:G:236:SER:N	2.54	0.41
1:G:264:GLU:OE2	1:G:264:GLU:HA	2.17	0.41
1:G:429:ASP:OD1	1:G:431:ARG:N	2.51	0.41
1:G:559:TYR:HA	1:G:560:PRO:HD2	1.74	0.41
1:H:66:PRO:CB	1:H:187:MET:HE1	2.51	0.41
1:H:93:HIS:HB3	1:H:95:TYR:HE1	1.84	0.41
1:H:246:MET:HE3	1:H:247:CYS:N	2.36	0.41
1:H:323:ILE:CD1	1:H:323:ILE:N	2.82	0.41
1:H:533:LEU:C	1:H:533:LEU:CD1	2.94	0.41
1:H:580:GLU:C	1:H:582:GLY:H	2.28	0.41
1:H:995:GLY:O	1:H:996:ASP:C	2.62	0.41
1:I:234:ASP:OD1	1:I:236:SER:HB3	2.20	0.41
1:I:265:THR:HG22	1:I:266:GLN:N	2.36	0.41
1:I:647:SER:OG	1:I:672:VAL:N	2.35	0.41
1:I:654:TRP:CE3	1:I:654:TRP:C	2.99	0.41
1:I:823:LEU:HA	1:I:823:LEU:HD23	1.73	0.41
1:I:894:ARG:NH1	1:I:919:ASP:C	2.79	0.41
1:J:18:ASN:OD1	1:J:19:PRO:HD2	2.20	0.41
1:J:49:GLN:C	1:J:51:LEU:H	2.28	0.41
1:J:141:ILE:HG12	1:J:142:ILE:H	1.86	0.41
1:J:234:ASP:OD1	1:J:236:SER:HB3	2.20	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:J:445:GLN:HE21	1:J:445:GLN:HB3	1.54	0.41
1:J:568:TRP:CD1	1:J:568:TRP:C	2.99	0.41
1:J:655:MET:O	1:J:655:MET:HG3	2.21	0.41
1:J:906:TYR:HB3	1:J:907:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1018:LEU:HD23	1:J:1018:LEU:HA	1.51	0.41
1:K:34:ALA:HB3	1:K:36:TRP:CE3	2.54	0.41
1:K:141:ILE:HG12	1:K:142:ILE:H	1.86	0.41
1:K:373:VAL:O	1:K:374:GLN:C	2.57	0.41
1:K:857:ARG:HH11	1:K:857:ARG:HG2	1.86	0.41
1:K:1018:LEU:HD22	1:K:1019:VAL:N	2.35	0.41
1:L:66:PRO:CB	1:L:187:MET:HE1	2.50	0.41
1:L:231:PHE:CD1	1:L:231:PHE:N	2.88	0.41
1:L:246:MET:HE3	1:L:247:CYS:N	2.36	0.41
1:L:429:ASP:OD1	1:L:431:ARG:N	2.51	0.41
1:L:546:LEU:HA	1:L:546:LEU:HD12	1.84	0.41
1:L:702:GLN:HA	1:L:703:PRO:HD2	1.84	0.41
1:L:896:ASN:HA	1:L:918:TRP:O	2.21	0.41
1:L:995:GLY:O	1:L:996:ASP:C	2.62	0.41
1:M:69:VAL:HG12	1:M:70:PRO:N	2.35	0.41
1:M:377:LEU:HD23	1:M:377:LEU:HA	1.90	0.41
1:M:432:TRP:O	1:M:433:LEU:C	2.64	0.41
1:M:533:LEU:C	1:M:533:LEU:CD1	2.94	0.41
1:M:668:VAL:HG13	1:M:669:PRO:CD	2.38	0.41
1:M:857:ARG:HG2	1:M:857:ARG:HH11	1.86	0.41
1:M:894:ARG:NH1	1:M:919:ASP:C	2.79	0.41
1:N:257:THR:HA	1:N:270:GLY:O	2.20	0.41
1:N:360:HIS:ND1	1:N:362:LEU:HB2	2.35	0.41
1:N:361:PRO:HB2	1:N:576:ILE:HD12	2.03	0.41
1:N:363:HIS:CD2	1:N:363:HIS:N	2.81	0.41
1:N:568:TRP:CD1	1:N:568:TRP:C	2.99	0.41
1:N:570:TRP:HD1	1:N:571:VAL:HG22	1.84	0.41
1:N:654:TRP:CE3	1:N:654:TRP:C	2.99	0.41
1:N:673:ALA:O	1:N:676:GLY:N	2.47	0.41
1:N:800:ARG:CZ	1:N:800:ARG:CB	2.98	0.41
1:O:471:LEU:HD23	1:O:471:LEU:HA	1.85	0.41
1:O:778:THR:CG2	1:O:887:GLN:H	2.32	0.41
1:O:894:ARG:NH1	1:O:919:ASP:C	2.79	0.41
1:P:49:GLN:CD	1:P:49:GLN:N	2.79	0.41
1:P:184:LEU:HD23	1:P:184:LEU:HA	1.84	0.41
1:P:255:ARG:NH1	1:P:255:ARG:CG	2.79	0.41
1:P:257:THR:OG1	1:P:316:HIS:HE1	2.03	0.41
1:P:533:LEU:C	1:P:533:LEU:CD1	2.94	0.41
1:P:894:ARG:NH1	1:P:919:ASP:C	2.79	0.41
1:A:395:HIS:HA	1:A:396:PRO:HD3	1.48	0.41
1:A:469:ASP:HB3	1:D:473:ARG:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LYS:O	1:A:523:TRP:C	2.61	0.41
1:A:654:TRP:CE3	1:A:654:TRP:C	2.99	0.41
1:A:772:ASP:OD1	1:A:772:ASP:N	2.30	0.41
1:B:429:ASP:O	1:B:432:TRP:N	2.44	0.41
1:B:429:ASP:OD2	1:B:431:ARG:NH1	2.54	0.41
1:C:35:SER:O	1:C:36:TRP:C	2.62	0.41
1:C:69:VAL:HG12	1:C:70:PRO:N	2.35	0.41
1:C:246:MET:HE3	1:C:247:CYS:N	2.36	0.41
1:C:900:LEU:HB2	1:C:939:CYS:O	2.20	0.41
1:D:234:ASP:OD1	1:D:236:SER:HB3	2.20	0.41
1:D:265:THR:HG22	1:D:266:GLN:N	2.36	0.41
1:D:548:GLY:O	1:D:549:PHE:C	2.63	0.41
1:D:696:LEU:CD1	1:D:697:THR:N	2.80	0.41
1:D:858:ILE:HG12	1:D:864:MET:HG3	2.03	0.41
1:E:10:VAL:C	1:E:12:GLN:N	2.79	0.41
1:E:395:HIS:HA	1:E:396:PRO:HD3	1.48	0.41
1:E:429:ASP:OD2	1:E:431:ARG:NH1	2.54	0.41
1:E:583:ASN:HA	1:E:584:PRO:HD3	1.79	0.41
1:E:858:ILE:HG12	1:E:864:MET:HG3	2.03	0.41
1:F:49:GLN:CD	1:F:49:GLN:N	2.79	0.41
1:F:363:HIS:CD2	1:F:363:HIS:N	2.81	0.41
1:F:645:ARG:NH2	1:F:650:GLU:OE2	2.48	0.41
1:F:901:GLY:HA3	1:F:902:PRO:HA	1.86	0.41
1:G:234:ASP:OD1	1:G:236:SER:HB3	2.20	0.41
1:G:475:ILE:O	1:G:476:LYS:C	2.63	0.41
1:G:654:TRP:CE3	1:G:654:TRP:C	2.99	0.41
1:G:745:MET:HA	1:G:745:MET:CE	2.44	0.41
1:H:49:GLN:CD	1:H:49:GLN:N	2.79	0.41
1:H:51:LEU:HD12	1:H:51:LEU:HA	1.84	0.41
1:H:184:LEU:HD23	1:H:184:LEU:HA	1.84	0.41
1:H:654:TRP:CE3	1:H:654:TRP:C	2.99	0.41
1:H:668:VAL:CG1	1:H:669:PRO:CD	2.99	0.41
1:J:694:LEU:HD12	1:J:694:LEU:HA	1.69	0.41
1:K:66:PRO:CB	1:K:187:MET:CE	2.99	0.41
1:K:69:VAL:HG12	1:K:70:PRO:N	2.35	0.41
1:K:141:ILE:C	1:K:142:ILE:HG13	2.46	0.41
1:K:230:ARG:O	1:K:238:ALA:HA	2.21	0.41
1:K:234:ASP:OD1	1:K:236:SER:HB3	2.20	0.41
1:L:102:ASN:ND2	1:L:201:ASP:CB	2.78	0.41
1:L:105:TYR:CE2	1:L:199:ASP:HB2	2.56	0.41
1:L:265:THR:HG22	1:L:266:GLN:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:580:GLU:CD	1:L:580:GLU:N	2.78	0.41
1:L:580:GLU:C	1:L:582:GLY:H	2.28	0.41
1:L:745:MET:CA	1:L:745:MET:CE	2.99	0.41
1:M:49:GLN:C	1:M:51:LEU:H	2.28	0.41
1:M:257:THR:HA	1:M:270:GLY:O	2.20	0.41
1:M:407:LEU:HD23	1:M:407:LEU:HA	1.89	0.41
1:N:31:PRO:HA	1:N:32:PRO:HD3	1.88	0.41
1:N:49:GLN:CD	1:N:49:GLN:N	2.79	0.41
1:N:257:THR:OG1	1:N:316:HIS:HE1	2.03	0.41
1:N:429:ASP:OD2	1:N:431:ARG:NH1	2.54	0.41
1:N:894:ARG:NH1	1:N:919:ASP:C	2.79	0.41
1:N:1020:TRP:CD1	1:N:1020:TRP:C	2.97	0.41
1:O:70:PRO:O	1:O:73:TRP:N	2.45	0.41
1:O:78:LEU:CB	1:O:79:PRO:CD	2.99	0.41
1:O:230:ARG:NH2	1:O:241:GLU:CD	2.79	0.41
1:O:234:ASP:OD1	1:O:236:SER:N	2.54	0.41
1:O:654:TRP:CE3	1:O:654:TRP:C	2.99	0.41
1:P:46:ARG:HB3	1:P:47:PRO:CD	2.50	0.41
1:P:475:ILE:O	1:P:476:LYS:C	2.63	0.41
1:P:513:PRO:O	1:P:514:ALA:HB3	2.20	0.41
1:P:658:LEU:HD12	1:P:658:LEU:HA	1.83	0.41
1:P:701:VAL:CG1	1:P:702:GLN:N	2.81	0.41
1:A:210:ARG:NH1	1:A:394:ASN:C	2.77	0.40
1:A:230:ARG:NH2	1:A:241:GLU:CD	2.79	0.40
1:A:265:THR:HG22	1:A:266:GLN:N	2.36	0.40
1:A:282:ARG:HH11	1:D:419:GLY:CA	2.34	0.40
1:B:134:LEU:HD21	1:B:177:LEU:HB2	2.04	0.40
1:B:230:ARG:NH2	1:B:241:GLU:CD	2.79	0.40
1:B:995:GLY:O	1:B:996:ASP:C	2.62	0.40
1:C:49:GLN:CD	1:C:49:GLN:N	2.79	0.40
1:C:429:ASP:OD2	1:C:431:ARG:NH1	2.54	0.40
1:C:694:LEU:O	1:C:722:LEU:N	2.51	0.40
1:C:900:LEU:HD23	1:C:900:LEU:HA	1.75	0.40
1:D:230:ARG:O	1:D:238:ALA:HA	2.22	0.40
1:D:308:LEU:HA	1:D:308:LEU:HD23	1.80	0.40
1:D:395:HIS:CE1	1:D:397:LEU:HB3	2.57	0.40
1:D:445:GLN:HE21	1:D:445:GLN:HB3	1.54	0.40
1:D:1020:TRP:CD1	1:D:1020:TRP:C	2.97	0.40
1:E:6:SER:OG	1:E:9:VAL:HB	2.22	0.40
1:E:282:ARG:HD3	1:H:418:HIS:O	2.21	0.40
1:F:522:LYS:O	1:F:523:TRP:C	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:822:LEU:HD12	1:F:823:LEU:H	1.80	0.40
1:G:105:TYR:CE2	1:G:199:ASP:HB2	2.57	0.40
1:G:242:ALA:O	1:G:290:THR:HA	2.22	0.40
1:G:531:ARG:O	1:G:561:ARG:NH1	2.46	0.40
1:G:655:MET:O	1:G:655:MET:HG3	2.21	0.40
1:G:701:VAL:HG12	1:G:702:GLN:H	1.83	0.40
1:H:35:SER:O	1:H:36:TRP:C	2.62	0.40
1:H:230:ARG:NH2	1:H:241:GLU:CD	2.79	0.40
1:H:668:VAL:HG13	1:H:669:PRO:CD	2.38	0.40
1:H:894:ARG:NH1	1:H:919:ASP:C	2.79	0.40
1:H:957:PHE:CD1	1:H:957:PHE:C	2.97	0.40
1:I:18:ASN:OD1	1:I:19:PRO:HD2	2.20	0.40
1:I:134:LEU:HD21	1:I:177:LEU:HB2	2.03	0.40
1:I:230:ARG:NH2	1:I:241:GLU:CD	2.79	0.40
1:I:599:ARG:HB2	1:I:600:GLN:H	1.40	0.40
1:J:66:PRO:CB	1:J:187:MET:CE	2.99	0.40
1:J:395:HIS:CE1	1:J:397:LEU:HB3	2.57	0.40
1:J:542:MET:HE3	1:J:601:PHE:HA	2.02	0.40
1:J:900:LEU:HB2	1:J:939:CYS:O	2.21	0.40
1:K:178:ARG:HH11	1:K:178:ARG:CB	2.33	0.40
1:K:482:ARG:HH11	1:K:482:ARG:HD2	1.71	0.40
1:L:147:ASN:HA	1:L:148:SER:HA	1.54	0.40
1:L:429:ASP:OD2	1:L:431:ARG:NH1	2.54	0.40
1:L:679:LEU:HD23	1:L:679:LEU:HA	1.26	0.40
1:L:957:PHE:CD1	1:L:957:PHE:C	2.97	0.40
1:M:230:ARG:O	1:M:238:ALA:HA	2.22	0.40
1:M:246:MET:HE3	1:M:247:CYS:N	2.36	0.40
1:M:282:ARG:HH11	1:P:419:GLY:C	2.29	0.40
1:M:858:ILE:HG12	1:M:864:MET:HG3	2.03	0.40
1:N:279:ILE:HD11	1:O:424:ASN:OD1	2.21	0.40
1:N:316:HIS:HA	1:N:323:ILE:HD12	1.99	0.40
1:N:513:PRO:O	1:N:514:ALA:HB3	2.20	0.40
1:O:69:VAL:HG12	1:O:70:PRO:N	2.35	0.40
1:O:242:ALA:O	1:O:290:THR:HA	2.22	0.40
1:O:655:MET:O	1:O:655:MET:HG3	2.21	0.40
1:O:701:VAL:HG12	1:O:702:GLN:H	1.83	0.40
1:O:878:HIS:HA	1:O:879:PRO:HD3	1.66	0.40
1:P:230:ARG:NH2	1:P:241:GLU:CD	2.79	0.40
1:P:360:HIS:ND1	1:P:362:LEU:HB2	2.35	0.40
1:P:857:ARG:HH11	1:P:857:ARG:HG2	1.86	0.40
1:A:134:LEU:HD21	1:A:177:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:LYS:HA	1:A:348:PRO:HD3	1.77	0.40
1:A:476:LYS:HD2	1:A:476:LYS:HA	1.81	0.40
1:A:894:ARG:NH1	1:A:919:ASP:C	2.79	0.40
1:B:49:GLN:CD	1:B:49:GLN:N	2.79	0.40
1:B:568:TRP:CD1	1:B:568:TRP:C	2.99	0.40
1:C:377:LEU:CD2	1:C:708:TRP:CA	2.99	0.40
1:C:713:HIS:C	1:C:714:ILE:HD13	2.46	0.40
1:C:894:ARG:NH1	1:C:919:ASP:C	2.79	0.40
1:D:65:ALA:CB	1:D:66:PRO:HD2	2.42	0.40
1:D:141:ILE:HG12	1:D:142:ILE:H	1.86	0.40
1:D:147:ASN:HB2	1:D:165:SER:HB3	2.02	0.40
1:D:246:MET:HE3	1:D:247:CYS:N	2.36	0.40
1:D:429:ASP:OD2	1:D:431:ARG:NH1	2.54	0.40
1:D:668:VAL:CG1	1:D:669:PRO:CD	2.99	0.40
1:E:900:LEU:HB2	1:E:939:CYS:O	2.21	0.40
1:F:6:SER:OG	1:F:9:VAL:HB	2.22	0.40
1:F:31:PRO:HA	1:F:32:PRO:HD3	1.88	0.40
1:F:141:ILE:C	1:F:142:ILE:HG13	2.46	0.40
1:F:246:MET:HE3	1:F:247:CYS:N	2.36	0.40
1:F:257:THR:OG1	1:F:316:HIS:HE1	2.03	0.40
1:F:745:MET:CA	1:F:745:MET:CE	2.99	0.40
1:F:858:ILE:HG12	1:F:864:MET:HG3	2.03	0.40
1:F:896:ASN:HA	1:F:918:TRP:O	2.21	0.40
1:F:900:LEU:HB2	1:F:939:CYS:O	2.21	0.40
1:G:395:HIS:CE1	1:G:397:LEU:HB3	2.56	0.40
1:H:46:ARG:HB3	1:H:47:PRO:CD	2.50	0.40
1:H:70:PRO:O	1:H:73:TRP:N	2.45	0.40
1:H:475:ILE:O	1:H:476:LYS:C	2.63	0.40
1:H:726:LEU:HA	1:H:726:LEU:HD23	1.65	0.40
1:H:878:HIS:HA	1:H:879:PRO:HD3	1.66	0.40
1:I:134:LEU:CD1	1:I:179:ALA:HA	2.51	0.40
1:J:10:VAL:C	1:J:12:GLN:N	2.79	0.40
1:J:134:LEU:CD1	1:J:179:ALA:HA	2.51	0.40
1:J:246:MET:HB3	1:J:274:PHE:CZ	2.57	0.40
1:J:479:ASP:HA	1:J:480:PRO:HD2	1.61	0.40
1:J:896:ASN:HA	1:J:918:TRP:O	2.21	0.40
1:J:931:PHE:CD2	1:J:931:PHE:C	2.98	0.40
1:K:246:MET:HB3	1:K:274:PHE:CZ	2.57	0.40
1:K:570:TRP:HD1	1:K:571:VAL:HG22	1.84	0.40
1:K:896:ASN:HA	1:K:918:TRP:O	2.21	0.40
1:L:134:LEU:HD21	1:L:177:LEU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:230:ARG:O	1:L:238:ALA:HA	2.21	0.40
1:L:234:ASP:OD1	1:L:236:SER:N	2.54	0.40
1:L:360:HIS:ND1	1:L:362:LEU:HB2	2.35	0.40
1:L:395:HIS:CE1	1:L:397:LEU:HB3	2.56	0.40
1:L:522:LYS:O	1:L:523:TRP:C	2.61	0.40
1:M:272:ALA:HA	1:M:273:PRO:HD3	1.76	0.40
1:M:323:ILE:CD1	1:M:323:ILE:N	2.82	0.40
1:N:265:THR:HG22	1:N:266:GLN:N	2.36	0.40
1:N:407:LEU:HD23	1:N:407:LEU:HA	1.89	0.40
1:N:822:LEU:HD12	1:N:823:LEU:H	1.80	0.40
1:N:857:ARG:HH11	1:N:857:ARG:HG2	1.86	0.40
1:O:69:VAL:HA	1:O:70:PRO:HD2	1.77	0.40
1:O:134:LEU:HD21	1:O:177:LEU:HB2	2.04	0.40
1:O:227:VAL:CG1	1:O:240:LEU:HD11	2.42	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:O:609:ALA:C	1:O:611:ARG:H	2.29	0.40
1:O:906:TYR:HB3	1:O:907:PRO:CD	2.50	0.40
1:P:105:TYR:CE2	1:P:199:ASP:HB2	2.57	0.40
1:P:134:LEU:CD1	1:P:179:ALA:HA	2.51	0.40
1:P:429:ASP:OD2	1:P:431:ARG:NH1	2.54	0.40
1:P:631:LEU:HD12	1:P:631:LEU:HA	1.81	0.40
1:P:749:ILE:N	1:P:749:ILE:CD1	2.78	0.40
1:A:78:LEU:CB	1:A:79:PRO:HD2	2.44	0.40
1:A:234:ASP:OD1	1:A:236:SER:HB3	2.20	0.40
1:A:246:MET:HB3	1:A:274:PHE:CZ	2.57	0.40
1:A:316:HIS:HA	1:A:323:ILE:HD12	1.99	0.40
1:A:361:PRO:HB2	1:A:576:ILE:HD12	2.03	0.40
1:A:726:LEU:HA	1:A:726:LEU:HD23	1.65	0.40
1:B:141:ILE:HG12	1:B:142:ILE:H	1.86	0.40
1:B:246:MET:HB3	1:B:274:PHE:CZ	2.57	0.40
1:B:609:ALA:C	1:B:611:ARG:H	2.29	0.40
1:B:682:LEU:HA	1:B:682:LEU:HD23	1.67	0.40
1:C:62:TRP:C	1:C:62:TRP:CE3	3.00	0.40
1:C:134:LEU:CD1	1:C:179:ALA:HA	2.51	0.40
1:C:141:ILE:HG12	1:C:142:ILE:H	1.86	0.40
1:D:6:SER:OG	1:D:9:VAL:HB	2.22	0.40
1:D:10:VAL:C	1:D:12:GLN:H	2.28	0.40
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.57	0.40
1:D:757:GLN:O	1:D:757:GLN:HG2	2.12	0.40
1:E:49:GLN:C	1:E:51:LEU:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:ASN:HB2	1:E:165:SER:HB3	2.02	0.40
1:F:48:SER:OG	1:F:50:GLN:HG2	2.22	0.40
1:F:62:TRP:C	1:F:62:TRP:CE3	3.00	0.40
1:F:66:PRO:CB	1:F:187:MET:CE	2.99	0.40
1:F:69:VAL:HA	1:F:70:PRO:HD2	1.77	0.40
1:F:230:ARG:O	1:F:238:ALA:HA	2.21	0.40
1:F:234:ASP:OD1	1:F:236:SER:HB3	2.20	0.40
1:F:391:HIS:ND1	1:F:412:GLU:OE1	2.44	0.40
1:F:1020:TRP:CD1	1:F:1020:TRP:C	2.97	0.40
1:G:134:LEU:HD21	1:G:177:LEU:HB2	2.04	0.40
1:G:134:LEU:CD1	1:G:179:ALA:HA	2.51	0.40
1:G:210:ARG:NH1	1:G:394:ASN:C	2.77	0.40
1:G:265:THR:HG22	1:G:266:GLN:N	2.36	0.40
1:G:906:TYR:HB3	1:G:907:PRO:CD	2.50	0.40
1:H:10:VAL:C	1:H:12:GLN:H	2.28	0.40
1:I:67:GLU:H	1:I:67:GLU:HG2	1.31	0.40
1:I:282:ARG:HH11	1:L:419:GLY:CA	2.34	0.40
1:I:395:HIS:CE1	1:I:397:LEU:HB3	2.56	0.40
1:I:475:ILE:O	1:I:476:LYS:C	2.63	0.40
1:I:702:GLN:HA	1:I:703:PRO:HD2	1.84	0.40
1:J:73:TRP:O	1:J:183:ARG:NH1	2.48	0.40
1:J:210:ARG:NH1	1:J:394:ASN:C	2.77	0.40
1:J:231:PHE:CD1	1:J:231:PHE:N	2.88	0.40
1:J:894:ARG:NH1	1:J:919:ASP:C	2.79	0.40
1:K:10:VAL:C	1:K:12:GLN:N	2.79	0.40
1:K:49:GLN:CD	1:K:49:GLN:N	2.79	0.40
1:K:894:ARG:NH1	1:K:919:ASP:C	2.79	0.40
1:K:906:TYR:OH	1:K:934:GLU:OE2	2.30	0.40
1:L:272:ALA:CB	1:L:273:PRO:CD	2.99	0.40
1:L:713:HIS:C	1:L:714:ILE:HD13	2.46	0.40
1:M:46:ARG:HB3	1:M:47:PRO:CD	2.50	0.40
1:M:361:PRO:HB2	1:M:576:ILE:HD12	2.03	0.40
1:M:655:MET:O	1:M:655:MET:HG3	2.21	0.40
1:M:745:MET:CA	1:M:745:MET:CE	2.99	0.40
1:N:141:ILE:C	1:N:142:ILE:HG13	2.46	0.40
1:N:178:ARG:HH11	1:N:178:ARG:CB	2.33	0.40
1:N:246:MET:HB3	1:N:274:PHE:CZ	2.57	0.40
1:N:395:HIS:CE1	1:N:397:LEU:HB3	2.56	0.40
1:N:679:LEU:HD23	1:N:679:LEU:HA	1.26	0.40
1:N:745:MET:CA	1:N:745:MET:CE	2.99	0.40
1:N:858:ILE:HG12	1:N:864:MET:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:390:SER:HA	1:O:391:HIS:HA	1.91	0.40
1:P:6:SER:OG	1:P:9:VAL:HB	2.22	0.40
1:P:583:ASN:HA	1:P:584:PRO:HD3	1.79	0.40
1:P:778:THR:HB	1:P:887:GLN:CB	2.48	0.40
1:A:10:VAL:C	1:A:12:GLN:H	2.29	0.40
1:A:227:VAL:CG1	1:A:240:LEU:HD11	2.42	0.40
1:A:234:ASP:OD1	1:A:236:SER:N	2.54	0.40
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.79	0.40
1:A:395:HIS:CE1	1:A:397:LEU:HB3	2.57	0.40
1:A:482:ARG:HH11	1:A:482:ARG:HD2	1.71	0.40
1:B:242:ALA:O	1:B:290:THR:HA	2.22	0.40
1:C:513:PRO:O	1:C:514:ALA:HB3	2.20	0.40
1:E:361:PRO:HB2	1:E:576:ILE:HD12	2.03	0.40
1:E:721:ARG:HE	1:E:721:ARG:HB3	1.69	0.40
1:F:134:LEU:CD1	1:F:179:ALA:HA	2.51	0.40
1:F:242:ALA:O	1:F:290:THR:HA	2.22	0.40
1:F:548:GLY:O	1:F:549:PHE:C	2.63	0.40
1:F:559:TYR:HA	1:F:560:PRO:HD2	1.74	0.40
1:F:757:GLN:O	1:F:757:GLN:HG2	2.12	0.40
1:G:609:ALA:C	1:G:611:ARG:H	2.29	0.40
1:H:395:HIS:CE1	1:H:397:LEU:HB3	2.56	0.40
1:H:421:VAL:O	1:H:425:ARG:NH1	2.46	0.40
1:I:49:GLN:CD	1:I:49:GLN:N	2.79	0.40
1:I:390:SER:HA	1:I:391:HIS:HA	1.91	0.40
1:I:685:LEU:HA	1:I:686:PRO:HD3	1.70	0.40
1:J:242:ALA:O	1:J:290:THR:HA	2.22	0.40
1:J:264:GLU:OE2	1:J:264:GLU:HA	2.17	0.40
1:J:463:GLY:O	1:J:486:TYR:OH	2.32	0.40
1:K:62:TRP:C	1:K:62:TRP:CE3	3.00	0.40
1:K:134:LEU:CD1	1:K:179:ALA:HA	2.51	0.40
1:K:225:PHE:C	1:K:226:HIS:CD2	3.00	0.40
1:K:231:PHE:CD1	1:K:231:PHE:N	2.88	0.40
1:K:254:LEU:O	1:K:255:ARG:NH1	2.54	0.40
1:K:360:HIS:HA	1:K:361:PRO:HD3	1.86	0.40
1:K:609:ALA:C	1:K:611:ARG:H	2.29	0.40
1:K:740:LEU:CD1	1:K:741:THR:N	2.80	0.40
1:L:230:ARG:NH2	1:L:241:GLU:CD	2.79	0.40
1:L:421:VAL:O	1:L:425:ARG:NH1	2.46	0.40
1:L:728:VAL:H	1:L:728:VAL:HG22	1.62	0.40
1:L:817:GLN:HE21	1:L:817:GLN:HB3	1.63	0.40
1:M:6:SER:OG	1:M:9:VAL:HB	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:282:ARG:HD3	1:P:420:MET:O	2.21	0.40
1:M:609:ALA:C	1:M:611:ARG:H	2.29	0.40
1:M:763:GLY:HA3	1:M:822:LEU:HD22	2.01	0.40
1:M:957:PHE:CD1	1:M:957:PHE:C	2.97	0.40
1:N:6:SER:OG	1:N:9:VAL:HB	2.22	0.40
1:N:62:TRP:C	1:N:62:TRP:CE3	3.00	0.40
1:N:102:ASN:ND2	1:N:201:ASP:CB	2.78	0.40
1:N:901:GLY:HA3	1:N:902:PRO:HA	1.86	0.40
1:O:395:HIS:CE1	1:O:397:LEU:HB3	2.56	0.40
1:O:722:LEU:HD23	1:O:722:LEU:HA	1.75	0.40
1:O:896:ASN:HA	1:O:918:TRP:O	2.21	0.40
1:P:225:PHE:C	1:P:226:HIS:CD2	3.00	0.40
1:P:995:GLY:O	1:P:996:ASP:C	2.62	0.40
1:A:43:ARG:HH11	1:A:43:ARG:CG	2.10	0.40
1:A:231:PHE:CD1	1:A:231:PHE:N	2.88	0.40
1:A:253:TYR:O	1:A:318:ALA:N	2.55	0.40
1:A:685:LEU:HA	1:A:686:PRO:HD3	1.70	0.40
1:B:105:TYR:CE2	1:B:199:ASP:HB2	2.57	0.40
1:B:391:HIS:ND1	1:B:412:GLU:OE1	2.44	0.40
1:B:548:GLY:O	1:B:549:PHE:C	2.63	0.40
1:B:726:LEU:HD23	1:B:726:LEU:HA	1.65	0.40
1:C:580:GLU:C	1:C:582:GLY:H	2.28	0.40
1:C:668:VAL:CG1	1:C:669:PRO:CD	2.99	0.40
1:E:221:GLN:H	1:E:221:GLN:HG2	1.70	0.40
1:E:230:ARG:O	1:E:238:ALA:HA	2.21	0.40
1:E:257:THR:HA	1:E:270:GLY:O	2.20	0.40
1:E:347:LYS:HA	1:E:348:PRO:HD3	1.77	0.40
1:E:377:LEU:CD2	1:E:708:TRP:CA	2.99	0.40
1:E:580:GLU:C	1:E:582:GLY:H	2.28	0.40
1:F:272:ALA:HA	1:F:273:PRO:HD3	1.76	0.40
1:F:429:ASP:O	1:F:432:TRP:N	2.44	0.40
1:F:694:LEU:O	1:F:722:LEU:N	2.51	0.40
1:G:246:MET:HE3	1:G:247:CYS:N	2.36	0.40
1:G:246:MET:HB3	1:G:274:PHE:CZ	2.57	0.40
1:G:542:MET:HE3	1:G:601:PHE:HA	2.02	0.40
1:H:57:GLU:HG2	1:H:83:THR:HG21	1.93	0.40
1:H:570:TRP:HD1	1:H:571:VAL:HG22	1.84	0.40
1:I:66:PRO:CB	1:I:187:MET:CE	2.99	0.40
1:I:254:LEU:O	1:I:255:ARG:NH1	2.54	0.40
1:I:957:PHE:CD1	1:I:957:PHE:C	2.97	0.40
1:I:1020:TRP:CD1	1:I:1020:TRP:C	2.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:62:TRP:C	1:J:62:TRP:CE3	3.00	0.40
1:J:102:ASN:ND2	1:J:201:ASP:CB	2.78	0.40
1:J:377:LEU:HD23	1:J:377:LEU:HA	1.90	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:J:722:LEU:HD23	1:J:722:LEU:HA	1.75	0.40
1:J:817:GLN:HE21	1:J:817:GLN:HB3	1.63	0.40
1:K:568:TRP:CD1	1:K:568:TRP:C	2.99	0.40
1:K:651:LEU:HD13	1:K:651:LEU:HA	1.51	0.40
1:K:745:MET:CA	1:K:745:MET:CE	2.99	0.40
1:K:822:LEU:HD12	1:K:823:LEU:H	1.80	0.40
1:K:900:LEU:HB2	1:K:939:CYS:O	2.21	0.40
1:L:66:PRO:CB	1:L:187:MET:CE	2.99	0.40
1:L:141:ILE:C	1:L:142:ILE:HG13	2.46	0.40
1:L:542:MET:HE3	1:L:601:PHE:HA	2.03	0.40
1:L:906:TYR:HB3	1:L:907:PRO:CD	2.50	0.40
1:M:10:VAL:C	1:M:12:GLN:H	2.28	0.40
1:M:48:SER:OG	1:M:50:GLN:HG2	2.22	0.40
1:M:147:ASN:HB2	1:M:165:SER:HB3	2.02	0.40
1:M:178:ARG:HH11	1:M:178:ARG:CB	2.33	0.40
1:M:242:ALA:O	1:M:290:THR:HA	2.22	0.40
1:M:246:MET:HB3	1:M:274:PHE:CZ	2.57	0.40
1:M:570:TRP:HD1	1:M:571:VAL:HG22	1.84	0.40
1:M:654:TRP:CE3	1:M:654:TRP:C	2.99	0.40
1:M:721:ARG:HE	1:M:721:ARG:HB3	1.69	0.40
1:M:1020:TRP:CD1	1:M:1020:TRP:C	2.97	0.40
1:N:230:ARG:O	1:N:238:ALA:HA	2.21	0.40
1:N:231:PHE:CD1	1:N:231:PHE:N	2.88	0.40
1:N:246:MET:HE3	1:N:247:CYS:N	2.36	0.40
1:N:817:GLN:HE21	1:N:817:GLN:HB3	1.63	0.40
1:O:10:VAL:C	1:O:12:GLN:N	2.79	0.40
1:O:35:SER:O	1:O:36:TRP:C	2.62	0.40
1:O:62:TRP:C	1:O:62:TRP:CE3	3.00	0.40
1:O:66:PRO:CB	1:O:187:MET:CE	2.99	0.40
1:O:246:MET:HE3	1:O:247:CYS:N	2.36	0.40
1:O:542:MET:HE3	1:O:601:PHE:HA	2.02	0.40
1:P:10:VAL:C	1:P:12:GLN:N	2.79	0.40
1:P:10:VAL:C	1:P:12:GLN:H	2.29	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:GLU:O	1:B:578:TYR:CG[2_555]	1.57	0.63
1:A:580:GLU:O	1:B:578:TYR:CB[2_555]	1.68	0.52
1:G:740:LEU:O	1:L:739:HIS:CD2[1_455]	1.94	0.26
1:A:580:GLU:O	1:B:578:TYR:CD1[2_555]	1.97	0.23
1:B:740:LEU:O	1:P:739:HIS:CD2[1_354]	2.09	0.11
1:F:80:GLU:OE2	5:I:2262:HOH:O[2_646]	2.10	0.10
1:B:739:HIS:NE2	1:P:738:PRO:O[1_354]	2.16	0.04
1:C:739:HIS:ND1	1:I:734:SER:O[1_655]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	B	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	C	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	D	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	E	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	F	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	G	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	H	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	I	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	J	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	K	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	L	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	M	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	N	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	O	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35
1	P	1018/1023 (100%)	956 (94%)	53 (5%)	9 (1%)	14	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	16288/16368 (100%)	15296 (94%)	848 (5%)	144 (1%)	14	35

All (144) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	SER
1	B	174	SER
1	C	174	SER
1	D	174	SER
1	E	174	SER
1	F	174	SER
1	G	174	SER
1	H	174	SER
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	A	46	ARG
1	A	164	ASP
1	A	461	GLU
1	B	46	ARG
1	B	164	ASP
1	B	461	GLU
1	C	46	ARG
1	C	164	ASP
1	C	461	GLU
1	D	46	ARG
1	D	164	ASP
1	D	461	GLU
1	E	46	ARG
1	E	164	ASP
1	E	461	GLU
1	F	46	ARG
1	F	164	ASP
1	F	461	GLU
1	G	46	ARG
1	G	164	ASP
1	G	461	GLU

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Mol	Chain	Res	Type
1	H	46	ARG
1	H	164	ASP
1	H	461	GLU
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	A	647	SER
1	B	647	SER
1	C	647	SER
1	D	647	SER
1	E	647	SER
1	E	690	SER
1	F	647	SER
1	G	647	SER
1	H	647	SER
1	H	690	SER
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	A	47	PRO
1	A	70	PRO
1	A	690	SER
1	B	47	PRO
1	B	70	PRO
1	B	690	SER
1	C	47	PRO
1	C	70	PRO
1	C	690	SER
1	D	47	PRO
1	D	70	PRO
1	D	690	SER
1	E	47	PRO
1	E	70	PRO
1	F	47	PRO
1	F	70	PRO
1	F	690	SER
1	G	47	PRO
1	G	70	PRO
1	G	690	SER
1	H	47	PRO
1	H	70	PRO
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

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Mol	Chain	Res	Type
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	A	79	PRO
1	B	79	PRO
1	C	79	PRO
1	D	79	PRO
1	E	79	PRO
1	F	79	PRO
1	G	79	PRO
1	H	79	PRO
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	A	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	B	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	C	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	D	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	E	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	F	872/872 (100%)	734 (84%)	138 (16%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	H	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	I	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	J	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	K	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	L	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	M	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	N	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	O	872/872 (100%)	734 (84%)	138 (16%)	2	7
1	P	872/872 (100%)	734 (84%)	138 (16%)	2	7
All	All	13952/13952 (100%)	11744 (84%)	2208 (16%)	2	7

All (2208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	9	VAL
1	A	11	LEU
1	A	13	ARG
1	A	24	LEU
1	A	37	ARG
1	A	38	ASN
1	A	39	SER
1	A	43	ARG
1	A	48	SER
1	A	49	GLN
1	A	50	GLN
1	A	52	ARG
1	A	54	LEU
1	A	57	GLU
1	A	67	GLU
1	A	71	GLU
1	A	72	SER
1	A	77	ASP
1	A	80	GLU
1	A	86	VAL
1	A	90	TRP
1	A	99	ILE

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Mol	Chain	Res	Type
1	A	102	ASN
1	A	107	ILE
1	A	114	VAL
1	A	116	THR
1	A	117	GLU
1	A	124	SER
1	A	125	LEU
1	A	128	ASN
1	A	136	GLU
1	A	141	ILE
1	A	165	SER
1	A	178	ARG
1	A	186	VAL
1	A	189	LEU
1	A	190	ARG
1	A	202	MET
1	A	210	ARG
1	A	211	ASP
1	A	213	SER
1	A	217	LYS
1	A	219	THR
1	A	230	ARG
1	A	237	ARG
1	A	241	GLU
1	A	246	MET
1	A	247	CYS
1	A	250	LEU
1	A	259	SER
1	A	264	GLU
1	A	267	VAL
1	A	277	GLU
1	A	279	ILE
1	A	282	ARG
1	A	293	LEU
1	A	299	LYS
1	A	310	ARG
1	A	312	VAL
1	A	314	GLU
1	A	333	ARG
1	A	336	ARG
1	A	347	LYS
1	A	370	GLN

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Mol	Chain	Res	Type
1	A	404	ARG
1	A	433	LEU
1	A	437	SER
1	A	438	GLU
1	A	445	GLN
1	A	448	ARG
1	A	461	GLU
1	A	473	ARG
1	A	477	SER
1	A	482	ARG
1	A	494	THR
1	A	519	SER
1	A	521	LYS
1	A	533	LEU
1	A	546	LEU
1	A	554	GLN
1	A	571	VAL
1	A	576	ILE
1	A	581	ASN
1	A	599	ARG
1	A	600	GLN
1	A	630	ARG
1	A	635	THR
1	A	651	LEU
1	A	652	LEU
1	A	655	MET
1	A	661	LYS
1	A	665	SER
1	A	667	GLU
1	A	672	VAL
1	A	681	GLU
1	A	684	GLU
1	A	690	SER
1	A	701	VAL
1	A	714	ILE
1	A	719	GLN
1	A	721	ARG
1	A	730	LEU
1	A	734	SER
1	A	737	ILE
1	A	743	SER
1	A	749	ILE

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Mol	Chain	Res	Type
1	A	755	ARG
1	A	768	MET
1	A	773	LYS
1	A	778	THR
1	A	781	ARG
1	A	797	GLU
1	A	799	THR
1	A	800	ARG
1	A	801	ILE
1	A	804	ASN
1	A	809	ARG
1	A	822	LEU
1	A	824	GLN
1	A	832	ASP
1	A	837	THR
1	A	857	ARG
1	A	867	THR
1	A	890	GLN
1	A	894	ARG
1	A	903[A]	GLN
1	A	903[B]	GLN
1	A	917	ARG
1	A	934	GLU
1	A	938	ARG
1	A	950	GLN
1	A	956	GLN
1	A	961	ARG
1	A	986	ILE
1	A	1006	GLU
1	A	1013	ARG
1	A	1018	LEU
1	B	3	ILE
1	B	9	VAL
1	B	11	LEU
1	B	13	ARG
1	B	24	LEU
1	B	37	ARG
1	B	38	ASN
1	B	39	SER
1	B	43	ARG
1	B	48	SER
1	B	49	GLN

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Mol	Chain	Res	Type
1	B	50	GLN
1	B	52	ARG
1	B	54	LEU
1	B	57	GLU
1	B	67	GLU
1	B	71	GLU
1	B	72	SER
1	B	77	ASP
1	B	80	GLU
1	B	86	VAL
1	B	90	TRP
1	B	99	ILE
1	B	102	ASN
1	B	107	ILE
1	B	114	VAL
1	B	116	THR
1	B	117	GLU
1	B	124	SER
1	B	125	LEU
1	B	128	ASN
1	B	136	GLU
1	B	141	ILE
1	B	165	SER
1	B	178	ARG
1	B	186	VAL
1	B	189	LEU
1	B	190	ARG
1	B	202	MET
1	B	210	ARG
1	B	211	ASP
1	B	213	SER
1	B	217	LYS
1	B	219	THR
1	B	230	ARG
1	B	237	ARG
1	B	241	GLU
1	B	246	MET
1	B	247	CYS
1	B	250	LEU
1	B	259	SER
1	B	264	GLU
1	B	267	VAL

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Mol	Chain	Res	Type
1	B	277	GLU
1	B	279	ILE
1	B	282	ARG
1	B	293	LEU
1	B	299	LYS
1	B	310	ARG
1	B	312	VAL
1	B	314	GLU
1	B	333	ARG
1	B	336	ARG
1	B	347	LYS
1	B	370	GLN
1	B	404	ARG
1	B	433	LEU
1	B	437	SER
1	B	438	GLU
1	B	445	GLN
1	B	448	ARG
1	B	461	GLU
1	B	473	ARG
1	B	477	SER
1	B	482	ARG
1	B	494	THR
1	B	519	SER
1	B	521	LYS
1	B	533	LEU
1	B	546	LEU
1	B	554	GLN
1	B	571	VAL
1	B	576	ILE
1	B	581	ASN
1	B	599	ARG
1	B	600	GLN
1	B	630	ARG
1	B	635	THR
1	B	651	LEU
1	B	652	LEU
1	B	655	MET
1	B	661	LYS
1	B	665	SER
1	B	667	GLU
1	B	672	VAL

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Mol	Chain	Res	Type
1	B	681	GLU
1	B	684	GLU
1	B	690	SER
1	B	701	VAL
1	B	714	ILE
1	B	719	GLN
1	B	721	ARG
1	B	730	LEU
1	B	734	SER
1	B	737	ILE
1	B	743	SER
1	B	749	ILE
1	B	755	ARG
1	B	768	MET
1	B	773	LYS
1	B	778	THR
1	B	781	ARG
1	B	797	GLU
1	B	799	THR
1	B	800	ARG
1	B	801	ILE
1	B	804	ASN
1	B	809	ARG
1	B	822	LEU
1	B	824	GLN
1	B	832	ASP
1	B	837	THR
1	B	857	ARG
1	B	867	THR
1	B	890	GLN
1	B	894	ARG
1	B	903[A]	GLN
1	B	903[B]	GLN
1	B	917	ARG
1	B	934	GLU
1	B	938	ARG
1	B	950	GLN
1	B	956	GLN
1	B	961	ARG
1	B	986	ILE
1	B	1006	GLU
1	B	1013	ARG

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Mol	Chain	Res	Type
1	B	1018	LEU
1	C	3	ILE
1	C	9	VAL
1	C	11	LEU
1	C	13	ARG
1	C	24	LEU
1	C	37	ARG
1	C	38	ASN
1	C	39	SER
1	C	43	ARG
1	C	48	SER
1	C	49	GLN
1	C	50	GLN
1	C	52	ARG
1	C	54	LEU
1	C	57	GLU
1	C	67	GLU
1	C	71	GLU
1	C	72	SER
1	C	77	ASP
1	C	80	GLU
1	C	86	VAL
1	C	90	TRP
1	C	99	ILE
1	C	102	ASN
1	C	107	ILE
1	C	114	VAL
1	C	116	THR
1	C	117	GLU
1	C	124	SER
1	C	125	LEU
1	C	128	ASN
1	C	136	GLU
1	C	141	ILE
1	C	165	SER
1	C	178	ARG
1	C	186	VAL
1	C	189	LEU
1	C	190	ARG
1	C	202	MET
1	C	210	ARG
1	C	211	ASP

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Mol	Chain	Res	Type
1	C	213	SER
1	C	217	LYS
1	C	219	THR
1	C	230	ARG
1	C	237	ARG
1	C	241	GLU
1	C	246	MET
1	C	247	CYS
1	C	250	LEU
1	C	259	SER
1	C	264	GLU
1	C	267	VAL
1	C	277	GLU
1	C	279	ILE
1	C	282	ARG
1	C	293	LEU
1	C	299	LYS
1	C	310	ARG
1	C	312	VAL
1	C	314	GLU
1	C	333	ARG
1	C	336	ARG
1	C	347	LYS
1	C	370	GLN
1	C	404	ARG
1	C	433	LEU
1	C	437	SER
1	C	438	GLU
1	C	445	GLN
1	C	448	ARG
1	C	461	GLU
1	C	473	ARG
1	C	477	SER
1	C	482	ARG
1	C	494	THR
1	C	519	SER
1	C	521	LYS
1	C	533	LEU
1	C	546	LEU
1	C	554	GLN
1	C	571	VAL
1	C	576	ILE

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Mol	Chain	Res	Type
1	C	581	ASN
1	C	599	ARG
1	C	600	GLN
1	C	630	ARG
1	C	635	THR
1	C	651	LEU
1	C	652	LEU
1	C	655	MET
1	C	661	LYS
1	C	665	SER
1	C	667	GLU
1	C	672	VAL
1	C	681	GLU
1	C	684	GLU
1	C	690	SER
1	C	701	VAL
1	C	714	ILE
1	C	719	GLN
1	C	721	ARG
1	C	730	LEU
1	C	734	SER
1	C	737	ILE
1	C	743	SER
1	C	749	ILE
1	C	755	ARG
1	C	768	MET
1	C	773	LYS
1	C	778	THR
1	C	781	ARG
1	C	797	GLU
1	C	799	THR
1	C	800	ARG
1	C	801	ILE
1	C	804	ASN
1	C	809	ARG
1	C	822	LEU
1	C	824	GLN
1	C	832	ASP
1	C	837	THR
1	C	857	ARG
1	C	867	THR
1	C	890	GLN

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Mol	Chain	Res	Type
1	C	894	ARG
1	C	903[A]	GLN
1	C	903[B]	GLN
1	C	917	ARG
1	C	934	GLU
1	C	938	ARG
1	C	950	GLN
1	C	956	GLN
1	C	961	ARG
1	C	986	ILE
1	C	1006	GLU
1	C	1013	ARG
1	C	1018	LEU
1	D	3	ILE
1	D	9	VAL
1	D	11	LEU
1	D	13	ARG
1	D	24	LEU
1	D	37	ARG
1	D	38	ASN
1	D	39	SER
1	D	43	ARG
1	D	48	SER
1	D	49	GLN
1	D	50	GLN
1	D	52	ARG
1	D	54	LEU
1	D	57	GLU
1	D	67	GLU
1	D	71	GLU
1	D	72	SER
1	D	77	ASP
1	D	80	GLU
1	D	86	VAL
1	D	90	TRP
1	D	99	ILE
1	D	102	ASN
1	D	107	ILE
1	D	114	VAL
1	D	116	THR
1	D	117	GLU
1	D	124	SER

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Mol	Chain	Res	Type
1	D	125	LEU
1	D	128	ASN
1	D	136	GLU
1	D	141	ILE
1	D	165	SER
1	D	178	ARG
1	D	186	VAL
1	D	189	LEU
1	D	190	ARG
1	D	202	MET
1	D	210	ARG
1	D	211	ASP
1	D	213	SER
1	D	217	LYS
1	D	219	THR
1	D	230	ARG
1	D	237	ARG
1	D	241	GLU
1	D	246	MET
1	D	247	CYS
1	D	250	LEU
1	D	259	SER
1	D	264	GLU
1	D	267	VAL
1	D	277	GLU
1	D	279	ILE
1	D	282	ARG
1	D	293	LEU
1	D	299	LYS
1	D	310	ARG
1	D	312	VAL
1	D	314	GLU
1	D	333	ARG
1	D	336	ARG
1	D	347	LYS
1	D	370	GLN
1	D	404	ARG
1	D	433	LEU
1	D	437	SER
1	D	438	GLU
1	D	445	GLN
1	D	448	ARG

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Mol	Chain	Res	Type
1	D	461	GLU
1	D	473	ARG
1	D	477	SER
1	D	482	ARG
1	D	494	THR
1	D	519	SER
1	D	521	LYS
1	D	533	LEU
1	D	546	LEU
1	D	554	GLN
1	D	571	VAL
1	D	576	ILE
1	D	581	ASN
1	D	599	ARG
1	D	600	GLN
1	D	630	ARG
1	D	635	THR
1	D	651	LEU
1	D	652	LEU
1	D	655	MET
1	D	661	LYS
1	D	665	SER
1	D	667	GLU
1	D	672	VAL
1	D	681	GLU
1	D	684	GLU
1	D	690	SER
1	D	701	VAL
1	D	714	ILE
1	D	719	GLN
1	D	721	ARG
1	D	730	LEU
1	D	734	SER
1	D	737	ILE
1	D	743	SER
1	D	749	ILE
1	D	755	ARG
1	D	768	MET
1	D	773	LYS
1	D	778	THR
1	D	781	ARG
1	D	797	GLU

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Mol	Chain	Res	Type
1	D	799	THR
1	D	800	ARG
1	D	801	ILE
1	D	804	ASN
1	D	809	ARG
1	D	822	LEU
1	D	824	GLN
1	D	832	ASP
1	D	837	THR
1	D	857	ARG
1	D	867	THR
1	D	890	GLN
1	D	894	ARG
1	D	903[A]	GLN
1	D	903[B]	GLN
1	D	917	ARG
1	D	934	GLU
1	D	938	ARG
1	D	950	GLN
1	D	956	GLN
1	D	961	ARG
1	D	986	ILE
1	D	1006	GLU
1	D	1013	ARG
1	D	1018	LEU
1	E	3	ILE
1	E	9	VAL
1	E	11	LEU
1	E	13	ARG
1	E	24	LEU
1	E	37	ARG
1	E	38	ASN
1	E	39	SER
1	E	43	ARG
1	E	48	SER
1	E	49	GLN
1	E	50	GLN
1	E	52	ARG
1	E	54	LEU
1	E	57	GLU
1	E	67	GLU
1	E	71	GLU

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Mol	Chain	Res	Type
1	E	72	SER
1	E	77	ASP
1	E	80	GLU
1	E	86	VAL
1	E	90	TRP
1	E	99	ILE
1	E	102	ASN
1	E	107	ILE
1	E	114	VAL
1	E	116	THR
1	E	117	GLU
1	E	124	SER
1	E	125	LEU
1	E	128	ASN
1	E	136	GLU
1	E	141	ILE
1	E	165	SER
1	E	178	ARG
1	E	186	VAL
1	E	189	LEU
1	E	190	ARG
1	E	202	MET
1	E	210	ARG
1	E	211	ASP
1	E	213	SER
1	E	217	LYS
1	E	219	THR
1	E	230	ARG
1	E	237	ARG
1	E	241	GLU
1	E	246	MET
1	E	247	CYS
1	E	250	LEU
1	E	259	SER
1	E	264	GLU
1	E	267	VAL
1	E	277	GLU
1	E	279	ILE
1	E	282	ARG
1	E	293	LEU
1	E	299	LYS
1	E	310	ARG

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Mol	Chain	Res	Type
1	E	312	VAL
1	E	314	GLU
1	E	333	ARG
1	E	336	ARG
1	E	347	LYS
1	E	370	GLN
1	E	404	ARG
1	E	433	LEU
1	E	437	SER
1	E	438	GLU
1	E	445	GLN
1	E	448	ARG
1	E	461	GLU
1	E	473	ARG
1	E	477	SER
1	E	482	ARG
1	E	494	THR
1	E	519	SER
1	E	521	LYS
1	E	533	LEU
1	E	546	LEU
1	E	554	GLN
1	E	571	VAL
1	E	576	ILE
1	E	581	ASN
1	E	599	ARG
1	E	600	GLN
1	E	630	ARG
1	E	635	THR
1	E	651	LEU
1	E	652	LEU
1	E	655	MET
1	E	661	LYS
1	E	665	SER
1	E	667	GLU
1	E	672	VAL
1	E	681	GLU
1	E	684	GLU
1	E	690	SER
1	E	701	VAL
1	E	714	ILE
1	E	719	GLN

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Mol	Chain	Res	Type
1	E	721	ARG
1	E	730	LEU
1	E	734	SER
1	E	737	ILE
1	E	743	SER
1	E	749	ILE
1	E	755	ARG
1	E	768	MET
1	E	773	LYS
1	E	778	THR
1	E	781	ARG
1	E	797	GLU
1	E	799	THR
1	E	800	ARG
1	E	801	ILE
1	E	804	ASN
1	E	809	ARG
1	E	822	LEU
1	E	824	GLN
1	E	832	ASP
1	E	837	THR
1	E	857	ARG
1	E	867	THR
1	E	890	GLN
1	E	894	ARG
1	E	903[A]	GLN
1	E	903[B]	GLN
1	E	917	ARG
1	E	934	GLU
1	E	938	ARG
1	E	950	GLN
1	E	956	GLN
1	E	961	ARG
1	E	986	ILE
1	E	1006	GLU
1	E	1013	ARG
1	E	1018	LEU
1	F	3	ILE
1	F	9	VAL
1	F	11	LEU
1	F	13	ARG
1	F	24	LEU

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Mol	Chain	Res	Type
1	F	37	ARG
1	F	38	ASN
1	F	39	SER
1	F	43	ARG
1	F	48	SER
1	F	49	GLN
1	F	50	GLN
1	F	52	ARG
1	F	54	LEU
1	F	57	GLU
1	F	67	GLU
1	F	71	GLU
1	F	72	SER
1	F	77	ASP
1	F	80	GLU
1	F	86	VAL
1	F	90	TRP
1	F	99	ILE
1	F	102	ASN
1	F	107	ILE
1	F	114	VAL
1	F	116	THR
1	F	117	GLU
1	F	124	SER
1	F	125	LEU
1	F	128	ASN
1	F	136	GLU
1	F	141	ILE
1	F	165	SER
1	F	178	ARG
1	F	186	VAL
1	F	189	LEU
1	F	190	ARG
1	F	202	MET
1	F	210	ARG
1	F	211	ASP
1	F	213	SER
1	F	217	LYS
1	F	219	THR
1	F	230	ARG
1	F	237	ARG
1	F	241	GLU

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Mol	Chain	Res	Type
1	F	246	MET
1	F	247	CYS
1	F	250	LEU
1	F	259	SER
1	F	264	GLU
1	F	267	VAL
1	F	277	GLU
1	F	279	ILE
1	F	282	ARG
1	F	293	LEU
1	F	299	LYS
1	F	310	ARG
1	F	312	VAL
1	F	314	GLU
1	F	333	ARG
1	F	336	ARG
1	F	347	LYS
1	F	370	GLN
1	F	404	ARG
1	F	433	LEU
1	F	437	SER
1	F	438	GLU
1	F	445	GLN
1	F	448	ARG
1	F	461	GLU
1	F	473	ARG
1	F	477	SER
1	F	482	ARG
1	F	494	THR
1	F	519	SER
1	F	521	LYS
1	F	533	LEU
1	F	546	LEU
1	F	554	GLN
1	F	571	VAL
1	F	576	ILE
1	F	581	ASN
1	F	599	ARG
1	F	600	GLN
1	F	630	ARG
1	F	635	THR
1	F	651	LEU

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Mol	Chain	Res	Type
1	F	652	LEU
1	F	655	MET
1	F	661	LYS
1	F	665	SER
1	F	667	GLU
1	F	672	VAL
1	F	681	GLU
1	F	684	GLU
1	F	690	SER
1	F	701	VAL
1	F	714	ILE
1	F	719	GLN
1	F	721	ARG
1	F	730	LEU
1	F	734	SER
1	F	737	ILE
1	F	743	SER
1	F	749	ILE
1	F	755	ARG
1	F	768	MET
1	F	773	LYS
1	F	778	THR
1	F	781	ARG
1	F	797	GLU
1	F	799	THR
1	F	800	ARG
1	F	801	ILE
1	F	804	ASN
1	F	809	ARG
1	F	822	LEU
1	F	824	GLN
1	F	832	ASP
1	F	837	THR
1	F	857	ARG
1	F	867	THR
1	F	890	GLN
1	F	894	ARG
1	F	903[A]	GLN
1	F	903[B]	GLN
1	F	917	ARG
1	F	934	GLU
1	F	938	ARG

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Mol	Chain	Res	Type
1	F	950	GLN
1	F	956	GLN
1	F	961	ARG
1	F	986	ILE
1	F	1006	GLU
1	F	1013	ARG
1	F	1018	LEU
1	G	3	ILE
1	G	9	VAL
1	G	11	LEU
1	G	13	ARG
1	G	24	LEU
1	G	37	ARG
1	G	38	ASN
1	G	39	SER
1	G	43	ARG
1	G	48	SER
1	G	49	GLN
1	G	50	GLN
1	G	52	ARG
1	G	54	LEU
1	G	57	GLU
1	G	67	GLU
1	G	71	GLU
1	G	72	SER
1	G	77	ASP
1	G	80	GLU
1	G	86	VAL
1	G	90	TRP
1	G	99	ILE
1	G	102	ASN
1	G	107	ILE
1	G	114	VAL
1	G	116	THR
1	G	117	GLU
1	G	124	SER
1	G	125	LEU
1	G	128	ASN
1	G	136	GLU
1	G	141	ILE
1	G	165	SER
1	G	178	ARG

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Mol	Chain	Res	Type
1	G	186	VAL
1	G	189	LEU
1	G	190	ARG
1	G	202	MET
1	G	210	ARG
1	G	211	ASP
1	G	213	SER
1	G	217	LYS
1	G	219	THR
1	G	230	ARG
1	G	237	ARG
1	G	241	GLU
1	G	246	MET
1	G	247	CYS
1	G	250	LEU
1	G	259	SER
1	G	264	GLU
1	G	267	VAL
1	G	277	GLU
1	G	279	ILE
1	G	282	ARG
1	G	293	LEU
1	G	299	LYS
1	G	310	ARG
1	G	312	VAL
1	G	314	GLU
1	G	333	ARG
1	G	336	ARG
1	G	347	LYS
1	G	370	GLN
1	G	404	ARG
1	G	433	LEU
1	G	437	SER
1	G	438	GLU
1	G	445	GLN
1	G	448	ARG
1	G	461	GLU
1	G	473	ARG
1	G	477	SER
1	G	482	ARG
1	G	494	THR
1	G	519	SER

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Mol	Chain	Res	Type
1	G	521	LYS
1	G	533	LEU
1	G	546	LEU
1	G	554	GLN
1	G	571	VAL
1	G	576	ILE
1	G	581	ASN
1	G	599	ARG
1	G	600	GLN
1	G	630	ARG
1	G	635	THR
1	G	651	LEU
1	G	652	LEU
1	G	655	MET
1	G	661	LYS
1	G	665	SER
1	G	667	GLU
1	G	672	VAL
1	G	681	GLU
1	G	684	GLU
1	G	690	SER
1	G	701	VAL
1	G	714	ILE
1	G	719	GLN
1	G	721	ARG
1	G	730	LEU
1	G	734	SER
1	G	737	ILE
1	G	743	SER
1	G	749	ILE
1	G	755	ARG
1	G	768	MET
1	G	773	LYS
1	G	778	THR
1	G	781	ARG
1	G	797	GLU
1	G	799	THR
1	G	800	ARG
1	G	801	ILE
1	G	804	ASN
1	G	809	ARG
1	G	822	LEU

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Mol	Chain	Res	Type
1	G	824	GLN
1	G	832	ASP
1	G	837	THR
1	G	857	ARG
1	G	867	THR
1	G	890	GLN
1	G	894	ARG
1	G	903[A]	GLN
1	G	903[B]	GLN
1	G	917	ARG
1	G	934	GLU
1	G	938	ARG
1	G	950	GLN
1	G	956	GLN
1	G	961	ARG
1	G	986	ILE
1	G	1006	GLU
1	G	1013	ARG
1	G	1018	LEU
1	H	3	ILE
1	H	9	VAL
1	H	11	LEU
1	H	13	ARG
1	H	24	LEU
1	H	37	ARG
1	H	38	ASN
1	H	39	SER
1	H	43	ARG
1	H	48	SER
1	H	49	GLN
1	H	50	GLN
1	H	52	ARG
1	H	54	LEU
1	H	57	GLU
1	H	67	GLU
1	H	71	GLU
1	H	72	SER
1	H	77	ASP
1	H	80	GLU
1	H	86	VAL
1	H	90	TRP
1	H	99	ILE

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Mol	Chain	Res	Type
1	H	102	ASN
1	H	107	ILE
1	H	114	VAL
1	H	116	THR
1	H	117	GLU
1	H	124	SER
1	H	125	LEU
1	H	128	ASN
1	H	136	GLU
1	H	141	ILE
1	H	165	SER
1	H	178	ARG
1	H	186	VAL
1	H	189	LEU
1	H	190	ARG
1	H	202	MET
1	H	210	ARG
1	H	211	ASP
1	H	213	SER
1	H	217	LYS
1	H	219	THR
1	H	230	ARG
1	H	237	ARG
1	H	241	GLU
1	H	246	MET
1	H	247	CYS
1	H	250	LEU
1	H	259	SER
1	H	264	GLU
1	H	267	VAL
1	H	277	GLU
1	H	279	ILE
1	H	282	ARG
1	H	293	LEU
1	H	299	LYS
1	H	310	ARG
1	H	312	VAL
1	H	314	GLU
1	H	333	ARG
1	H	336	ARG
1	H	347	LYS
1	H	370	GLN

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Mol	Chain	Res	Type
1	H	404	ARG
1	H	433	LEU
1	H	437	SER
1	H	438	GLU
1	H	445	GLN
1	H	448	ARG
1	H	461	GLU
1	H	473	ARG
1	H	477	SER
1	H	482	ARG
1	H	494	THR
1	H	519	SER
1	H	521	LYS
1	H	533	LEU
1	H	546	LEU
1	H	554	GLN
1	H	571	VAL
1	H	576	ILE
1	H	581	ASN
1	H	599	ARG
1	H	600	GLN
1	H	630	ARG
1	H	635	THR
1	H	651	LEU
1	H	652	LEU
1	H	655	MET
1	H	661	LYS
1	H	665	SER
1	H	667	GLU
1	H	672	VAL
1	H	681	GLU
1	H	684	GLU
1	H	690	SER
1	H	701	VAL
1	H	714	ILE
1	H	719	GLN
1	H	721	ARG
1	H	730	LEU
1	H	734	SER
1	H	737	ILE
1	H	743	SER
1	H	749	ILE

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Mol	Chain	Res	Type
1	H	755	ARG
1	H	768	MET
1	H	773	LYS
1	H	778	THR
1	H	781	ARG
1	H	797	GLU
1	H	799	THR
1	H	800	ARG
1	H	801	ILE
1	H	804	ASN
1	H	809	ARG
1	H	822	LEU
1	H	824	GLN
1	H	832	ASP
1	H	837	THR
1	H	857	ARG
1	H	867	THR
1	H	890	GLN
1	H	894	ARG
1	H	903[A]	GLN
1	H	903[B]	GLN
1	H	917	ARG
1	H	934	GLU
1	H	938	ARG
1	H	950	GLN
1	H	956	GLN
1	H	961	ARG
1	H	986	ILE
1	H	1006	GLU
1	H	1013	ARG
1	H	1018	LEU
1	I	3	ILE
1	I	9	VAL
1	I	11	LEU
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

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Mol	Chain	Res	Type
1	I	50	GLN
1	I	52	ARG
1	I	54	LEU
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	86	VAL
1	I	90	TRP
1	I	99	ILE
1	I	102	ASN
1	I	107	ILE
1	I	114	VAL
1	I	116	THR
1	I	117	GLU
1	I	124	SER
1	I	125	LEU
1	I	128	ASN
1	I	136	GLU
1	I	141	ILE
1	I	165	SER
1	I	178	ARG
1	I	186	VAL
1	I	189	LEU
1	I	190	ARG
1	I	202	MET
1	I	210	ARG
1	I	211	ASP
1	I	213	SER
1	I	217	LYS
1	I	219	THR
1	I	230	ARG
1	I	237	ARG
1	I	241	GLU
1	I	246	MET
1	I	247	CYS
1	I	250	LEU
1	I	259	SER
1	I	264	GLU
1	I	267	VAL

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Mol	Chain	Res	Type
1	I	277	GLU
1	I	279	ILE
1	I	282	ARG
1	I	293	LEU
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	404	ARG
1	I	433	LEU
1	I	437	SER
1	I	438	GLU
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	576	ILE
1	I	581	ASN
1	I	599	ARG
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	667	GLU
1	I	672	VAL

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Mol	Chain	Res	Type
1	I	681	GLU
1	I	684	GLU
1	I	690	SER
1	I	701	VAL
1	I	714	ILE
1	I	719	GLN
1	I	721	ARG
1	I	730	LEU
1	I	734	SER
1	I	737	ILE
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	890	GLN
1	I	894	ARG
1	I	903[A]	GLN
1	I	903[B]	GLN
1	I	917	ARG
1	I	934	GLU
1	I	938	ARG
1	I	950	GLN
1	I	956	GLN
1	I	961	ARG
1	I	986	ILE
1	I	1006	GLU
1	I	1013	ARG

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Mol	Chain	Res	Type
1	I	1018	LEU
1	J	3	ILE
1	J	9	VAL
1	J	11	LEU
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	54	LEU
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	86	VAL
1	J	90	TRP
1	J	99	ILE
1	J	102	ASN
1	J	107	ILE
1	J	114	VAL
1	J	116	THR
1	J	117	GLU
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	186	VAL
1	J	189	LEU
1	J	190	ARG
1	J	202	MET
1	J	210	ARG
1	J	211	ASP

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Mol	Chain	Res	Type
1	J	213	SER
1	J	217	LYS
1	J	219	THR
1	J	230	ARG
1	J	237	ARG
1	J	241	GLU
1	J	246	MET
1	J	247	CYS
1	J	250	LEU
1	J	259	SER
1	J	264	GLU
1	J	267	VAL
1	J	277	GLU
1	J	279	ILE
1	J	282	ARG
1	J	293	LEU
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	404	ARG
1	J	433	LEU
1	J	437	SER
1	J	438	GLU
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	576	ILE

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Mol	Chain	Res	Type
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	667	GLU
1	J	672	VAL
1	J	681	GLU
1	J	684	GLU
1	J	690	SER
1	J	701	VAL
1	J	714	ILE
1	J	719	GLN
1	J	721	ARG
1	J	730	LEU
1	J	734	SER
1	J	737	ILE
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	890	GLN

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Mol	Chain	Res	Type
1	J	894	ARG
1	J	903[A]	GLN
1	J	903[B]	GLN
1	J	917	ARG
1	J	934	GLU
1	J	938	ARG
1	J	950	GLN
1	J	956	GLN
1	J	961	ARG
1	J	986	ILE
1	J	1006	GLU
1	J	1013	ARG
1	J	1018	LEU
1	K	3	ILE
1	K	9	VAL
1	K	11	LEU
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
1	K	52	ARG
1	K	54	LEU
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	86	VAL
1	K	90	TRP
1	K	99	ILE
1	K	102	ASN
1	K	107	ILE
1	K	114	VAL
1	K	116	THR
1	K	117	GLU
1	K	124	SER

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Mol	Chain	Res	Type
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	186	VAL
1	K	189	LEU
1	K	190	ARG
1	K	202	MET
1	K	210	ARG
1	K	211	ASP
1	K	213	SER
1	K	217	LYS
1	K	219	THR
1	K	230	ARG
1	K	237	ARG
1	K	241	GLU
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	293	LEU
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	404	ARG
1	K	433	LEU
1	K	437	SER
1	K	438	GLU
1	K	445	GLN
1	K	448	ARG

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Mol	Chain	Res	Type
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	576	ILE
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	667	GLU
1	K	672	VAL
1	K	681	GLU
1	K	684	GLU
1	K	690	SER
1	K	701	VAL
1	K	714	ILE
1	K	719	GLN
1	K	721	ARG
1	K	730	LEU
1	K	734	SER
1	K	737	ILE
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

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Mol	Chain	Res	Type
1	K	799	THR
1	K	800	ARG
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	890	GLN
1	K	894	ARG
1	K	903[A]	GLN
1	K	903[B]	GLN
1	K	917	ARG
1	K	934	GLU
1	K	938	ARG
1	K	950	GLN
1	K	956	GLN
1	K	961	ARG
1	K	986	ILE
1	K	1006	GLU
1	K	1013	ARG
1	K	1018	LEU
1	L	3	ILE
1	L	9	VAL
1	L	11	LEU
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	54	LEU
1	L	57	GLU
1	L	67	GLU
1	L	71	GLU

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Mol	Chain	Res	Type
1	L	72	SER
1	L	77	ASP
1	L	80	GLU
1	L	86	VAL
1	L	90	TRP
1	L	99	ILE
1	L	102	ASN
1	L	107	ILE
1	L	114	VAL
1	L	116	THR
1	L	117	GLU
1	L	124	SER
1	L	125	LEU
1	L	128	ASN
1	L	136	GLU
1	L	141	ILE
1	L	165	SER
1	L	178	ARG
1	L	186	VAL
1	L	189	LEU
1	L	190	ARG
1	L	202	MET
1	L	210	ARG
1	L	211	ASP
1	L	213	SER
1	L	217	LYS
1	L	219	THR
1	L	230	ARG
1	L	237	ARG
1	L	241	GLU
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	293	LEU
1	L	299	LYS
1	L	310	ARG

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Mol	Chain	Res	Type
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	404	ARG
1	L	433	LEU
1	L	437	SER
1	L	438	GLU
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
1	L	571	VAL
1	L	576	ILE
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	667	GLU
1	L	672	VAL
1	L	681	GLU
1	L	684	GLU
1	L	690	SER
1	L	701	VAL
1	L	714	ILE
1	L	719	GLN

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Mol	Chain	Res	Type
1	L	721	ARG
1	L	730	LEU
1	L	734	SER
1	L	737	ILE
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	890	GLN
1	L	894	ARG
1	L	903[A]	GLN
1	L	903[B]	GLN
1	L	917	ARG
1	L	934	GLU
1	L	938	ARG
1	L	950	GLN
1	L	956	GLN
1	L	961	ARG
1	L	986	ILE
1	L	1006	GLU
1	L	1013	ARG
1	L	1018	LEU
1	M	3	ILE
1	M	9	VAL
1	M	11	LEU
1	M	13	ARG
1	M	24	LEU

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Mol	Chain	Res	Type
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	54	LEU
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	86	VAL
1	M	90	TRP
1	M	99	ILE
1	M	102	ASN
1	M	107	ILE
1	M	114	VAL
1	M	116	THR
1	M	117	GLU
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	186	VAL
1	M	189	LEU
1	M	190	ARG
1	M	202	MET
1	M	210	ARG
1	M	211	ASP
1	M	213	SER
1	M	217	LYS
1	M	219	THR
1	M	230	ARG
1	M	237	ARG
1	M	241	GLU

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Mol	Chain	Res	Type
1	M	246	MET
1	M	247	CYS
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	293	LEU
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	404	ARG
1	M	433	LEU
1	M	437	SER
1	M	438	GLU
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	576	ILE
1	M	581	ASN
1	M	599	ARG
1	M	600	GLN
1	M	630	ARG
1	M	635	THR
1	M	651	LEU

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Mol	Chain	Res	Type
1	M	652	LEU
1	M	655	MET
1	M	661	LYS
1	M	665	SER
1	M	667	GLU
1	M	672	VAL
1	M	681	GLU
1	M	684	GLU
1	M	690	SER
1	M	701	VAL
1	M	714	ILE
1	M	719	GLN
1	M	721	ARG
1	M	730	LEU
1	M	734	SER
1	M	737	ILE
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	890	GLN
1	M	894	ARG
1	M	903[A]	GLN
1	M	903[B]	GLN
1	M	917	ARG
1	M	934	GLU
1	M	938	ARG

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Mol	Chain	Res	Type
1	M	950	GLN
1	M	956	GLN
1	M	961	ARG
1	M	986	ILE
1	M	1006	GLU
1	M	1013	ARG
1	M	1018	LEU
1	N	3	ILE
1	N	9	VAL
1	N	11	LEU
1	N	13	ARG
1	N	24	LEU
1	N	37	ARG
1	N	38	ASN
1	N	39	SER
1	N	43	ARG
1	N	48	SER
1	N	49	GLN
1	N	50	GLN
1	N	52	ARG
1	N	54	LEU
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	86	VAL
1	N	90	TRP
1	N	99	ILE
1	N	102	ASN
1	N	107	ILE
1	N	114	VAL
1	N	116	THR
1	N	117	GLU
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

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Mol	Chain	Res	Type
1	N	186	VAL
1	N	189	LEU
1	N	190	ARG
1	N	202	MET
1	N	210	ARG
1	N	211	ASP
1	N	213	SER
1	N	217	LYS
1	N	219	THR
1	N	230	ARG
1	N	237	ARG
1	N	241	GLU
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	293	LEU
1	N	299	LYS
1	N	310	ARG
1	N	312	VAL
1	N	314	GLU
1	N	333	ARG
1	N	336	ARG
1	N	347	LYS
1	N	370	GLN
1	N	404	ARG
1	N	433	LEU
1	N	437	SER
1	N	438	GLU
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

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Mol	Chain	Res	Type
1	N	521	LYS
1	N	533	LEU
1	N	546	LEU
1	N	554	GLN
1	N	571	VAL
1	N	576	ILE
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	667	GLU
1	N	672	VAL
1	N	681	GLU
1	N	684	GLU
1	N	690	SER
1	N	701	VAL
1	N	714	ILE
1	N	719	GLN
1	N	721	ARG
1	N	730	LEU
1	N	734	SER
1	N	737	ILE
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
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

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Mol	Chain	Res	Type
1	N	824	GLN
1	N	832	ASP
1	N	837	THR
1	N	857	ARG
1	N	867	THR
1	N	890	GLN
1	N	894	ARG
1	N	903[A]	GLN
1	N	903[B]	GLN
1	N	917	ARG
1	N	934	GLU
1	N	938	ARG
1	N	950	GLN
1	N	956	GLN
1	N	961	ARG
1	N	986	ILE
1	N	1006	GLU
1	N	1013	ARG
1	N	1018	LEU
1	O	3	ILE
1	O	9	VAL
1	O	11	LEU
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	54	LEU
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	86	VAL
1	O	90	TRP
1	O	99	ILE

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Mol	Chain	Res	Type
1	O	102	ASN
1	O	107	ILE
1	O	114	VAL
1	O	116	THR
1	O	117	GLU
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	186	VAL
1	O	189	LEU
1	O	190	ARG
1	O	202	MET
1	O	210	ARG
1	O	211	ASP
1	O	213	SER
1	O	217	LYS
1	O	219	THR
1	O	230	ARG
1	O	237	ARG
1	O	241	GLU
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	293	LEU
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

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Mol	Chain	Res	Type
1	O	404	ARG
1	O	433	LEU
1	O	437	SER
1	O	438	GLU
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
1	O	533	LEU
1	O	546	LEU
1	O	554	GLN
1	O	571	VAL
1	O	576	ILE
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	667	GLU
1	O	672	VAL
1	O	681	GLU
1	O	684	GLU
1	O	690	SER
1	O	701	VAL
1	O	714	ILE
1	O	719	GLN
1	O	721	ARG
1	O	730	LEU
1	O	734	SER
1	O	737	ILE
1	O	743	SER
1	O	749	ILE

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Mol	Chain	Res	Type
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	890	GLN
1	O	894	ARG
1	O	903[A]	GLN
1	O	903[B]	GLN
1	O	917	ARG
1	O	934	GLU
1	O	938	ARG
1	O	950	GLN
1	O	956	GLN
1	O	961	ARG
1	O	986	ILE
1	O	1006	GLU
1	O	1013	ARG
1	O	1018	LEU
1	P	3	ILE
1	P	9	VAL
1	P	11	LEU
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

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Mol	Chain	Res	Type
1	P	50	GLN
1	P	52	ARG
1	P	54	LEU
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	86	VAL
1	P	90	TRP
1	P	99	ILE
1	P	102	ASN
1	P	107	ILE
1	P	114	VAL
1	P	116	THR
1	P	117	GLU
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	186	VAL
1	P	189	LEU
1	P	190	ARG
1	P	202	MET
1	P	210	ARG
1	P	211	ASP
1	P	213	SER
1	P	217	LYS
1	P	219	THR
1	P	230	ARG
1	P	237	ARG
1	P	241	GLU
1	P	246	MET
1	P	247	CYS
1	P	250	LEU
1	P	259	SER
1	P	264	GLU
1	P	267	VAL

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Mol	Chain	Res	Type
1	P	277	GLU
1	P	279	ILE
1	P	282	ARG
1	P	293	LEU
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	404	ARG
1	P	433	LEU
1	P	437	SER
1	P	438	GLU
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	576	ILE
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
1	P	665	SER
1	P	667	GLU
1	P	672	VAL

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Mol	Chain	Res	Type
1	P	681	GLU
1	P	684	GLU
1	P	690	SER
1	P	701	VAL
1	P	714	ILE
1	P	719	GLN
1	P	721	ARG
1	P	730	LEU
1	P	734	SER
1	P	737	ILE
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	890	GLN
1	P	894	ARG
1	P	903[A]	GLN
1	P	903[B]	GLN
1	P	917	ARG
1	P	934	GLU
1	P	938	ARG
1	P	950	GLN
1	P	956	GLN
1	P	961	ARG
1	P	986	ILE
1	P	1006	GLU
1	P	1013	ARG

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Mol	Chain	Res	Type
1	P	1018	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (379) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	102	ASN
1	A	128	ASN
1	A	221	GLN
1	A	226	HIS
1	A	262	GLN
1	A	316	HIS
1	A	363	HIS
1	A	382	ASN
1	A	394	ASN
1	A	445	GLN
1	A	467	ASN
1	A	485	GLN
1	A	597	ASN
1	A	624	GLN
1	A	634	GLN
1	A	739	HIS
1	A	761	GLN
1	A	783	GLN
1	A	817	GLN
1	A	949	HIS
1	A	977	HIS
1	A	990	HIS
1	A	1017	GLN
1	B	49	GLN
1	B	102	ASN
1	B	128	ASN
1	B	221	GLN
1	B	226	HIS
1	B	262	GLN
1	B	316	HIS
1	B	363	HIS
1	B	382	ASN
1	B	394	ASN
1	B	445	GLN
1	B	467	ASN
1	B	597	ASN

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Mol	Chain	Res	Type
1	B	624	GLN
1	B	634	GLN
1	B	739	HIS
1	B	761	GLN
1	B	783	GLN
1	B	817	GLN
1	B	949	HIS
1	B	977	HIS
1	B	990	HIS
1	B	1017	GLN
1	C	49	GLN
1	C	89	ASN
1	C	102	ASN
1	C	128	ASN
1	C	221	GLN
1	C	226	HIS
1	C	262	GLN
1	C	316	HIS
1	C	363	HIS
1	C	382	ASN
1	C	394	ASN
1	C	445	GLN
1	C	467	ASN
1	C	485	GLN
1	C	597	ASN
1	C	624	GLN
1	C	634	GLN
1	C	739	HIS
1	C	761	GLN
1	C	783	GLN
1	C	817	GLN
1	C	949	HIS
1	C	977	HIS
1	C	990	HIS
1	C	1017	GLN
1	D	49	GLN
1	D	102	ASN
1	D	128	ASN
1	D	221	GLN
1	D	226	HIS
1	D	262	GLN
1	D	316	HIS

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Mol	Chain	Res	Type
1	D	363	HIS
1	D	382	ASN
1	D	394	ASN
1	D	445	GLN
1	D	467	ASN
1	D	485	GLN
1	D	597	ASN
1	D	624	GLN
1	D	634	GLN
1	D	761	GLN
1	D	783	GLN
1	D	817	GLN
1	D	949	HIS
1	D	977	HIS
1	D	990	HIS
1	D	1017	GLN
1	E	49	GLN
1	E	102	ASN
1	E	128	ASN
1	E	221	GLN
1	E	226	HIS
1	E	262	GLN
1	E	316	HIS
1	E	363	HIS
1	E	382	ASN
1	E	394	ASN
1	E	445	GLN
1	E	467	ASN
1	E	597	ASN
1	E	624	GLN
1	E	634	GLN
1	E	702	GLN
1	E	761	GLN
1	E	783	GLN
1	E	817	GLN
1	E	949	HIS
1	E	977	HIS
1	E	990	HIS
1	E	1017	GLN
1	F	49	GLN
1	F	102	ASN
1	F	128	ASN

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Mol	Chain	Res	Type
1	F	221	GLN
1	F	226	HIS
1	F	262	GLN
1	F	316	HIS
1	F	363	HIS
1	F	382	ASN
1	F	394	ASN
1	F	445	GLN
1	F	467	ASN
1	F	485	GLN
1	F	597	ASN
1	F	624	GLN
1	F	634	GLN
1	F	739	HIS
1	F	761	GLN
1	F	783	GLN
1	F	817	GLN
1	F	949	HIS
1	F	977	HIS
1	F	990	HIS
1	F	1017	GLN
1	G	49	GLN
1	G	102	ASN
1	G	128	ASN
1	G	221	GLN
1	G	226	HIS
1	G	316	HIS
1	G	363	HIS
1	G	382	ASN
1	G	394	ASN
1	G	445	GLN
1	G	467	ASN
1	G	485	GLN
1	G	597	ASN
1	G	624	GLN
1	G	634	GLN
1	G	739	HIS
1	G	761	GLN
1	G	783	GLN
1	G	817	GLN
1	G	949	HIS
1	G	977	HIS

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Mol	Chain	Res	Type
1	G	990	HIS
1	G	1017	GLN
1	H	49	GLN
1	H	102	ASN
1	H	128	ASN
1	H	221	GLN
1	H	226	HIS
1	H	262	GLN
1	H	316	HIS
1	H	382	ASN
1	H	394	ASN
1	H	445	GLN
1	H	467	ASN
1	H	485	GLN
1	H	597	ASN
1	H	624	GLN
1	H	634	GLN
1	H	739	HIS
1	H	761	GLN
1	H	783	GLN
1	H	817	GLN
1	H	949	HIS
1	H	977	HIS
1	H	990	HIS
1	H	1017	GLN
1	I	49	GLN
1	I	102	ASN
1	I	128	ASN
1	I	221	GLN
1	I	226	HIS
1	I	262	GLN
1	I	316	HIS
1	I	382	ASN
1	I	394	ASN
1	I	445	GLN
1	I	467	ASN
1	I	485	GLN
1	I	597	ASN
1	I	624	GLN
1	I	634	GLN
1	I	739	HIS
1	I	761	GLN

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Mol	Chain	Res	Type
1	I	783	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	262	GLN
1	J	316	HIS
1	J	363	HIS
1	J	382	ASN
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	783	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
1	K	221	GLN
1	K	226	HIS
1	K	262	GLN
1	K	316	HIS
1	K	363	HIS
1	K	382	ASN
1	K	394	ASN
1	K	445	GLN
1	K	467	ASN
1	K	597	ASN

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Mol	Chain	Res	Type
1	K	624	GLN
1	K	634	GLN
1	K	702	GLN
1	K	739	HIS
1	K	761	GLN
1	K	783	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	89	ASN
1	L	102	ASN
1	L	128	ASN
1	L	221	GLN
1	L	226	HIS
1	L	262	GLN
1	L	316	HIS
1	L	363	HIS
1	L	382	ASN
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	702	GLN
1	L	739	HIS
1	L	761	GLN
1	L	783	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	89	ASN
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	262	GLN
1	M	316	HIS
1	M	382	ASN
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	702	GLN
1	M	739	HIS
1	M	761	GLN
1	M	783	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	89	ASN
1	N	102	ASN
1	N	128	ASN
1	N	221	GLN
1	N	226	HIS
1	N	262	GLN
1	N	316	HIS
1	N	363	HIS
1	N	382	ASN
1	N	394	ASN
1	N	445	GLN
1	N	467	ASN
1	N	485	GLN
1	N	597	ASN
1	N	624	GLN
1	N	634	GLN
1	N	739	HIS
1	N	761	GLN
1	N	783	GLN
1	N	817	GLN
1	N	949	HIS
1	N	977	HIS
1	N	990	HIS

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Mol	Chain	Res	Type
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	262	GLN
1	O	316	HIS
1	O	363	HIS
1	O	382	ASN
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	702	GLN
1	O	739	HIS
1	O	761	GLN
1	O	783	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	262	GLN
1	P	316	HIS
1	P	382	ASN
1	P	394	ASN
1	P	445	GLN
1	P	467	ASN
1	P	597	ASN
1	P	624	GLN
1	P	634	GLN
1	P	702	GLN
1	P	739	HIS
1	P	761	GLN

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Mol	Chain	Res	Type
1	P	783	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 molecules in this entry.

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

48 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	H	748	1	8,9,10	0.92	0	6,9,11	1.62	2 (33%)
1	CME	M	1021	1	8,9,10	0.67	0	6,9,11	1.51	1 (16%)
1	CME	B	748	1	8,9,10	0.92	0	6,9,11	1.62	2 (33%)
1	CME	I	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	P	914	1	8,9,10	0.93	0	6,9,11	1.58	1 (16%)
1	CME	I	748	1	8,9,10	0.93	0	6,9,11	1.62	2 (33%)
1	CME	N	748	1	8,9,10	0.93	0	6,9,11	1.62	2 (33%)
1	CME	P	748	1	8,9,10	0.93	0	6,9,11	1.62	2 (33%)
1	CME	N	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)
1	CME	E	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	C	748	1	8,9,10	0.92	0	6,9,11	1.62	2 (33%)
1	CME	K	914	1	8,9,10	0.93	0	6,9,11	1.58	1 (16%)
1	CME	C	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)
1	CME	K	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CME	C	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	J	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)
1	CME	D	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)
1	CME	L	748	1	8,9,10	0.92	0	6,9,11	1.61	2 (33%)
1	CME	G	914	1	8,9,10	0.93	0	6,9,11	1.58	1 (16%)
1	CME	I	914	1	8,9,10	0.92	0	6,9,11	1.58	1 (16%)
1	CME	E	914	1	8,9,10	0.93	0	6,9,11	1.58	1 (16%)
1	CME	O	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)
1	CME	O	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	G	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	H	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)
1	CME	J	748	1	8,9,10	0.93	0	6,9,11	1.62	2 (33%)
1	CME	L	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	A	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)
1	CME	D	1021	1	8,9,10	0.67	0	6,9,11	1.52	1 (16%)
1	CME	J	1021	1	8,9,10	0.67	0	6,9,11	1.52	1 (16%)
1	CME	K	748	1	8,9,10	0.93	0	6,9,11	1.61	2 (33%)
1	CME	H	1021	1	8,9,10	0.67	0	6,9,11	1.52	1 (16%)
1	CME	B	914	1	8,9,10	0.93	0	6,9,11	1.58	1 (16%)
1	CME	F	748	1	8,9,10	0.93	0	6,9,11	1.62	2 (33%)
1	CME	M	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)
1	CME	D	748	1	8,9,10	0.93	0	6,9,11	1.62	2 (33%)
1	CME	F	914	1	8,9,10	0.92	0	6,9,11	1.58	1 (16%)
1	CME	L	914	1	8,9,10	0.93	0	6,9,11	1.57	1 (16%)
1	CME	B	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	G	748	1	8,9,10	0.92	0	6,9,11	1.62	2 (33%)
1	CME	N	1021	1	8,9,10	0.67	0	6,9,11	1.52	1 (16%)
1	CME	P	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	A	748	1	8,9,10	0.92	0	6,9,11	1.62	2 (33%)
1	CME	O	748	1	8,9,10	0.93	0	6,9,11	1.62	2 (33%)
1	CME	M	748	1	8,9,10	0.92	0	6,9,11	1.62	2 (33%)
1	CME	A	1021	1	8,9,10	0.66	0	6,9,11	1.52	1 (16%)
1	CME	F	1021	1	8,9,10	0.67	0	6,9,11	1.51	1 (16%)
1	CME	E	748	1	8,9,10	0.92	0	6,9,11	1.62	2 (33%)

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	H	748	1	-	4/5/8/10	-
1	CME	M	1021	1	-	5/5/8/10	-
1	CME	B	748	1	-	4/5/8/10	-
1	CME	I	1021	1	-	5/5/8/10	-
1	CME	P	914	1	-	3/5/8/10	-
1	CME	I	748	1	-	4/5/8/10	-
1	CME	N	748	1	-	4/5/8/10	-
1	CME	P	748	1	-	4/5/8/10	-
1	CME	N	914	1	-	3/5/8/10	-
1	CME	E	1021	1	-	5/5/8/10	-
1	CME	C	748	1	-	4/5/8/10	-
1	CME	K	914	1	-	3/5/8/10	-
1	CME	C	914	1	-	3/5/8/10	-
1	CME	K	1021	1	-	5/5/8/10	-
1	CME	C	1021	1	-	5/5/8/10	-
1	CME	J	914	1	-	3/5/8/10	-
1	CME	D	914	1	-	3/5/8/10	-
1	CME	L	748	1	-	4/5/8/10	-
1	CME	G	914	1	-	3/5/8/10	-
1	CME	I	914	1	-	3/5/8/10	-
1	CME	E	914	1	-	2/5/8/10	-
1	CME	O	914	1	-	3/5/8/10	-
1	CME	O	1021	1	-	5/5/8/10	-
1	CME	G	1021	1	-	5/5/8/10	-
1	CME	H	914	1	-	3/5/8/10	-
1	CME	J	748	1	-	4/5/8/10	-
1	CME	L	1021	1	-	5/5/8/10	-
1	CME	A	914	1	-	3/5/8/10	-
1	CME	D	1021	1	-	5/5/8/10	-
1	CME	J	1021	1	-	5/5/8/10	-
1	CME	K	748	1	-	4/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	H	1021	1	-	5/5/8/10	-
1	CME	B	914	1	-	3/5/8/10	-
1	CME	F	748	1	-	4/5/8/10	-
1	CME	M	914	1	-	3/5/8/10	-
1	CME	D	748	1	-	4/5/8/10	-
1	CME	F	914	1	-	2/5/8/10	-
1	CME	L	914	1	-	2/5/8/10	-
1	CME	B	1021	1	-	5/5/8/10	-
1	CME	G	748	1	-	4/5/8/10	-
1	CME	N	1021	1	-	5/5/8/10	-
1	CME	P	1021	1	-	5/5/8/10	-
1	CME	A	748	1	-	4/5/8/10	-
1	CME	O	748	1	-	4/5/8/10	-
1	CME	M	748	1	-	4/5/8/10	-
1	CME	A	1021	1	-	5/5/8/10	-
1	CME	F	1021	1	-	5/5/8/10	-
1	CME	E	748	1	-	4/5/8/10	-

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	914	CME	CB-SG-SD	-3.45	94.94	103.86
1	I	914	CME	CB-SG-SD	-3.44	94.95	103.86
1	E	914	CME	CB-SG-SD	-3.44	94.95	103.86
1	K	914	CME	CB-SG-SD	-3.44	94.95	103.86
1	F	914	CME	CB-SG-SD	-3.44	94.95	103.86
1	B	914	CME	CB-SG-SD	-3.44	94.96	103.86
1	P	914	CME	CB-SG-SD	-3.44	94.96	103.86
1	M	914	CME	CB-SG-SD	-3.44	94.96	103.86
1	D	914	CME	CB-SG-SD	-3.44	94.97	103.86
1	A	914	CME	CB-SG-SD	-3.43	94.97	103.86
1	O	914	CME	CB-SG-SD	-3.43	94.97	103.86
1	L	914	CME	CB-SG-SD	-3.43	94.97	103.86
1	C	914	CME	CB-SG-SD	-3.43	94.97	103.86
1	H	914	CME	CB-SG-SD	-3.43	94.98	103.86
1	N	914	CME	CB-SG-SD	-3.43	94.98	103.86
1	J	914	CME	CB-SG-SD	-3.43	94.98	103.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	1021	CME	CB-CA-C	-2.50	104.01	110.80
1	O	1021	CME	CB-CA-C	-2.50	104.01	110.80
1	C	1021	CME	CB-CA-C	-2.50	104.02	110.80
1	N	1021	CME	CB-CA-C	-2.50	104.02	110.80
1	J	1021	CME	CB-CA-C	-2.49	104.03	110.80
1	B	1021	CME	CB-CA-C	-2.49	104.03	110.80
1	H	1021	CME	CB-CA-C	-2.49	104.03	110.80
1	K	1021	CME	CB-CA-C	-2.49	104.03	110.80
1	D	1021	CME	CB-CA-C	-2.49	104.03	110.80
1	E	1021	CME	CB-CA-C	-2.49	104.04	110.80
1	I	1021	CME	CB-CA-C	-2.49	104.04	110.80
1	A	1021	CME	CB-CA-C	-2.49	104.05	110.80
1	F	1021	CME	CB-CA-C	-2.48	104.07	110.80
1	L	1021	CME	CB-CA-C	-2.48	104.07	110.80
1	G	1021	CME	CB-CA-C	-2.48	104.08	110.80
1	M	1021	CME	CB-CA-C	-2.47	104.08	110.80
1	M	748	CME	CA-CB-SG	-2.36	104.79	114.45
1	P	748	CME	CA-CB-SG	-2.35	104.80	114.45
1	H	748	CME	CA-CB-SG	-2.35	104.81	114.45
1	B	748	CME	CA-CB-SG	-2.35	104.81	114.45
1	L	748	CME	CA-CB-SG	-2.35	104.82	114.45
1	C	748	CME	CA-CB-SG	-2.35	104.82	114.45
1	J	748	CME	CA-CB-SG	-2.35	104.83	114.45
1	G	748	CME	CA-CB-SG	-2.35	104.83	114.45
1	N	748	CME	CA-CB-SG	-2.35	104.83	114.45
1	D	748	CME	CA-CB-SG	-2.35	104.83	114.45
1	E	748	CME	CA-CB-SG	-2.34	104.84	114.45
1	O	748	CME	CA-CB-SG	-2.34	104.84	114.45
1	K	748	CME	CA-CB-SG	-2.34	104.84	114.45
1	I	748	CME	CA-CB-SG	-2.34	104.85	114.45
1	F	748	CME	CA-CB-SG	-2.34	104.85	114.45
1	A	748	CME	CA-CB-SG	-2.34	104.85	114.45
1	E	748	CME	CE-SD-SG	-2.06	94.43	103.46
1	P	748	CME	CE-SD-SG	-2.05	94.45	103.46
1	L	748	CME	CE-SD-SG	-2.05	94.45	103.46
1	I	748	CME	CE-SD-SG	-2.05	94.45	103.46
1	B	748	CME	CE-SD-SG	-2.05	94.45	103.46
1	F	748	CME	CE-SD-SG	-2.05	94.45	103.46
1	O	748	CME	CE-SD-SG	-2.05	94.45	103.46
1	K	748	CME	CE-SD-SG	-2.05	94.46	103.46
1	J	748	CME	CE-SD-SG	-2.05	94.46	103.46
1	C	748	CME	CE-SD-SG	-2.05	94.47	103.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	748	CME	CE-SD-SG	-2.05	94.47	103.46
1	M	748	CME	CE-SD-SG	-2.05	94.47	103.46
1	N	748	CME	CE-SD-SG	-2.05	94.47	103.46
1	A	748	CME	CE-SD-SG	-2.05	94.47	103.46
1	D	748	CME	CE-SD-SG	-2.05	94.47	103.46
1	H	748	CME	CE-SD-SG	-2.04	94.48	103.46

There are no chirality outliers.

All (189) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	748	CME	SD-CE-CZ-OH
1	A	1021	CME	N-CA-CB-SG
1	A	1021	CME	SD-CE-CZ-OH
1	B	748	CME	SD-CE-CZ-OH
1	B	1021	CME	N-CA-CB-SG
1	B	1021	CME	SD-CE-CZ-OH
1	C	748	CME	SD-CE-CZ-OH
1	C	1021	CME	N-CA-CB-SG
1	C	1021	CME	SD-CE-CZ-OH
1	D	748	CME	SD-CE-CZ-OH
1	D	1021	CME	N-CA-CB-SG
1	D	1021	CME	SD-CE-CZ-OH
1	E	748	CME	SD-CE-CZ-OH
1	E	1021	CME	N-CA-CB-SG
1	E	1021	CME	SD-CE-CZ-OH
1	F	748	CME	SD-CE-CZ-OH
1	F	1021	CME	N-CA-CB-SG
1	F	1021	CME	SD-CE-CZ-OH
1	G	748	CME	SD-CE-CZ-OH
1	G	1021	CME	N-CA-CB-SG
1	G	1021	CME	SD-CE-CZ-OH
1	H	748	CME	SD-CE-CZ-OH
1	H	1021	CME	N-CA-CB-SG
1	H	1021	CME	SD-CE-CZ-OH
1	I	748	CME	SD-CE-CZ-OH
1	I	1021	CME	N-CA-CB-SG
1	I	1021	CME	SD-CE-CZ-OH
1	J	748	CME	SD-CE-CZ-OH
1	J	1021	CME	N-CA-CB-SG
1	J	1021	CME	SD-CE-CZ-OH
1	K	748	CME	SD-CE-CZ-OH

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Mol	Chain	Res	Type	Atoms
1	K	1021	CME	N-CA-CB-SG
1	K	1021	CME	SD-CE-CZ-OH
1	L	748	CME	SD-CE-CZ-OH
1	L	1021	CME	N-CA-CB-SG
1	L	1021	CME	SD-CE-CZ-OH
1	M	748	CME	SD-CE-CZ-OH
1	M	1021	CME	N-CA-CB-SG
1	M	1021	CME	SD-CE-CZ-OH
1	N	748	CME	SD-CE-CZ-OH
1	N	1021	CME	N-CA-CB-SG
1	N	1021	CME	SD-CE-CZ-OH
1	O	748	CME	SD-CE-CZ-OH
1	O	1021	CME	N-CA-CB-SG
1	O	1021	CME	SD-CE-CZ-OH
1	P	748	CME	SD-CE-CZ-OH
1	P	1021	CME	N-CA-CB-SG
1	P	1021	CME	SD-CE-CZ-OH
1	A	1021	CME	CE-SD-SG-CB
1	B	1021	CME	CE-SD-SG-CB
1	C	1021	CME	CE-SD-SG-CB
1	D	1021	CME	CE-SD-SG-CB
1	E	1021	CME	CE-SD-SG-CB
1	F	1021	CME	CE-SD-SG-CB
1	G	1021	CME	CE-SD-SG-CB
1	H	1021	CME	CE-SD-SG-CB
1	I	1021	CME	CE-SD-SG-CB
1	J	1021	CME	CE-SD-SG-CB
1	K	1021	CME	CE-SD-SG-CB
1	L	1021	CME	CE-SD-SG-CB
1	M	1021	CME	CE-SD-SG-CB
1	N	1021	CME	CE-SD-SG-CB
1	O	1021	CME	CE-SD-SG-CB
1	P	1021	CME	CE-SD-SG-CB
1	A	748	CME	CE-SD-SG-CB
1	B	748	CME	CE-SD-SG-CB
1	C	748	CME	CE-SD-SG-CB
1	D	748	CME	CE-SD-SG-CB
1	E	748	CME	CE-SD-SG-CB
1	F	748	CME	CE-SD-SG-CB
1	G	748	CME	CE-SD-SG-CB
1	H	748	CME	CE-SD-SG-CB
1	I	748	CME	CE-SD-SG-CB

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Mol	Chain	Res	Type	Atoms
1	J	748	CME	CE-SD-SG-CB
1	K	748	CME	CE-SD-SG-CB
1	L	748	CME	CE-SD-SG-CB
1	M	748	CME	CE-SD-SG-CB
1	N	748	CME	CE-SD-SG-CB
1	O	748	CME	CE-SD-SG-CB
1	P	748	CME	CE-SD-SG-CB
1	A	914	CME	SD-CE-CZ-OH
1	B	914	CME	SD-CE-CZ-OH
1	C	914	CME	SD-CE-CZ-OH
1	D	914	CME	SD-CE-CZ-OH
1	E	914	CME	SD-CE-CZ-OH
1	F	914	CME	SD-CE-CZ-OH
1	G	914	CME	SD-CE-CZ-OH
1	H	914	CME	SD-CE-CZ-OH
1	I	914	CME	SD-CE-CZ-OH
1	J	914	CME	SD-CE-CZ-OH
1	K	914	CME	SD-CE-CZ-OH
1	L	914	CME	SD-CE-CZ-OH
1	M	914	CME	SD-CE-CZ-OH
1	N	914	CME	SD-CE-CZ-OH
1	O	914	CME	SD-CE-CZ-OH
1	P	914	CME	SD-CE-CZ-OH
1	A	914	CME	CA-CB-SG-SD
1	B	914	CME	CA-CB-SG-SD
1	C	914	CME	CA-CB-SG-SD
1	D	914	CME	CA-CB-SG-SD
1	E	914	CME	CA-CB-SG-SD
1	F	914	CME	CA-CB-SG-SD
1	G	914	CME	CA-CB-SG-SD
1	H	914	CME	CA-CB-SG-SD
1	I	914	CME	CA-CB-SG-SD
1	J	914	CME	CA-CB-SG-SD
1	K	914	CME	CA-CB-SG-SD
1	L	914	CME	CA-CB-SG-SD
1	M	914	CME	CA-CB-SG-SD
1	N	914	CME	CA-CB-SG-SD
1	O	914	CME	CA-CB-SG-SD
1	P	914	CME	CA-CB-SG-SD
1	A	748	CME	N-CA-CB-SG
1	B	748	CME	N-CA-CB-SG
1	C	748	CME	N-CA-CB-SG

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Mol	Chain	Res	Type	Atoms
1	D	748	CME	N-CA-CB-SG
1	E	748	CME	N-CA-CB-SG
1	F	748	CME	N-CA-CB-SG
1	G	748	CME	N-CA-CB-SG
1	H	748	CME	N-CA-CB-SG
1	I	748	CME	N-CA-CB-SG
1	J	748	CME	N-CA-CB-SG
1	K	748	CME	N-CA-CB-SG
1	L	748	CME	N-CA-CB-SG
1	M	748	CME	N-CA-CB-SG
1	N	748	CME	N-CA-CB-SG
1	O	748	CME	N-CA-CB-SG
1	P	748	CME	N-CA-CB-SG
1	A	748	CME	CZ-CE-SD-SG
1	A	914	CME	CZ-CE-SD-SG
1	A	1021	CME	CZ-CE-SD-SG
1	B	748	CME	CZ-CE-SD-SG
1	B	914	CME	CZ-CE-SD-SG
1	B	1021	CME	CZ-CE-SD-SG
1	C	748	CME	CZ-CE-SD-SG
1	C	914	CME	CZ-CE-SD-SG
1	C	1021	CME	CZ-CE-SD-SG
1	D	748	CME	CZ-CE-SD-SG
1	D	914	CME	CZ-CE-SD-SG
1	D	1021	CME	CZ-CE-SD-SG
1	E	748	CME	CZ-CE-SD-SG
1	E	1021	CME	CZ-CE-SD-SG
1	F	748	CME	CZ-CE-SD-SG
1	F	1021	CME	CZ-CE-SD-SG
1	G	748	CME	CZ-CE-SD-SG
1	G	914	CME	CZ-CE-SD-SG
1	G	1021	CME	CZ-CE-SD-SG
1	H	748	CME	CZ-CE-SD-SG
1	H	914	CME	CZ-CE-SD-SG
1	H	1021	CME	CZ-CE-SD-SG
1	I	748	CME	CZ-CE-SD-SG
1	I	914	CME	CZ-CE-SD-SG
1	I	1021	CME	CZ-CE-SD-SG
1	J	748	CME	CZ-CE-SD-SG
1	J	914	CME	CZ-CE-SD-SG
1	J	1021	CME	CZ-CE-SD-SG
1	K	748	CME	CZ-CE-SD-SG

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Mol	Chain	Res	Type	Atoms
1	K	914	CME	CZ-CE-SD-SG
1	K	1021	CME	CZ-CE-SD-SG
1	L	748	CME	CZ-CE-SD-SG
1	L	1021	CME	CZ-CE-SD-SG
1	M	748	CME	CZ-CE-SD-SG
1	M	914	CME	CZ-CE-SD-SG
1	M	1021	CME	CZ-CE-SD-SG
1	N	748	CME	CZ-CE-SD-SG
1	N	914	CME	CZ-CE-SD-SG
1	N	1021	CME	CZ-CE-SD-SG
1	O	748	CME	CZ-CE-SD-SG
1	O	914	CME	CZ-CE-SD-SG
1	O	1021	CME	CZ-CE-SD-SG
1	P	748	CME	CZ-CE-SD-SG
1	P	914	CME	CZ-CE-SD-SG
1	P	1021	CME	CZ-CE-SD-SG
1	A	1021	CME	CA-CB-SG-SD
1	B	1021	CME	CA-CB-SG-SD
1	C	1021	CME	CA-CB-SG-SD
1	D	1021	CME	CA-CB-SG-SD
1	E	1021	CME	CA-CB-SG-SD
1	F	1021	CME	CA-CB-SG-SD
1	G	1021	CME	CA-CB-SG-SD
1	H	1021	CME	CA-CB-SG-SD
1	I	1021	CME	CA-CB-SG-SD
1	J	1021	CME	CA-CB-SG-SD
1	K	1021	CME	CA-CB-SG-SD
1	L	1021	CME	CA-CB-SG-SD
1	M	1021	CME	CA-CB-SG-SD
1	N	1021	CME	CA-CB-SG-SD
1	O	1021	CME	CA-CB-SG-SD
1	P	1021	CME	CA-CB-SG-SD

There are no ring outliers.

32 monomers are involved in 136 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	748	CME	2	0
1	M	1021	CME	6	0
1	B	748	CME	2	0
1	I	1021	CME	7	0
1	I	748	CME	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	N	748	CME	2	0
1	P	748	CME	2	0
1	E	1021	CME	7	0
1	C	748	CME	2	0
1	K	1021	CME	6	0
1	C	1021	CME	6	0
1	L	748	CME	2	0
1	O	1021	CME	7	0
1	G	1021	CME	7	0
1	J	748	CME	2	0
1	L	1021	CME	6	0
1	D	1021	CME	6	0
1	J	1021	CME	7	0
1	K	748	CME	2	0
1	H	1021	CME	6	0
1	F	748	CME	2	0
1	D	748	CME	2	0
1	B	1021	CME	7	0
1	G	748	CME	2	0
1	N	1021	CME	7	0
1	P	1021	CME	6	0
1	A	748	CME	2	0
1	O	748	CME	2	0
1	M	748	CME	2	0
1	A	1021	CME	7	0
1	F	1021	CME	6	0
1	E	748	CME	2	0

5.5 Carbohydrates

32 monosaccharides 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	$\# Z > 2$
2	BGC	Q	1	2	12,12,12	0.65	0	17,17,17	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2FG	Q	2	2,4	11,11,12	0.88	0	12,15,17	1.35	2 (16%)
2	BGC	R	1	2	12,12,12	0.65	0	17,17,17	0.71	0
2	2FG	R	2	2,4	11,11,12	0.88	0	12,15,17	1.36	2 (16%)
2	BGC	S	1	2	12,12,12	0.66	0	17,17,17	0.72	0
2	2FG	S	2	2,4	11,11,12	0.88	0	12,15,17	1.37	2 (16%)
2	BGC	T	1	2	12,12,12	0.65	0	17,17,17	0.72	0
2	2FG	T	2	2,4	11,11,12	0.87	0	12,15,17	1.36	2 (16%)
2	BGC	U	1	2	12,12,12	0.66	0	17,17,17	0.72	0
2	2FG	U	2	2,4	11,11,12	0.88	0	12,15,17	1.36	2 (16%)
2	BGC	V	1	2	12,12,12	0.66	0	17,17,17	0.72	0
2	2FG	V	2	2,4	11,11,12	0.89	0	12,15,17	1.35	2 (16%)
2	BGC	W	1	2	12,12,12	0.66	0	17,17,17	0.72	0
2	2FG	W	2	2,4	11,11,12	0.90	0	12,15,17	1.35	2 (16%)
2	BGC	X	1	2	12,12,12	0.66	0	17,17,17	0.72	0
2	2FG	X	2	2,4	11,11,12	0.88	0	12,15,17	1.35	2 (16%)
2	BGC	Y	1	2	12,12,12	0.66	0	17,17,17	0.72	0
2	2FG	Y	2	2,4	11,11,12	0.87	0	12,15,17	1.37	2 (16%)
2	BGC	Z	1	2	12,12,12	0.66	0	17,17,17	0.72	0
2	2FG	Z	2	2,4	11,11,12	0.89	0	12,15,17	1.35	2 (16%)
2	BGC	a	1	2	12,12,12	0.65	0	17,17,17	0.72	0
2	2FG	a	2	2,4	11,11,12	0.87	0	12,15,17	1.36	2 (16%)
2	BGC	b	1	2	12,12,12	0.66	0	17,17,17	0.73	0
2	2FG	b	2	2,4	11,11,12	0.87	0	12,15,17	1.36	2 (16%)
2	BGC	c	1	2	12,12,12	0.65	0	17,17,17	0.72	0
2	2FG	c	2	2,4	11,11,12	0.88	0	12,15,17	1.37	2 (16%)
2	BGC	d	1	2	12,12,12	0.65	0	17,17,17	0.72	0
2	2FG	d	2	2,4	11,11,12	0.88	0	12,15,17	1.35	2 (16%)
2	BGC	e	1	2	12,12,12	0.65	0	17,17,17	0.72	0
2	2FG	e	2	2,4	11,11,12	0.87	0	12,15,17	1.37	2 (16%)
2	BGC	f	1	2	12,12,12	0.66	0	17,17,17	0.72	0
2	2FG	f	2	2,4	11,11,12	0.88	0	12,15,17	1.36	2 (16%)

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	BGC	Q	1	2	-	2/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2FG	Q	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	R	1	2	-	2/2/22/22	0/1/1/1
2	2FG	R	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	S	1	2	-	2/2/22/22	0/1/1/1
2	2FG	S	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	T	1	2	-	2/2/22/22	0/1/1/1
2	2FG	T	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	U	1	2	-	2/2/22/22	0/1/1/1
2	2FG	U	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	V	1	2	-	2/2/22/22	0/1/1/1
2	2FG	V	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	W	1	2	-	2/2/22/22	0/1/1/1
2	2FG	W	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	X	1	2	-	2/2/22/22	0/1/1/1
2	2FG	X	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	Y	1	2	-	2/2/22/22	0/1/1/1
2	2FG	Y	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	Z	1	2	-	2/2/22/22	0/1/1/1
2	2FG	Z	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	a	1	2	-	2/2/22/22	0/1/1/1
2	2FG	a	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	b	1	2	-	2/2/22/22	0/1/1/1
2	2FG	b	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	c	1	2	-	2/2/22/22	0/1/1/1
2	2FG	c	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	d	1	2	-	2/2/22/22	0/1/1/1
2	2FG	d	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	e	1	2	-	2/2/22/22	0/1/1/1
2	2FG	e	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	f	1	2	-	2/2/22/22	0/1/1/1
2	2FG	f	2	2,4	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	2	2FG	C2-C3-C4	-3.48	105.39	109.59
2	e	2	2FG	C2-C3-C4	-3.47	105.40	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	2	2FG	C2-C3-C4	-3.47	105.40	109.59
2	S	2	2FG	C2-C3-C4	-3.46	105.42	109.59
2	T	2	2FG	C2-C3-C4	-3.46	105.42	109.59
2	c	2	2FG	C2-C3-C4	-3.46	105.42	109.59
2	f	2	2FG	C2-C3-C4	-3.44	105.44	109.59
2	R	2	2FG	C2-C3-C4	-3.44	105.44	109.59
2	b	2	2FG	C2-C3-C4	-3.44	105.44	109.59
2	d	2	2FG	C2-C3-C4	-3.44	105.44	109.59
2	Z	2	2FG	C2-C3-C4	-3.44	105.45	109.59
2	V	2	2FG	C2-C3-C4	-3.43	105.45	109.59
2	a	2	2FG	C2-C3-C4	-3.43	105.45	109.59
2	W	2	2FG	C2-C3-C4	-3.43	105.46	109.59
2	X	2	2FG	C2-C3-C4	-3.42	105.46	109.59
2	Q	2	2FG	C2-C3-C4	-3.41	105.48	109.59
2	c	2	2FG	F2-C2-C1	-2.25	106.49	108.26
2	S	2	2FG	F2-C2-C1	-2.23	106.51	108.26
2	e	2	2FG	F2-C2-C1	-2.22	106.51	108.26
2	Y	2	2FG	F2-C2-C1	-2.21	106.52	108.26
2	T	2	2FG	F2-C2-C1	-2.21	106.52	108.26
2	a	2	2FG	F2-C2-C1	-2.21	106.52	108.26
2	b	2	2FG	F2-C2-C1	-2.21	106.52	108.26
2	f	2	2FG	F2-C2-C1	-2.19	106.53	108.26
2	R	2	2FG	F2-C2-C1	-2.19	106.54	108.26
2	U	2	2FG	F2-C2-C1	-2.18	106.54	108.26
2	X	2	2FG	F2-C2-C1	-2.17	106.55	108.26
2	Q	2	2FG	F2-C2-C1	-2.16	106.56	108.26
2	d	2	2FG	F2-C2-C1	-2.16	106.56	108.26
2	W	2	2FG	F2-C2-C1	-2.15	106.57	108.26
2	Z	2	2FG	F2-C2-C1	-2.15	106.57	108.26
2	V	2	2FG	F2-C2-C1	-2.14	106.58	108.26

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	1	BGC	O5-C5-C6-O6
2	R	1	BGC	O5-C5-C6-O6
2	T	1	BGC	O5-C5-C6-O6
2	b	1	BGC	O5-C5-C6-O6
2	c	1	BGC	O5-C5-C6-O6
2	e	1	BGC	O5-C5-C6-O6
2	f	1	BGC	O5-C5-C6-O6

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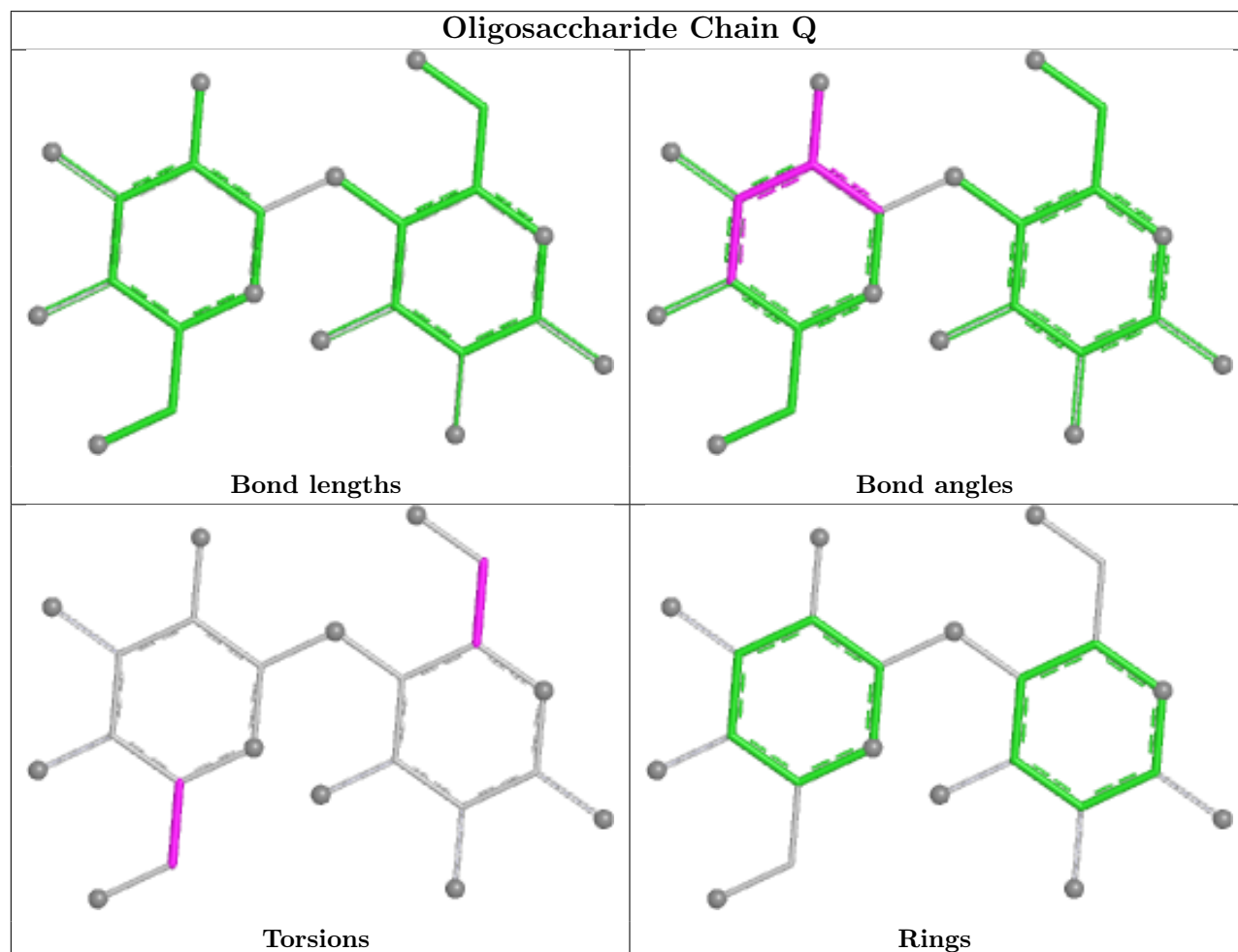
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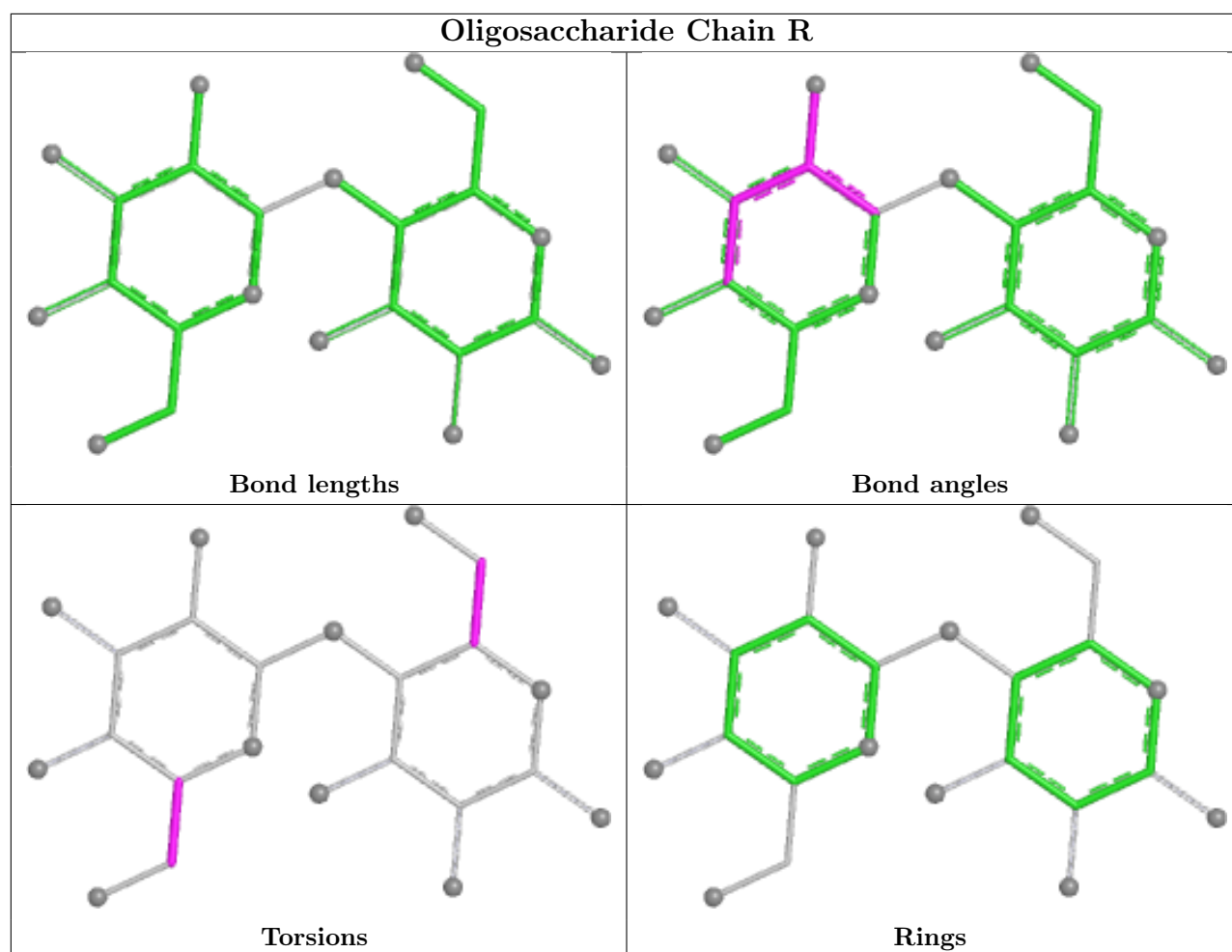
Mol	Chain	Res	Type	Atoms
2	S	1	BGC	O5-C5-C6-O6
2	U	1	BGC	O5-C5-C6-O6
2	V	1	BGC	O5-C5-C6-O6
2	W	1	BGC	O5-C5-C6-O6
2	X	1	BGC	O5-C5-C6-O6
2	Y	1	BGC	O5-C5-C6-O6
2	Z	1	BGC	O5-C5-C6-O6
2	a	1	BGC	O5-C5-C6-O6
2	d	1	BGC	O5-C5-C6-O6
2	Q	1	BGC	C4-C5-C6-O6
2	R	1	BGC	C4-C5-C6-O6
2	S	1	BGC	C4-C5-C6-O6
2	T	1	BGC	C4-C5-C6-O6
2	U	1	BGC	C4-C5-C6-O6
2	V	1	BGC	C4-C5-C6-O6
2	W	1	BGC	C4-C5-C6-O6
2	Y	1	BGC	C4-C5-C6-O6
2	Z	1	BGC	C4-C5-C6-O6
2	a	1	BGC	C4-C5-C6-O6
2	b	1	BGC	C4-C5-C6-O6
2	c	1	BGC	C4-C5-C6-O6
2	d	1	BGC	C4-C5-C6-O6
2	e	1	BGC	C4-C5-C6-O6
2	f	1	BGC	C4-C5-C6-O6
2	X	1	BGC	C4-C5-C6-O6
2	Q	2	2FG	O5-C5-C6-O6
2	R	2	2FG	O5-C5-C6-O6
2	S	2	2FG	O5-C5-C6-O6
2	T	2	2FG	O5-C5-C6-O6
2	U	2	2FG	O5-C5-C6-O6
2	V	2	2FG	O5-C5-C6-O6
2	W	2	2FG	O5-C5-C6-O6
2	X	2	2FG	O5-C5-C6-O6
2	Y	2	2FG	O5-C5-C6-O6
2	Z	2	2FG	O5-C5-C6-O6
2	a	2	2FG	O5-C5-C6-O6
2	b	2	2FG	O5-C5-C6-O6
2	c	2	2FG	O5-C5-C6-O6
2	d	2	2FG	O5-C5-C6-O6
2	e	2	2FG	O5-C5-C6-O6
2	f	2	2FG	O5-C5-C6-O6

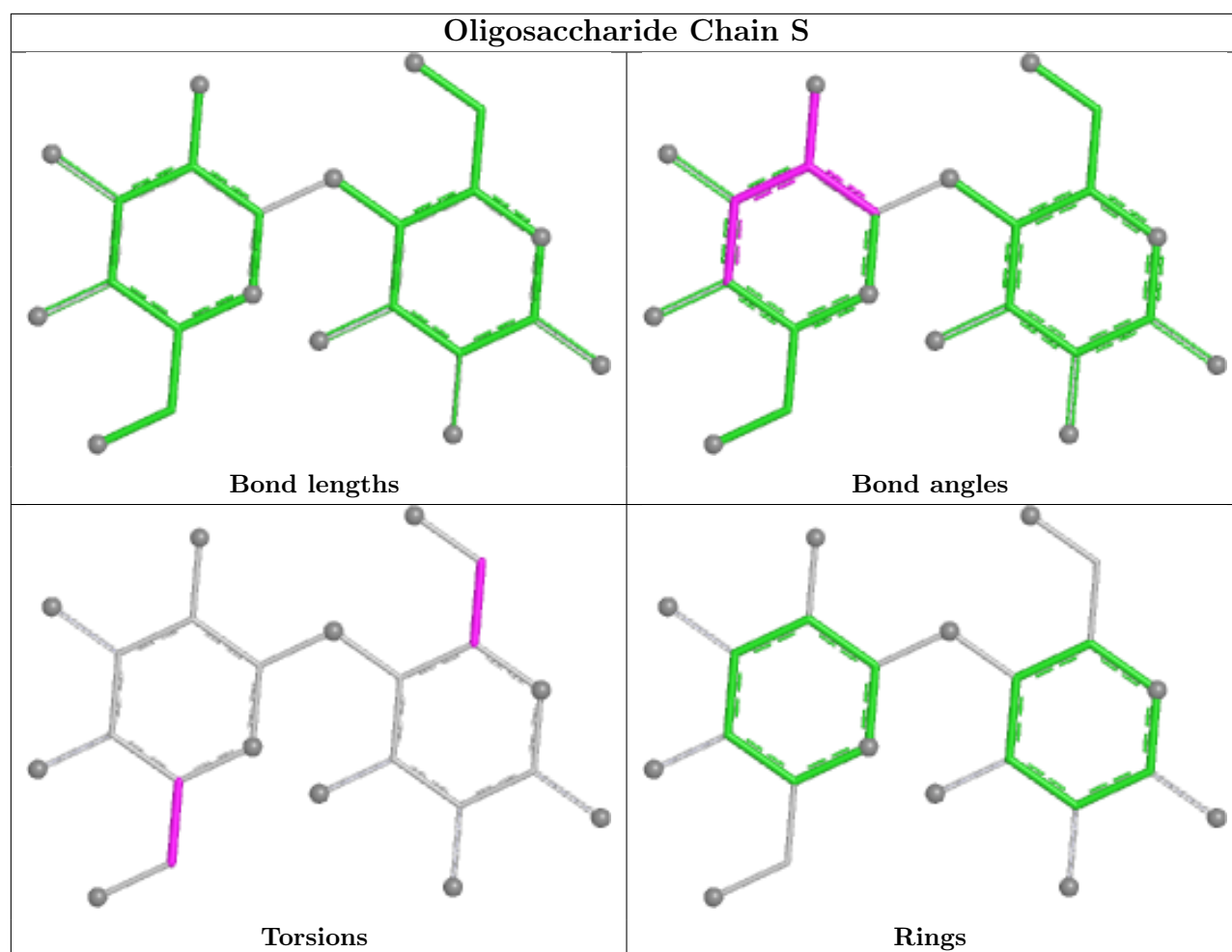
There are no ring outliers.

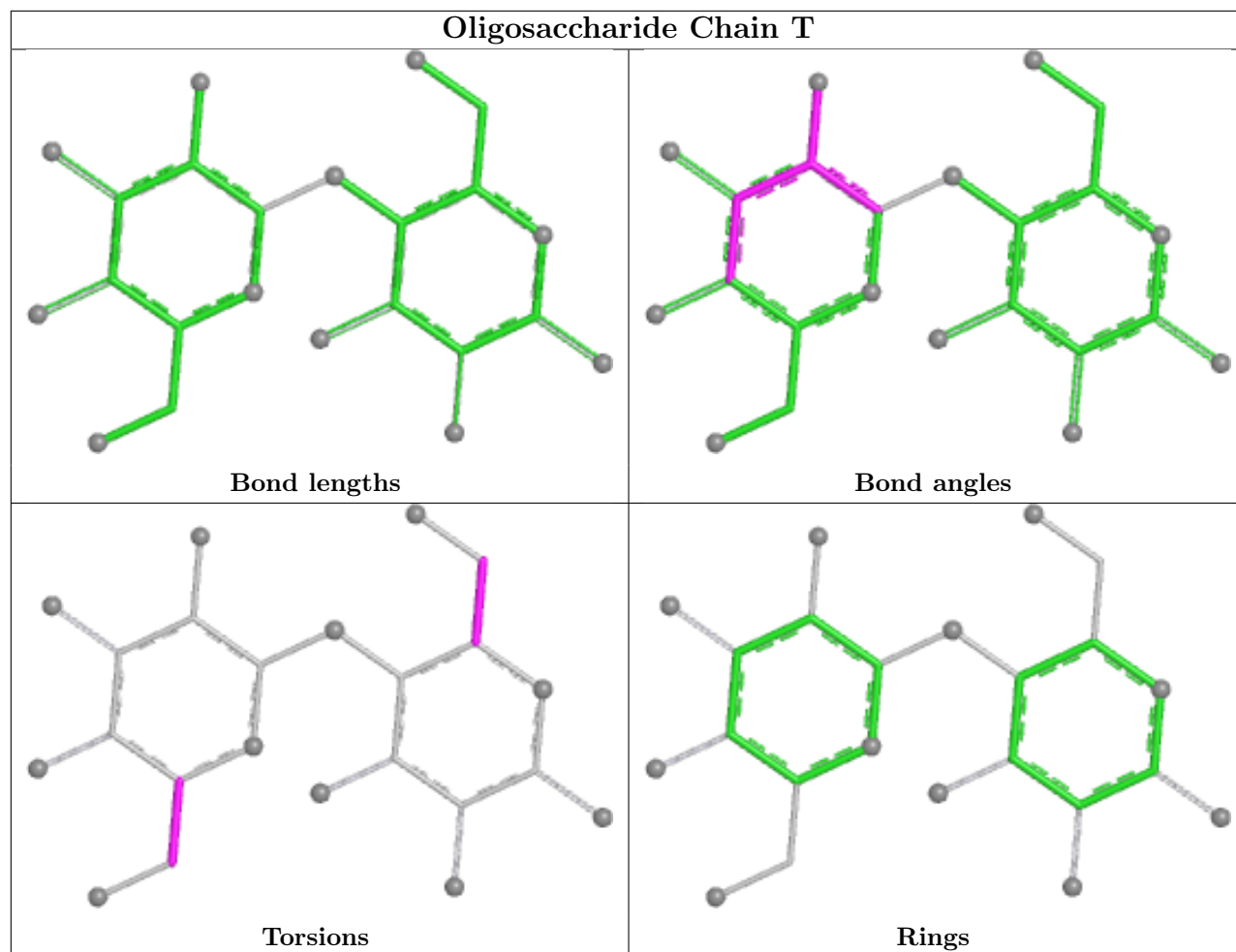
No monomer is involved in short contacts.

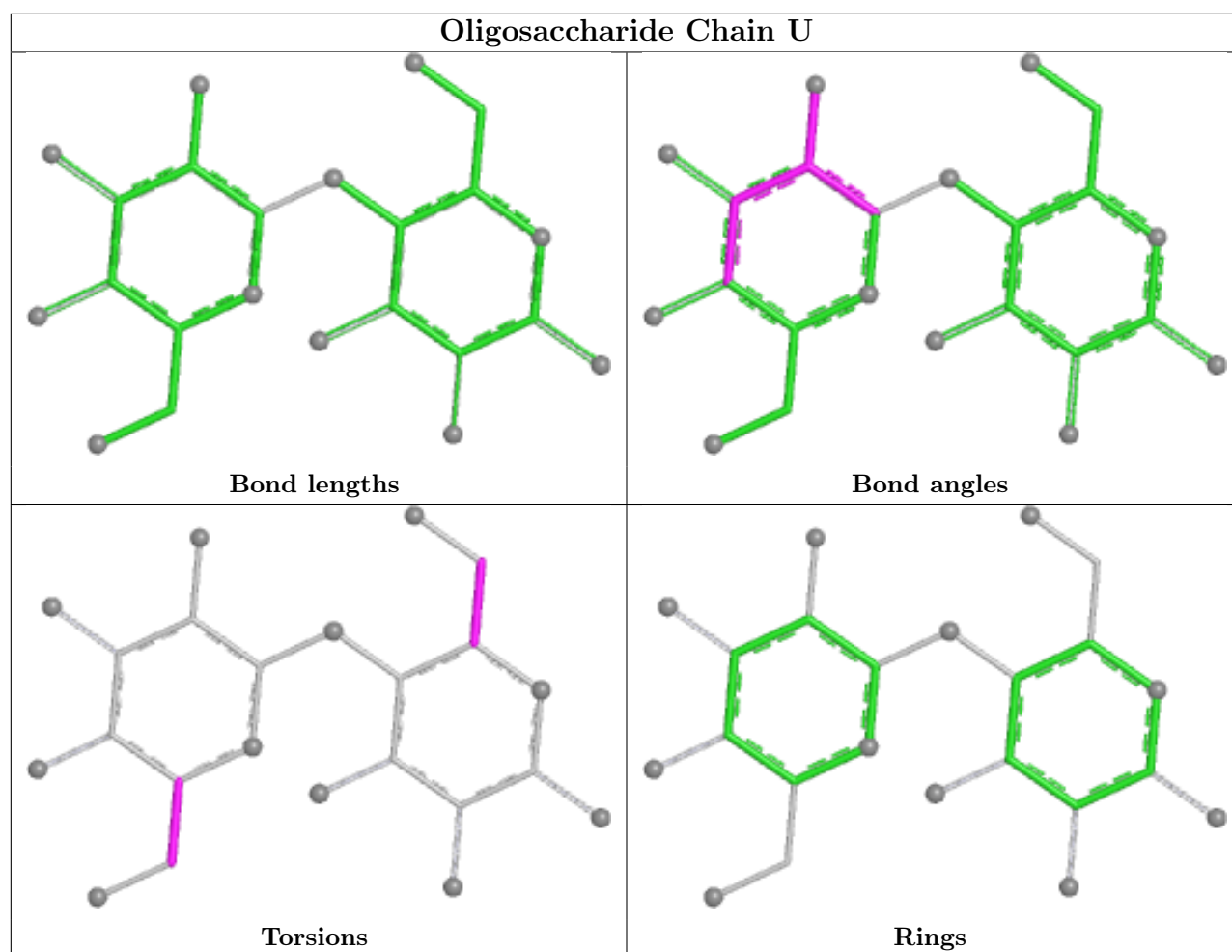
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



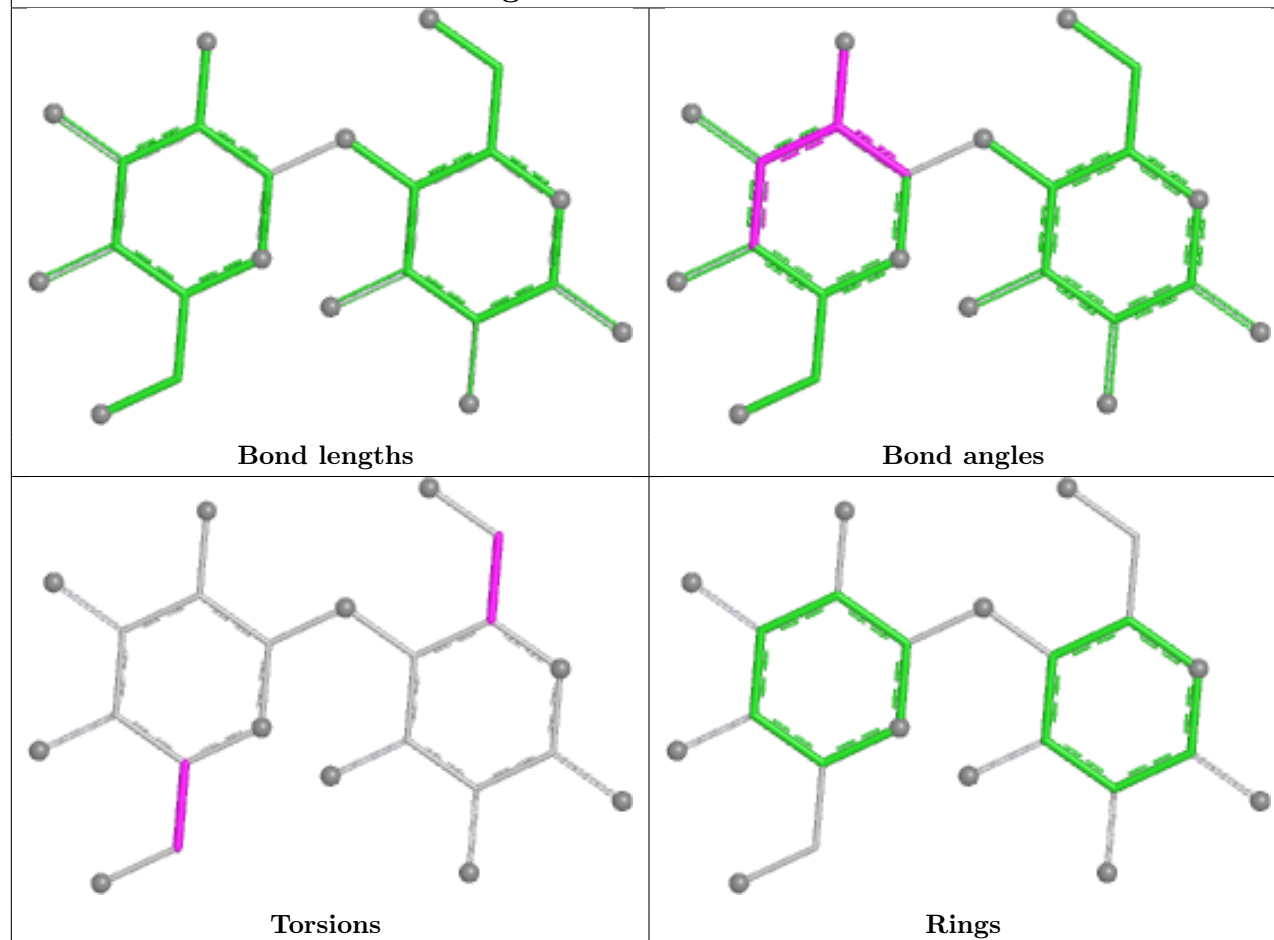


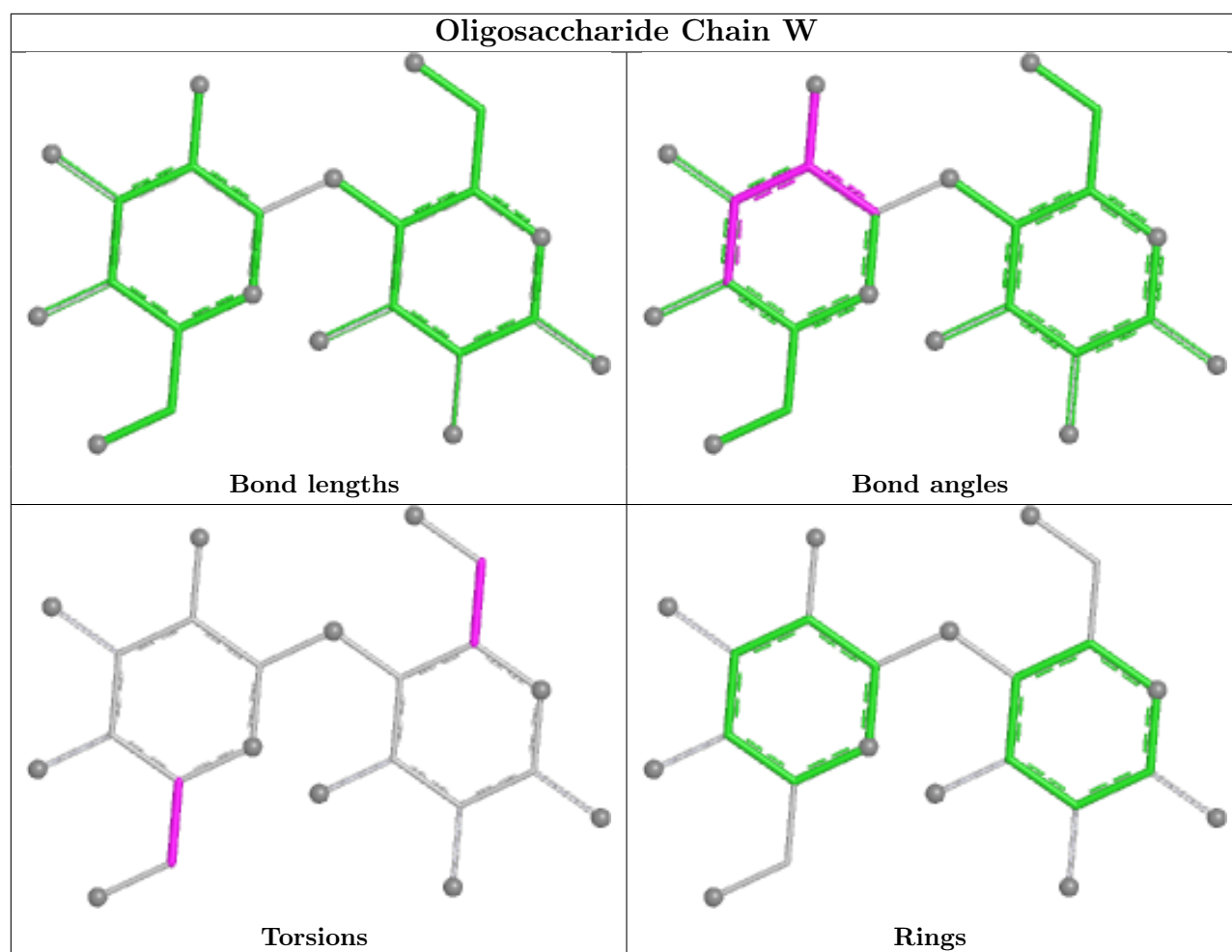


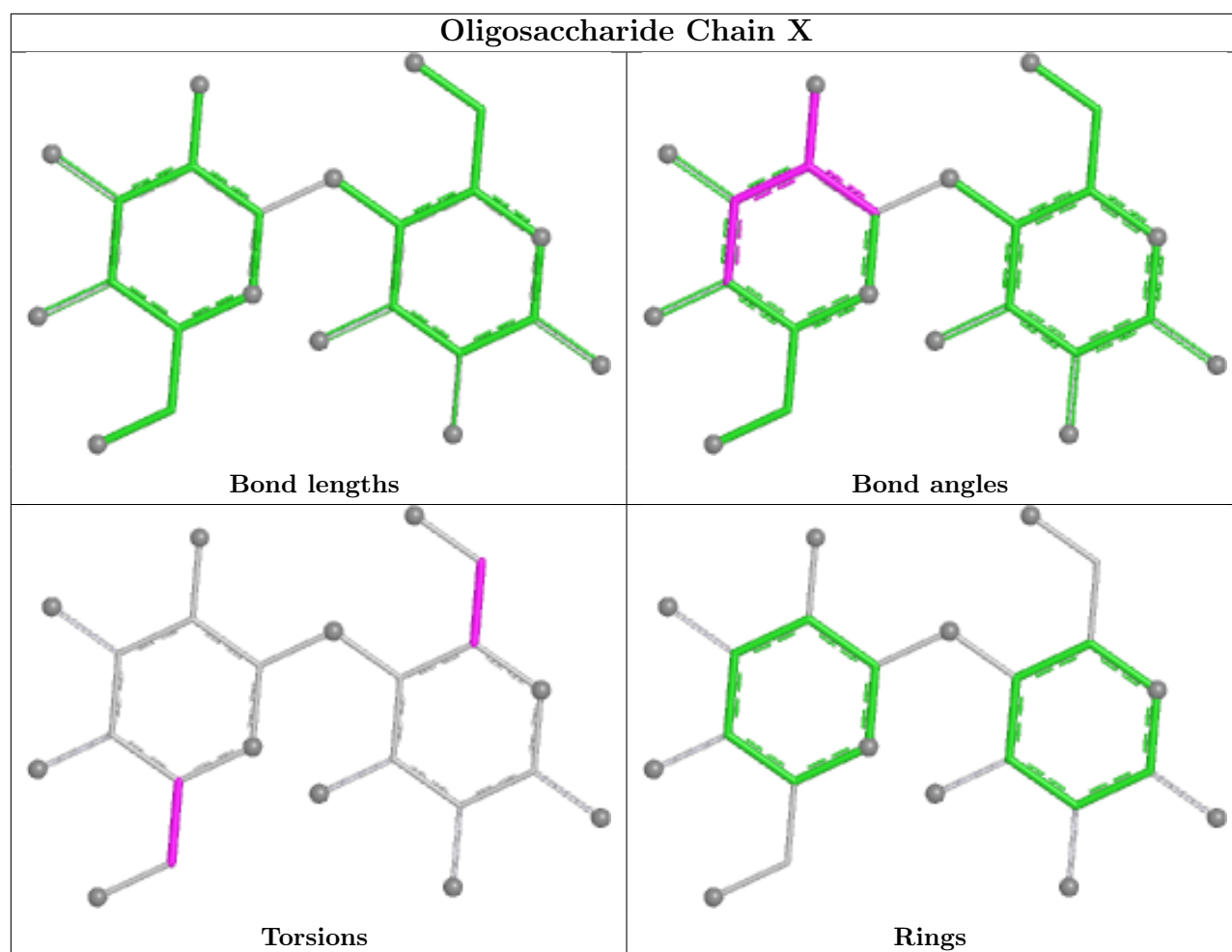


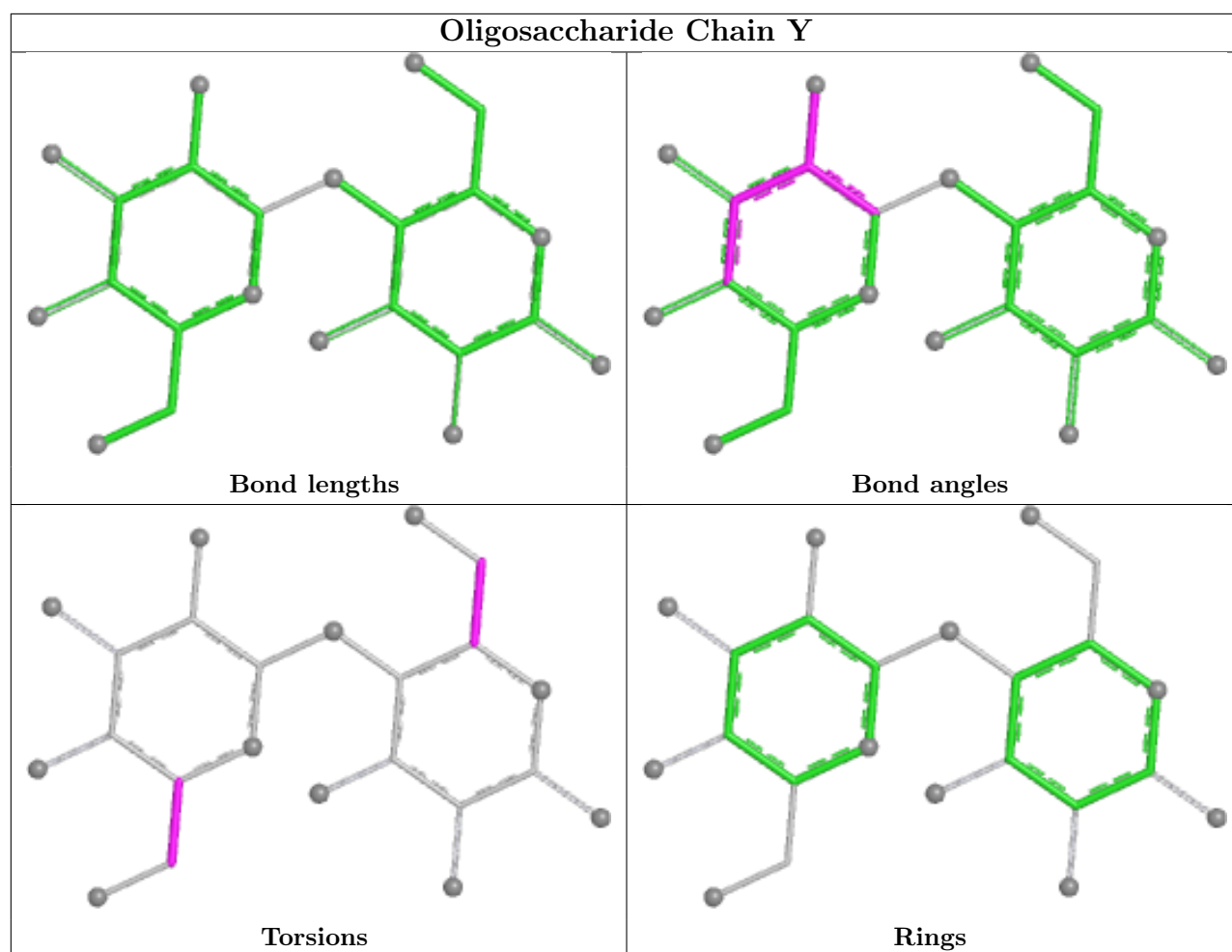


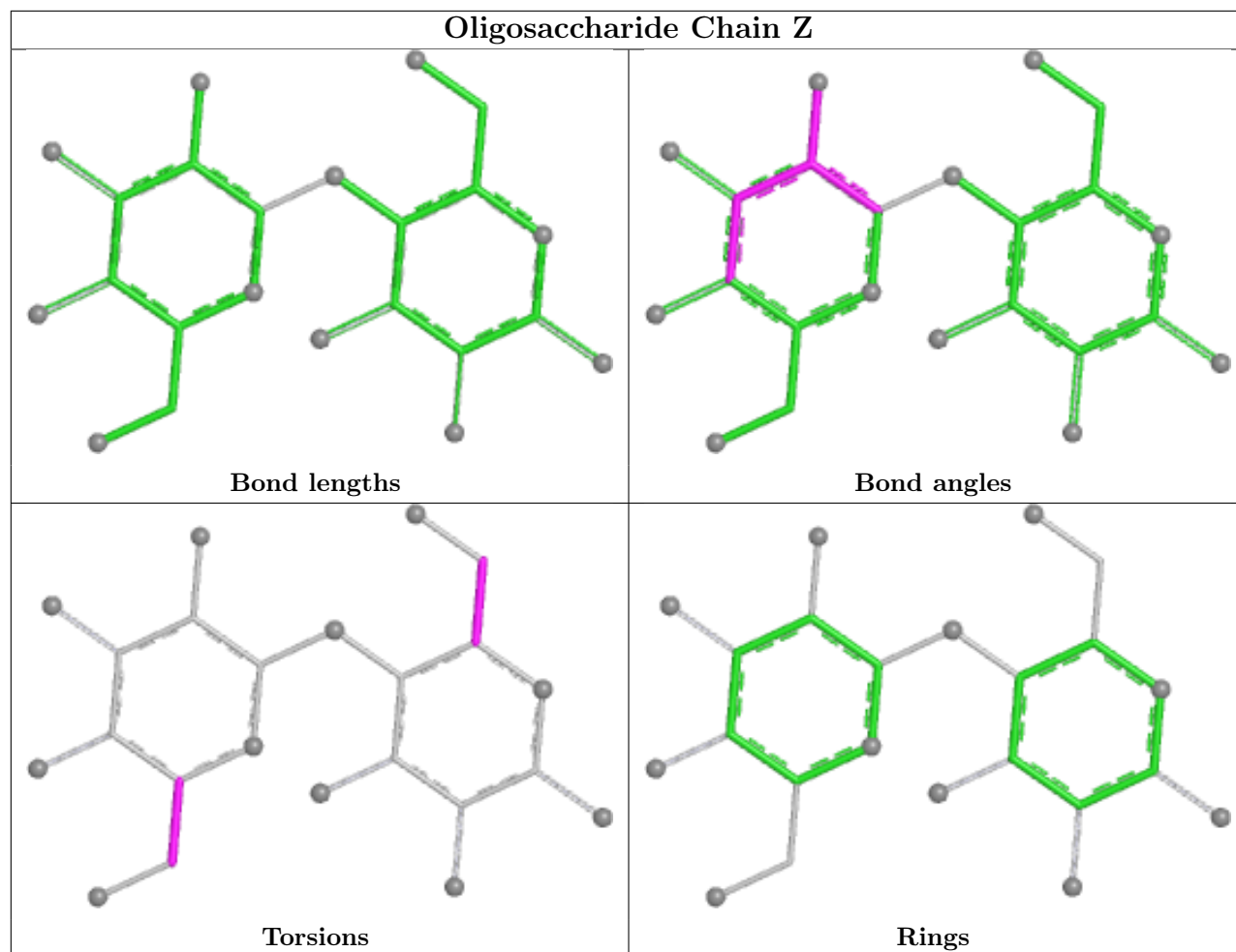
Oligosaccharide Chain V

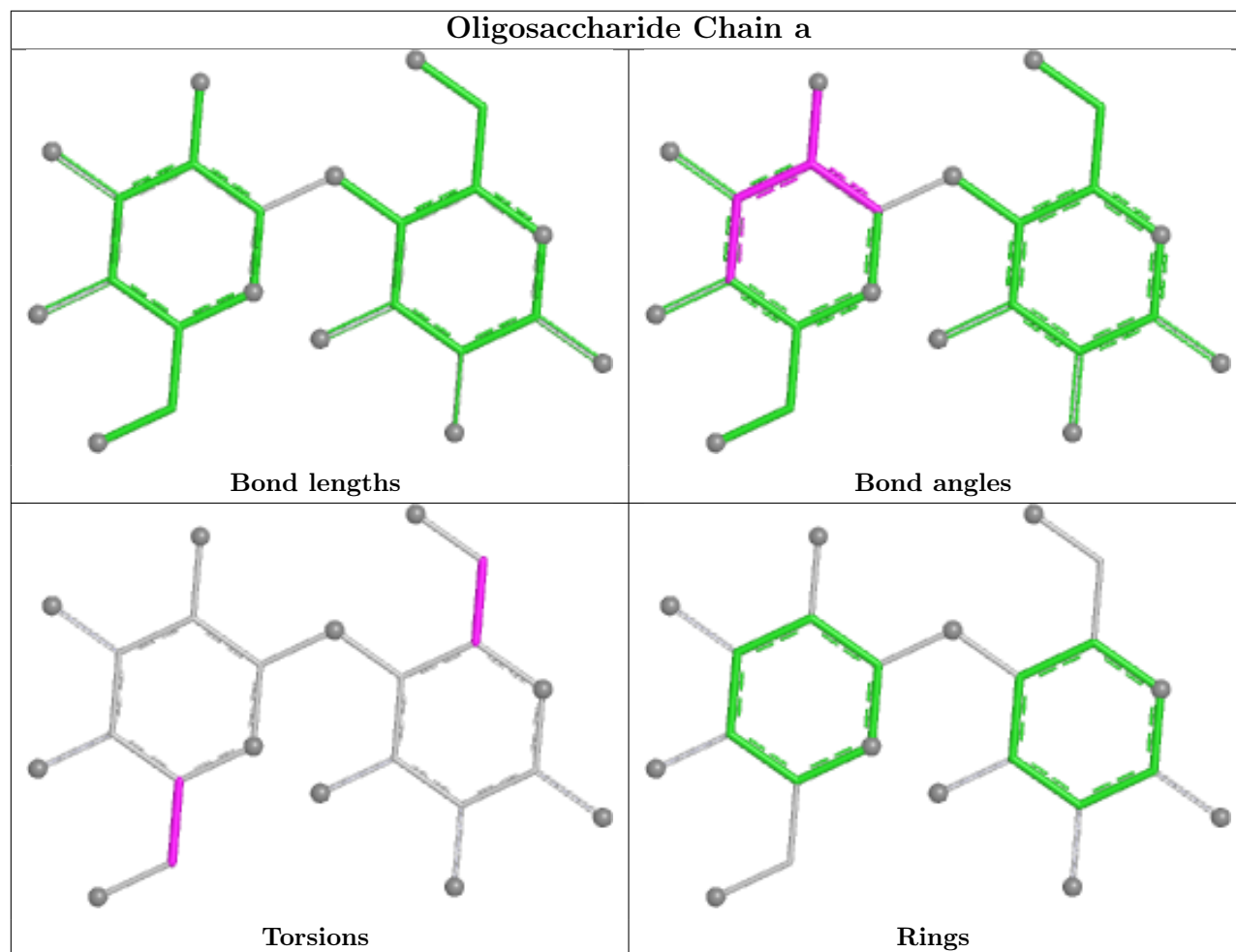


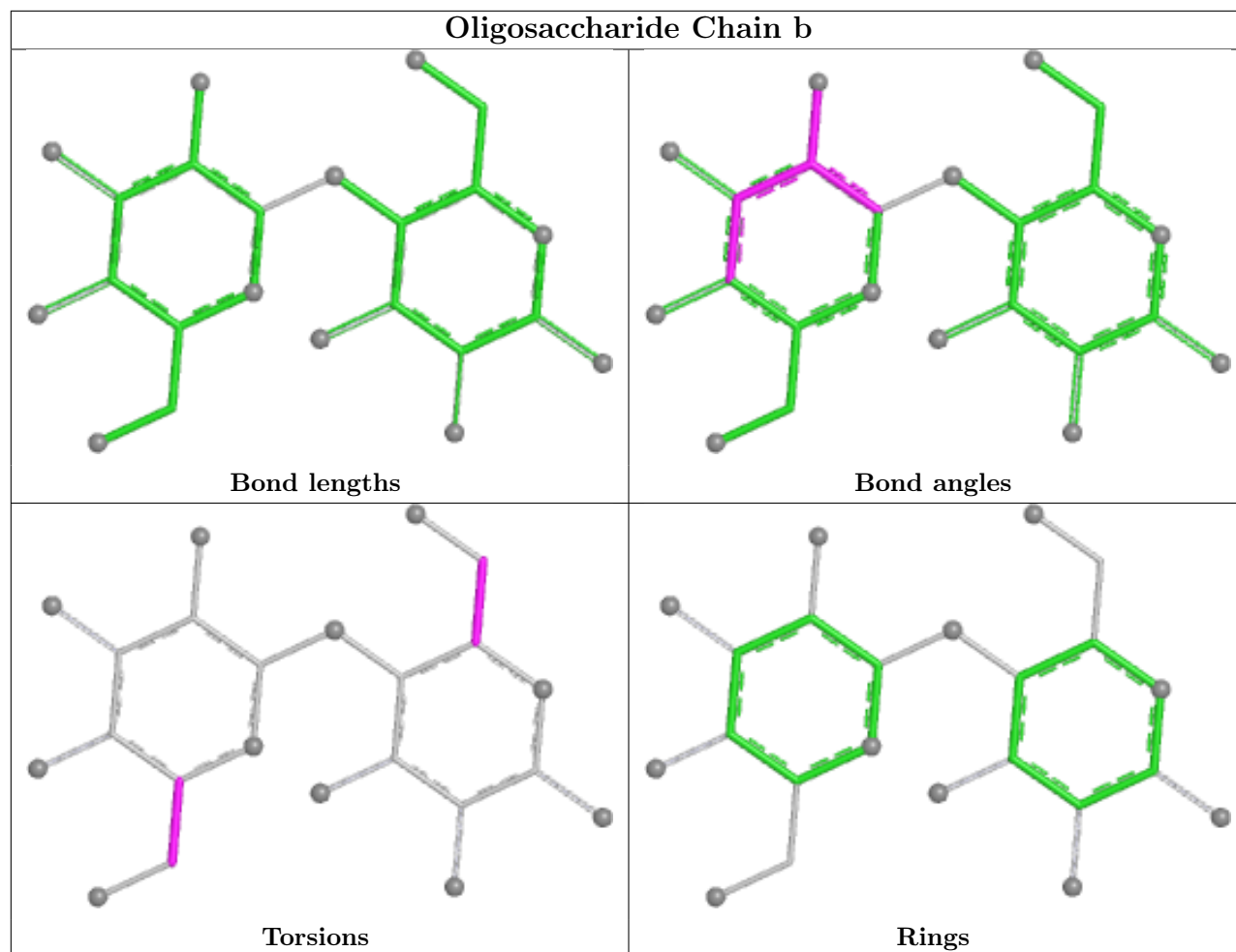


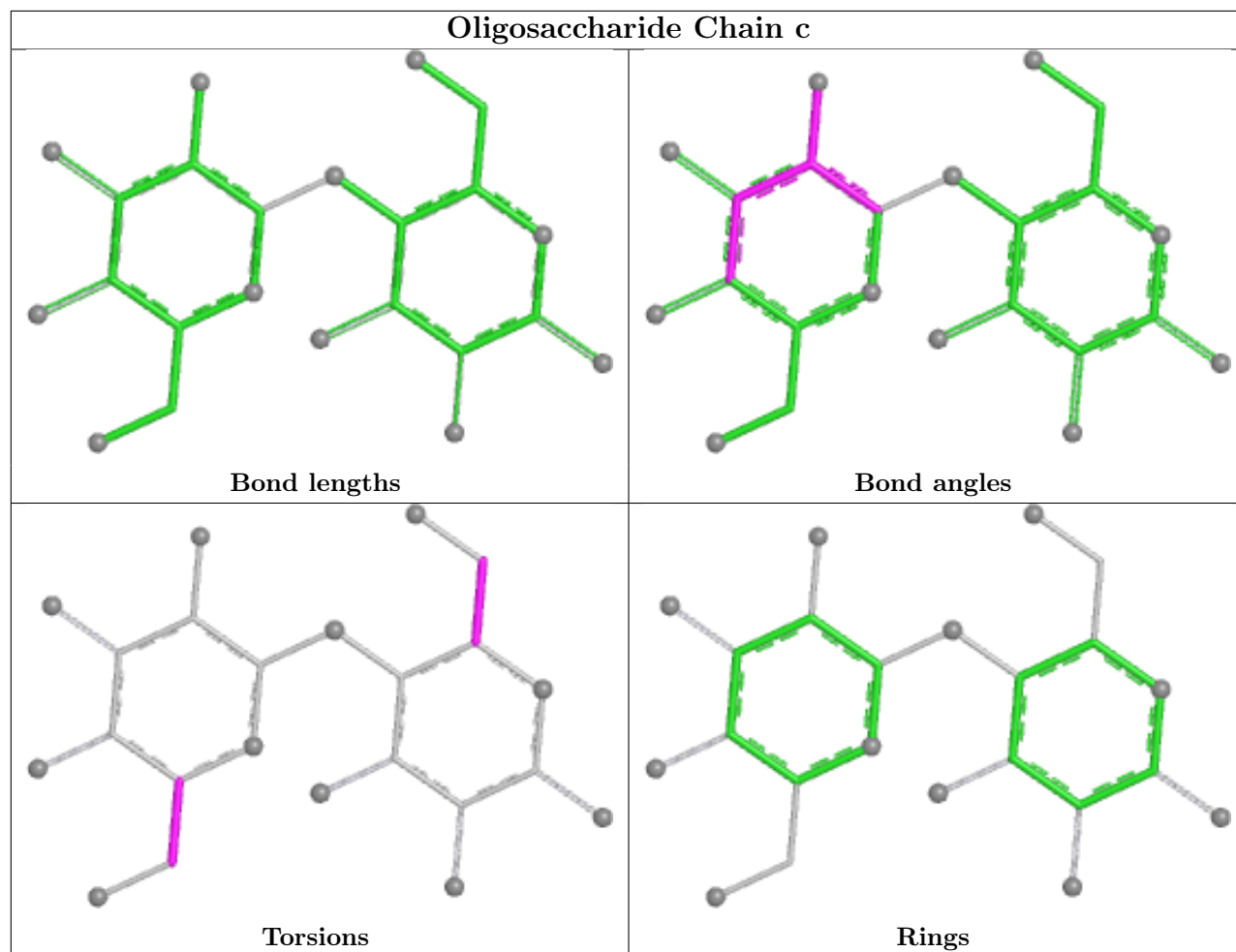


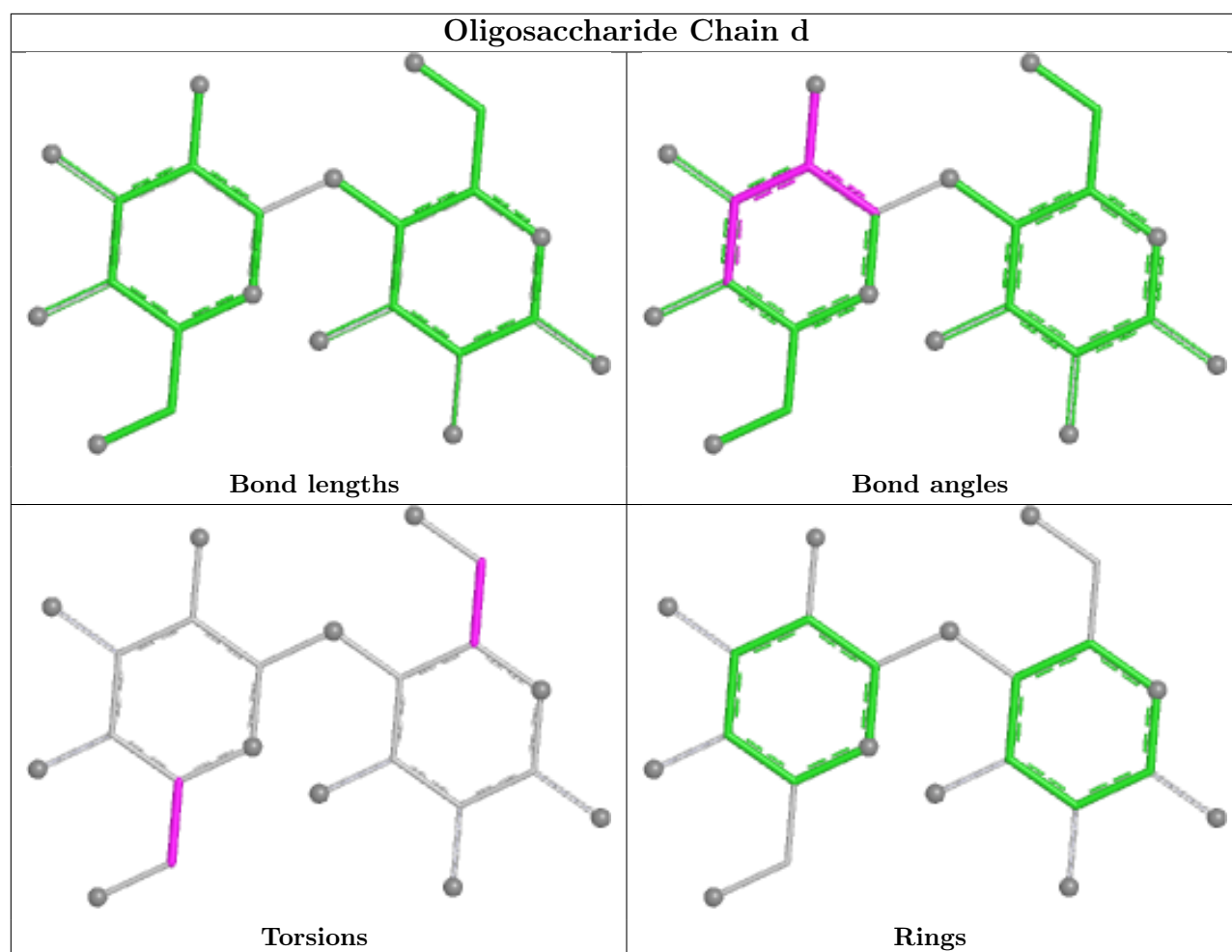


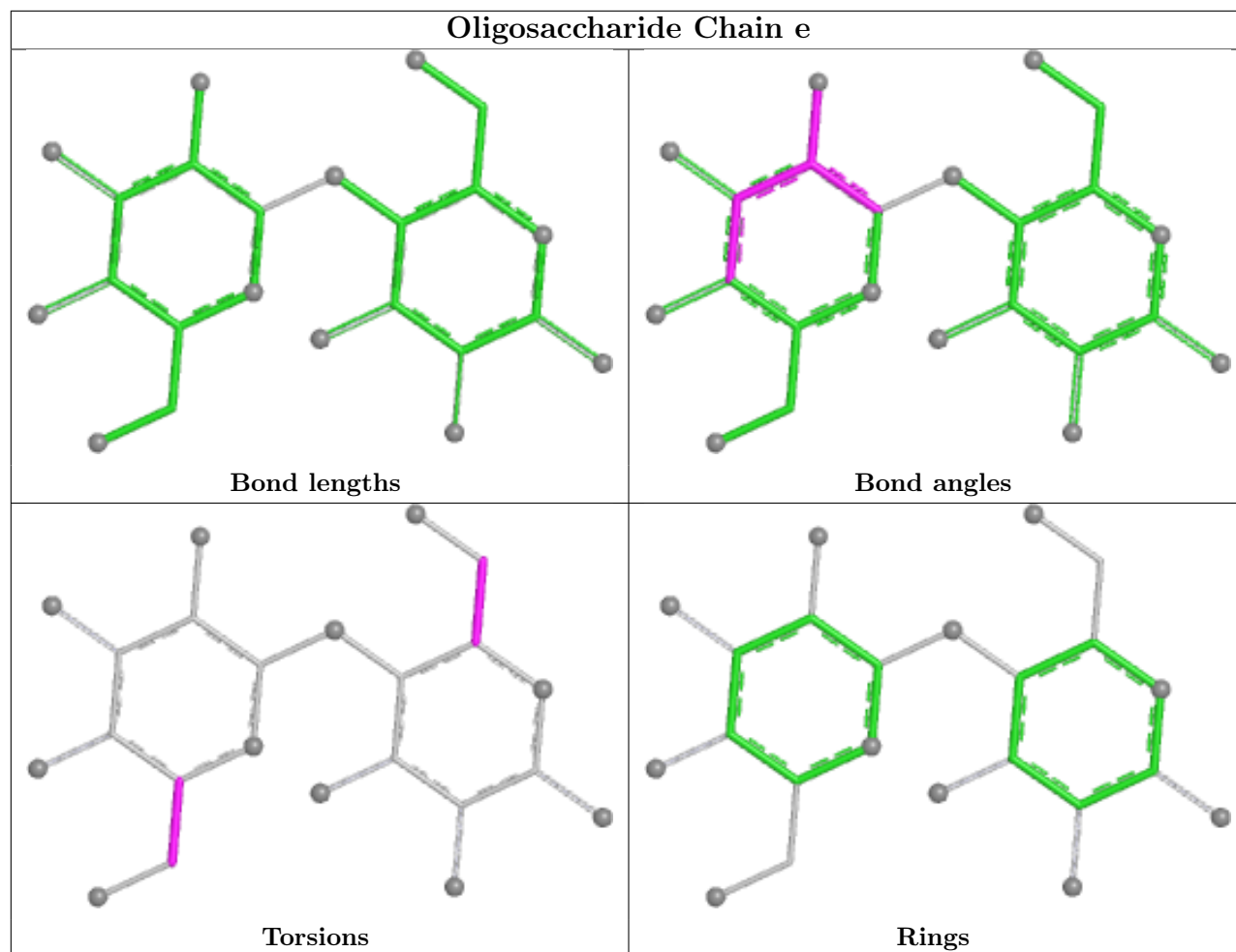


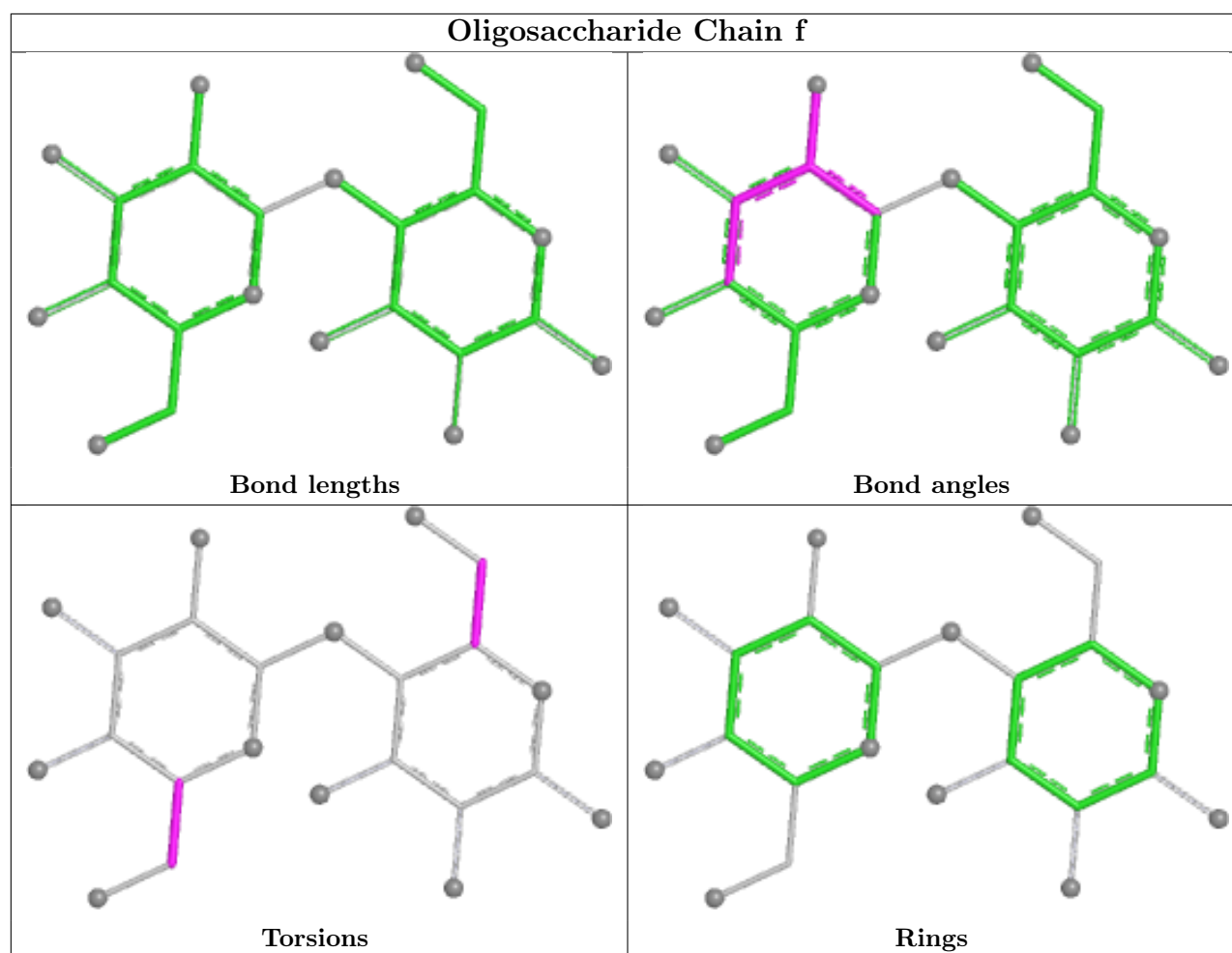












5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 64 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1018/1023 (99%)	-0.08	24 (2%)	59	56	2, 23, 63, 99	2 (0%)
1	B	1018/1023 (99%)	-0.13	14 (1%)	73	72	1, 21, 61, 98	2 (0%)
1	C	1018/1023 (99%)	-0.11	22 (2%)	62	59	1, 21, 61, 98	2 (0%)
1	D	1018/1023 (99%)	0.22	39 (3%)	44	40	10, 31, 69, 100	2 (0%)
1	E	1018/1023 (99%)	0.93	119 (11%)	9	7	27, 48, 83, 100	2 (0%)
1	F	1018/1023 (99%)	-0.03	20 (1%)	65	62	8, 28, 67, 100	2 (0%)
1	G	1018/1023 (99%)	-0.00	15 (1%)	72	70	8, 28, 68, 100	2 (0%)
1	H	1018/1023 (99%)	0.48	48 (4%)	36	33	18, 38, 75, 100	2 (0%)
1	I	1018/1023 (99%)	0.14	22 (2%)	62	59	11, 32, 70, 100	2 (0%)
1	J	1018/1023 (99%)	-0.05	16 (1%)	70	68	10, 30, 69, 100	2 (0%)
1	K	1018/1023 (99%)	0.32	17 (1%)	69	67	24, 45, 81, 100	2 (0%)
1	L	1018/1023 (99%)	0.50	42 (4%)	41	37	25, 45, 81, 100	2 (0%)
1	M	1018/1023 (99%)	1.16	166 (16%)	4	4	27, 48, 83, 100	2 (0%)
1	N	1018/1023 (99%)	0.19	31 (3%)	52	49	16, 36, 74, 100	2 (0%)
1	O	1018/1023 (99%)	0.31	23 (2%)	61	58	21, 42, 78, 100	2 (0%)
1	P	1018/1023 (99%)	1.72	359 (35%)	1	1	37, 60, 91, 100	2 (0%)
All	All	16288/16368 (99%)	0.35	977 (5%)	27	24	1, 37, 76, 100	32 (0%)

All (977) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	582	GLY	8.7
1	P	739	HIS	6.4
1	P	364	GLY	5.8
1	I	735	HIS	5.7
1	A	580	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	581	ASN	5.5
1	P	575	LEU	5.5
1	P	684	GLU	5.2
1	P	149	ALA	5.1
1	P	133	TRP	5.1
1	P	683	PRO	4.9
1	M	162	GLY	4.9
1	P	143	PHE	4.9
1	P	204	ARG	4.8
1	M	596	PRO	4.8
1	E	160	GLY	4.7
1	P	86	VAL	4.7
1	L	739	HIS	4.6
1	P	685	LEU	4.6
1	F	581	ASN	4.5
1	P	405	TYR	4.5
1	E	173	LEU	4.5
1	B	582	GLY	4.5
1	M	177	LEU	4.3
1	E	596	PRO	4.3
1	M	735	HIS	4.3
1	H	582	GLY	4.3
1	E	364	GLY	4.3
1	P	81	ALA	4.3
1	P	609	ALA	4.3
1	F	75	GLU	4.2
1	A	682	LEU	4.2
1	L	682	LEU	4.2
1	D	736	ALA	4.2
1	P	325	ALA	4.2
1	A	131	GLU	4.2
1	M	325	ALA	4.1
1	P	634	GLN	4.1
1	P	596	PRO	4.1
1	P	585	TRP	4.1
1	P	316	HIS	4.1
1	M	116	THR	4.1
1	E	140	ARG	4.0
1	D	735	HIS	4.0
1	P	414	ASN	4.0
1	H	149	ALA	4.0
1	M	160	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	579	ASP	4.0
1	P	209	PHE	3.9
1	L	733	ALA	3.9
1	M	734	SER	3.9
1	F	744	GLU	3.9
1	E	77	ASP	3.9
1	E	123	TYR	3.9
1	P	129	VAL	3.9
1	P	73	TRP	3.8
1	E	84	VAL	3.8
1	A	583	ASN	3.8
1	P	725	ASN	3.8
1	M	123	TYR	3.8
1	P	794	GLY	3.8
1	L	685	LEU	3.8
1	M	195	SER	3.8
1	K	731	PRO	3.8
1	P	115	PRO	3.8
1	L	3	ILE	3.7
1	P	315	LEU	3.7
1	M	149	ALA	3.7
1	P	689	GLU	3.7
1	P	121	GLY	3.7
1	P	923	SER	3.7
1	P	105	TYR	3.6
1	P	191	TRP	3.6
1	E	179	ALA	3.6
1	M	173	LEU	3.6
1	P	3	ILE	3.6
1	P	101	THR	3.6
1	N	581	ASN	3.6
1	E	73	TRP	3.6
1	P	158	TRP	3.6
1	M	247	CYS	3.6
1	M	69	VAL	3.6
1	M	73	TRP	3.6
1	D	744	GLU	3.6
1	P	656	VAL	3.6
1	P	96	ASP	3.5
1	E	74	LEU	3.5
1	M	38	ASN	3.5
1	P	58	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	P	173	LEU	3.5
1	P	728	VAL	3.5
1	B	739	HIS	3.5
1	L	116	THR	3.5
1	M	832	ASP	3.5
1	P	284	GLY	3.5
1	P	723	ALA	3.5
1	P	111	PRO	3.5
1	E	710	GLU	3.5
1	A	685	LEU	3.5
1	E	7	LEU	3.5
1	P	215	LEU	3.5
1	P	317	THR	3.5
1	P	185	ALA	3.5
1	O	744	GLU	3.5
1	M	15	ASP	3.4
1	P	970	THR	3.4
1	E	65	ALA	3.4
1	M	736	ALA	3.4
1	P	361	PRO	3.4
1	K	739	HIS	3.4
1	E	60	PHE	3.4
1	E	36	TRP	3.4
1	D	734	SER	3.4
1	C	742	THR	3.4
1	P	4	THR	3.4
1	H	160	GLY	3.4
1	P	70	PRO	3.4
1	P	60	PHE	3.4
1	B	584	PRO	3.4
1	M	320	GLY	3.4
1	E	76	CYS	3.4
1	P	54	LEU	3.4
1	P	360	HIS	3.4
1	P	799	THR	3.3
1	E	162	GLY	3.3
1	P	359	HIS	3.3
1	P	92	MET	3.3
1	E	143	PHE	3.3
1	M	795	VAL	3.3
1	P	930	VAL	3.3
1	P	222	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	P	798	ALA	3.3
1	P	45	ASP	3.3
1	P	186	VAL	3.3
1	E	136	GLU	3.3
1	E	689	GLU	3.3
1	E	459	GLY	3.3
1	D	747	PHE	3.3
1	M	129	VAL	3.3
1	E	131	GLU	3.3
1	G	829	THR	3.3
1	K	596	PRO	3.3
1	P	7	LEU	3.3
1	N	745	MET	3.3
1	P	687	GLN	3.3
1	M	312	VAL	3.3
1	P	85	VAL	3.3
1	A	832	ASP	3.3
1	M	76	CYS	3.2
1	P	74	LEU	3.2
1	P	729	THR	3.2
1	P	195	SER	3.2
1	B	581	ASN	3.2
1	O	128	ASN	3.2
1	G	580	GLU	3.2
1	M	219	THR	3.2
1	P	34	ALA	3.2
1	P	272	ALA	3.2
1	L	60	PHE	3.2
1	M	99	ILE	3.2
1	B	832	ASP	3.2
1	E	177	LEU	3.2
1	F	689	GLU	3.2
1	A	596	PRO	3.2
1	L	735	HIS	3.2
1	M	427	THR	3.2
1	J	743	SER	3.2
1	F	734	SER	3.2
1	B	737	ILE	3.2
1	P	141	ILE	3.2
1	C	581	ASN	3.1
1	N	583	ASN	3.1
1	E	66	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	L	4	THR	3.1
1	P	848	THR	3.1
1	P	279	ILE	3.1
1	H	581	ASN	3.1
1	M	572	ASP	3.1
1	E	575	LEU	3.1
1	P	177	LEU	3.1
1	M	136	GLU	3.1
1	P	131	GLU	3.1
1	P	98	PRO	3.1
1	P	899	GLY	3.1
1	K	733	ALA	3.1
1	M	39	SER	3.1
1	P	672	VAL	3.1
1	F	832	ASP	3.1
1	P	594	ASP	3.1
1	A	799	THR	3.1
1	P	714	ILE	3.1
1	M	9	VAL	3.1
1	P	162	GLY	3.1
1	E	29	ALA	3.1
1	M	603	MET	3.1
1	O	760	ARG	3.1
1	D	582	GLY	3.0
1	A	179	ALA	3.0
1	M	246	MET	3.0
1	P	179	ALA	3.0
1	P	36	TRP	3.0
1	P	708	TRP	3.0
1	P	679	LEU	3.0
1	P	920	LEU	3.0
1	P	55	ASN	3.0
1	M	737	ILE	3.0
1	M	742	THR	3.0
1	M	114	VAL	3.0
1	H	133	TRP	3.0
1	P	398	TRP	3.0
1	P	654	TRP	3.0
1	P	897	TRP	3.0
1	C	39	SER	3.0
1	M	134	LEU	3.0
1	P	206	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	N	744	GLU	3.0
1	P	688	PRO	3.0
1	P	140	ARG	3.0
1	P	749	ILE	3.0
1	P	664	ALA	3.0
1	P	313	VAL	3.0
1	P	608	PHE	3.0
1	C	734	SER	3.0
1	M	314	GLU	3.0
1	P	48	SER	3.0
1	P	124	SER	3.0
1	P	766	SER	3.0
1	P	59	ARG	3.0
1	P	635	THR	3.0
1	M	274	PHE	3.0
1	P	63	PHE	3.0
1	P	84	VAL	3.0
1	J	735	HIS	2.9
1	M	646	HIS	2.9
1	P	216	HIS	2.9
1	E	52	ARG	2.9
1	F	252	ASP	2.9
1	N	319	ASP	2.9
1	P	190	ARG	2.9
1	P	447	ASP	2.9
1	E	798	ALA	2.9
1	M	691	ALA	2.9
1	E	127	PHE	2.9
1	P	189	LEU	2.9
1	P	663	LEU	2.9
1	B	583	ASN	2.9
1	E	158	TRP	2.9
1	N	135	GLN	2.9
1	M	248	GLY	2.9
1	L	97	ALA	2.9
1	P	217	LYS	2.9
1	P	254	LEU	2.9
1	H	216	HIS	2.9
1	E	361	PRO	2.9
1	P	47	PRO	2.9
1	D	745	MET	2.9
1	E	16	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	P	203	TRP	2.9
1	P	210	ARG	2.9
1	H	583	ASN	2.9
1	M	582	GLY	2.9
1	K	732	ALA	2.9
1	M	798	ALA	2.9
1	P	691	ALA	2.9
1	H	195	SER	2.8
1	P	147	ASN	2.8
1	P	323	ILE	2.8
1	L	61	ALA	2.8
1	P	652	LEU	2.8
1	P	694	LEU	2.8
1	P	732	ALA	2.8
1	E	176	PHE	2.8
1	J	580	GLU	2.8
1	P	902	PRO	2.8
1	L	734	SER	2.8
1	M	6	SER	2.8
1	P	543	GLY	2.8
1	E	152	LEU	2.8
1	L	123	TYR	2.8
1	P	214	LEU	2.8
1	P	122	CYS	2.8
1	P	175	ALA	2.8
1	P	840	HIS	2.8
1	O	596	PRO	2.8
1	O	686	PRO	2.8
1	M	16	TRP	2.8
1	P	90	TRP	2.8
1	I	581	ASN	2.8
1	E	78	LEU	2.8
1	P	947	GLY	2.8
1	H	130	ASP	2.8
1	P	65	ALA	2.8
1	P	95	TYR	2.8
1	P	335	VAL	2.8
1	P	392	TYR	2.8
1	P	932	PRO	2.8
1	E	262	GLN	2.8
1	E	208	ILE	2.8
1	M	3	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	734	SER	2.8
1	P	722	LEU	2.8
1	M	117	GLU	2.8
1	J	13	ARG	2.8
1	P	669	PRO	2.7
1	P	576	ILE	2.7
1	P	35	SER	2.7
1	L	590	GLY	2.7
1	P	391	HIS	2.7
1	E	34	ALA	2.7
1	G	832	ASP	2.7
1	J	252	ASP	2.7
1	L	681	GLU	2.7
1	M	594	ASP	2.7
1	O	249	GLU	2.7
1	P	244	VAL	2.7
1	P	281	GLU	2.7
1	P	650	GLU	2.7
1	H	3	ILE	2.7
1	M	189	LEU	2.7
1	M	426	LEU	2.7
1	P	751	LEU	2.7
1	E	133	TRP	2.7
1	E	202	MET	2.7
1	P	153	TRP	2.7
1	A	178	ARG	2.7
1	A	681	GLU	2.7
1	C	744	GLU	2.7
1	C	747	PHE	2.7
1	E	193	ASP	2.7
1	P	116	THR	2.7
1	P	572	ASP	2.7
1	M	686	PRO	2.7
1	P	218	PRO	2.7
1	P	376	ILE	2.7
1	P	205	MET	2.7
1	F	743	SER	2.7
1	G	582	GLY	2.7
1	H	800	ARG	2.7
1	N	580	GLU	2.7
1	P	178	ARG	2.7
1	H	81	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	101	THR	2.7
1	M	179	ALA	2.7
1	P	69	VAL	2.7
1	P	627	PHE	2.7
1	P	738	PRO	2.7
1	P	100	TYR	2.7
1	P	737	ILE	2.7
1	H	140	ARG	2.7
1	M	710	GLU	2.7
1	P	690	SER	2.7
1	P	918	TRP	2.7
1	P	971	SER	2.7
1	K	892	ALA	2.7
1	M	127	PHE	2.7
1	M	601	PHE	2.7
1	M	829	THR	2.7
1	P	657	ALA	2.7
1	D	596	PRO	2.7
1	N	746	ASP	2.7
1	P	584	PRO	2.7
1	P	138	GLN	2.6
1	M	100	TYR	2.6
1	E	189	LEU	2.6
1	P	670	LEU	2.6
1	M	59	ARG	2.6
1	D	136	GLU	2.6
1	M	577	LYS	2.6
1	A	732	ALA	2.6
1	E	48	SER	2.6
1	E	733	ALA	2.6
1	M	66	PRO	2.6
1	M	361	PRO	2.6
1	P	139	THR	2.6
1	P	422	PRO	2.6
1	D	832	ASP	2.6
1	E	100	TYR	2.6
1	P	362	LEU	2.6
1	P	900	LEU	2.6
1	F	76	CYS	2.6
1	P	14	ARG	2.6
1	P	446	ARG	2.6
1	H	364	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	581	ASN	2.6
1	I	736	ALA	2.6
1	P	146	VAL	2.6
1	P	274	PHE	2.6
1	P	705	ALA	2.6
1	P	595	THR	2.6
1	E	15	ASP	2.6
1	E	99	ILE	2.6
1	L	134	LEU	2.6
1	M	152	LEU	2.6
1	P	682	LEU	2.6
1	P	962	TYR	2.6
1	M	442	ARG	2.6
1	M	218	PRO	2.6
1	D	799	THR	2.6
1	H	4	THR	2.6
1	M	727	SER	2.6
1	K	832	ASP	2.6
1	P	130	ASP	2.6
1	E	279	ILE	2.6
1	E	134	LEU	2.6
1	M	392	TYR	2.6
1	P	797	GLU	2.6
1	F	81	ALA	2.6
1	P	9	VAL	2.6
1	O	583	ASN	2.6
1	P	327	ALA	2.6
1	A	135	GLN	2.6
1	L	761	GLN	2.6
1	M	139	THR	2.5
1	P	49	GLN	2.6
1	H	73	TRP	2.5
1	N	734	SER	2.5
1	P	570	TRP	2.5
1	P	960	SER	2.5
1	M	801	ILE	2.5
1	E	13	ARG	2.5
1	P	418	HIS	2.5
1	H	744	GLU	2.5
1	O	136	GLU	2.5
1	E	275	GLY	2.5
1	P	676	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	P	451	PRO	2.5
1	G	179	ALA	2.5
1	K	664	ALA	2.5
1	L	798	ALA	2.5
1	M	657	ALA	2.5
1	N	664	ALA	2.5
1	J	742	THR	2.5
1	E	367	MET	2.5
1	E	746	ASP	2.5
1	P	134	LEU	2.5
1	P	356	ARG	2.5
1	P	651	LEU	2.5
1	D	819	GLU	2.5
1	P	309	TYR	2.5
1	M	180	GLY	2.5
1	L	686	PRO	2.5
1	M	688	PRO	2.5
1	A	733	ALA	2.5
1	M	200	GLN	2.5
1	N	798	ALA	2.5
1	M	220	THR	2.5
1	P	545	SER	2.5
1	P	586	SER	2.5
1	P	861	SER	2.5
1	C	746	ASP	2.5
1	I	832	ASP	2.5
1	I	1023	LYS	2.5
1	J	319	ASP	2.5
1	O	75	GLU	2.5
1	P	314	GLU	2.5
1	P	750	GLU	2.5
1	A	180	GLY	2.5
1	P	590	GLY	2.5
1	L	683	PRO	2.5
1	C	761	GLN	2.5
1	E	81	ALA	2.5
1	E	327	ALA	2.5
1	G	723	ALA	2.5
1	M	113	PHE	2.5
1	M	733	ALA	2.5
1	N	747	PHE	2.5
1	P	176	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	P	221	GLN	2.5
1	P	22	THR	2.5
1	P	38	ASN	2.5
1	M	575	LEU	2.5
1	N	13	ARG	2.5
1	F	319	ASP	2.5
1	M	77	ASP	2.5
1	N	832	ASP	2.5
1	P	301	TRP	2.5
1	P	591	ASP	2.5
1	P	653[A]	HIS	2.5
1	K	136	GLU	2.5
1	P	285	TYR	2.5
1	P	940	GLY	2.5
1	E	688	PRO	2.5
1	L	596	PRO	2.5
1	L	687	GLN	2.5
1	M	135	GLN	2.5
1	C	664	ALA	2.5
1	P	61	ALA	2.5
1	P	912	ALA	2.5
1	F	742	THR	2.4
1	L	76	CYS	2.4
1	M	174	SER	2.4
1	P	39	SER	2.4
1	B	735	HIS	2.4
1	E	832	ASP	2.4
1	M	133	TRP	2.4
1	M	158	TRP	2.4
1	H	136	GLU	2.4
1	E	79	PRO	2.4
1	G	180	GLY	2.4
1	O	731	PRO	2.4
1	C	253	TYR	2.4
1	H	578	TYR	2.4
1	D	687	GLN	2.4
1	E	1023	LYS	2.4
1	P	289	VAL	2.4
1	D	798	ALA	2.4
1	O	732	ALA	2.4
1	P	820	ALA	2.4
1	D	829	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	595	THR	2.4
1	N	59	ARG	2.4
1	O	178	ARG	2.4
1	E	583	ASN	2.4
1	I	102	ASN	2.4
1	M	315	LEU	2.4
1	M	322	LEU	2.4
1	M	714	ILE	2.4
1	M	751	LEU	2.4
1	G	124	SER	2.4
1	M	93	HIS	2.4
1	K	594	ASP	2.4
1	M	602	CYS	2.4
1	O	77	ASP	2.4
1	P	247	CYS	2.4
1	A	136	GLU	2.4
1	M	744	GLU	2.4
1	P	170	GLU	2.4
1	P	326	GLU	2.4
1	P	187	MET	2.4
1	P	928	PRO	2.4
1	L	634	GLN	2.4
1	P	10	VAL	2.4
1	P	578	TYR	2.4
1	D	179	ALA	2.4
1	G	732	ALA	2.4
1	M	34	ALA	2.4
1	M	512	PHE	2.4
1	E	595	THR	2.4
1	L	177	LEU	2.4
1	M	967	LEU	2.4
1	N	742	THR	2.4
1	P	397	LEU	2.4
1	M	460	ASN	2.4
1	P	89	ASN	2.4
1	P	935	ASN	2.4
1	G	735	HIS	2.4
1	N	735	HIS	2.4
1	M	665	SER	2.4
1	P	632	SER	2.4
1	D	77	ASP	2.4
1	E	191	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	16	TRP	2.4
1	H	832	ASP	2.4
1	J	744	GLU	2.4
1	P	832	ASP	2.4
1	C	582	GLY	2.4
1	H	162	GLY	2.4
1	L	137	GLY	2.4
1	M	115	PRO	2.4
1	D	761	GLN	2.4
1	J	129	VAL	2.4
1	M	289	VAL	2.4
1	H	13	ARG	2.4
1	I	733	ALA	2.4
1	I	800	ARG	2.4
1	O	13	ARG	2.4
1	P	97	ALA	2.4
1	P	225	PHE	2.4
1	P	747	PHE	2.4
1	H	78	LEU	2.4
1	A	735	HIS	2.4
1	J	581	ASN	2.4
1	P	102	ASN	2.4
1	M	797	GLU	2.4
1	P	681	GLU	2.4
1	P	367	MET	2.4
1	P	443	MET	2.4
1	P	106	PRO	2.4
1	P	686	PRO	2.4
1	M	846	GLY	2.4
1	O	162	GLY	2.4
1	H	135	GLN	2.4
1	N	668	VAL	2.4
1	P	239	VAL	2.4
1	P	701	VAL	2.4
1	E	150	PHE	2.4
1	L	732	ALA	2.4
1	M	60	PHE	2.4
1	P	821	ALA	2.4
1	E	321	THR	2.3
1	H	220	THR	2.3
1	M	363	HIS	2.3
1	E	55	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	55	ASN	2.3
1	A	689	GLU	2.3
1	C	689	GLU	2.3
1	M	170	GLU	2.3
1	P	296	GLU	2.3
1	M	598	ASP	2.3
1	F	59	ARG	2.3
1	L	370	GLN	2.3
1	M	687	GLN	2.3
1	P	771	GLY	2.3
1	P	43	ARG	2.3
1	M	10	VAL	2.3
1	P	312	VAL	2.3
1	D	758	PHE	2.3
1	E	736	ALA	2.3
1	H	736	ALA	2.3
1	I	685	LEU	2.3
1	P	311	ALA	2.3
1	D	739	HIS	2.3
1	M	704	ASN	2.3
1	P	382	ASN	2.3
1	C	580	GLU	2.3
1	D	580	GLU	2.3
1	E	744	GLU	2.3
1	F	745	MET	2.3
1	I	744	GLU	2.3
1	E	164	ASP	2.3
1	H	259	SER	2.3
1	I	734	SER	2.3
1	L	132	SER	2.3
1	M	259	SER	2.3
1	O	743	SER	2.3
1	P	598	ASP	2.3
1	I	13	ARG	2.3
1	M	237	ARG	2.3
1	E	86	VAL	2.3
1	M	159	VAL	2.3
1	P	895	VAL	2.3
1	D	733	ALA	2.3
1	P	125	LEU	2.3
1	I	737	ILE	2.3
1	O	801	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	216	HIS	2.3
1	P	646	HIS	2.3
1	P	126	THR	2.3
1	E	195	SER	2.3
1	J	130	ASP	2.3
1	K	39	SER	2.3
1	M	130	ASP	2.3
1	M	193	ASP	2.3
1	M	746	ASP	2.3
1	L	364	GLY	2.3
1	P	160	GLY	2.3
1	A	84	VAL	2.3
1	M	421	VAL	2.3
1	P	76	CYS	2.3
1	P	354	VAL	2.3
1	P	366	VAL	2.3
1	E	747	PHE	2.3
1	H	189	LEU	2.3
1	P	127	PHE	2.3
1	P	184	LEU	2.3
1	L	81	ALA	2.3
1	M	833	ALA	2.3
1	P	541	ALA	2.3
1	P	636	ILE	2.3
1	P	801	ILE	2.3
1	P	959	ILE	2.3
1	C	745	MET	2.3
1	E	83	THR	2.3
1	M	848	THR	2.3
1	N	799	THR	2.3
1	O	742	THR	2.3
1	P	219	THR	2.3
1	E	253	TYR	2.3
1	P	503	TYR	2.3
1	P	41	GLU	2.3
1	P	136	GLU	2.3
1	E	89	ASN	2.3
1	C	13	ARG	2.3
1	C	743	SER	2.3
1	E	130	ASP	2.3
1	E	178	ARG	2.3
1	E	237	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	572	ASP	2.3
1	H	579	ASP	2.3
1	K	124	SER	2.3
1	M	213	SER	2.3
1	P	13	ARG	2.3
1	P	403	ASP	2.3
1	N	761	GLN	2.3
1	P	50	GLN	2.3
1	P	262	GLN	2.3
1	D	589	GLY	2.3
1	E	582	GLY	2.3
1	L	133	TRP	2.3
1	P	194	GLY	2.3
1	E	54	LEU	2.3
1	E	315	LEU	2.3
1	M	638	VAL	2.3
1	P	322	LEU	2.3
1	P	726	LEU	2.3
1	B	179	ALA	2.2
1	C	733	ALA	2.2
1	I	179	ALA	2.2
1	M	151	HIS	2.2
1	M	44	THR	2.2
1	B	181	GLU	2.2
1	F	580	GLU	2.2
1	P	929	TYR	2.2
1	L	128	ASN	2.2
1	E	59	ARG	2.2
1	N	178	ARG	2.2
1	P	630	ARG	2.2
1	M	574	SER	2.2
1	P	192	SER	2.2
1	P	266	GLN	2.2
1	P	390	SER	2.2
1	P	890	GLN	2.2
1	E	751	LEU	2.2
1	P	62	TRP	2.2
1	P	261	TRP	2.2
1	P	258	VAL	2.2
1	P	267	VAL	2.2
1	P	484	VAL	2.2
1	P	868	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	737	ILE	2.2
1	H	143	PHE	2.2
1	P	142	ILE	2.2
1	P	601	PHE	2.2
1	I	97	ALA	2.2
1	K	735	HIS	2.2
1	P	858	ILE	2.2
1	N	825	CYS	2.2
1	E	75	GLU	2.2
1	E	116	THR	2.2
1	L	684	GLU	2.2
1	M	75	GLU	2.2
1	M	229	THR	2.2
1	P	982	THR	2.2
1	F	253	TYR	2.2
1	E	190	ARG	2.2
1	M	178	ARG	2.2
1	M	809	ARG	2.2
1	P	128	ASN	2.2
1	M	47	PRO	2.2
1	M	422	PRO	2.2
1	H	23	GLN	2.2
1	F	582	GLY	2.2
1	M	419	GLY	2.2
1	M	660	GLY	2.2
1	N	39	SER	2.2
1	P	617	LEU	2.2
1	P	696	LEU	2.2
1	E	571	VAL	2.2
1	P	109	VAL	2.2
1	P	668	VAL	2.2
1	C	735	HIS	2.2
1	D	3	ILE	2.2
1	D	737	ILE	2.2
1	P	107	ILE	2.2
1	H	34	ALA	2.2
1	O	179	ALA	2.2
1	F	57	GLU	2.2
1	N	321	THR	2.2
1	E	46	ARG	2.2
1	M	140	ARG	2.2
1	A	686	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	23	GLN	2.2
1	B	1023	LYS	2.2
1	D	740	LEU	2.2
1	D	846	GLY	2.2
1	I	746	ASP	2.2
1	M	27	LEU	2.2
1	M	48	SER	2.2
1	M	329	ASP	2.2
1	M	663	LEU	2.2
1	N	685	LEU	2.2
1	P	193	ASP	2.2
1	P	574	SER	2.2
1	P	933	SER	2.2
1	K	133	TRP	2.2
1	M	323	ILE	2.2
1	N	3	ILE	2.2
1	P	208	ILE	2.2
1	H	116	THR	2.2
1	M	400	THR	2.2
1	M	799	THR	2.2
1	P	220	THR	2.2
1	L	59	ARG	2.2
1	M	46	ARG	2.2
1	D	581	ASN	2.2
1	E	115	PRO	2.2
1	G	581	ASN	2.2
1	H	38	ASN	2.2
1	L	688	PRO	2.2
1	M	725	ASN	2.2
1	O	687	GLN	2.2
1	A	134	LEU	2.2
1	C	685	LEU	2.2
1	M	167	LEU	2.2
1	M	276	GLY	2.2
1	P	426	LEU	2.2
1	P	740	LEU	2.2
1	L	96	ASP	2.2
1	O	832	ASP	2.2
1	P	919	ASP	2.2
1	G	734	SER	2.2
1	C	3	ILE	2.2
1	E	151	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	801	ILE	2.2
1	M	186	VAL	2.2
1	P	477	SER	2.2
1	P	974	HIS	2.2
1	P	673	ALA	2.1
1	P	717	TRP	2.1
1	E	157	ARG	2.1
1	H	219	THR	2.1
1	P	321	THR	2.1
1	P	425	ARG	2.1
1	E	64	PRO	2.1
1	I	596	PRO	2.1
1	P	64	PRO	2.1
1	L	102	ASN	2.1
1	O	1023	LYS	2.1
1	P	597	ASN	2.1
1	P	600	GLN	2.1
1	P	604	ASN	2.1
1	P	775	GLN	2.1
1	E	215	LEU	2.1
1	J	745	MET	2.1
1	P	922	LEU	2.1
1	D	283	GLY	2.1
1	P	463	GLY	2.1
1	P	901	GLY	2.1
1	E	735	HIS	2.1
1	E	35	SER	2.1
1	P	269	SER	2.1
1	K	63	PHE	2.1
1	H	681	GLU	2.1
1	P	16	TRP	2.1
1	P	324	GLU	2.1
1	P	448	ARG	2.1
1	H	799	THR	2.1
1	P	618	THR	2.1
1	M	1023	LYS	2.1
1	P	112	PRO	2.1
1	D	964	GLN	2.1
1	I	78	LEU	2.1
1	M	581	ASN	2.1
1	M	745	MET	2.1
1	O	581	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	546	LEU	2.1
1	E	263	GLY	2.1
1	H	180	GLY	2.1
1	I	180	GLY	2.1
1	M	463	GLY	2.1
1	E	653[A]	HIS	2.1
1	F	130	ASP	2.1
1	M	319	ASP	2.1
1	H	960	SER	2.1
1	J	318	ALA	2.1
1	L	689	GLU	2.1
1	C	760	ARG	2.1
1	D	760	ARG	2.1
1	M	398	TRP	2.1
1	P	52	ARG	2.1
1	P	404	ARG	2.1
1	P	298	PRO	2.1
1	M	370	GLN	2.1
1	N	49	GLN	2.1
1	P	702	GLN	2.1
1	H	134	LEU	2.1
1	C	583	ASN	2.1
1	D	583	ASN	2.1
1	E	704	ASN	2.1
1	H	128	ASN	2.1
1	M	25	ASN	2.1
1	P	25	ASN	2.1
1	P	297	ASN	2.1
1	P	581	ASN	2.1
1	P	958	ASN	2.1
1	B	180	GLY	2.1
1	E	357	HIS	2.1
1	M	84	VAL	2.1
1	E	954	ASP	2.1
1	D	689	GLU	2.1
1	E	609	ALA	2.1
1	E	734	SER	2.1
1	E	819	GLU	2.1
1	E	833	ALA	2.1
1	H	178	ARG	2.1
1	I	325	ALA	2.1
1	P	715	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	249	GLU	2.1
1	P	166	ARG	2.1
1	E	203	TRP	2.1
1	P	756	TRP	2.1
1	P	806	TRP	2.1
1	P	842	TRP	2.1
1	P	530	THR	2.1
1	E	218	PRO	2.1
1	E	135	GLN	2.1
1	H	177	LEU	2.1
1	P	377	LEU	2.1
1	I	247	CYS	2.1
1	I	276	GLY	2.1
1	P	283	GLY	2.1
1	B	578	TYR	2.1
1	P	99	ILE	2.1
1	P	770	ILE	2.1
1	H	895	VAL	2.1
1	P	571	VAL	2.1
1	P	834	VAL	2.1
1	D	579	ASP	2.0
1	D	594	ASP	2.0
1	E	96	ASP	2.0
1	E	659	ASP	2.0
1	J	832	ASP	2.0
1	L	594	ASP	2.0
1	L	832	ASP	2.0
1	M	13	ARG	2.0
1	M	96	ASP	2.0
1	M	143	PHE	2.1
1	M	772	ASP	2.0
1	P	164	ASP	2.0
1	P	171	PHE	2.1
1	H	65	ALA	2.0
1	K	131	GLU	2.0
1	M	800	ARG	2.0
1	P	416	GLU	2.0
1	L	48	SER	2.0
1	P	978	ALA	2.0
1	E	299	LYS	2.0
1	M	203	TRP	2.0
1	M	729	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	P	948	PRO	2.0
1	F	583	ASN	2.0
1	M	89	ASN	2.0
1	P	232	ASN	2.0
1	P	357	HIS	2.0
1	P	395	HIS	2.0
1	N	248	GLY	2.0
1	P	137	GLY	2.0
1	P	660	GLY	2.0
1	P	680	ILE	2.0
1	P	752	GLY	2.0
1	D	253	TYR	2.0
1	G	668	VAL	2.0
1	H	76	CYS	2.0
1	P	123	TYR	2.0
1	D	800	ARG	2.0
1	G	178	ARG	2.0
1	N	46	ARG	2.0
1	D	732	ALA	2.0
1	E	591	ASP	2.0
1	E	661	LYS	2.0
1	J	733	ALA	2.0
1	N	820	ALA	2.0
1	P	68	ALA	2.0
1	P	201	ASP	2.0
1	P	818	ALA	2.0
1	E	39	SER	2.0
1	M	169	SER	2.0
1	M	367	MET	2.0
1	P	271	THR	2.0
1	P	1020	TRP	2.0
1	E	214	LEU	2.0
1	H	74	LEU	2.0
1	M	11	LEU	2.0
1	P	308	LEU	2.0
1	P	903[A]	GLN	2.0
1	P	976	LEU	2.0
1	P	1022	GLN	2.0
1	K	128	ASN	2.0
1	M	118	ASN	2.0
1	N	38	ASN	2.0
1	P	712	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	P	981	GLY	2.0
1	B	84	VAL	2.0
1	D	84	VAL	2.0
1	E	188	VAL	2.0
1	P	103	VAL	2.0
1	P	159	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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CME	P	914	10/11	0.72	0.22	54,62,98,100	0
1	CME	P	1021	10/11	0.77	0.19	72,87,100,100	0
1	CME	P	748	10/11	0.81	0.17	68,80,100,100	0
1	CME	M	748	10/11	0.83	0.18	56,68,100,100	0
1	CME	O	748	10/11	0.84	0.24	50,62,95,100	0
1	CME	L	748	10/11	0.85	0.16	53,65,99,100	0
1	CME	B	1021	10/11	0.85	0.17	33,49,84,97	0
1	CME	K	1021	10/11	0.85	0.13	57,73,100,100	0
1	CME	L	1021	10/11	0.86	0.12	57,73,100,100	0
1	CME	J	1021	10/11	0.86	0.16	42,58,93,100	0
1	CME	M	914	10/11	0.87	0.14	42,50,86,92	0
1	CME	N	1021	10/11	0.87	0.14	48,64,99,100	0
1	CME	E	748	10/11	0.87	0.20	56,68,100,100	0
1	CME	G	1021	10/11	0.87	0.14	41,56,91,100	0
1	CME	I	748	10/11	0.87	0.16	40,52,85,97	0
1	CME	B	748	10/11	0.87	0.14	29,41,75,86	0
1	CME	N	748	10/11	0.88	0.18	44,56,90,100	0
1	CME	H	1021	10/11	0.88	0.13	50,66,100,100	0
1	CME	C	1021	10/11	0.88	0.14	33,49,84,97	0
1	CME	J	748	10/11	0.88	0.14	38,50,84,95	0
1	CME	D	748	10/11	0.88	0.17	39,51,84,95	0
1	CME	K	748	10/11	0.88	0.14	53,65,98,100	0
1	CME	E	1021	10/11	0.89	0.16	60,76,100,100	0
1	CME	F	748	10/11	0.89	0.14	36,48,81,93	0
1	CME	F	1021	10/11	0.89	0.12	40,56,91,100	0
1	CME	D	1021	10/11	0.89	0.16	43,58,93,100	0
1	CME	C	748	10/11	0.90	0.15	29,41,74,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CME	H	748	10/11	0.90	0.14	46,58,92,100	0
1	CME	O	1021	10/11	0.90	0.13	54,69,100,100	0
1	CME	A	1021	10/11	0.90	0.12	35,50,85,99	0
1	CME	M	1021	10/11	0.90	0.16	60,75,100,100	0
1	CME	L	914	10/11	0.90	0.13	40,47,84,89	0
1	CME	I	1021	10/11	0.91	0.12	44,60,94,100	0
1	CME	A	748	10/11	0.91	0.14	31,43,76,87	0
1	CME	A	914	10/11	0.92	0.11	17,25,61,67	0
1	CME	K	914	10/11	0.92	0.11	40,47,84,89	0
1	CME	G	748	10/11	0.92	0.13	37,48,82,93	0
1	CME	E	914	10/11	0.92	0.14	42,50,87,92	0
1	CME	J	914	10/11	0.93	0.11	25,32,69,75	0
1	CME	I	914	10/11	0.93	0.11	26,34,70,76	0
1	CME	N	914	10/11	0.94	0.10	31,38,75,81	0
1	CME	O	914	10/11	0.94	0.10	36,44,80,86	0
1	CME	H	914	10/11	0.94	0.10	33,40,77,82	0
1	CME	F	914	10/11	0.95	0.10	23,30,67,72	0
1	CME	D	914	10/11	0.95	0.11	25,33,69,75	0
1	CME	B	914	10/11	0.95	0.09	16,23,60,66	0
1	CME	G	914	10/11	0.95	0.09	23,31,67,73	0
1	CME	C	914	10/11	0.96	0.09	16,23,60,65	0

6.3 Carbohydrates ⓘ

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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2FG	X	2	11/12	0.67	0.22	56,61,72,78	0
2	2FG	U	2	11/12	0.85	0.21	66,71,82,88	0
2	BGC	Z	1	12/12	0.85	0.14	50,65,82,99	0
2	BGC	R	1	12/12	0.86	0.15	41,56,73,90	0
2	2FG	Q	2	11/12	0.86	0.16	40,46,57,63	0
2	BGC	W	1	12/12	0.87	0.18	48,63,80,97	0
2	BGC	T	1	12/12	0.87	0.14	50,65,82,99	0
2	BGC	Y	1	12/12	0.87	0.14	51,67,84,100	0
2	BGC	S	1	12/12	0.87	0.13	41,56,73,89	0
2	2FG	R	2	11/12	0.88	0.13	39,44,55,61	0
2	2FG	S	2	11/12	0.89	0.14	39,44,55,61	0
2	BGC	V	1	12/12	0.89	0.13	48,63,80,96	0

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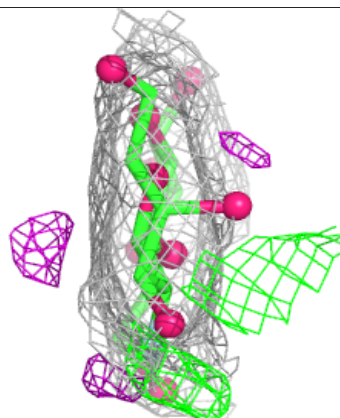
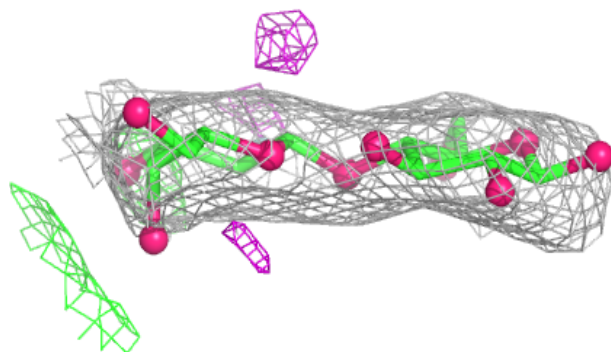
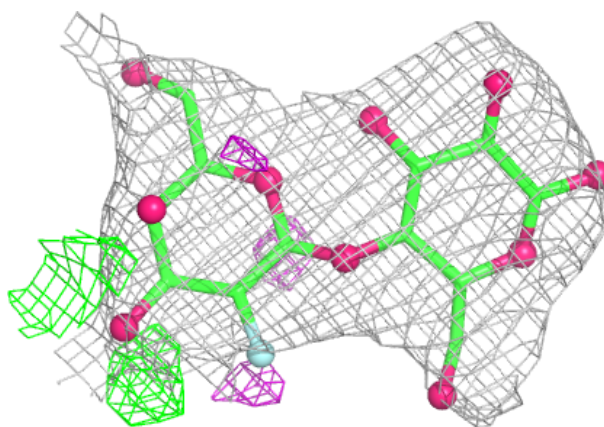
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	X	1	12/12	0.90	0.13	58,73,90,100	0
2	2FG	Y	2	11/12	0.90	0.13	49,55,66,72	0
2	2FG	V	2	11/12	0.90	0.14	46,51,62,68	0
2	2FG	Z	2	11/12	0.90	0.13	48,53,64,70	0
2	BGC	U	1	12/12	0.91	0.15	67,83,100,100	0
2	2FG	W	2	11/12	0.91	0.12	46,51,63,68	0
2	BGC	Q	1	12/12	0.92	0.11	42,57,74,91	0
2	2FG	T	2	11/12	0.95	0.10	48,54,65,71	0
2	BGC	a	1	12/12	-	-	65,80,97,100	0
2	2FG	a	2	11/12	-	-	63,68,79,85	0
2	BGC	b	1	12/12	-	-	65,80,97,100	0
2	2FG	b	2	11/12	-	-	63,68,79,85	0
2	BGC	c	1	12/12	-	-	67,82,99,100	0
2	2FG	c	2	11/12	-	-	65,71,82,88	0
2	BGC	d	1	12/12	-	-	56,71,88,100	0
2	2FG	d	2	11/12	-	-	54,59,70,76	0
2	BGC	e	1	12/12	-	-	61,76,93,100	0
2	2FG	e	2	11/12	-	-	59,65,76,82	0
2	BGC	f	1	12/12	-	-	79,94,100,100	0
2	2FG	f	2	11/12	-	-	77,83,94,100	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

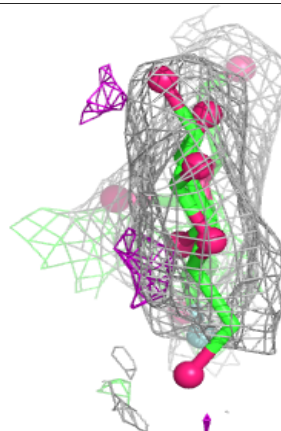
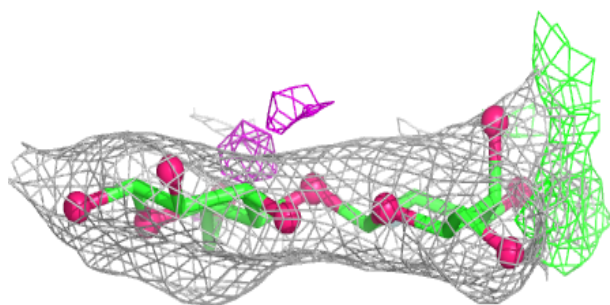
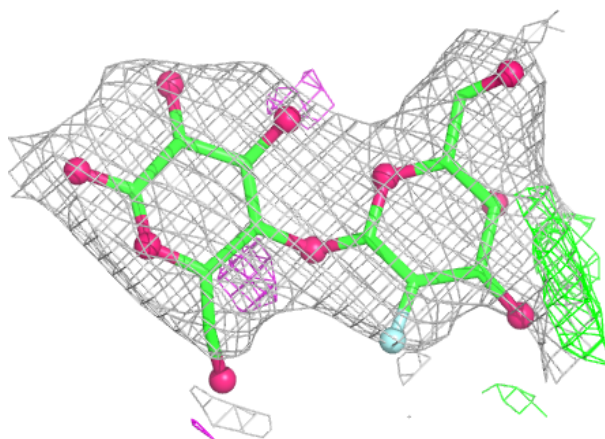
Electron density around Chain Q:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



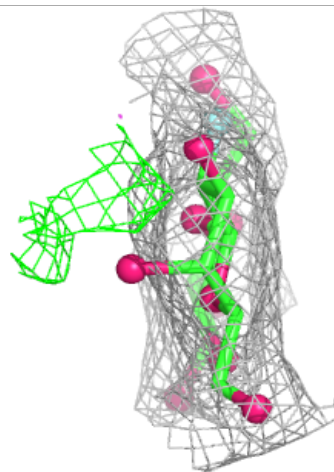
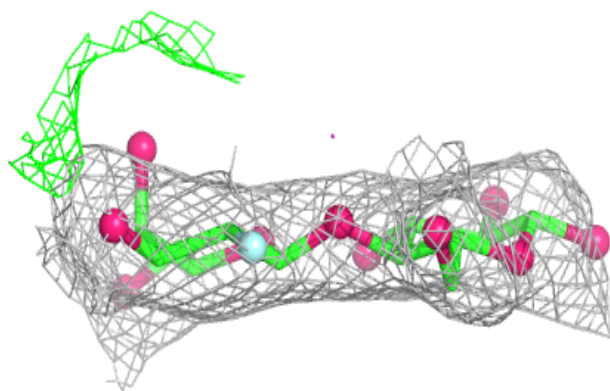
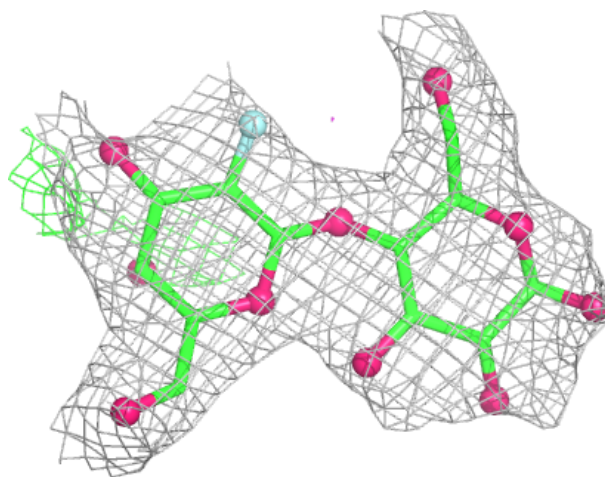
Electron density around Chain R:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



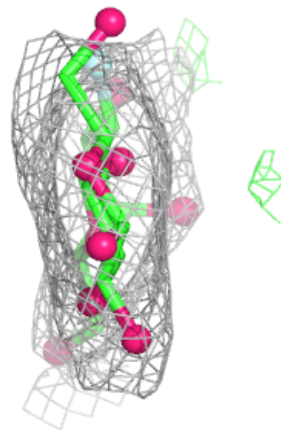
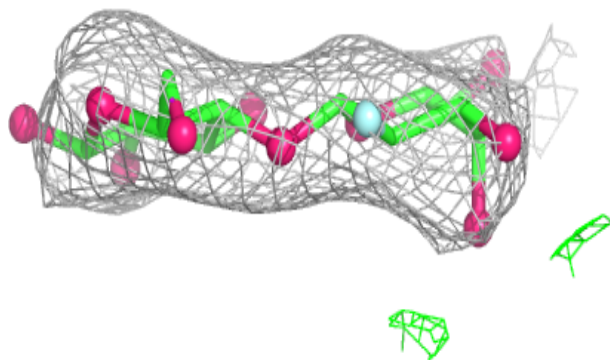
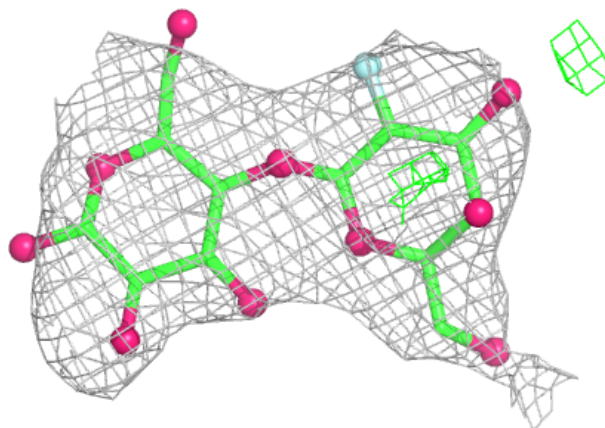
Electron density around Chain S:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



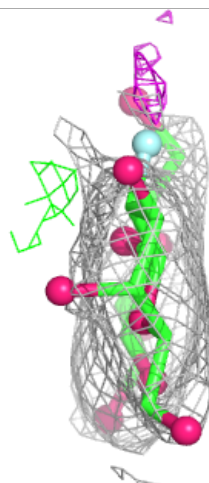
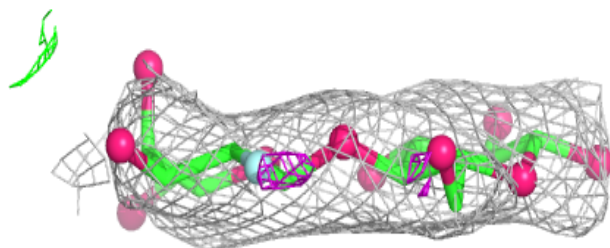
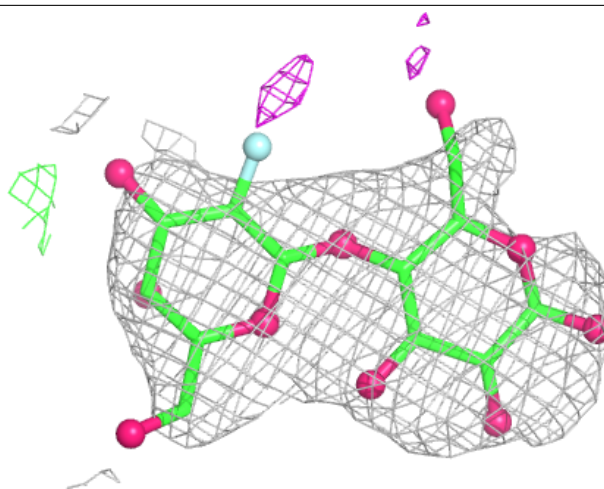
Electron density around Chain T:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



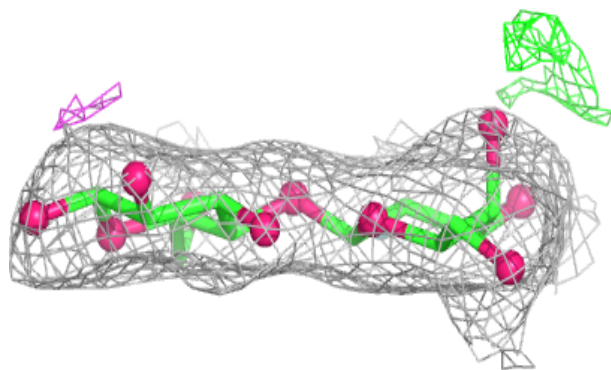
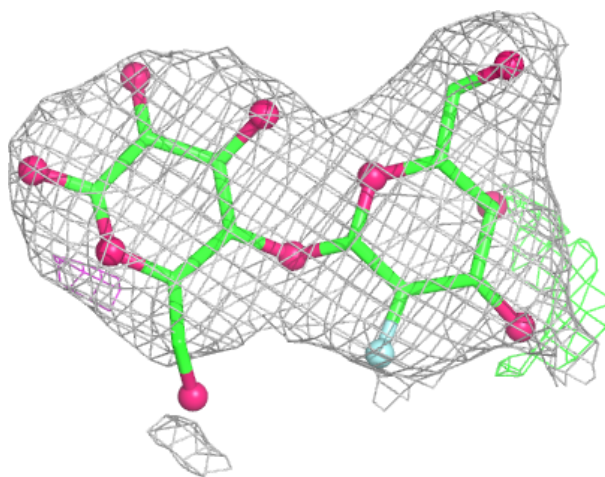
Electron density around Chain U:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



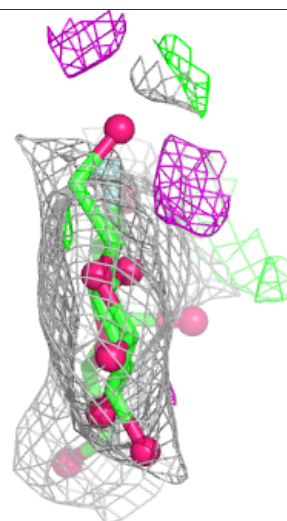
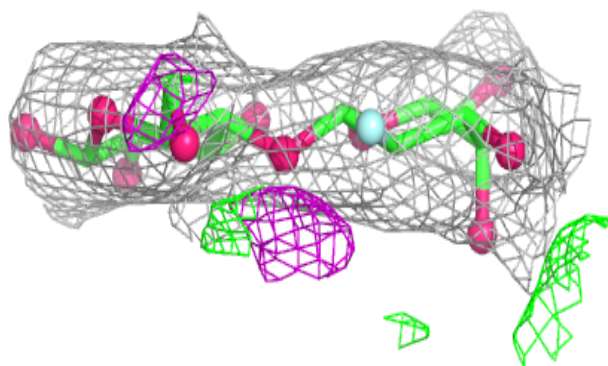
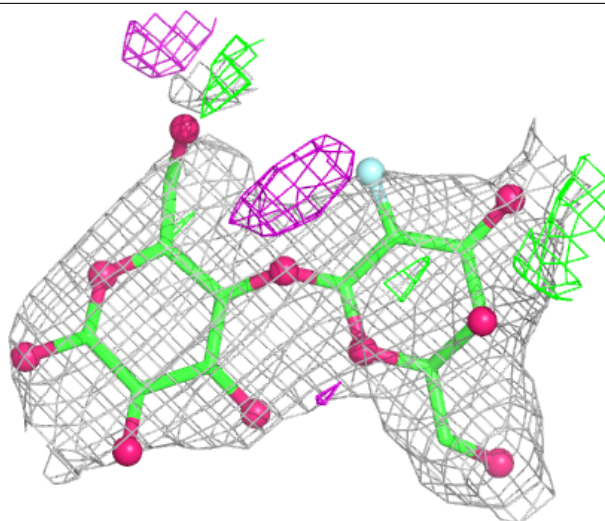
Electron density around Chain V:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



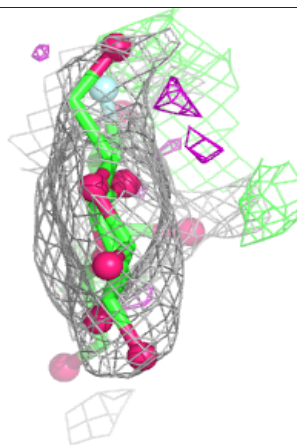
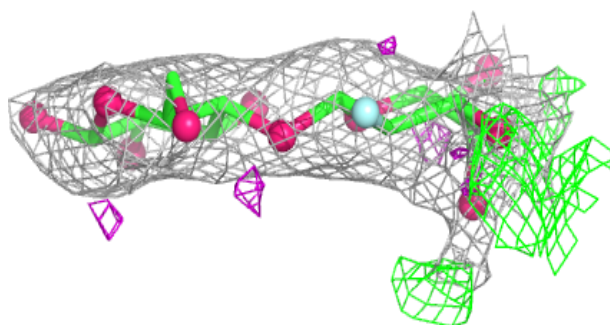
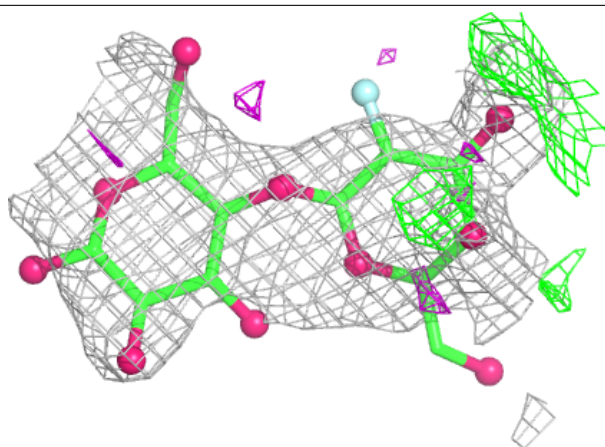
Electron density around Chain W:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



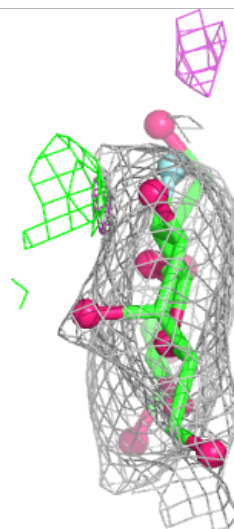
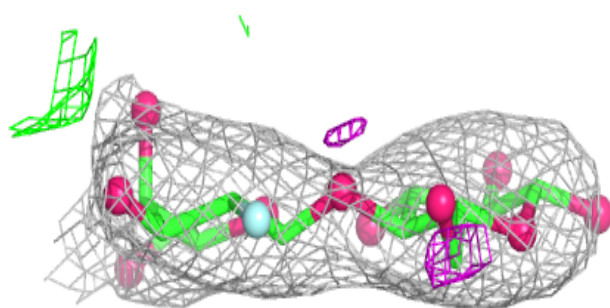
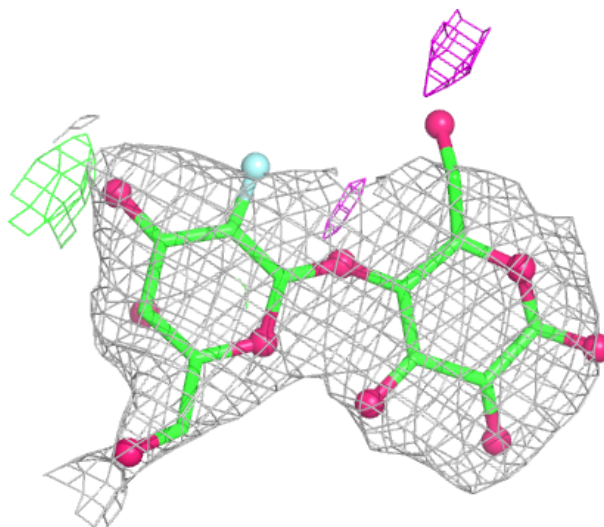
Electron density around Chain X:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



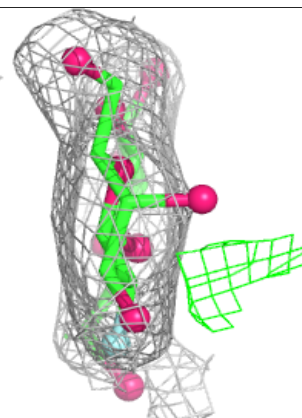
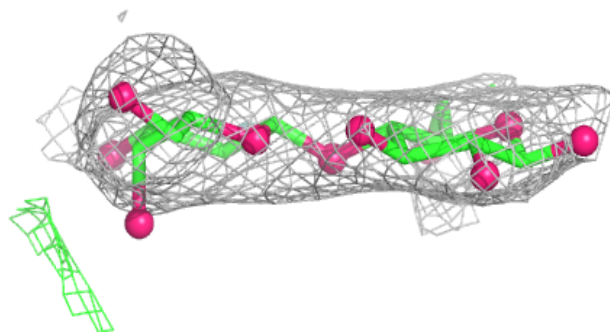
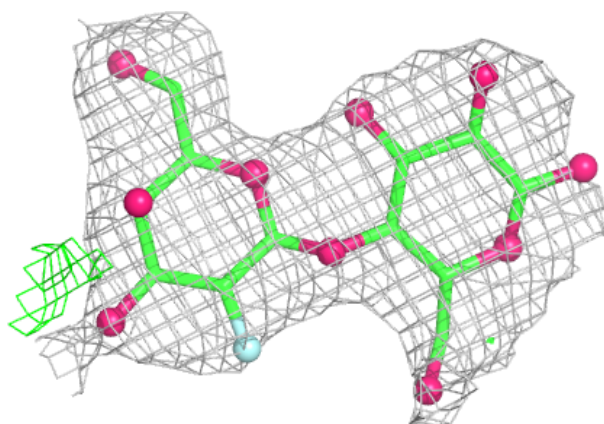
Electron density around Chain Y:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



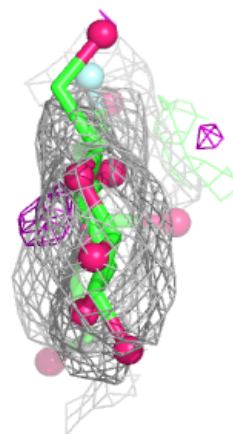
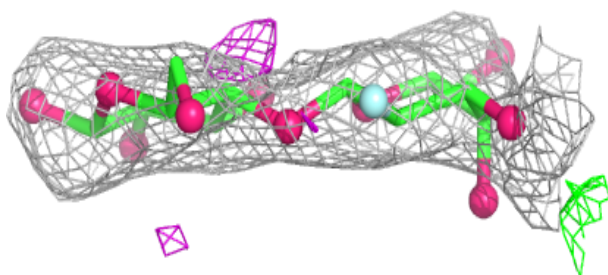
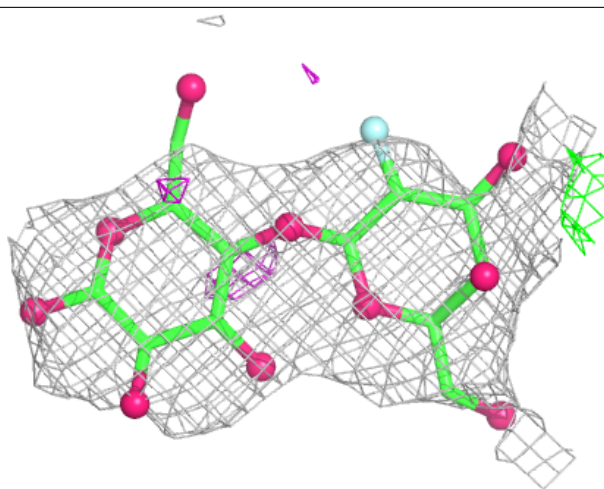
Electron density around Chain Z:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



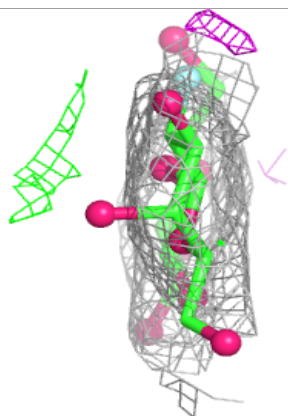
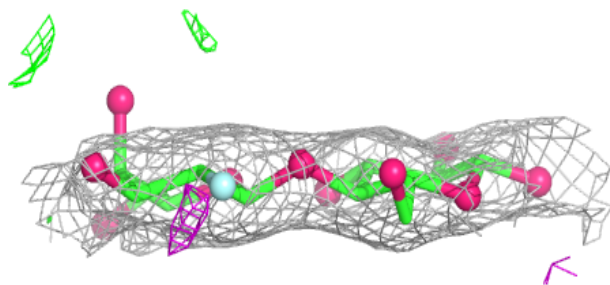
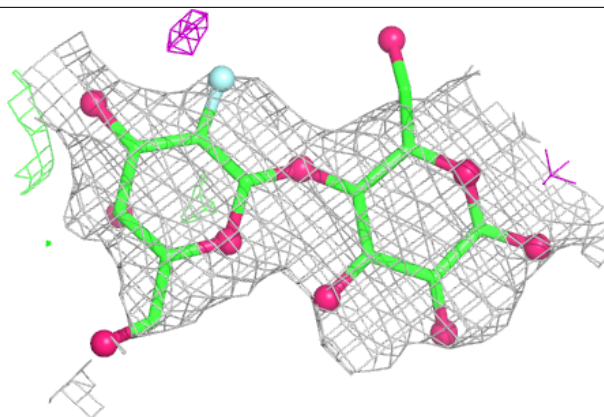
Electron density around Chain a:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

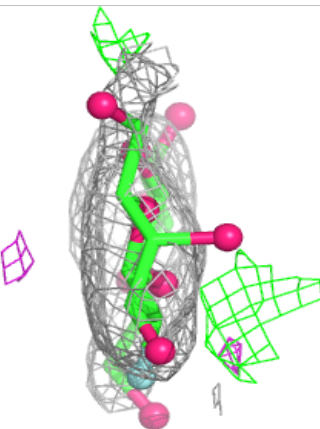
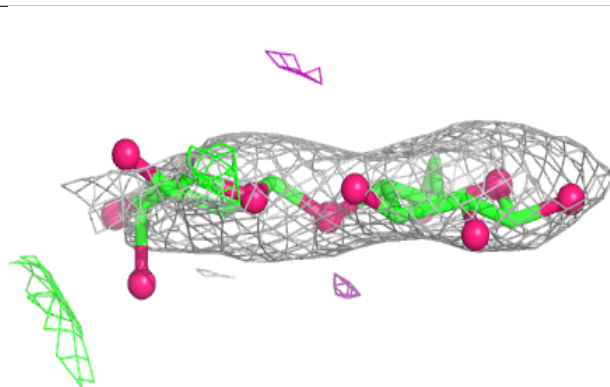
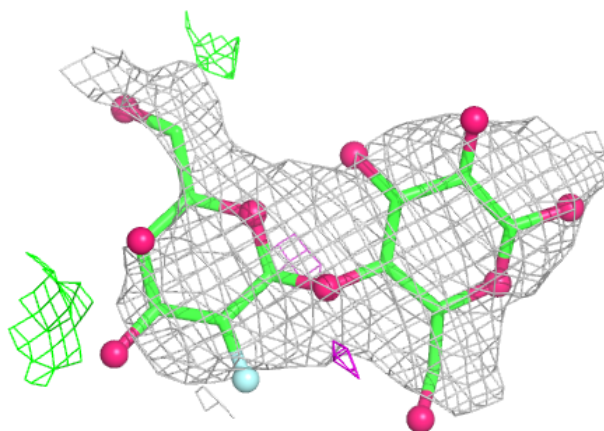


Electron density around Chain b:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

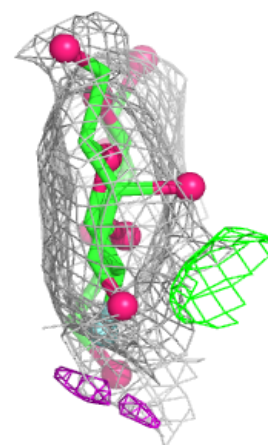
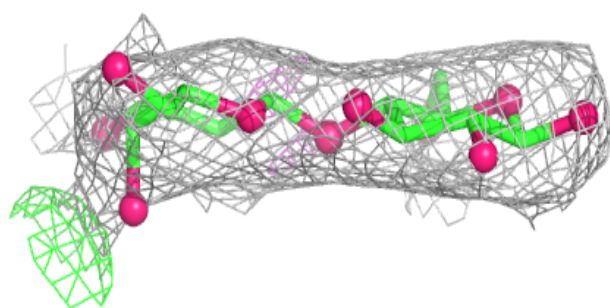
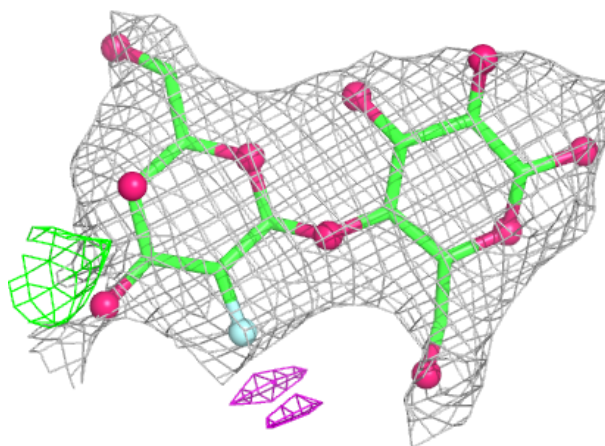
**Electron density around Chain c:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



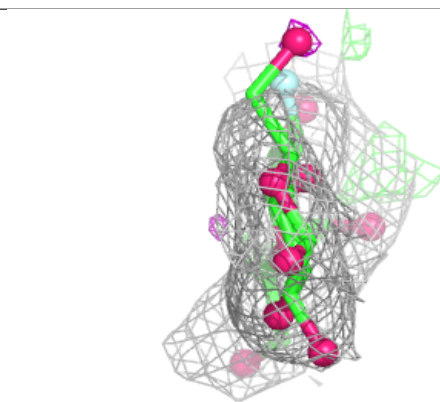
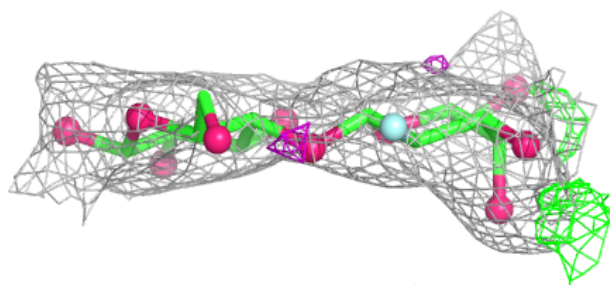
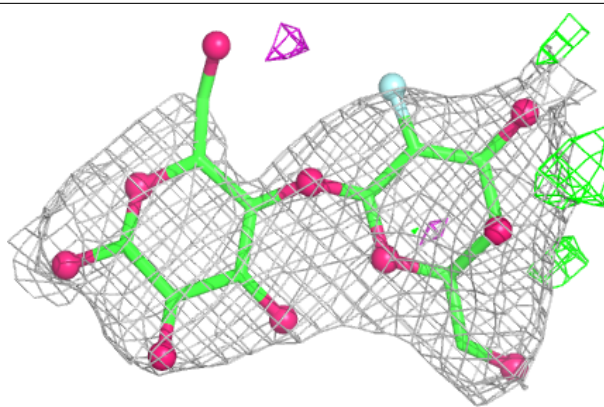
Electron density around Chain d:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

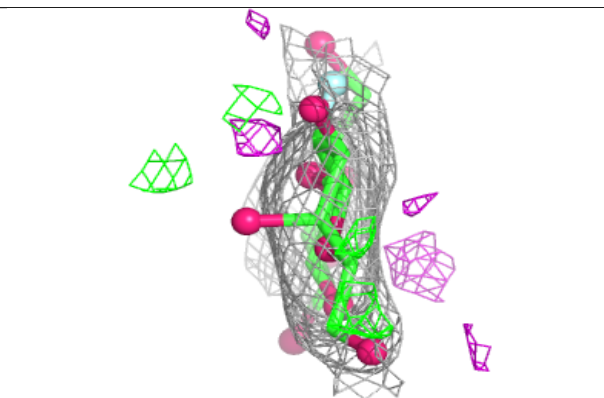
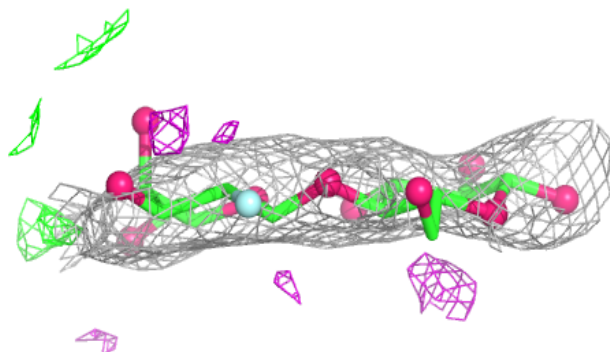
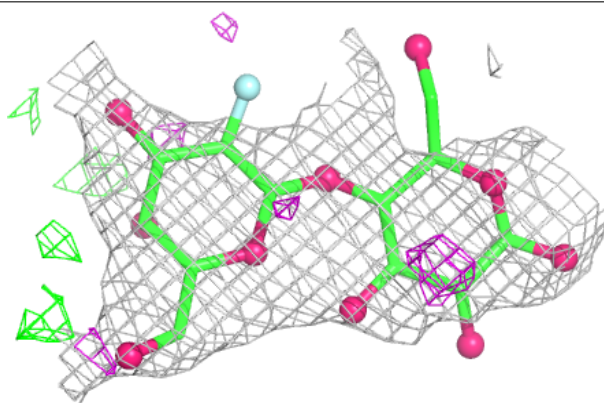


Electron density around Chain e:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain f:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NA	L	2004	1/1	0.71	0.18	53,53,53,53	0
4	NA	M	2004	1/1	0.78	0.20	55,55,55,55	0
4	NA	O	2005	1/1	0.80	0.10	37,37,37,37	0
4	NA	P	2004	1/1	0.80	0.16	67,67,67,67	0
4	NA	D	2004	1/1	0.83	0.09	38,38,38,38	0
4	NA	K	2004	1/1	0.83	0.12	53,53,53,53	0
4	NA	D	2005	1/1	0.85	0.08	26,26,26,26	0
4	NA	J	2004	1/1	0.86	0.13	38,38,38,38	0
4	NA	J	2005	1/1	0.87	0.06	25,25,25,25	0
3	MG	P	2002	1/1	0.87	0.18	60,60,60,60	0
3	MG	E	2003	1/1	0.88	0.10	42,42,42,42	0
3	MG	L	2003	1/1	0.88	0.11	39,39,39,39	0
3	MG	C	2003	1/1	0.89	0.12	15,15,15,15	0
4	NA	O	2004	1/1	0.89	0.10	49,49,49,49	0
3	MG	M	2002	1/1	0.89	0.14	48,48,48,48	0
3	MG	H	2003	1/1	0.89	0.06	32,32,32,32	0
4	NA	I	2005	1/1	0.90	0.09	27,27,27,27	0
3	MG	I	2003	1/1	0.90	0.09	26,26,26,26	0
4	NA	E	2004	1/1	0.90	0.20	55,55,55,55	0
4	NA	N	2004	1/1	0.91	0.10	44,44,44,44	0
3	MG	G	2002	1/1	0.91	0.20	29,29,29,29	0
3	MG	H	2002	1/1	0.91	0.24	39,39,39,39	0
3	MG	L	2002	1/1	0.91	0.17	46,46,46,46	0
3	MG	F	2003	1/1	0.92	0.11	22,22,22,22	0
4	NA	A	2004	1/1	0.92	0.07	30,30,30,30	0
4	NA	C	2005	1/1	0.92	0.06	16,16,16,16	0
3	MG	A	2002	1/1	0.92	0.08	23,23,23,23	0
3	MG	J	2002	1/1	0.93	0.08	31,31,31,31	0
3	MG	G	2003	1/1	0.93	0.08	22,22,22,22	0
4	NA	G	2004	1/1	0.93	0.07	36,36,36,36	0
4	NA	M	2005	1/1	0.93	0.10	43,43,43,43	0
4	NA	K	2005	1/1	0.94	0.04	40,40,40,40	0
4	NA	F	2004	1/1	0.94	0.14	36,36,36,36	0
3	MG	F	2002	1/1	0.94	0.17	29,29,29,29	0
4	NA	H	2004	1/1	0.94	0.12	46,46,46,46	0
3	MG	E	2002	1/1	0.94	0.15	48,48,48,48	0
4	NA	N	2005	1/1	0.94	0.10	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	N	2003	1/1	0.94	0.06	30,30,30,30	0
3	MG	C	2002	1/1	0.94	0.15	22,22,22,22	0
3	MG	P	2003	1/1	0.94	0.07	53,53,53,53	0
3	MG	O	2003	1/1	0.95	0.08	35,35,35,35	0
3	MG	D	2003	1/1	0.95	0.07	24,24,24,24	0
4	NA	E	2005	1/1	0.95	0.09	43,43,43,43	0
3	MG	O	2002	1/1	0.95	0.18	42,42,42,42	0
4	NA	F	2005	1/1	0.95	0.05	23,23,23,23	0
4	NA	P	2005	1/1	0.95	0.12	55,55,55,55	0
4	NA	G	2005	1/1	0.96	0.04	24,24,24,24	0
3	MG	N	2002	1/1	0.96	0.12	37,37,37,37	0
3	MG	I	2002	1/1	0.96	0.15	32,32,32,32	0
3	MG	D	2002	1/1	0.96	0.11	31,31,31,31	0
4	NA	A	2005	1/1	0.96	0.05	18,18,18,18	0
4	NA	B	2005	1/1	0.96	0.10	16,16,16,16	0
4	NA	C	2004	1/1	0.96	0.08	29,29,29,29	0
3	MG	B	2003	1/1	0.96	0.08	15,15,15,15	0
3	MG	B	2002	1/1	0.97	0.17	22,22,22,22	0
3	MG	J	2003	1/1	0.97	0.11	24,24,24,24	0
3	MG	M	2003	1/1	0.97	0.15	41,41,41,41	0
3	MG	K	2002	1/1	0.97	0.16	45,45,45,45	0
3	MG	K	2003	1/1	0.97	0.05	39,39,39,39	0
4	NA	L	2005	1/1	0.97	0.08	40,40,40,40	0
3	MG	A	2003	1/1	0.97	0.09	16,16,16,16	0
4	NA	H	2005	1/1	0.98	0.06	33,33,33,33	0
4	NA	B	2004	1/1	0.98	0.06	29,29,29,29	0
4	NA	I	2004	1/1	0.99	0.06	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.