



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 09:44 PM UTC

PDB ID : 4V41 / pdb_00004v41
Title : E. COLI (LAC Z) BETA-GALACTOSIDASE (NCS CONSTRAINED MONOMER-MONOCLINIC)
Authors : Juers, D.H.; Jacobson, R.H.; Wigley, D.; Zhang, X.J.; Huber, R.E.; Tronrud, D.E.; Matthews, B.W.
Deposited on : 2000-06-07
Resolution : 2.50 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:

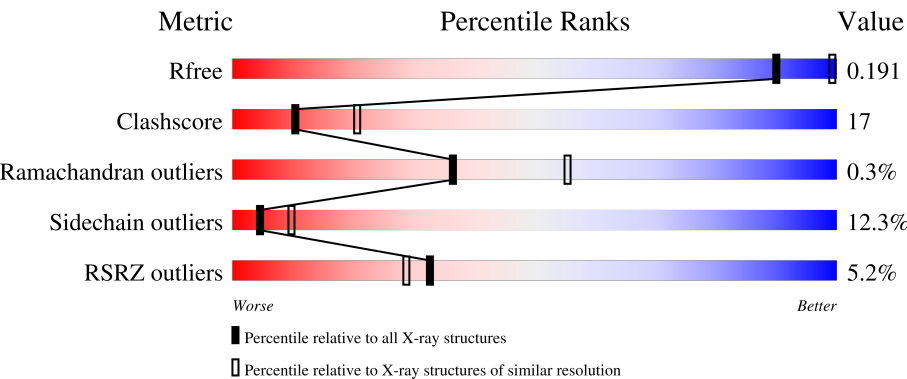
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.50 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.



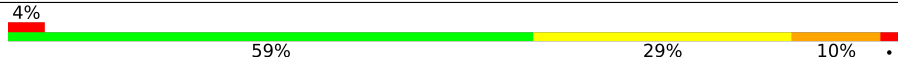
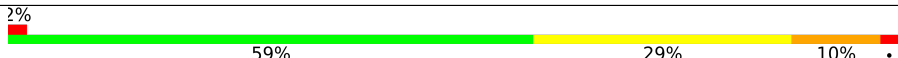
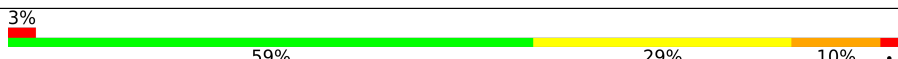
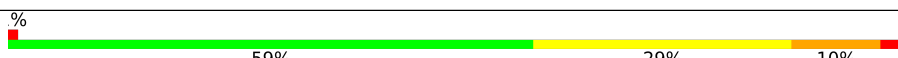
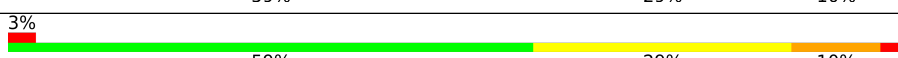
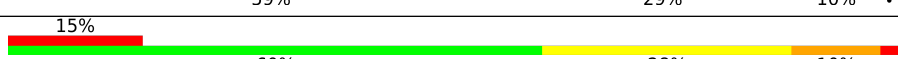
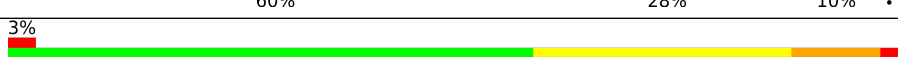
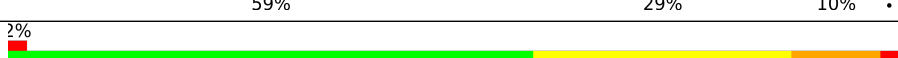
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	4% 60%28%10%
1	B	1023	4% 60%29%10%
1	C	1023	3% 58%30%10%
1	D	1023	4% 60%28%10%
1	E	1023	5% 59%29%9%

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 138704 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	5	0
			8232	5201	1462	1528	41			
1	B	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	C	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	D	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	E	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	F	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	G	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	H	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	I	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	J	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	K	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	L	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	M	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	N	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	O	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	1528	41			
1	P	1021	Total	C	N	O	S	0	5	0
			8232	5201	1462	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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

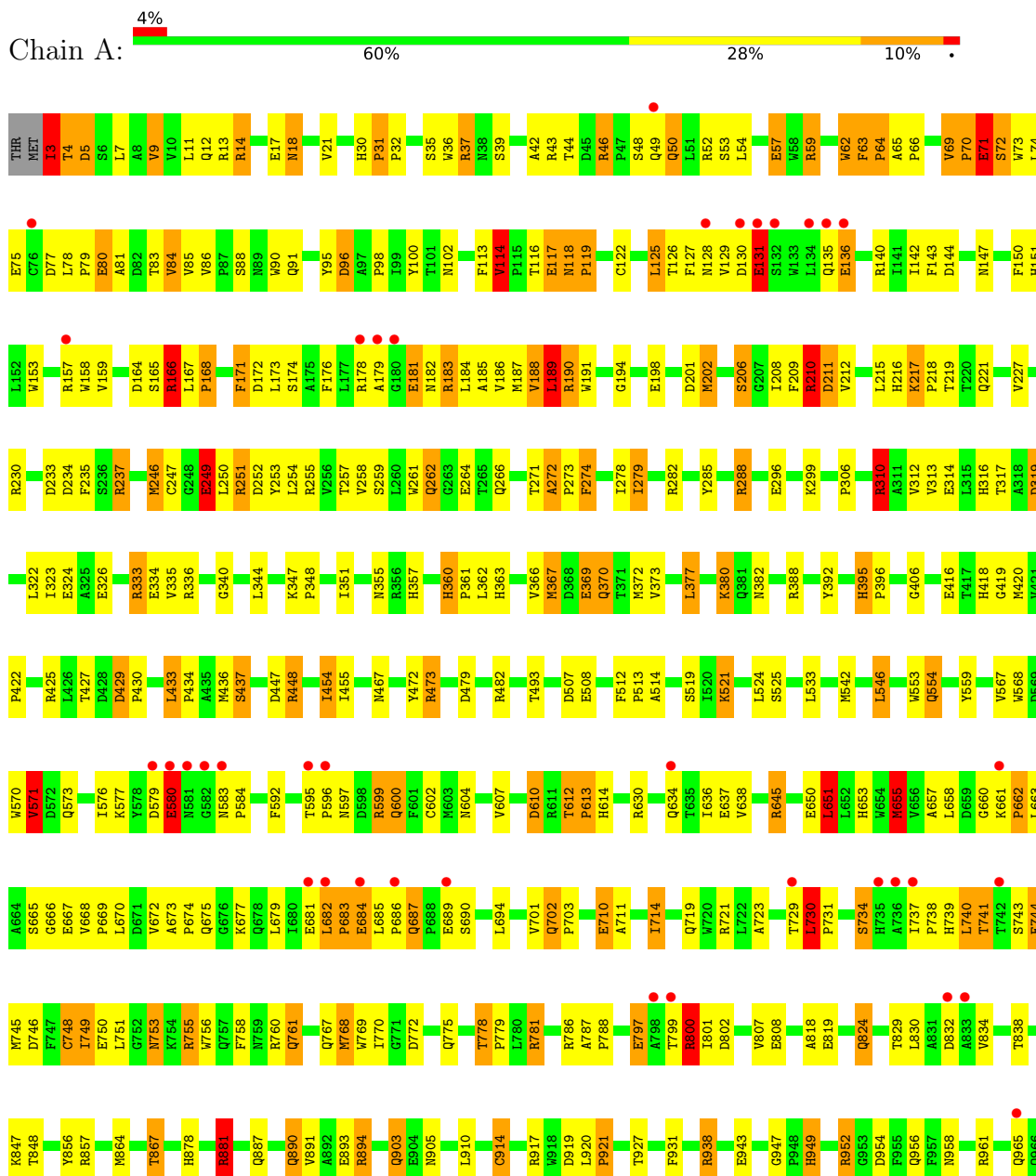
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	434	Total O 434 434	0	0
3	B	436	Total O 436 436	0	0
3	C	433	Total O 433 433	0	0
3	D	437	Total O 437 437	0	0
3	E	435	Total O 435 435	0	0
3	F	436	Total O 436 436	0	0
3	G	434	Total O 434 434	0	0
3	H	435	Total O 435 435	0	0
3	I	434	Total O 434 434	0	0
3	J	436	Total O 436 436	0	0
3	K	435	Total O 435 435	0	0
3	L	435	Total O 435 435	0	0
3	M	434	Total O 434 434	0	0
3	N	436	Total O 436 436	0	0
3	O	433	Total O 433 433	0	0
3	P	437	Total O 437 437	0	0

3 Residue-property plots [i](#)

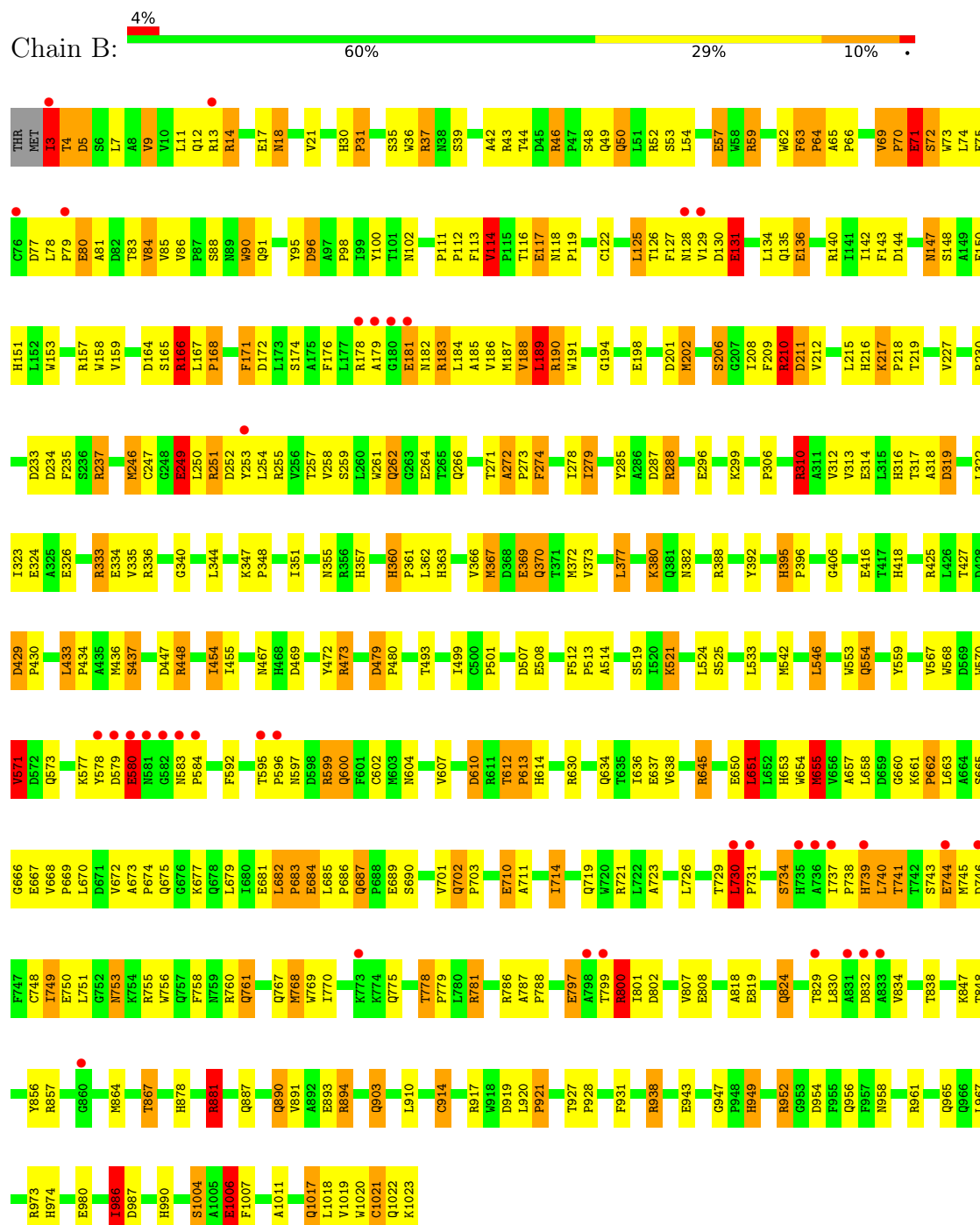
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



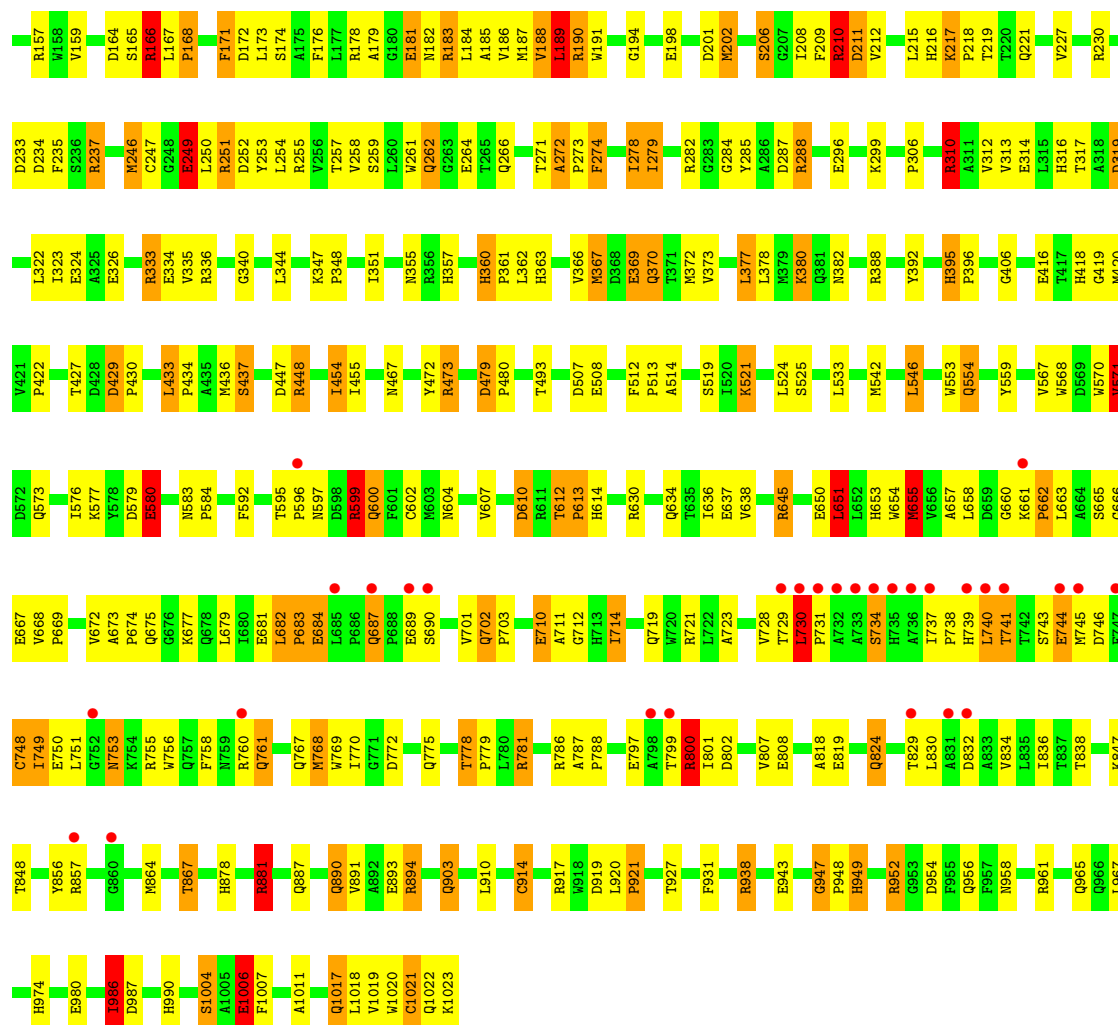


● Molecule 1: BETA-GALACTOSIDASE

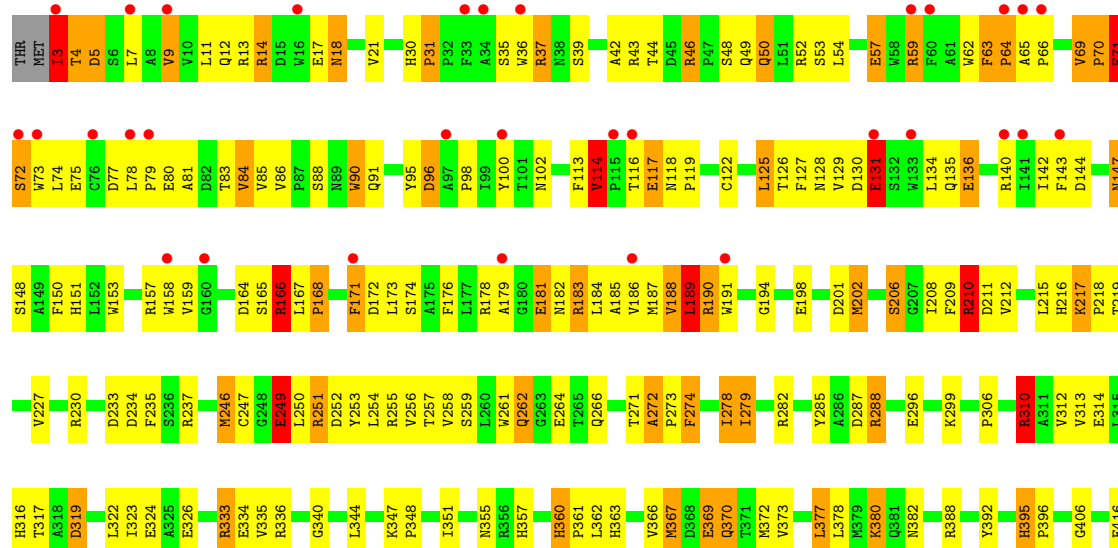


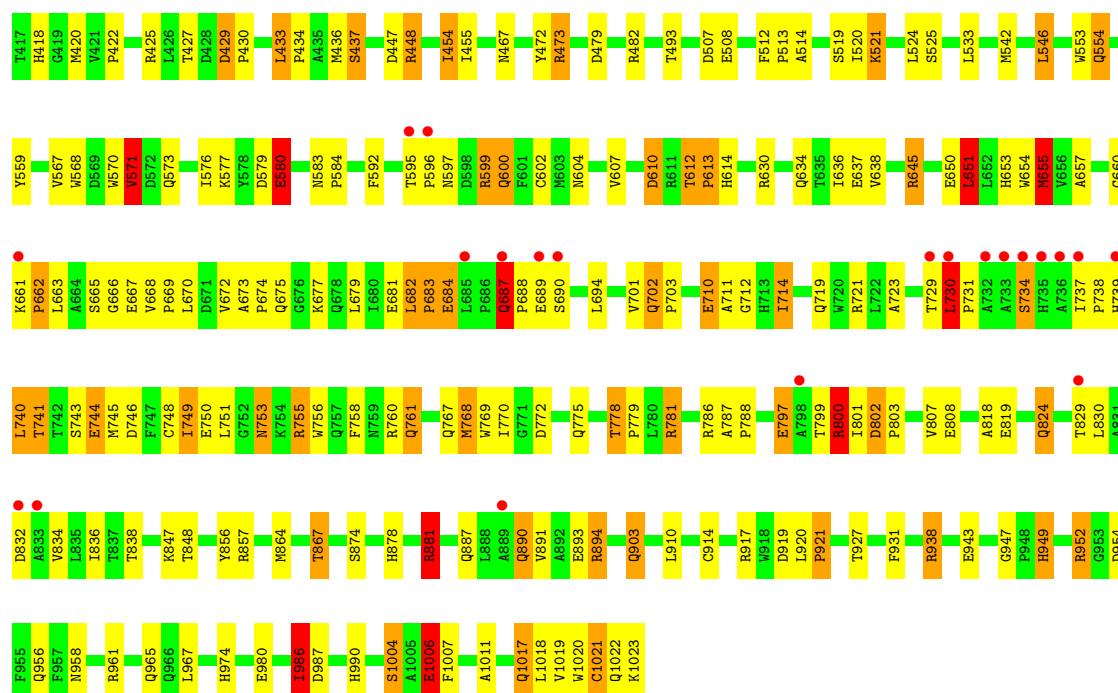
● Molecule 1: BETA-GALACTOSIDASE



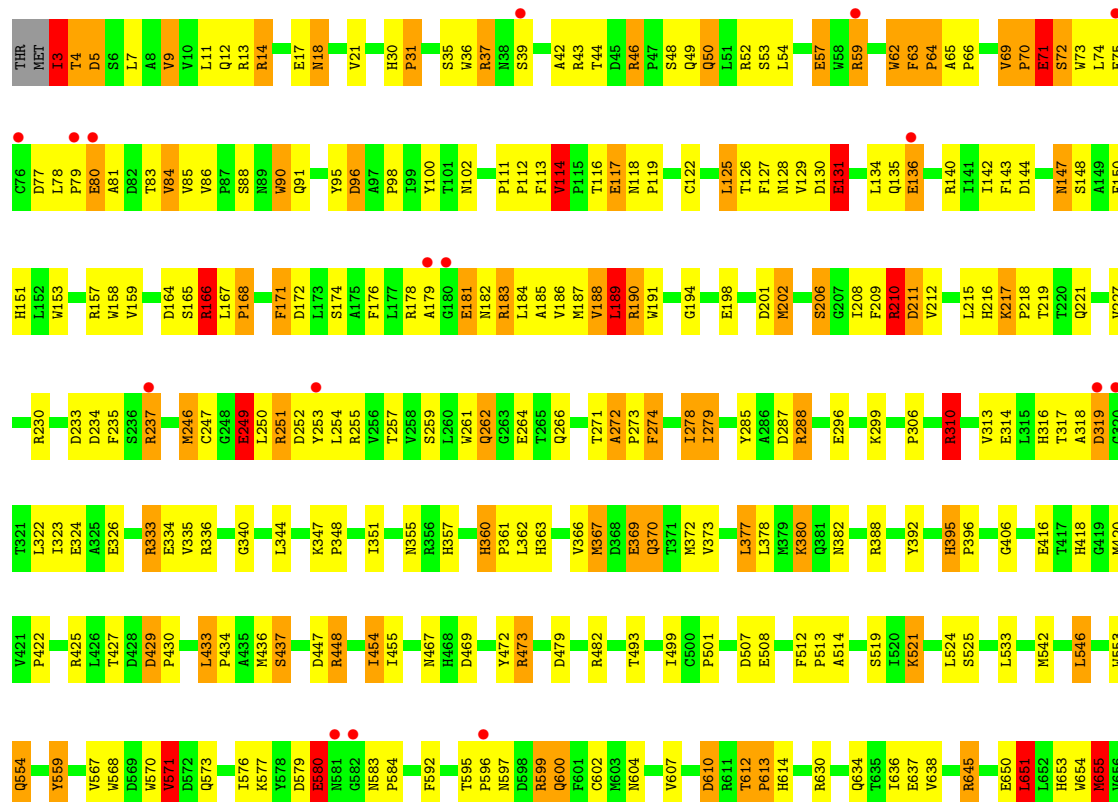


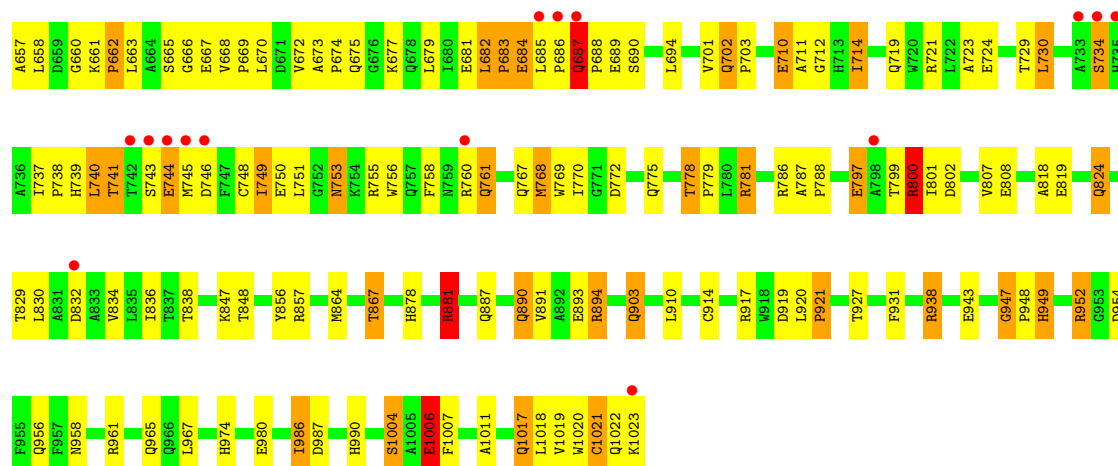
● Molecule 1: BETA-GALACTOSIDASE



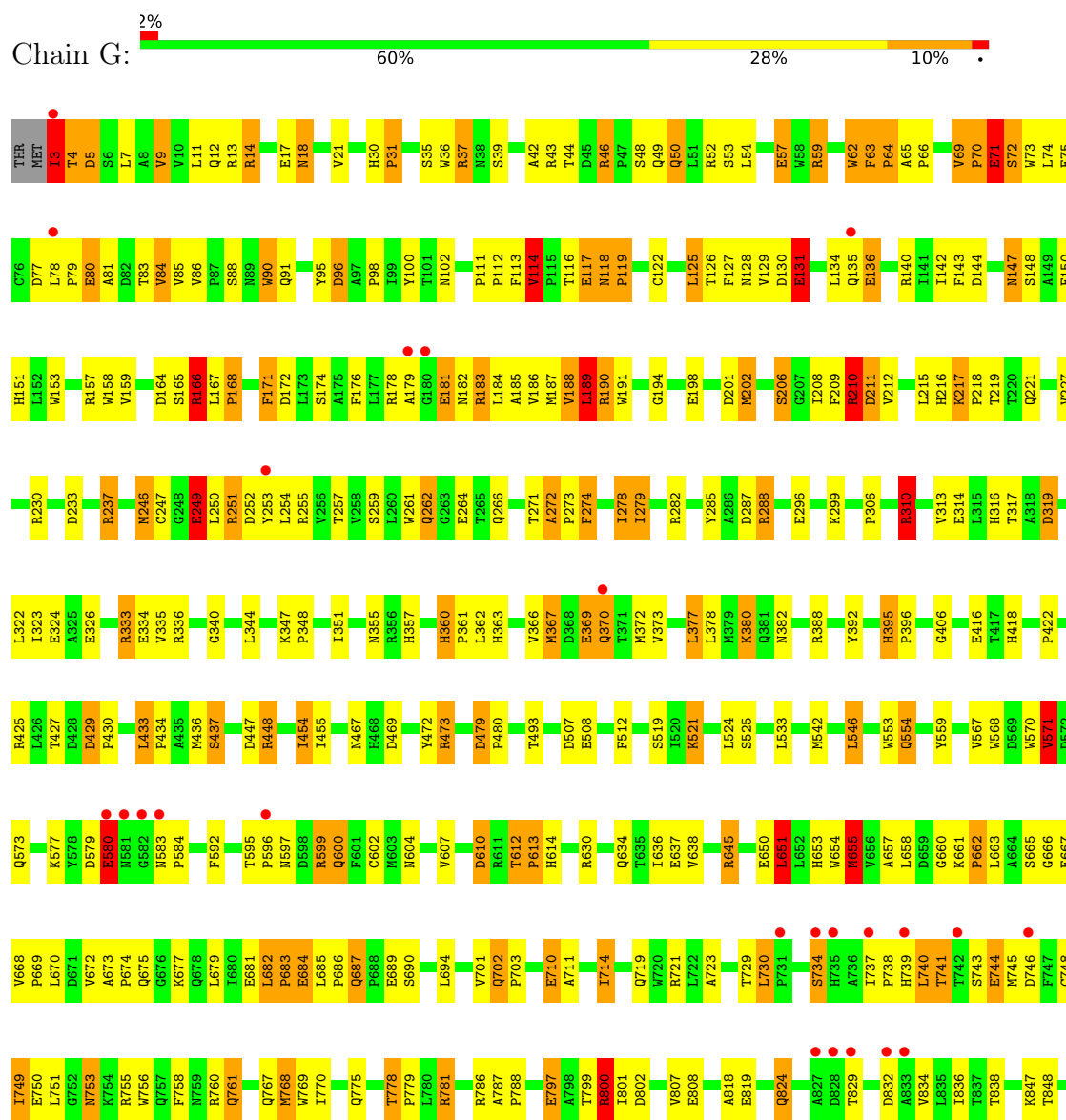


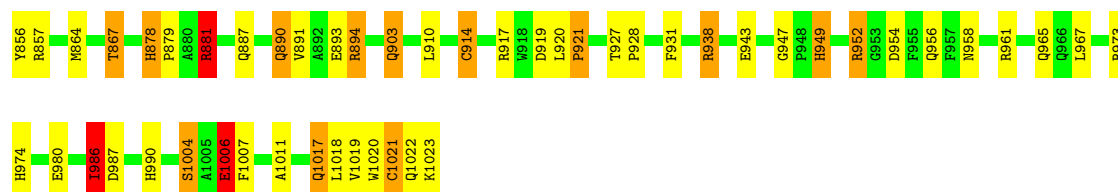
• Molecule 1: BETA-GALACTOSIDASE



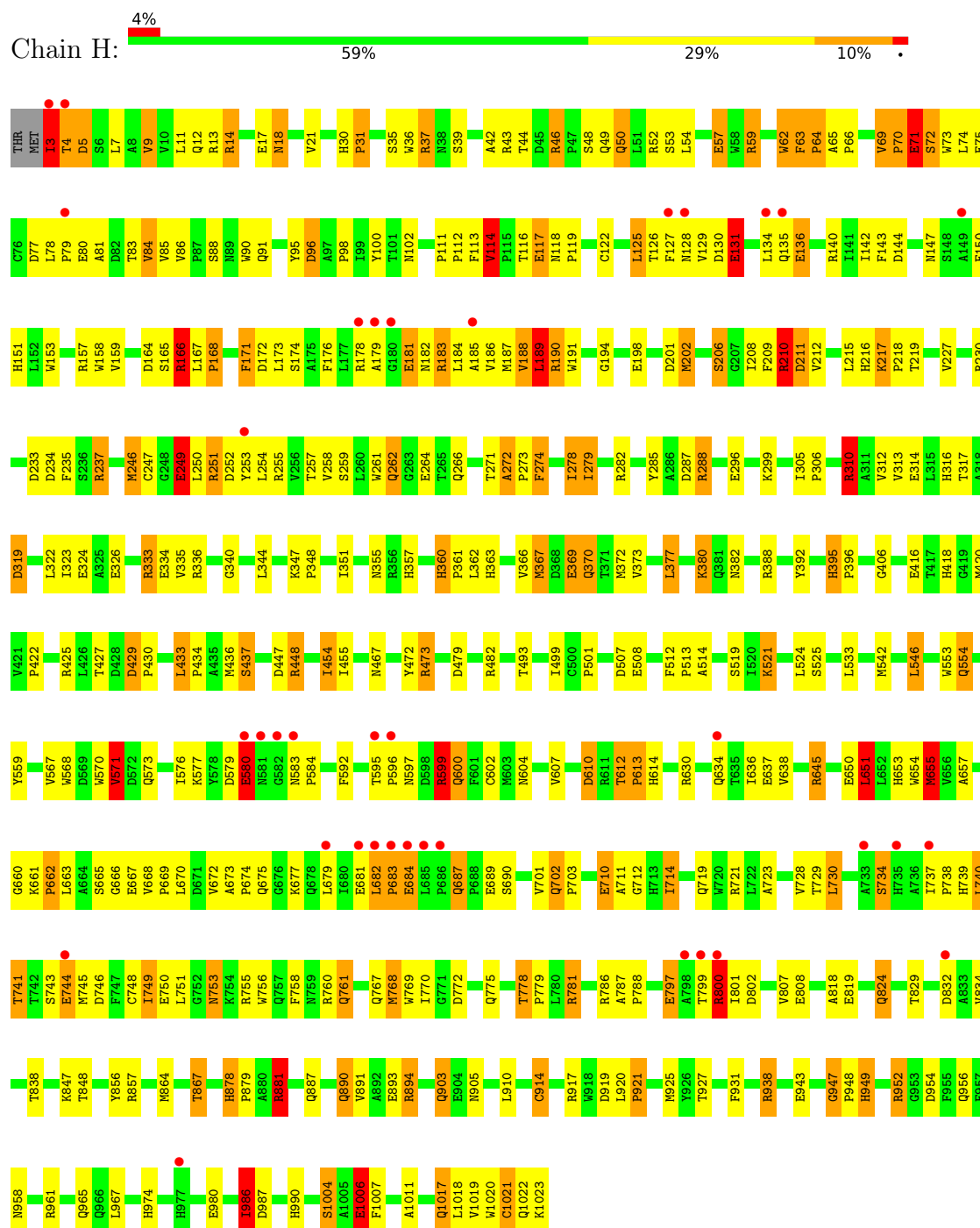


• Molecule 1: BETA-GALACTOSIDASE

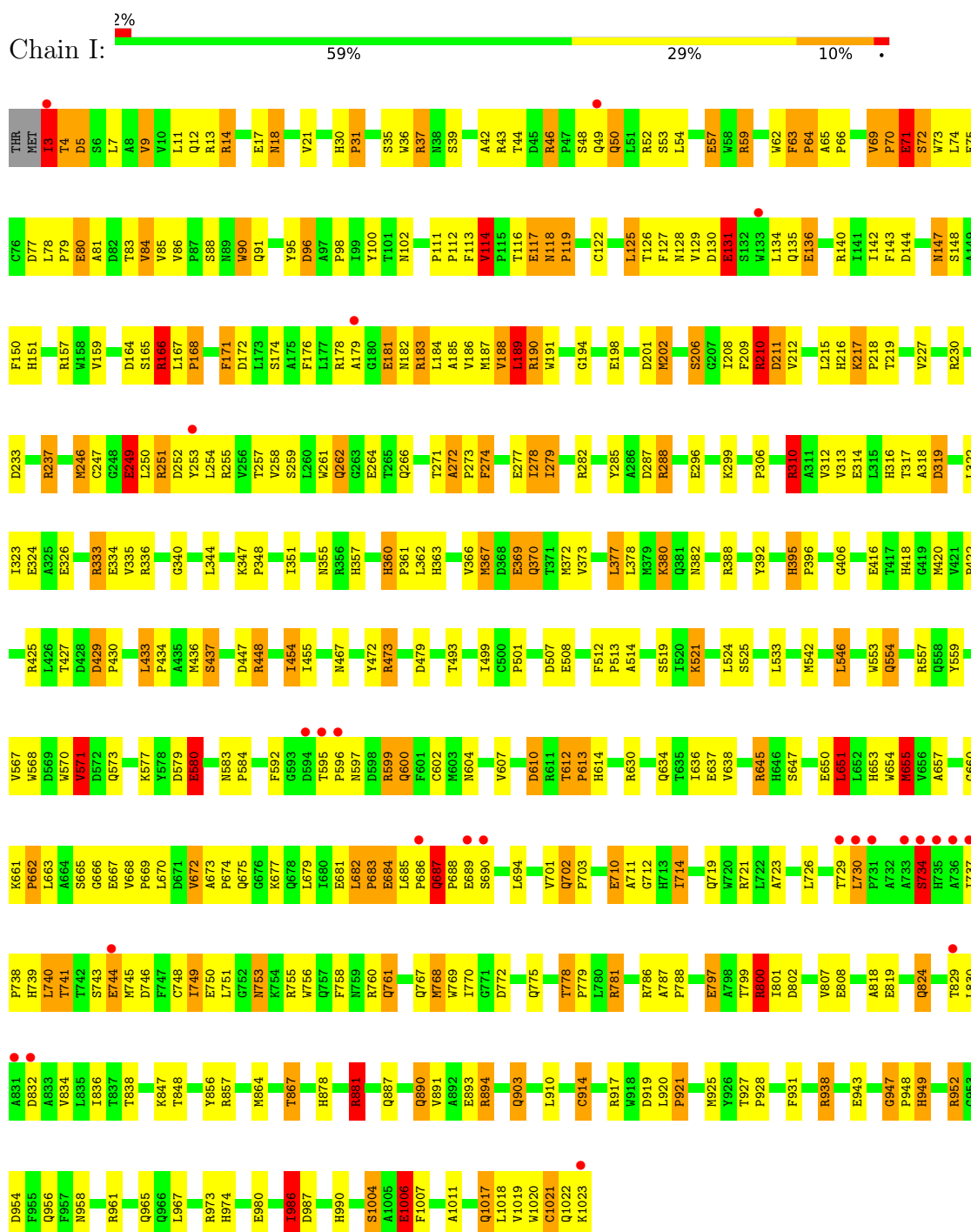




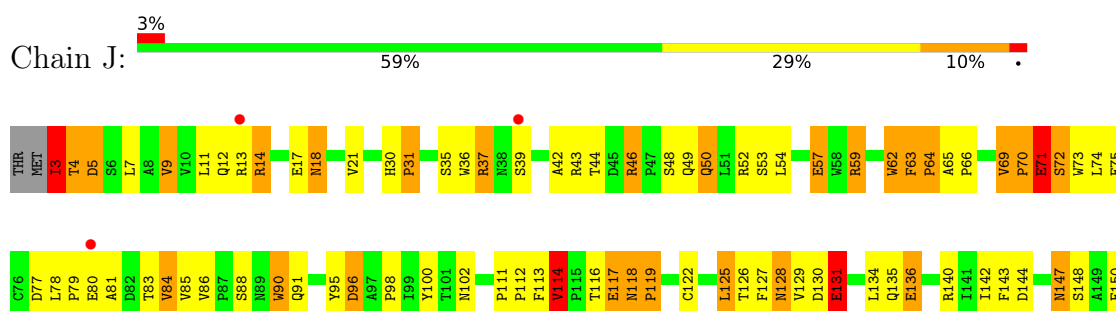
• Molecule 1: BETA-GALACTOSIDASE

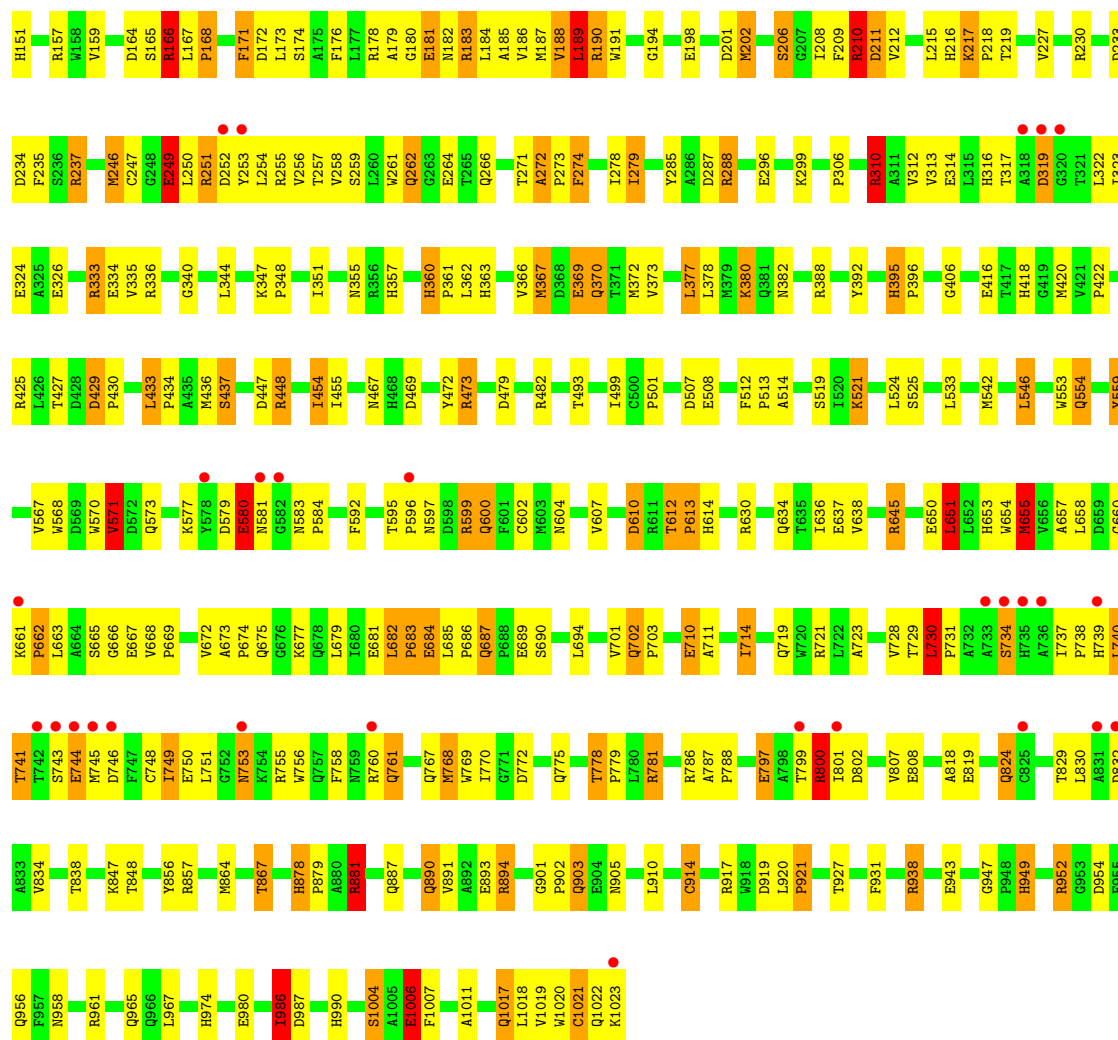


• Molecule 1: BETA-GALACTOSIDASE

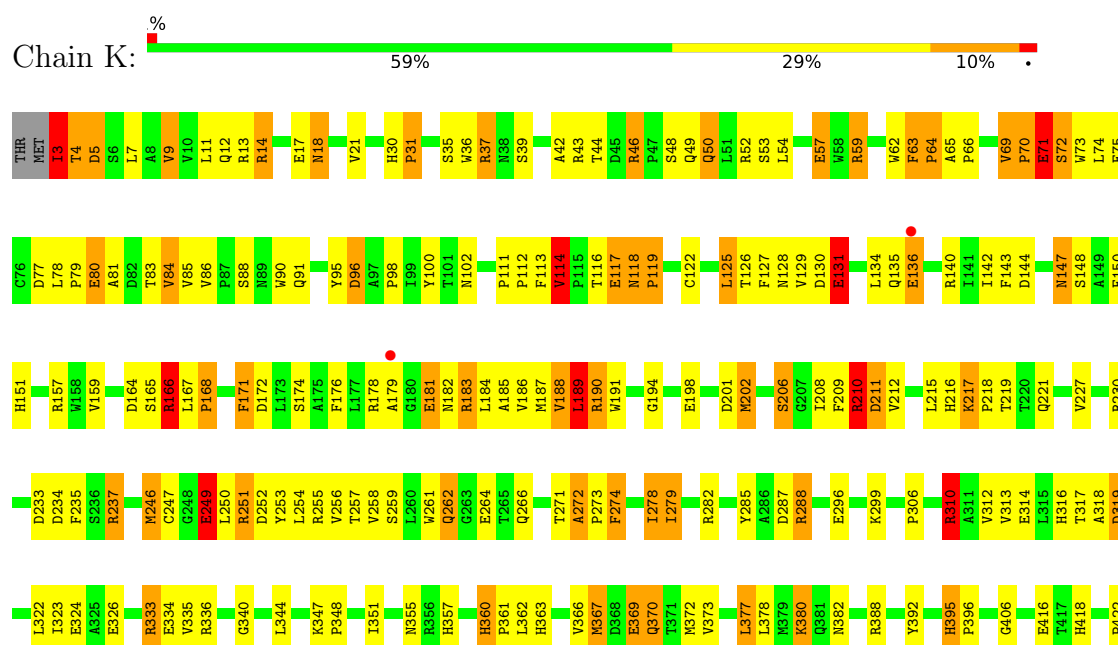


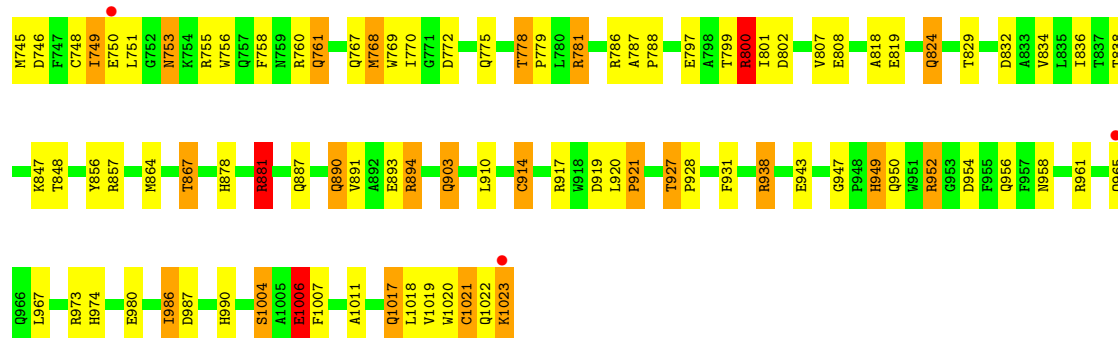
• Molecule 1: BETA-GALACTOSIDASE



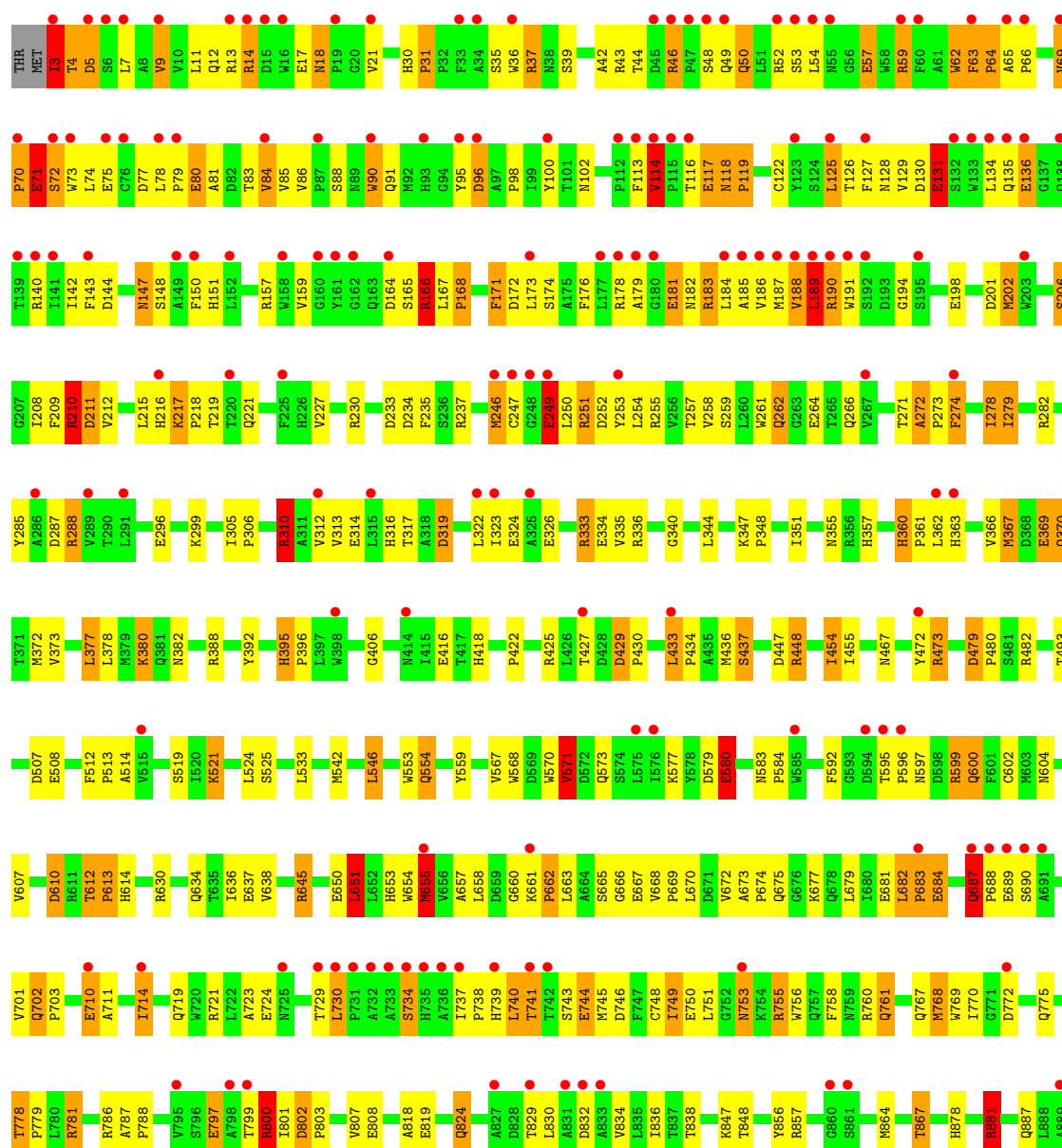


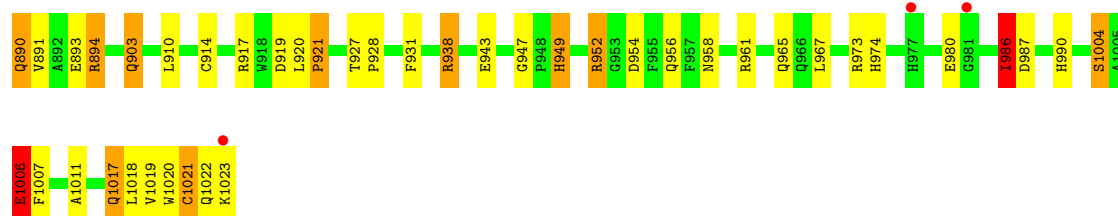
• Molecule 1: BETA-GALACTOSIDASE



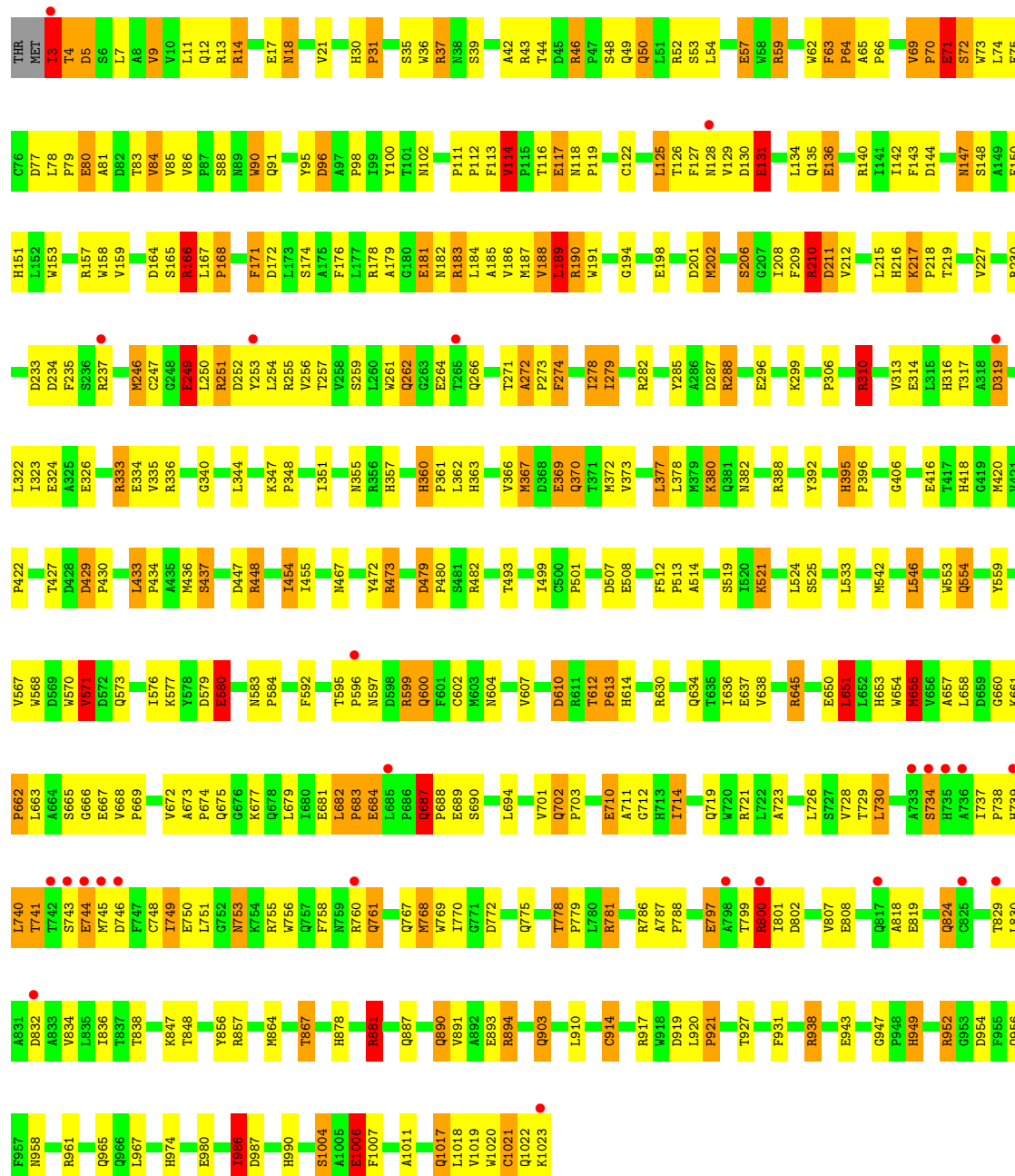


• Molecule 1: BETA-GALACTOSIDASE

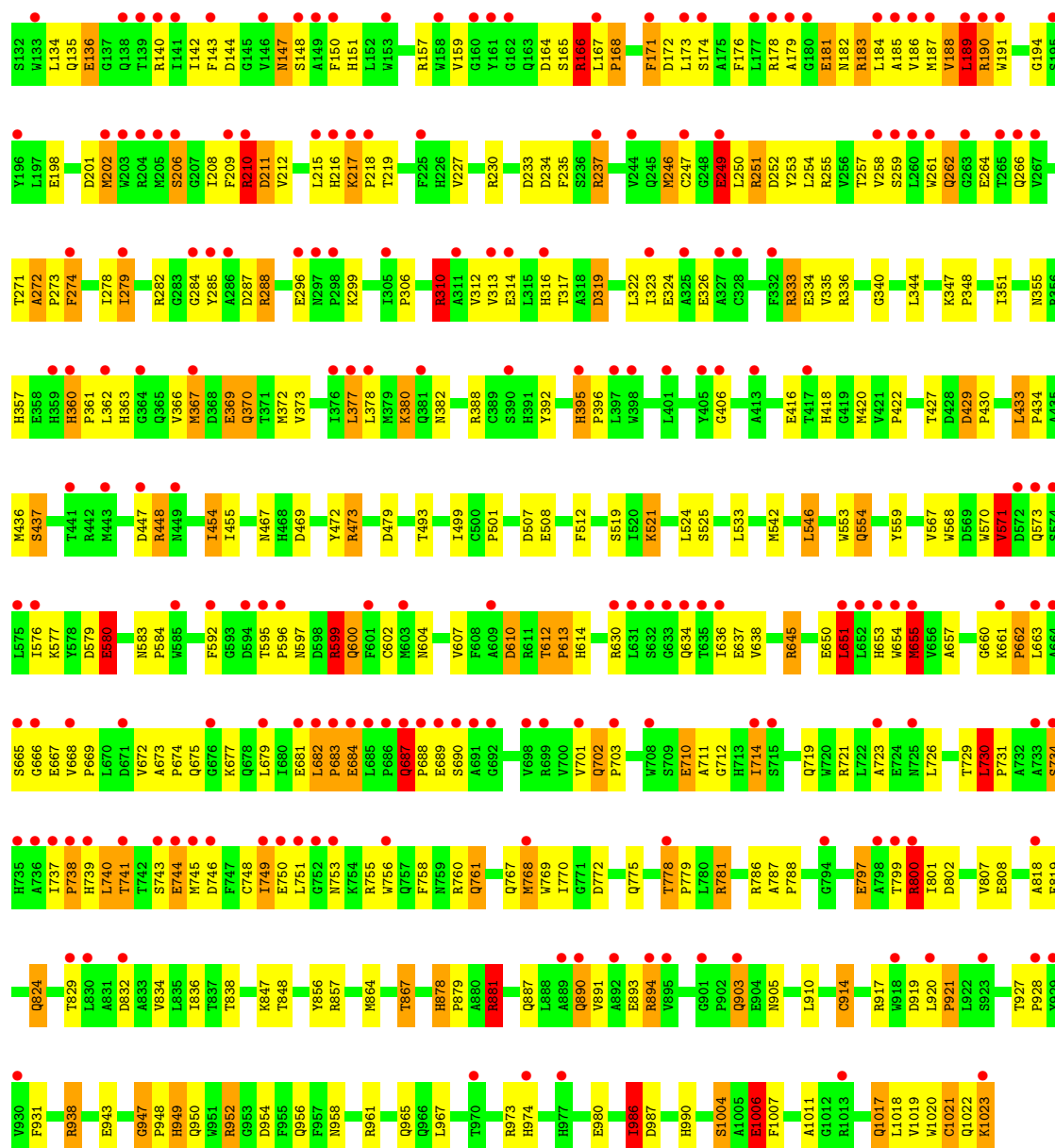




• Molecule 1: BETA-GALACTOSIDASE



• Molecule 1: BETA-GALACTOSIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.90Å 207.50Å 509.90Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50 200.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	71.0 ((Not available)-2.50) 72.7 (200.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.00Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.199 , 0.207 0.184 , 0.191	Depositor DCC
R_{free} test set	1680 reflections (0.28%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 100.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	138704	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% 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: CME, MG

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	1.47	37/8472 (0.4%)	1.85	177/11553 (1.5%)
1	B	1.47	37/8472 (0.4%)	1.85	179/11553 (1.5%)
1	C	1.47	39/8472 (0.5%)	1.85	180/11553 (1.6%)
1	D	1.47	36/8472 (0.4%)	1.85	182/11553 (1.6%)
1	E	1.47	37/8472 (0.4%)	1.85	179/11553 (1.5%)
1	F	1.47	37/8472 (0.4%)	1.85	180/11553 (1.6%)
1	G	1.47	37/8472 (0.4%)	1.85	180/11553 (1.6%)
1	H	1.47	36/8472 (0.4%)	1.85	182/11553 (1.6%)
1	I	1.47	38/8472 (0.4%)	1.85	180/11553 (1.6%)
1	J	1.47	38/8472 (0.4%)	1.85	180/11553 (1.6%)
1	K	1.47	36/8472 (0.4%)	1.85	180/11553 (1.6%)
1	L	1.47	36/8472 (0.4%)	1.85	178/11553 (1.5%)
1	M	1.47	37/8472 (0.4%)	1.85	179/11553 (1.5%)
1	N	1.47	35/8472 (0.4%)	1.85	180/11553 (1.6%)
1	O	1.47	37/8472 (0.4%)	1.85	182/11553 (1.6%)
1	P	1.47	37/8472 (0.4%)	1.85	178/11553 (1.5%)
All	All	1.47	590/135552 (0.4%)	1.85	2876/184848 (1.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	0
1	B	2	0
1	C	2	0
1	D	2	0
1	E	2	0
1	F	2	0
1	G	2	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	2	0
1	I	2	0
1	J	2	0
1	K	2	0
1	L	2	0
1	M	2	0
1	N	2	0
1	O	2	0
1	P	2	0
All	All	32	0

All (590) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	118	ASN	N-CA	-9.04	1.38	1.46
1	K	118	ASN	N-CA	-9.02	1.38	1.46
1	C	118	ASN	N-CA	-9.00	1.38	1.46
1	B	118	ASN	N-CA	-8.98	1.38	1.46
1	M	118	ASN	N-CA	-8.98	1.38	1.46
1	F	118	ASN	N-CA	-8.97	1.38	1.46
1	J	118	ASN	N-CA	-8.97	1.38	1.46
1	P	118	ASN	N-CA	-8.97	1.38	1.46
1	D	118	ASN	N-CA	-8.96	1.38	1.46
1	O	118	ASN	N-CA	-8.95	1.38	1.46
1	G	118	ASN	N-CA	-8.94	1.38	1.46
1	I	118	ASN	N-CA	-8.94	1.38	1.46
1	N	118	ASN	N-CA	-8.93	1.38	1.46
1	A	118	ASN	N-CA	-8.92	1.38	1.46
1	H	118	ASN	N-CA	-8.88	1.38	1.46
1	L	118	ASN	N-CA	-8.87	1.38	1.46
1	C	249	GLU	CD-OE2	7.13	1.38	1.25
1	O	249	GLU	CD-OE2	7.12	1.38	1.25
1	H	249	GLU	CD-OE2	7.11	1.38	1.25
1	J	249	GLU	CD-OE2	7.11	1.38	1.25
1	P	249	GLU	CD-OE2	7.11	1.38	1.25
1	I	249	GLU	CD-OE2	7.11	1.38	1.25
1	B	249	GLU	CD-OE2	7.10	1.38	1.25
1	F	249	GLU	CD-OE2	7.10	1.38	1.25
1	D	249	GLU	CD-OE2	7.09	1.38	1.25
1	A	249	GLU	CD-OE2	7.09	1.38	1.25
1	N	249	GLU	CD-OE2	7.08	1.38	1.25
1	K	249	GLU	CD-OE2	7.08	1.38	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	249	GLU	CD-OE2	7.07	1.38	1.25
1	M	249	GLU	CD-OE2	7.07	1.38	1.25
1	L	249	GLU	CD-OE2	7.06	1.38	1.25
1	G	249	GLU	CD-OE2	7.06	1.38	1.25
1	O	117	GLU	C-N	-6.97	1.28	1.33
1	P	479	ASP	C-N	-6.93	1.26	1.34
1	H	117	GLU	C-N	-6.92	1.28	1.33
1	N	117	GLU	C-N	-6.89	1.28	1.33
1	J	479	ASP	C-N	-6.86	1.26	1.34
1	P	117	GLU	C-N	-6.86	1.28	1.33
1	L	117	GLU	C-N	-6.85	1.28	1.33
1	M	117	GLU	C-N	-6.85	1.28	1.33
1	E	479	ASP	C-N	-6.85	1.26	1.34
1	D	117	GLU	C-N	-6.84	1.28	1.33
1	I	479	ASP	C-N	-6.84	1.26	1.34
1	K	117	GLU	C-N	-6.84	1.28	1.33
1	I	117	GLU	C-N	-6.83	1.28	1.33
1	M	744	GLU	CD-OE2	6.83	1.38	1.25
1	L	479	ASP	C-N	-6.83	1.26	1.34
1	L	744	GLU	CD-OE2	6.83	1.38	1.25
1	B	117	GLU	C-N	-6.82	1.28	1.33
1	A	479	ASP	C-N	-6.82	1.26	1.34
1	B	479	ASP	C-N	-6.82	1.26	1.34
1	C	117	GLU	C-N	-6.82	1.28	1.33
1	G	117	GLU	C-N	-6.82	1.28	1.33
1	K	744	GLU	CD-OE2	6.82	1.38	1.25
1	H	479	ASP	C-N	-6.82	1.26	1.34
1	N	479	ASP	C-N	-6.81	1.26	1.34
1	H	744	GLU	CD-OE2	6.81	1.38	1.25
1	F	479	ASP	C-N	-6.80	1.26	1.34
1	J	744	GLU	CD-OE2	6.80	1.38	1.25
1	C	744	GLU	CD-OE2	6.80	1.38	1.25
1	G	479	ASP	C-N	-6.80	1.26	1.34
1	O	479	ASP	C-N	-6.79	1.26	1.34
1	B	744	GLU	CD-OE2	6.79	1.38	1.25
1	G	744	GLU	CD-OE2	6.79	1.38	1.25
1	D	744	GLU	CD-OE2	6.79	1.38	1.25
1	E	744	GLU	CD-OE2	6.79	1.38	1.25
1	A	744	GLU	CD-OE2	6.78	1.38	1.25
1	E	117	GLU	C-N	-6.78	1.28	1.33
1	F	117	GLU	C-N	-6.78	1.28	1.33
1	K	479	ASP	C-N	-6.78	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	744	GLU	CD-OE2	6.78	1.38	1.25
1	F	744	GLU	CD-OE2	6.77	1.38	1.25
1	M	479	ASP	C-N	-6.77	1.26	1.34
1	D	479	ASP	C-N	-6.77	1.26	1.34
1	O	744	GLU	CD-OE2	6.76	1.38	1.25
1	C	479	ASP	C-N	-6.76	1.26	1.34
1	C	151	HIS	ND1-CE1	6.76	1.39	1.32
1	I	151	HIS	ND1-CE1	6.75	1.39	1.32
1	N	151	HIS	ND1-CE1	6.75	1.39	1.32
1	D	151	HIS	ND1-CE1	6.75	1.39	1.32
1	N	744	GLU	CD-OE2	6.75	1.38	1.25
1	F	151	HIS	ND1-CE1	6.74	1.39	1.32
1	I	744	GLU	CD-OE2	6.74	1.38	1.25
1	K	151	HIS	ND1-CE1	6.74	1.39	1.32
1	P	151	HIS	ND1-CE1	6.74	1.39	1.32
1	A	117	GLU	C-N	-6.73	1.28	1.33
1	J	117	GLU	C-N	-6.72	1.28	1.33
1	H	151	HIS	ND1-CE1	6.72	1.39	1.32
1	G	151	HIS	ND1-CE1	6.71	1.39	1.32
1	J	151	HIS	ND1-CE1	6.71	1.39	1.32
1	A	151	HIS	ND1-CE1	6.71	1.39	1.32
1	B	151	HIS	ND1-CE1	6.71	1.39	1.32
1	E	151	HIS	ND1-CE1	6.70	1.39	1.32
1	O	151	HIS	ND1-CE1	6.67	1.39	1.32
1	E	737	ILE	N-CA	-6.66	1.40	1.46
1	L	151	HIS	ND1-CE1	6.65	1.39	1.32
1	M	151	HIS	ND1-CE1	6.65	1.39	1.32
1	H	737	ILE	N-CA	-6.63	1.40	1.46
1	L	737	ILE	N-CA	-6.61	1.40	1.46
1	J	737	ILE	N-CA	-6.61	1.40	1.46
1	A	737	ILE	N-CA	-6.60	1.40	1.46
1	C	737	ILE	N-CA	-6.59	1.40	1.46
1	F	737	ILE	N-CA	-6.58	1.40	1.46
1	B	737	ILE	N-CA	-6.57	1.41	1.46
1	P	737	ILE	N-CA	-6.57	1.41	1.46
1	D	737	ILE	N-CA	-6.57	1.41	1.46
1	N	737	ILE	N-CA	-6.56	1.41	1.46
1	O	737	ILE	N-CA	-6.55	1.41	1.46
1	M	737	ILE	N-CA	-6.54	1.41	1.46
1	I	737	ILE	N-CA	-6.54	1.41	1.46
1	G	737	ILE	N-CA	-6.53	1.41	1.46
1	K	737	ILE	N-CA	-6.52	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	689	GLU	CD-OE2	6.30	1.37	1.25
1	D	737	ILE	CA-CB	-6.29	1.48	1.55
1	I	737	ILE	CA-CB	-6.29	1.48	1.55
1	F	737	ILE	CA-CB	-6.29	1.48	1.55
1	L	737	ILE	CA-CB	-6.29	1.48	1.55
1	F	689	GLU	CD-OE2	6.29	1.37	1.25
1	K	737	ILE	CA-CB	-6.28	1.48	1.55
1	C	689	GLU	CD-OE2	6.28	1.37	1.25
1	B	737	ILE	CA-CB	-6.27	1.48	1.55
1	B	689	GLU	CD-OE2	6.26	1.37	1.25
1	O	737	ILE	CA-CB	-6.26	1.48	1.55
1	A	689	GLU	CD-OE2	6.25	1.37	1.25
1	J	737	ILE	CA-CB	-6.25	1.48	1.55
1	P	689	GLU	CD-OE2	6.25	1.37	1.25
1	E	689	GLU	CD-OE2	6.25	1.37	1.25
1	D	689	GLU	CD-OE2	6.25	1.37	1.25
1	E	737	ILE	CA-CB	-6.24	1.48	1.55
1	L	689	GLU	CD-OE2	6.24	1.37	1.25
1	M	737	ILE	CA-CB	-6.24	1.48	1.55
1	C	737	ILE	CA-CB	-6.24	1.48	1.55
1	J	689	GLU	CD-OE2	6.24	1.37	1.25
1	O	689	GLU	CD-OE2	6.24	1.37	1.25
1	M	689	GLU	CD-OE2	6.24	1.37	1.25
1	I	689	GLU	CD-OE2	6.23	1.37	1.25
1	H	689	GLU	CD-OE2	6.23	1.37	1.25
1	K	689	GLU	CD-OE2	6.23	1.37	1.25
1	N	737	ILE	CA-CB	-6.23	1.48	1.55
1	P	737	ILE	CA-CB	-6.23	1.48	1.55
1	G	689	GLU	CD-OE2	6.23	1.37	1.25
1	A	737	ILE	CA-CB	-6.22	1.48	1.55
1	H	737	ILE	CA-CB	-6.21	1.48	1.55
1	G	737	ILE	CA-CB	-6.21	1.48	1.55
1	I	819	GLU	CD-OE2	6.20	1.37	1.25
1	G	819	GLU	CD-OE2	6.19	1.37	1.25
1	H	819	GLU	CD-OE2	6.19	1.37	1.25
1	M	819	GLU	CD-OE2	6.19	1.37	1.25
1	E	819	GLU	CD-OE2	6.18	1.37	1.25
1	C	819	GLU	CD-OE2	6.18	1.37	1.25
1	L	819	GLU	CD-OE2	6.18	1.37	1.25
1	A	819	GLU	CD-OE2	6.17	1.37	1.25
1	O	819	GLU	CD-OE2	6.17	1.37	1.25
1	K	819	GLU	CD-OE2	6.17	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	819	GLU	CD-OE2	6.16	1.37	1.25
1	N	819	GLU	CD-OE2	6.16	1.37	1.25
1	B	819	GLU	CD-OE2	6.16	1.37	1.25
1	F	819	GLU	CD-OE2	6.14	1.37	1.25
1	P	819	GLU	CD-OE2	6.14	1.37	1.25
1	J	819	GLU	CD-OE2	6.13	1.37	1.25
1	J	662	PRO	CA-C	-6.07	1.46	1.52
1	E	662	PRO	CA-C	-6.06	1.46	1.52
1	G	75	GLU	CD-OE2	6.05	1.36	1.25
1	L	75	GLU	CD-OE2	6.05	1.36	1.25
1	J	75	GLU	CD-OE2	6.05	1.36	1.25
1	M	662	PRO	CA-C	-6.05	1.46	1.52
1	O	75	GLU	CD-OE2	6.05	1.36	1.25
1	M	75	GLU	CD-OE2	6.05	1.36	1.25
1	C	800	ARG	NE-CZ	6.04	1.39	1.33
1	I	75	GLU	CD-OE2	6.04	1.36	1.25
1	I	662	PRO	CA-C	-6.04	1.46	1.52
1	B	75	GLU	CD-OE2	6.03	1.36	1.25
1	B	800	ARG	NE-CZ	6.03	1.39	1.33
1	C	75	GLU	CD-OE2	6.03	1.36	1.25
1	E	75	GLU	CD-OE2	6.03	1.36	1.25
1	N	75	GLU	CD-OE2	6.03	1.36	1.25
1	O	800	ARG	NE-CZ	6.03	1.39	1.33
1	A	75	GLU	CD-OE2	6.03	1.36	1.25
1	F	75	GLU	CD-OE2	6.03	1.36	1.25
1	A	662	PRO	CA-C	-6.03	1.46	1.52
1	D	75	GLU	CD-OE2	6.03	1.36	1.25
1	B	662	PRO	CA-C	-6.02	1.46	1.52
1	I	800	ARG	NE-CZ	6.01	1.39	1.33
1	O	662	PRO	CA-C	-6.01	1.46	1.52
1	L	800	ARG	NE-CZ	6.01	1.39	1.33
1	H	75	GLU	CD-OE2	6.00	1.36	1.25
1	P	662	PRO	CA-C	-6.00	1.46	1.52
1	F	662	PRO	CA-C	-6.00	1.46	1.52
1	P	75	GLU	CD-OE2	6.00	1.36	1.25
1	N	662	PRO	CA-C	-6.00	1.46	1.52
1	A	800	ARG	NE-CZ	6.00	1.39	1.33
1	G	800	ARG	NE-CZ	6.00	1.39	1.33
1	K	75	GLU	CD-OE2	6.00	1.36	1.25
1	H	800	ARG	NE-CZ	5.99	1.39	1.33
1	N	800	ARG	NE-CZ	5.99	1.39	1.33
1	J	800	ARG	NE-CZ	5.99	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	800	ARG	NE-CZ	5.98	1.39	1.33
1	K	662	PRO	CA-C	-5.97	1.46	1.52
1	L	662	PRO	CA-C	-5.97	1.46	1.52
1	M	800	ARG	NE-CZ	5.97	1.39	1.33
1	C	662	PRO	CA-C	-5.96	1.46	1.52
1	P	800	ARG	NE-CZ	5.96	1.39	1.33
1	F	800	ARG	NE-CZ	5.95	1.39	1.33
1	H	288	ARG	C-N	-5.94	1.27	1.33
1	G	662	PRO	CA-C	-5.94	1.46	1.52
1	G	288	ARG	C-N	-5.93	1.27	1.33
1	K	800	ARG	NE-CZ	5.93	1.39	1.33
1	D	288	ARG	C-N	-5.93	1.27	1.33
1	D	662	PRO	CA-C	-5.93	1.46	1.52
1	H	662	PRO	CA-C	-5.92	1.46	1.52
1	F	288	ARG	C-N	-5.92	1.27	1.33
1	E	800	ARG	NE-CZ	5.92	1.39	1.33
1	O	288	ARG	C-N	-5.90	1.27	1.33
1	A	288	ARG	C-N	-5.90	1.27	1.33
1	I	288	ARG	C-N	-5.89	1.27	1.33
1	J	288	ARG	C-N	-5.89	1.27	1.33
1	N	288	ARG	C-N	-5.89	1.27	1.33
1	B	288	ARG	C-N	-5.88	1.27	1.33
1	P	288	ARG	C-N	-5.86	1.27	1.33
1	J	63	PHE	C-N	-5.85	1.26	1.34
1	L	288	ARG	C-N	-5.85	1.27	1.33
1	K	288	ARG	C-N	-5.85	1.27	1.33
1	C	288	ARG	C-N	-5.84	1.27	1.33
1	E	288	ARG	C-N	-5.84	1.27	1.33
1	N	63	PHE	C-N	-5.84	1.26	1.34
1	F	580	GLU	CD-OE2	5.84	1.36	1.25
1	D	63	PHE	C-N	-5.84	1.26	1.34
1	D	580	GLU	CD-OE2	5.83	1.36	1.25
1	M	63	PHE	C-N	-5.82	1.26	1.34
1	O	63	PHE	C-N	-5.82	1.26	1.34
1	P	63	PHE	C-N	-5.82	1.26	1.34
1	C	580	GLU	CD-OE2	5.82	1.36	1.25
1	F	63	PHE	C-N	-5.81	1.26	1.34
1	I	580	GLU	CD-OE2	5.81	1.36	1.25
1	L	63	PHE	C-N	-5.81	1.26	1.34
1	I	63	PHE	C-N	-5.81	1.26	1.34
1	K	63	PHE	C-N	-5.81	1.26	1.34
1	B	63	PHE	C-N	-5.80	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	580	GLU	CD-OE2	5.80	1.36	1.25
1	M	580	GLU	CD-OE2	5.80	1.36	1.25
1	L	580	GLU	CD-OE2	5.80	1.36	1.25
1	M	288	ARG	C-N	-5.80	1.27	1.33
1	E	580	GLU	CD-OE2	5.79	1.36	1.25
1	A	580	GLU	CD-OE2	5.79	1.36	1.25
1	N	580	GLU	CD-OE2	5.79	1.36	1.25
1	E	63	PHE	C-N	-5.79	1.26	1.34
1	G	580	GLU	CD-OE2	5.78	1.36	1.25
1	K	580	GLU	CD-OE2	5.78	1.36	1.25
1	O	580	GLU	CD-OE2	5.78	1.36	1.25
1	H	580	GLU	CD-OE2	5.77	1.36	1.25
1	J	580	GLU	CD-OE2	5.77	1.36	1.25
1	G	63	PHE	C-N	-5.77	1.26	1.34
1	P	580	GLU	CD-OE2	5.77	1.36	1.25
1	H	63	PHE	C-N	-5.75	1.26	1.34
1	A	63	PHE	C-N	-5.74	1.26	1.34
1	C	63	PHE	C-N	-5.74	1.26	1.34
1	I	131	GLU	CD-OE2	5.70	1.36	1.25
1	C	131	GLU	CD-OE2	5.70	1.36	1.25
1	H	131	GLU	CD-OE2	5.70	1.36	1.25
1	E	131	GLU	CD-OE2	5.68	1.36	1.25
1	P	131	GLU	CD-OE2	5.68	1.36	1.25
1	G	131	GLU	CD-OE2	5.68	1.36	1.25
1	A	131	GLU	CD-OE2	5.67	1.36	1.25
1	B	131	GLU	CD-OE2	5.66	1.36	1.25
1	F	131	GLU	CD-OE2	5.66	1.36	1.25
1	J	131	GLU	CD-OE2	5.66	1.36	1.25
1	D	131	GLU	CD-OE2	5.66	1.36	1.25
1	K	131	GLU	CD-OE2	5.66	1.36	1.25
1	O	131	GLU	CD-OE2	5.65	1.36	1.25
1	M	131	GLU	CD-OE2	5.65	1.36	1.25
1	N	131	GLU	CD-OE2	5.64	1.36	1.25
1	L	131	GLU	CD-OE2	5.63	1.36	1.25
1	G	980	GLU	CD-OE2	5.58	1.35	1.25
1	N	980	GLU	CD-OE2	5.58	1.35	1.25
1	M	980	GLU	CD-OE2	5.58	1.35	1.25
1	B	980	GLU	CD-OE2	5.57	1.35	1.25
1	M	252	ASP	CG-OD2	5.56	1.35	1.25
1	E	980	GLU	CD-OE2	5.55	1.35	1.25
1	D	980	GLU	CD-OE2	5.55	1.35	1.25
1	F	980	GLU	CD-OE2	5.55	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	252	ASP	CG-OD2	5.55	1.35	1.25
1	A	980	GLU	CD-OE2	5.55	1.35	1.25
1	B	252	ASP	CG-OD2	5.54	1.35	1.25
1	O	980	GLU	CD-OE2	5.54	1.35	1.25
1	O	252	ASP	CG-OD2	5.54	1.35	1.25
1	H	980	GLU	CD-OE2	5.53	1.35	1.25
1	L	980	GLU	CD-OE2	5.52	1.35	1.25
1	F	252	ASP	CG-OD2	5.52	1.35	1.25
1	I	980	GLU	CD-OE2	5.52	1.35	1.25
1	J	980	GLU	CD-OE2	5.52	1.35	1.25
1	I	252	ASP	CG-OD2	5.52	1.35	1.25
1	L	252	ASP	CG-OD2	5.52	1.35	1.25
1	D	684	GLU	CD-OE2	5.52	1.35	1.25
1	C	980	GLU	CD-OE2	5.51	1.35	1.25
1	H	252	ASP	CG-OD2	5.51	1.35	1.25
1	E	252	ASP	CG-OD2	5.51	1.35	1.25
1	K	980	GLU	CD-OE2	5.51	1.35	1.25
1	P	739	HIS	N-CA	-5.51	1.39	1.46
1	A	252	ASP	CG-OD2	5.50	1.35	1.25
1	P	980	GLU	CD-OE2	5.50	1.35	1.25
1	K	252	ASP	CG-OD2	5.50	1.35	1.25
1	N	252	ASP	CG-OD2	5.50	1.35	1.25
1	C	252	ASP	CG-OD2	5.49	1.35	1.25
1	D	252	ASP	CG-OD2	5.49	1.35	1.25
1	G	252	ASP	CG-OD2	5.49	1.35	1.25
1	G	684	GLU	CD-OE2	5.49	1.35	1.25
1	J	252	ASP	CG-OD2	5.48	1.35	1.25
1	O	684	GLU	CD-OE2	5.48	1.35	1.25
1	K	684	GLU	CD-OE2	5.48	1.35	1.25
1	M	684	GLU	CD-OE2	5.48	1.35	1.25
1	P	684	GLU	CD-OE2	5.48	1.35	1.25
1	A	684	GLU	CD-OE2	5.48	1.35	1.25
1	F	684	GLU	CD-OE2	5.48	1.35	1.25
1	G	739	HIS	N-CA	-5.48	1.39	1.46
1	N	684	GLU	CD-OE2	5.47	1.35	1.25
1	K	739	HIS	N-CA	-5.47	1.39	1.46
1	E	739	HIS	N-CA	-5.47	1.39	1.46
1	L	684	GLU	CD-OE2	5.47	1.35	1.25
1	C	684	GLU	CD-OE2	5.46	1.35	1.25
1	B	684	GLU	CD-OE2	5.46	1.35	1.25
1	L	739	HIS	N-CA	-5.46	1.39	1.46
1	I	684	GLU	CD-OE2	5.46	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	684	GLU	CD-OE2	5.45	1.35	1.25
1	M	739	HIS	N-CA	-5.45	1.39	1.46
1	A	739	HIS	N-CA	-5.45	1.39	1.46
1	E	684	GLU	CD-OE2	5.44	1.35	1.25
1	F	454	ILE	CA-CB	-5.44	1.48	1.54
1	H	454	ILE	CA-CB	-5.44	1.48	1.54
1	J	684	GLU	CD-OE2	5.44	1.35	1.25
1	N	739	HIS	N-CA	-5.43	1.39	1.46
1	C	739	HIS	N-CA	-5.43	1.39	1.46
1	F	739	HIS	N-CA	-5.43	1.39	1.46
1	I	739	HIS	N-CA	-5.43	1.39	1.46
1	N	454	ILE	CA-CB	-5.43	1.48	1.54
1	C	454	ILE	CA-CB	-5.43	1.48	1.54
1	B	454	ILE	CA-CB	-5.43	1.48	1.54
1	O	636	ILE	CA-CB	-5.43	1.47	1.54
1	B	739	HIS	N-CA	-5.42	1.39	1.46
1	L	636	ILE	CA-CB	-5.42	1.47	1.54
1	H	636	ILE	CA-CB	-5.42	1.47	1.54
1	K	454	ILE	CA-CB	-5.42	1.48	1.54
1	I	454	ILE	CA-CB	-5.42	1.48	1.54
1	D	454	ILE	CA-CB	-5.42	1.48	1.54
1	J	454	ILE	CA-CB	-5.42	1.48	1.54
1	H	739	HIS	N-CA	-5.42	1.39	1.46
1	J	636	ILE	CA-CB	-5.41	1.47	1.54
1	E	454	ILE	CA-CB	-5.41	1.48	1.54
1	A	454	ILE	CA-CB	-5.41	1.48	1.54
1	M	454	ILE	CA-CB	-5.41	1.48	1.54
1	M	296	GLU	CD-OE2	5.40	1.35	1.25
1	L	454	ILE	CA-CB	-5.40	1.48	1.54
1	J	739	HIS	N-CA	-5.40	1.39	1.46
1	I	636	ILE	CA-CB	-5.40	1.47	1.54
1	P	454	ILE	CA-CB	-5.40	1.48	1.54
1	N	296	GLU	CD-OE2	5.39	1.35	1.25
1	D	739	HIS	N-CA	-5.38	1.39	1.46
1	H	296	GLU	CD-OE2	5.38	1.35	1.25
1	O	296	GLU	CD-OE2	5.38	1.35	1.25
1	B	296	GLU	CD-OE2	5.38	1.35	1.25
1	G	296	GLU	CD-OE2	5.38	1.35	1.25
1	G	454	ILE	CA-CB	-5.38	1.48	1.54
1	A	296	GLU	CD-OE2	5.38	1.35	1.25
1	C	296	GLU	CD-OE2	5.38	1.35	1.25
1	E	296	GLU	CD-OE2	5.38	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	296	GLU	CD-OE2	5.37	1.35	1.25
1	G	636	ILE	CA-CB	-5.37	1.48	1.54
1	K	636	ILE	CA-CB	-5.37	1.48	1.54
1	O	454	ILE	CA-CB	-5.37	1.48	1.54
1	C	181	GLU	CD-OE2	5.37	1.35	1.25
1	L	296	GLU	CD-OE2	5.37	1.35	1.25
1	D	181	GLU	CD-OE2	5.37	1.35	1.25
1	J	296	GLU	CD-OE2	5.37	1.35	1.25
1	K	296	GLU	CD-OE2	5.37	1.35	1.25
1	O	739	HIS	N-CA	-5.37	1.39	1.46
1	I	296	GLU	CD-OE2	5.37	1.35	1.25
1	A	636	ILE	CA-CB	-5.36	1.48	1.54
1	D	296	GLU	CD-OE2	5.36	1.35	1.25
1	H	181	GLU	CD-OE2	5.36	1.35	1.25
1	N	636	ILE	CA-CB	-5.36	1.48	1.54
1	N	181	GLU	CD-OE2	5.36	1.35	1.25
1	P	296	GLU	CD-OE2	5.36	1.35	1.25
1	E	636	ILE	CA-CB	-5.36	1.48	1.54
1	I	181	GLU	CD-OE2	5.36	1.35	1.25
1	P	636	ILE	CA-CB	-5.36	1.48	1.54
1	J	181	GLU	CD-OE2	5.35	1.35	1.25
1	C	636	ILE	CA-CB	-5.35	1.48	1.54
1	A	181	GLU	CD-OE2	5.34	1.35	1.25
1	K	181	GLU	CD-OE2	5.34	1.35	1.25
1	G	181	GLU	CD-OE2	5.33	1.35	1.25
1	I	208	ILE	CA-C	-5.33	1.47	1.53
1	B	181	GLU	CD-OE2	5.33	1.35	1.25
1	F	636	ILE	CA-CB	-5.33	1.48	1.54
1	M	181	GLU	CD-OE2	5.33	1.35	1.25
1	O	181	GLU	CD-OE2	5.33	1.35	1.25
1	E	181	GLU	CD-OE2	5.32	1.35	1.25
1	F	181	GLU	CD-OE2	5.32	1.35	1.25
1	L	181	GLU	CD-OE2	5.32	1.35	1.25
1	D	636	ILE	CA-CB	-5.32	1.48	1.54
1	G	136	GLU	CD-OE2	5.32	1.35	1.25
1	L	136	GLU	CD-OE2	5.31	1.35	1.25
1	M	208	ILE	CA-C	-5.31	1.47	1.53
1	O	136	GLU	CD-OE2	5.30	1.35	1.25
1	B	636	ILE	CA-CB	-5.30	1.48	1.54
1	P	181	GLU	CD-OE2	5.30	1.35	1.25
1	C	208	ILE	CA-C	-5.30	1.47	1.53
1	K	136	GLU	CD-OE2	5.29	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	208	ILE	CA-C	-5.29	1.47	1.53
1	G	208	ILE	CA-C	-5.29	1.47	1.53
1	M	636	ILE	CA-CB	-5.29	1.48	1.54
1	B	208	ILE	CA-C	-5.29	1.47	1.53
1	B	136	GLU	CD-OE2	5.28	1.35	1.25
1	L	208	ILE	CA-C	-5.28	1.47	1.53
1	E	136	GLU	CD-OE2	5.28	1.35	1.25
1	J	208	ILE	CA-C	-5.28	1.47	1.53
1	D	136	GLU	CD-OE2	5.28	1.35	1.25
1	A	208	ILE	CA-C	-5.27	1.47	1.53
1	N	31	PRO	C-N	-5.27	1.27	1.33
1	O	208	ILE	CA-C	-5.27	1.47	1.53
1	E	208	ILE	CA-C	-5.27	1.47	1.53
1	F	136	GLU	CD-OE2	5.27	1.35	1.25
1	H	662	PRO	C-O	-5.27	1.18	1.23
1	A	136	GLU	CD-OE2	5.27	1.35	1.25
1	F	208	ILE	CA-C	-5.27	1.47	1.53
1	H	31	PRO	C-N	-5.27	1.27	1.33
1	C	136	GLU	CD-OE2	5.26	1.35	1.25
1	F	662	PRO	C-O	-5.26	1.18	1.23
1	N	662	PRO	C-O	-5.26	1.18	1.23
1	P	136	GLU	CD-OE2	5.26	1.35	1.25
1	H	208	ILE	CA-C	-5.26	1.47	1.53
1	J	136	GLU	CD-OE2	5.26	1.35	1.25
1	C	31	PRO	C-N	-5.25	1.27	1.33
1	I	136	GLU	CD-OE2	5.25	1.35	1.25
1	K	208	ILE	CA-C	-5.25	1.47	1.53
1	D	208	ILE	CA-C	-5.25	1.47	1.53
1	I	662	PRO	C-O	-5.25	1.18	1.23
1	H	136	GLU	CD-OE2	5.25	1.35	1.25
1	M	31	PRO	C-N	-5.24	1.27	1.33
1	P	31	PRO	C-N	-5.24	1.27	1.33
1	N	136	GLU	CD-OE2	5.24	1.35	1.25
1	D	31	PRO	C-N	-5.24	1.27	1.33
1	L	31	PRO	C-N	-5.24	1.27	1.33
1	C	662	PRO	C-O	-5.24	1.18	1.23
1	G	31	PRO	C-N	-5.22	1.27	1.33
1	E	710	GLU	CD-OE2	5.22	1.35	1.25
1	A	31	PRO	C-N	-5.22	1.27	1.33
1	N	710	GLU	CD-OE2	5.22	1.35	1.25
1	G	662	PRO	C-O	-5.22	1.18	1.23
1	K	662	PRO	C-O	-5.22	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	136	GLU	CD-OE2	5.22	1.35	1.25
1	P	710	GLU	CD-OE2	5.21	1.35	1.25
1	F	710	GLU	CD-OE2	5.21	1.35	1.25
1	N	208	ILE	CA-C	-5.20	1.47	1.53
1	J	31	PRO	C-N	-5.20	1.27	1.33
1	B	31	PRO	C-N	-5.20	1.27	1.33
1	K	31	PRO	C-N	-5.20	1.27	1.33
1	H	710	GLU	CD-OE2	5.20	1.35	1.25
1	O	710	GLU	CD-OE2	5.20	1.35	1.25
1	J	710	GLU	CD-OE2	5.19	1.35	1.25
1	L	710	GLU	CD-OE2	5.19	1.35	1.25
1	M	710	GLU	CD-OE2	5.19	1.35	1.25
1	P	662	PRO	C-O	-5.19	1.18	1.23
1	D	662	PRO	C-O	-5.19	1.18	1.23
1	F	31	PRO	C-N	-5.19	1.27	1.33
1	G	710	GLU	CD-OE2	5.19	1.35	1.25
1	I	710	GLU	CD-OE2	5.19	1.35	1.25
1	O	70	PRO	C-O	5.19	1.28	1.23
1	O	31	PRO	C-N	-5.19	1.27	1.33
1	A	710	GLU	CD-OE2	5.18	1.35	1.25
1	J	662	PRO	C-O	-5.18	1.18	1.23
1	E	662	PRO	C-O	-5.18	1.18	1.23
1	H	70	PRO	C-O	5.18	1.28	1.23
1	K	710	GLU	CD-OE2	5.17	1.35	1.25
1	F	1019	VAL	CA-CB	-5.17	1.48	1.54
1	D	710	GLU	CD-OE2	5.17	1.35	1.25
1	B	662	PRO	C-O	-5.17	1.18	1.23
1	J	1019	VAL	CA-CB	-5.17	1.48	1.54
1	I	31	PRO	C-N	-5.17	1.27	1.33
1	I	70	PRO	C-O	5.17	1.28	1.23
1	C	710	GLU	CD-OE2	5.16	1.35	1.25
1	M	662	PRO	C-O	-5.16	1.18	1.23
1	C	288	ARG	CA-C	-5.15	1.46	1.52
1	E	31	PRO	C-N	-5.15	1.27	1.33
1	P	70	PRO	C-O	5.15	1.28	1.23
1	B	710	GLU	CD-OE2	5.15	1.35	1.25
1	I	1019	VAL	CA-CB	-5.15	1.48	1.54
1	L	662	PRO	C-O	-5.14	1.18	1.23
1	C	1019	VAL	CA-CB	-5.14	1.48	1.54
1	M	288	ARG	CA-C	-5.14	1.46	1.52
1	N	1019	VAL	CA-CB	-5.14	1.48	1.54
1	A	662	PRO	C-O	-5.14	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	70	PRO	C-O	5.13	1.28	1.23
1	G	288	ARG	CA-C	-5.13	1.46	1.52
1	H	264	GLU	CD-OE2	5.13	1.35	1.25
1	O	662	PRO	C-O	-5.13	1.18	1.23
1	M	70	PRO	C-O	5.13	1.28	1.23
1	P	1019	VAL	CA-CB	-5.13	1.48	1.54
1	E	70	PRO	C-O	5.12	1.28	1.23
1	I	288	ARG	CA-C	-5.12	1.46	1.52
1	F	288	ARG	CA-C	-5.12	1.46	1.52
1	N	264	GLU	CD-OE2	5.12	1.35	1.25
1	G	70	PRO	C-O	5.12	1.28	1.23
1	K	264	GLU	CD-OE2	5.12	1.35	1.25
1	C	264	GLU	CD-OE2	5.12	1.35	1.25
1	G	264	GLU	CD-OE2	5.12	1.35	1.25
1	O	264	GLU	CD-OE2	5.12	1.35	1.25
1	J	264	GLU	CD-OE2	5.12	1.35	1.25
1	G	1019	VAL	CA-CB	-5.11	1.48	1.54
1	M	1019	VAL	CA-CB	-5.11	1.48	1.54
1	B	1019	VAL	CA-CB	-5.11	1.48	1.54
1	D	264	GLU	CD-OE2	5.11	1.35	1.25
1	E	288	ARG	CA-C	-5.11	1.46	1.52
1	D	740	LEU	C-O	-5.11	1.17	1.23
1	E	1019	VAL	CA-CB	-5.11	1.48	1.54
1	O	1019	VAL	CA-CB	-5.11	1.48	1.54
1	B	288	ARG	CA-C	-5.10	1.46	1.52
1	H	1019	VAL	CA-CB	-5.10	1.48	1.54
1	K	740	LEU	C-O	-5.10	1.17	1.23
1	P	264	GLU	CD-OE2	5.10	1.35	1.25
1	A	1019	VAL	CA-CB	-5.10	1.48	1.54
1	K	1019	VAL	CA-CB	-5.10	1.48	1.54
1	L	70	PRO	C-O	5.10	1.28	1.23
1	A	70	PRO	C-O	5.10	1.28	1.23
1	D	70	PRO	C-O	5.10	1.28	1.23
1	K	70	PRO	C-O	5.09	1.28	1.23
1	N	70	PRO	C-O	5.09	1.28	1.23
1	M	264	GLU	CD-OE2	5.09	1.35	1.25
1	B	264	GLU	CD-OE2	5.09	1.35	1.25
1	D	288	ARG	CA-C	-5.09	1.46	1.52
1	L	1019	VAL	CA-CB	-5.09	1.48	1.54
1	A	264	GLU	CD-OE2	5.09	1.35	1.25
1	L	264	GLU	CD-OE2	5.08	1.35	1.25
1	G	740	LEU	C-O	-5.08	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	264	GLU	CD-OE2	5.08	1.34	1.25
1	A	288	ARG	CA-C	-5.08	1.46	1.52
1	E	264	GLU	CD-OE2	5.08	1.34	1.25
1	P	740	LEU	C-O	-5.07	1.17	1.23
1	D	319	ASP	CG-OD2	5.07	1.34	1.25
1	F	264	GLU	CD-OE2	5.07	1.34	1.25
1	P	319	ASP	CG-OD2	5.07	1.34	1.25
1	J	70	PRO	C-O	5.07	1.28	1.23
1	I	740	LEU	C-O	-5.06	1.17	1.23
1	H	740	LEU	C-O	-5.06	1.17	1.23
1	L	288	ARG	CA-C	-5.06	1.46	1.52
1	P	288	ARG	CA-C	-5.06	1.46	1.52
1	A	740	LEU	C-O	-5.05	1.17	1.23
1	B	740	LEU	C-O	-5.05	1.17	1.23
1	L	319	ASP	CG-OD2	5.05	1.34	1.25
1	C	319	ASP	CG-OD2	5.05	1.34	1.25
1	F	70	PRO	C-O	5.05	1.28	1.23
1	H	319	ASP	CG-OD2	5.05	1.34	1.25
1	F	740	LEU	C-O	-5.05	1.17	1.23
1	M	797	GLU	CD-OE2	5.05	1.34	1.25
1	M	740	LEU	C-O	-5.04	1.17	1.23
1	J	256	VAL	CA-C	-5.04	1.46	1.52
1	J	797	GLU	CD-OE2	5.04	1.34	1.25
1	O	740	LEU	C-O	-5.04	1.17	1.23
1	C	740	LEU	C-O	-5.04	1.17	1.23
1	E	319	ASP	CG-OD2	5.04	1.34	1.25
1	E	256	VAL	CA-C	-5.04	1.46	1.52
1	A	319	ASP	CG-OD2	5.03	1.34	1.25
1	N	797	GLU	CD-OE2	5.03	1.34	1.25
1	N	319	ASP	CG-OD2	5.03	1.34	1.25
1	O	319	ASP	CG-OD2	5.03	1.34	1.25
1	C	277	GLU	CD-OE2	5.03	1.34	1.25
1	B	70	PRO	C-O	5.03	1.28	1.23
1	F	797	GLU	CD-OE2	5.03	1.34	1.25
1	G	797	GLU	CD-OE2	5.03	1.34	1.25
1	J	288	ARG	CA-C	-5.03	1.46	1.52
1	J	319	ASP	CG-OD2	5.03	1.34	1.25
1	I	277	GLU	CD-OE2	5.03	1.34	1.25
1	K	319	ASP	CG-OD2	5.03	1.34	1.25
1	L	740	LEU	C-O	-5.03	1.17	1.23
1	B	319	ASP	CG-OD2	5.02	1.34	1.25
1	C	256	VAL	CA-C	-5.02	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	825	CYS	CA-C	-5.02	1.48	1.53
1	A	797	GLU	CD-OE2	5.02	1.34	1.25
1	O	797	GLU	CD-OE2	5.02	1.34	1.25
1	G	319	ASP	CG-OD2	5.02	1.34	1.25
1	H	797	GLU	CD-OE2	5.02	1.34	1.25
1	B	797	GLU	CD-OE2	5.01	1.34	1.25
1	D	1019	VAL	CA-CB	-5.01	1.48	1.54
1	F	319	ASP	CG-OD2	5.01	1.34	1.25
1	I	797	GLU	CD-OE2	5.01	1.34	1.25
1	P	797	GLU	CD-OE2	5.01	1.34	1.25
1	O	508	GLU	CD-OE2	5.01	1.34	1.25
1	K	797	GLU	CD-OE2	5.01	1.34	1.25
1	E	797	GLU	CD-OE2	5.01	1.34	1.25
1	I	319	ASP	CG-OD2	5.01	1.34	1.25
1	J	740	LEU	C-O	-5.01	1.17	1.23
1	M	319	ASP	CG-OD2	5.01	1.34	1.25

All (2876) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	571	VAL	CB-CA-C	-10.10	95.27	110.82
1	L	571	VAL	CB-CA-C	-10.10	95.27	110.82
1	F	571	VAL	CB-CA-C	-10.09	95.28	110.82
1	E	571	VAL	CB-CA-C	-10.09	95.28	110.82
1	M	571	VAL	CB-CA-C	-10.08	95.29	110.82
1	C	571	VAL	CB-CA-C	-10.08	95.30	110.82
1	A	571	VAL	CB-CA-C	-10.08	95.30	110.82
1	O	571	VAL	CB-CA-C	-10.08	95.30	110.82
1	H	571	VAL	CB-CA-C	-10.07	95.31	110.82
1	K	571	VAL	CB-CA-C	-10.07	95.31	110.82
1	G	571	VAL	CB-CA-C	-10.07	95.31	110.82
1	I	571	VAL	CB-CA-C	-10.07	95.32	110.82
1	B	571	VAL	CB-CA-C	-10.06	95.32	110.82
1	D	571	VAL	CB-CA-C	-10.06	95.32	110.82
1	N	571	VAL	CB-CA-C	-10.05	95.35	110.82
1	J	571	VAL	CB-CA-C	-10.04	95.35	110.82
1	J	95	TYR	N-CA-C	9.55	121.69	111.28
1	D	95	TYR	N-CA-C	9.55	121.69	111.28
1	M	95	TYR	N-CA-C	9.54	121.68	111.28
1	E	95	TYR	N-CA-C	9.54	121.67	111.28
1	K	95	TYR	N-CA-C	9.53	121.67	111.28
1	L	95	TYR	N-CA-C	9.52	121.66	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	95	TYR	N-CA-C	9.52	121.65	111.28
1	G	95	TYR	N-CA-C	9.52	121.65	111.28
1	A	95	TYR	N-CA-C	9.51	121.65	111.28
1	O	95	TYR	N-CA-C	9.51	121.64	111.28
1	F	95	TYR	N-CA-C	9.50	121.64	111.28
1	H	95	TYR	N-CA-C	9.50	121.63	111.28
1	P	95	TYR	N-CA-C	9.50	121.63	111.28
1	B	95	TYR	N-CA-C	9.49	121.62	111.28
1	C	95	TYR	N-CA-C	9.48	121.61	111.28
1	N	95	TYR	N-CA-C	9.47	121.61	111.28
1	D	249	GLU	N-CA-CB	9.25	124.13	110.35
1	K	249	GLU	N-CA-CB	9.25	124.13	110.35
1	E	249	GLU	N-CA-CB	9.25	124.13	110.35
1	A	249	GLU	N-CA-CB	9.24	124.12	110.35
1	B	249	GLU	N-CA-CB	9.24	124.11	110.35
1	F	249	GLU	N-CA-CB	9.24	124.11	110.35
1	O	249	GLU	N-CA-CB	9.24	124.11	110.35
1	G	249	GLU	N-CA-CB	9.23	124.10	110.35
1	N	249	GLU	N-CA-CB	9.22	124.09	110.35
1	C	249	GLU	N-CA-CB	9.22	124.08	110.35
1	L	249	GLU	N-CA-CB	9.22	124.08	110.35
1	P	249	GLU	N-CA-CB	9.22	124.08	110.35
1	M	249	GLU	N-CA-CB	9.21	124.08	110.35
1	H	249	GLU	N-CA-CB	9.20	124.06	110.35
1	I	249	GLU	N-CA-CB	9.20	124.06	110.35
1	J	249	GLU	N-CA-CB	9.19	124.04	110.35
1	K	1018	LEU	CB-CA-C	-8.90	91.31	110.45
1	D	1018	LEU	CB-CA-C	-8.90	91.31	110.45
1	E	1018	LEU	CB-CA-C	-8.89	91.33	110.45
1	C	1018	LEU	CB-CA-C	-8.89	91.34	110.45
1	L	1018	LEU	CB-CA-C	-8.89	91.34	110.45
1	A	1018	LEU	CB-CA-C	-8.88	91.35	110.45
1	F	1018	LEU	CB-CA-C	-8.89	91.35	110.45
1	P	1018	LEU	CB-CA-C	-8.89	91.35	110.45
1	M	1018	LEU	CB-CA-C	-8.88	91.35	110.45
1	O	1018	LEU	CB-CA-C	-8.88	91.35	110.45
1	B	1018	LEU	CB-CA-C	-8.88	91.35	110.45
1	H	1018	LEU	CB-CA-C	-8.88	91.35	110.45
1	G	1018	LEU	CB-CA-C	-8.88	91.36	110.45
1	I	1018	LEU	CB-CA-C	-8.88	91.37	110.45
1	J	1018	LEU	CB-CA-C	-8.87	91.37	110.45
1	N	1018	LEU	CB-CA-C	-8.86	91.41	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	363	HIS	CA-CB-CG	-8.83	104.97	113.80
1	G	363	HIS	CA-CB-CG	-8.81	104.99	113.80
1	F	363	HIS	CA-CB-CG	-8.81	104.99	113.80
1	C	363	HIS	CA-CB-CG	-8.80	105.00	113.80
1	A	363	HIS	CA-CB-CG	-8.79	105.01	113.80
1	B	363	HIS	CA-CB-CG	-8.79	105.01	113.80
1	H	363	HIS	CA-CB-CG	-8.78	105.02	113.80
1	P	363	HIS	CA-CB-CG	-8.78	105.02	113.80
1	N	363	HIS	CA-CB-CG	-8.78	105.02	113.80
1	K	363	HIS	CA-CB-CG	-8.78	105.03	113.80
1	J	363	HIS	CA-CB-CG	-8.77	105.03	113.80
1	L	363	HIS	CA-CB-CG	-8.77	105.03	113.80
1	O	363	HIS	CA-CB-CG	-8.77	105.03	113.80
1	M	363	HIS	CA-CB-CG	-8.76	105.04	113.80
1	E	363	HIS	CA-CB-CG	-8.74	105.06	113.80
1	D	363	HIS	CA-CB-CG	-8.73	105.07	113.80
1	K	949	HIS	CA-CB-CG	-8.50	105.30	113.80
1	G	949	HIS	CA-CB-CG	-8.49	105.31	113.80
1	O	949	HIS	CA-CB-CG	-8.48	105.32	113.80
1	D	949	HIS	CA-CB-CG	-8.48	105.32	113.80
1	B	949	HIS	CA-CB-CG	-8.47	105.33	113.80
1	E	949	HIS	CA-CB-CG	-8.47	105.33	113.80
1	A	949	HIS	CA-CB-CG	-8.47	105.33	113.80
1	J	949	HIS	CA-CB-CG	-8.47	105.33	113.80
1	F	949	HIS	CA-CB-CG	-8.46	105.34	113.80
1	M	949	HIS	CA-CB-CG	-8.46	105.33	113.80
1	J	612	THR	CA-C-N	8.46	128.47	119.76
1	J	612	THR	C-N-CA	8.46	128.47	119.76
1	N	949	HIS	CA-CB-CG	-8.46	105.34	113.80
1	C	949	HIS	CA-CB-CG	-8.46	105.34	113.80
1	H	949	HIS	CA-CB-CG	-8.46	105.34	113.80
1	E	612	THR	CA-C-N	8.45	128.46	119.76
1	E	612	THR	C-N-CA	8.45	128.46	119.76
1	I	949	HIS	CA-CB-CG	-8.45	105.35	113.80
1	L	949	HIS	CA-CB-CG	-8.45	105.35	113.80
1	M	612	THR	CA-C-N	8.44	128.45	119.76
1	M	612	THR	C-N-CA	8.44	128.45	119.76
1	H	612	THR	CA-C-N	8.42	128.44	119.76
1	H	612	THR	C-N-CA	8.42	128.44	119.76
1	P	949	HIS	CA-CB-CG	-8.42	105.38	113.80
1	B	612	THR	CA-C-N	8.42	128.43	119.76
1	B	612	THR	C-N-CA	8.42	128.43	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	166	ARG	N-CA-CB	8.41	123.06	110.53
1	C	612	THR	CA-C-N	8.41	128.42	119.76
1	C	612	THR	C-N-CA	8.41	128.42	119.76
1	I	612	THR	CA-C-N	8.41	128.42	119.76
1	I	612	THR	C-N-CA	8.41	128.42	119.76
1	N	612	THR	CA-C-N	8.41	128.42	119.76
1	N	612	THR	C-N-CA	8.41	128.42	119.76
1	E	166	ARG	N-CA-CB	8.40	123.05	110.53
1	M	63	PHE	CA-C-N	8.40	128.05	119.56
1	M	63	PHE	C-N-CA	8.40	128.05	119.56
1	G	612	THR	CA-C-N	8.40	128.41	119.76
1	G	612	THR	C-N-CA	8.40	128.41	119.76
1	J	166	ARG	N-CA-CB	8.40	123.05	110.53
1	A	612	THR	CA-C-N	8.39	128.41	119.76
1	A	612	THR	C-N-CA	8.39	128.41	119.76
1	C	166	ARG	N-CA-CB	8.39	123.04	110.53
1	D	63	PHE	CA-C-N	8.39	128.04	119.56
1	D	63	PHE	C-N-CA	8.39	128.04	119.56
1	D	612	THR	CA-C-N	8.39	128.41	119.76
1	D	612	THR	C-N-CA	8.39	128.41	119.76
1	G	166	ARG	N-CA-CB	8.39	123.04	110.53
1	L	166	ARG	N-CA-CB	8.39	123.04	110.53
1	N	166	ARG	N-CA-CB	8.39	123.03	110.53
1	O	63	PHE	CA-C-N	8.39	128.03	119.56
1	O	63	PHE	C-N-CA	8.39	128.03	119.56
1	O	612	THR	CA-C-N	8.39	128.40	119.76
1	O	612	THR	C-N-CA	8.39	128.40	119.76
1	I	63	PHE	CA-C-N	8.39	128.03	119.56
1	I	63	PHE	C-N-CA	8.39	128.03	119.56
1	I	166	ARG	N-CA-CB	8.39	123.03	110.53
1	O	166	ARG	N-CA-CB	8.39	123.03	110.53
1	A	166	ARG	N-CA-CB	8.38	123.02	110.53
1	P	166	ARG	N-CA-CB	8.38	123.02	110.53
1	K	612	THR	CA-C-N	8.37	128.39	119.76
1	K	612	THR	C-N-CA	8.37	128.39	119.76
1	A	63	PHE	CA-C-N	8.37	128.02	119.56
1	A	63	PHE	C-N-CA	8.37	128.02	119.56
1	B	166	ARG	N-CA-CB	8.37	123.00	110.53
1	J	63	PHE	CA-C-N	8.37	128.02	119.56
1	J	63	PHE	C-N-CA	8.37	128.02	119.56
1	L	612	THR	CA-C-N	8.37	128.38	119.76
1	L	612	THR	C-N-CA	8.37	128.38	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	166	ARG	N-CA-CB	8.37	123.00	110.53
1	L	63	PHE	CA-C-N	8.37	128.01	119.56
1	L	63	PHE	C-N-CA	8.37	128.01	119.56
1	F	166	ARG	N-CA-CB	8.36	122.99	110.53
1	H	63	PHE	CA-C-N	8.36	128.01	119.56
1	H	63	PHE	C-N-CA	8.36	128.01	119.56
1	N	63	PHE	CA-C-N	8.36	128.00	119.56
1	N	63	PHE	C-N-CA	8.36	128.00	119.56
1	F	612	THR	CA-C-N	8.35	128.36	119.76
1	F	612	THR	C-N-CA	8.35	128.36	119.76
1	M	166	ARG	N-CA-CB	8.35	122.97	110.53
1	P	612	THR	CA-C-N	8.35	128.36	119.76
1	P	612	THR	C-N-CA	8.35	128.36	119.76
1	E	63	PHE	CA-C-N	8.35	127.99	119.56
1	E	63	PHE	C-N-CA	8.35	127.99	119.56
1	C	63	PHE	CA-C-N	8.35	127.99	119.56
1	C	63	PHE	C-N-CA	8.35	127.99	119.56
1	D	166	ARG	N-CA-CB	8.35	122.96	110.53
1	B	63	PHE	CA-C-N	8.34	127.99	119.56
1	B	63	PHE	C-N-CA	8.34	127.99	119.56
1	K	63	PHE	CA-C-N	8.34	127.98	119.56
1	K	63	PHE	C-N-CA	8.34	127.98	119.56
1	F	63	PHE	CA-C-N	8.32	127.96	119.56
1	F	63	PHE	C-N-CA	8.32	127.96	119.56
1	G	63	PHE	CA-C-N	8.31	127.95	119.56
1	G	63	PHE	C-N-CA	8.31	127.95	119.56
1	P	63	PHE	CA-C-N	8.30	127.95	119.56
1	P	63	PHE	C-N-CA	8.30	127.95	119.56
1	C	181	GLU	N-CA-C	8.23	121.69	109.59
1	D	181	GLU	N-CA-C	8.23	121.69	109.59
1	H	181	GLU	N-CA-C	8.22	121.68	109.59
1	B	181	GLU	N-CA-C	8.22	121.68	109.59
1	E	181	GLU	N-CA-C	8.22	121.67	109.59
1	J	181	GLU	N-CA-C	8.22	121.67	109.59
1	I	181	GLU	N-CA-C	8.21	121.67	109.59
1	K	181	GLU	N-CA-C	8.21	121.66	109.59
1	A	181	GLU	N-CA-C	8.21	121.66	109.59
1	O	181	GLU	N-CA-C	8.20	121.65	109.59
1	M	181	GLU	N-CA-C	8.20	121.65	109.59
1	N	181	GLU	N-CA-C	8.20	121.65	109.59
1	P	181	GLU	N-CA-C	8.20	121.64	109.59
1	L	181	GLU	N-CA-C	8.20	121.64	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	181	GLU	N-CA-C	8.18	121.61	109.59
1	G	181	GLU	N-CA-C	8.18	121.62	109.59
1	K	113	PHE	CA-CB-CG	-8.16	105.64	113.80
1	I	113	PHE	CA-CB-CG	-8.16	105.64	113.80
1	M	113	PHE	CA-CB-CG	-8.16	105.64	113.80
1	E	113	PHE	CA-CB-CG	-8.15	105.65	113.80
1	B	113	PHE	CA-CB-CG	-8.15	105.65	113.80
1	K	210	ARG	CD-NE-CZ	8.15	135.81	124.40
1	H	113	PHE	CA-CB-CG	-8.15	105.65	113.80
1	L	210	ARG	CD-NE-CZ	8.15	135.81	124.40
1	I	210	ARG	CD-NE-CZ	8.15	135.80	124.40
1	H	210	ARG	CD-NE-CZ	8.14	135.80	124.40
1	F	113	PHE	CA-CB-CG	-8.14	105.66	113.80
1	O	210	ARG	CD-NE-CZ	8.14	135.79	124.40
1	G	113	PHE	CA-CB-CG	-8.13	105.67	113.80
1	N	210	ARG	CD-NE-CZ	8.13	135.79	124.40
1	C	113	PHE	CA-CB-CG	-8.13	105.67	113.80
1	C	210	ARG	CD-NE-CZ	8.13	135.78	124.40
1	F	210	ARG	CD-NE-CZ	8.13	135.78	124.40
1	L	113	PHE	CA-CB-CG	-8.13	105.67	113.80
1	A	210	ARG	CD-NE-CZ	8.13	135.78	124.40
1	A	113	PHE	CA-CB-CG	-8.12	105.67	113.80
1	B	210	ARG	CD-NE-CZ	8.12	135.77	124.40
1	P	210	ARG	CD-NE-CZ	8.12	135.77	124.40
1	D	113	PHE	CA-CB-CG	-8.12	105.68	113.80
1	D	210	ARG	CD-NE-CZ	8.12	135.77	124.40
1	G	210	ARG	CD-NE-CZ	8.12	135.76	124.40
1	E	210	ARG	CD-NE-CZ	8.11	135.76	124.40
1	J	210	ARG	CD-NE-CZ	8.11	135.75	124.40
1	M	210	ARG	CD-NE-CZ	8.11	135.76	124.40
1	J	113	PHE	CA-CB-CG	-8.10	105.70	113.80
1	N	113	PHE	CA-CB-CG	-8.10	105.70	113.80
1	P	113	PHE	CA-CB-CG	-8.10	105.70	113.80
1	L	306	PRO	N-CA-CB	8.10	107.92	102.25
1	O	113	PHE	CA-CB-CG	-8.10	105.70	113.80
1	M	306	PRO	N-CA-CB	8.09	107.92	102.25
1	B	114	VAL	N-CA-CB	-8.09	99.89	111.21
1	E	114	VAL	N-CA-CB	-8.08	99.90	111.21
1	G	447	ASP	N-CA-C	8.08	123.35	113.17
1	H	114	VAL	N-CA-CB	-8.08	99.90	111.21
1	P	114	VAL	N-CA-CB	-8.08	99.90	111.21
1	P	306	PRO	N-CA-CB	8.08	107.91	102.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	306	PRO	N-CA-CB	8.08	107.91	102.25
1	J	447	ASP	N-CA-C	8.08	123.35	113.17
1	E	306	PRO	N-CA-CB	8.07	107.90	102.25
1	H	447	ASP	N-CA-C	8.07	123.34	113.17
1	N	114	VAL	N-CA-CB	-8.07	99.91	111.21
1	O	114	VAL	N-CA-CB	-8.07	99.91	111.21
1	D	447	ASP	N-CA-C	8.07	123.33	113.17
1	D	114	VAL	N-CA-CB	-8.06	99.92	111.21
1	I	447	ASP	N-CA-C	8.06	123.33	113.17
1	J	114	VAL	N-CA-CB	-8.06	99.92	111.21
1	K	114	VAL	N-CA-CB	-8.06	99.92	111.21
1	K	447	ASP	N-CA-C	8.06	123.33	113.17
1	N	306	PRO	N-CA-CB	8.06	107.89	102.25
1	M	447	ASP	N-CA-C	8.06	123.33	113.17
1	A	114	VAL	N-CA-CB	-8.06	99.93	111.21
1	F	447	ASP	N-CA-C	8.06	123.32	113.17
1	I	114	VAL	N-CA-CB	-8.06	99.93	111.21
1	L	447	ASP	N-CA-C	8.06	123.32	113.17
1	O	306	PRO	N-CA-CB	8.06	107.89	102.25
1	F	114	VAL	N-CA-CB	-8.05	99.94	111.21
1	H	306	PRO	N-CA-CB	8.05	107.88	102.25
1	I	306	PRO	N-CA-CB	8.05	107.88	102.25
1	B	447	ASP	N-CA-C	8.05	123.31	113.17
1	C	306	PRO	N-CA-CB	8.04	107.88	102.25
1	G	114	VAL	N-CA-CB	-8.04	99.95	111.21
1	K	306	PRO	N-CA-CB	8.04	107.88	102.25
1	O	447	ASP	N-CA-C	8.04	123.31	113.17
1	E	447	ASP	N-CA-C	8.04	123.30	113.17
1	C	114	VAL	N-CA-CB	-8.04	99.96	111.21
1	N	447	ASP	N-CA-C	8.04	123.30	113.17
1	A	447	ASP	N-CA-C	8.04	123.30	113.17
1	A	306	PRO	N-CA-CB	8.03	107.87	102.25
1	L	114	VAL	N-CA-CB	-8.03	99.96	111.21
1	M	114	VAL	N-CA-CB	-8.03	99.97	111.21
1	P	447	ASP	N-CA-C	8.03	123.29	113.17
1	J	306	PRO	N-CA-CB	8.03	107.87	102.25
1	C	448	ARG	NE-CZ-NH2	-8.03	111.98	119.20
1	G	306	PRO	N-CA-CB	8.02	107.87	102.25
1	C	447	ASP	N-CA-C	8.01	123.26	113.17
1	D	306	PRO	N-CA-CB	8.01	107.86	102.25
1	B	306	PRO	N-CA-CB	8.01	107.86	102.25
1	G	448	ARG	NE-CZ-NH2	-8.00	112.00	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	448	ARG	NE-CZ-NH2	-7.99	112.01	119.20
1	L	448	ARG	NE-CZ-NH2	-7.99	112.01	119.20
1	H	448	ARG	NE-CZ-NH2	-7.98	112.02	119.20
1	N	448	ARG	NE-CZ-NH2	-7.97	112.02	119.20
1	I	448	ARG	NE-CZ-NH2	-7.97	112.03	119.20
1	A	448	ARG	NE-CZ-NH2	-7.97	112.03	119.20
1	F	448	ARG	NE-CZ-NH2	-7.97	112.03	119.20
1	B	448	ARG	NE-CZ-NH2	-7.96	112.03	119.20
1	K	448	ARG	NE-CZ-NH2	-7.96	112.03	119.20
1	M	448	ARG	NE-CZ-NH2	-7.96	112.04	119.20
1	E	448	ARG	NE-CZ-NH2	-7.95	112.04	119.20
1	O	448	ARG	NE-CZ-NH2	-7.95	112.05	119.20
1	J	448	ARG	NE-CZ-NH2	-7.94	112.05	119.20
1	P	448	ARG	NE-CZ-NH2	-7.94	112.06	119.20
1	I	210	ARG	NE-CZ-NH1	7.84	129.34	121.50
1	L	210	ARG	NE-CZ-NH1	7.84	129.34	121.50
1	J	210	ARG	NE-CZ-NH1	7.83	129.33	121.50
1	M	210	ARG	NE-CZ-NH1	7.82	129.31	121.50
1	H	881	ARG	NE-CZ-NH2	-7.81	112.17	119.20
1	J	881	ARG	NE-CZ-NH2	-7.81	112.17	119.20
1	K	881	ARG	NE-CZ-NH2	-7.81	112.17	119.20
1	G	210	ARG	NE-CZ-NH1	7.80	129.30	121.50
1	P	210	ARG	NE-CZ-NH1	7.80	129.30	121.50
1	D	210	ARG	NE-CZ-NH1	7.80	129.30	121.50
1	A	210	ARG	NE-CZ-NH1	7.80	129.30	121.50
1	H	210	ARG	NE-CZ-NH1	7.79	129.29	121.50
1	L	881	ARG	NE-CZ-NH2	-7.79	112.19	119.20
1	C	210	ARG	NE-CZ-NH1	7.79	129.29	121.50
1	E	210	ARG	NE-CZ-NH1	7.79	129.29	121.50
1	C	881	ARG	NE-CZ-NH2	-7.78	112.19	119.20
1	N	881	ARG	NE-CZ-NH2	-7.78	112.20	119.20
1	P	881	ARG	NE-CZ-NH2	-7.78	112.20	119.20
1	F	881	ARG	NE-CZ-NH2	-7.78	112.20	119.20
1	G	881	ARG	NE-CZ-NH2	-7.78	112.20	119.20
1	B	881	ARG	NE-CZ-NH2	-7.77	112.20	119.20
1	F	210	ARG	NE-CZ-NH1	7.77	129.27	121.50
1	E	881	ARG	NE-CZ-NH2	-7.76	112.21	119.20
1	N	210	ARG	NE-CZ-NH1	7.76	129.26	121.50
1	A	881	ARG	NE-CZ-NH2	-7.76	112.22	119.20
1	K	210	ARG	NE-CZ-NH1	7.76	129.26	121.50
1	O	210	ARG	NE-CZ-NH1	7.75	129.25	121.50
1	M	881	ARG	NE-CZ-NH2	-7.75	112.22	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	ARG	NE-CZ-NH1	7.75	129.25	121.50
1	J	4	THR	N-CA-C	-7.74	103.84	113.28
1	D	881	ARG	NE-CZ-NH2	-7.73	112.24	119.20
1	I	881	ARG	NE-CZ-NH2	-7.73	112.24	119.20
1	O	881	ARG	NE-CZ-NH2	-7.73	112.24	119.20
1	F	4	THR	N-CA-C	-7.72	103.86	113.28
1	L	4	THR	N-CA-C	-7.71	103.87	113.28
1	M	4	THR	N-CA-C	-7.71	103.87	113.28
1	C	4	THR	N-CA-C	-7.71	103.87	113.28
1	H	4	THR	N-CA-C	-7.71	103.87	113.28
1	D	4	THR	N-CA-C	-7.71	103.88	113.28
1	I	4	THR	N-CA-C	-7.71	103.88	113.28
1	H	570	TRP	N-CA-C	7.70	119.58	111.03
1	P	4	THR	N-CA-C	-7.70	103.89	113.28
1	A	4	THR	N-CA-C	-7.70	103.89	113.28
1	P	570	TRP	N-CA-C	7.69	119.57	111.03
1	E	4	THR	N-CA-C	-7.69	103.90	113.28
1	O	570	TRP	N-CA-C	7.69	119.56	111.03
1	B	570	TRP	N-CA-C	7.69	119.56	111.03
1	G	4	THR	N-CA-C	-7.69	103.90	113.28
1	E	570	TRP	N-CA-C	7.69	119.56	111.03
1	L	570	TRP	N-CA-C	7.68	119.56	111.03
1	N	4	THR	N-CA-C	-7.68	103.91	113.28
1	O	4	THR	N-CA-C	-7.68	103.91	113.28
1	M	570	TRP	N-CA-C	7.67	119.55	111.03
1	K	4	THR	N-CA-C	-7.67	103.92	113.28
1	K	570	TRP	N-CA-C	7.66	119.53	111.03
1	N	570	TRP	N-CA-C	7.66	119.53	111.03
1	F	570	TRP	N-CA-C	7.66	119.53	111.03
1	I	570	TRP	N-CA-C	7.65	119.53	111.03
1	B	4	THR	N-CA-C	-7.65	103.95	113.28
1	J	570	TRP	N-CA-C	7.64	119.52	111.03
1	G	570	TRP	N-CA-C	7.64	119.51	111.03
1	D	570	TRP	N-CA-C	7.63	119.50	111.03
1	C	570	TRP	N-CA-C	7.62	119.49	111.03
1	A	570	TRP	N-CA-C	7.61	119.47	111.03
1	N	980	GLU	N-CA-C	7.56	120.18	111.11
1	E	980	GLU	N-CA-C	7.55	120.18	111.11
1	G	980	GLU	N-CA-C	7.55	120.17	111.11
1	O	980	GLU	N-CA-C	7.55	120.17	111.11
1	L	980	GLU	N-CA-C	7.55	120.17	111.11
1	A	980	GLU	N-CA-C	7.54	120.16	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	980	GLU	N-CA-C	7.53	120.14	111.11
1	K	980	GLU	N-CA-C	7.53	120.15	111.11
1	M	980	GLU	N-CA-C	7.53	120.14	111.11
1	B	360	HIS	CA-CB-CG	-7.53	106.27	113.80
1	I	980	GLU	N-CA-C	7.53	120.14	111.11
1	P	980	GLU	N-CA-C	7.53	120.14	111.11
1	J	980	GLU	N-CA-C	7.53	120.14	111.11
1	B	980	GLU	N-CA-C	7.52	120.14	111.11
1	F	980	GLU	N-CA-C	7.52	120.14	111.11
1	H	360	HIS	CA-CB-CG	-7.52	106.28	113.80
1	D	980	GLU	N-CA-C	7.52	120.14	111.11
1	C	980	GLU	N-CA-C	7.52	120.13	111.11
1	A	360	HIS	CA-CB-CG	-7.51	106.28	113.80
1	C	360	HIS	CA-CB-CG	-7.50	106.30	113.80
1	L	360	HIS	CA-CB-CG	-7.50	106.30	113.80
1	P	360	HIS	CA-CB-CG	-7.50	106.30	113.80
1	M	360	HIS	CA-CB-CG	-7.50	106.30	113.80
1	J	360	HIS	CA-CB-CG	-7.49	106.31	113.80
1	E	360	HIS	CA-CB-CG	-7.49	106.31	113.80
1	K	360	HIS	CA-CB-CG	-7.49	106.31	113.80
1	B	84	VAL	N-CA-CB	-7.48	99.87	112.44
1	G	84	VAL	N-CA-CB	-7.48	99.87	112.44
1	G	360	HIS	CA-CB-CG	-7.48	106.32	113.80
1	D	360	HIS	CA-CB-CG	-7.47	106.33	113.80
1	O	84	VAL	N-CA-CB	-7.47	99.89	112.44
1	F	84	VAL	N-CA-CB	-7.47	99.89	112.44
1	C	84	VAL	N-CA-CB	-7.47	99.89	112.44
1	I	360	HIS	CA-CB-CG	-7.46	106.34	113.80
1	K	84	VAL	N-CA-CB	-7.46	99.90	112.44
1	P	84	VAL	N-CA-CB	-7.46	99.90	112.44
1	N	360	HIS	CA-CB-CG	-7.46	106.34	113.80
1	A	84	VAL	N-CA-CB	-7.46	99.91	112.44
1	E	84	VAL	N-CA-CB	-7.46	99.91	112.44
1	F	360	HIS	CA-CB-CG	-7.46	106.34	113.80
1	L	84	VAL	N-CA-CB	-7.46	99.91	112.44
1	D	84	VAL	N-CA-CB	-7.45	99.92	112.44
1	I	84	VAL	N-CA-CB	-7.45	99.92	112.44
1	M	84	VAL	N-CA-CB	-7.45	99.92	112.44
1	H	84	VAL	N-CA-CB	-7.45	99.93	112.44
1	N	84	VAL	N-CA-CB	-7.45	99.93	112.44
1	J	84	VAL	N-CA-CB	-7.44	99.94	112.44
1	O	360	HIS	CA-CB-CG	-7.44	106.36	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	610	ASP	CA-CB-CG	7.43	120.03	112.60
1	P	610	ASP	CA-CB-CG	7.42	120.02	112.60
1	L	1004	SER	N-CA-CB	7.42	120.86	110.17
1	N	1004	SER	N-CA-CB	7.42	120.86	110.17
1	F	610	ASP	CA-CB-CG	7.42	120.02	112.60
1	E	938	ARG	NE-CZ-NH2	-7.41	112.53	119.20
1	L	610	ASP	CA-CB-CG	7.41	120.01	112.60
1	N	610	ASP	CA-CB-CG	7.41	120.01	112.60
1	A	938	ARG	NE-CZ-NH2	-7.41	112.53	119.20
1	F	1004	SER	N-CA-CB	7.41	120.84	110.17
1	M	938	ARG	NE-CZ-NH2	-7.41	112.53	119.20
1	B	610	ASP	CA-CB-CG	7.41	120.00	112.60
1	G	610	ASP	CA-CB-CG	7.40	120.00	112.60
1	H	610	ASP	CA-CB-CG	7.40	120.00	112.60
1	M	209	PHE	CA-CB-CG	-7.40	106.40	113.80
1	A	1004	SER	N-CA-CB	7.40	120.82	110.17
1	O	1004	SER	N-CA-CB	7.40	120.82	110.17
1	F	209	PHE	CA-CB-CG	-7.39	106.41	113.80
1	F	938	ARG	NE-CZ-NH2	-7.39	112.55	119.20
1	P	1004	SER	N-CA-CB	7.39	120.81	110.17
1	D	610	ASP	CA-CB-CG	7.39	119.99	112.60
1	D	938	ARG	NE-CZ-NH2	-7.39	112.55	119.20
1	E	1004	SER	N-CA-CB	7.39	120.81	110.17
1	B	1004	SER	N-CA-CB	7.39	120.81	110.17
1	I	938	ARG	NE-CZ-NH2	-7.38	112.55	119.20
1	K	610	ASP	CA-CB-CG	7.38	119.98	112.60
1	L	209	PHE	CA-CB-CG	-7.38	106.42	113.80
1	H	209	PHE	CA-CB-CG	-7.38	106.42	113.80
1	O	938	ARG	NE-CZ-NH2	-7.38	112.56	119.20
1	I	1004	SER	N-CA-CB	7.38	120.79	110.17
1	K	1004	SER	N-CA-CB	7.38	120.80	110.17
1	A	610	ASP	CA-CB-CG	7.38	119.98	112.60
1	B	209	PHE	CA-CB-CG	-7.38	106.42	113.80
1	D	1004	SER	N-CA-CB	7.38	120.79	110.17
1	G	1004	SER	N-CA-CB	7.38	120.79	110.17
1	I	610	ASP	CA-CB-CG	7.38	119.97	112.60
1	E	610	ASP	CA-CB-CG	7.37	119.97	112.60
1	J	610	ASP	CA-CB-CG	7.37	119.97	112.60
1	P	209	PHE	CA-CB-CG	-7.37	106.43	113.80
1	C	209	PHE	CA-CB-CG	-7.37	106.43	113.80
1	M	610	ASP	CA-CB-CG	7.37	119.97	112.60
1	O	209	PHE	CA-CB-CG	-7.37	106.43	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	610	ASP	CA-CB-CG	7.37	119.97	112.60
1	J	938	ARG	NE-CZ-NH2	-7.37	112.57	119.20
1	L	46	ARG	CA-CB-CG	-7.36	99.37	114.10
1	H	938	ARG	NE-CZ-NH2	-7.36	112.58	119.20
1	I	46	ARG	CA-CB-CG	-7.36	99.38	114.10
1	G	938	ARG	NE-CZ-NH2	-7.36	112.58	119.20
1	O	46	ARG	CA-CB-CG	-7.36	99.39	114.10
1	C	938	ARG	NE-CZ-NH2	-7.35	112.58	119.20
1	P	938	ARG	NE-CZ-NH2	-7.35	112.58	119.20
1	A	209	PHE	CA-CB-CG	-7.35	106.45	113.80
1	I	209	PHE	CA-CB-CG	-7.35	106.45	113.80
1	M	46	ARG	CA-CB-CG	-7.35	99.39	114.10
1	H	46	ARG	CA-CB-CG	-7.35	99.40	114.10
1	C	1004	SER	N-CA-CB	7.35	120.84	110.04
1	G	46	ARG	CA-CB-CG	-7.35	99.41	114.10
1	N	209	PHE	CA-CB-CG	-7.35	106.45	113.80
1	B	46	ARG	CA-CB-CG	-7.34	99.41	114.10
1	K	938	ARG	NE-CZ-NH2	-7.34	112.59	119.20
1	N	938	ARG	NE-CZ-NH2	-7.34	112.59	119.20
1	K	209	PHE	CA-CB-CG	-7.34	106.46	113.80
1	H	1004	SER	N-CA-CB	7.34	120.83	110.04
1	A	46	ARG	CA-CB-CG	-7.34	99.42	114.10
1	E	46	ARG	CA-CB-CG	-7.34	99.43	114.10
1	J	46	ARG	CA-CB-CG	-7.34	99.43	114.10
1	J	209	PHE	CA-CB-CG	-7.34	106.46	113.80
1	J	1004	SER	N-CA-CB	7.34	120.82	110.04
1	P	46	ARG	CA-CB-CG	-7.34	99.43	114.10
1	C	46	ARG	CA-CB-CG	-7.33	99.43	114.10
1	M	1004	SER	N-CA-CB	7.33	120.82	110.04
1	F	46	ARG	CA-CB-CG	-7.33	99.44	114.10
1	N	46	ARG	CA-CB-CG	-7.33	99.44	114.10
1	D	46	ARG	CA-CB-CG	-7.32	99.45	114.10
1	B	938	ARG	NE-CZ-NH2	-7.32	112.61	119.20
1	D	209	PHE	CA-CB-CG	-7.32	106.48	113.80
1	E	209	PHE	CA-CB-CG	-7.32	106.48	113.80
1	G	209	PHE	CA-CB-CG	-7.31	106.49	113.80
1	K	46	ARG	CA-CB-CG	-7.31	99.48	114.10
1	L	938	ARG	NE-CZ-NH2	-7.30	112.63	119.20
1	I	448	ARG	N-CA-C	7.21	121.77	113.19
1	E	448	ARG	N-CA-C	7.18	121.74	113.19
1	D	448	ARG	N-CA-C	7.18	121.73	113.19
1	B	448	ARG	N-CA-C	7.17	121.73	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	802	ASP	CA-C-N	7.17	126.85	119.82
1	L	802	ASP	C-N-CA	7.17	126.85	119.82
1	B	802	ASP	CA-C-N	7.17	126.85	119.82
1	B	802	ASP	C-N-CA	7.17	126.85	119.82
1	G	448	ARG	N-CA-C	7.17	121.72	113.19
1	M	448	ARG	N-CA-C	7.17	121.72	113.19
1	J	802	ASP	CA-C-N	7.17	126.84	119.82
1	J	802	ASP	C-N-CA	7.17	126.84	119.82
1	A	448	ARG	N-CA-C	7.16	121.71	113.19
1	F	448	ARG	N-CA-C	7.15	121.70	113.19
1	C	448	ARG	N-CA-C	7.15	121.70	113.19
1	J	448	ARG	N-CA-C	7.15	121.70	113.19
1	O	448	ARG	N-CA-C	7.15	121.70	113.19
1	P	448	ARG	N-CA-C	7.15	121.69	113.19
1	L	448	ARG	N-CA-C	7.14	121.69	113.19
1	N	448	ARG	N-CA-C	7.14	121.69	113.19
1	I	802	ASP	CA-C-N	7.14	126.82	119.82
1	I	802	ASP	C-N-CA	7.14	126.82	119.82
1	K	448	ARG	N-CA-C	7.14	121.69	113.19
1	H	802	ASP	CA-C-N	7.14	126.82	119.82
1	H	802	ASP	C-N-CA	7.14	126.82	119.82
1	G	802	ASP	CA-C-N	7.14	126.81	119.82
1	G	802	ASP	C-N-CA	7.14	126.81	119.82
1	P	802	ASP	CA-C-N	7.14	126.81	119.82
1	P	802	ASP	C-N-CA	7.14	126.81	119.82
1	H	448	ARG	N-CA-C	7.14	121.68	113.19
1	A	802	ASP	CA-C-N	7.13	126.81	119.82
1	A	802	ASP	C-N-CA	7.13	126.81	119.82
1	O	802	ASP	CA-C-N	7.13	126.81	119.82
1	O	802	ASP	C-N-CA	7.13	126.81	119.82
1	C	802	ASP	CA-C-N	7.13	126.80	119.82
1	C	802	ASP	C-N-CA	7.13	126.80	119.82
1	E	802	ASP	CA-C-N	7.13	126.80	119.82
1	E	802	ASP	C-N-CA	7.13	126.80	119.82
1	K	802	ASP	CA-C-N	7.12	126.80	119.82
1	K	802	ASP	C-N-CA	7.12	126.80	119.82
1	M	802	ASP	CA-C-N	7.12	126.80	119.82
1	M	802	ASP	C-N-CA	7.12	126.80	119.82
1	N	802	ASP	CA-C-N	7.12	126.80	119.82
1	N	802	ASP	C-N-CA	7.12	126.80	119.82
1	F	802	ASP	CA-C-N	7.11	126.79	119.82
1	F	802	ASP	C-N-CA	7.11	126.79	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	802	ASP	CA-C-N	7.07	126.74	119.82
1	D	802	ASP	C-N-CA	7.07	126.74	119.82
1	N	614	HIS	N-CA-C	-7.02	100.95	110.36
1	M	614	HIS	N-CA-C	-7.01	100.96	110.36
1	A	233	ASP	CA-CB-CG	7.01	119.61	112.60
1	I	614	HIS	N-CA-C	-7.00	100.97	110.36
1	P	614	HIS	N-CA-C	-7.00	100.97	110.36
1	K	614	HIS	N-CA-C	-7.00	100.98	110.36
1	F	614	HIS	N-CA-C	-7.00	100.98	110.36
1	B	233	ASP	CA-CB-CG	7.00	119.60	112.60
1	I	77	ASP	N-CA-CB	7.00	120.33	110.04
1	C	614	HIS	N-CA-C	-7.00	100.99	110.36
1	D	614	HIS	N-CA-C	-6.99	100.99	110.36
1	K	233	ASP	CA-CB-CG	6.99	119.59	112.60
1	J	77	ASP	N-CA-CB	6.99	120.32	110.04
1	C	77	ASP	N-CA-CB	6.99	120.31	110.04
1	D	77	ASP	N-CA-CB	6.99	120.31	110.04
1	E	614	HIS	N-CA-C	-6.99	101.00	110.36
1	O	614	HIS	N-CA-C	-6.99	101.00	110.36
1	C	210	ARG	NE-CZ-NH2	-6.99	112.91	119.20
1	D	210	ARG	NE-CZ-NH2	-6.99	112.91	119.20
1	D	233	ASP	CA-CB-CG	6.99	119.58	112.60
1	F	77	ASP	N-CA-CB	6.99	120.31	110.04
1	J	614	HIS	N-CA-C	-6.99	101.00	110.36
1	A	614	HIS	N-CA-C	-6.98	101.00	110.36
1	J	210	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	M	77	ASP	N-CA-CB	6.98	120.30	110.04
1	G	614	HIS	N-CA-C	-6.98	101.01	110.36
1	H	614	HIS	N-CA-C	-6.98	101.01	110.36
1	L	614	HIS	N-CA-C	-6.98	101.00	110.36
1	H	233	ASP	CA-CB-CG	6.98	119.58	112.60
1	A	210	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	B	614	HIS	N-CA-C	-6.98	101.01	110.36
1	H	77	ASP	N-CA-CB	6.98	120.30	110.04
1	O	77	ASP	N-CA-CB	6.98	120.30	110.04
1	G	17	GLU	N-CA-CB	6.97	121.83	111.51
1	N	233	ASP	CA-CB-CG	6.97	119.57	112.60
1	A	77	ASP	N-CA-CB	6.97	120.29	110.04
1	G	77	ASP	N-CA-CB	6.97	120.29	110.04
1	L	233	ASP	CA-CB-CG	6.97	119.57	112.60
1	E	77	ASP	N-CA-CB	6.97	120.28	110.04
1	P	210	ARG	NE-CZ-NH2	-6.97	112.93	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	210	ARG	NE-CZ-NH2	-6.97	112.93	119.20
1	J	233	ASP	CA-CB-CG	6.97	119.57	112.60
1	C	233	ASP	CA-CB-CG	6.96	119.56	112.60
1	N	77	ASP	N-CA-CB	6.96	120.28	110.04
1	P	233	ASP	CA-CB-CG	6.96	119.56	112.60
1	G	210	ARG	NE-CZ-NH2	-6.96	112.94	119.20
1	I	233	ASP	CA-CB-CG	6.96	119.56	112.60
1	P	77	ASP	N-CA-CB	6.96	120.28	110.04
1	K	77	ASP	N-CA-CB	6.96	120.27	110.04
1	E	210	ARG	NE-CZ-NH2	-6.95	112.94	119.20
1	F	233	ASP	CA-CB-CG	6.95	119.55	112.60
1	B	77	ASP	N-CA-CB	6.95	120.25	110.04
1	E	233	ASP	CA-CB-CG	6.95	119.55	112.60
1	H	17	GLU	N-CA-CB	6.95	121.79	111.51
1	K	17	GLU	N-CA-CB	6.94	121.78	111.51
1	B	210	ARG	NE-CZ-NH2	-6.94	112.95	119.20
1	D	17	GLU	N-CA-CB	6.94	121.78	111.51
1	F	17	GLU	N-CA-CB	6.94	121.78	111.51
1	B	17	GLU	N-CA-CB	6.94	121.78	111.51
1	O	210	ARG	NE-CZ-NH2	-6.94	112.96	119.20
1	L	77	ASP	N-CA-CB	6.93	120.23	110.04
1	M	233	ASP	CA-CB-CG	6.93	119.53	112.60
1	O	17	GLU	N-CA-CB	6.93	121.77	111.51
1	P	17	GLU	N-CA-CB	6.93	121.77	111.51
1	M	17	GLU	N-CA-CB	6.93	121.77	111.51
1	M	210	ARG	NE-CZ-NH2	-6.93	112.96	119.20
1	A	17	GLU	N-CA-CB	6.93	121.77	111.51
1	J	17	GLU	N-CA-CB	6.93	121.77	111.51
1	L	210	ARG	NE-CZ-NH2	-6.93	112.96	119.20
1	G	233	ASP	CA-CB-CG	6.93	119.53	112.60
1	O	233	ASP	CA-CB-CG	6.93	119.53	112.60
1	N	17	GLU	N-CA-CB	6.92	121.76	111.51
1	N	210	ARG	NE-CZ-NH2	-6.92	112.97	119.20
1	L	17	GLU	N-CA-CB	6.92	121.76	111.51
1	C	17	GLU	N-CA-CB	6.92	121.75	111.51
1	I	17	GLU	N-CA-CB	6.92	121.75	111.51
1	I	210	ARG	NE-CZ-NH2	-6.92	112.98	119.20
1	K	210	ARG	NE-CZ-NH2	-6.90	112.99	119.20
1	G	395	HIS	CA-C-O	6.90	126.23	119.75
1	E	17	GLU	N-CA-CB	6.90	121.72	111.51
1	F	210	ARG	NE-CZ-NH2	-6.89	113.00	119.20
1	B	395	HIS	CA-C-O	6.87	126.21	119.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	395	HIS	CA-C-O	6.87	126.21	119.75
1	D	395	HIS	CA-C-O	6.87	126.20	119.75
1	J	395	HIS	CA-C-O	6.87	126.20	119.75
1	K	395	HIS	CA-C-O	6.86	126.20	119.75
1	L	395	HIS	CA-C-O	6.86	126.19	119.75
1	A	395	HIS	CA-C-O	6.83	126.17	119.75
1	P	395	HIS	CA-C-O	6.82	126.16	119.75
1	O	395	HIS	CA-C-O	6.82	126.16	119.75
1	C	395	HIS	CA-C-O	6.81	126.15	119.75
1	I	395	HIS	CA-C-O	6.80	126.15	119.75
1	H	395	HIS	CA-C-O	6.79	126.14	119.75
1	F	395	HIS	CA-C-O	6.79	126.13	119.75
1	N	395	HIS	CA-C-O	6.78	126.13	119.75
1	E	395	HIS	CA-C-O	6.75	126.10	119.75
1	J	739	HIS	CA-CB-CG	-6.72	107.08	113.80
1	L	739	HIS	CA-CB-CG	-6.72	107.08	113.80
1	F	739	HIS	CA-CB-CG	-6.71	107.09	113.80
1	L	938	ARG	CD-NE-CZ	6.71	133.80	124.40
1	I	739	HIS	CA-CB-CG	-6.71	107.09	113.80
1	N	739	HIS	CA-CB-CG	-6.71	107.09	113.80
1	G	739	HIS	CA-CB-CG	-6.71	107.09	113.80
1	B	938	ARG	CD-NE-CZ	6.71	133.79	124.40
1	K	938	ARG	CD-NE-CZ	6.71	133.79	124.40
1	K	739	HIS	CA-CB-CG	-6.70	107.10	113.80
1	B	739	HIS	CA-CB-CG	-6.70	107.10	113.80
1	N	938	ARG	CD-NE-CZ	6.70	133.78	124.40
1	O	739	HIS	CA-CB-CG	-6.70	107.10	113.80
1	A	739	HIS	CA-CB-CG	-6.70	107.10	113.80
1	C	739	HIS	CA-CB-CG	-6.70	107.10	113.80
1	A	938	ARG	CD-NE-CZ	6.69	133.77	124.40
1	C	938	ARG	CD-NE-CZ	6.69	133.77	124.40
1	E	739	HIS	CA-CB-CG	-6.69	107.11	113.80
1	D	739	HIS	CA-CB-CG	-6.69	107.11	113.80
1	G	938	ARG	CD-NE-CZ	6.69	133.76	124.40
1	H	739	HIS	CA-CB-CG	-6.68	107.11	113.80
1	N	147	ASN	CA-CB-CG	6.68	119.28	112.60
1	P	938	ARG	CD-NE-CZ	6.68	133.75	124.40
1	J	938	ARG	CD-NE-CZ	6.68	133.75	124.40
1	O	938	ARG	CD-NE-CZ	6.68	133.75	124.40
1	M	739	HIS	CA-CB-CG	-6.67	107.12	113.80
1	E	938	ARG	CD-NE-CZ	6.67	133.74	124.40
1	M	938	ARG	CD-NE-CZ	6.67	133.74	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	938	ARG	CD-NE-CZ	6.66	133.73	124.40
1	D	938	ARG	CD-NE-CZ	6.66	133.72	124.40
1	H	938	ARG	CD-NE-CZ	6.66	133.72	124.40
1	F	938	ARG	CD-NE-CZ	6.66	133.72	124.40
1	D	147	ASN	CA-CB-CG	6.65	119.25	112.60
1	P	739	HIS	CA-CB-CG	-6.64	107.16	113.80
1	I	147	ASN	CA-CB-CG	6.63	119.23	112.60
1	P	147	ASN	CA-CB-CG	6.62	119.22	112.60
1	O	147	ASN	CA-CB-CG	6.62	119.22	112.60
1	F	147	ASN	CA-CB-CG	6.62	119.22	112.60
1	H	147	ASN	CA-CB-CG	6.62	119.22	112.60
1	K	147	ASN	CA-CB-CG	6.61	119.21	112.60
1	E	147	ASN	CA-CB-CG	6.61	119.21	112.60
1	G	147	ASN	CA-CB-CG	6.61	119.21	112.60
1	L	147	ASN	CA-CB-CG	6.60	119.20	112.60
1	B	147	ASN	CA-CB-CG	6.60	119.20	112.60
1	M	147	ASN	CA-CB-CG	6.60	119.20	112.60
1	A	147	ASN	CA-CB-CG	6.59	119.19	112.60
1	C	147	ASN	CA-CB-CG	6.59	119.19	112.60
1	P	769	TRP	CB-CA-C	-6.58	96.36	109.33
1	B	769	TRP	CB-CA-C	-6.58	96.36	109.33
1	P	613	PRO	CB-CA-C	-6.58	102.97	111.46
1	I	769	TRP	CB-CA-C	-6.58	96.37	109.33
1	A	769	TRP	CB-CA-C	-6.58	96.38	109.33
1	E	613	PRO	CB-CA-C	-6.58	102.98	111.46
1	H	613	PRO	CB-CA-C	-6.58	102.98	111.46
1	J	769	TRP	CB-CA-C	-6.58	96.38	109.33
1	J	147	ASN	CA-CB-CG	6.57	119.17	112.60
1	I	613	PRO	CB-CA-C	-6.57	102.98	111.46
1	N	613	PRO	CB-CA-C	-6.57	102.99	111.46
1	O	769	TRP	CB-CA-C	-6.57	96.39	109.33
1	E	769	TRP	CB-CA-C	-6.56	96.40	109.33
1	G	769	TRP	CB-CA-C	-6.56	96.40	109.33
1	K	769	TRP	CB-CA-C	-6.56	96.40	109.33
1	D	613	PRO	CB-CA-C	-6.56	103.00	111.46
1	L	769	TRP	CB-CA-C	-6.56	96.41	109.33
1	D	769	TRP	CB-CA-C	-6.56	96.42	109.33
1	F	613	PRO	CB-CA-C	-6.56	103.00	111.46
1	J	613	PRO	CB-CA-C	-6.56	103.00	111.46
1	N	769	TRP	CB-CA-C	-6.56	96.41	109.33
1	A	613	PRO	CB-CA-C	-6.55	103.01	111.46
1	C	769	TRP	CB-CA-C	-6.55	96.42	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	769	TRP	CB-CA-C	-6.55	96.42	109.33
1	G	613	PRO	CB-CA-C	-6.55	103.00	111.46
1	H	769	TRP	CB-CA-C	-6.55	96.42	109.33
1	M	769	TRP	CB-CA-C	-6.55	96.42	109.33
1	O	613	PRO	CB-CA-C	-6.55	103.01	111.46
1	C	613	PRO	CB-CA-C	-6.54	103.02	111.46
1	C	881	ARG	NE-CZ-NH1	6.54	128.04	121.50
1	B	613	PRO	CB-CA-C	-6.54	103.03	111.46
1	K	613	PRO	CB-CA-C	-6.53	103.04	111.46
1	D	938	ARG	N-CA-CB	6.53	122.09	110.80
1	G	881	ARG	NE-CZ-NH1	6.53	128.03	121.50
1	L	613	PRO	CB-CA-C	-6.53	103.04	111.46
1	M	613	PRO	CB-CA-C	-6.52	103.05	111.46
1	N	938	ARG	N-CA-CB	6.52	122.08	110.80
1	F	881	ARG	NE-CZ-NH1	6.52	128.02	121.50
1	N	881	ARG	NE-CZ-NH1	6.52	128.02	121.50
1	M	938	ARG	N-CA-CB	6.51	122.07	110.80
1	E	938	ARG	N-CA-CB	6.51	122.06	110.80
1	I	938	ARG	N-CA-CB	6.51	122.06	110.80
1	G	938	ARG	N-CA-CB	6.50	122.05	110.80
1	L	881	ARG	NE-CZ-NH1	6.50	128.00	121.50
1	K	938	ARG	N-CA-CB	6.50	122.05	110.80
1	O	938	ARG	N-CA-CB	6.50	122.05	110.80
1	B	881	ARG	NE-CZ-NH1	6.50	128.00	121.50
1	H	938	ARG	N-CA-CB	6.50	122.04	110.80
1	C	938	ARG	N-CA-CB	6.50	122.04	110.80
1	H	881	ARG	NE-CZ-NH1	6.50	128.00	121.50
1	J	938	ARG	N-CA-CB	6.50	122.04	110.80
1	M	881	ARG	NE-CZ-NH1	6.49	127.99	121.50
1	O	881	ARG	NE-CZ-NH1	6.49	127.99	121.50
1	F	938	ARG	N-CA-CB	6.49	122.02	110.80
1	J	881	ARG	NE-CZ-NH1	6.49	127.99	121.50
1	A	938	ARG	N-CA-CB	6.49	122.02	110.80
1	B	938	ARG	N-CA-CB	6.49	122.02	110.80
1	L	150	PHE	N-CA-C	6.48	118.37	108.52
1	L	938	ARG	N-CA-CB	6.48	122.01	110.80
1	P	938	ARG	N-CA-CB	6.48	122.00	110.80
1	F	150	PHE	N-CA-C	6.48	118.36	108.52
1	K	881	ARG	NE-CZ-NH1	6.48	127.98	121.50
1	D	150	PHE	N-CA-C	6.47	118.36	108.52
1	A	881	ARG	NE-CZ-NH1	6.47	127.97	121.50
1	O	150	PHE	N-CA-C	6.47	118.35	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	118	ASN	CA-C-O	6.47	127.71	120.34
1	C	687	GLN	CA-C-N	6.46	126.48	119.89
1	C	687	GLN	C-N-CA	6.46	126.48	119.89
1	P	687	GLN	CA-C-N	6.46	126.48	119.89
1	P	687	GLN	C-N-CA	6.46	126.48	119.89
1	E	881	ARG	NE-CZ-NH1	6.46	127.96	121.50
1	H	150	PHE	N-CA-C	6.46	118.34	108.52
1	B	150	PHE	N-CA-C	6.46	118.34	108.52
1	E	150	PHE	N-CA-C	6.46	118.34	108.52
1	O	687	GLN	CA-C-N	6.46	126.48	119.89
1	O	687	GLN	C-N-CA	6.46	126.48	119.89
1	A	150	PHE	N-CA-C	6.46	118.34	108.52
1	P	150	PHE	N-CA-C	6.46	118.34	108.52
1	D	734	SER	N-CA-C	-6.46	100.13	110.14
1	F	687	GLN	CA-C-N	6.46	126.47	119.89
1	F	687	GLN	C-N-CA	6.46	126.47	119.89
1	G	150	PHE	N-CA-C	6.46	118.33	108.52
1	J	150	PHE	N-CA-C	6.46	118.33	108.52
1	I	150	PHE	N-CA-C	6.45	118.32	108.52
1	K	118	ASN	CA-C-O	6.45	127.69	120.34
1	K	150	PHE	N-CA-C	6.44	118.31	108.52
1	N	150	PHE	N-CA-C	6.44	118.31	108.52
1	O	118	ASN	CA-C-O	6.44	127.68	120.34
1	M	150	PHE	N-CA-C	6.44	118.31	108.52
1	P	881	ARG	NE-CZ-NH1	6.44	127.94	121.50
1	M	734	SER	N-CA-C	-6.44	100.16	110.14
1	J	734	SER	N-CA-C	-6.44	100.17	110.14
1	C	150	PHE	N-CA-C	6.43	118.30	108.52
1	E	687	GLN	CA-C-N	6.43	126.45	119.89
1	E	687	GLN	C-N-CA	6.43	126.45	119.89
1	B	734	SER	N-CA-C	-6.43	100.17	110.14
1	F	734	SER	N-CA-C	-6.43	100.18	110.14
1	P	781	ARG	N-CA-C	6.43	118.84	109.07
1	J	118	ASN	CA-C-O	6.43	127.67	120.34
1	J	687	GLN	CA-C-N	6.43	126.44	119.89
1	J	687	GLN	C-N-CA	6.43	126.44	119.89
1	M	687	GLN	CA-C-N	6.43	126.44	119.89
1	M	687	GLN	C-N-CA	6.43	126.44	119.89
1	D	687	GLN	CA-C-N	6.42	126.44	119.89
1	D	687	GLN	C-N-CA	6.42	126.44	119.89
1	M	72	SER	O-C-N	6.42	128.93	122.12
1	A	687	GLN	CA-C-N	6.42	126.44	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	687	GLN	C-N-CA	6.42	126.44	119.89
1	A	734	SER	N-CA-C	-6.42	100.19	110.14
1	H	687	GLN	CA-C-N	6.42	126.44	119.89
1	H	687	GLN	C-N-CA	6.42	126.44	119.89
1	P	734	SER	N-CA-C	-6.42	100.19	110.14
1	C	734	SER	N-CA-C	-6.42	100.19	110.14
1	G	734	SER	N-CA-C	-6.42	100.19	110.14
1	N	781	ARG	N-CA-C	6.42	118.83	109.07
1	I	881	ARG	NE-CZ-NH1	6.42	127.92	121.50
1	N	687	GLN	CA-C-N	6.42	126.44	119.89
1	N	687	GLN	C-N-CA	6.42	126.44	119.89
1	E	781	ARG	N-CA-C	6.42	118.82	109.07
1	H	781	ARG	N-CA-C	6.42	118.82	109.07
1	I	734	SER	N-CA-C	-6.42	100.19	110.14
1	L	734	SER	N-CA-C	-6.42	100.20	110.14
1	N	734	SER	N-CA-C	-6.42	100.20	110.14
1	L	781	ARG	N-CA-C	6.41	118.82	109.07
1	E	931	PHE	CB-CA-C	6.41	116.52	110.17
1	I	781	ARG	N-CA-C	6.41	118.82	109.07
1	K	687	GLN	CA-C-N	6.41	126.43	119.89
1	K	687	GLN	C-N-CA	6.41	126.43	119.89
1	K	734	SER	N-CA-C	-6.41	100.20	110.14
1	J	781	ARG	N-CA-C	6.41	118.81	109.07
1	F	781	ARG	N-CA-C	6.40	118.80	109.07
1	O	734	SER	N-CA-C	-6.40	100.22	110.14
1	A	781	ARG	N-CA-C	6.40	118.80	109.07
1	M	118	ASN	CA-C-O	6.40	127.64	120.34
1	M	781	ARG	N-CA-C	6.40	118.80	109.07
1	D	781	ARG	N-CA-C	6.40	118.80	109.07
1	D	881	ARG	NE-CZ-NH1	6.40	127.90	121.50
1	E	734	SER	N-CA-C	-6.40	100.22	110.14
1	G	118	ASN	CA-C-O	6.40	127.63	120.34
1	O	781	ARG	N-CA-C	6.40	118.80	109.07
1	A	72	SER	O-C-N	6.40	128.90	122.12
1	B	781	ARG	N-CA-C	6.40	118.79	109.07
1	H	734	SER	N-CA-C	-6.40	100.23	110.14
1	G	687	GLN	CA-C-N	6.39	126.41	119.89
1	G	687	GLN	C-N-CA	6.39	126.41	119.89
1	P	118	ASN	CA-C-O	6.39	127.63	120.34
1	C	781	ARG	N-CA-C	6.39	118.79	109.07
1	D	72	SER	O-C-N	6.39	128.90	122.12
1	K	756	TRP	CA-C-N	-6.39	113.98	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	756	TRP	C-N-CA	-6.39	113.98	122.99
1	N	118	ASN	CA-C-O	6.39	127.63	120.34
1	P	931	PHE	CB-CA-C	6.39	116.50	110.17
1	B	118	ASN	CA-C-O	6.39	127.63	120.34
1	K	781	ARG	N-CA-C	6.39	118.78	109.07
1	D	118	ASN	CA-C-O	6.39	127.62	120.34
1	L	931	PHE	CB-CA-C	6.39	116.49	110.17
1	M	931	PHE	CB-CA-C	6.39	116.49	110.17
1	N	756	TRP	CA-C-N	-6.39	113.98	122.99
1	N	756	TRP	C-N-CA	-6.39	113.98	122.99
1	B	687	GLN	CA-C-N	6.38	126.40	119.89
1	B	687	GLN	C-N-CA	6.38	126.40	119.89
1	E	72	SER	O-C-N	6.38	128.89	122.12
1	F	118	ASN	CA-C-O	6.38	127.62	120.34
1	F	756	TRP	CA-C-N	-6.38	113.99	122.99
1	F	756	TRP	C-N-CA	-6.38	113.99	122.99
1	I	756	TRP	CA-C-N	-6.38	113.99	122.99
1	I	756	TRP	C-N-CA	-6.38	113.99	122.99
1	I	118	ASN	CA-C-O	6.38	127.62	120.34
1	B	931	PHE	CB-CA-C	6.38	116.49	110.17
1	L	72	SER	O-C-N	6.38	128.88	122.12
1	H	931	PHE	CB-CA-C	6.38	116.48	110.17
1	O	72	SER	O-C-N	6.38	128.88	122.12
1	C	72	SER	O-C-N	6.38	128.88	122.12
1	A	118	ASN	CA-C-O	6.37	127.61	120.34
1	B	72	SER	O-C-N	6.37	128.88	122.12
1	C	931	PHE	CB-CA-C	6.37	116.48	110.17
1	F	931	PHE	CB-CA-C	6.37	116.48	110.17
1	G	72	SER	O-C-N	6.37	128.88	122.12
1	J	72	SER	O-C-N	6.37	128.88	122.12
1	J	931	PHE	CB-CA-C	6.37	116.48	110.17
1	O	931	PHE	CB-CA-C	6.37	116.48	110.17
1	B	756	TRP	CA-C-N	-6.37	114.01	122.99
1	B	756	TRP	C-N-CA	-6.37	114.01	122.99
1	C	118	ASN	CA-C-O	6.37	127.60	120.34
1	G	781	ARG	N-CA-C	6.37	118.75	109.07
1	A	931	PHE	CB-CA-C	6.37	116.47	110.17
1	C	787	ALA	CA-C-N	6.37	126.39	119.90
1	C	787	ALA	C-N-CA	6.37	126.39	119.90
1	P	72	SER	O-C-N	6.37	128.87	122.12
1	E	118	ASN	CA-C-O	6.36	127.59	120.34
1	L	687	GLN	CA-C-N	6.36	126.38	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	687	GLN	C-N-CA	6.36	126.38	119.89
1	G	787	ALA	CA-C-N	6.36	126.39	119.90
1	G	787	ALA	C-N-CA	6.36	126.39	119.90
1	I	687	GLN	CA-C-N	6.36	126.38	119.89
1	I	687	GLN	C-N-CA	6.36	126.38	119.89
1	L	118	ASN	CA-C-O	6.36	127.59	120.34
1	C	756	TRP	CA-C-N	-6.36	114.03	122.99
1	C	756	TRP	C-N-CA	-6.36	114.03	122.99
1	I	72	SER	O-C-N	6.36	128.86	122.12
1	L	756	TRP	CA-C-N	-6.36	114.03	122.99
1	L	756	TRP	C-N-CA	-6.36	114.03	122.99
1	A	756	TRP	CA-C-N	-6.35	114.03	122.99
1	A	756	TRP	C-N-CA	-6.35	114.03	122.99
1	E	756	TRP	CA-C-N	-6.35	114.03	122.99
1	E	756	TRP	C-N-CA	-6.35	114.03	122.99
1	K	787	ALA	CA-C-N	6.35	126.38	119.90
1	K	787	ALA	C-N-CA	6.35	126.38	119.90
1	J	756	TRP	CA-C-N	-6.35	114.03	122.99
1	J	756	TRP	C-N-CA	-6.35	114.03	122.99
1	M	787	ALA	CA-C-N	6.35	126.37	119.90
1	M	787	ALA	C-N-CA	6.35	126.37	119.90
1	K	931	PHE	CB-CA-C	6.35	116.45	110.17
1	D	756	TRP	CA-C-N	-6.34	114.04	122.99
1	D	756	TRP	C-N-CA	-6.34	114.04	122.99
1	D	931	PHE	CB-CA-C	6.34	116.45	110.17
1	N	72	SER	O-C-N	6.34	128.84	122.12
1	G	756	TRP	CA-C-N	-6.34	114.05	122.99
1	G	756	TRP	C-N-CA	-6.34	114.05	122.99
1	E	69	VAL	N-CA-CB	6.34	115.97	110.08
1	H	72	SER	O-C-N	6.34	128.84	122.12
1	P	756	TRP	CA-C-N	-6.34	114.05	122.99
1	P	756	TRP	C-N-CA	-6.34	114.05	122.99
1	G	931	PHE	CB-CA-C	6.34	116.44	110.17
1	H	433	LEU	CA-C-O	6.34	124.94	118.73
1	J	787	ALA	CA-C-N	6.34	126.36	119.90
1	J	787	ALA	C-N-CA	6.34	126.36	119.90
1	O	756	TRP	CA-C-N	-6.34	114.06	122.99
1	O	756	TRP	C-N-CA	-6.34	114.06	122.99
1	D	69	VAL	N-CA-CB	6.33	115.97	110.08
1	O	787	ALA	CA-C-N	6.33	126.36	119.90
1	O	787	ALA	C-N-CA	6.33	126.36	119.90
1	F	72	SER	O-C-N	6.33	128.83	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	931	PHE	CB-CA-C	6.33	116.44	110.17
1	H	756	TRP	CA-C-N	-6.33	114.07	122.99
1	H	756	TRP	C-N-CA	-6.33	114.07	122.99
1	I	931	PHE	CB-CA-C	6.33	116.43	110.17
1	M	756	TRP	CA-C-N	-6.33	114.07	122.99
1	M	756	TRP	C-N-CA	-6.33	114.07	122.99
1	A	787	ALA	CA-C-N	6.32	126.35	119.90
1	A	787	ALA	C-N-CA	6.32	126.35	119.90
1	D	787	ALA	CA-C-N	6.32	126.35	119.90
1	D	787	ALA	C-N-CA	6.32	126.35	119.90
1	K	72	SER	O-C-N	6.32	128.82	122.12
1	I	69	VAL	N-CA-CB	6.32	115.96	110.08
1	J	433	LEU	CA-C-O	6.32	124.92	118.73
1	E	787	ALA	CA-C-N	6.32	126.35	119.90
1	E	787	ALA	C-N-CA	6.32	126.35	119.90
1	P	69	VAL	N-CA-CB	6.32	115.96	110.08
1	C	433	LEU	CA-C-O	6.31	124.92	118.73
1	B	69	VAL	N-CA-CB	6.31	115.95	110.08
1	F	787	ALA	CA-C-N	6.31	126.33	119.90
1	F	787	ALA	C-N-CA	6.31	126.33	119.90
1	E	433	LEU	CA-C-O	6.30	124.91	118.73
1	E	559	TYR	CA-C-O	6.30	127.48	119.54
1	H	787	ALA	CA-C-N	6.30	126.33	119.90
1	H	787	ALA	C-N-CA	6.30	126.33	119.90
1	K	69	VAL	N-CA-CB	6.30	115.94	110.08
1	D	433	LEU	CA-C-O	6.30	124.91	118.73
1	I	559	TYR	CA-C-O	6.30	127.48	119.54
1	J	69	VAL	N-CA-CB	6.30	115.94	110.08
1	N	433	LEU	CA-C-O	6.30	124.90	118.73
1	L	787	ALA	CA-C-N	6.29	126.32	119.90
1	L	787	ALA	C-N-CA	6.29	126.32	119.90
1	G	433	LEU	CA-C-O	6.29	124.89	118.73
1	K	559	TYR	CA-C-O	6.29	127.47	119.54
1	H	69	VAL	N-CA-CB	6.29	115.93	110.08
1	I	787	ALA	CA-C-N	6.29	126.31	119.90
1	I	787	ALA	C-N-CA	6.29	126.31	119.90
1	L	559	TYR	CA-C-O	6.29	127.46	119.54
1	B	433	LEU	CA-C-O	6.29	124.89	118.73
1	A	69	VAL	N-CA-CB	6.28	115.92	110.08
1	A	433	LEU	CA-C-O	6.28	124.89	118.73
1	O	433	LEU	CA-C-O	6.28	124.89	118.73
1	N	559	TYR	CA-C-O	6.28	127.46	119.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	559	TYR	CA-C-O	6.28	127.45	119.54
1	C	69	VAL	N-CA-CB	6.28	115.92	110.08
1	M	559	TYR	CA-C-O	6.28	127.45	119.54
1	O	69	VAL	N-CA-CB	6.28	115.92	110.08
1	N	69	VAL	N-CA-CB	6.28	115.92	110.08
1	P	433	LEU	CA-C-O	6.28	124.88	118.73
1	K	433	LEU	CA-C-O	6.28	124.88	118.73
1	F	69	VAL	N-CA-CB	6.28	115.92	110.08
1	I	433	LEU	CA-C-O	6.27	124.88	118.73
1	L	433	LEU	CA-C-O	6.27	124.88	118.73
1	M	433	LEU	CA-C-O	6.27	124.88	118.73
1	L	69	VAL	N-CA-CB	6.27	115.91	110.08
1	A	559	TYR	CA-C-O	6.27	127.44	119.54
1	B	787	ALA	CA-C-N	6.27	126.29	119.90
1	B	787	ALA	C-N-CA	6.27	126.29	119.90
1	P	559	TYR	CA-C-O	6.27	127.44	119.54
1	F	433	LEU	CA-C-O	6.27	124.87	118.73
1	P	787	ALA	CA-C-N	6.27	126.29	119.90
1	P	787	ALA	C-N-CA	6.27	126.29	119.90
1	F	559	TYR	CA-C-O	6.26	127.43	119.54
1	J	559	TYR	CA-C-O	6.26	127.43	119.54
1	G	559	TYR	CA-C-O	6.26	127.43	119.54
1	H	559	TYR	CA-C-O	6.26	127.43	119.54
1	N	787	ALA	CA-C-N	6.26	126.28	119.90
1	N	787	ALA	C-N-CA	6.26	126.28	119.90
1	M	69	VAL	N-CA-CB	6.26	115.90	110.08
1	C	559	TYR	CA-C-O	6.26	127.42	119.54
1	G	69	VAL	N-CA-CB	6.25	115.90	110.08
1	D	559	TYR	CA-C-O	6.25	127.41	119.54
1	O	559	TYR	CA-C-O	6.25	127.41	119.54
1	C	788	PRO	N-CA-CB	6.24	108.74	103.25
1	K	788	PRO	N-CA-CB	6.24	108.74	103.25
1	O	788	PRO	N-CA-CB	6.22	108.73	103.25
1	G	788	PRO	N-CA-CB	6.21	108.72	103.25
1	A	788	PRO	N-CA-CB	6.20	108.71	103.25
1	H	186	VAL	CA-C-N	-6.20	114.78	122.84
1	H	186	VAL	C-N-CA	-6.20	114.78	122.84
1	D	788	PRO	N-CA-CB	6.20	108.71	103.25
1	E	186	VAL	CA-C-N	-6.20	114.78	122.84
1	E	186	VAL	C-N-CA	-6.20	114.78	122.84
1	P	788	PRO	N-CA-CB	6.20	108.70	103.25
1	J	788	PRO	N-CA-CB	6.20	108.70	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	788	PRO	N-CA-CB	6.19	108.70	103.25
1	P	186	VAL	CA-C-N	-6.18	114.80	122.84
1	P	186	VAL	C-N-CA	-6.18	114.80	122.84
1	L	788	PRO	N-CA-CB	6.18	108.69	103.25
1	M	788	PRO	N-CA-CB	6.18	108.69	103.25
1	B	788	PRO	N-CA-CB	6.18	108.69	103.25
1	I	702	GLN	CA-C-N	6.18	125.39	118.97
1	I	702	GLN	C-N-CA	6.18	125.39	118.97
1	I	788	PRO	N-CA-CB	6.18	108.69	103.25
1	I	186	VAL	CA-C-N	-6.17	114.81	122.84
1	I	186	VAL	C-N-CA	-6.17	114.81	122.84
1	B	186	VAL	CA-C-N	-6.17	114.82	122.84
1	B	186	VAL	C-N-CA	-6.17	114.82	122.84
1	C	186	VAL	CA-C-N	-6.17	114.82	122.84
1	C	186	VAL	C-N-CA	-6.17	114.82	122.84
1	E	788	PRO	N-CA-CB	6.17	108.68	103.25
1	F	186	VAL	CA-C-N	-6.17	114.82	122.84
1	F	186	VAL	C-N-CA	-6.17	114.82	122.84
1	O	186	VAL	CA-C-N	-6.17	114.82	122.84
1	O	186	VAL	C-N-CA	-6.17	114.82	122.84
1	H	878	HIS	CA-CB-CG	-6.16	107.64	113.80
1	I	878	HIS	CA-CB-CG	-6.16	107.64	113.80
1	K	186	VAL	CA-C-N	-6.16	114.83	122.84
1	K	186	VAL	C-N-CA	-6.16	114.83	122.84
1	A	186	VAL	CA-C-N	-6.16	114.84	122.84
1	A	186	VAL	C-N-CA	-6.16	114.84	122.84
1	D	186	VAL	CA-C-N	-6.15	114.84	122.84
1	D	186	VAL	C-N-CA	-6.15	114.84	122.84
1	J	878	HIS	CA-CB-CG	-6.15	107.65	113.80
1	A	702	GLN	CA-C-N	6.15	125.37	118.97
1	A	702	GLN	C-N-CA	6.15	125.37	118.97
1	C	702	GLN	CA-C-N	6.15	125.37	118.97
1	C	702	GLN	C-N-CA	6.15	125.37	118.97
1	C	878	HIS	CA-CB-CG	-6.15	107.65	113.80
1	F	788	PRO	N-CA-CB	6.15	108.66	103.25
1	K	878	HIS	CA-CB-CG	-6.15	107.65	113.80
1	D	702	GLN	CA-C-N	6.15	125.36	118.97
1	D	702	GLN	C-N-CA	6.15	125.36	118.97
1	M	186	VAL	CA-C-N	-6.14	114.85	122.84
1	M	186	VAL	C-N-CA	-6.14	114.85	122.84
1	N	788	PRO	N-CA-CB	6.14	108.66	103.25
1	D	878	HIS	CA-CB-CG	-6.14	107.66	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	186	VAL	CA-C-N	-6.14	114.86	122.84
1	L	186	VAL	C-N-CA	-6.14	114.86	122.84
1	L	166	ARG	NE-CZ-NH1	6.14	127.64	121.50
1	N	702	GLN	CA-C-N	6.14	125.35	118.97
1	N	702	GLN	C-N-CA	6.14	125.35	118.97
1	O	878	HIS	CA-CB-CG	-6.14	107.66	113.80
1	E	878	HIS	CA-CB-CG	-6.14	107.66	113.80
1	G	186	VAL	CA-C-N	-6.14	114.86	122.84
1	G	186	VAL	C-N-CA	-6.14	114.86	122.84
1	J	186	VAL	CA-C-N	-6.14	114.86	122.84
1	J	186	VAL	C-N-CA	-6.14	114.86	122.84
1	A	878	HIS	CA-CB-CG	-6.13	107.67	113.80
1	O	166	ARG	NE-CZ-NH1	6.13	127.63	121.50
1	I	166	ARG	NE-CZ-NH1	6.13	127.63	121.50
1	N	186	VAL	CA-C-N	-6.13	114.87	122.84
1	N	186	VAL	C-N-CA	-6.13	114.87	122.84
1	E	702	GLN	CA-C-N	6.13	125.35	118.97
1	E	702	GLN	C-N-CA	6.13	125.35	118.97
1	G	878	HIS	CA-CB-CG	-6.13	107.67	113.80
1	P	702	GLN	CA-C-N	6.13	125.34	118.97
1	P	702	GLN	C-N-CA	6.13	125.34	118.97
1	M	878	HIS	CA-CB-CG	-6.12	107.67	113.80
1	B	702	GLN	CA-C-N	6.12	125.34	118.97
1	B	702	GLN	C-N-CA	6.12	125.34	118.97
1	H	702	GLN	CA-C-N	6.12	125.34	118.97
1	H	702	GLN	C-N-CA	6.12	125.34	118.97
1	J	702	GLN	CA-C-N	6.12	125.34	118.97
1	J	702	GLN	C-N-CA	6.12	125.34	118.97
1	O	554	GLN	CB-CG-CD	-6.12	102.19	112.60
1	B	878	HIS	CA-CB-CG	-6.12	107.68	113.80
1	E	554	GLN	CB-CG-CD	-6.12	102.20	112.60
1	H	554	GLN	CB-CG-CD	-6.12	102.20	112.60
1	L	927	THR	CA-C-O	6.12	125.22	119.59
1	O	702	GLN	CA-C-N	6.12	125.33	118.97
1	O	702	GLN	C-N-CA	6.12	125.33	118.97
1	B	927	THR	CA-C-O	6.11	125.21	119.59
1	H	761	GLN	CA-CB-CG	-6.11	101.88	114.10
1	L	761	GLN	CA-CB-CG	-6.11	101.87	114.10
1	C	554	GLN	CB-CG-CD	-6.11	102.21	112.60
1	I	927	THR	CA-C-O	6.11	125.21	119.59
1	L	702	GLN	CA-C-N	6.11	125.33	118.97
1	L	702	GLN	C-N-CA	6.11	125.33	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	878	HIS	CA-CB-CG	-6.11	107.69	113.80
1	K	702	GLN	CA-C-N	6.11	125.33	118.97
1	K	702	GLN	C-N-CA	6.11	125.33	118.97
1	C	927	THR	CA-C-O	6.11	125.21	119.59
1	D	166	ARG	NE-CZ-NH1	6.11	127.61	121.50
1	F	702	GLN	CA-C-N	6.11	125.32	118.97
1	F	702	GLN	C-N-CA	6.11	125.32	118.97
1	N	927	THR	CA-C-O	6.11	125.21	119.59
1	P	761	GLN	CA-CB-CG	-6.11	101.89	114.10
1	B	554	GLN	CB-CG-CD	-6.11	102.22	112.60
1	C	761	GLN	CA-CB-CG	-6.11	101.89	114.10
1	G	927	THR	CA-C-O	6.11	125.21	119.59
1	O	761	GLN	CA-CB-CG	-6.11	101.89	114.10
1	J	927	THR	CA-C-O	6.10	125.21	119.59
1	E	761	GLN	CA-CB-CG	-6.10	101.89	114.10
1	J	761	GLN	CA-CB-CG	-6.10	101.89	114.10
1	K	166	ARG	NE-CZ-NH1	6.10	127.60	121.50
1	P	554	GLN	CB-CG-CD	-6.10	102.22	112.60
1	C	166	ARG	NE-CZ-NH1	6.10	127.60	121.50
1	E	166	ARG	NE-CZ-NH1	6.10	127.60	121.50
1	I	395	HIS	CA-C-N	6.10	126.28	119.32
1	I	395	HIS	C-N-CA	6.10	126.28	119.32
1	I	761	GLN	CA-CB-CG	-6.10	101.90	114.10
1	N	878	HIS	CA-CB-CG	-6.10	107.70	113.80
1	A	761	GLN	CA-CB-CG	-6.10	101.91	114.10
1	G	761	GLN	CA-CB-CG	-6.10	101.90	114.10
1	K	761	GLN	CA-CB-CG	-6.10	101.91	114.10
1	M	927	THR	CA-C-O	6.10	125.20	119.59
1	A	554	GLN	CB-CG-CD	-6.09	102.24	112.60
1	F	927	THR	CA-C-O	6.09	125.20	119.59
1	G	702	GLN	CA-C-N	6.09	125.31	118.97
1	G	702	GLN	C-N-CA	6.09	125.31	118.97
1	A	927	THR	CA-C-O	6.09	125.19	119.59
1	E	395	HIS	CA-C-N	6.09	126.27	119.32
1	E	395	HIS	C-N-CA	6.09	126.27	119.32
1	H	395	HIS	CA-C-N	6.09	126.27	119.32
1	H	395	HIS	C-N-CA	6.09	126.27	119.32
1	J	166	ARG	NE-CZ-NH1	6.09	127.59	121.50
1	N	554	GLN	CB-CG-CD	-6.09	102.24	112.60
1	B	761	GLN	CA-CB-CG	-6.09	101.92	114.10
1	D	761	GLN	CA-CB-CG	-6.09	101.92	114.10
1	L	554	GLN	CB-CG-CD	-6.09	102.24	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	166	ARG	NE-CZ-NH1	6.09	127.59	121.50
1	A	166	ARG	NE-CZ-NH1	6.09	127.59	121.50
1	N	166	ARG	NE-CZ-NH1	6.09	127.59	121.50
1	M	554	GLN	CB-CG-CD	-6.09	102.25	112.60
1	J	554	GLN	CB-CG-CD	-6.09	102.25	112.60
1	F	761	GLN	CA-CB-CG	-6.08	101.93	114.10
1	K	395	HIS	CA-C-N	6.08	126.26	119.32
1	K	395	HIS	C-N-CA	6.08	126.26	119.32
1	K	554	GLN	CB-CG-CD	-6.08	102.25	112.60
1	M	761	GLN	CA-CB-CG	-6.08	101.93	114.10
1	D	554	GLN	CB-CG-CD	-6.08	102.26	112.60
1	G	554	GLN	CB-CG-CD	-6.08	102.26	112.60
1	N	761	GLN	CA-CB-CG	-6.08	101.93	114.10
1	E	927	THR	CA-C-O	6.08	125.19	119.59
1	G	166	ARG	NE-CZ-NH1	6.08	127.58	121.50
1	M	702	GLN	CA-C-N	6.08	125.30	118.97
1	M	702	GLN	C-N-CA	6.08	125.30	118.97
1	D	927	THR	CA-C-O	6.08	125.18	119.59
1	H	166	ARG	NE-CZ-NH1	6.08	127.58	121.50
1	H	927	THR	CA-C-O	6.08	125.18	119.59
1	L	878	HIS	CA-CB-CG	-6.08	107.72	113.80
1	P	878	HIS	CA-CB-CG	-6.08	107.72	113.80
1	D	395	HIS	CA-C-N	6.07	126.24	119.32
1	D	395	HIS	C-N-CA	6.07	126.24	119.32
1	I	554	GLN	CB-CG-CD	-6.07	102.28	112.60
1	O	927	THR	CA-C-O	6.07	125.17	119.59
1	F	166	ARG	NE-CZ-NH1	6.07	127.57	121.50
1	B	166	ARG	NE-CZ-NH1	6.06	127.56	121.50
1	P	166	ARG	NE-CZ-NH1	6.06	127.56	121.50
1	B	395	HIS	CA-C-N	6.06	126.23	119.32
1	B	395	HIS	C-N-CA	6.06	126.23	119.32
1	F	554	GLN	CB-CG-CD	-6.06	102.30	112.60
1	P	395	HIS	CA-C-N	6.06	126.23	119.32
1	P	395	HIS	C-N-CA	6.06	126.23	119.32
1	P	927	THR	CA-C-O	6.06	125.16	119.59
1	K	927	THR	CA-C-O	6.05	125.16	119.59
1	A	395	HIS	CA-C-N	6.05	126.22	119.32
1	A	395	HIS	C-N-CA	6.05	126.22	119.32
1	K	96	ASP	N-CA-CB	6.05	120.80	111.24
1	B	335	VAL	CB-CA-C	-6.05	102.13	110.96
1	N	335	VAL	CB-CA-C	-6.05	102.13	110.96
1	G	395	HIS	CA-C-N	6.04	126.21	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	395	HIS	C-N-CA	6.04	126.21	119.32
1	K	335	VAL	CB-CA-C	-6.04	102.13	110.96
1	F	96	ASP	N-CA-CB	6.04	120.79	111.24
1	F	395	HIS	CA-C-N	6.04	126.21	119.32
1	F	395	HIS	C-N-CA	6.04	126.21	119.32
1	D	335	VAL	CB-CA-C	-6.04	102.14	110.96
1	B	740	LEU	O-C-N	-6.04	116.18	122.94
1	C	395	HIS	CA-C-N	6.04	126.20	119.32
1	C	395	HIS	C-N-CA	6.04	126.20	119.32
1	N	395	HIS	CA-C-N	6.04	126.20	119.32
1	N	395	HIS	C-N-CA	6.04	126.20	119.32
1	O	335	VAL	CB-CA-C	-6.04	102.14	110.96
1	A	335	VAL	CB-CA-C	-6.04	102.15	110.96
1	F	335	VAL	CB-CA-C	-6.04	102.14	110.96
1	G	335	VAL	CB-CA-C	-6.04	102.15	110.96
1	C	335	VAL	CB-CA-C	-6.04	102.15	110.96
1	J	395	HIS	CA-C-N	6.04	126.20	119.32
1	J	395	HIS	C-N-CA	6.04	126.20	119.32
1	L	335	VAL	CB-CA-C	-6.04	102.15	110.96
1	J	96	ASP	N-CA-CB	6.03	120.77	111.24
1	J	335	VAL	CB-CA-C	-6.03	102.15	110.96
1	H	335	VAL	CB-CA-C	-6.03	102.15	110.96
1	I	335	VAL	CB-CA-C	-6.03	102.15	110.96
1	E	335	VAL	CB-CA-C	-6.03	102.16	110.96
1	L	96	ASP	N-CA-CB	6.03	120.77	111.24
1	H	96	ASP	N-CA-CB	6.03	120.76	111.24
1	C	96	ASP	N-CA-CB	6.03	120.76	111.24
1	L	395	HIS	CA-C-N	6.02	126.19	119.32
1	L	395	HIS	C-N-CA	6.02	126.19	119.32
1	G	96	ASP	N-CA-CB	6.02	120.75	111.24
1	M	395	HIS	CA-C-N	6.02	126.18	119.32
1	M	395	HIS	C-N-CA	6.02	126.18	119.32
1	D	96	ASP	N-CA-CB	6.02	120.75	111.24
1	M	335	VAL	CB-CA-C	-6.02	102.17	110.96
1	A	96	ASP	N-CA-CB	6.02	120.75	111.24
1	B	96	ASP	N-CA-CB	6.02	120.75	111.24
1	P	96	ASP	N-CA-CB	6.01	120.74	111.24
1	P	335	VAL	CB-CA-C	-6.01	102.18	110.96
1	F	740	LEU	O-C-N	-6.01	116.21	122.94
1	M	96	ASP	N-CA-CB	6.01	120.74	111.24
1	O	395	HIS	CA-C-N	6.01	126.17	119.32
1	O	395	HIS	C-N-CA	6.01	126.17	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	740	LEU	O-C-N	-6.01	116.21	122.94
1	I	96	ASP	N-CA-CB	6.00	120.73	111.24
1	L	740	LEU	O-C-N	-6.00	116.22	122.94
1	N	96	ASP	N-CA-CB	6.00	120.73	111.24
1	G	740	LEU	O-C-N	-6.00	116.22	122.94
1	O	96	ASP	N-CA-CB	6.00	120.72	111.24
1	D	740	LEU	O-C-N	-6.00	116.23	122.94
1	P	740	LEU	O-C-N	-5.99	116.23	122.94
1	C	740	LEU	O-C-N	-5.99	116.23	122.94
1	M	740	LEU	O-C-N	-5.98	116.24	122.94
1	E	740	LEU	O-C-N	-5.97	116.25	122.94
1	I	740	LEU	O-C-N	-5.97	116.25	122.94
1	A	740	LEU	O-C-N	-5.97	116.25	122.94
1	G	118	ASN	CB-CA-C	5.97	119.25	111.01
1	D	118	ASN	CB-CA-C	5.97	119.24	111.01
1	J	740	LEU	O-C-N	-5.97	116.26	122.94
1	K	740	LEU	O-C-N	-5.97	116.26	122.94
1	L	118	ASN	CB-CA-C	5.96	119.24	111.01
1	I	118	ASN	CB-CA-C	5.96	119.24	111.01
1	E	118	ASN	CB-CA-C	5.96	119.23	111.01
1	J	118	ASN	CB-CA-C	5.96	119.23	111.01
1	M	118	ASN	CB-CA-C	5.96	119.23	111.01
1	B	729	THR	O-C-N	5.95	130.66	123.16
1	B	687	GLN	O-C-N	5.95	126.64	121.34
1	A	118	ASN	CB-CA-C	5.95	119.22	111.01
1	C	729	THR	N-CA-CB	5.95	120.37	110.85
1	P	729	THR	O-C-N	5.95	130.66	123.16
1	P	118	ASN	CB-CA-C	5.95	119.22	111.01
1	F	729	THR	N-CA-CB	5.95	120.36	110.85
1	I	729	THR	N-CA-CB	5.95	120.36	110.85
1	N	729	THR	N-CA-CB	5.95	120.36	110.85
1	O	740	LEU	O-C-N	-5.95	116.28	122.94
1	B	118	ASN	CB-CA-C	5.94	119.21	111.01
1	C	118	ASN	CB-CA-C	5.94	119.21	111.01
1	D	729	THR	O-C-N	5.94	130.65	123.16
1	H	118	ASN	CB-CA-C	5.94	119.21	111.01
1	K	310	ARG	N-CA-CB	5.94	119.90	110.57
1	F	166	ARG	N-CA-C	5.94	120.68	113.38
1	B	729	THR	N-CA-CB	5.93	120.35	110.85
1	D	166	ARG	N-CA-C	5.93	120.68	113.38
1	M	729	THR	O-C-N	5.93	130.64	123.16
1	M	729	THR	N-CA-CB	5.93	120.34	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	740	LEU	O-C-N	-5.93	116.30	122.94
1	H	166	ARG	N-CA-C	5.93	120.67	113.38
1	K	729	THR	O-C-N	5.93	130.63	123.16
1	N	729	THR	O-C-N	5.93	130.63	123.16
1	O	310	ARG	N-CA-CB	5.93	119.88	110.57
1	O	729	THR	O-C-N	5.93	130.63	123.16
1	A	729	THR	O-C-N	5.93	130.63	123.16
1	C	729	THR	O-C-N	5.93	130.63	123.16
1	D	310	ARG	N-CA-CB	5.93	119.88	110.57
1	J	729	THR	N-CA-CB	5.93	120.33	110.85
1	O	118	ASN	CB-CA-C	5.93	119.19	111.01
1	O	729	THR	N-CA-CB	5.92	120.33	110.85
1	B	310	ARG	N-CA-CB	5.92	119.87	110.57
1	C	166	ARG	N-CA-C	5.92	120.66	113.38
1	L	729	THR	O-C-N	5.92	130.62	123.16
1	L	729	THR	N-CA-CB	5.92	120.33	110.85
1	P	729	THR	N-CA-CB	5.92	120.33	110.85
1	G	729	THR	N-CA-CB	5.92	120.32	110.85
1	N	687	GLN	O-C-N	5.92	126.61	121.34
1	F	340	GLY	CA-C-N	-5.92	113.52	122.81
1	F	340	GLY	C-N-CA	-5.92	113.52	122.81
1	N	118	ASN	CB-CA-C	5.92	119.18	111.01
1	I	166	ARG	N-CA-C	5.92	120.66	113.38
1	I	687	GLN	O-C-N	5.92	126.61	121.34
1	J	729	THR	O-C-N	5.92	130.62	123.16
1	O	166	ARG	N-CA-C	5.92	120.66	113.38
1	D	729	THR	N-CA-CB	5.92	120.31	110.85
1	H	729	THR	N-CA-CB	5.92	120.31	110.85
1	F	118	ASN	CB-CA-C	5.91	119.17	111.01
1	K	729	THR	N-CA-CB	5.91	120.31	110.85
1	D	340	GLY	CA-C-N	-5.91	113.53	122.81
1	D	340	GLY	C-N-CA	-5.91	113.53	122.81
1	C	310	ARG	N-CA-CB	5.91	119.85	110.57
1	E	729	THR	N-CA-CB	5.91	120.31	110.85
1	I	729	THR	O-C-N	5.91	130.61	123.16
1	M	166	ARG	N-CA-C	5.91	120.65	113.38
1	D	687	GLN	O-C-N	5.91	126.60	121.34
1	E	818	ALA	O-C-N	5.91	129.83	122.86
1	P	818	ALA	O-C-N	5.91	129.83	122.86
1	G	183	ARG	CD-NE-CZ	-5.91	116.13	124.40
1	H	729	THR	O-C-N	5.91	130.60	123.16
1	K	340	GLY	CA-C-N	-5.91	113.54	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	340	GLY	C-N-CA	-5.91	113.54	122.81
1	N	310	ARG	N-CA-CB	5.91	119.84	110.57
1	A	310	ARG	N-CA-CB	5.90	119.84	110.57
1	F	183	ARG	CD-NE-CZ	-5.90	116.13	124.40
1	A	166	ARG	N-CA-C	5.90	120.64	113.38
1	C	340	GLY	CA-C-N	-5.90	113.54	122.81
1	C	340	GLY	C-N-CA	-5.90	113.54	122.81
1	F	729	THR	O-C-N	5.90	130.60	123.16
1	G	274	PHE	CA-CB-CG	-5.90	107.90	113.80
1	H	687	GLN	O-C-N	5.90	126.59	121.34
1	G	729	THR	O-C-N	5.90	130.60	123.16
1	N	818	ALA	O-C-N	5.90	129.82	122.86
1	B	166	ARG	N-CA-C	5.90	120.64	113.38
1	G	818	ALA	O-C-N	5.90	129.82	122.86
1	O	818	ALA	O-C-N	5.90	129.82	122.86
1	P	166	ARG	N-CA-C	5.90	120.63	113.38
1	P	183	ARG	CD-NE-CZ	-5.90	116.14	124.40
1	J	340	GLY	CA-C-N	-5.90	113.55	122.81
1	J	340	GLY	C-N-CA	-5.90	113.55	122.81
1	K	118	ASN	CB-CA-C	5.90	119.15	111.01
1	A	340	GLY	CA-C-N	-5.89	113.56	122.81
1	A	340	GLY	C-N-CA	-5.89	113.56	122.81
1	B	818	ALA	O-C-N	5.89	129.81	122.86
1	D	183	ARG	CD-NE-CZ	-5.89	116.15	124.40
1	M	818	ALA	O-C-N	5.89	129.82	122.86
1	A	687	GLN	O-C-N	5.89	126.58	121.34
1	A	729	THR	N-CA-CB	5.89	120.28	110.85
1	E	310	ARG	N-CA-CB	5.89	119.82	110.57
1	G	310	ARG	N-CA-CB	5.89	119.82	110.57
1	H	310	ARG	N-CA-CB	5.89	119.82	110.57
1	I	310	ARG	N-CA-CB	5.89	119.82	110.57
1	K	687	GLN	O-C-N	5.89	126.58	121.34
1	N	166	ARG	N-CA-C	5.89	120.63	113.38
1	B	183	ARG	CD-NE-CZ	-5.89	116.15	124.40
1	C	183	ARG	CD-NE-CZ	-5.89	116.15	124.40
1	G	166	ARG	N-CA-C	5.89	120.63	113.38
1	J	166	ARG	N-CA-C	5.89	120.63	113.38
1	K	183	ARG	CD-NE-CZ	-5.89	116.15	124.40
1	L	340	GLY	CA-C-N	-5.89	113.56	122.81
1	L	340	GLY	C-N-CA	-5.89	113.56	122.81
1	M	183	ARG	CD-NE-CZ	-5.89	116.15	124.40
1	O	340	GLY	CA-C-N	-5.89	113.56	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	340	GLY	C-N-CA	-5.89	113.56	122.81
1	E	166	ARG	N-CA-C	5.89	120.62	113.38
1	F	310	ARG	N-CA-CB	5.89	119.82	110.57
1	L	166	ARG	N-CA-C	5.89	120.62	113.38
1	M	310	ARG	N-CA-CB	5.89	119.82	110.57
1	P	310	ARG	N-CA-CB	5.89	119.82	110.57
1	E	729	THR	O-C-N	5.89	130.58	123.16
1	L	310	ARG	N-CA-CB	5.89	119.81	110.57
1	L	687	GLN	O-C-N	5.89	126.58	121.34
1	H	189	LEU	N-CA-CB	5.88	120.22	110.63
1	I	183	ARG	CD-NE-CZ	-5.88	116.16	124.40
1	K	166	ARG	N-CA-C	5.88	120.62	113.38
1	A	183	ARG	CD-NE-CZ	-5.88	116.17	124.40
1	E	687	GLN	O-C-N	5.88	126.57	121.34
1	H	183	ARG	CD-NE-CZ	-5.88	116.17	124.40
1	I	189	LEU	N-CA-CB	5.88	120.22	110.63
1	I	340	GLY	CA-C-N	-5.88	113.58	122.81
1	I	340	GLY	C-N-CA	-5.88	113.58	122.81
1	N	274	PHE	CA-CB-CG	-5.88	107.92	113.80
1	E	340	GLY	CA-C-N	-5.88	113.58	122.81
1	E	340	GLY	C-N-CA	-5.88	113.58	122.81
1	J	310	ARG	N-CA-CB	5.88	119.80	110.57
1	M	340	GLY	CA-C-N	-5.88	113.58	122.81
1	M	340	GLY	C-N-CA	-5.88	113.58	122.81
1	P	189	LEU	N-CA-CB	5.88	120.21	110.63
1	D	818	ALA	O-C-N	5.88	129.79	122.86
1	D	274	PHE	CA-CB-CG	-5.88	107.92	113.80
1	A	818	ALA	O-C-N	5.87	129.79	122.86
1	D	189	LEU	N-CA-CB	5.87	120.20	110.63
1	E	183	ARG	CD-NE-CZ	-5.87	116.18	124.40
1	G	687	GLN	O-C-N	5.87	126.56	121.34
1	I	818	ALA	O-C-N	5.87	129.79	122.86
1	N	340	GLY	CA-C-N	-5.87	113.59	122.81
1	N	340	GLY	C-N-CA	-5.87	113.59	122.81
1	P	340	GLY	CA-C-N	-5.87	113.59	122.81
1	P	340	GLY	C-N-CA	-5.87	113.59	122.81
1	F	818	ALA	O-C-N	5.87	129.79	122.86
1	E	189	LEU	N-CA-CB	5.87	120.20	110.63
1	J	189	LEU	N-CA-CB	5.87	120.20	110.63
1	J	818	ALA	O-C-N	5.87	129.78	122.86
1	M	687	GLN	O-C-N	5.87	126.56	121.34
1	O	183	ARG	CD-NE-CZ	-5.87	116.18	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	LEU	N-CA-CB	5.87	120.19	110.63
1	J	687	GLN	O-C-N	5.87	126.56	121.34
1	F	189	LEU	N-CA-CB	5.87	120.19	110.63
1	F	274	PHE	CA-CB-CG	-5.87	107.93	113.80
1	I	274	PHE	CA-CB-CG	-5.87	107.93	113.80
1	O	687	GLN	O-C-N	5.87	126.56	121.34
1	C	818	ALA	O-C-N	5.86	129.78	122.86
1	O	189	LEU	N-CA-CB	5.86	120.19	110.63
1	G	340	GLY	CA-C-N	-5.86	113.61	122.81
1	G	340	GLY	C-N-CA	-5.86	113.61	122.81
1	M	189	LEU	N-CA-CB	5.86	120.19	110.63
1	F	18	ASN	CA-C-N	5.86	125.96	119.87
1	F	18	ASN	C-N-CA	5.86	125.96	119.87
1	H	340	GLY	CA-C-N	-5.86	113.62	122.81
1	H	340	GLY	C-N-CA	-5.86	113.62	122.81
1	K	189	LEU	N-CA-CB	5.86	120.17	110.63
1	N	189	LEU	N-CA-CB	5.86	120.17	110.63
1	A	189	LEU	N-CA-CB	5.85	120.17	110.63
1	J	183	ARG	CD-NE-CZ	-5.85	116.20	124.40
1	C	189	LEU	N-CA-CB	5.85	120.17	110.63
1	M	18	ASN	CA-C-N	5.85	125.96	119.87
1	M	18	ASN	C-N-CA	5.85	125.96	119.87
1	G	189	LEU	N-CA-CB	5.85	120.17	110.63
1	O	274	PHE	CA-CB-CG	-5.85	107.95	113.80
1	B	274	PHE	CA-CB-CG	-5.85	107.95	113.80
1	L	818	ALA	O-C-N	5.85	129.76	122.86
1	A	274	PHE	CA-CB-CG	-5.85	107.95	113.80
1	J	274	PHE	CA-CB-CG	-5.85	107.95	113.80
1	B	18	ASN	CA-C-N	5.85	125.95	119.87
1	B	18	ASN	C-N-CA	5.85	125.95	119.87
1	C	18	ASN	CA-C-N	5.85	125.95	119.87
1	C	18	ASN	C-N-CA	5.85	125.95	119.87
1	H	274	PHE	CA-CB-CG	-5.85	107.95	113.80
1	N	183	ARG	CD-NE-CZ	-5.85	116.22	124.40
1	B	340	GLY	CA-C-N	-5.84	113.63	122.81
1	B	340	GLY	C-N-CA	-5.84	113.63	122.81
1	K	274	PHE	CA-CB-CG	-5.84	107.95	113.80
1	L	189	LEU	N-CA-CB	5.84	120.16	110.63
1	K	818	ALA	O-C-N	5.84	129.75	122.86
1	L	274	PHE	CA-CB-CG	-5.84	107.96	113.80
1	C	274	PHE	CA-CB-CG	-5.84	107.96	113.80
1	M	274	PHE	CA-CB-CG	-5.84	107.96	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	183	ARG	CD-NE-CZ	-5.84	116.22	124.40
1	N	18	ASN	CA-C-N	5.84	125.94	119.87
1	N	18	ASN	C-N-CA	5.84	125.94	119.87
1	P	274	PHE	CA-CB-CG	-5.84	107.96	113.80
1	E	274	PHE	CA-CB-CG	-5.84	107.96	113.80
1	E	18	ASN	CA-C-N	5.83	125.94	119.87
1	E	18	ASN	C-N-CA	5.83	125.94	119.87
1	J	18	ASN	CA-C-N	5.83	125.94	119.87
1	J	18	ASN	C-N-CA	5.83	125.94	119.87
1	P	18	ASN	CA-C-N	5.83	125.94	119.87
1	P	18	ASN	C-N-CA	5.83	125.94	119.87
1	F	687	GLN	O-C-N	5.83	126.53	121.34
1	G	18	ASN	CA-C-N	5.83	125.93	119.87
1	G	18	ASN	C-N-CA	5.83	125.93	119.87
1	H	818	ALA	O-C-N	5.83	129.74	122.86
1	E	159	VAL	N-CA-C	5.82	116.57	111.56
1	I	18	ASN	CA-C-N	5.82	125.92	119.87
1	I	18	ASN	C-N-CA	5.82	125.92	119.87
1	P	687	GLN	O-C-N	5.82	126.52	121.34
1	A	18	ASN	CA-C-N	5.82	125.92	119.87
1	A	18	ASN	C-N-CA	5.82	125.92	119.87
1	K	18	ASN	CA-C-N	5.81	125.91	119.87
1	K	18	ASN	C-N-CA	5.81	125.91	119.87
1	D	18	ASN	CA-C-N	5.80	125.90	119.87
1	D	18	ASN	C-N-CA	5.80	125.90	119.87
1	G	159	VAL	N-CA-C	5.80	116.55	111.56
1	H	159	VAL	N-CA-C	5.80	116.55	111.56
1	C	687	GLN	O-C-N	5.80	126.50	121.34
1	A	159	VAL	N-CA-C	5.79	116.54	111.56
1	L	159	VAL	N-CA-C	5.79	116.54	111.56
1	F	986	ILE	CB-CA-C	-5.79	103.15	111.19
1	B	159	VAL	N-CA-C	5.78	116.53	111.56
1	H	18	ASN	CA-C-N	5.78	125.88	119.87
1	H	18	ASN	C-N-CA	5.78	125.88	119.87
1	K	986	ILE	CB-CA-C	-5.78	103.16	111.19
1	N	159	VAL	N-CA-C	5.78	116.53	111.56
1	C	986	ILE	CB-CA-C	-5.78	103.16	111.19
1	I	159	VAL	N-CA-C	5.77	116.53	111.56
1	L	18	ASN	CA-C-N	5.77	125.87	119.87
1	L	18	ASN	C-N-CA	5.77	125.87	119.87
1	H	313	VAL	CB-CA-C	-5.76	103.50	110.99
1	I	986	ILE	CB-CA-C	-5.76	103.18	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	159	VAL	N-CA-C	5.76	116.52	111.56
1	O	159	VAL	N-CA-C	5.76	116.52	111.56
1	J	986	ILE	CB-CA-C	-5.76	103.18	111.19
1	G	986	ILE	CB-CA-C	-5.76	103.18	111.19
1	O	18	ASN	CA-C-N	5.76	125.86	119.87
1	O	18	ASN	C-N-CA	5.76	125.86	119.87
1	C	142	ILE	N-CA-C	5.76	116.16	107.75
1	P	159	VAL	N-CA-C	5.76	116.51	111.56
1	A	986	ILE	CB-CA-C	-5.76	103.19	111.19
1	C	159	VAL	N-CA-C	5.76	116.51	111.56
1	N	986	ILE	CB-CA-C	-5.76	103.19	111.19
1	P	986	ILE	CB-CA-C	-5.76	103.19	111.19
1	D	986	ILE	CB-CA-C	-5.75	103.19	111.19
1	D	159	VAL	N-CA-C	5.75	116.51	111.56
1	J	159	VAL	N-CA-C	5.75	116.51	111.56
1	P	262	GLN	OE1-CD-NE2	5.75	128.35	122.60
1	D	142	ILE	N-CA-C	5.75	116.15	107.75
1	K	159	VAL	N-CA-C	5.75	116.51	111.56
1	F	262	GLN	OE1-CD-NE2	5.75	128.35	122.60
1	I	262	GLN	OE1-CD-NE2	5.75	128.35	122.60
1	B	986	ILE	CB-CA-C	-5.75	103.20	111.19
1	F	159	VAL	N-CA-C	5.75	116.50	111.56
1	L	974	HIS	CA-CB-CG	-5.75	108.05	113.80
1	M	986	ILE	CB-CA-C	-5.74	103.21	111.19
1	E	986	ILE	CB-CA-C	-5.74	103.21	111.19
1	F	974	HIS	CA-CB-CG	-5.74	108.06	113.80
1	H	986	ILE	CB-CA-C	-5.74	103.21	111.19
1	P	974	HIS	CA-CB-CG	-5.73	108.07	113.80
1	G	313	VAL	CB-CA-C	-5.73	103.55	110.99
1	L	986	ILE	CB-CA-C	-5.73	103.23	111.19
1	O	986	ILE	CB-CA-C	-5.73	103.23	111.19
1	K	262	GLN	OE1-CD-NE2	5.73	128.33	122.60
1	H	974	HIS	CA-CB-CG	-5.72	108.08	113.80
1	I	974	HIS	CA-CB-CG	-5.72	108.08	113.80
1	E	313	VAL	CB-CA-C	-5.72	103.55	110.99
1	H	262	GLN	OE1-CD-NE2	5.72	128.32	122.60
1	C	313	VAL	CB-CA-C	-5.72	103.56	110.99
1	O	974	HIS	CA-CB-CG	-5.72	108.08	113.80
1	K	974	HIS	CA-CB-CG	-5.72	108.08	113.80
1	D	313	VAL	CB-CA-C	-5.72	103.56	110.99
1	I	313	VAL	CB-CA-C	-5.72	103.56	110.99
1	J	262	GLN	OE1-CD-NE2	5.72	128.32	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	VAL	CB-CA-C	-5.71	103.56	110.99
1	B	313	VAL	CB-CA-C	-5.71	103.57	110.99
1	L	262	GLN	OE1-CD-NE2	5.71	128.31	122.60
1	P	313	VAL	CB-CA-C	-5.71	103.56	110.99
1	E	262	GLN	OE1-CD-NE2	5.71	128.31	122.60
1	F	313	VAL	CB-CA-C	-5.71	103.57	110.99
1	E	974	HIS	CA-CB-CG	-5.71	108.09	113.80
1	O	313	VAL	CB-CA-C	-5.71	103.57	110.99
1	A	974	HIS	CA-CB-CG	-5.71	108.09	113.80
1	L	313	VAL	CB-CA-C	-5.71	103.57	110.99
1	N	974	HIS	CA-CB-CG	-5.70	108.10	113.80
1	M	313	VAL	CB-CA-C	-5.70	103.58	110.99
1	N	313	VAL	CB-CA-C	-5.70	103.58	110.99
1	C	974	HIS	CA-CB-CG	-5.70	108.10	113.80
1	E	96	ASP	N-CA-CB	5.70	120.73	111.21
1	I	382	ASN	CA-CB-CG	-5.70	106.90	112.60
1	K	313	VAL	CB-CA-C	-5.70	103.58	110.99
1	J	974	HIS	CA-CB-CG	-5.69	108.11	113.80
1	H	382	ASN	CA-CB-CG	-5.69	106.91	112.60
1	A	262	GLN	OE1-CD-NE2	5.69	128.29	122.60
1	B	974	HIS	CA-CB-CG	-5.69	108.11	113.80
1	D	382	ASN	CA-CB-CG	-5.69	106.91	112.60
1	I	142	ILE	N-CA-C	5.69	116.19	107.77
1	J	313	VAL	CB-CA-C	-5.69	103.60	110.99
1	O	262	GLN	OE1-CD-NE2	5.68	128.28	122.60
1	G	974	HIS	CA-CB-CG	-5.68	108.12	113.80
1	D	262	GLN	OE1-CD-NE2	5.68	128.28	122.60
1	N	262	GLN	OE1-CD-NE2	5.68	128.28	122.60
1	M	974	HIS	CA-CB-CG	-5.68	108.12	113.80
1	F	1007	PHE	CA-CB-CG	-5.68	108.12	113.80
1	J	142	ILE	N-CA-C	5.68	116.17	107.77
1	C	262	GLN	OE1-CD-NE2	5.67	128.27	122.60
1	M	142	ILE	N-CA-C	5.67	116.17	107.77
1	D	974	HIS	CA-CB-CG	-5.67	108.13	113.80
1	J	1007	PHE	CA-CB-CG	-5.67	108.13	113.80
1	L	142	ILE	N-CA-C	5.67	116.16	107.77
1	M	262	GLN	OE1-CD-NE2	5.67	128.27	122.60
1	E	1007	PHE	CA-CB-CG	-5.67	108.13	113.80
1	H	142	ILE	N-CA-C	5.67	116.16	107.77
1	H	655	MET	N-CA-C	5.67	117.02	108.46
1	M	1007	PHE	CA-CB-CG	-5.67	108.13	113.80
1	P	655	MET	N-CA-C	5.67	117.01	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	ILE	N-CA-C	5.66	116.15	107.77
1	I	655	MET	N-CA-C	5.66	117.01	108.46
1	J	655	MET	N-CA-C	5.66	117.01	108.46
1	L	382	ASN	CA-CB-CG	-5.66	106.94	112.60
1	N	142	ILE	N-CA-C	5.66	116.15	107.77
1	D	655	MET	N-CA-C	5.66	117.00	108.46
1	G	1007	PHE	CA-CB-CG	-5.66	108.14	113.80
1	E	655	MET	N-CA-C	5.66	117.00	108.46
1	F	142	ILE	N-CA-C	5.66	116.14	107.77
1	F	179	ALA	N-CA-CB	5.66	118.60	110.06
1	M	655	MET	N-CA-C	5.66	117.00	108.46
1	B	262	GLN	OE1-CD-NE2	5.65	128.25	122.60
1	E	142	ILE	N-CA-C	5.65	116.14	107.77
1	O	1007	PHE	CA-CB-CG	-5.65	108.15	113.80
1	G	142	ILE	N-CA-C	5.65	116.13	107.77
1	K	142	ILE	N-CA-C	5.65	116.14	107.77
1	O	382	ASN	CA-CB-CG	-5.65	106.95	112.60
1	A	655	MET	N-CA-C	5.65	116.99	108.46
1	B	655	MET	N-CA-C	5.65	116.99	108.46
1	L	655	MET	N-CA-C	5.65	116.99	108.46
1	O	142	ILE	N-CA-C	5.65	116.13	107.77
1	P	142	ILE	N-CA-C	5.65	116.13	107.77
1	C	655	MET	N-CA-C	5.65	116.99	108.46
1	J	553	TRP	CA-CB-CG	-5.65	102.87	113.60
1	B	382	ASN	CA-CB-CG	-5.65	106.95	112.60
1	F	655	MET	N-CA-C	5.65	116.99	108.46
1	G	655	MET	N-CA-C	5.65	116.99	108.46
1	K	655	MET	N-CA-C	5.65	116.99	108.46
1	B	142	ILE	N-CA-C	5.65	116.13	107.77
1	C	553	TRP	CA-CB-CG	-5.65	102.87	113.60
1	B	553	TRP	CA-CB-CG	-5.64	102.88	113.60
1	E	382	ASN	CA-CB-CG	-5.64	106.96	112.60
1	K	1007	PHE	CA-CB-CG	-5.64	108.16	113.80
1	A	382	ASN	CA-CB-CG	-5.64	106.96	112.60
1	E	553	TRP	CA-CB-CG	-5.64	102.88	113.60
1	M	179	ALA	N-CA-CB	5.64	118.58	110.06
1	M	382	ASN	CA-CB-CG	-5.64	106.96	112.60
1	G	382	ASN	CA-CB-CG	-5.64	106.96	112.60
1	O	179	ALA	N-CA-CB	5.64	118.57	110.06
1	J	179	ALA	N-CA-CB	5.64	118.57	110.06
1	G	262	GLN	OE1-CD-NE2	5.63	128.24	122.60
1	O	655	MET	N-CA-C	5.63	116.97	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	382	ASN	CA-CB-CG	-5.63	106.97	112.60
1	G	179	ALA	N-CA-CB	5.63	118.56	110.06
1	I	553	TRP	CA-CB-CG	-5.63	102.90	113.60
1	K	179	ALA	N-CA-CB	5.63	118.56	110.06
1	A	1007	PHE	CA-CB-CG	-5.63	108.17	113.80
1	D	553	TRP	CA-CB-CG	-5.63	102.91	113.60
1	H	1007	PHE	CA-CB-CG	-5.63	108.17	113.80
1	K	382	ASN	CA-CB-CG	-5.63	106.97	112.60
1	L	179	ALA	N-CA-CB	5.63	118.56	110.06
1	N	382	ASN	CA-CB-CG	-5.63	106.97	112.60
1	P	382	ASN	CA-CB-CG	-5.63	106.97	112.60
1	C	1007	PHE	CA-CB-CG	-5.63	108.17	113.80
1	F	382	ASN	CA-CB-CG	-5.63	106.97	112.60
1	L	1007	PHE	CA-CB-CG	-5.63	108.17	113.80
1	K	553	TRP	CA-CB-CG	-5.62	102.91	113.60
1	A	179	ALA	N-CA-CB	5.62	118.55	110.06
1	E	179	ALA	N-CA-CB	5.62	118.55	110.06
1	N	655	MET	N-CA-C	5.62	116.95	108.46
1	N	1007	PHE	CA-CB-CG	-5.62	108.18	113.80
1	P	553	TRP	CA-CB-CG	-5.62	102.92	113.60
1	A	553	TRP	CA-CB-CG	-5.62	102.92	113.60
1	M	553	TRP	CA-CB-CG	-5.62	102.92	113.60
1	F	553	TRP	CA-CB-CG	-5.62	102.92	113.60
1	O	553	TRP	CA-CB-CG	-5.62	102.92	113.60
1	N	553	TRP	CA-CB-CG	-5.62	102.93	113.60
1	H	179	ALA	N-CA-CB	5.62	118.54	110.06
1	H	553	TRP	CA-CB-CG	-5.62	102.93	113.60
1	I	1007	PHE	CA-CB-CG	-5.61	108.19	113.80
1	C	382	ASN	CA-CB-CG	-5.61	106.99	112.60
1	D	734	SER	CA-C-N	-5.61	113.28	122.54
1	D	734	SER	C-N-CA	-5.61	113.28	122.54
1	C	179	ALA	N-CA-CB	5.61	118.53	110.06
1	L	553	TRP	CA-CB-CG	-5.61	102.94	113.60
1	C	734	SER	CA-C-N	-5.61	113.29	122.54
1	C	734	SER	C-N-CA	-5.61	113.29	122.54
1	D	1007	PHE	CA-CB-CG	-5.61	108.19	113.80
1	N	179	ALA	N-CA-CB	5.61	118.53	110.06
1	B	179	ALA	N-CA-CB	5.60	118.52	110.06
1	D	938	ARG	NE-CZ-NH1	5.60	127.10	121.50
1	G	553	TRP	CA-CB-CG	-5.60	102.96	113.60
1	D	179	ALA	N-CA-CB	5.60	118.51	110.06
1	J	734	SER	CA-C-N	-5.60	113.31	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	734	SER	C-N-CA	-5.60	113.31	122.54
1	O	734	SER	CA-C-N	-5.59	113.31	122.54
1	O	734	SER	C-N-CA	-5.59	113.31	122.54
1	B	734	SER	CA-C-N	-5.59	113.31	122.54
1	B	734	SER	C-N-CA	-5.59	113.31	122.54
1	E	210	ARG	N-CA-CB	5.59	120.32	111.43
1	I	179	ALA	N-CA-CB	5.59	118.50	110.06
1	D	210	ARG	N-CA-CB	5.59	120.31	111.43
1	P	734	SER	CA-C-N	-5.59	113.32	122.54
1	P	734	SER	C-N-CA	-5.59	113.32	122.54
1	E	734	SER	CA-C-N	-5.59	113.32	122.54
1	E	734	SER	C-N-CA	-5.59	113.32	122.54
1	L	734	SER	CA-C-N	-5.58	113.33	122.54
1	L	734	SER	C-N-CA	-5.58	113.33	122.54
1	P	210	ARG	N-CA-CB	5.58	120.31	111.43
1	P	980	GLU	CA-C-N	-5.58	110.46	121.41
1	P	980	GLU	C-N-CA	-5.58	110.46	121.41
1	A	734	SER	CA-C-N	-5.58	113.33	122.54
1	A	734	SER	C-N-CA	-5.58	113.33	122.54
1	E	938	ARG	NE-CZ-NH1	5.58	127.08	121.50
1	G	734	SER	CA-C-N	-5.58	113.33	122.54
1	G	734	SER	C-N-CA	-5.58	113.33	122.54
1	I	734	SER	CA-C-N	-5.58	113.33	122.54
1	I	734	SER	C-N-CA	-5.58	113.33	122.54
1	J	210	ARG	N-CA-CB	5.58	120.31	111.43
1	K	734	SER	CA-C-N	-5.58	113.33	122.54
1	K	734	SER	C-N-CA	-5.58	113.33	122.54
1	P	179	ALA	N-CA-CB	5.58	118.49	110.06
1	M	734	SER	CA-C-N	-5.58	113.33	122.54
1	M	734	SER	C-N-CA	-5.58	113.33	122.54
1	N	734	SER	CA-C-N	-5.58	113.33	122.54
1	N	734	SER	C-N-CA	-5.58	113.33	122.54
1	B	1007	PHE	CA-CB-CG	-5.58	108.22	113.80
1	F	938	ARG	NE-CZ-NH1	5.58	127.08	121.50
1	N	210	ARG	N-CA-CB	5.58	120.30	111.43
1	O	980	GLU	CA-C-N	-5.58	110.48	121.41
1	O	980	GLU	C-N-CA	-5.58	110.48	121.41
1	A	210	ARG	N-CA-CB	5.57	120.29	111.43
1	B	210	ARG	N-CA-CB	5.57	120.29	111.43
1	C	210	ARG	N-CA-CB	5.57	120.29	111.43
1	G	210	ARG	N-CA-CB	5.57	120.29	111.43
1	J	147	ASN	N-CA-CB	-5.57	101.32	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	210	ARG	N-CA-CB	5.57	120.29	111.43
1	M	147	ASN	N-CA-CB	-5.57	101.32	110.68
1	B	675	GLN	OE1-CD-NE2	5.57	128.17	122.60
1	H	734	SER	CA-C-N	-5.57	113.35	122.54
1	H	734	SER	C-N-CA	-5.57	113.35	122.54
1	I	980	GLU	CA-C-N	-5.57	110.49	121.41
1	I	980	GLU	C-N-CA	-5.57	110.49	121.41
1	J	675	GLN	OE1-CD-NE2	5.57	128.17	122.60
1	L	147	ASN	N-CA-CB	-5.57	101.32	110.68
1	B	938	ARG	NE-CZ-NH1	5.57	127.07	121.50
1	G	147	ASN	N-CA-CB	-5.57	101.32	110.68
1	H	980	GLU	CA-C-N	-5.57	110.50	121.41
1	H	980	GLU	C-N-CA	-5.57	110.50	121.41
1	J	980	GLU	CA-C-N	-5.57	110.49	121.41
1	J	980	GLU	C-N-CA	-5.57	110.49	121.41
1	E	675	GLN	OE1-CD-NE2	5.57	128.17	122.60
1	I	210	ARG	N-CA-CB	5.57	120.28	111.43
1	M	938	ARG	NE-CZ-NH1	5.57	127.07	121.50
1	F	210	ARG	N-CA-CB	5.57	120.28	111.43
1	H	210	ARG	N-CA-CB	5.57	120.28	111.43
1	K	210	ARG	N-CA-CB	5.57	120.28	111.43
1	K	980	GLU	CA-C-N	-5.57	110.50	121.41
1	K	980	GLU	C-N-CA	-5.57	110.50	121.41
1	O	210	ARG	N-CA-CB	5.57	120.28	111.43
1	N	980	GLU	CA-C-N	-5.56	110.50	121.41
1	N	980	GLU	C-N-CA	-5.56	110.50	121.41
1	A	147	ASN	N-CA-CB	-5.56	101.33	110.68
1	E	980	GLU	CA-C-N	-5.56	110.51	121.41
1	E	980	GLU	C-N-CA	-5.56	110.51	121.41
1	I	147	ASN	N-CA-CB	-5.56	101.33	110.68
1	M	980	GLU	CA-C-N	-5.56	110.51	121.41
1	M	980	GLU	C-N-CA	-5.56	110.51	121.41
1	P	1007	PHE	CA-CB-CG	-5.56	108.24	113.80
1	A	980	GLU	CA-C-N	-5.56	110.51	121.41
1	A	980	GLU	C-N-CA	-5.56	110.51	121.41
1	F	734	SER	CA-C-N	-5.56	113.36	122.54
1	F	734	SER	C-N-CA	-5.56	113.36	122.54
1	M	210	ARG	N-CA-CB	5.56	120.27	111.43
1	I	938	ARG	NE-CZ-NH1	5.56	127.06	121.50
1	A	675	GLN	OE1-CD-NE2	5.56	128.16	122.60
1	G	675	GLN	OE1-CD-NE2	5.56	128.16	122.60
1	O	938	ARG	NE-CZ-NH1	5.56	127.06	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	ASN	N-CA-CB	-5.55	101.35	110.68
1	C	938	ARG	NE-CZ-NH1	5.55	127.05	121.50
1	H	938	ARG	NE-CZ-NH1	5.55	127.05	121.50
1	L	980	GLU	CA-C-N	-5.55	110.52	121.41
1	L	980	GLU	C-N-CA	-5.55	110.52	121.41
1	C	675	GLN	OE1-CD-NE2	5.55	128.15	122.60
1	C	980	GLU	CA-C-N	-5.55	110.53	121.41
1	C	980	GLU	C-N-CA	-5.55	110.53	121.41
1	B	980	GLU	CA-C-N	-5.55	110.53	121.41
1	B	980	GLU	C-N-CA	-5.55	110.53	121.41
1	C	147	ASN	N-CA-CB	-5.55	101.35	110.68
1	F	980	GLU	CA-C-N	-5.55	110.53	121.41
1	F	980	GLU	C-N-CA	-5.55	110.53	121.41
1	G	980	GLU	CA-C-N	-5.55	110.53	121.41
1	G	980	GLU	C-N-CA	-5.55	110.53	121.41
1	O	675	GLN	OE1-CD-NE2	5.55	128.15	122.60
1	D	980	GLU	CA-C-N	-5.55	110.53	121.41
1	D	980	GLU	C-N-CA	-5.55	110.53	121.41
1	F	147	ASN	N-CA-CB	-5.55	101.36	110.68
1	I	168	PRO	CB-CA-C	-5.55	104.31	111.46
1	O	147	ASN	N-CA-CB	-5.55	101.36	110.68
1	P	938	ARG	NE-CZ-NH1	5.55	127.05	121.50
1	C	954	ASP	CA-CB-CG	-5.54	107.06	112.60
1	A	938	ARG	NE-CZ-NH1	5.54	127.04	121.50
1	D	147	ASN	N-CA-CB	-5.54	101.37	110.68
1	L	62	TRP	N-CA-CB	-5.54	101.60	111.08
1	D	675	GLN	OE1-CD-NE2	5.54	128.14	122.60
1	J	954	ASP	CA-CB-CG	-5.54	107.06	112.60
1	K	147	ASN	N-CA-CB	-5.54	101.37	110.68
1	K	938	ARG	NE-CZ-NH1	5.54	127.04	121.50
1	O	954	ASP	CA-CB-CG	-5.54	107.06	112.60
1	H	147	ASN	N-CA-CB	-5.54	101.37	110.68
1	I	62	TRP	N-CA-CB	-5.54	101.61	111.08
1	M	168	PRO	CB-CA-C	-5.54	104.31	111.46
1	N	62	TRP	N-CA-CB	-5.54	101.61	111.08
1	P	147	ASN	N-CA-CB	-5.54	101.38	110.68
1	E	147	ASN	N-CA-CB	-5.54	101.38	110.68
1	C	168	PRO	CB-CA-C	-5.53	104.32	111.46
1	D	71	GLU	CB-CA-C	5.53	121.43	110.42
1	F	71	GLU	CB-CA-C	5.53	121.43	110.42
1	K	168	PRO	CB-CA-C	-5.53	104.32	111.46
1	H	675	GLN	OE1-CD-NE2	5.53	128.13	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	PRO	CB-CA-C	-5.53	104.33	111.46
1	E	348	PRO	CB-CA-C	-5.53	104.64	111.11
1	G	938	ARG	NE-CZ-NH1	5.53	127.03	121.50
1	O	348	PRO	CB-CA-C	-5.53	104.64	111.11
1	P	62	TRP	N-CA-CB	-5.53	101.63	111.08
1	P	954	ASP	CA-CB-CG	-5.53	107.07	112.60
1	G	71	GLU	CB-CA-C	5.53	121.42	110.42
1	J	62	TRP	N-CA-CB	-5.53	101.63	111.08
1	M	62	TRP	N-CA-CB	-5.53	101.63	111.08
1	N	147	ASN	N-CA-CB	-5.53	101.40	110.68
1	M	675	GLN	OE1-CD-NE2	5.52	128.12	122.60
1	O	71	GLU	CB-CA-C	5.52	121.41	110.42
1	D	168	PRO	CB-CA-C	-5.52	104.34	111.46
1	G	168	PRO	CB-CA-C	-5.52	104.33	111.46
1	N	348	PRO	CB-CA-C	-5.52	104.65	111.11
1	N	938	ARG	NE-CZ-NH1	5.52	127.02	121.50
1	O	508	GLU	CB-CA-C	-5.52	100.17	109.50
1	F	954	ASP	CA-CB-CG	-5.52	107.08	112.60
1	J	168	PRO	CB-CA-C	-5.52	104.34	111.46
1	L	938	ARG	NE-CZ-NH1	5.52	127.02	121.50
1	D	508	GLU	CB-CA-C	-5.52	100.17	109.50
1	D	683	PRO	CB-CA-C	-5.52	104.00	111.12
1	E	168	PRO	CB-CA-C	-5.52	104.34	111.46
1	J	71	GLU	CB-CA-C	5.52	121.40	110.42
1	L	71	GLU	CB-CA-C	5.52	121.40	110.42
1	L	954	ASP	CA-CB-CG	-5.52	107.08	112.60
1	O	62	TRP	N-CA-CB	-5.52	101.64	111.08
1	A	62	TRP	N-CA-CB	-5.52	101.64	111.08
1	A	168	PRO	CB-CA-C	-5.52	104.34	111.46
1	H	62	TRP	N-CA-CB	-5.52	101.65	111.08
1	I	675	GLN	OE1-CD-NE2	5.52	128.12	122.60
1	L	168	PRO	CB-CA-C	-5.52	104.34	111.46
1	N	967	LEU	CA-C-O	5.52	126.59	120.63
1	P	675	GLN	OE1-CD-NE2	5.52	128.12	122.60
1	F	62	TRP	N-CA-CB	-5.52	101.65	111.08
1	J	938	ARG	NE-CZ-NH1	5.52	127.02	121.50
1	K	62	TRP	N-CA-CB	-5.52	101.65	111.08
1	K	683	PRO	CB-CA-C	-5.52	104.00	111.12
1	N	168	PRO	CB-CA-C	-5.52	104.34	111.46
1	G	62	TRP	N-CA-CB	-5.51	101.65	111.08
1	J	738	PRO	N-CA-CB	5.51	108.57	103.39
1	A	71	GLU	CB-CA-C	5.51	121.39	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	71	GLU	CB-CA-C	5.51	121.39	110.42
1	E	71	GLU	CB-CA-C	5.51	121.39	110.42
1	G	348	PRO	CB-CA-C	-5.51	104.66	111.11
1	I	508	GLU	CB-CA-C	-5.51	100.19	109.50
1	N	954	ASP	CA-CB-CG	-5.51	107.09	112.60
1	A	954	ASP	CA-CB-CG	-5.51	107.09	112.60
1	B	348	PRO	CB-CA-C	-5.51	104.66	111.11
1	C	683	PRO	CB-CA-C	-5.51	104.01	111.12
1	D	62	TRP	N-CA-CB	-5.51	101.66	111.08
1	H	168	PRO	CB-CA-C	-5.51	104.35	111.46
1	L	675	GLN	OE1-CD-NE2	5.51	128.11	122.60
1	O	683	PRO	CB-CA-C	-5.51	104.01	111.12
1	C	348	PRO	CB-CA-C	-5.51	104.67	111.11
1	F	683	PRO	CB-CA-C	-5.51	104.02	111.12
1	P	508	GLU	CB-CA-C	-5.51	100.19	109.50
1	C	62	TRP	N-CA-CB	-5.50	101.67	111.08
1	G	508	GLU	CB-CA-C	-5.50	100.20	109.50
1	K	71	GLU	CB-CA-C	5.50	121.38	110.42
1	O	168	PRO	CB-CA-C	-5.50	104.36	111.46
1	A	508	GLU	CB-CA-C	-5.50	100.20	109.50
1	B	954	ASP	CA-CB-CG	-5.50	107.10	112.60
1	E	62	TRP	N-CA-CB	-5.50	101.67	111.08
1	F	508	GLU	CB-CA-C	-5.50	100.20	109.50
1	H	71	GLU	CB-CA-C	5.50	121.37	110.42
1	I	348	PRO	CB-CA-C	-5.50	104.67	111.11
1	I	524	LEU	CB-CA-C	-5.50	100.45	110.63
1	L	348	PRO	CB-CA-C	-5.50	104.67	111.11
1	M	71	GLU	CB-CA-C	5.50	121.37	110.42
1	P	71	GLU	CB-CA-C	5.50	121.37	110.42
1	P	168	PRO	CB-CA-C	-5.50	104.36	111.46
1	H	508	GLU	CB-CA-C	-5.50	100.20	109.50
1	M	508	GLU	CB-CA-C	-5.50	100.20	109.50
1	J	508	GLU	CB-CA-C	-5.50	100.20	109.50
1	B	683	PRO	CB-CA-C	-5.50	104.03	111.12
1	D	954	ASP	CA-CB-CG	-5.50	107.10	112.60
1	F	348	PRO	CB-CA-C	-5.50	104.68	111.11
1	I	71	GLU	CB-CA-C	5.50	121.36	110.42
1	N	675	GLN	OE1-CD-NE2	5.50	128.10	122.60
1	L	508	GLU	CB-CA-C	-5.50	100.21	109.50
1	N	508	GLU	CB-CA-C	-5.50	100.21	109.50
1	B	62	TRP	N-CA-CB	-5.49	101.69	111.08
1	F	168	PRO	CB-CA-C	-5.49	104.37	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	675	GLN	OE1-CD-NE2	5.49	128.09	122.60
1	F	967	LEU	CA-C-O	5.49	126.56	120.63
1	H	967	LEU	CA-C-O	5.49	126.56	120.63
1	I	683	PRO	CB-CA-C	-5.49	104.03	111.12
1	J	683	PRO	CB-CA-C	-5.49	104.03	111.12
1	A	683	PRO	CB-CA-C	-5.49	104.03	111.12
1	P	738	PRO	N-CA-CB	5.49	108.55	103.39
1	C	738	PRO	N-CA-CB	5.49	108.55	103.39
1	G	683	PRO	CB-CA-C	-5.49	104.04	111.12
1	N	683	PRO	CB-CA-C	-5.49	104.04	111.12
1	D	738	PRO	N-CA-CB	5.49	108.55	103.39
1	E	508	GLU	CB-CA-C	-5.49	100.22	109.50
1	H	348	PRO	CB-CA-C	-5.49	104.69	111.11
1	H	524	LEU	CB-CA-C	-5.49	100.47	110.63
1	H	683	PRO	CB-CA-C	-5.49	104.04	111.12
1	N	71	GLU	CB-CA-C	5.49	121.34	110.42
1	B	524	LEU	CB-CA-C	-5.49	100.48	110.63
1	A	348	PRO	CB-CA-C	-5.49	104.69	111.11
1	B	71	GLU	CB-CA-C	5.49	121.33	110.42
1	D	348	PRO	CB-CA-C	-5.49	104.69	111.11
1	J	524	LEU	CB-CA-C	-5.49	100.48	110.63
1	K	508	GLU	CB-CA-C	-5.49	100.23	109.50
1	O	524	LEU	CB-CA-C	-5.49	100.48	110.63
1	P	348	PRO	CB-CA-C	-5.49	104.69	111.11
1	P	683	PRO	CB-CA-C	-5.49	104.04	111.12
1	P	524	LEU	CB-CA-C	-5.48	100.48	110.63
1	B	508	GLU	CB-CA-C	-5.48	100.23	109.50
1	E	683	PRO	CB-CA-C	-5.48	104.05	111.12
1	F	524	LEU	CB-CA-C	-5.48	100.49	110.63
1	I	954	ASP	CA-CB-CG	-5.48	107.12	112.60
1	K	675	GLN	OE1-CD-NE2	5.48	128.08	122.60
1	L	524	LEU	CB-CA-C	-5.48	100.49	110.63
1	L	683	PRO	CB-CA-C	-5.48	104.05	111.12
1	M	524	LEU	CB-CA-C	-5.48	100.49	110.63
1	A	524	LEU	CB-CA-C	-5.48	100.49	110.63
1	C	508	GLU	CB-CA-C	-5.48	100.24	109.50
1	G	954	ASP	CA-CB-CG	-5.48	107.12	112.60
1	H	954	ASP	CA-CB-CG	-5.48	107.12	112.60
1	M	954	ASP	CA-CB-CG	-5.48	107.12	112.60
1	D	524	LEU	CB-CA-C	-5.48	100.50	110.63
1	D	967	LEU	CA-C-O	5.48	126.55	120.63
1	I	967	LEU	CA-C-O	5.48	126.55	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	683	PRO	CB-CA-C	-5.48	104.06	111.12
1	P	967	LEU	CA-C-O	5.48	126.54	120.63
1	C	524	LEU	CB-CA-C	-5.47	100.50	110.63
1	H	738	PRO	N-CA-CB	5.47	108.54	103.39
1	M	738	PRO	N-CA-CB	5.47	108.54	103.39
1	G	524	LEU	CB-CA-C	-5.47	100.51	110.63
1	J	710	GLU	CB-CA-C	-5.47	100.17	110.51
1	K	524	LEU	CB-CA-C	-5.47	100.51	110.63
1	I	710	GLU	CB-CA-C	-5.47	100.17	110.51
1	O	710	GLU	CB-CA-C	-5.47	100.17	110.51
1	D	710	GLU	CB-CA-C	-5.47	100.18	110.51
1	J	348	PRO	CB-CA-C	-5.47	104.72	111.11
1	L	967	LEU	CA-C-O	5.47	126.53	120.63
1	E	524	LEU	CB-CA-C	-5.46	100.52	110.63
1	E	710	GLU	CB-CA-C	-5.46	100.18	110.51
1	C	710	GLU	CB-CA-C	-5.46	100.19	110.51
1	K	348	PRO	CB-CA-C	-5.46	104.72	111.11
1	A	967	LEU	CA-C-O	5.46	126.53	120.63
1	B	710	GLU	CB-CA-C	-5.46	100.19	110.51
1	C	967	LEU	CA-C-O	5.46	126.53	120.63
1	N	524	LEU	CB-CA-C	-5.46	100.53	110.63
1	O	967	LEU	CA-C-O	5.46	126.53	120.63
1	P	710	GLU	CB-CA-C	-5.46	100.19	110.51
1	A	710	GLU	CB-CA-C	-5.46	100.19	110.51
1	N	710	GLU	CB-CA-C	-5.46	100.19	110.51
1	G	710	GLU	CB-CA-C	-5.46	100.19	110.51
1	M	710	GLU	CB-CA-C	-5.46	100.19	110.51
1	B	967	LEU	CA-C-O	5.46	126.52	120.63
1	F	710	GLU	CB-CA-C	-5.46	100.20	110.51
1	I	750	GLU	N-CA-CB	-5.46	101.44	111.37
1	M	348	PRO	CB-CA-C	-5.46	104.73	111.11
1	N	738	PRO	N-CA-CB	5.46	108.52	103.39
1	E	954	ASP	CA-CB-CG	-5.46	107.14	112.60
1	K	954	ASP	CA-CB-CG	-5.46	107.14	112.60
1	A	738	PRO	N-CA-CB	5.45	108.52	103.39
1	E	738	PRO	N-CA-CB	5.45	108.52	103.39
1	E	967	LEU	CA-C-O	5.45	126.52	120.63
1	I	738	PRO	N-CA-CB	5.45	108.52	103.39
1	G	967	LEU	CA-C-O	5.45	126.52	120.63
1	L	144	ASP	CA-CB-CG	-5.45	107.15	112.60
1	L	710	GLU	CB-CA-C	-5.45	100.20	110.51
1	N	750	GLU	N-CA-CB	-5.45	101.45	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	738	PRO	N-CA-CB	5.45	108.51	103.39
1	J	750	GLU	N-CA-CB	-5.45	101.45	111.37
1	B	750	GLU	N-CA-CB	-5.45	101.46	111.37
1	H	750	GLU	N-CA-CB	-5.45	101.46	111.37
1	M	750	GLU	N-CA-CB	-5.45	101.46	111.37
1	H	775	GLN	CA-C-N	-5.44	114.26	122.81
1	H	775	GLN	C-N-CA	-5.44	114.26	122.81
1	P	750	GLU	N-CA-CB	-5.44	101.46	111.37
1	G	750	GLU	N-CA-CB	-5.44	101.47	111.37
1	B	738	PRO	N-CA-CB	5.44	108.50	103.39
1	F	738	PRO	N-CA-CB	5.44	108.50	103.39
1	G	775	GLN	CA-C-N	-5.44	114.27	122.81
1	G	775	GLN	C-N-CA	-5.44	114.27	122.81
1	J	775	GLN	CA-C-N	-5.44	114.27	122.81
1	J	775	GLN	C-N-CA	-5.44	114.27	122.81
1	L	738	PRO	N-CA-CB	5.44	108.50	103.39
1	O	143	PHE	CB-CA-C	-5.44	102.08	110.78
1	O	738	PRO	N-CA-CB	5.44	108.50	103.39
1	E	750	GLU	N-CA-CB	-5.44	101.47	111.37
1	H	710	GLU	CB-CA-C	-5.44	100.23	110.51
1	K	710	GLU	CB-CA-C	-5.44	100.23	110.51
1	K	750	GLU	N-CA-CB	-5.44	101.48	111.37
1	F	750	GLU	N-CA-CB	-5.43	101.48	111.37
1	I	143	PHE	CB-CA-C	-5.43	102.09	110.78
1	L	750	GLU	N-CA-CB	-5.43	101.48	111.37
1	M	144	ASP	CA-CB-CG	-5.43	107.17	112.60
1	D	775	GLN	CA-C-N	-5.43	114.28	122.81
1	D	775	GLN	C-N-CA	-5.43	114.28	122.81
1	E	144	ASP	CA-CB-CG	-5.43	107.17	112.60
1	K	144	ASP	CA-CB-CG	-5.43	107.17	112.60
1	A	750	GLU	N-CA-CB	-5.43	101.49	111.37
1	C	750	GLU	N-CA-CB	-5.43	101.49	111.37
1	I	144	ASP	CA-CB-CG	-5.43	107.17	112.60
1	J	967	LEU	CA-C-O	5.43	126.49	120.63
1	M	967	LEU	CA-C-O	5.43	126.49	120.63
1	O	750	GLU	N-CA-CB	-5.43	101.49	111.37
1	I	212	VAL	N-CA-CB	5.42	118.90	111.41
1	K	738	PRO	N-CA-CB	5.42	108.49	103.39
1	F	143	PHE	CB-CA-C	-5.42	102.10	110.78
1	G	144	ASP	CA-CB-CG	-5.42	107.18	112.60
1	L	775	GLN	CA-C-N	-5.42	114.30	122.81
1	L	775	GLN	C-N-CA	-5.42	114.30	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	143	PHE	CB-CA-C	-5.42	102.10	110.78
1	C	144	ASP	CA-CB-CG	-5.42	107.18	112.60
1	J	64	PRO	CB-CA-C	-5.42	103.76	111.68
1	K	967	LEU	CA-C-O	5.42	126.48	120.63
1	I	938	ARG	CG-CD-NE	-5.42	100.08	112.00
1	N	143	PHE	CB-CA-C	-5.42	102.11	110.78
1	O	212	VAL	N-CA-CB	5.42	118.89	111.41
1	A	144	ASP	CA-CB-CG	-5.42	107.18	112.60
1	B	64	PRO	CB-CA-C	-5.42	103.77	111.68
1	B	144	ASP	CA-CB-CG	-5.42	107.18	112.60
1	D	143	PHE	CB-CA-C	-5.42	102.11	110.78
1	M	775	GLN	CA-C-N	-5.42	114.31	122.81
1	M	775	GLN	C-N-CA	-5.42	114.31	122.81
1	P	64	PRO	CB-CA-C	-5.42	103.77	111.68
1	A	143	PHE	CB-CA-C	-5.41	102.12	110.78
1	A	775	GLN	CA-C-N	-5.41	114.31	122.81
1	A	775	GLN	C-N-CA	-5.41	114.31	122.81
1	B	143	PHE	CB-CA-C	-5.41	102.12	110.78
1	J	143	PHE	CB-CA-C	-5.41	102.12	110.78
1	L	212	VAL	N-CA-CB	5.41	118.88	111.41
1	M	143	PHE	CB-CA-C	-5.41	102.12	110.78
1	E	775	GLN	CA-C-N	-5.41	114.31	122.81
1	E	775	GLN	C-N-CA	-5.41	114.31	122.81
1	D	750	GLU	N-CA-CB	-5.41	101.52	111.37
1	E	961	ARG	CA-C-N	-5.41	114.83	122.94
1	E	961	ARG	C-N-CA	-5.41	114.83	122.94
1	H	938	ARG	CG-CD-NE	-5.41	100.10	112.00
1	O	775	GLN	CA-C-N	-5.41	114.32	122.81
1	O	775	GLN	C-N-CA	-5.41	114.32	122.81
1	O	938	ARG	CG-CD-NE	-5.41	100.10	112.00
1	I	542	MET	N-CA-C	5.41	117.05	108.67
1	J	938	ARG	CG-CD-NE	-5.41	100.11	112.00
1	K	775	GLN	CA-C-N	-5.41	114.32	122.81
1	K	775	GLN	C-N-CA	-5.41	114.32	122.81
1	M	64	PRO	CB-CA-C	-5.41	103.79	111.68
1	N	212	VAL	N-CA-CB	5.41	118.87	111.41
1	O	64	PRO	CB-CA-C	-5.41	103.79	111.68
1	P	144	ASP	CA-CB-CG	-5.41	107.19	112.60
1	P	775	GLN	CA-C-N	-5.41	114.32	122.81
1	P	775	GLN	C-N-CA	-5.41	114.32	122.81
1	E	938	ARG	CG-CD-NE	-5.40	100.11	112.00
1	C	64	PRO	CB-CA-C	-5.40	103.79	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	938	ARG	CG-CD-NE	-5.40	100.11	112.00
1	H	144	ASP	CA-CB-CG	-5.40	107.20	112.60
1	L	143	PHE	CB-CA-C	-5.40	102.14	110.78
1	N	144	ASP	CA-CB-CG	-5.40	107.20	112.60
1	O	682	LEU	CA-C-O	5.40	124.73	120.19
1	B	775	GLN	CA-C-N	-5.40	114.33	122.81
1	B	775	GLN	C-N-CA	-5.40	114.33	122.81
1	G	938	ARG	CG-CD-NE	-5.40	100.12	112.00
1	J	144	ASP	CA-CB-CG	-5.40	107.20	112.60
1	N	961	ARG	CA-C-N	-5.40	114.84	122.94
1	N	961	ARG	C-N-CA	-5.40	114.84	122.94
1	E	64	PRO	CB-CA-C	-5.40	103.80	111.68
1	I	961	ARG	CA-C-N	-5.40	114.84	122.94
1	I	961	ARG	C-N-CA	-5.40	114.84	122.94
1	O	542	MET	N-CA-C	5.40	117.04	108.67
1	A	938	ARG	CG-CD-NE	-5.40	100.13	112.00
1	F	775	GLN	CA-C-N	-5.40	114.34	122.81
1	F	775	GLN	C-N-CA	-5.40	114.34	122.81
1	H	143	PHE	CB-CA-C	-5.40	102.14	110.78
1	K	143	PHE	CB-CA-C	-5.40	102.14	110.78
1	M	938	ARG	CG-CD-NE	-5.40	100.13	112.00
1	A	212	VAL	N-CA-CB	5.40	118.86	111.41
1	G	143	PHE	CB-CA-C	-5.40	102.15	110.78
1	M	212	VAL	N-CA-CB	5.40	118.86	111.41
1	N	775	GLN	CA-C-N	-5.40	114.34	122.81
1	N	775	GLN	C-N-CA	-5.40	114.34	122.81
1	C	775	GLN	CA-C-N	-5.39	114.34	122.81
1	C	775	GLN	C-N-CA	-5.39	114.34	122.81
1	F	212	VAL	N-CA-CB	5.39	118.86	111.41
1	F	682	LEU	CA-C-O	5.39	124.72	120.19
1	F	938	ARG	CG-CD-NE	-5.39	100.13	112.00
1	H	64	PRO	CB-CA-C	-5.39	103.80	111.68
1	B	212	VAL	N-CA-CB	5.39	118.85	111.41
1	I	775	GLN	CA-C-N	-5.39	114.34	122.81
1	I	775	GLN	C-N-CA	-5.39	114.34	122.81
1	L	938	ARG	CG-CD-NE	-5.39	100.13	112.00
1	N	938	ARG	CG-CD-NE	-5.39	100.14	112.00
1	E	212	VAL	N-CA-CB	5.39	118.85	111.41
1	P	961	ARG	CA-C-N	-5.39	114.85	122.94
1	P	961	ARG	C-N-CA	-5.39	114.85	122.94
1	G	212	VAL	N-CA-CB	5.39	118.85	111.41
1	O	961	ARG	CA-C-N	-5.39	114.86	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	961	ARG	C-N-CA	-5.39	114.86	122.94
1	K	938	ARG	CG-CD-NE	-5.39	100.15	112.00
1	A	961	ARG	CA-C-N	-5.39	114.86	122.94
1	A	961	ARG	C-N-CA	-5.39	114.86	122.94
1	E	143	PHE	CB-CA-C	-5.39	102.16	110.78
1	I	64	PRO	CB-CA-C	-5.39	103.81	111.68
1	L	961	ARG	CA-C-N	-5.39	114.86	122.94
1	L	961	ARG	C-N-CA	-5.39	114.86	122.94
1	M	542	MET	N-CA-C	5.39	117.02	108.67
1	C	143	PHE	CB-CA-C	-5.38	102.16	110.78
1	J	961	ARG	CA-C-N	-5.38	114.86	122.94
1	J	961	ARG	C-N-CA	-5.38	114.86	122.94
1	L	682	LEU	CA-C-O	5.38	124.71	120.19
1	P	938	ARG	CG-CD-NE	-5.38	100.15	112.00
1	C	542	MET	N-CA-C	5.38	117.01	108.67
1	D	144	ASP	CA-CB-CG	-5.38	107.22	112.60
1	F	64	PRO	CB-CA-C	-5.38	103.82	111.68
1	G	64	PRO	CB-CA-C	-5.38	103.82	111.68
1	C	938	ARG	CG-CD-NE	-5.38	100.16	112.00
1	G	542	MET	N-CA-C	5.38	117.01	108.67
1	K	961	ARG	CA-C-N	-5.38	114.87	122.94
1	K	961	ARG	C-N-CA	-5.38	114.87	122.94
1	L	542	MET	N-CA-C	5.38	117.01	108.67
1	B	961	ARG	CA-C-N	-5.38	114.87	122.94
1	B	961	ARG	C-N-CA	-5.38	114.87	122.94
1	P	212	VAL	N-CA-CB	5.38	118.83	111.41
1	J	212	VAL	N-CA-CB	5.38	118.83	111.41
1	M	961	ARG	CA-C-N	-5.38	114.87	122.94
1	M	961	ARG	C-N-CA	-5.38	114.87	122.94
1	B	542	MET	N-CA-C	5.38	117.00	108.67
1	B	938	ARG	CG-CD-NE	-5.38	100.17	112.00
1	C	961	ARG	CA-C-N	-5.38	114.88	122.94
1	C	961	ARG	C-N-CA	-5.38	114.88	122.94
1	D	961	ARG	CA-C-N	-5.38	114.88	122.94
1	D	961	ARG	C-N-CA	-5.38	114.88	122.94
1	F	961	ARG	CA-C-N	-5.38	114.87	122.94
1	F	961	ARG	C-N-CA	-5.38	114.87	122.94
1	M	682	LEU	CA-C-O	5.38	124.71	120.19
1	N	64	PRO	CB-CA-C	-5.38	103.83	111.68
1	D	212	VAL	N-CA-CB	5.37	118.82	111.41
1	D	682	LEU	CA-C-O	5.37	124.70	120.19
1	I	947	GLY	CA-C-N	5.37	125.84	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	947	GLY	C-N-CA	5.37	125.84	120.04
1	J	1011	ALA	N-CA-C	5.37	119.10	112.54
1	N	542	MET	N-CA-C	5.37	117.00	108.67
1	B	682	LEU	CA-C-O	5.37	124.70	120.19
1	D	64	PRO	CB-CA-C	-5.37	103.84	111.68
1	K	64	PRO	CB-CA-C	-5.37	103.84	111.68
1	G	961	ARG	CA-C-N	-5.37	114.89	122.94
1	G	961	ARG	C-N-CA	-5.37	114.89	122.94
1	O	144	ASP	CA-CB-CG	-5.37	107.23	112.60
1	C	212	VAL	N-CA-CB	5.37	118.81	111.41
1	E	542	MET	N-CA-C	5.37	116.99	108.67
1	F	144	ASP	CA-CB-CG	-5.37	107.23	112.60
1	H	212	VAL	N-CA-CB	5.37	118.81	111.41
1	H	961	ARG	CA-C-N	-5.37	114.89	122.94
1	H	961	ARG	C-N-CA	-5.37	114.89	122.94
1	N	1011	ALA	N-CA-C	5.37	119.09	112.54
1	A	542	MET	N-CA-C	5.36	116.98	108.67
1	F	1011	ALA	N-CA-C	5.36	119.08	112.54
1	B	369	GLU	N-CA-C	5.36	117.55	111.11
1	K	212	VAL	N-CA-CB	5.36	118.81	111.41
1	P	542	MET	N-CA-C	5.36	116.98	108.67
1	K	682	LEU	CA-C-O	5.36	124.69	120.19
1	A	1011	ALA	N-CA-C	5.36	119.08	112.54
1	D	542	MET	N-CA-C	5.36	116.97	108.67
1	F	947	GLY	CA-C-N	5.36	125.83	120.04
1	F	947	GLY	C-N-CA	5.36	125.83	120.04
1	K	542	MET	N-CA-C	5.36	116.97	108.67
1	F	542	MET	N-CA-C	5.36	116.97	108.67
1	H	542	MET	N-CA-C	5.36	116.97	108.67
1	O	1011	ALA	N-CA-C	5.36	119.07	112.54
1	D	1011	ALA	N-CA-C	5.35	119.07	112.54
1	H	369	GLU	N-CA-C	5.35	117.53	111.11
1	A	64	PRO	CB-CA-C	-5.35	103.86	111.68
1	I	369	GLU	N-CA-C	5.35	117.53	111.11
1	B	1011	ALA	N-CA-C	5.35	119.07	112.54
1	J	542	MET	N-CA-C	5.35	116.96	108.67
1	L	947	GLY	CA-C-N	5.35	125.82	120.04
1	L	947	GLY	C-N-CA	5.35	125.82	120.04
1	E	1011	ALA	N-CA-C	5.35	119.06	112.54
1	L	64	PRO	CB-CA-C	-5.35	103.87	111.68
1	K	1011	ALA	N-CA-C	5.35	119.06	112.54
1	D	947	GLY	CA-C-N	5.34	125.81	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	947	GLY	C-N-CA	5.34	125.81	120.04
1	L	1011	ALA	N-CA-C	5.34	119.06	112.54
1	C	1011	ALA	N-CA-C	5.34	119.06	112.54
1	E	369	GLU	N-CA-C	5.34	117.52	111.11
1	E	682	LEU	CA-C-O	5.34	124.68	120.19
1	L	369	GLU	N-CA-C	5.34	117.52	111.11
1	O	369	GLU	N-CA-C	5.34	117.52	111.11
1	A	682	LEU	CA-C-O	5.34	124.68	120.19
1	G	1011	ALA	N-CA-C	5.34	119.05	112.54
1	I	1011	ALA	N-CA-C	5.34	119.06	112.54
1	P	682	LEU	CA-C-O	5.34	124.67	120.19
1	C	947	GLY	CA-C-N	5.34	125.80	120.04
1	C	947	GLY	C-N-CA	5.34	125.80	120.04
1	A	369	GLU	N-CA-C	5.33	117.51	111.11
1	H	947	GLY	CA-C-N	5.33	125.80	120.04
1	H	947	GLY	C-N-CA	5.33	125.80	120.04
1	N	369	GLU	N-CA-C	5.33	117.51	111.11
1	P	369	GLU	N-CA-C	5.33	117.51	111.11
1	M	369	GLU	N-CA-C	5.33	117.51	111.11
1	M	1011	ALA	N-CA-C	5.33	119.04	112.54
1	P	1011	ALA	N-CA-C	5.33	119.04	112.54
1	J	682	LEU	CA-C-O	5.32	124.66	120.19
1	I	310	ARG	CA-C-N	-5.32	115.48	122.99
1	I	310	ARG	C-N-CA	-5.32	115.48	122.99
1	C	682	LEU	CA-C-O	5.32	124.66	120.19
1	A	947	GLY	CA-C-N	5.32	125.78	120.04
1	A	947	GLY	C-N-CA	5.32	125.78	120.04
1	H	1011	ALA	N-CA-C	5.32	119.03	112.54
1	N	947	GLY	CA-C-N	5.32	125.78	120.04
1	N	947	GLY	C-N-CA	5.32	125.78	120.04
1	N	310	ARG	CA-C-N	-5.32	115.49	122.99
1	N	310	ARG	C-N-CA	-5.32	115.49	122.99
1	F	369	GLU	N-CA-C	5.31	117.49	111.11
1	K	947	GLY	CA-C-N	5.31	125.78	120.04
1	K	947	GLY	C-N-CA	5.31	125.78	120.04
1	G	947	GLY	CA-C-N	5.31	125.78	120.04
1	G	947	GLY	C-N-CA	5.31	125.78	120.04
1	H	682	LEU	CA-C-O	5.31	124.65	120.19
1	L	310	ARG	CA-C-N	-5.31	115.50	122.99
1	L	310	ARG	C-N-CA	-5.31	115.50	122.99
1	D	369	GLU	N-CA-C	5.31	117.48	111.11
1	K	369	GLU	N-CA-C	5.31	117.48	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	1006	GLU	CG-CD-OE2	-5.31	106.19	118.40
1	E	947	GLY	CA-C-N	5.31	125.77	120.04
1	E	947	GLY	C-N-CA	5.31	125.77	120.04
1	G	682	LEU	CA-C-O	5.31	124.65	120.19
1	I	682	LEU	CA-C-O	5.31	124.65	120.19
1	E	508	GLU	CA-CB-CG	5.30	124.71	114.10
1	H	508	GLU	CA-CB-CG	5.30	124.71	114.10
1	K	508	GLU	CA-CB-CG	5.30	124.71	114.10
1	M	947	GLY	CA-C-N	5.30	125.77	120.04
1	M	947	GLY	C-N-CA	5.30	125.77	120.04
1	B	272	ALA	CA-C-N	5.30	126.47	119.84
1	B	272	ALA	C-N-CA	5.30	126.47	119.84
1	B	947	GLY	CA-C-N	5.30	125.77	120.04
1	B	947	GLY	C-N-CA	5.30	125.77	120.04
1	E	1006	GLU	CG-CD-OE2	-5.30	106.21	118.40
1	G	369	GLU	N-CA-C	5.30	117.47	111.11
1	J	1006	GLU	CG-CD-OE2	-5.30	106.20	118.40
1	B	1006	GLU	CG-CD-OE2	-5.30	106.21	118.40
1	C	369	GLU	N-CA-C	5.30	117.47	111.11
1	P	1006	GLU	CG-CD-OE2	-5.30	106.21	118.40
1	N	508	GLU	CA-CB-CG	5.30	124.70	114.10
1	N	682	LEU	CA-C-O	5.30	124.64	120.19
1	A	98	PRO	N-CA-C	-5.30	102.84	111.68
1	B	310	ARG	CA-C-N	-5.30	115.52	122.99
1	B	310	ARG	C-N-CA	-5.30	115.52	122.99
1	C	508	GLU	CA-CB-CG	5.30	124.69	114.10
1	I	272	ALA	CA-C-N	5.30	126.46	119.84
1	I	272	ALA	C-N-CA	5.30	126.46	119.84
1	J	369	GLU	N-CA-C	5.30	117.47	111.11
1	L	272	ALA	CA-C-N	5.29	126.46	119.84
1	L	272	ALA	C-N-CA	5.29	126.46	119.84
1	I	508	GLU	CA-CB-CG	5.29	124.69	114.10
1	O	272	ALA	CA-C-N	5.29	126.46	119.84
1	O	272	ALA	C-N-CA	5.29	126.46	119.84
1	F	1006	GLU	CG-CD-OE2	-5.29	106.23	118.40
1	L	508	GLU	CA-CB-CG	5.29	124.68	114.10
1	P	947	GLY	CA-C-N	5.29	125.75	120.04
1	P	947	GLY	C-N-CA	5.29	125.75	120.04
1	A	508	GLU	CA-CB-CG	5.29	124.68	114.10
1	A	1006	GLU	CG-CD-OE2	-5.29	106.23	118.40
1	K	310	ARG	CA-C-N	-5.29	115.53	122.99
1	K	310	ARG	C-N-CA	-5.29	115.53	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	508	GLU	CA-CB-CG	5.29	124.68	114.10
1	F	508	GLU	CA-CB-CG	5.29	124.68	114.10
1	J	98	PRO	N-CA-C	-5.29	102.85	111.68
1	M	272	ALA	CA-C-N	5.29	126.45	119.84
1	M	272	ALA	C-N-CA	5.29	126.45	119.84
1	A	272	ALA	CA-C-N	5.29	126.45	119.84
1	A	272	ALA	C-N-CA	5.29	126.45	119.84
1	C	272	ALA	CA-C-N	5.29	126.45	119.84
1	C	272	ALA	C-N-CA	5.29	126.45	119.84
1	D	1006	GLU	CG-CD-OE2	-5.29	106.24	118.40
1	G	1006	GLU	CG-CD-OE2	-5.29	106.24	118.40
1	C	310	ARG	CA-C-N	-5.28	115.54	122.99
1	C	310	ARG	C-N-CA	-5.28	115.54	122.99
1	C	1006	GLU	CG-CD-OE2	-5.28	106.25	118.40
1	I	1006	GLU	CG-CD-OE2	-5.28	106.25	118.40
1	J	947	GLY	CA-C-N	5.28	125.75	120.04
1	J	947	GLY	C-N-CA	5.28	125.75	120.04
1	N	1006	GLU	CG-CD-OE2	-5.28	106.25	118.40
1	M	508	GLU	CA-CB-CG	5.28	124.66	114.10
1	K	739	HIS	N-CA-CB	-5.28	102.41	110.65
1	K	1006	GLU	CG-CD-OE2	-5.28	106.25	118.40
1	P	508	GLU	CA-CB-CG	5.28	124.66	114.10
1	D	272	ALA	CA-C-N	5.28	126.44	119.84
1	D	272	ALA	C-N-CA	5.28	126.44	119.84
1	G	310	ARG	CA-C-N	-5.28	115.55	122.99
1	G	310	ARG	C-N-CA	-5.28	115.55	122.99
1	J	508	GLU	CA-CB-CG	5.28	124.66	114.10
1	O	508	GLU	CA-CB-CG	5.28	124.66	114.10
1	J	310	ARG	CA-C-N	-5.28	115.55	122.99
1	J	310	ARG	C-N-CA	-5.28	115.55	122.99
1	L	1006	GLU	CG-CD-OE2	-5.28	106.27	118.40
1	P	272	ALA	CA-C-N	5.28	126.43	119.84
1	P	272	ALA	C-N-CA	5.28	126.43	119.84
1	H	272	ALA	CA-C-N	5.27	126.43	119.84
1	H	272	ALA	C-N-CA	5.27	126.43	119.84
1	K	272	ALA	CA-C-N	5.27	126.43	119.84
1	K	272	ALA	C-N-CA	5.27	126.43	119.84
1	A	310	ARG	CA-C-N	-5.27	115.56	122.99
1	A	310	ARG	C-N-CA	-5.27	115.56	122.99
1	B	370	GLN	N-CA-CB	-5.27	102.37	110.01
1	H	1006	GLU	CG-CD-OE2	-5.27	106.28	118.40
1	M	739	HIS	N-CA-CB	-5.27	102.43	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	958	ASN	N-CA-CB	5.27	121.33	111.53
1	D	508	GLU	CA-CB-CG	5.27	124.64	114.10
1	L	370	GLN	N-CA-CB	-5.27	102.37	110.01
1	M	1006	GLU	CG-CD-OE2	-5.27	106.29	118.40
1	B	98	PRO	N-CA-C	-5.27	102.89	111.68
1	C	370	GLN	N-CA-CB	-5.27	102.38	110.01
1	C	723	ALA	O-C-N	5.26	128.79	123.26
1	B	739	HIS	N-CA-CB	-5.26	102.44	110.65
1	G	508	GLU	CA-CB-CG	5.26	124.63	114.10
1	N	739	HIS	N-CA-CB	-5.26	102.44	110.65
1	D	739	HIS	N-CA-CB	-5.26	102.44	110.65
1	P	98	PRO	N-CA-C	-5.26	102.89	111.68
1	A	739	HIS	N-CA-CB	-5.26	102.45	110.65
1	H	370	GLN	N-CA-CB	-5.26	102.38	110.01
1	O	310	ARG	CA-C-N	-5.26	115.58	122.99
1	O	310	ARG	C-N-CA	-5.26	115.58	122.99
1	P	739	HIS	N-CA-CB	-5.26	102.44	110.65
1	C	98	PRO	N-CA-C	-5.26	102.90	111.68
1	F	98	PRO	N-CA-C	-5.26	102.90	111.68
1	J	272	ALA	CA-C-N	5.26	126.41	119.84
1	J	272	ALA	C-N-CA	5.26	126.41	119.84
1	D	310	ARG	CA-C-N	-5.26	115.58	122.99
1	D	310	ARG	C-N-CA	-5.26	115.58	122.99
1	E	98	PRO	N-CA-C	-5.26	102.90	111.68
1	E	272	ALA	CA-C-N	5.26	126.41	119.84
1	E	272	ALA	C-N-CA	5.26	126.41	119.84
1	E	739	HIS	N-CA-CB	-5.26	102.45	110.65
1	F	272	ALA	CA-C-N	5.26	126.41	119.84
1	F	272	ALA	C-N-CA	5.26	126.41	119.84
1	I	98	PRO	N-CA-C	-5.26	102.90	111.68
1	N	272	ALA	CA-C-N	5.26	126.41	119.84
1	N	272	ALA	C-N-CA	5.26	126.41	119.84
1	O	739	HIS	N-CA-CB	-5.26	102.45	110.65
1	D	98	PRO	N-CA-C	-5.25	102.90	111.68
1	E	958	ASN	N-CA-CB	5.25	121.30	111.53
1	G	739	HIS	N-CA-CB	-5.25	102.45	110.65
1	H	98	PRO	N-CA-C	-5.25	102.91	111.68
1	J	370	GLN	N-CA-CB	-5.25	102.39	110.01
1	O	98	PRO	N-CA-C	-5.25	102.91	111.68
1	O	947	GLY	CA-C-N	5.25	125.71	120.04
1	O	947	GLY	C-N-CA	5.25	125.71	120.04
1	C	739	HIS	N-CA-CB	-5.25	102.46	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	98	PRO	N-CA-C	-5.25	102.91	111.68
1	M	723	ALA	O-C-N	5.25	128.77	123.26
1	E	5	ASP	CA-C-O	5.25	125.63	119.28
1	H	739	HIS	N-CA-CB	-5.25	102.46	110.65
1	O	370	GLN	N-CA-CB	-5.25	102.40	110.01
1	D	370	GLN	N-CA-CB	-5.25	102.40	110.01
1	E	370	GLN	N-CA-CB	-5.25	102.40	110.01
1	F	370	GLN	N-CA-CB	-5.25	102.40	110.01
1	G	272	ALA	CA-C-N	5.25	126.40	119.84
1	G	272	ALA	C-N-CA	5.25	126.40	119.84
1	N	98	PRO	N-CA-C	-5.25	102.91	111.68
1	F	739	HIS	N-CA-CB	-5.25	102.47	110.65
1	J	739	HIS	N-CA-CB	-5.25	102.47	110.65
1	L	739	HIS	N-CA-CB	-5.25	102.47	110.65
1	C	188	VAL	N-CA-C	5.25	115.86	108.36
1	M	310	ARG	CA-C-N	-5.25	115.59	122.99
1	M	310	ARG	C-N-CA	-5.25	115.59	122.99
1	F	310	ARG	CA-C-N	-5.24	115.60	122.99
1	F	310	ARG	C-N-CA	-5.24	115.60	122.99
1	I	370	GLN	N-CA-CB	-5.24	102.41	110.01
1	O	723	ALA	O-C-N	5.24	128.76	123.26
1	P	310	ARG	CA-C-N	-5.24	115.60	122.99
1	P	310	ARG	C-N-CA	-5.24	115.60	122.99
1	P	958	ASN	N-CA-CB	5.24	121.28	111.53
1	A	958	ASN	N-CA-CB	5.24	121.28	111.53
1	N	958	ASN	N-CA-CB	5.24	121.28	111.53
1	B	958	ASN	N-CA-CB	5.24	121.28	111.53
1	F	723	ALA	O-C-N	5.24	128.76	123.26
1	G	98	PRO	N-CA-C	-5.24	102.93	111.68
1	G	958	ASN	N-CA-CB	5.24	121.28	111.53
1	J	188	VAL	N-CA-C	5.24	115.85	108.36
1	M	370	GLN	N-CA-CB	-5.24	102.41	110.01
1	O	5	ASP	CA-C-O	5.24	125.62	119.28
1	O	958	ASN	N-CA-CB	5.24	121.28	111.53
1	F	958	ASN	N-CA-CB	5.24	121.28	111.53
1	L	5	ASP	CA-C-O	5.24	125.62	119.28
1	N	370	GLN	N-CA-CB	-5.24	102.42	110.01
1	K	723	ALA	O-C-N	5.24	128.76	123.26
1	L	98	PRO	N-CA-C	-5.24	102.94	111.68
1	D	5	ASP	CA-C-O	5.24	125.62	119.28
1	D	188	VAL	N-CA-C	5.24	115.85	108.36
1	G	370	GLN	N-CA-CB	-5.24	102.42	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	310	ARG	CA-C-N	-5.24	115.61	122.99
1	H	310	ARG	C-N-CA	-5.24	115.61	122.99
1	J	921	PRO	CB-CA-C	-5.24	103.14	110.63
1	K	592	PHE	CA-CB-CG	-5.24	108.56	113.80
1	I	739	HIS	N-CA-CB	-5.23	102.48	110.65
1	G	5	ASP	CA-C-O	5.23	125.61	119.28
1	H	188	VAL	N-CA-C	5.23	115.84	108.36
1	H	958	ASN	N-CA-CB	5.23	121.26	111.53
1	K	370	GLN	N-CA-CB	-5.23	102.42	110.01
1	N	5	ASP	CA-C-O	5.23	125.61	119.28
1	P	723	ALA	O-C-N	5.23	128.75	123.26
1	L	958	ASN	N-CA-CB	5.23	121.26	111.53
1	P	370	GLN	N-CA-CB	-5.23	102.43	110.01
1	I	958	ASN	N-CA-CB	5.23	121.25	111.53
1	K	958	ASN	N-CA-CB	5.23	121.25	111.53
1	A	370	GLN	N-CA-CB	-5.23	102.43	110.01
1	I	5	ASP	CA-C-O	5.23	125.60	119.28
1	A	723	ALA	O-C-N	5.22	128.75	123.26
1	D	958	ASN	N-CA-CB	5.22	121.25	111.53
1	F	5	ASP	CA-C-O	5.22	125.60	119.28
1	M	98	PRO	N-CA-C	-5.22	102.96	111.68
1	F	921	PRO	CB-CA-C	-5.22	103.16	110.63
1	J	958	ASN	N-CA-CB	5.22	121.25	111.53
1	P	921	PRO	CB-CA-C	-5.22	103.16	110.63
1	A	5	ASP	CA-C-O	5.22	125.60	119.28
1	B	5	ASP	CA-C-O	5.22	125.59	119.28
1	B	592	PHE	CA-CB-CG	-5.22	108.58	113.80
1	K	3	ILE	CA-CB-CG2	-5.22	101.63	110.50
1	K	5	ASP	CA-C-O	5.22	125.60	119.28
1	P	188	VAL	N-CA-C	5.22	115.82	108.36
1	D	592	PHE	CA-CB-CG	-5.22	108.58	113.80
1	G	188	VAL	N-CA-C	5.22	115.82	108.36
1	J	429	ASP	CA-C-N	5.22	125.52	119.47
1	J	429	ASP	C-N-CA	5.22	125.52	119.47
1	L	723	ALA	O-C-N	5.22	128.74	123.26
1	B	188	VAL	N-CA-C	5.22	115.82	108.36
1	C	3	ILE	CA-CB-CG2	-5.22	101.63	110.50
1	J	5	ASP	CA-C-O	5.22	125.59	119.28
1	E	723	ALA	O-C-N	5.21	128.74	123.26
1	E	310	ARG	CA-C-N	-5.21	115.64	122.99
1	E	310	ARG	C-N-CA	-5.21	115.64	122.99
1	I	921	PRO	CB-CA-C	-5.21	103.18	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	5	ASP	CA-C-O	5.21	125.59	119.28
1	M	958	ASN	N-CA-CB	5.21	121.22	111.53
1	H	5	ASP	CA-C-O	5.21	125.58	119.28
1	L	3	ILE	CA-CB-CG2	-5.21	101.64	110.50
1	M	188	VAL	N-CA-C	5.21	115.81	108.36
1	N	3	ILE	CA-CB-CG2	-5.21	101.64	110.50
1	A	188	VAL	N-CA-C	5.21	115.81	108.36
1	B	723	ALA	O-C-N	5.21	128.73	123.26
1	F	188	VAL	N-CA-C	5.21	115.81	108.36
1	O	592	PHE	CA-CB-CG	-5.21	108.59	113.80
1	C	5	ASP	CA-C-O	5.21	125.58	119.28
1	J	592	PHE	CA-CB-CG	-5.21	108.59	113.80
1	N	723	ALA	O-C-N	5.21	128.73	123.26
1	P	5	ASP	CA-C-O	5.21	125.58	119.28
1	A	592	PHE	CA-CB-CG	-5.20	108.60	113.80
1	F	3	ILE	CA-CB-CG2	-5.20	101.66	110.50
1	I	723	ALA	O-C-N	5.20	128.72	123.26
1	J	723	ALA	O-C-N	5.20	128.72	123.26
1	C	921	PRO	CB-CA-C	-5.20	103.19	110.63
1	H	1006	GLU	CB-CA-C	-5.20	98.82	110.21
1	K	95	TYR	O-C-N	5.20	127.63	122.12
1	M	3	ILE	CA-CB-CG2	-5.20	101.66	110.50
1	B	429	ASP	CA-C-N	5.20	125.50	119.47
1	B	429	ASP	C-N-CA	5.20	125.50	119.47
1	E	1006	GLU	CB-CA-C	-5.20	98.83	110.21
1	H	512	PHE	CB-CA-C	-5.20	100.90	109.27
1	J	95	TYR	O-C-N	5.20	127.63	122.12
1	M	592	PHE	CA-CB-CG	-5.20	108.60	113.80
1	A	921	PRO	CB-CA-C	-5.20	103.20	110.63
1	P	95	TYR	O-C-N	5.20	127.63	122.12
1	D	723	ALA	O-C-N	5.20	128.72	123.26
1	I	3	ILE	CA-CB-CG2	-5.19	101.67	110.50
1	J	3	ILE	CA-CB-CG2	-5.19	101.67	110.50
1	K	188	VAL	N-CA-C	5.19	115.79	108.36
1	K	921	PRO	CB-CA-C	-5.19	103.20	110.63
1	N	95	TYR	O-C-N	5.19	127.62	122.12
1	B	921	PRO	CB-CA-C	-5.19	103.20	110.63
1	H	723	ALA	O-C-N	5.19	128.71	123.26
1	P	3	ILE	CA-CB-CG2	-5.19	101.67	110.50
1	A	3	ILE	CA-CB-CG2	-5.19	101.67	110.50
1	B	3	ILE	CA-CB-CG2	-5.19	101.68	110.50
1	E	188	VAL	N-CA-C	5.19	115.78	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	3	ILE	CA-CB-CG2	-5.19	101.68	110.50
1	H	592	PHE	CA-CB-CG	-5.19	108.61	113.80
1	N	592	PHE	CA-CB-CG	-5.19	108.61	113.80
1	O	921	PRO	CB-CA-C	-5.19	103.21	110.63
1	I	592	PHE	CA-CB-CG	-5.19	108.61	113.80
1	M	95	TYR	O-C-N	5.19	127.62	122.12
1	H	921	PRO	CB-CA-C	-5.19	103.21	110.63
1	L	592	PHE	CA-CB-CG	-5.19	108.61	113.80
1	O	3	ILE	CA-CB-CG2	-5.19	101.68	110.50
1	E	472	TYR	CA-C-O	5.19	126.27	120.82
1	P	592	PHE	CA-CB-CG	-5.19	108.61	113.80
1	D	512	PHE	CB-CA-C	-5.18	100.92	109.27
1	E	921	PRO	CB-CA-C	-5.18	103.22	110.63
1	G	723	ALA	O-C-N	5.18	128.70	123.26
1	H	3	ILE	CA-CB-CG2	-5.18	101.69	110.50
1	L	921	PRO	CB-CA-C	-5.18	103.22	110.63
1	C	592	PHE	CA-CB-CG	-5.18	108.62	113.80
1	D	921	PRO	CB-CA-C	-5.18	103.22	110.63
1	G	1006	GLU	CB-CA-C	-5.18	98.86	110.21
1	N	472	TYR	CA-C-O	5.18	126.26	120.82
1	L	1006	GLU	CB-CA-C	-5.18	98.86	110.21
1	M	1006	GLU	CB-CA-C	-5.18	98.86	110.21
1	O	188	VAL	N-CA-C	5.18	115.77	108.36
1	P	1006	GLU	CB-CA-C	-5.18	98.86	110.21
1	A	1006	GLU	CB-CA-C	-5.18	98.87	110.21
1	E	592	PHE	CA-CB-CG	-5.18	108.62	113.80
1	F	512	PHE	CB-CA-C	-5.18	100.93	109.27
1	K	472	TYR	CA-C-O	5.18	126.26	120.82
1	N	921	PRO	CB-CA-C	-5.18	103.22	110.63
1	O	714	ILE	CB-CA-C	-5.18	104.69	110.96
1	B	1006	GLU	CB-CA-C	-5.18	98.87	110.21
1	L	188	VAL	N-CA-C	5.18	115.77	108.36
1	B	714	ILE	CB-CA-C	-5.18	104.70	110.96
1	E	3	ILE	CA-CB-CG2	-5.18	101.70	110.50
1	G	921	PRO	CB-CA-C	-5.18	103.23	110.63
1	H	95	TYR	O-C-N	5.18	127.61	122.12
1	C	1006	GLU	CB-CA-C	-5.17	98.88	110.21
1	I	714	ILE	CB-CA-C	-5.17	104.70	110.96
1	I	1006	GLU	CB-CA-C	-5.17	98.88	110.21
1	N	1006	GLU	CB-CA-C	-5.17	98.88	110.21
1	D	429	ASP	CA-C-N	5.17	125.47	119.47
1	D	429	ASP	C-N-CA	5.17	125.47	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	512	PHE	CB-CA-C	-5.17	100.94	109.27
1	F	592	PHE	CA-CB-CG	-5.17	108.63	113.80
1	I	188	VAL	N-CA-C	5.17	115.76	108.36
1	K	1006	GLU	CB-CA-C	-5.17	98.89	110.21
1	O	429	ASP	CA-C-N	5.17	125.47	119.47
1	O	429	ASP	C-N-CA	5.17	125.47	119.47
1	P	429	ASP	CA-C-N	5.17	125.47	119.47
1	P	429	ASP	C-N-CA	5.17	125.47	119.47
1	A	429	ASP	CA-C-N	5.17	125.47	119.47
1	A	429	ASP	C-N-CA	5.17	125.47	119.47
1	D	1006	GLU	CB-CA-C	-5.17	98.90	110.21
1	F	95	TYR	O-C-N	5.17	127.60	122.12
1	J	1006	GLU	CB-CA-C	-5.17	98.90	110.21
1	C	95	TYR	O-C-N	5.16	127.59	122.12
1	F	1006	GLU	CB-CA-C	-5.16	98.90	110.21
1	G	592	PHE	CA-CB-CG	-5.16	108.64	113.80
1	P	472	TYR	CA-C-O	5.16	126.24	120.82
1	E	429	ASP	CA-C-N	5.16	125.46	119.47
1	E	429	ASP	C-N-CA	5.16	125.46	119.47
1	N	188	VAL	N-CA-C	5.16	115.74	108.36
1	O	1006	GLU	CB-CA-C	-5.16	98.91	110.21
1	D	3	ILE	CA-CB-CG2	-5.16	101.73	110.50
1	G	95	TYR	O-C-N	5.16	127.59	122.12
1	M	429	ASP	CA-C-N	5.16	125.45	119.47
1	M	429	ASP	C-N-CA	5.16	125.45	119.47
1	B	472	TYR	CA-C-O	5.16	126.24	120.82
1	K	351	ILE	N-CA-C	5.16	116.17	108.54
1	L	95	TYR	O-C-N	5.16	127.59	122.12
1	L	512	PHE	CB-CA-C	-5.16	100.97	109.27
1	N	429	ASP	CA-C-N	5.16	125.45	119.47
1	N	429	ASP	C-N-CA	5.16	125.45	119.47
1	O	95	TYR	O-C-N	5.16	127.59	122.12
1	E	95	TYR	O-C-N	5.16	127.59	122.12
1	E	512	PHE	CB-CA-C	-5.16	100.97	109.27
1	J	512	PHE	CB-CA-C	-5.16	100.97	109.27
1	M	472	TYR	CA-C-O	5.16	126.23	120.82
1	M	921	PRO	CB-CA-C	-5.16	103.26	110.63
1	A	512	PHE	CB-CA-C	-5.15	100.97	109.27
1	G	472	TYR	CA-C-O	5.15	126.23	120.82
1	G	512	PHE	CB-CA-C	-5.15	100.98	109.27
1	H	890	GLN	N-CA-CB	-5.15	102.99	110.36
1	P	512	PHE	CB-CA-C	-5.15	100.97	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	429	ASP	CA-C-N	5.15	125.44	119.47
1	K	429	ASP	C-N-CA	5.15	125.44	119.47
1	K	512	PHE	CB-CA-C	-5.15	100.98	109.27
1	L	472	TYR	CA-C-O	5.15	126.23	120.82
1	N	512	PHE	CB-CA-C	-5.15	100.98	109.27
1	C	351	ILE	N-CA-C	5.15	116.16	108.54
1	I	429	ASP	CA-C-N	5.15	125.44	119.47
1	I	429	ASP	C-N-CA	5.15	125.44	119.47
1	I	472	TYR	CA-C-O	5.15	126.23	120.82
1	C	512	PHE	CB-CA-C	-5.15	100.98	109.27
1	D	95	TYR	O-C-N	5.15	127.58	122.12
1	E	651	LEU	CB-CA-C	-5.15	100.29	109.71
1	I	512	PHE	CB-CA-C	-5.15	100.98	109.27
1	P	714	ILE	CB-CA-C	-5.15	104.73	110.96
1	G	351	ILE	N-CA-C	5.15	116.16	108.54
1	P	890	GLN	N-CA-CB	-5.15	103.00	110.36
1	C	714	ILE	CB-CA-C	-5.14	104.73	110.96
1	F	429	ASP	CA-C-N	5.14	125.44	119.47
1	F	429	ASP	C-N-CA	5.14	125.44	119.47
1	G	714	ILE	CB-CA-C	-5.14	104.73	110.96
1	O	512	PHE	CB-CA-C	-5.14	100.99	109.27
1	O	651	LEU	CB-CA-C	-5.14	100.30	109.71
1	E	351	ILE	N-CA-C	5.14	116.15	108.54
1	H	472	TYR	CA-C-O	5.14	126.22	120.82
1	F	472	TYR	CA-C-O	5.14	126.22	120.82
1	K	714	ILE	CB-CA-C	-5.14	104.74	110.96
1	M	714	ILE	CB-CA-C	-5.14	104.74	110.96
1	C	651	LEU	CB-CA-C	-5.14	100.31	109.71
1	A	472	TYR	CA-C-O	5.14	126.22	120.82
1	I	95	TYR	O-C-N	5.14	127.57	122.12
1	C	429	ASP	CA-C-N	5.14	125.43	119.47
1	C	429	ASP	C-N-CA	5.14	125.43	119.47
1	F	890	GLN	N-CA-CB	-5.14	103.02	110.36
1	I	890	GLN	N-CA-CB	-5.14	103.02	110.36
1	C	890	GLN	N-CA-CB	-5.13	103.02	110.36
1	F	651	LEU	CB-CA-C	-5.13	100.31	109.71
1	H	429	ASP	CA-C-N	5.13	125.43	119.47
1	H	429	ASP	C-N-CA	5.13	125.43	119.47
1	L	429	ASP	CA-C-N	5.13	125.43	119.47
1	L	429	ASP	C-N-CA	5.13	125.43	119.47
1	M	512	PHE	CB-CA-C	-5.13	101.00	109.27
1	M	890	GLN	N-CA-CB	-5.13	103.02	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	651	LEU	CB-CA-C	-5.13	100.31	109.71
1	D	651	LEU	CB-CA-C	-5.13	100.32	109.71
1	N	714	ILE	CB-CA-C	-5.13	104.75	110.96
1	N	890	GLN	N-CA-CB	-5.13	103.02	110.36
1	A	714	ILE	CB-CA-C	-5.13	104.75	110.96
1	A	890	GLN	N-CA-CB	-5.13	103.02	110.36
1	B	890	GLN	N-CA-CB	-5.13	103.02	110.36
1	B	95	TYR	O-C-N	5.13	127.56	122.12
1	F	351	ILE	N-CA-C	5.13	116.13	108.54
1	H	351	ILE	N-CA-C	5.13	116.13	108.54
1	J	714	ILE	CB-CA-C	-5.13	104.75	110.96
1	K	651	LEU	CB-CA-C	-5.13	100.33	109.71
1	L	758	PHE	CA-CB-CG	-5.13	108.67	113.80
1	H	714	ILE	CB-CA-C	-5.13	104.76	110.96
1	J	890	GLN	N-CA-CB	-5.13	103.03	110.36
1	K	890	GLN	N-CA-CB	-5.13	103.03	110.36
1	N	651	LEU	CB-CA-C	-5.13	100.33	109.71
1	J	651	LEU	CB-CA-C	-5.12	100.33	109.71
1	A	95	TYR	O-C-N	5.12	127.55	122.12
1	A	651	LEU	CB-CA-C	-5.12	100.33	109.71
1	B	351	ILE	N-CA-C	5.12	116.12	108.54
1	D	472	TYR	CA-C-O	5.12	126.20	120.82
1	H	651	LEU	CB-CA-C	-5.12	100.33	109.71
1	L	890	GLN	N-CA-CB	-5.12	103.03	110.36
1	B	651	LEU	CB-CA-C	-5.12	100.34	109.71
1	E	714	ILE	CB-CA-C	-5.12	104.76	110.96
1	G	651	LEU	CB-CA-C	-5.12	100.34	109.71
1	I	651	LEU	CB-CA-C	-5.12	100.34	109.71
1	E	890	GLN	N-CA-CB	-5.12	103.04	110.36
1	A	351	ILE	N-CA-C	5.12	116.12	108.54
1	C	448	ARG	CA-C-N	-5.12	114.09	122.54
1	C	448	ARG	C-N-CA	-5.12	114.09	122.54
1	I	135	GLN	N-CA-CB	5.12	117.59	110.07
1	J	135	GLN	N-CA-CB	5.12	117.59	110.07
1	L	351	ILE	N-CA-C	5.12	116.12	108.54
1	P	448	ARG	CA-C-N	-5.12	114.09	122.54
1	P	448	ARG	C-N-CA	-5.12	114.09	122.54
1	C	730	LEU	O-C-N	5.12	127.64	121.60
1	O	351	ILE	N-CA-C	5.12	116.11	108.54
1	M	758	PHE	CA-CB-CG	-5.12	108.68	113.80
1	I	730	LEU	O-C-N	5.11	127.63	121.60
1	L	448	ARG	CA-C-N	-5.11	114.10	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	448	ARG	C-N-CA	-5.11	114.10	122.54
1	L	651	LEU	CB-CA-C	-5.11	100.35	109.71
1	L	714	ILE	CB-CA-C	-5.11	104.77	110.96
1	B	135	GLN	N-CA-CB	5.11	117.58	110.07
1	F	714	ILE	CB-CA-C	-5.11	104.77	110.96
1	G	429	ASP	CA-C-N	5.11	125.40	119.47
1	G	429	ASP	C-N-CA	5.11	125.40	119.47
1	P	351	ILE	N-CA-C	5.11	116.11	108.54
1	F	448	ARG	CA-C-N	-5.11	114.11	122.54
1	F	448	ARG	C-N-CA	-5.11	114.11	122.54
1	M	135	GLN	N-CA-CB	5.11	117.58	110.07
1	O	890	GLN	N-CA-CB	-5.11	103.05	110.36
1	P	599	ARG	N-CA-C	5.11	116.08	108.31
1	P	758	PHE	CA-CB-CG	-5.11	108.69	113.80
1	C	135	GLN	N-CA-CB	5.11	117.58	110.07
1	D	448	ARG	CA-C-N	-5.11	114.11	122.54
1	D	448	ARG	C-N-CA	-5.11	114.11	122.54
1	N	135	GLN	N-CA-CB	5.11	117.58	110.07
1	C	472	TYR	CA-C-O	5.11	126.18	120.82
1	E	135	GLN	N-CA-CB	5.11	117.58	110.07
1	N	351	ILE	N-CA-C	5.11	116.10	108.54
1	A	135	GLN	N-CA-CB	5.11	117.57	110.07
1	F	758	PHE	CA-CB-CG	-5.11	108.69	113.80
1	J	472	TYR	CA-C-O	5.11	126.18	120.82
1	L	721	ARG	N-CA-CB	5.11	118.75	110.17
1	M	651	LEU	CB-CA-C	-5.11	100.36	109.71
1	D	135	GLN	N-CA-CB	5.10	117.57	110.07
1	D	351	ILE	N-CA-C	5.10	116.09	108.54
1	G	890	GLN	N-CA-CB	-5.10	103.06	110.36
1	M	351	ILE	N-CA-C	5.10	116.09	108.54
1	J	351	ILE	N-CA-C	5.10	116.09	108.54
1	O	472	TYR	CA-C-O	5.10	126.18	120.82
1	A	448	ARG	CA-C-N	-5.10	114.12	122.54
1	A	448	ARG	C-N-CA	-5.10	114.12	122.54
1	D	890	GLN	N-CA-CB	-5.10	103.07	110.36
1	G	730	LEU	O-C-N	5.10	127.62	121.60
1	M	448	ARG	CA-C-N	-5.10	114.12	122.54
1	M	448	ARG	C-N-CA	-5.10	114.12	122.54
1	K	135	GLN	N-CA-CB	5.10	117.56	110.07
1	D	714	ILE	CB-CA-C	-5.09	104.80	110.96
1	L	135	GLN	N-CA-CB	5.09	117.56	110.07
1	N	721	ARG	N-CA-CB	5.09	118.73	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	448	ARG	CA-C-N	-5.09	114.13	122.54
1	O	448	ARG	C-N-CA	-5.09	114.13	122.54
1	O	758	PHE	CA-CB-CG	-5.09	108.70	113.80
1	N	448	ARG	CA-C-N	-5.09	114.14	122.54
1	N	448	ARG	C-N-CA	-5.09	114.14	122.54
1	N	758	PHE	CA-CB-CG	-5.09	108.71	113.80
1	F	721	ARG	N-CA-CB	5.09	118.72	110.17
1	G	135	GLN	N-CA-CB	5.09	117.55	110.07
1	J	758	PHE	CA-CB-CG	-5.09	108.71	113.80
1	G	448	ARG	CA-C-N	-5.09	114.14	122.54
1	G	448	ARG	C-N-CA	-5.09	114.14	122.54
1	K	448	ARG	CA-C-N	-5.09	114.14	122.54
1	K	448	ARG	C-N-CA	-5.09	114.14	122.54
1	M	730	LEU	O-C-N	5.09	127.61	121.60
1	O	135	GLN	N-CA-CB	5.09	117.55	110.07
1	B	448	ARG	CA-C-N	-5.09	114.15	122.54
1	B	448	ARG	C-N-CA	-5.09	114.15	122.54
1	D	730	LEU	O-C-N	5.09	127.60	121.60
1	H	135	GLN	N-CA-CB	5.09	117.55	110.07
1	I	351	ILE	N-CA-C	5.09	116.07	108.54
1	P	135	GLN	N-CA-CB	5.09	117.55	110.07
1	P	721	ARG	N-CA-CB	5.09	118.72	110.17
1	B	730	LEU	O-C-N	5.09	127.60	121.60
1	H	448	ARG	CA-C-N	-5.09	114.15	122.54
1	H	448	ARG	C-N-CA	-5.09	114.15	122.54
1	I	448	ARG	CA-C-N	-5.09	114.15	122.54
1	I	448	ARG	C-N-CA	-5.09	114.15	122.54
1	F	135	GLN	N-CA-CB	5.08	117.54	110.07
1	H	599	ARG	N-CA-C	5.08	116.04	108.31
1	K	730	LEU	O-C-N	5.08	127.60	121.60
1	D	758	PHE	CA-CB-CG	-5.08	108.72	113.80
1	G	758	PHE	CA-CB-CG	-5.08	108.72	113.80
1	H	206	SER	N-CA-CB	5.08	119.29	111.46
1	C	721	ARG	N-CA-CB	5.08	118.70	110.17
1	H	730	LEU	O-C-N	5.08	127.59	121.60
1	H	721	ARG	N-CA-CB	5.08	118.70	110.17
1	D	599	ARG	N-CA-C	5.08	116.02	108.31
1	G	721	ARG	N-CA-CB	5.08	118.69	110.17
1	J	721	ARG	N-CA-CB	5.08	118.70	110.17
1	O	730	LEU	O-C-N	5.08	127.59	121.60
1	A	721	ARG	N-CA-CB	5.07	118.69	110.17
1	A	758	PHE	CA-CB-CG	-5.07	108.73	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	448	ARG	CA-C-N	-5.07	114.17	122.54
1	E	448	ARG	C-N-CA	-5.07	114.17	122.54
1	M	206	SER	N-CA-CB	5.07	119.27	111.46
1	C	758	PHE	CA-CB-CG	-5.07	108.73	113.80
1	D	172	ASP	CA-C-N	-5.07	113.49	122.26
1	D	172	ASP	C-N-CA	-5.07	113.49	122.26
1	K	721	ARG	N-CA-CB	5.07	118.69	110.17
1	D	721	ARG	N-CA-CB	5.07	118.69	110.17
1	E	758	PHE	CA-CB-CG	-5.07	108.73	113.80
1	F	206	SER	N-CA-CB	5.07	119.27	111.46
1	L	142	ILE	CB-CA-C	-5.07	103.57	110.42
1	N	206	SER	N-CA-CB	5.07	119.27	111.46
1	J	730	LEU	O-C-N	5.07	127.58	121.60
1	L	730	LEU	O-C-N	5.07	127.58	121.60
1	A	730	LEU	O-C-N	5.07	127.58	121.60
1	B	206	SER	N-CA-CB	5.07	119.26	111.46
1	K	206	SER	N-CA-CB	5.07	119.26	111.46
1	G	702	GLN	CA-C-O	5.07	123.81	119.71
1	P	206	SER	N-CA-CB	5.07	119.26	111.46
1	B	721	ARG	N-CA-CB	5.06	118.68	110.17
1	C	206	SER	N-CA-CB	5.06	119.26	111.46
1	J	448	ARG	CA-C-N	-5.06	114.19	122.54
1	J	448	ARG	C-N-CA	-5.06	114.19	122.54
1	N	142	ILE	CB-CA-C	-5.06	103.58	110.42
1	F	142	ILE	CB-CA-C	-5.06	103.59	110.42
1	J	142	ILE	CB-CA-C	-5.06	103.58	110.42
1	J	206	SER	N-CA-CB	5.06	119.26	111.46
1	K	758	PHE	CA-CB-CG	-5.06	108.74	113.80
1	O	142	ILE	CB-CA-C	-5.06	103.58	110.42
1	P	142	ILE	CB-CA-C	-5.06	103.58	110.42
1	G	142	ILE	CB-CA-C	-5.06	103.59	110.42
1	I	758	PHE	CA-CB-CG	-5.06	108.74	113.80
1	O	172	ASP	CA-C-N	-5.06	113.50	122.26
1	O	172	ASP	C-N-CA	-5.06	113.50	122.26
1	C	702	GLN	CA-C-O	5.06	123.81	119.71
1	I	721	ARG	N-CA-CB	5.06	118.67	110.17
1	A	206	SER	N-CA-CB	5.06	119.25	111.46
1	E	96	ASP	N-CA-C	-5.06	101.76	108.74
1	H	758	PHE	CA-CB-CG	-5.05	108.75	113.80
1	K	142	ILE	CB-CA-C	-5.05	103.60	110.42
1	M	721	ARG	N-CA-CB	5.05	118.66	110.17
1	O	206	SER	N-CA-CB	5.05	119.24	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	744	GLU	CA-C-N	5.05	130.55	121.66
1	B	744	GLU	C-N-CA	5.05	130.55	121.66
1	C	172	ASP	CA-C-N	-5.05	113.52	122.26
1	C	172	ASP	C-N-CA	-5.05	113.52	122.26
1	E	730	LEU	O-C-N	5.05	127.56	121.60
1	A	142	ILE	CB-CA-C	-5.05	103.60	110.42
1	I	744	GLU	CA-C-N	5.05	130.55	121.66
1	I	744	GLU	C-N-CA	5.05	130.55	121.66
1	N	730	LEU	O-C-N	5.05	127.56	121.60
1	E	142	ILE	CB-CA-C	-5.05	103.60	110.42
1	I	142	ILE	CB-CA-C	-5.05	103.60	110.42
1	M	142	ILE	CB-CA-C	-5.05	103.60	110.42
1	N	278	ILE	CA-C-N	-5.05	116.13	121.84
1	N	278	ILE	C-N-CA	-5.05	116.13	121.84
1	O	721	ARG	N-CA-CB	5.05	118.65	110.17
1	E	721	ARG	N-CA-CB	5.05	118.65	110.17
1	O	472	TYR	N-CA-CB	-5.05	102.69	110.01
1	H	172	ASP	CA-C-N	-5.05	113.53	122.26
1	H	172	ASP	C-N-CA	-5.05	113.53	122.26
1	M	278	ILE	CA-C-N	-5.05	116.14	121.84
1	M	278	ILE	C-N-CA	-5.05	116.14	121.84
1	B	758	PHE	CA-CB-CG	-5.04	108.76	113.80
1	C	744	GLU	CA-C-N	5.04	130.54	121.66
1	C	744	GLU	C-N-CA	5.04	130.54	121.66
1	D	206	SER	N-CA-CB	5.04	119.23	111.46
1	H	142	ILE	CB-CA-C	-5.04	103.61	110.42
1	H	702	GLN	CA-C-O	5.04	123.80	119.71
1	I	206	SER	N-CA-CB	5.04	119.22	111.46
1	I	278	ILE	CA-C-N	-5.04	116.14	121.84
1	I	278	ILE	C-N-CA	-5.04	116.14	121.84
1	P	172	ASP	CA-C-N	-5.04	113.54	122.26
1	P	172	ASP	C-N-CA	-5.04	113.54	122.26
1	G	472	TYR	N-CA-CB	-5.04	102.70	110.01
1	B	367	MET	CG-SD-CE	-5.04	89.81	100.90
1	B	472	TYR	N-CA-CB	-5.04	102.70	110.01
1	E	367	MET	CG-SD-CE	-5.04	89.81	100.90
1	K	702	GLN	CA-C-O	5.04	123.79	119.71
1	L	206	SER	N-CA-CB	5.04	119.22	111.46
1	M	172	ASP	CA-C-N	-5.04	113.54	122.26
1	M	172	ASP	C-N-CA	-5.04	113.54	122.26
1	N	744	GLU	CA-C-N	5.04	130.53	121.66
1	N	744	GLU	C-N-CA	5.04	130.53	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	278	ILE	CA-C-N	-5.04	116.15	121.84
1	D	278	ILE	C-N-CA	-5.04	116.15	121.84
1	F	367	MET	CG-SD-CE	-5.04	89.82	100.90
1	J	172	ASP	CA-C-N	-5.04	113.55	122.26
1	J	172	ASP	C-N-CA	-5.04	113.55	122.26
1	O	278	ILE	CA-C-N	-5.04	116.15	121.84
1	O	278	ILE	C-N-CA	-5.04	116.15	121.84
1	O	744	GLU	CA-C-N	5.04	130.53	121.66
1	O	744	GLU	C-N-CA	5.04	130.53	121.66
1	B	142	ILE	CB-CA-C	-5.04	103.62	110.42
1	E	206	SER	N-CA-CB	5.04	119.22	111.46
1	G	206	SER	N-CA-CB	5.04	119.22	111.46
1	G	744	GLU	CA-C-N	5.04	130.52	121.66
1	G	744	GLU	C-N-CA	5.04	130.52	121.66
1	H	367	MET	CG-SD-CE	-5.04	89.82	100.90
1	H	472	TYR	N-CA-CB	-5.04	102.71	110.01
1	I	172	ASP	CA-C-N	-5.04	113.55	122.26
1	I	172	ASP	C-N-CA	-5.04	113.55	122.26
1	K	367	MET	CG-SD-CE	-5.04	89.82	100.90
1	L	172	ASP	CA-C-N	-5.04	113.55	122.26
1	L	172	ASP	C-N-CA	-5.04	113.55	122.26
1	A	172	ASP	CA-C-N	-5.03	113.55	122.26
1	A	172	ASP	C-N-CA	-5.03	113.55	122.26
1	G	172	ASP	CA-C-N	-5.03	113.55	122.26
1	G	172	ASP	C-N-CA	-5.03	113.55	122.26
1	N	172	ASP	CA-C-N	-5.03	113.55	122.26
1	N	172	ASP	C-N-CA	-5.03	113.55	122.26
1	D	142	ILE	CB-CA-C	-5.03	103.62	110.77
1	D	367	MET	CG-SD-CE	-5.03	89.83	100.90
1	H	744	GLU	CA-C-N	5.03	130.52	121.66
1	H	744	GLU	C-N-CA	5.03	130.52	121.66
1	C	278	ILE	CA-C-N	-5.03	116.16	121.84
1	C	278	ILE	C-N-CA	-5.03	116.16	121.84
1	E	278	ILE	CA-C-N	-5.03	116.16	121.84
1	E	278	ILE	C-N-CA	-5.03	116.16	121.84
1	F	702	GLN	CA-C-O	5.03	123.78	119.71
1	J	744	GLU	CA-C-N	5.03	130.51	121.66
1	J	744	GLU	C-N-CA	5.03	130.51	121.66
1	K	744	GLU	CA-C-N	5.03	130.51	121.66
1	K	744	GLU	C-N-CA	5.03	130.51	121.66
1	P	730	LEU	O-C-N	5.03	127.53	121.60
1	A	351	ILE	CB-CA-C	-5.03	105.20	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	MET	CG-SD-CE	-5.03	89.84	100.90
1	B	351	ILE	CB-CA-C	-5.03	105.20	111.08
1	D	702	GLN	CA-C-O	5.03	123.78	119.71
1	E	172	ASP	CA-C-N	-5.03	113.56	122.26
1	E	172	ASP	C-N-CA	-5.03	113.56	122.26
1	J	367	MET	CG-SD-CE	-5.03	89.84	100.90
1	J	472	TYR	N-CA-CB	-5.03	102.72	110.01
1	O	728	VAL	CA-C-N	-5.03	114.78	122.87
1	O	728	VAL	C-N-CA	-5.03	114.78	122.87
1	P	367	MET	CG-SD-CE	-5.03	89.84	100.90
1	A	744	GLU	CA-C-N	5.03	130.50	121.66
1	A	744	GLU	C-N-CA	5.03	130.50	121.66
1	C	367	MET	CG-SD-CE	-5.03	89.84	100.90
1	E	744	GLU	CA-C-N	5.03	130.50	121.66
1	E	744	GLU	C-N-CA	5.03	130.50	121.66
1	F	744	GLU	CA-C-N	5.03	130.50	121.66
1	F	744	GLU	C-N-CA	5.03	130.50	121.66
1	L	367	MET	CG-SD-CE	-5.03	89.84	100.90
1	M	744	GLU	CA-C-N	5.03	130.50	121.66
1	M	744	GLU	C-N-CA	5.03	130.50	121.66
1	O	367	MET	CG-SD-CE	-5.03	89.84	100.90
1	P	744	GLU	CA-C-N	5.03	130.50	121.66
1	P	744	GLU	C-N-CA	5.03	130.50	121.66
1	I	472	TYR	N-CA-CB	-5.02	102.72	110.01
1	L	150	PHE	CA-CB-CG	-5.02	108.78	113.80
1	N	367	MET	CG-SD-CE	-5.02	89.85	100.90
1	P	472	TYR	N-CA-CB	-5.02	102.72	110.01
1	F	172	ASP	CA-C-N	-5.02	113.57	122.26
1	F	172	ASP	C-N-CA	-5.02	113.57	122.26
1	I	367	MET	CG-SD-CE	-5.02	89.85	100.90
1	L	351	ILE	CB-CA-C	-5.02	105.20	111.08
1	O	702	GLN	CA-C-O	5.02	123.78	119.71
1	F	278	ILE	CA-C-N	-5.02	116.17	121.84
1	F	278	ILE	C-N-CA	-5.02	116.17	121.84
1	G	278	ILE	CA-C-N	-5.02	116.17	121.84
1	G	278	ILE	C-N-CA	-5.02	116.17	121.84
1	D	744	GLU	CA-C-N	5.02	130.49	121.66
1	D	744	GLU	C-N-CA	5.02	130.49	121.66
1	J	150	PHE	CA-CB-CG	-5.02	108.78	113.80
1	K	172	ASP	CA-C-N	-5.02	113.58	122.26
1	K	172	ASP	C-N-CA	-5.02	113.58	122.26
1	C	142	ILE	CB-CA-C	-5.02	103.64	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	740	LEU	N-CA-C	5.02	117.95	110.52
1	D	472	TYR	N-CA-CB	-5.02	102.73	110.01
1	D	728	VAL	CA-C-N	-5.02	114.79	122.87
1	D	728	VAL	C-N-CA	-5.02	114.79	122.87
1	G	351	ILE	CB-CA-C	-5.02	105.21	111.08
1	K	278	ILE	CA-C-N	-5.02	116.17	121.84
1	K	278	ILE	C-N-CA	-5.02	116.17	121.84
1	F	150	PHE	CA-CB-CG	-5.02	108.78	113.80
1	G	367	MET	CG-SD-CE	-5.02	89.86	100.90
1	M	367	MET	CG-SD-CE	-5.02	89.86	100.90
1	C	472	TYR	N-CA-CB	-5.01	102.74	110.01
1	I	150	PHE	CA-CB-CG	-5.01	108.79	113.80
1	L	728	VAL	CA-C-N	-5.01	114.80	122.87
1	L	728	VAL	C-N-CA	-5.01	114.80	122.87
1	M	351	ILE	CB-CA-C	-5.01	105.22	111.08
1	A	472	TYR	N-CA-CB	-5.01	102.74	110.01
1	B	249	GLU	O-C-N	5.01	129.05	122.68
1	B	740	LEU	N-CA-C	5.01	117.94	110.52
1	F	730	LEU	O-C-N	5.01	127.51	121.60
1	H	278	ILE	CA-C-N	-5.01	116.18	121.84
1	H	278	ILE	C-N-CA	-5.01	116.18	121.84
1	N	472	TYR	N-CA-CB	-5.01	102.74	110.01
1	B	172	ASP	CA-C-N	-5.01	113.59	122.26
1	B	172	ASP	C-N-CA	-5.01	113.59	122.26
1	E	472	TYR	N-CA-CB	-5.01	102.75	110.01
1	J	702	GLN	CA-C-O	5.01	123.77	119.71
1	M	472	TYR	N-CA-CB	-5.01	102.75	110.01
1	N	728	VAL	CA-C-N	-5.01	114.81	122.87
1	N	728	VAL	C-N-CA	-5.01	114.81	122.87
1	H	728	VAL	CA-C-N	-5.01	114.81	122.87
1	H	728	VAL	C-N-CA	-5.01	114.81	122.87
1	P	351	ILE	CB-CA-C	-5.00	105.22	111.08
1	F	472	TYR	N-CA-CB	-5.00	102.75	110.01
1	L	702	GLN	CA-C-O	5.00	123.76	119.71
1	O	150	PHE	CA-CB-CG	-5.00	108.80	113.80
1	I	740	LEU	N-CA-C	5.00	117.92	110.52
1	J	728	VAL	CA-C-N	-5.00	114.82	122.87
1	J	728	VAL	C-N-CA	-5.00	114.82	122.87
1	K	728	VAL	CA-C-N	-5.00	114.82	122.87
1	K	728	VAL	C-N-CA	-5.00	114.82	122.87

All (32) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	166	ARG	CA
1	A	249	GLU	CA
1	B	166	ARG	CA
1	B	249	GLU	CA
1	C	166	ARG	CA
1	C	249	GLU	CA
1	D	166	ARG	CA
1	D	249	GLU	CA
1	E	166	ARG	CA
1	E	249	GLU	CA
1	F	166	ARG	CA
1	F	249	GLU	CA
1	G	166	ARG	CA
1	G	249	GLU	CA
1	H	166	ARG	CA
1	H	249	GLU	CA
1	I	166	ARG	CA
1	I	249	GLU	CA
1	J	166	ARG	CA
1	J	249	GLU	CA
1	K	166	ARG	CA
1	K	249	GLU	CA
1	L	166	ARG	CA
1	L	249	GLU	CA
1	M	166	ARG	CA
1	M	249	GLU	CA
1	N	166	ARG	CA
1	N	249	GLU	CA
1	O	166	ARG	CA
1	O	249	GLU	CA
1	P	166	ARG	CA
1	P	249	GLU	CA

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	8232	0	7817	279	3
1	B	8232	0	7817	274	4
1	C	8232	0	7817	272	1
1	D	8232	0	7817	286	0
1	E	8232	0	7817	278	0
1	F	8232	0	7817	283	0
1	G	8232	0	7817	277	0
1	H	8232	0	7817	274	0
1	I	8232	0	7817	282	1
1	J	8232	0	7817	284	0
1	K	8232	0	7817	284	0
1	L	8232	0	7817	274	0
1	M	8232	0	7817	284	0
1	N	8232	0	7817	278	0
1	O	8232	0	7817	279	0
1	P	8232	0	7817	282	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
3	A	434	0	0	13	0
3	B	436	0	0	13	0
3	C	433	0	0	13	0
3	D	437	0	0	13	0
3	E	435	0	0	13	0
3	F	436	0	0	13	0
3	G	434	0	0	13	0
3	H	435	0	0	13	0
3	I	434	0	0	13	0
3	J	436	0	0	13	0
3	K	435	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	435	0	0	13	0
3	M	434	0	0	13	0
3	N	436	0	0	13	0
3	O	433	0	0	13	0
3	P	437	0	0	13	0
All	All	138704	0	125072	4364	5

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 17.

All (4364) 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:H:427:THR:HA	1:H:436:MET:HE1	1.17	1.17
1:I:427:THR:HA	1:I:436:MET:HE1	1.17	1.17
1:P:427:THR:HA	1:P:436:MET:HE1	1.17	1.16
1:O:427:THR:HA	1:O:436:MET:HE1	1.17	1.16
1:B:427:THR:HA	1:B:436:MET:HE1	1.17	1.15
1:G:427:THR:HA	1:G:436:MET:HE1	1.17	1.15
1:N:427:THR:HA	1:N:436:MET:HE1	1.17	1.13
1:A:427:THR:HA	1:A:436:MET:HE1	1.17	1.12
1:J:427:THR:HA	1:J:436:MET:HE1	1.17	1.12
1:C:427:THR:HA	1:C:436:MET:HE1	1.17	1.12
1:F:427:THR:HA	1:F:436:MET:HE1	1.17	1.12
1:M:427:THR:HA	1:M:436:MET:HE1	1.17	1.11
1:K:427:THR:HA	1:K:436:MET:HE1	1.17	1.11
1:E:427:THR:HA	1:E:436:MET:HE1	1.17	1.10
1:D:427:THR:HA	1:D:436:MET:HE1	1.17	1.09
1:L:427:THR:HA	1:L:436:MET:HE1	1.17	1.09
1:E:436:MET:HE3	1:E:467:ASN:HD22	1.31	0.96
1:N:436:MET:HE3	1:N:467:ASN:HD22	1.31	0.96
1:D:436:MET:HE3	1:D:467:ASN:HD22	1.31	0.95
1:F:436:MET:HE3	1:F:467:ASN:HD22	1.31	0.95
1:M:436:MET:HE3	1:M:467:ASN:HD22	1.31	0.95
1:L:436:MET:HE3	1:L:467:ASN:HD22	1.31	0.95
1:K:436:MET:HE3	1:K:467:ASN:HD22	1.31	0.95
1:C:436:MET:HE3	1:C:467:ASN:HD22	1.31	0.94
1:G:436:MET:HE3	1:G:467:ASN:HD22	1.31	0.94
1:I:436:MET:HE3	1:I:467:ASN:HD22	1.31	0.94
1:A:436:MET:HE3	1:A:467:ASN:HD22	1.31	0.94
1:B:525:SER:HB3	3:B:3101:HOH:O	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:436:MET:HE3	1:J:467:ASN:HD22	1.31	0.92
1:B:436:MET:HE3	1:B:467:ASN:HD22	1.31	0.92
1:H:436:MET:HE3	1:H:467:ASN:HD22	1.31	0.92
1:O:436:MET:HE3	1:O:467:ASN:HD22	1.31	0.92
1:P:436:MET:HE3	1:P:467:ASN:HD22	1.31	0.92
1:D:427:THR:HA	1:D:436:MET:CE	2.02	0.89
1:L:427:THR:HA	1:L:436:MET:CE	2.02	0.89
1:G:427:THR:HA	1:G:436:MET:CE	2.02	0.89
1:C:427:THR:HA	1:C:436:MET:CE	2.02	0.89
1:N:427:THR:HA	1:N:436:MET:CE	2.02	0.89
1:F:427:THR:HA	1:F:436:MET:CE	2.02	0.89
1:A:427:THR:HA	1:A:436:MET:CE	2.02	0.88
1:E:427:THR:HA	1:E:436:MET:CE	2.02	0.88
1:B:427:THR:HA	1:B:436:MET:CE	2.03	0.88
1:I:427:THR:HA	1:I:436:MET:CE	2.02	0.88
1:J:427:THR:HA	1:J:436:MET:CE	2.03	0.88
1:M:427:THR:HA	1:M:436:MET:CE	2.02	0.88
1:N:595:THR:HG23	1:N:596:PRO:HA	1.57	0.87
1:O:427:THR:HA	1:O:436:MET:CE	2.02	0.87
1:K:427:THR:HA	1:K:436:MET:CE	2.02	0.87
1:F:595:THR:HG23	1:F:596:PRO:HA	1.57	0.87
1:H:595:THR:HG23	1:H:596:PRO:HA	1.57	0.87
1:P:595:THR:HG23	1:P:596:PRO:HA	1.57	0.87
1:P:427:THR:HA	1:P:436:MET:CE	2.02	0.87
1:K:525:SER:HB3	3:K:4178:HOH:O	1.74	0.87
1:E:595:THR:HG23	1:E:596:PRO:HA	1.57	0.86
1:M:595:THR:HG23	1:M:596:PRO:HA	1.57	0.86
1:A:595:THR:HG23	1:A:596:PRO:HA	1.57	0.86
1:H:427:THR:HA	1:H:436:MET:CE	2.02	0.86
1:C:595:THR:HG23	1:C:596:PRO:HA	1.57	0.86
1:J:745:MET:HE2	1:J:745:MET:HA	1.58	0.86
1:K:595:THR:HG23	1:K:596:PRO:HA	1.57	0.86
1:D:745:MET:HA	1:D:745:MET:HE2	1.58	0.85
1:E:745:MET:HE2	1:E:745:MET:HA	1.58	0.85
1:L:595:THR:HG23	1:L:596:PRO:HA	1.57	0.85
1:B:595:THR:HG23	1:B:596:PRO:HA	1.57	0.85
1:D:595:THR:HG23	1:D:596:PRO:HA	1.57	0.85
1:O:525:SER:HB3	3:O:3528:HOH:O	1.76	0.85
1:M:745:MET:HE2	1:M:745:MET:HA	1.58	0.85
1:A:745:MET:HE2	1:A:745:MET:HA	1.58	0.85
1:I:745:MET:HE2	1:I:745:MET:HA	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:745:MET:HA	1:O:745:MET:HE2	1.58	0.85
1:I:595:THR:HG23	1:I:596:PRO:HA	1.57	0.84
1:G:595:THR:HG23	1:G:596:PRO:HA	1.57	0.84
1:K:745:MET:HE2	1:K:745:MET:HA	1.58	0.84
1:B:745:MET:HE2	1:B:745:MET:HA	1.58	0.84
1:G:745:MET:HA	1:G:745:MET:HE2	1.58	0.84
1:J:595:THR:HG23	1:J:596:PRO:HA	1.57	0.84
1:O:595:THR:HG23	1:O:596:PRO:HA	1.57	0.84
1:M:525:SER:HB3	3:M:4424:HOH:O	1.76	0.84
1:L:745:MET:HA	1:L:745:MET:HE2	1.58	0.84
1:F:745:MET:HE2	1:F:745:MET:HA	1.58	0.84
1:N:745:MET:HE2	1:N:745:MET:HA	1.58	0.84
1:H:745:MET:HE2	1:H:745:MET:HA	1.58	0.83
1:J:856:TYR:HD2	1:J:864:MET:HE2	1.44	0.83
1:P:856:TYR:HD2	1:P:864:MET:HE2	1.44	0.83
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.58	0.83
1:P:745:MET:HE2	1:P:745:MET:HA	1.58	0.83
1:H:525:SER:HB3	3:H:4178:HOH:O	1.77	0.83
1:H:856:TYR:HD2	1:H:864:MET:HE2	1.44	0.83
1:C:745:MET:HE2	1:C:745:MET:HA	1.58	0.83
1:A:856:TYR:HD2	1:A:864:MET:HE2	1.44	0.82
1:B:856:TYR:HD2	1:B:864:MET:HE2	1.44	0.82
1:E:856:TYR:HD2	1:E:864:MET:HE2	1.44	0.82
1:F:856:TYR:HD2	1:F:864:MET:HE2	1.44	0.82
1:L:856:TYR:HD2	1:L:864:MET:HE2	1.44	0.82
1:D:856:TYR:HD2	1:D:864:MET:HE2	1.44	0.82
1:K:856:TYR:HD2	1:K:864:MET:HE2	1.44	0.82
1:N:856:TYR:HD2	1:N:864:MET:HE2	1.44	0.82
1:I:856:TYR:HD2	1:I:864:MET:HE2	1.44	0.81
1:M:856:TYR:HD2	1:M:864:MET:HE2	1.44	0.81
1:O:856:TYR:HD2	1:O:864:MET:HE2	1.44	0.81
1:G:856:TYR:HD2	1:G:864:MET:HE2	1.44	0.81
1:A:282:ARG:HD3	1:D:420:MET:O	1.81	0.81
1:C:856:TYR:HD2	1:C:864:MET:HE2	1.44	0.81
1:C:436:MET:CE	1:C:467:ASN:HD22	1.95	0.80
1:F:436:MET:CE	1:F:467:ASN:HD22	1.95	0.80
1:N:436:MET:CE	1:N:467:ASN:HD22	1.95	0.80
1:D:436:MET:CE	1:D:467:ASN:HD22	1.95	0.80
1:M:436:MET:CE	1:M:467:ASN:HD22	1.95	0.80
1:E:436:MET:CE	1:E:467:ASN:HD22	1.95	0.80
1:I:436:MET:CE	1:I:467:ASN:HD22	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:MET:CE	1:A:467:ASN:HD22	1.95	0.79
1:I:525:SER:HB3	3:I:4424:HOH:O	1.81	0.79
1:L:525:SER:HB3	3:L:3107:HOH:O	1.81	0.79
1:I:316:HIS:HA	1:I:323:ILE:HD12	1.66	0.78
1:K:436:MET:CE	1:K:467:ASN:HD22	1.95	0.78
1:L:436:MET:CE	1:L:467:ASN:HD22	1.95	0.78
1:P:436:MET:CE	1:P:467:ASN:HD22	1.95	0.78
1:D:316:HIS:HA	1:D:323:ILE:HD12	1.66	0.78
1:H:436:MET:CE	1:H:467:ASN:HD22	1.95	0.78
1:B:436:MET:CE	1:B:467:ASN:HD22	1.95	0.78
1:P:316:HIS:HA	1:P:323:ILE:HD12	1.66	0.78
1:J:436:MET:CE	1:J:467:ASN:HD22	1.95	0.78
1:O:436:MET:CE	1:O:467:ASN:HD22	1.95	0.78
1:C:316:HIS:HA	1:C:323:ILE:HD12	1.66	0.78
1:L:316:HIS:HA	1:L:323:ILE:HD12	1.66	0.78
1:G:436:MET:CE	1:G:467:ASN:HD22	1.95	0.78
1:J:316:HIS:HA	1:J:323:ILE:HD12	1.66	0.78
1:K:316:HIS:HA	1:K:323:ILE:HD12	1.66	0.78
1:H:316:HIS:HA	1:H:323:ILE:HD12	1.66	0.77
1:B:316:HIS:HA	1:B:323:ILE:HD12	1.66	0.77
1:G:525:SER:HB3	3:G:3531:HOH:O	1.85	0.77
1:E:316:HIS:HA	1:E:323:ILE:HD12	1.66	0.77
1:G:316:HIS:HA	1:G:323:ILE:HD12	1.66	0.77
1:O:316:HIS:HA	1:O:323:ILE:HD12	1.66	0.77
1:J:285:TYR:HB3	1:J:288:ARG:HG3	1.67	0.76
1:B:285:TYR:HB3	1:B:288:ARG:HG3	1.67	0.76
1:E:525:SER:HB3	3:E:4426:HOH:O	1.85	0.76
1:L:949:HIS:CD2	1:L:1020:TRP:HE1	2.04	0.76
1:A:316:HIS:HA	1:A:323:ILE:HD12	1.66	0.76
1:M:316:HIS:HA	1:M:323:ILE:HD12	1.66	0.76
1:I:949:HIS:CD2	1:I:1020:TRP:HE1	2.04	0.76
1:L:57:GLU:HG2	1:L:83:THR:CG2	2.16	0.76
1:B:949:HIS:CD2	1:B:1020:TRP:HE1	2.04	0.76
1:J:57:GLU:HG2	1:J:83:THR:CG2	2.16	0.76
1:N:316:HIS:HA	1:N:323:ILE:HD12	1.66	0.76
1:O:57:GLU:HG2	1:O:83:THR:CG2	2.16	0.76
1:E:57:GLU:HG2	1:E:83:THR:CG2	2.16	0.76
1:K:285:TYR:HB3	1:K:288:ARG:HG3	1.68	0.76
1:N:949:HIS:CD2	1:N:1020:TRP:HE1	2.04	0.76
1:F:316:HIS:HA	1:F:323:ILE:HD12	1.66	0.76
1:F:949:HIS:CD2	1:F:1020:TRP:HE1	2.04	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:949:HIS:CD2	1:J:1020:TRP:HE1	2.04	0.76
1:M:57:GLU:HG2	1:M:83:THR:CG2	2.16	0.76
1:D:57:GLU:HG2	1:D:83:THR:CG2	2.16	0.75
1:D:525:SER:HB3	3:D:3109:HOH:O	1.86	0.75
1:K:57:GLU:HG2	1:K:83:THR:CG2	2.16	0.75
1:L:285:TYR:HB3	1:L:288:ARG:HG3	1.68	0.75
1:A:949:HIS:CD2	1:A:1020:TRP:HE1	2.04	0.75
1:C:949:HIS:CD2	1:C:1020:TRP:HE1	2.04	0.75
1:G:949:HIS:CD2	1:G:1020:TRP:HE1	2.04	0.75
1:H:57:GLU:HG2	1:H:83:THR:CG2	2.16	0.75
1:I:285:TYR:HB3	1:I:288:ARG:HG3	1.67	0.75
1:P:57:GLU:HG2	1:P:83:THR:CG2	2.16	0.75
1:A:57:GLU:HG2	1:A:83:THR:CG2	2.16	0.75
1:C:57:GLU:HG2	1:C:83:THR:CG2	2.16	0.75
1:F:285:TYR:HB3	1:F:288:ARG:HG3	1.67	0.75
1:G:57:GLU:HG2	1:G:83:THR:CG2	2.16	0.75
1:I:57:GLU:HG2	1:I:83:THR:CG2	2.16	0.75
1:M:949:HIS:CD2	1:M:1020:TRP:HE1	2.04	0.75
1:O:949:HIS:CD2	1:O:1020:TRP:HE1	2.04	0.75
1:F:701:VAL:O	1:F:703:PRO:HD3	1.86	0.75
1:K:701:VAL:O	1:K:703:PRO:HD3	1.87	0.75
1:N:285:TYR:HB3	1:N:288:ARG:HG3	1.68	0.75
1:N:525:SER:HB3	3:N:3102:HOH:O	1.87	0.75
1:A:701:VAL:O	1:A:703:PRO:HD3	1.86	0.75
1:H:285:TYR:HB3	1:H:288:ARG:HG3	1.68	0.75
1:B:701:VAL:O	1:B:703:PRO:HD3	1.86	0.75
1:C:701:VAL:O	1:C:703:PRO:HD3	1.86	0.75
1:D:78:LEU:HB3	1:D:79:PRO:HD2	1.69	0.75
1:D:701:VAL:O	1:D:703:PRO:HD3	1.86	0.75
1:E:949:HIS:CD2	1:E:1020:TRP:HE1	2.04	0.75
1:H:701:VAL:O	1:H:703:PRO:HD3	1.86	0.75
1:I:701:VAL:O	1:I:703:PRO:HD3	1.86	0.75
1:P:285:TYR:HB3	1:P:288:ARG:HG3	1.67	0.75
1:J:78:LEU:HB3	1:J:79:PRO:HD2	1.69	0.75
1:P:949:HIS:CD2	1:P:1020:TRP:HE1	2.04	0.75
1:B:57:GLU:HG2	1:B:83:THR:CG2	2.16	0.75
1:D:949:HIS:CD2	1:D:1020:TRP:HE1	2.04	0.75
1:N:57:GLU:HG2	1:N:83:THR:CG2	2.16	0.75
1:A:285:TYR:HB3	1:A:288:ARG:HG3	1.68	0.74
1:G:285:TYR:HB3	1:G:288:ARG:HG3	1.68	0.74
1:K:78:LEU:HB3	1:K:79:PRO:HD2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:285:TYR:HB3	1:O:288:ARG:HG3	1.67	0.74
1:P:701:VAL:O	1:P:703:PRO:HD3	1.86	0.74
1:C:78:LEU:HB3	1:C:79:PRO:HD2	1.69	0.74
1:C:285:TYR:HB3	1:C:288:ARG:HG3	1.67	0.74
1:E:78:LEU:HB3	1:E:79:PRO:HD2	1.69	0.74
1:E:285:TYR:HB3	1:E:288:ARG:HG3	1.68	0.74
1:K:949:HIS:CD2	1:K:1020:TRP:HE1	2.04	0.74
1:F:57:GLU:HG2	1:F:83:THR:CG2	2.16	0.74
1:G:701:VAL:O	1:G:703:PRO:HD3	1.86	0.74
1:P:525:SER:HB3	3:P:3107:HOH:O	1.86	0.74
1:P:78:LEU:HB3	1:P:79:PRO:HD2	1.69	0.74
1:H:78:LEU:HB3	1:H:79:PRO:HD2	1.69	0.74
1:L:701:VAL:O	1:L:703:PRO:HD3	1.86	0.74
1:M:285:TYR:HB3	1:M:288:ARG:HG3	1.68	0.74
1:E:189:LEU:N	1:E:189:LEU:HD23	2.03	0.74
1:J:189:LEU:N	1:J:189:LEU:HD23	2.03	0.74
1:M:78:LEU:HB3	1:M:79:PRO:HD2	1.69	0.74
1:M:189:LEU:N	1:M:189:LEU:HD23	2.03	0.74
1:K:189:LEU:N	1:K:189:LEU:HD23	2.03	0.74
1:M:701:VAL:O	1:M:703:PRO:HD3	1.86	0.74
1:N:701:VAL:O	1:N:703:PRO:HD3	1.86	0.74
1:B:78:LEU:HB3	1:B:79:PRO:HD2	1.69	0.74
1:I:78:LEU:HB3	1:I:79:PRO:HD2	1.69	0.74
1:J:701:VAL:O	1:J:703:PRO:HD3	1.87	0.74
1:P:316:HIS:HA	1:P:323:ILE:CD1	2.18	0.74
1:D:285:TYR:HB3	1:D:288:ARG:HG3	1.68	0.73
1:L:568:TRP:HE1	1:L:604:ASN:HD22	1.37	0.73
1:A:189:LEU:HD23	1:A:189:LEU:N	2.03	0.73
1:H:316:HIS:HA	1:H:323:ILE:CD1	2.19	0.73
1:J:568:TRP:HE1	1:J:604:ASN:HD22	1.36	0.73
1:B:189:LEU:N	1:B:189:LEU:HD23	2.03	0.73
1:E:316:HIS:HA	1:E:323:ILE:CD1	2.18	0.73
1:E:701:VAL:O	1:E:703:PRO:HD3	1.86	0.73
1:F:78:LEU:HB3	1:F:79:PRO:HD2	1.69	0.73
1:H:949:HIS:CD2	1:H:1020:TRP:HE1	2.04	0.73
1:K:316:HIS:HA	1:K:323:ILE:CD1	2.18	0.73
1:L:78:LEU:HB3	1:L:79:PRO:HD2	1.69	0.73
1:M:316:HIS:HA	1:M:323:ILE:CD1	2.19	0.73
1:L:189:LEU:N	1:L:189:LEU:HD23	2.03	0.73
1:M:278:ILE:HD12	1:M:278:ILE:H	1.54	0.73
1:N:78:LEU:HB3	1:N:79:PRO:HD2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:316:HIS:HA	1:O:323:ILE:CD1	2.18	0.73
1:A:316:HIS:HA	1:A:323:ILE:CD1	2.18	0.73
1:B:316:HIS:HA	1:B:323:ILE:CD1	2.18	0.73
1:C:316:HIS:HA	1:C:323:ILE:CD1	2.18	0.73
1:E:278:ILE:HD12	1:E:278:ILE:H	1.54	0.73
1:G:316:HIS:HA	1:G:323:ILE:CD1	2.19	0.73
1:I:316:HIS:HA	1:I:323:ILE:CD1	2.18	0.73
1:P:189:LEU:N	1:P:189:LEU:HD23	2.03	0.73
1:H:189:LEU:N	1:H:189:LEU:HD23	2.03	0.73
1:L:316:HIS:HA	1:L:323:ILE:CD1	2.18	0.73
1:C:189:LEU:N	1:C:189:LEU:HD23	2.03	0.73
1:D:894:ARG:NH2	1:D:921:PRO:HD3	2.04	0.73
1:J:316:HIS:HA	1:J:323:ILE:CD1	2.18	0.73
1:E:568:TRP:HE1	1:E:604:ASN:HD22	1.36	0.73
1:K:894:ARG:NH2	1:K:921:PRO:HD3	2.04	0.73
1:L:278:ILE:H	1:L:278:ILE:HD12	1.54	0.73
1:M:568:TRP:HE1	1:M:604:ASN:HD22	1.37	0.73
1:N:189:LEU:HD23	1:N:189:LEU:N	2.03	0.73
1:O:78:LEU:HB3	1:O:79:PRO:HD2	1.69	0.73
1:A:78:LEU:HB3	1:A:79:PRO:HD2	1.69	0.73
1:F:189:LEU:HD23	1:F:189:LEU:N	2.03	0.73
1:G:78:LEU:HB3	1:G:79:PRO:HD2	1.69	0.73
1:M:282:ARG:HD3	1:P:420:MET:O	1.88	0.73
1:E:894:ARG:NH2	1:E:921:PRO:HD3	2.04	0.73
1:G:189:LEU:N	1:G:189:LEU:HD23	2.03	0.73
1:I:568:TRP:HE1	1:I:604:ASN:HD22	1.37	0.73
1:J:894:ARG:NH2	1:J:921:PRO:HD3	2.04	0.73
1:G:894:ARG:NH2	1:G:921:PRO:HD3	2.04	0.72
1:H:278:ILE:HD12	1:H:278:ILE:H	1.54	0.72
1:K:568:TRP:HE1	1:K:604:ASN:HD22	1.36	0.72
1:O:894:ARG:NH2	1:O:921:PRO:HD3	2.04	0.72
1:C:278:ILE:H	1:C:278:ILE:HD12	1.54	0.72
1:D:189:LEU:N	1:D:189:LEU:HD23	2.03	0.72
1:O:701:VAL:O	1:O:703:PRO:HD3	1.86	0.72
1:L:894:ARG:NH2	1:L:921:PRO:HD3	2.04	0.72
1:A:894:ARG:NH2	1:A:921:PRO:HD3	2.04	0.72
1:F:316:HIS:HA	1:F:323:ILE:CD1	2.18	0.72
1:F:894:ARG:NH2	1:F:921:PRO:HD3	2.04	0.72
1:N:316:HIS:HA	1:N:323:ILE:CD1	2.18	0.72
1:C:894:ARG:NH2	1:C:921:PRO:HD3	2.04	0.72
1:D:316:HIS:HA	1:D:323:ILE:CD1	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:894:ARG:NH2	1:M:921:PRO:HD3	2.04	0.72
1:B:278:ILE:H	1:B:278:ILE:HD12	1.54	0.72
1:N:894:ARG:NH2	1:N:921:PRO:HD3	2.04	0.72
1:P:278:ILE:HD12	1:P:278:ILE:H	1.54	0.72
1:A:568:TRP:HE1	1:A:604:ASN:HD22	1.36	0.72
1:B:894:ARG:NH2	1:B:921:PRO:HD3	2.04	0.72
1:H:894:ARG:NH2	1:H:921:PRO:HD3	2.04	0.72
1:C:568:TRP:HE1	1:C:604:ASN:HD22	1.37	0.72
1:I:189:LEU:HD23	1:I:189:LEU:N	2.03	0.72
1:O:189:LEU:N	1:O:189:LEU:HD23	2.03	0.72
1:P:894:ARG:NH2	1:P:921:PRO:HD3	2.04	0.72
1:I:278:ILE:H	1:I:278:ILE:HD12	1.54	0.72
1:M:425:ARG:NH2	1:P:287:ASP:OD2	2.23	0.72
1:B:568:TRP:HE1	1:B:604:ASN:HD22	1.37	0.72
1:C:7:LEU:CD1	1:C:74:LEU:HD11	2.20	0.72
1:C:183:ARG:HD3	3:C:4254:HOH:O	1.90	0.72
1:D:278:ILE:H	1:D:278:ILE:HD12	1.54	0.72
1:O:278:ILE:H	1:O:278:ILE:HD12	1.54	0.72
1:F:7:LEU:CD1	1:F:74:LEU:HD11	2.20	0.71
1:F:278:ILE:H	1:F:278:ILE:HD12	1.54	0.71
1:M:7:LEU:CD1	1:M:74:LEU:HD11	2.20	0.71
1:M:425:ARG:HH22	1:P:287:ASP:CG	1.98	0.71
1:K:7:LEU:CD1	1:K:74:LEU:HD11	2.20	0.71
1:N:278:ILE:H	1:N:278:ILE:HD12	1.54	0.71
1:E:7:LEU:CD1	1:E:74:LEU:HD11	2.20	0.71
1:I:894:ARG:NH2	1:I:921:PRO:HD3	2.04	0.71
1:K:278:ILE:H	1:K:278:ILE:HD12	1.54	0.71
1:N:7:LEU:CD1	1:N:74:LEU:HD11	2.20	0.71
1:A:278:ILE:H	1:A:278:ILE:HD12	1.54	0.71
1:J:7:LEU:CD1	1:J:74:LEU:HD11	2.20	0.71
1:N:183:ARG:HD3	3:N:3360:HOH:O	1.90	0.71
1:P:568:TRP:HE1	1:P:604:ASN:HD22	1.36	0.71
1:B:7:LEU:CD1	1:B:74:LEU:HD11	2.20	0.71
1:E:183:ARG:HD3	3:E:4253:HOH:O	1.90	0.71
1:A:7:LEU:CD1	1:A:74:LEU:HD11	2.20	0.71
1:D:1021:CME:HE2	1:D:1021:CME:C	2.21	0.71
1:G:7:LEU:CD1	1:G:74:LEU:HD11	2.20	0.71
1:G:278:ILE:H	1:G:278:ILE:HD12	1.54	0.71
1:O:7:LEU:CD1	1:O:74:LEU:HD11	2.20	0.71
1:F:1021:CME:C	1:F:1021:CME:HE2	2.21	0.71
1:N:568:TRP:HE1	1:N:604:ASN:HD22	1.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ARG:HD3	3:D:3366:HOH:O	1.90	0.71
1:D:568:TRP:HE1	1:D:604:ASN:HD22	1.37	0.71
1:H:568:TRP:HE1	1:H:604:ASN:HD22	1.36	0.71
1:I:7:LEU:CD1	1:I:74:LEU:HD11	2.20	0.71
1:L:183:ARG:HD3	3:L:3363:HOH:O	1.90	0.71
1:P:7:LEU:CD1	1:P:74:LEU:HD11	2.20	0.71
1:F:568:TRP:HE1	1:F:604:ASN:HD22	1.37	0.71
1:L:7:LEU:CD1	1:L:74:LEU:HD11	2.20	0.70
1:M:183:ARG:HD3	3:M:4253:HOH:O	1.90	0.70
1:E:1021:CME:C	1:E:1021:CME:HE2	2.21	0.70
1:G:183:ARG:HD3	3:G:3357:HOH:O	1.90	0.70
1:H:7:LEU:CD1	1:H:74:LEU:HD11	2.20	0.70
1:K:1021:CME:C	1:K:1021:CME:HE2	2.21	0.70
1:L:1021:CME:HE2	1:L:1021:CME:C	2.21	0.70
1:O:183:ARG:HD3	3:O:3357:HOH:O	1.90	0.70
1:K:183:ARG:HD3	3:K:4254:HOH:O	1.90	0.70
1:B:183:ARG:HD3	3:B:3357:HOH:O	1.90	0.70
1:D:7:LEU:CD1	1:D:74:LEU:HD11	2.20	0.70
1:F:183:ARG:HD3	3:F:3359:HOH:O	1.90	0.70
1:J:183:ARG:HD3	3:J:3360:HOH:O	1.90	0.70
1:A:1021:CME:C	1:A:1021:CME:HE2	2.21	0.70
1:N:1021:CME:C	1:N:1021:CME:HE2	2.21	0.70
1:G:568:TRP:HE1	1:G:604:ASN:HD22	1.36	0.70
1:J:278:ILE:H	1:J:278:ILE:HD12	1.54	0.70
1:C:1021:CME:C	1:C:1021:CME:HE2	2.21	0.70
1:O:568:TRP:HE1	1:O:604:ASN:HD22	1.37	0.70
1:I:1021:CME:C	1:I:1021:CME:HE2	2.21	0.70
1:P:1021:CME:C	1:P:1021:CME:HE2	2.21	0.70
1:P:183:ARG:HD3	3:P:3365:HOH:O	1.90	0.70
1:I:183:ARG:HD3	3:I:4252:HOH:O	1.90	0.70
1:J:579:ASP:OD1	1:J:583:ASN:HB2	1.92	0.70
1:M:579:ASP:OD1	1:M:583:ASN:HB2	1.92	0.70
1:B:1021:CME:C	1:B:1021:CME:HE2	2.21	0.69
1:E:579:ASP:OD1	1:E:583:ASN:HB2	1.92	0.69
1:G:166:ARG:HG3	1:G:392:TYR:HB2	1.74	0.69
1:K:254:LEU:C	1:K:255:ARG:HG2	2.17	0.69
1:P:166:ARG:HG3	1:P:392:TYR:HB2	1.74	0.69
1:A:183:ARG:HD3	3:A:4254:HOH:O	1.90	0.69
1:B:579:ASP:OD1	1:B:583:ASN:HB2	1.92	0.69
1:D:166:ARG:HG3	1:D:392:TYR:HB2	1.74	0.69
1:K:579:ASP:OD1	1:K:583:ASN:HB2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:166:ARG:HG3	1:O:392:TYR:HB2	1.74	0.69
1:P:579:ASP:OD1	1:P:583:ASN:HB2	1.93	0.69
1:G:579:ASP:OD1	1:G:583:ASN:HB2	1.92	0.69
1:H:166:ARG:HG3	1:H:392:TYR:HB2	1.74	0.69
1:H:254:LEU:C	1:H:255:ARG:HG2	2.17	0.69
1:C:579:ASP:OD1	1:C:583:ASN:HB2	1.92	0.69
1:G:254:LEU:C	1:G:255:ARG:HG2	2.17	0.69
1:K:63:PHE:HB3	1:K:64:PRO:HD2	1.75	0.69
1:O:1021:CME:HE2	1:O:1021:CME:C	2.21	0.69
1:G:1021:CME:C	1:G:1021:CME:HE2	2.21	0.69
1:H:183:ARG:HD3	3:H:4254:HOH:O	1.90	0.69
1:I:63:PHE:HB3	1:I:64:PRO:HD2	1.75	0.69
1:A:425:ARG:HH22	1:D:287:ASP:CG	2.01	0.69
1:B:166:ARG:HG3	1:B:392:TYR:HB2	1.74	0.69
1:L:254:LEU:C	1:L:255:ARG:HG2	2.17	0.69
1:P:254:LEU:C	1:P:255:ARG:HG2	2.17	0.69
1:F:579:ASP:OD1	1:F:583:ASN:HB2	1.92	0.69
1:I:254:LEU:C	1:I:255:ARG:HG2	2.17	0.69
1:A:254:LEU:C	1:A:255:ARG:HG2	2.17	0.69
1:A:579:ASP:OD1	1:A:583:ASN:HB2	1.92	0.69
1:B:254:LEU:C	1:B:255:ARG:HG2	2.17	0.69
1:F:434:PRO:HB3	1:G:434:PRO:HB3	1.74	0.69
1:G:63:PHE:HB3	1:G:64:PRO:HD2	1.75	0.69
1:H:1021:CME:C	1:H:1021:CME:HE2	2.21	0.69
1:J:1021:CME:C	1:J:1021:CME:HE2	2.21	0.69
1:N:166:ARG:HG3	1:N:392:TYR:HB2	1.74	0.69
1:O:63:PHE:HB3	1:O:64:PRO:HD2	1.75	0.69
1:O:579:ASP:OD1	1:O:583:ASN:HB2	1.92	0.69
1:B:919:ASP:O	1:B:920:LEU:HD23	1.93	0.69
1:E:254:LEU:C	1:E:255:ARG:HG2	2.17	0.69
1:F:166:ARG:HG3	1:F:392:TYR:HB2	1.74	0.69
1:N:287:ASP:CG	1:O:425:ARG:HH22	2.01	0.69
1:B:63:PHE:HB3	1:B:64:PRO:HD2	1.75	0.69
1:C:166:ARG:HG3	1:C:392:TYR:HB2	1.74	0.69
1:E:166:ARG:HG3	1:E:392:TYR:HB2	1.74	0.69
1:J:166:ARG:HG3	1:J:392:TYR:HB2	1.74	0.69
1:O:952:ARG:NH1	1:O:952:ARG:HG2	2.08	0.69
1:A:63:PHE:HB3	1:A:64:PRO:HD2	1.75	0.68
1:J:952:ARG:NH1	1:J:952:ARG:HG2	2.08	0.68
1:L:579:ASP:OD1	1:L:583:ASN:HB2	1.92	0.68
1:M:1021:CME:C	1:M:1021:CME:HE2	2.21	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:579:ASP:OD1	1:N:583:ASN:HB2	1.92	0.68
1:P:952:ARG:NH1	1:P:952:ARG:HG2	2.08	0.68
1:C:525:SER:HB3	3:C:4178:HOH:O	1.91	0.68
1:D:254:LEU:C	1:D:255:ARG:HG2	2.17	0.68
1:F:254:LEU:C	1:F:255:ARG:HG2	2.17	0.68
1:G:919:ASP:O	1:G:920:LEU:HD23	1.93	0.68
1:H:952:ARG:NH1	1:H:952:ARG:HG2	2.08	0.68
1:L:952:ARG:HG2	1:L:952:ARG:NH1	2.08	0.68
1:A:919:ASP:O	1:A:920:LEU:HD23	1.93	0.68
1:D:919:ASP:O	1:D:920:LEU:HD23	1.94	0.68
1:I:166:ARG:HG3	1:I:392:TYR:HB2	1.74	0.68
1:J:254:LEU:C	1:J:255:ARG:HG2	2.17	0.68
1:L:166:ARG:HG3	1:L:392:TYR:HB2	1.74	0.68
1:N:254:LEU:C	1:N:255:ARG:HG2	2.17	0.68
1:A:952:ARG:HG2	1:A:952:ARG:NH1	2.08	0.68
1:I:919:ASP:O	1:I:920:LEU:HD23	1.93	0.68
1:O:254:LEU:C	1:O:255:ARG:HG2	2.17	0.68
1:O:919:ASP:O	1:O:920:LEU:HD23	1.93	0.68
1:F:856:TYR:CD2	1:F:864:MET:HE2	2.29	0.68
1:H:919:ASP:O	1:H:920:LEU:HD23	1.94	0.68
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.74	0.68
1:J:63:PHE:HB3	1:J:64:PRO:HD2	1.75	0.68
1:M:166:ARG:HG3	1:M:392:TYR:HB2	1.74	0.68
1:N:919:ASP:O	1:N:920:LEU:HD23	1.94	0.68
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.75	0.68
1:E:919:ASP:O	1:E:920:LEU:HD23	1.93	0.68
1:I:579:ASP:OD1	1:I:583:ASN:HB2	1.92	0.68
1:L:63:PHE:HB3	1:L:64:PRO:HD2	1.75	0.68
1:B:43:ARG:HG2	1:B:43:ARG:HH11	1.59	0.68
1:H:43:ARG:HG2	1:H:43:ARG:HH11	1.59	0.68
1:I:920:LEU:HB3	1:I:921:PRO:HD2	1.76	0.68
1:M:254:LEU:C	1:M:255:ARG:HG2	2.17	0.68
1:O:917:ARG:HH22	1:O:943:GLU:CD	2.02	0.68
1:F:917:ARG:HH22	1:F:943:GLU:CD	2.02	0.68
1:G:890:GLN:HG3	1:G:891:VAL:N	2.09	0.68
1:I:890:GLN:HG3	1:I:891:VAL:N	2.09	0.68
1:J:43:ARG:HH11	1:J:43:ARG:HG2	1.59	0.68
1:A:890:GLN:HG3	1:A:891:VAL:N	2.09	0.68
1:C:917:ARG:HH22	1:C:943:GLU:CD	2.02	0.68
1:D:579:ASP:OD1	1:D:583:ASN:HB2	1.92	0.68
1:J:919:ASP:O	1:J:920:LEU:HD23	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:43:ARG:HG2	1:O:43:ARG:HH11	1.59	0.68
1:C:43:ARG:HG2	1:C:43:ARG:HH11	1.59	0.67
1:C:254:LEU:C	1:C:255:ARG:HG2	2.17	0.67
1:F:919:ASP:O	1:F:920:LEU:HD23	1.94	0.67
1:G:952:ARG:NH1	1:G:952:ARG:HG2	2.08	0.67
1:H:579:ASP:OD1	1:H:583:ASN:HB2	1.92	0.67
1:I:952:ARG:HG2	1:I:952:ARG:NH1	2.08	0.67
1:L:917:ARG:HH22	1:L:943:GLU:CD	2.02	0.67
1:L:919:ASP:O	1:L:920:LEU:HD23	1.93	0.67
1:M:919:ASP:O	1:M:920:LEU:HD23	1.94	0.67
1:P:43:ARG:HG2	1:P:43:ARG:HH11	1.59	0.67
1:A:917:ARG:HH22	1:A:943:GLU:CD	2.02	0.67
1:I:917:ARG:HH22	1:I:943:GLU:CD	2.02	0.67
1:K:917:ARG:HH22	1:K:943:GLU:CD	2.02	0.67
1:L:856:TYR:CD2	1:L:864:MET:HE2	2.29	0.67
1:P:919:ASP:O	1:P:920:LEU:HD23	1.94	0.67
1:E:43:ARG:HG2	1:E:43:ARG:HH11	1.59	0.67
1:G:43:ARG:HG2	1:G:43:ARG:HH11	1.59	0.67
1:K:166:ARG:HG3	1:K:392:TYR:HB2	1.74	0.67
1:M:43:ARG:HG2	1:M:43:ARG:HH11	1.59	0.67
1:N:890:GLN:HG3	1:N:891:VAL:N	2.09	0.67
1:C:856:TYR:CD2	1:C:864:MET:HE2	2.29	0.67
1:C:952:ARG:HG2	1:C:952:ARG:NH1	2.08	0.67
1:E:920:LEU:HB3	1:E:921:PRO:HD2	1.76	0.67
1:J:890:GLN:HG3	1:J:891:VAL:N	2.09	0.67
1:K:919:ASP:O	1:K:920:LEU:HD23	1.94	0.67
1:L:920:LEU:HB3	1:L:921:PRO:HD2	1.76	0.67
1:M:63:PHE:HB3	1:M:64:PRO:HD2	1.75	0.67
1:M:920:LEU:HB3	1:M:921:PRO:HD2	1.76	0.67
1:B:920:LEU:HB3	1:B:921:PRO:HD2	1.76	0.67
1:C:63:PHE:HB3	1:C:64:PRO:HD2	1.75	0.67
1:D:917:ARG:HH22	1:D:943:GLU:CD	2.02	0.67
1:E:63:PHE:HB3	1:E:64:PRO:HD2	1.75	0.67
1:N:952:ARG:HG2	1:N:952:ARG:NH1	2.08	0.67
1:O:856:TYR:CD2	1:O:864:MET:HE2	2.29	0.67
1:E:952:ARG:NH1	1:E:952:ARG:HG2	2.08	0.67
1:F:43:ARG:HG2	1:F:43:ARG:HH11	1.59	0.67
1:G:920:LEU:HB3	1:G:921:PRO:HD2	1.76	0.67
1:H:63:PHE:HB3	1:H:64:PRO:HD2	1.75	0.67
1:M:917:ARG:HH22	1:M:943:GLU:CD	2.02	0.67
1:N:43:ARG:HG2	1:N:43:ARG:HH11	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:920:LEU:HB3	1:O:921:PRO:HD2	1.76	0.67
1:G:917:ARG:HH22	1:G:943:GLU:CD	2.02	0.67
1:K:920:LEU:HB3	1:K:921:PRO:HD2	1.76	0.67
1:E:917:ARG:HH22	1:E:943:GLU:CD	2.02	0.67
1:F:63:PHE:HB3	1:F:64:PRO:HD2	1.75	0.67
1:F:890:GLN:HG3	1:F:891:VAL:N	2.09	0.67
1:F:952:ARG:HG2	1:F:952:ARG:NH1	2.08	0.67
1:K:952:ARG:HG2	1:K:952:ARG:NH1	2.08	0.67
1:M:7:LEU:HD13	1:M:74:LEU:HD11	1.77	0.67
1:M:952:ARG:NH1	1:M:952:ARG:HG2	2.08	0.67
1:N:63:PHE:HB3	1:N:64:PRO:HD2	1.75	0.67
1:A:43:ARG:HG2	1:A:43:ARG:HH11	1.59	0.67
1:B:278:ILE:HD12	1:B:278:ILE:N	2.10	0.67
1:C:919:ASP:O	1:C:920:LEU:HD23	1.94	0.67
1:E:7:LEU:HD13	1:E:74:LEU:HD11	1.77	0.67
1:F:920:LEU:HB3	1:F:921:PRO:HD2	1.76	0.67
1:H:890:GLN:HG3	1:H:891:VAL:N	2.09	0.67
1:H:917:ARG:HH22	1:H:943:GLU:CD	2.02	0.67
1:J:278:ILE:HD12	1:J:278:ILE:N	2.10	0.67
1:K:43:ARG:HG2	1:K:43:ARG:HH11	1.59	0.67
1:P:278:ILE:HD12	1:P:278:ILE:N	2.10	0.67
1:B:917:ARG:HH22	1:B:943:GLU:CD	2.02	0.66
1:D:952:ARG:HG2	1:D:952:ARG:NH1	2.08	0.66
1:G:278:ILE:HD12	1:G:278:ILE:N	2.10	0.66
1:H:278:ILE:HD12	1:H:278:ILE:N	2.10	0.66
1:L:43:ARG:HG2	1:L:43:ARG:HH11	1.59	0.66
1:L:952:ARG:HG2	1:L:952:ARG:HH11	1.61	0.66
1:N:856:TYR:CD2	1:N:864:MET:HE2	2.29	0.66
1:N:920:LEU:HB3	1:N:921:PRO:HD2	1.76	0.66
1:O:278:ILE:HD12	1:O:278:ILE:N	2.10	0.66
1:A:7:LEU:HD13	1:A:74:LEU:HD11	1.77	0.66
1:I:278:ILE:HD12	1:I:278:ILE:N	2.10	0.66
1:J:920:LEU:HB3	1:J:921:PRO:HD2	1.76	0.66
1:L:278:ILE:HD12	1:L:278:ILE:N	2.10	0.66
1:M:278:ILE:HD12	1:M:278:ILE:N	2.10	0.66
1:B:952:ARG:HG2	1:B:952:ARG:HH11	1.61	0.66
1:F:278:ILE:HD12	1:F:278:ILE:N	2.10	0.66
1:K:278:ILE:HD12	1:K:278:ILE:N	2.10	0.66
1:N:278:ILE:HD12	1:N:278:ILE:N	2.10	0.66
1:N:917:ARG:HH22	1:N:943:GLU:CD	2.02	0.66
1:A:418:HIS:O	1:D:282:ARG:HD2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:890:GLN:HG3	1:C:891:VAL:N	2.09	0.66
1:C:952:ARG:HG2	1:C:952:ARG:HH11	1.61	0.66
1:E:278:ILE:HD12	1:E:278:ILE:N	2.10	0.66
1:I:43:ARG:HG2	1:I:43:ARG:HH11	1.59	0.66
1:J:917:ARG:HH22	1:J:943:GLU:CD	2.02	0.66
1:L:890:GLN:HG3	1:L:891:VAL:N	2.09	0.66
1:O:890:GLN:HG3	1:O:891:VAL:N	2.09	0.66
1:P:63:PHE:HB3	1:P:64:PRO:HD2	1.75	0.66
1:P:917:ARG:HH22	1:P:943:GLU:CD	2.02	0.66
1:D:278:ILE:HD12	1:D:278:ILE:N	2.10	0.66
1:H:7:LEU:HD13	1:H:74:LEU:HD11	1.77	0.66
1:K:856:TYR:CD2	1:K:864:MET:HE2	2.29	0.66
1:B:890:GLN:HG3	1:B:891:VAL:N	2.09	0.66
1:B:952:ARG:HG2	1:B:952:ARG:NH1	2.08	0.66
1:D:43:ARG:HG2	1:D:43:ARG:HH11	1.59	0.66
1:D:856:TYR:CD2	1:D:864:MET:HE2	2.29	0.66
1:D:890:GLN:HG3	1:D:891:VAL:N	2.09	0.66
1:P:7:LEU:HD13	1:P:74:LEU:HD11	1.77	0.66
1:A:525:SER:HB3	3:A:4178:HOH:O	1.94	0.66
1:D:7:LEU:HD13	1:D:74:LEU:HD11	1.77	0.66
1:J:7:LEU:HD13	1:J:74:LEU:HD11	1.77	0.66
1:L:7:LEU:HD13	1:L:74:LEU:HD11	1.77	0.66
1:C:920:LEU:HB3	1:C:921:PRO:HD2	1.76	0.66
1:E:952:ARG:HG2	1:E:952:ARG:HH11	1.61	0.66
1:J:434:PRO:HB3	1:K:434:PRO:HB3	1.76	0.66
1:M:890:GLN:HG3	1:M:891:VAL:N	2.09	0.66
1:N:952:ARG:HG2	1:N:952:ARG:HH11	1.61	0.66
1:P:890:GLN:HG3	1:P:891:VAL:N	2.09	0.66
1:A:278:ILE:HD12	1:A:278:ILE:N	2.10	0.66
1:C:278:ILE:HD12	1:C:278:ILE:N	2.10	0.66
1:M:952:ARG:HG2	1:M:952:ARG:HH11	1.61	0.66
1:N:43:ARG:HG2	1:N:43:ARG:NH1	2.11	0.66
1:A:920:LEU:HB3	1:A:921:PRO:HD2	1.76	0.66
1:D:43:ARG:HG2	1:D:43:ARG:NH1	2.11	0.66
1:D:952:ARG:HG2	1:D:952:ARG:HH11	1.61	0.66
1:O:43:ARG:HG2	1:O:43:ARG:NH1	2.11	0.66
1:P:856:TYR:CD2	1:P:864:MET:HE2	2.29	0.66
1:P:952:ARG:HG2	1:P:952:ARG:HH11	1.60	0.66
1:D:920:LEU:HB3	1:D:921:PRO:HD2	1.76	0.65
1:P:43:ARG:HG2	1:P:43:ARG:NH1	2.11	0.65
1:P:920:LEU:HB3	1:P:921:PRO:HD2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:ARG:HG2	1:E:43:ARG:NH1	2.11	0.65
1:F:525:SER:HB3	3:F:3102:HOH:O	1.95	0.65
1:F:952:ARG:HG2	1:F:952:ARG:HH11	1.61	0.65
1:H:43:ARG:HG2	1:H:43:ARG:NH1	2.11	0.65
1:J:334:GLU:OE1	1:J:336:ARG:NH1	2.30	0.65
1:K:890:GLN:HG3	1:K:891:VAL:N	2.09	0.65
1:A:117:GLU:OE1	1:A:117:GLU:N	2.29	0.65
1:D:7:LEU:N	1:D:71:GLU:OE2	2.30	0.65
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.30	0.65
1:H:59:ARG:NH2	1:H:81:ALA:O	2.30	0.65
1:H:952:ARG:HG2	1:H:952:ARG:HH11	1.61	0.65
1:K:43:ARG:HG2	1:K:43:ARG:NH1	2.11	0.65
1:A:334:GLU:OE1	1:A:336:ARG:NH1	2.30	0.65
1:B:7:LEU:N	1:B:71:GLU:OE2	2.30	0.65
1:F:7:LEU:N	1:F:71:GLU:OE2	2.30	0.65
1:I:7:LEU:N	1:I:71:GLU:OE2	2.30	0.65
1:J:7:LEU:N	1:J:71:GLU:OE2	2.30	0.65
1:K:952:ARG:HG2	1:K:952:ARG:HH11	1.61	0.65
1:L:334:GLU:OE1	1:L:336:ARG:NH1	2.30	0.65
1:P:59:ARG:NH2	1:P:81:ALA:O	2.30	0.65
1:A:43:ARG:HG2	1:A:43:ARG:NH1	2.11	0.65
1:B:7:LEU:HD13	1:B:74:LEU:HD11	1.77	0.65
1:E:856:TYR:CD2	1:E:864:MET:HE2	2.29	0.65
1:E:890:GLN:HG3	1:E:891:VAL:N	2.09	0.65
1:I:681:GLU:HA	1:I:681:GLU:OE2	1.97	0.65
1:M:43:ARG:HG2	1:M:43:ARG:NH1	2.11	0.65
1:O:7:LEU:HD13	1:O:74:LEU:HD11	1.77	0.65
1:H:920:LEU:HB3	1:H:921:PRO:HD2	1.76	0.65
1:I:59:ARG:NH2	1:I:81:ALA:O	2.30	0.65
1:I:427:THR:CA	1:I:436:MET:HE1	2.12	0.65
1:L:7:LEU:N	1:L:71:GLU:OE2	2.30	0.65
1:F:334:GLU:OE1	1:F:336:ARG:NH1	2.30	0.65
1:J:59:ARG:NH2	1:J:81:ALA:O	2.30	0.65
1:J:952:ARG:HG2	1:J:952:ARG:HH11	1.61	0.65
1:K:7:LEU:N	1:K:71:GLU:OE2	2.30	0.65
1:M:117:GLU:OE1	1:M:117:GLU:N	2.29	0.65
1:N:334:GLU:OE1	1:N:336:ARG:NH1	2.30	0.65
1:B:59:ARG:NH2	1:B:81:ALA:O	2.30	0.65
1:B:856:TYR:CD2	1:B:864:MET:HE2	2.29	0.65
1:C:7:LEU:N	1:C:71:GLU:OE2	2.30	0.65
1:C:681:GLU:HA	1:C:681:GLU:OE2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:GLU:OE1	1:E:117:GLU:N	2.29	0.65
1:E:334:GLU:OE1	1:E:336:ARG:NH1	2.30	0.65
1:G:7:LEU:HD13	1:G:74:LEU:HD11	1.77	0.65
1:H:856:TYR:CD2	1:H:864:MET:HE2	2.29	0.65
1:N:7:LEU:HD13	1:N:74:LEU:HD11	1.77	0.65
1:F:43:ARG:HG2	1:F:43:ARG:NH1	2.11	0.65
1:F:59:ARG:NH2	1:F:81:ALA:O	2.30	0.65
1:J:43:ARG:HG2	1:J:43:ARG:NH1	2.11	0.65
1:J:856:TYR:CD2	1:J:864:MET:HE2	2.29	0.65
1:L:59:ARG:NH2	1:L:81:ALA:O	2.30	0.65
1:A:952:ARG:HG2	1:A:952:ARG:HH11	1.61	0.64
1:B:43:ARG:HG2	1:B:43:ARG:NH1	2.11	0.64
1:C:59:ARG:NH2	1:C:81:ALA:O	2.30	0.64
1:D:917:ARG:NH2	1:D:943:GLU:OE1	2.30	0.64
1:G:43:ARG:HG2	1:G:43:ARG:NH1	2.11	0.64
1:G:952:ARG:HG2	1:G:952:ARG:HH11	1.61	0.64
1:J:917:ARG:NH2	1:J:943:GLU:OE1	2.30	0.64
1:M:334:GLU:OE1	1:M:336:ARG:NH1	2.30	0.64
1:N:59:ARG:NH2	1:N:81:ALA:O	2.30	0.64
1:P:7:LEU:N	1:P:71:GLU:OE2	2.30	0.64
1:A:59:ARG:NH2	1:A:81:ALA:O	2.30	0.64
1:C:334:GLU:OE1	1:C:336:ARG:NH1	2.30	0.64
1:C:917:ARG:NH2	1:C:943:GLU:OE1	2.30	0.64
1:F:7:LEU:HD13	1:F:74:LEU:HD11	1.77	0.64
1:F:753:ASN:OD1	1:F:753:ASN:N	2.30	0.64
1:H:7:LEU:N	1:H:71:GLU:OE2	2.30	0.64
1:L:43:ARG:HG2	1:L:43:ARG:NH1	2.11	0.64
1:O:917:ARG:NH2	1:O:943:GLU:OE1	2.30	0.64
1:A:7:LEU:N	1:A:71:GLU:OE2	2.30	0.64
1:A:856:TYR:CD2	1:A:864:MET:HE2	2.29	0.64
1:B:334:GLU:OE1	1:B:336:ARG:NH1	2.30	0.64
1:G:917:ARG:NH2	1:G:943:GLU:OE1	2.30	0.64
1:K:334:GLU:OE1	1:K:336:ARG:NH1	2.30	0.64
1:M:279:ILE:HD11	1:P:422:PRO:HG2	1.79	0.64
1:N:753:ASN:OD1	1:N:753:ASN:N	2.30	0.64
1:E:7:LEU:N	1:E:71:GLU:OE2	2.30	0.64
1:G:59:ARG:NH2	1:G:81:ALA:O	2.30	0.64
1:G:334:GLU:OE1	1:G:336:ARG:NH1	2.30	0.64
1:L:917:ARG:NH2	1:L:943:GLU:OE1	2.30	0.64
1:N:287:ASP:OD2	1:O:425:ARG:NH2	2.30	0.64
1:N:917:ARG:NH2	1:N:943:GLU:OE1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:334:GLU:OE1	1:O:336:ARG:NH1	2.30	0.64
1:F:917:ARG:NH2	1:F:943:GLU:OE1	2.30	0.64
1:I:7:LEU:HD13	1:I:74:LEU:HD11	1.77	0.64
1:I:952:ARG:HG2	1:I:952:ARG:HH11	1.61	0.64
1:J:117:GLU:N	1:J:117:GLU:OE1	2.29	0.64
1:C:117:GLU:OE1	1:C:117:GLU:N	2.29	0.64
1:G:681:GLU:HA	1:G:681:GLU:OE2	1.97	0.64
1:H:917:ARG:NH2	1:H:943:GLU:OE1	2.30	0.64
1:I:334:GLU:OE1	1:I:336:ARG:NH1	2.30	0.64
1:P:917:ARG:NH2	1:P:943:GLU:OE1	2.30	0.64
1:C:43:ARG:HG2	1:C:43:ARG:NH1	2.11	0.64
1:H:334:GLU:OE1	1:H:336:ARG:NH1	2.30	0.64
1:I:917:ARG:NH2	1:I:943:GLU:OE1	2.30	0.64
1:M:7:LEU:N	1:M:71:GLU:OE2	2.30	0.64
1:M:59:ARG:NH2	1:M:81:ALA:O	2.30	0.64
1:B:917:ARG:NH2	1:B:943:GLU:OE1	2.30	0.64
1:C:7:LEU:HD13	1:C:74:LEU:HD11	1.77	0.64
1:E:59:ARG:NH2	1:E:81:ALA:O	2.30	0.64
1:I:43:ARG:HG2	1:I:43:ARG:NH1	2.11	0.64
1:J:525:SER:HB3	3:J:3103:HOH:O	1.97	0.64
1:N:7:LEU:N	1:N:71:GLU:OE2	2.30	0.64
1:O:7:LEU:N	1:O:71:GLU:OE2	2.30	0.64
1:P:334:GLU:OE1	1:P:336:ARG:NH1	2.30	0.64
1:G:7:LEU:N	1:G:71:GLU:OE2	2.30	0.64
1:O:59:ARG:NH2	1:O:81:ALA:O	2.30	0.64
1:O:681:GLU:OE2	1:O:681:GLU:HA	1.97	0.64
1:B:681:GLU:HA	1:B:681:GLU:OE2	1.97	0.64
1:D:59:ARG:NH2	1:D:81:ALA:O	2.30	0.64
1:D:681:GLU:OE2	1:D:681:GLU:HA	1.97	0.64
1:K:59:ARG:NH2	1:K:81:ALA:O	2.30	0.64
1:M:856:TYR:CD2	1:M:864:MET:HE2	2.29	0.64
1:M:917:ARG:NH2	1:M:943:GLU:OE1	2.30	0.64
1:O:427:THR:CA	1:O:436:MET:HE1	2.12	0.64
1:E:129:VAL:HG23	1:E:182:ASN:HD22	1.63	0.63
1:K:117:GLU:OE1	1:K:117:GLU:N	2.29	0.63
1:F:117:GLU:OE1	1:F:117:GLU:N	2.29	0.63
1:A:917:ARG:NH2	1:A:943:GLU:OE1	2.30	0.63
1:G:856:TYR:CD2	1:G:864:MET:HE2	2.29	0.63
1:J:129:VAL:HG23	1:J:182:ASN:HD22	1.63	0.63
1:K:7:LEU:HD13	1:K:74:LEU:HD11	1.77	0.63
1:K:917:ARG:NH2	1:K:943:GLU:OE1	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:129:VAL:HG23	1:L:182:ASN:HD22	1.63	0.63
1:P:681:GLU:HA	1:P:681:GLU:OE2	1.97	0.63
1:A:427:THR:CA	1:A:436:MET:HE1	2.12	0.63
1:D:129:VAL:HG23	1:D:182:ASN:HD22	1.63	0.63
1:J:681:GLU:HA	1:J:681:GLU:OE2	1.97	0.63
1:K:681:GLU:HA	1:K:681:GLU:OE2	1.97	0.63
1:O:129:VAL:HG23	1:O:182:ASN:HD22	1.63	0.63
1:P:117:GLU:OE1	1:P:117:GLU:N	2.29	0.63
1:E:917:ARG:NH2	1:E:943:GLU:OE1	2.30	0.63
1:H:129:VAL:HG23	1:H:182:ASN:HD22	1.63	0.63
1:M:129:VAL:HG23	1:M:182:ASN:HD22	1.64	0.63
1:N:681:GLU:HA	1:N:681:GLU:OE2	1.97	0.63
1:E:681:GLU:HA	1:E:681:GLU:OE2	1.97	0.63
1:L:681:GLU:OE2	1:L:681:GLU:HA	1.97	0.63
1:M:681:GLU:HA	1:M:681:GLU:OE2	1.97	0.63
1:A:681:GLU:HA	1:A:681:GLU:OE2	1.97	0.63
1:F:681:GLU:HA	1:F:681:GLU:OE2	1.97	0.63
1:E:66:PRO:HB3	1:E:187:MET:CE	2.29	0.63
1:F:66:PRO:HB3	1:F:187:MET:CE	2.29	0.63
1:G:129:VAL:HG23	1:G:182:ASN:HD22	1.63	0.63
1:N:66:PRO:HB3	1:N:187:MET:CE	2.29	0.63
1:P:129:VAL:HG23	1:P:182:ASN:HD22	1.63	0.63
1:A:129:VAL:HG23	1:A:182:ASN:HD22	1.63	0.62
1:J:66:PRO:HB3	1:J:187:MET:CE	2.29	0.62
1:K:129:VAL:HG23	1:K:182:ASN:HD22	1.63	0.62
1:C:66:PRO:HB3	1:C:187:MET:CE	2.29	0.62
1:O:952:ARG:HG2	1:O:952:ARG:HH11	1.60	0.62
1:B:66:PRO:HB3	1:B:187:MET:CE	2.29	0.62
1:J:753:ASN:OD1	1:J:753:ASN:N	2.30	0.62
1:C:129:VAL:HG23	1:C:182:ASN:HD22	1.63	0.62
1:F:129:VAL:HG23	1:F:182:ASN:HD22	1.63	0.62
1:M:66:PRO:HB3	1:M:187:MET:CE	2.30	0.62
1:O:66:PRO:HB3	1:O:187:MET:CE	2.29	0.62
1:D:66:PRO:HB3	1:D:187:MET:CE	2.30	0.62
1:G:66:PRO:HB3	1:G:187:MET:CE	2.29	0.62
1:H:681:GLU:HA	1:H:681:GLU:OE2	1.97	0.62
1:I:856:TYR:CD2	1:I:864:MET:HE2	2.29	0.62
1:N:129:VAL:HG23	1:N:182:ASN:HD22	1.63	0.62
1:B:129:VAL:HG23	1:B:182:ASN:HD22	1.63	0.62
1:L:66:PRO:HB3	1:L:187:MET:CE	2.29	0.62
1:A:66:PRO:HB3	1:A:187:MET:CE	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:117:GLU:OE1	1:I:117:GLU:N	2.29	0.62
1:N:30:HIS:ND1	1:N:31:PRO:O	2.30	0.62
1:H:117:GLU:OE1	1:H:117:GLU:N	2.29	0.62
1:K:66:PRO:HB3	1:K:187:MET:CE	2.29	0.62
1:K:753:ASN:OD1	1:K:753:ASN:N	2.30	0.62
1:L:427:THR:CA	1:L:436:MET:HE1	2.12	0.61
1:H:66:PRO:HB3	1:H:187:MET:CE	2.29	0.61
1:I:129:VAL:HG23	1:I:182:ASN:HD22	1.63	0.61
1:P:66:PRO:HB3	1:P:187:MET:CE	2.29	0.61
1:I:66:PRO:HB3	1:I:187:MET:CE	2.29	0.61
1:A:30:HIS:ND1	1:A:31:PRO:O	2.30	0.61
1:L:634:GLN:O	1:L:682:LEU:HB2	2.01	0.61
1:A:425:ARG:NH2	1:D:287:ASP:OD2	2.34	0.61
1:A:749:ILE:CD1	1:A:834:VAL:HG11	2.31	0.61
1:E:749:ILE:CD1	1:E:834:VAL:HG11	2.31	0.61
1:F:749:ILE:CD1	1:F:834:VAL:HG11	2.31	0.61
1:I:30:HIS:ND1	1:I:31:PRO:O	2.30	0.61
1:I:749:ILE:CD1	1:I:834:VAL:HG11	2.31	0.61
1:L:753:ASN:OD1	1:L:753:ASN:N	2.30	0.61
1:M:749:ILE:CD1	1:M:834:VAL:HG11	2.31	0.61
1:N:749:ILE:CD1	1:N:834:VAL:HG11	2.31	0.61
1:C:749:ILE:CD1	1:C:834:VAL:HG11	2.31	0.61
1:K:427:THR:CA	1:K:436:MET:HE1	2.12	0.61
1:L:1020:TRP:HD1	1:L:1021:CME:N	1.99	0.61
1:F:129:VAL:HG23	1:F:182:ASN:ND2	2.16	0.61
1:G:634:GLN:O	1:G:682:LEU:HB2	2.01	0.61
1:G:749:ILE:CD1	1:G:834:VAL:HG11	2.31	0.61
1:H:634:GLN:O	1:H:682:LEU:HB2	2.01	0.61
1:N:129:VAL:HG23	1:N:182:ASN:ND2	2.16	0.61
1:O:129:VAL:HG23	1:O:182:ASN:ND2	2.16	0.61
1:O:749:ILE:CD1	1:O:834:VAL:HG11	2.31	0.61
1:O:1020:TRP:HD1	1:O:1021:CME:N	1.99	0.61
1:C:634:GLN:O	1:C:682:LEU:HB2	2.01	0.61
1:F:1020:TRP:HD1	1:F:1021:CME:N	1.99	0.61
1:P:1020:TRP:HD1	1:P:1021:CME:N	1.99	0.61
1:C:1020:TRP:HD1	1:C:1021:CME:N	1.99	0.61
1:D:117:GLU:OE1	1:D:117:GLU:N	2.29	0.61
1:D:1020:TRP:HD1	1:D:1021:CME:N	1.99	0.60
1:L:129:VAL:HG23	1:L:182:ASN:ND2	2.16	0.60
1:L:749:ILE:CD1	1:L:834:VAL:HG11	2.31	0.60
1:N:1020:TRP:HD1	1:N:1021:CME:N	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:634:GLN:O	1:O:682:LEU:HB2	2.01	0.60
1:P:634:GLN:O	1:P:682:LEU:HB2	2.01	0.60
1:A:129:VAL:HG23	1:A:182:ASN:ND2	2.16	0.60
1:B:129:VAL:HG23	1:B:182:ASN:ND2	2.16	0.60
1:D:749:ILE:CD1	1:D:834:VAL:HG11	2.31	0.60
1:E:129:VAL:HG23	1:E:182:ASN:ND2	2.16	0.60
1:H:749:ILE:CD1	1:H:834:VAL:HG11	2.31	0.60
1:J:634:GLN:O	1:J:682:LEU:HB2	2.01	0.60
1:K:1020:TRP:HD1	1:K:1021:CME:N	1.99	0.60
1:B:634:GLN:O	1:B:682:LEU:HB2	2.01	0.60
1:C:129:VAL:HG23	1:C:182:ASN:ND2	2.16	0.60
1:G:117:GLU:N	1:G:117:GLU:OE1	2.29	0.60
1:H:30:HIS:ND1	1:H:31:PRO:O	2.30	0.60
1:H:1020:TRP:HD1	1:H:1021:CME:N	1.99	0.60
1:K:749:ILE:CD1	1:K:834:VAL:HG11	2.31	0.60
1:N:682:LEU:HD22	1:N:683:PRO:HD2	1.84	0.60
1:O:682:LEU:HD22	1:O:683:PRO:HD2	1.83	0.60
1:D:30:HIS:ND1	1:D:31:PRO:O	2.30	0.60
1:F:682:LEU:HD22	1:F:683:PRO:HD2	1.84	0.60
1:K:634:GLN:O	1:K:682:LEU:HB2	2.01	0.60
1:K:682:LEU:HD22	1:K:683:PRO:HD2	1.84	0.60
1:L:682:LEU:HD22	1:L:683:PRO:HD2	1.83	0.60
1:M:129:VAL:HG23	1:M:182:ASN:ND2	2.16	0.60
1:P:682:LEU:HD22	1:P:683:PRO:HD2	1.84	0.60
1:C:333:ARG:NH2	3:C:4202:HOH:O	2.31	0.60
1:C:682:LEU:HD22	1:C:683:PRO:HD2	1.84	0.60
1:G:129:VAL:HG23	1:G:182:ASN:ND2	2.16	0.60
1:G:682:LEU:HD22	1:G:683:PRO:HD2	1.83	0.60
1:H:129:VAL:HG23	1:H:182:ASN:ND2	2.16	0.60
1:H:682:LEU:HD22	1:H:683:PRO:HD2	1.83	0.60
1:I:1020:TRP:HD1	1:I:1021:CME:N	1.99	0.60
1:J:749:ILE:CD1	1:J:834:VAL:HG11	2.31	0.60
1:O:117:GLU:OE1	1:O:117:GLU:N	2.29	0.60
1:B:749:ILE:CD1	1:B:834:VAL:HG11	2.31	0.60
1:E:634:GLN:O	1:E:682:LEU:HB2	2.01	0.60
1:F:634:GLN:O	1:F:682:LEU:HB2	2.01	0.60
1:G:322:LEU:HD23	1:G:324:GLU:N	2.17	0.60
1:G:1020:TRP:HD1	1:G:1021:CME:N	1.99	0.60
1:I:682:LEU:HD22	1:I:683:PRO:HD2	1.83	0.60
1:L:178:ARG:NH1	1:L:181:GLU:O	2.35	0.60
1:A:634:GLN:O	1:A:682:LEU:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1020:TRP:HD1	1:B:1021:CME:N	1.99	0.60
1:D:634:GLN:O	1:D:682:LEU:HB2	2.01	0.60
1:F:178:ARG:NH1	1:F:181:GLU:O	2.35	0.60
1:J:88:SER:HA	1:J:366:VAL:HG21	1.84	0.60
1:K:129:VAL:HG23	1:K:182:ASN:ND2	2.16	0.60
1:M:178:ARG:NH1	1:M:181:GLU:O	2.35	0.60
1:N:634:GLN:O	1:N:682:LEU:HB2	2.01	0.60
1:O:322:LEU:HD23	1:O:324:GLU:N	2.17	0.60
1:A:88:SER:HA	1:A:366:VAL:HG21	1.84	0.60
1:E:322:LEU:HD23	1:E:324:GLU:N	2.17	0.60
1:H:360:HIS:CE1	1:H:362:LEU:HB2	2.37	0.60
1:K:178:ARG:NH1	1:K:181:GLU:O	2.35	0.60
1:N:322:LEU:HD23	1:N:324:GLU:N	2.17	0.60
1:P:322:LEU:HD23	1:P:324:GLU:N	2.17	0.60
1:A:1020:TRP:HD1	1:A:1021:CME:N	1.99	0.60
1:B:178:ARG:NH1	1:B:181:GLU:O	2.35	0.60
1:B:322:LEU:HD23	1:B:324:GLU:N	2.17	0.60
1:C:88:SER:HA	1:C:366:VAL:HG21	1.84	0.60
1:D:178:ARG:NH1	1:D:181:GLU:O	2.35	0.60
1:H:322:LEU:HD23	1:H:324:GLU:N	2.17	0.60
1:I:178:ARG:NH1	1:I:181:GLU:O	2.35	0.60
1:K:577:LYS:O	1:K:584:PRO:HA	2.02	0.60
1:L:577:LYS:O	1:L:584:PRO:HA	2.02	0.60
1:M:682:LEU:HD22	1:M:683:PRO:HD2	1.83	0.60
1:M:753:ASN:OD1	1:M:753:ASN:N	2.30	0.60
1:P:577:LYS:O	1:P:584:PRO:HA	2.02	0.60
1:A:577:LYS:O	1:A:584:PRO:HA	2.02	0.60
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.37	0.60
1:D:129:VAL:HG23	1:D:182:ASN:ND2	2.16	0.60
1:H:577:LYS:O	1:H:584:PRO:HA	2.02	0.60
1:J:322:LEU:HD23	1:J:324:GLU:N	2.17	0.60
1:K:88:SER:HA	1:K:366:VAL:HG21	1.84	0.60
1:K:333:ARG:NH2	3:K:4202:HOH:O	2.31	0.60
1:K:360:HIS:CE1	1:K:362:LEU:HB2	2.37	0.60
1:L:117:GLU:OE1	1:L:117:GLU:N	2.29	0.60
1:N:360:HIS:CE1	1:N:362:LEU:HB2	2.37	0.60
1:E:178:ARG:NH1	1:E:181:GLU:O	2.35	0.59
1:E:753:ASN:OD1	1:E:753:ASN:N	2.30	0.59
1:F:30:HIS:ND1	1:F:31:PRO:O	2.30	0.59
1:F:360:HIS:CE1	1:F:362:LEU:HB2	2.37	0.59
1:G:178:ARG:NH1	1:G:181:GLU:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:577:LYS:O	1:G:584:PRO:HA	2.02	0.59
1:J:682:LEU:HD22	1:J:683:PRO:HD2	1.83	0.59
1:L:322:LEU:HD23	1:L:324:GLU:N	2.17	0.59
1:M:88:SER:HA	1:M:366:VAL:HG21	1.84	0.59
1:N:178:ARG:NH1	1:N:181:GLU:O	2.35	0.59
1:N:427:THR:CA	1:N:436:MET:HE1	2.12	0.59
1:N:577:LYS:O	1:N:584:PRO:HA	2.02	0.59
1:P:129:VAL:HG23	1:P:182:ASN:ND2	2.16	0.59
1:D:322:LEU:HD23	1:D:324:GLU:N	2.17	0.59
1:I:129:VAL:HG23	1:I:182:ASN:ND2	2.16	0.59
1:I:322:LEU:HD23	1:I:324:GLU:N	2.17	0.59
1:M:322:LEU:HD23	1:M:324:GLU:N	2.17	0.59
1:O:178:ARG:NH1	1:O:181:GLU:O	2.35	0.59
1:O:577:LYS:O	1:O:584:PRO:HA	2.02	0.59
1:P:178:ARG:NH1	1:P:181:GLU:O	2.35	0.59
1:P:360:HIS:CE1	1:P:362:LEU:HB2	2.37	0.59
1:A:322:LEU:HD23	1:A:324:GLU:N	2.17	0.59
1:B:786:ARG:HH11	1:B:990:HIS:CE1	2.21	0.59
1:D:360:HIS:CE1	1:D:362:LEU:HB2	2.37	0.59
1:E:786:ARG:HH11	1:E:990:HIS:CE1	2.21	0.59
1:E:1020:TRP:HD1	1:E:1021:CME:N	1.99	0.59
1:F:287:ASP:OD2	1:G:425:ARG:NH2	2.35	0.59
1:F:577:LYS:O	1:F:584:PRO:HA	2.02	0.59
1:G:88:SER:HA	1:G:366:VAL:HG21	1.84	0.59
1:H:178:ARG:NH1	1:H:181:GLU:O	2.35	0.59
1:I:634:GLN:O	1:I:682:LEU:HB2	2.01	0.59
1:J:129:VAL:HG23	1:J:182:ASN:ND2	2.16	0.59
1:J:178:ARG:NH1	1:J:181:GLU:O	2.35	0.59
1:J:360:HIS:CE1	1:J:362:LEU:HB2	2.37	0.59
1:J:786:ARG:HH11	1:J:990:HIS:CE1	2.21	0.59
1:J:1020:TRP:HD1	1:J:1021:CME:N	1.99	0.59
1:K:322:LEU:HD23	1:K:324:GLU:N	2.17	0.59
1:N:117:GLU:OE1	1:N:117:GLU:N	2.29	0.59
1:O:88:SER:HA	1:O:366:VAL:HG21	1.84	0.59
1:A:178:ARG:NH1	1:A:181:GLU:O	2.35	0.59
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.37	0.59
1:A:682:LEU:HD22	1:A:683:PRO:HD2	1.84	0.59
1:A:786:ARG:HH11	1:A:990:HIS:CE1	2.21	0.59
1:B:577:LYS:O	1:B:584:PRO:HA	2.02	0.59
1:D:682:LEU:HD22	1:D:683:PRO:HD2	1.83	0.59
1:E:88:SER:HA	1:E:366:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:682:LEU:HD22	1:E:683:PRO:HD2	1.83	0.59
1:G:360:HIS:CE1	1:G:362:LEU:HB2	2.37	0.59
1:M:1020:TRP:HD1	1:M:1021:CME:N	1.99	0.59
1:N:894:ARG:NH1	1:N:919:ASP:OD2	2.36	0.59
1:B:894:ARG:NH1	1:B:919:ASP:OD2	2.36	0.59
1:C:178:ARG:NH1	1:C:181:GLU:O	2.35	0.59
1:C:427:THR:CA	1:C:436:MET:HE1	2.12	0.59
1:C:894:ARG:NH1	1:C:919:ASP:OD2	2.36	0.59
1:F:894:ARG:NH1	1:F:919:ASP:OD2	2.36	0.59
1:G:786:ARG:HH11	1:G:990:HIS:CE1	2.21	0.59
1:I:333:ARG:NH2	3:I:4200:HOH:O	2.31	0.59
1:L:786:ARG:HH11	1:L:990:HIS:CE1	2.21	0.59
1:N:786:ARG:HH11	1:N:990:HIS:CE1	2.21	0.59
1:O:786:ARG:HH11	1:O:990:HIS:CE1	2.21	0.59
1:B:682:LEU:HD22	1:B:683:PRO:HD2	1.84	0.59
1:C:322:LEU:HD23	1:C:324:GLU:N	2.17	0.59
1:C:577:LYS:O	1:C:584:PRO:HA	2.02	0.59
1:F:427:THR:CA	1:F:436:MET:HE1	2.12	0.59
1:F:786:ARG:HH11	1:F:990:HIS:CE1	2.21	0.59
1:H:786:ARG:HH11	1:H:990:HIS:CE1	2.21	0.59
1:I:577:LYS:O	1:I:584:PRO:HA	2.02	0.59
1:L:88:SER:HA	1:L:366:VAL:HG21	1.84	0.59
1:P:749:ILE:CD1	1:P:834:VAL:HG11	2.31	0.59
1:B:117:GLU:OE1	1:B:117:GLU:N	2.29	0.59
1:G:894:ARG:NH1	1:G:919:ASP:OD2	2.36	0.59
1:H:88:SER:HA	1:H:366:VAL:HG21	1.84	0.59
1:B:333:ARG:NH2	3:B:3305:HOH:O	2.31	0.59
1:I:786:ARG:HH11	1:I:990:HIS:CE1	2.21	0.59
1:K:894:ARG:NH1	1:K:919:ASP:OD2	2.36	0.59
1:M:894:ARG:NH1	1:M:919:ASP:OD2	2.36	0.59
1:N:745:MET:HE2	1:N:745:MET:CA	2.32	0.59
1:C:249:GLU:OE1	1:C:251:ARG:NH1	2.34	0.59
1:D:786:ARG:HH11	1:D:990:HIS:CE1	2.21	0.59
1:D:786:ARG:HH11	1:D:990:HIS:HE1	1.51	0.59
1:F:322:LEU:HD23	1:F:324:GLU:N	2.17	0.59
1:J:894:ARG:NH1	1:J:919:ASP:OD2	2.36	0.59
1:L:894:ARG:NH1	1:L:919:ASP:OD2	2.36	0.59
1:M:746:ASP:HA	1:M:760:ARG:HG3	1.85	0.59
1:N:333:ARG:NH2	3:N:3308:HOH:O	2.31	0.59
1:P:786:ARG:HH11	1:P:990:HIS:CE1	2.21	0.59
1:A:746:ASP:HA	1:A:760:ARG:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:753:ASN:OD1	1:D:753:ASN:N	2.30	0.59
1:E:746:ASP:HA	1:E:760:ARG:HG3	1.85	0.59
1:I:88:SER:HA	1:I:366:VAL:HG21	1.84	0.59
1:I:360:HIS:CE1	1:I:362:LEU:HB2	2.37	0.59
1:M:577:LYS:O	1:M:584:PRO:HA	2.02	0.59
1:A:786:ARG:HH11	1:A:990:HIS:HE1	1.50	0.58
1:C:360:HIS:CE1	1:C:362:LEU:HB2	2.37	0.58
1:D:577:LYS:O	1:D:584:PRO:HA	2.02	0.58
1:E:894:ARG:NH1	1:E:919:ASP:OD2	2.36	0.58
1:F:88:SER:HA	1:F:366:VAL:HG21	1.84	0.58
1:F:746:ASP:HA	1:F:760:ARG:HG3	1.85	0.58
1:I:745:MET:HE2	1:I:745:MET:CA	2.32	0.58
1:J:377:LEU:N	1:J:377:LEU:HD23	2.18	0.58
1:J:427:THR:CA	1:J:436:MET:HE1	2.12	0.58
1:N:746:ASP:HA	1:N:760:ARG:HG3	1.85	0.58
1:O:360:HIS:CE1	1:O:362:LEU:HB2	2.37	0.58
1:E:360:HIS:CE1	1:E:362:LEU:HB2	2.37	0.58
1:E:786:ARG:HH11	1:E:990:HIS:HE1	1.50	0.58
1:L:746:ASP:HA	1:L:760:ARG:HG3	1.85	0.58
1:M:634:GLN:O	1:M:682:LEU:HB2	2.01	0.58
1:P:88:SER:HA	1:P:366:VAL:HG21	1.84	0.58
1:P:786:ARG:HH11	1:P:990:HIS:HE1	1.50	0.58
1:B:287:ASP:OD2	1:C:425:ARG:NH2	2.36	0.58
1:C:786:ARG:HH11	1:C:990:HIS:CE1	2.21	0.58
1:D:88:SER:HA	1:D:366:VAL:HG21	1.84	0.58
1:D:745:MET:HE2	1:D:745:MET:CA	2.32	0.58
1:E:577:LYS:O	1:E:584:PRO:HA	2.02	0.58
1:H:786:ARG:HH11	1:H:990:HIS:HE1	1.50	0.58
1:H:894:ARG:NH1	1:H:919:ASP:OD2	2.36	0.58
1:I:746:ASP:HA	1:I:760:ARG:HG3	1.85	0.58
1:J:436:MET:HE3	1:J:467:ASN:ND2	2.13	0.58
1:N:88:SER:HA	1:N:366:VAL:HG21	1.84	0.58
1:O:894:ARG:NH1	1:O:919:ASP:OD2	2.36	0.58
1:D:746:ASP:HA	1:D:760:ARG:HG3	1.85	0.58
1:G:272:ALA:HB1	1:G:273:PRO:HD2	1.86	0.58
1:J:745:MET:HE2	1:J:745:MET:CA	2.32	0.58
1:J:746:ASP:HA	1:J:760:ARG:HG3	1.85	0.58
1:L:166:ARG:HD3	3:L:3144:HOH:O	2.04	0.58
1:M:360:HIS:CE1	1:M:362:LEU:HB2	2.37	0.58
1:O:272:ALA:HB1	1:O:273:PRO:HD2	1.86	0.58
1:D:427:THR:CA	1:D:436:MET:HE1	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:ARG:NH2	3:E:4201:HOH:O	2.31	0.58
1:F:166:ARG:HD3	3:F:3140:HOH:O	2.04	0.58
1:N:166:ARG:HD3	3:N:3141:HOH:O	2.04	0.58
1:P:894:ARG:NH1	1:P:919:ASP:OD2	2.36	0.58
1:G:166:ARG:HD3	3:G:3138:HOH:O	2.04	0.58
1:I:377:LEU:N	1:I:377:LEU:HD23	2.19	0.58
1:J:249:GLU:OE1	1:J:251:ARG:NH1	2.34	0.58
1:J:577:LYS:O	1:J:584:PRO:HA	2.02	0.58
1:L:272:ALA:HB1	1:L:273:PRO:HD2	1.86	0.58
1:L:360:HIS:CE1	1:L:362:LEU:HB2	2.37	0.58
1:M:786:ARG:HH11	1:M:990:HIS:HE1	1.50	0.58
1:M:786:ARG:HH11	1:M:990:HIS:CE1	2.21	0.58
1:B:88:SER:HA	1:B:366:VAL:HG21	1.84	0.58
1:E:434:PRO:HB3	1:H:434:PRO:HB3	1.84	0.58
1:G:249:GLU:OE1	1:G:251:ARG:NH1	2.34	0.58
1:I:894:ARG:NH1	1:I:919:ASP:OD2	2.36	0.58
1:J:786:ARG:HH11	1:J:990:HIS:HE1	1.51	0.58
1:O:249:GLU:OE1	1:O:251:ARG:NH1	2.34	0.58
1:A:249:GLU:OE1	1:A:251:ARG:NH1	2.34	0.58
1:A:377:LEU:N	1:A:377:LEU:HD23	2.18	0.58
1:B:377:LEU:N	1:B:377:LEU:HD23	2.18	0.58
1:E:745:MET:HE2	1:E:745:MET:CA	2.32	0.58
1:H:746:ASP:HA	1:H:760:ARG:HG3	1.86	0.58
1:I:272:ALA:HB1	1:I:273:PRO:HD2	1.86	0.58
1:J:272:ALA:HB1	1:J:273:PRO:HD2	1.86	0.58
1:K:597:ASN:HD22	1:K:599:ARG:H	1.52	0.58
1:K:786:ARG:HH11	1:K:990:HIS:CE1	2.21	0.58
1:L:597:ASN:HD22	1:L:599:ARG:H	1.52	0.58
1:M:333:ARG:NH2	3:M:4201:HOH:O	2.31	0.58
1:A:894:ARG:NH1	1:A:919:ASP:OD2	2.36	0.58
1:B:272:ALA:HB1	1:B:273:PRO:HD2	1.86	0.58
1:B:786:ARG:HH11	1:B:990:HIS:HE1	1.51	0.58
1:C:166:ARG:HD3	3:C:4034:HOH:O	2.04	0.58
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.85	0.58
1:E:597:ASN:HD22	1:E:599:ARG:H	1.52	0.58
1:K:786:ARG:HH11	1:K:990:HIS:HE1	1.51	0.58
1:M:377:LEU:N	1:M:377:LEU:HD23	2.19	0.58
1:M:830:LEU:HD11	1:N:830:LEU:HD11	1.86	0.58
1:N:377:LEU:HD23	1:N:377:LEU:N	2.19	0.58
1:N:420:MET:O	1:O:282:ARG:HD3	2.03	0.58
1:A:272:ALA:HB1	1:A:273:PRO:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:597:ASN:HD22	1:D:599:ARG:H	1.52	0.58
1:F:272:ALA:HB1	1:F:273:PRO:HD2	1.86	0.58
1:G:668:VAL:HG13	1:G:669:PRO:HD2	1.86	0.58
1:N:272:ALA:HB1	1:N:273:PRO:HD2	1.86	0.58
1:P:166:ARG:HG3	1:P:392:TYR:CB	2.34	0.58
1:P:746:ASP:HA	1:P:760:ARG:HG3	1.85	0.58
1:A:333:ARG:NH2	3:A:4202:HOH:O	2.31	0.57
1:B:166:ARG:HD3	3:B:3139:HOH:O	2.04	0.57
1:C:753:ASN:OD1	1:C:753:ASN:N	2.30	0.57
1:C:786:ARG:HH11	1:C:990:HIS:HE1	1.50	0.57
1:K:272:ALA:HB1	1:K:273:PRO:HD2	1.86	0.57
1:L:377:LEU:N	1:L:377:LEU:HD23	2.18	0.57
1:M:597:ASN:HD22	1:M:599:ARG:H	1.52	0.57
1:O:436:MET:HE3	1:O:467:ASN:ND2	2.13	0.57
1:O:668:VAL:HG13	1:O:669:PRO:HD2	1.87	0.57
1:A:668:VAL:HG13	1:A:669:PRO:HD2	1.87	0.57
1:I:668:VAL:HG13	1:I:669:PRO:HD2	1.87	0.57
1:L:30:HIS:ND1	1:L:31:PRO:O	2.30	0.57
1:M:249:GLU:OE1	1:M:251:ARG:NH1	2.34	0.57
1:E:166:ARG:HD3	3:E:4034:HOH:O	2.04	0.57
1:M:166:ARG:HG3	1:M:392:TYR:CB	2.34	0.57
1:N:434:PRO:HB3	1:O:434:PRO:HB3	1.85	0.57
1:N:662:PRO:C	1:N:663:LEU:HD23	2.30	0.57
1:B:597:ASN:HD22	1:B:599:ARG:H	1.52	0.57
1:B:668:VAL:HG13	1:B:669:PRO:HD2	1.86	0.57
1:C:272:ALA:HB1	1:C:273:PRO:HD2	1.86	0.57
1:D:662:PRO:C	1:D:663:LEU:HD23	2.30	0.57
1:E:166:ARG:HG3	1:E:392:TYR:CB	2.34	0.57
1:F:662:PRO:C	1:F:663:LEU:HD23	2.30	0.57
1:G:377:LEU:N	1:G:377:LEU:HD23	2.18	0.57
1:J:662:PRO:C	1:J:663:LEU:HD23	2.30	0.57
1:O:377:LEU:N	1:O:377:LEU:HD23	2.18	0.57
1:C:668:VAL:HG13	1:C:669:PRO:HD2	1.87	0.57
1:D:166:ARG:HD3	3:D:3147:HOH:O	2.04	0.57
1:D:377:LEU:N	1:D:377:LEU:HD23	2.18	0.57
1:L:662:PRO:C	1:L:663:LEU:HD23	2.30	0.57
1:L:668:VAL:HG13	1:L:669:PRO:HD2	1.86	0.57
1:P:597:ASN:HD22	1:P:599:ARG:H	1.52	0.57
1:A:279:ILE:HD11	1:D:422:PRO:HG2	1.86	0.57
1:B:662:PRO:C	1:B:663:LEU:HD23	2.30	0.57
1:C:377:LEU:HD23	1:C:377:LEU:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:662:PRO:C	1:E:663:LEU:HD23	2.30	0.57
1:G:166:ARG:HG3	1:G:392:TYR:CB	2.34	0.57
1:G:746:ASP:HA	1:G:760:ARG:HG3	1.85	0.57
1:I:279:ILE:HD11	1:L:422:PRO:HG2	1.85	0.57
1:O:166:ARG:HG3	1:O:392:TYR:CB	2.34	0.57
1:O:746:ASP:HA	1:O:760:ARG:HG3	1.85	0.57
1:G:662:PRO:C	1:G:663:LEU:HD23	2.30	0.57
1:H:166:ARG:HG3	1:H:392:TYR:CB	2.34	0.57
1:I:166:ARG:HG3	1:I:392:TYR:CB	2.34	0.57
1:I:786:ARG:HH11	1:I:990:HIS:HE1	1.50	0.57
1:J:30:HIS:ND1	1:J:31:PRO:O	2.30	0.57
1:K:30:HIS:ND1	1:K:31:PRO:O	2.30	0.57
1:N:166:ARG:HG3	1:N:392:TYR:CB	2.34	0.57
1:N:436:MET:HE3	1:N:467:ASN:ND2	2.13	0.57
1:N:668:VAL:HG13	1:N:669:PRO:HD2	1.87	0.57
1:O:333:ARG:NH2	3:O:3305:HOH:O	2.31	0.57
1:A:597:ASN:HD22	1:A:599:ARG:H	1.52	0.57
1:A:662:PRO:C	1:A:663:LEU:HD23	2.30	0.57
1:B:166:ARG:HG3	1:B:392:TYR:CB	2.34	0.57
1:B:249:GLU:OE1	1:B:251:ARG:NH1	2.34	0.57
1:F:668:VAL:HG13	1:F:669:PRO:HD2	1.86	0.57
1:F:786:ARG:HH11	1:F:990:HIS:HE1	1.50	0.57
1:G:333:ARG:NH2	3:G:3305:HOH:O	2.31	0.57
1:H:436:MET:HE3	1:H:467:ASN:ND2	2.13	0.57
1:I:166:ARG:HD3	3:I:4034:HOH:O	2.04	0.57
1:K:166:ARG:HD3	3:K:4034:HOH:O	2.04	0.57
1:P:166:ARG:HD3	3:P:3146:HOH:O	2.04	0.57
1:D:166:ARG:HG3	1:D:392:TYR:CB	2.34	0.57
1:D:249:GLU:OE1	1:D:251:ARG:NH1	2.34	0.57
1:D:894:ARG:NH1	1:D:919:ASP:OD2	2.36	0.57
1:E:63:PHE:CB	1:E:64:PRO:HD2	2.34	0.57
1:F:166:ARG:HG3	1:F:392:TYR:CB	2.34	0.57
1:F:436:MET:HE3	1:F:467:ASN:ND2	2.13	0.57
1:J:597:ASN:HD22	1:J:599:ARG:H	1.52	0.57
1:P:662:PRO:C	1:P:663:LEU:HD23	2.30	0.57
1:C:30:HIS:ND1	1:C:31:PRO:O	2.30	0.57
1:C:662:PRO:C	1:C:663:LEU:HD23	2.30	0.57
1:E:249:GLU:OE1	1:E:251:ARG:NH1	2.34	0.57
1:H:662:PRO:C	1:H:663:LEU:HD23	2.30	0.57
1:J:166:ARG:HD3	3:J:3141:HOH:O	2.04	0.57
1:J:422:PRO:HG2	1:K:279:ILE:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:272:ALA:HB1	1:M:273:PRO:HD2	1.86	0.57
1:O:166:ARG:HD3	3:O:3138:HOH:O	2.04	0.57
1:P:272:ALA:HB1	1:P:273:PRO:HD2	1.86	0.57
1:B:949:HIS:HD2	1:B:1020:TRP:HE1	1.53	0.56
1:C:745:MET:HE2	1:C:745:MET:CA	2.32	0.56
1:H:597:ASN:HD22	1:H:599:ARG:H	1.52	0.56
1:H:668:VAL:HG13	1:H:669:PRO:HD2	1.86	0.56
1:N:249:GLU:OE1	1:N:251:ARG:NH1	2.34	0.56
1:P:30:HIS:ND1	1:P:31:PRO:O	2.30	0.56
1:A:166:ARG:HG3	1:A:392:TYR:CB	2.34	0.56
1:A:166:ARG:HD3	3:A:4034:HOH:O	2.04	0.56
1:F:249:GLU:OE1	1:F:251:ARG:NH1	2.35	0.56
1:F:287:ASP:CG	1:G:425:ARG:HH22	2.12	0.56
1:I:662:PRO:C	1:I:663:LEU:HD23	2.30	0.56
1:L:786:ARG:HH11	1:L:990:HIS:HE1	1.50	0.56
1:B:30:HIS:ND1	1:B:31:PRO:O	2.30	0.56
1:C:166:ARG:HG3	1:C:392:TYR:CB	2.34	0.56
1:C:597:ASN:HD22	1:C:599:ARG:H	1.52	0.56
1:D:272:ALA:HB1	1:D:273:PRO:HD2	1.86	0.56
1:F:377:LEU:HD23	1:F:377:LEU:N	2.19	0.56
1:H:166:ARG:HD3	3:H:4034:HOH:O	2.04	0.56
1:K:166:ARG:HG3	1:K:392:TYR:CB	2.34	0.56
1:K:377:LEU:N	1:K:377:LEU:HD23	2.18	0.56
1:L:166:ARG:HG3	1:L:392:TYR:CB	2.34	0.56
1:L:949:HIS:HD2	1:L:1020:TRP:HE1	1.53	0.56
1:M:166:ARG:HD3	3:M:4034:HOH:O	2.04	0.56
1:N:786:ARG:HH11	1:N:990:HIS:HE1	1.51	0.56
1:P:436:MET:HE3	1:P:467:ASN:ND2	2.13	0.56
1:B:316:HIS:HD2	1:B:317:THR:O	1.89	0.56
1:D:316:HIS:HD2	1:D:317:THR:O	1.89	0.56
1:D:668:VAL:HG13	1:D:669:PRO:HD2	1.87	0.56
1:G:316:HIS:HD2	1:G:317:THR:O	1.89	0.56
1:H:272:ALA:HB1	1:H:273:PRO:HD2	1.86	0.56
1:H:333:ARG:NH2	3:H:4202:HOH:O	2.31	0.56
1:M:662:PRO:C	1:M:663:LEU:HD23	2.30	0.56
1:O:30:HIS:ND1	1:O:31:PRO:O	2.30	0.56
1:O:662:PRO:C	1:O:663:LEU:HD23	2.30	0.56
1:A:436:MET:HE3	1:A:467:ASN:ND2	2.13	0.56
1:B:746:ASP:HA	1:B:760:ARG:HG3	1.85	0.56
1:E:30:HIS:ND1	1:E:31:PRO:O	2.30	0.56
1:E:316:HIS:HD2	1:E:317:THR:O	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:427:THR:CA	1:E:436:MET:HE1	2.12	0.56
1:H:493:THR:HG23	3:H:4019:HOH:O	2.06	0.56
1:I:645:ARG:NH2	1:I:650:GLU:OE1	2.39	0.56
1:K:493:THR:HG23	3:K:4019:HOH:O	2.06	0.56
1:M:434:PRO:HB3	1:P:434:PRO:HB3	1.87	0.56
1:N:316:HIS:HD2	1:N:317:THR:O	1.89	0.56
1:P:493:THR:HG23	3:P:3131:HOH:O	2.06	0.56
1:A:316:HIS:HD2	1:A:317:THR:O	1.89	0.56
1:E:202:MET:HE3	1:E:357:HIS:CE1	2.41	0.56
1:E:377:LEU:N	1:E:377:LEU:HD23	2.18	0.56
1:E:645:ARG:NH2	1:E:650:GLU:OE1	2.39	0.56
1:F:493:THR:HG23	3:F:3125:HOH:O	2.06	0.56
1:G:786:ARG:HH11	1:G:990:HIS:HE1	1.50	0.56
1:H:202:MET:HE3	1:H:357:HIS:CE1	2.41	0.56
1:M:316:HIS:HD2	1:M:317:THR:O	1.89	0.56
1:M:745:MET:HE2	1:M:745:MET:CA	2.32	0.56
1:D:949:HIS:HD2	1:D:1020:TRP:HE1	1.53	0.56
1:E:272:ALA:HB1	1:E:273:PRO:HD2	1.86	0.56
1:F:202:MET:HE3	1:F:357:HIS:CE1	2.41	0.56
1:I:63:PHE:CB	1:I:64:PRO:HD2	2.34	0.56
1:I:202:MET:HE3	1:I:357:HIS:CE1	2.41	0.56
1:K:746:ASP:HA	1:K:760:ARG:HG3	1.85	0.56
1:O:597:ASN:HD22	1:O:599:ARG:H	1.52	0.56
1:O:786:ARG:HH11	1:O:990:HIS:HE1	1.51	0.56
1:P:645:ARG:NH2	1:P:650:GLU:OE1	2.39	0.56
1:P:668:VAL:HG13	1:P:669:PRO:HD2	1.87	0.56
1:D:202:MET:HE3	1:D:357:HIS:CE1	2.41	0.56
1:D:645:ARG:NH2	1:D:650:GLU:OE1	2.39	0.56
1:G:597:ASN:HD22	1:G:599:ARG:H	1.52	0.56
1:I:493:THR:HG23	3:I:4019:HOH:O	2.06	0.56
1:I:753:ASN:OD1	1:I:753:ASN:N	2.30	0.56
1:K:662:PRO:C	1:K:663:LEU:HD23	2.30	0.56
1:M:202:MET:HE3	1:M:357:HIS:CE1	2.41	0.56
1:P:202:MET:HE3	1:P:357:HIS:CE1	2.41	0.56
1:A:202:MET:HE3	1:A:357:HIS:CE1	2.41	0.56
1:C:202:MET:HE3	1:C:357:HIS:CE1	2.41	0.56
1:C:595:THR:HG23	1:C:596:PRO:CA	2.35	0.56
1:F:63:PHE:CB	1:F:64:PRO:HD2	2.34	0.56
1:F:597:ASN:HD22	1:F:599:ARG:H	1.52	0.56
1:H:377:LEU:N	1:H:377:LEU:HD23	2.19	0.56
1:I:894:ARG:HD3	1:I:919:ASP:OD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:493:THR:HG23	3:M:4019:HOH:O	2.06	0.56
1:O:745:MET:HE2	1:O:745:MET:CA	2.32	0.56
1:P:377:LEU:N	1:P:377:LEU:HD23	2.18	0.56
1:A:493:THR:HG23	3:A:4019:HOH:O	2.06	0.56
1:A:894:ARG:HD3	1:A:919:ASP:OD2	2.06	0.56
1:B:202:MET:HE3	1:B:357:HIS:CE1	2.41	0.56
1:F:645:ARG:NH2	1:F:650:GLU:OE1	2.39	0.56
1:J:645:ARG:NH2	1:J:650:GLU:OE1	2.39	0.56
1:L:770:ILE:HD11	1:L:1022:GLN:HG2	1.88	0.56
1:N:63:PHE:CB	1:N:64:PRO:HD2	2.34	0.56
1:N:597:ASN:HD22	1:N:599:ARG:H	1.52	0.56
1:N:645:ARG:NH2	1:N:650:GLU:OE1	2.39	0.56
1:O:202:MET:HE3	1:O:357:HIS:CE1	2.41	0.56
1:P:316:HIS:HD2	1:P:317:THR:O	1.89	0.56
1:P:333:ARG:NH2	3:P:3313:HOH:O	2.31	0.56
1:F:333:ARG:NH2	3:F:3307:HOH:O	2.31	0.55
1:G:427:THR:CA	1:G:436:MET:HE1	2.12	0.55
1:H:316:HIS:HD2	1:H:317:THR:O	1.89	0.55
1:J:166:ARG:HG3	1:J:392:TYR:CB	2.34	0.55
1:J:493:THR:HG23	3:J:3126:HOH:O	2.06	0.55
1:K:436:MET:HE3	1:K:467:ASN:ND2	2.13	0.55
1:L:894:ARG:HD3	1:L:919:ASP:OD2	2.06	0.55
1:O:645:ARG:NH2	1:O:650:GLU:OE1	2.39	0.55
1:C:316:HIS:HD2	1:C:317:THR:O	1.89	0.55
1:D:333:ARG:NH2	3:D:3314:HOH:O	2.31	0.55
1:D:493:THR:HG23	3:D:3132:HOH:O	2.06	0.55
1:G:770:ILE:HD11	1:G:1022:GLN:HG2	1.88	0.55
1:J:316:HIS:HD2	1:J:317:THR:O	1.89	0.55
1:J:668:VAL:HG13	1:J:669:PRO:HD2	1.87	0.55
1:K:645:ARG:NH2	1:K:650:GLU:OE1	2.39	0.55
1:K:745:MET:HE2	1:K:745:MET:CA	2.32	0.55
1:L:645:ARG:NH2	1:L:650:GLU:OE1	2.39	0.55
1:M:645:ARG:NH2	1:M:650:GLU:OE1	2.39	0.55
1:N:493:THR:HG23	3:N:3126:HOH:O	2.06	0.55
1:O:316:HIS:HD2	1:O:317:THR:O	1.89	0.55
1:A:645:ARG:NH2	1:A:650:GLU:OE1	2.39	0.55
1:B:645:ARG:NH2	1:B:650:GLU:OE1	2.39	0.55
1:H:249:GLU:OE1	1:H:251:ARG:NH1	2.35	0.55
1:H:645:ARG:NH2	1:H:650:GLU:OE1	2.39	0.55
1:H:894:ARG:HD3	1:H:919:ASP:OD2	2.06	0.55
1:K:668:VAL:HG13	1:K:669:PRO:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:427:THR:CA	1:M:436:MET:HE1	2.12	0.55
1:M:668:VAL:HG13	1:M:669:PRO:HD2	1.87	0.55
1:O:493:THR:HG23	3:O:3123:HOH:O	2.06	0.55
1:O:770:ILE:HD11	1:O:1022:GLN:HG2	1.88	0.55
1:C:493:THR:HG23	3:C:4019:HOH:O	2.06	0.55
1:C:894:ARG:HD3	1:C:919:ASP:OD2	2.06	0.55
1:D:360:HIS:ND1	1:D:361:PRO:HD2	2.22	0.55
1:D:894:ARG:HD3	1:D:919:ASP:OD2	2.06	0.55
1:F:949:HIS:HD2	1:F:1020:TRP:HE1	1.53	0.55
1:G:645:ARG:NH2	1:G:650:GLU:OE1	2.39	0.55
1:H:360:HIS:ND1	1:H:361:PRO:HD2	2.22	0.55
1:J:824:GLN:O	1:J:838:THR:HA	2.07	0.55
1:K:824:GLN:O	1:K:838:THR:HA	2.07	0.55
1:L:316:HIS:HD2	1:L:317:THR:O	1.89	0.55
1:L:493:THR:HG23	3:L:3129:HOH:O	2.06	0.55
1:L:745:MET:HE2	1:L:745:MET:CA	2.32	0.55
1:O:894:ARG:HD3	1:O:919:ASP:OD2	2.06	0.55
1:P:249:GLU:OE1	1:P:251:ARG:NH1	2.34	0.55
1:P:824:GLN:O	1:P:838:THR:HA	2.07	0.55
1:A:422:PRO:HG2	1:D:279:ILE:CD1	2.37	0.55
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.89	0.55
1:E:360:HIS:ND1	1:E:361:PRO:HD2	2.22	0.55
1:F:745:MET:HE2	1:F:745:MET:CA	2.32	0.55
1:H:824:GLN:O	1:H:838:THR:HA	2.07	0.55
1:I:824:GLN:O	1:I:838:THR:HA	2.07	0.55
1:J:360:HIS:ND1	1:J:361:PRO:HD2	2.22	0.55
1:J:894:ARG:HD3	1:J:919:ASP:OD2	2.06	0.55
1:N:949:HIS:HD2	1:N:1020:TRP:HE1	1.53	0.55
1:O:824:GLN:O	1:O:838:THR:HA	2.07	0.55
1:P:360:HIS:ND1	1:P:361:PRO:HD2	2.22	0.55
1:A:360:HIS:ND1	1:A:361:PRO:HD2	2.22	0.55
1:B:894:ARG:HD3	1:B:919:ASP:OD2	2.06	0.55
1:D:436:MET:HE3	1:D:467:ASN:ND2	2.13	0.55
1:G:949:HIS:HD2	1:G:1020:TRP:HE1	1.53	0.55
1:K:43:ARG:NH1	1:K:44:THR:HG23	2.22	0.55
1:K:202:MET:HE3	1:K:357:HIS:CE1	2.41	0.55
1:K:894:ARG:HD3	1:K:919:ASP:OD2	2.06	0.55
1:O:651:LEU:HD12	1:O:668:VAL:O	2.07	0.55
1:A:770:ILE:HD11	1:A:1022:GLN:HG2	1.88	0.55
1:B:824:GLN:O	1:B:838:THR:HA	2.07	0.55
1:C:645:ARG:NH2	1:C:650:GLU:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:651:LEU:HD12	1:D:668:VAL:O	2.07	0.55
1:E:668:VAL:HG13	1:E:669:PRO:HD2	1.87	0.55
1:F:651:LEU:HD12	1:F:668:VAL:O	2.07	0.55
1:G:202:MET:HE3	1:G:357:HIS:CE1	2.41	0.55
1:G:651:LEU:HD12	1:G:668:VAL:O	2.07	0.55
1:J:770:ILE:HD11	1:J:1022:GLN:HG2	1.88	0.55
1:L:202:MET:HE3	1:L:357:HIS:CE1	2.41	0.55
1:N:43:ARG:NH1	1:N:44:THR:HG23	2.22	0.55
1:O:360:HIS:ND1	1:O:361:PRO:HD2	2.22	0.55
1:A:422:PRO:HG2	1:D:279:ILE:HD11	1.89	0.55
1:B:287:ASP:CG	1:C:425:ARG:HH22	2.14	0.55
1:B:493:THR:HG23	3:B:3124:HOH:O	2.06	0.55
1:C:43:ARG:NH1	1:C:44:THR:HG23	2.22	0.55
1:F:43:ARG:NH1	1:F:44:THR:HG23	2.22	0.55
1:F:894:ARG:HD3	1:F:919:ASP:OD2	2.06	0.55
1:G:824:GLN:O	1:G:838:THR:HA	2.07	0.55
1:I:597:ASN:HD22	1:I:599:ARG:H	1.52	0.55
1:J:43:ARG:NH1	1:J:44:THR:HG23	2.22	0.55
1:M:30:HIS:ND1	1:M:31:PRO:O	2.30	0.55
1:M:651:LEU:HD12	1:M:668:VAL:O	2.07	0.55
1:N:894:ARG:HD3	1:N:919:ASP:OD2	2.06	0.55
1:C:824:GLN:O	1:C:838:THR:HA	2.07	0.55
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.89	0.55
1:D:770:ILE:HD11	1:D:1022:GLN:HG2	1.88	0.55
1:E:43:ARG:NH1	1:E:44:THR:HG23	2.22	0.55
1:E:493:THR:HG23	3:E:4019:HOH:O	2.06	0.55
1:E:651:LEU:HD12	1:E:668:VAL:O	2.07	0.55
1:F:316:HIS:HD2	1:F:317:THR:O	1.89	0.55
1:F:433:LEU:HB3	1:F:434:PRO:HD3	1.89	0.55
1:G:433:LEU:HB3	1:G:434:PRO:HD3	1.89	0.55
1:G:745:MET:HE2	1:G:745:MET:CA	2.32	0.55
1:I:316:HIS:HD2	1:I:317:THR:O	1.89	0.55
1:I:360:HIS:ND1	1:I:361:PRO:HD2	2.22	0.55
1:I:433:LEU:HB3	1:I:434:PRO:HD3	1.89	0.55
1:L:740:LEU:HD12	1:L:741:THR:H	1.72	0.55
1:N:433:LEU:HB3	1:N:434:PRO:HD3	1.89	0.55
1:P:43:ARG:NH1	1:P:44:THR:HG23	2.22	0.55
1:P:949:HIS:HD2	1:P:1020:TRP:HE1	1.53	0.55
1:B:770:ILE:HD11	1:B:1022:GLN:HG2	1.88	0.55
1:E:436:MET:HE3	1:E:467:ASN:ND2	2.13	0.55
1:G:894:ARG:HD3	1:G:919:ASP:OD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:436:MET:HE3	1:L:467:ASN:ND2	2.13	0.55
1:L:651:LEU:HD12	1:L:668:VAL:O	2.07	0.55
1:M:824:GLN:O	1:M:838:THR:HA	2.07	0.55
1:M:894:ARG:HD3	1:M:919:ASP:OD2	2.06	0.55
1:N:279:ILE:HD11	1:O:422:PRO:HG2	1.89	0.55
1:N:360:HIS:ND1	1:N:361:PRO:HD2	2.22	0.55
1:O:433:LEU:HB3	1:O:434:PRO:HD3	1.89	0.55
1:C:949:HIS:HD2	1:C:1020:TRP:HE1	1.53	0.54
1:E:894:ARG:HD3	1:E:919:ASP:OD2	2.06	0.54
1:H:43:ARG:NH1	1:H:44:THR:HG23	2.22	0.54
1:H:651:LEU:HD12	1:H:668:VAL:O	2.07	0.54
1:J:202:MET:HE3	1:J:357:HIS:CE1	2.41	0.54
1:J:740:LEU:HD12	1:J:741:THR:H	1.72	0.54
1:K:360:HIS:ND1	1:K:361:PRO:HD2	2.22	0.54
1:K:433:LEU:HB3	1:K:434:PRO:HD3	1.89	0.54
1:M:43:ARG:NH1	1:M:44:THR:HG23	2.22	0.54
1:P:651:LEU:HD12	1:P:668:VAL:O	2.07	0.54
1:A:651:LEU:HD12	1:A:668:VAL:O	2.07	0.54
1:B:43:ARG:NH1	1:B:44:THR:HG23	2.22	0.54
1:B:745:MET:HE2	1:B:745:MET:CA	2.32	0.54
1:D:43:ARG:NH1	1:D:44:THR:HG23	2.22	0.54
1:I:43:ARG:NH1	1:I:44:THR:HG23	2.22	0.54
1:I:249:GLU:OE1	1:I:251:ARG:NH1	2.34	0.54
1:I:254:LEU:O	1:I:255:ARG:HG2	2.08	0.54
1:I:651:LEU:HD12	1:I:668:VAL:O	2.07	0.54
1:J:433:LEU:HB3	1:J:434:PRO:HD3	1.89	0.54
1:K:740:LEU:HD12	1:K:741:THR:H	1.73	0.54
1:L:254:LEU:O	1:L:255:ARG:HG2	2.08	0.54
1:L:433:LEU:HB3	1:L:434:PRO:HD3	1.89	0.54
1:N:651:LEU:HD12	1:N:668:VAL:O	2.07	0.54
1:O:125:LEU:HG	1:O:126:THR:N	2.23	0.54
1:P:125:LEU:HG	1:P:126:THR:N	2.23	0.54
1:P:254:LEU:O	1:P:255:ARG:HG2	2.08	0.54
1:B:651:LEU:HD12	1:B:668:VAL:O	2.07	0.54
1:B:740:LEU:HD12	1:B:741:THR:H	1.72	0.54
1:F:125:LEU:HG	1:F:126:THR:N	2.23	0.54
1:F:167:LEU:HB3	1:F:168:PRO:HD2	1.90	0.54
1:F:824:GLN:O	1:F:838:THR:HA	2.07	0.54
1:G:254:LEU:O	1:G:255:ARG:HG2	2.08	0.54
1:G:360:HIS:ND1	1:G:361:PRO:HD2	2.22	0.54
1:G:740:LEU:HD12	1:G:741:THR:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:420:MET:O	1:L:282:ARG:HD3	2.08	0.54
1:J:333:ARG:NH2	3:J:3308:HOH:O	2.31	0.54
1:L:167:LEU:HB3	1:L:168:PRO:HD2	1.90	0.54
1:N:167:LEU:HB3	1:N:168:PRO:HD2	1.90	0.54
1:N:202:MET:HE3	1:N:357:HIS:CE1	2.41	0.54
1:A:254:LEU:O	1:A:255:ARG:HG2	2.08	0.54
1:D:254:LEU:O	1:D:255:ARG:HG2	2.08	0.54
1:G:30:HIS:ND1	1:G:31:PRO:O	2.30	0.54
1:G:493:THR:HG23	3:G:3123:HOH:O	2.06	0.54
1:H:770:ILE:HD11	1:H:1022:GLN:HG2	1.88	0.54
1:I:167:LEU:HB3	1:I:168:PRO:HD2	1.90	0.54
1:I:740:LEU:HD12	1:I:741:THR:H	1.73	0.54
1:L:824:GLN:O	1:L:838:THR:HA	2.07	0.54
1:P:167:LEU:HB3	1:P:168:PRO:HD2	1.90	0.54
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.43	0.54
1:A:595:THR:HG23	1:A:596:PRO:CA	2.35	0.54
1:A:824:GLN:O	1:A:838:THR:HA	2.07	0.54
1:C:651:LEU:HD12	1:C:668:VAL:O	2.07	0.54
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.43	0.54
1:F:360:HIS:ND1	1:F:361:PRO:HD2	2.22	0.54
1:G:73:TRP:CE2	1:G:122:CYS:HB3	2.43	0.54
1:H:63:PHE:CB	1:H:64:PRO:HD2	2.34	0.54
1:H:125:LEU:HG	1:H:126:THR:N	2.23	0.54
1:J:322:LEU:HD23	1:J:322:LEU:C	2.33	0.54
1:M:167:LEU:HB3	1:M:168:PRO:HD2	1.90	0.54
1:M:436:MET:HE3	1:M:467:ASN:ND2	2.13	0.54
1:O:73:TRP:CE2	1:O:122:CYS:HB3	2.43	0.54
1:P:73:TRP:CE2	1:P:122:CYS:HB3	2.43	0.54
1:P:894:ARG:HD3	1:P:919:ASP:OD2	2.06	0.54
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.89	0.54
1:B:188:VAL:C	1:B:189:LEU:HD23	2.33	0.54
1:B:436:MET:HE3	1:B:467:ASN:ND2	2.13	0.54
1:F:254:LEU:O	1:F:255:ARG:HG2	2.08	0.54
1:F:770:ILE:HD11	1:F:1022:GLN:HG2	1.88	0.54
1:G:43:ARG:NH1	1:G:44:THR:HG23	2.22	0.54
1:H:167:LEU:HB3	1:H:168:PRO:HD2	1.90	0.54
1:J:50:GLN:O	1:J:215:LEU:HA	2.08	0.54
1:J:127:PHE:HE2	1:J:184:LEU:HG	1.73	0.54
1:J:254:LEU:O	1:J:255:ARG:HG2	2.08	0.54
1:K:322:LEU:HD23	1:K:322:LEU:C	2.33	0.54
1:K:651:LEU:HD12	1:K:668:VAL:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:360:HIS:ND1	1:L:361:PRO:HD2	2.22	0.54
1:N:254:LEU:O	1:N:255:ARG:HG2	2.08	0.54
1:N:770:ILE:HD11	1:N:1022:GLN:HG2	1.88	0.54
1:P:63:PHE:CB	1:P:64:PRO:HD2	2.34	0.54
1:B:167:LEU:HB3	1:B:168:PRO:HD2	1.90	0.54
1:B:427:THR:CA	1:B:436:MET:HE1	2.12	0.54
1:C:50:GLN:O	1:C:215:LEU:HA	2.08	0.54
1:C:436:MET:HE3	1:C:467:ASN:ND2	2.13	0.54
1:D:322:LEU:HD23	1:D:322:LEU:C	2.33	0.54
1:D:824:GLN:O	1:D:838:THR:HA	2.07	0.54
1:F:50:GLN:O	1:F:215:LEU:HA	2.08	0.54
1:H:73:TRP:CE2	1:H:122:CYS:HB3	2.43	0.54
1:I:322:LEU:HD23	1:I:322:LEU:C	2.33	0.54
1:L:50:GLN:O	1:L:215:LEU:HA	2.08	0.54
1:L:333:ARG:NH2	3:L:3311:HOH:O	2.31	0.54
1:N:188:VAL:C	1:N:189:LEU:HD23	2.33	0.54
1:P:433:LEU:HB3	1:P:434:PRO:HD3	1.89	0.54
1:P:745:MET:HE2	1:P:745:MET:CA	2.32	0.54
1:B:254:LEU:O	1:B:255:ARG:HG2	2.08	0.54
1:C:167:LEU:HB3	1:C:168:PRO:HD2	1.90	0.54
1:C:254:LEU:O	1:C:255:ARG:HG2	2.08	0.54
1:C:770:ILE:HD11	1:C:1022:GLN:HG2	1.88	0.54
1:D:595:THR:HG23	1:D:596:PRO:CA	2.35	0.54
1:F:322:LEU:HD23	1:F:322:LEU:C	2.33	0.54
1:I:770:ILE:HD11	1:I:1022:GLN:HG2	1.88	0.54
1:J:125:LEU:HG	1:J:126:THR:N	2.23	0.54
1:J:651:LEU:HD12	1:J:668:VAL:O	2.07	0.54
1:K:316:HIS:HD2	1:K:317:THR:O	1.89	0.54
1:M:254:LEU:O	1:M:255:ARG:HG2	2.08	0.54
1:M:433:LEU:HB3	1:M:434:PRO:HD3	1.89	0.54
1:N:322:LEU:HD23	1:N:322:LEU:C	2.33	0.54
1:A:127:PHE:HE2	1:A:184:LEU:HG	1.73	0.54
1:A:745:MET:HE2	1:A:745:MET:CA	2.32	0.54
1:C:37:ARG:NH2	1:C:218:PRO:HD3	2.23	0.54
1:C:73:TRP:CE2	1:C:122:CYS:HB3	2.43	0.54
1:E:167:LEU:HB3	1:E:168:PRO:HD2	1.90	0.54
1:H:127:PHE:HE2	1:H:184:LEU:HG	1.73	0.54
1:H:254:LEU:O	1:H:255:ARG:HG2	2.08	0.54
1:L:249:GLU:OE1	1:L:251:ARG:NH1	2.34	0.54
1:M:360:HIS:ND1	1:M:361:PRO:HD2	2.22	0.54
1:O:43:ARG:NH1	1:O:44:THR:HG23	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:740:LEU:HD12	1:O:741:THR:H	1.73	0.54
1:A:167:LEU:HB3	1:A:168:PRO:HD2	1.90	0.54
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.43	0.54
1:B:322:LEU:HD23	1:B:323:ILE:N	2.23	0.54
1:B:360:HIS:ND1	1:B:361:PRO:HD2	2.22	0.54
1:C:127:PHE:HE2	1:C:184:LEU:HG	1.73	0.54
1:E:125:LEU:HG	1:E:126:THR:N	2.23	0.54
1:G:188:VAL:C	1:G:189:LEU:HD23	2.33	0.54
1:H:50:GLN:O	1:H:215:LEU:HA	2.08	0.54
1:J:287:ASP:OD2	1:K:425:ARG:NH2	2.41	0.54
1:L:43:ARG:NH1	1:L:44:THR:HG23	2.22	0.54
1:L:322:LEU:HD23	1:L:323:ILE:N	2.23	0.54
1:N:127:PHE:HE2	1:N:184:LEU:HG	1.73	0.54
1:N:824:GLN:O	1:N:838:THR:HA	2.07	0.54
1:P:770:ILE:HD11	1:P:1022:GLN:HG2	1.88	0.54
1:A:37:ARG:NH2	1:A:218:PRO:HD3	2.24	0.53
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.89	0.53
1:C:322:LEU:HD23	1:C:322:LEU:C	2.33	0.53
1:C:740:LEU:HD12	1:C:741:THR:H	1.73	0.53
1:D:50:GLN:O	1:D:215:LEU:HA	2.08	0.53
1:E:433:LEU:HB3	1:E:434:PRO:HD3	1.89	0.53
1:F:37:ARG:NH2	1:F:218:PRO:HD3	2.23	0.53
1:F:322:LEU:HD23	1:F:323:ILE:N	2.23	0.53
1:F:740:LEU:HD12	1:F:741:THR:H	1.72	0.53
1:H:322:LEU:HD23	1:H:323:ILE:N	2.23	0.53
1:H:740:LEU:HD12	1:H:741:THR:H	1.72	0.53
1:K:127:PHE:HE2	1:K:184:LEU:HG	1.73	0.53
1:L:188:VAL:C	1:L:189:LEU:HD23	2.33	0.53
1:L:322:LEU:HD23	1:L:322:LEU:C	2.33	0.53
1:M:50:GLN:O	1:M:215:LEU:HA	2.08	0.53
1:N:73:TRP:CE2	1:N:122:CYS:HB3	2.43	0.53
1:N:125:LEU:HG	1:N:126:THR:N	2.23	0.53
1:O:37:ARG:NH2	1:O:218:PRO:HD3	2.23	0.53
1:O:50:GLN:O	1:O:215:LEU:HA	2.08	0.53
1:O:188:VAL:C	1:O:189:LEU:HD23	2.33	0.53
1:P:50:GLN:O	1:P:215:LEU:HA	2.08	0.53
1:P:127:PHE:HE2	1:P:184:LEU:HG	1.73	0.53
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.73	0.53
1:C:125:LEU:HG	1:C:126:THR:N	2.23	0.53
1:C:322:LEU:HD23	1:C:323:ILE:N	2.23	0.53
1:E:254:LEU:O	1:E:255:ARG:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:TRP:CE2	1:F:122:CYS:HB3	2.43	0.53
1:G:50:GLN:O	1:G:215:LEU:HA	2.08	0.53
1:I:188:VAL:C	1:I:189:LEU:HD23	2.33	0.53
1:I:282:ARG:HD3	1:L:420:MET:O	2.08	0.53
1:K:770:ILE:HD11	1:K:1022:GLN:HG2	1.89	0.53
1:L:73:TRP:CE2	1:L:122:CYS:HB3	2.43	0.53
1:M:125:LEU:HG	1:M:126:THR:N	2.23	0.53
1:N:37:ARG:NH2	1:N:218:PRO:HD3	2.23	0.53
1:N:740:LEU:HD12	1:N:741:THR:H	1.73	0.53
1:O:254:LEU:O	1:O:255:ARG:HG2	2.08	0.53
1:P:188:VAL:C	1:P:189:LEU:HD23	2.33	0.53
1:A:703:PRO:O	1:A:711:ALA:HB1	2.09	0.53
1:B:369:GLU:O	1:B:373:VAL:HG23	2.09	0.53
1:C:63:PHE:CB	1:C:64:PRO:HD2	2.34	0.53
1:D:37:ARG:NH2	1:D:218:PRO:HD3	2.23	0.53
1:D:322:LEU:HD23	1:D:323:ILE:N	2.23	0.53
1:E:770:ILE:HD11	1:E:1022:GLN:HG2	1.88	0.53
1:F:422:PRO:HG2	1:G:279:ILE:HD11	1.90	0.53
1:G:167:LEU:HB3	1:G:168:PRO:HD2	1.90	0.53
1:G:322:LEU:HD23	1:G:323:ILE:N	2.23	0.53
1:G:703:PRO:O	1:G:711:ALA:HB1	2.09	0.53
1:H:433:LEU:HB3	1:H:434:PRO:HD3	1.89	0.53
1:H:745:MET:HE2	1:H:745:MET:CA	2.32	0.53
1:I:127:PHE:HE2	1:I:184:LEU:HG	1.73	0.53
1:J:167:LEU:HB3	1:J:168:PRO:HD2	1.90	0.53
1:J:369:GLU:O	1:J:373:VAL:HG23	2.09	0.53
1:K:125:LEU:HG	1:K:126:THR:N	2.23	0.53
1:L:127:PHE:HE2	1:L:184:LEU:HG	1.73	0.53
1:M:770:ILE:HD11	1:M:1022:GLN:HG2	1.88	0.53
1:N:703:PRO:O	1:N:711:ALA:HB1	2.09	0.53
1:P:703:PRO:O	1:P:711:ALA:HB1	2.09	0.53
1:A:50:GLN:O	1:A:215:LEU:HA	2.08	0.53
1:A:673:ALA:HB1	1:A:674:PRO:HD2	1.91	0.53
1:B:703:PRO:O	1:B:711:ALA:HB1	2.09	0.53
1:D:703:PRO:O	1:D:711:ALA:HB1	2.09	0.53
1:G:37:ARG:NH2	1:G:218:PRO:HD3	2.23	0.53
1:G:125:LEU:HG	1:G:126:THR:N	2.23	0.53
1:H:703:PRO:O	1:H:711:ALA:HB1	2.09	0.53
1:L:369:GLU:O	1:L:373:VAL:HG23	2.09	0.53
1:P:740:LEU:HD12	1:P:741:THR:H	1.73	0.53
1:E:127:PHE:HE2	1:E:184:LEU:HG	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:PHE:HE2	1:F:184:LEU:HG	1.73	0.53
1:G:369:GLU:O	1:G:373:VAL:HG23	2.09	0.53
1:I:369:GLU:O	1:I:373:VAL:HG23	2.09	0.53
1:O:167:LEU:HB3	1:O:168:PRO:HD2	1.90	0.53
1:O:673:ALA:HB1	1:O:674:PRO:HD2	1.91	0.53
1:P:37:ARG:NH2	1:P:218:PRO:HD3	2.23	0.53
1:A:43:ARG:NH1	1:A:44:THR:HG23	2.22	0.53
1:A:125:LEU:HG	1:A:126:THR:N	2.23	0.53
1:B:473:ARG:HD2	1:C:469:ASP:HB3	1.90	0.53
1:C:360:HIS:ND1	1:C:361:PRO:HD2	2.22	0.53
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.91	0.53
1:E:69:VAL:HG13	1:E:70:PRO:HD2	1.91	0.53
1:E:703:PRO:O	1:E:711:ALA:HB1	2.09	0.53
1:G:673:ALA:HB1	1:G:674:PRO:HD2	1.91	0.53
1:H:37:ARG:NH2	1:H:218:PRO:HD3	2.24	0.53
1:I:703:PRO:O	1:I:711:ALA:HB1	2.09	0.53
1:J:322:LEU:HD23	1:J:323:ILE:N	2.23	0.53
1:K:50:GLN:O	1:K:215:LEU:HA	2.08	0.53
1:M:740:LEU:HD12	1:M:741:THR:H	1.72	0.53
1:N:422:PRO:HG2	1:O:279:ILE:HD11	1.89	0.53
1:O:322:LEU:HD23	1:O:323:ILE:N	2.23	0.53
1:O:369:GLU:O	1:O:373:VAL:HG23	2.09	0.53
1:P:322:LEU:HD23	1:P:323:ILE:N	2.24	0.53
1:A:282:ARG:NH1	1:D:419:GLY:O	2.41	0.53
1:E:740:LEU:HD12	1:E:741:THR:H	1.73	0.53
1:E:824:GLN:O	1:E:838:THR:HA	2.07	0.53
1:H:673:ALA:HB1	1:H:674:PRO:HD2	1.91	0.53
1:J:188:VAL:C	1:J:189:LEU:HD23	2.33	0.53
1:K:322:LEU:HD23	1:K:323:ILE:N	2.23	0.53
1:M:37:ARG:NH2	1:M:218:PRO:HD3	2.23	0.53
1:M:69:VAL:HG13	1:M:70:PRO:HD2	1.91	0.53
1:M:127:PHE:HE2	1:M:184:LEU:HG	1.73	0.53
1:N:673:ALA:HB1	1:N:674:PRO:HD2	1.91	0.53
1:A:63:PHE:CB	1:A:64:PRO:HD2	2.34	0.53
1:A:322:LEU:HD23	1:A:322:LEU:C	2.33	0.53
1:A:740:LEU:HD12	1:A:741:THR:H	1.73	0.53
1:D:167:LEU:HB3	1:D:168:PRO:HD2	1.90	0.53
1:D:369:GLU:O	1:D:373:VAL:HG23	2.09	0.53
1:E:37:ARG:NH2	1:E:218:PRO:HD3	2.24	0.53
1:E:73:TRP:CE2	1:E:122:CYS:HB3	2.43	0.53
1:E:322:LEU:HD23	1:E:322:LEU:C	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:322:LEU:HD23	1:G:322:LEU:C	2.33	0.53
1:I:125:LEU:HG	1:I:126:THR:N	2.23	0.53
1:I:436:MET:HE3	1:I:467:ASN:ND2	2.13	0.53
1:J:703:PRO:O	1:J:711:ALA:HB1	2.09	0.53
1:K:188:VAL:C	1:K:189:LEU:HD23	2.33	0.53
1:L:37:ARG:NH2	1:L:218:PRO:HD3	2.23	0.53
1:M:322:LEU:HD23	1:M:322:LEU:C	2.33	0.53
1:M:673:ALA:HB1	1:M:674:PRO:HD2	1.91	0.53
1:M:703:PRO:O	1:M:711:ALA:HB1	2.09	0.53
1:N:322:LEU:HD23	1:N:323:ILE:N	2.23	0.53
1:O:703:PRO:O	1:O:711:ALA:HB1	2.09	0.53
1:A:322:LEU:HD23	1:A:323:ILE:N	2.23	0.53
1:B:322:LEU:HD23	1:B:322:LEU:C	2.33	0.53
1:B:651:LEU:CD1	1:B:669:PRO:HA	2.39	0.53
1:F:188:VAL:C	1:F:189:LEU:HD23	2.33	0.53
1:H:369:GLU:O	1:H:373:VAL:HG23	2.09	0.53
1:I:50:GLN:O	1:I:215:LEU:HA	2.08	0.53
1:I:73:TRP:CE2	1:I:122:CYS:HB3	2.43	0.53
1:I:651:LEU:CD1	1:I:669:PRO:HA	2.39	0.53
1:J:949:HIS:HD2	1:J:1020:TRP:HE1	1.53	0.53
1:K:254:LEU:O	1:K:255:ARG:HG2	2.08	0.53
1:M:73:TRP:CE2	1:M:122:CYS:HB3	2.43	0.53
1:M:369:GLU:O	1:M:373:VAL:HG23	2.09	0.53
1:A:369:GLU:O	1:A:373:VAL:HG23	2.09	0.53
1:D:69:VAL:HG13	1:D:70:PRO:HD2	1.91	0.53
1:E:50:GLN:O	1:E:215:LEU:HA	2.08	0.53
1:E:673:ALA:HB1	1:E:674:PRO:HD2	1.91	0.53
1:I:673:ALA:HB1	1:I:674:PRO:HD2	1.91	0.53
1:J:37:ARG:NH2	1:J:218:PRO:HD3	2.23	0.53
1:J:69:VAL:HG13	1:J:70:PRO:HD2	1.91	0.53
1:J:673:ALA:HB1	1:J:674:PRO:HD2	1.91	0.53
1:K:37:ARG:NH2	1:K:218:PRO:HD3	2.24	0.53
1:L:651:LEU:CD1	1:L:669:PRO:HA	2.39	0.53
1:M:7:LEU:HD13	1:M:74:LEU:CD1	2.39	0.53
1:N:279:ILE:CD1	1:O:422:PRO:HG2	2.39	0.53
1:O:7:LEU:HD13	1:O:74:LEU:CD1	2.39	0.53
1:O:322:LEU:HD23	1:O:322:LEU:C	2.33	0.53
1:O:949:HIS:HD2	1:O:1020:TRP:HE1	1.53	0.53
1:P:369:GLU:O	1:P:373:VAL:HG23	2.09	0.53
1:P:651:LEU:CD1	1:P:669:PRO:HA	2.39	0.53
1:P:673:ALA:HB1	1:P:674:PRO:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:GLN:O	1:B:215:LEU:HA	2.08	0.52
1:B:69:VAL:HG13	1:B:70:PRO:HD2	1.91	0.52
1:C:682:LEU:CD2	1:C:683:PRO:HD2	2.39	0.52
1:E:322:LEU:HD23	1:E:323:ILE:N	2.23	0.52
1:E:422:PRO:HG2	1:H:279:ILE:HD11	1.91	0.52
1:F:210:ARG:HD3	3:F:3141:HOH:O	2.10	0.52
1:F:673:ALA:HB1	1:F:674:PRO:HD2	1.91	0.52
1:G:127:PHE:HE2	1:G:184:LEU:HG	1.73	0.52
1:J:651:LEU:CD1	1:J:669:PRO:HA	2.39	0.52
1:K:651:LEU:CD1	1:K:669:PRO:HA	2.39	0.52
1:L:673:ALA:HB1	1:L:674:PRO:HD2	1.91	0.52
1:L:703:PRO:O	1:L:711:ALA:HB1	2.09	0.52
1:N:369:GLU:O	1:N:373:VAL:HG23	2.09	0.52
1:P:278:ILE:H	1:P:278:ILE:CD1	2.22	0.52
1:P:322:LEU:HD23	1:P:322:LEU:C	2.33	0.52
1:A:188:VAL:C	1:A:189:LEU:HD23	2.33	0.52
1:C:369:GLU:O	1:C:373:VAL:HG23	2.09	0.52
1:D:127:PHE:HE2	1:D:184:LEU:HG	1.73	0.52
1:E:7:LEU:HD13	1:E:74:LEU:CD1	2.40	0.52
1:E:420:MET:O	1:H:282:ARG:HD3	2.10	0.52
1:F:703:PRO:O	1:F:711:ALA:HB1	2.09	0.52
1:H:188:VAL:C	1:H:189:LEU:HD23	2.33	0.52
1:H:322:LEU:HD23	1:H:322:LEU:C	2.33	0.52
1:H:651:LEU:CD1	1:H:669:PRO:HA	2.39	0.52
1:I:682:LEU:CD2	1:I:683:PRO:HD2	2.39	0.52
1:J:73:TRP:CE2	1:J:122:CYS:HB3	2.43	0.52
1:J:210:ARG:HD3	3:J:3142:HOH:O	2.09	0.52
1:K:369:GLU:O	1:K:373:VAL:HG23	2.09	0.52
1:M:322:LEU:HD23	1:M:323:ILE:N	2.23	0.52
1:M:651:LEU:CD1	1:M:669:PRO:HA	2.39	0.52
1:A:420:MET:O	1:D:282:ARG:HD3	2.09	0.52
1:A:949:HIS:HD2	1:A:1020:TRP:HE1	1.53	0.52
1:B:910:LEU:C	1:B:910:LEU:HD12	2.35	0.52
1:C:7:LEU:HD13	1:C:74:LEU:CD1	2.39	0.52
1:C:188:VAL:C	1:C:189:LEU:HD23	2.33	0.52
1:C:651:LEU:CD1	1:C:669:PRO:HA	2.39	0.52
1:D:740:LEU:HD12	1:D:741:THR:H	1.72	0.52
1:H:251:ARG:HB3	1:H:253:TYR:CE2	2.45	0.52
1:K:69:VAL:HG13	1:K:70:PRO:HD2	1.91	0.52
1:K:167:LEU:HB3	1:K:168:PRO:HD2	1.90	0.52
1:L:125:LEU:HG	1:L:126:THR:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:210:ARG:HD3	3:L:3145:HOH:O	2.09	0.52
1:N:50:GLN:O	1:N:215:LEU:HA	2.08	0.52
1:P:251:ARG:HB3	1:P:253:TYR:CE2	2.45	0.52
1:B:37:ARG:NH2	1:B:218:PRO:HD3	2.24	0.52
1:B:673:ALA:HB1	1:B:674:PRO:HD2	1.91	0.52
1:C:210:ARG:HD3	3:C:4035:HOH:O	2.10	0.52
1:D:910:LEU:C	1:D:910:LEU:HD12	2.35	0.52
1:I:434:PRO:HB3	1:L:434:PRO:HB3	1.90	0.52
1:J:910:LEU:C	1:J:910:LEU:HD12	2.35	0.52
1:K:73:TRP:CE2	1:K:122:CYS:HB3	2.43	0.52
1:A:682:LEU:CD2	1:A:683:PRO:HD2	2.39	0.52
1:F:7:LEU:HD13	1:F:74:LEU:CD1	2.39	0.52
1:F:251:ARG:HB3	1:F:253:TYR:CE2	2.45	0.52
1:F:369:GLU:O	1:F:373:VAL:HG23	2.09	0.52
1:H:7:LEU:HD13	1:H:74:LEU:CD1	2.39	0.52
1:I:830:LEU:HD11	1:J:830:LEU:HD11	1.91	0.52
1:M:682:LEU:CD2	1:M:683:PRO:HD2	2.39	0.52
1:N:416:GLU:OE1	1:N:418:HIS:HB2	2.10	0.52
1:A:910:LEU:C	1:A:910:LEU:HD12	2.35	0.52
1:C:645:ARG:HH22	1:C:650:GLU:CD	2.18	0.52
1:D:210:ARG:HD3	3:D:3148:HOH:O	2.09	0.52
1:D:682:LEU:CD2	1:D:683:PRO:HD2	2.39	0.52
1:E:910:LEU:C	1:E:910:LEU:HD12	2.35	0.52
1:F:645:ARG:HH22	1:F:650:GLU:CD	2.18	0.52
1:H:682:LEU:CD2	1:H:683:PRO:HD2	2.39	0.52
1:I:322:LEU:HD23	1:I:323:ILE:N	2.23	0.52
1:J:682:LEU:CD2	1:J:683:PRO:HD2	2.39	0.52
1:K:7:LEU:HD13	1:K:74:LEU:CD1	2.40	0.52
1:K:251:ARG:HB3	1:K:253:TYR:CE2	2.45	0.52
1:K:701:VAL:HG22	1:K:714:ILE:CD1	2.40	0.52
1:K:703:PRO:O	1:K:711:ALA:HB1	2.09	0.52
1:L:251:ARG:HB3	1:L:253:TYR:CE2	2.45	0.52
1:L:910:LEU:C	1:L:910:LEU:HD12	2.35	0.52
1:M:188:VAL:C	1:M:189:LEU:HD23	2.33	0.52
1:O:127:PHE:HE2	1:O:184:LEU:HG	1.73	0.52
1:A:419:GLY:C	1:D:282:ARG:HH11	2.16	0.52
1:B:701:VAL:HG22	1:B:714:ILE:CD1	2.40	0.52
1:C:416:GLU:OE1	1:C:418:HIS:HB2	2.10	0.52
1:C:701:VAL:HG22	1:C:714:ILE:CD1	2.40	0.52
1:C:703:PRO:O	1:C:711:ALA:HB1	2.09	0.52
1:D:188:VAL:C	1:D:189:LEU:HD23	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:VAL:C	1:E:189:LEU:HD23	2.33	0.52
1:G:651:LEU:CD1	1:G:669:PRO:HA	2.39	0.52
1:K:910:LEU:C	1:K:910:LEU:HD12	2.35	0.52
1:M:194:GLY:O	1:M:198:GLU:HG3	2.10	0.52
1:M:416:GLU:OE1	1:M:418:HIS:HB2	2.10	0.52
1:O:251:ARG:HB3	1:O:253:TYR:CE2	2.45	0.52
1:O:645:ARG:HH22	1:O:650:GLU:CD	2.18	0.52
1:O:701:VAL:HG22	1:O:714:ILE:CD1	2.40	0.52
1:O:910:LEU:C	1:O:910:LEU:HD12	2.35	0.52
1:P:910:LEU:C	1:P:910:LEU:HD12	2.35	0.52
1:B:125:LEU:HG	1:B:126:THR:N	2.23	0.52
1:B:194:GLY:O	1:B:198:GLU:HG3	2.10	0.52
1:B:595:THR:HG23	1:B:596:PRO:CA	2.35	0.52
1:B:645:ARG:HH22	1:B:650:GLU:CD	2.18	0.52
1:D:125:LEU:HG	1:D:126:THR:N	2.23	0.52
1:E:701:VAL:HG22	1:E:714:ILE:CD1	2.40	0.52
1:G:701:VAL:HG22	1:G:714:ILE:CD1	2.40	0.52
1:H:194:GLY:O	1:H:198:GLU:HG3	2.10	0.52
1:H:210:ARG:HD3	3:H:4035:HOH:O	2.09	0.52
1:H:910:LEU:C	1:H:910:LEU:HD12	2.35	0.52
1:I:7:LEU:HD13	1:I:74:LEU:CD1	2.39	0.52
1:I:69:VAL:HG13	1:I:70:PRO:HD2	1.91	0.52
1:K:210:ARG:HD3	3:K:4035:HOH:O	2.09	0.52
1:L:69:VAL:HG13	1:L:70:PRO:HD2	1.91	0.52
1:N:651:LEU:CD1	1:N:669:PRO:HA	2.39	0.52
1:P:416:GLU:OE1	1:P:418:HIS:HB2	2.10	0.52
1:A:7:LEU:HD13	1:A:74:LEU:CD1	2.39	0.52
1:A:251:ARG:HB3	1:A:253:TYR:CE2	2.45	0.52
1:B:251:ARG:HB3	1:B:253:TYR:CE2	2.45	0.52
1:B:881:ARG:HD3	1:B:987:ASP:OD1	2.10	0.52
1:C:910:LEU:C	1:C:910:LEU:HD12	2.35	0.52
1:D:645:ARG:HH22	1:D:650:GLU:CD	2.18	0.52
1:E:416:GLU:OE1	1:E:418:HIS:HB2	2.10	0.52
1:H:753:ASN:OD1	1:H:753:ASN:N	2.30	0.52
1:I:194:GLY:O	1:I:198:GLU:HG3	2.10	0.52
1:L:645:ARG:HH22	1:L:650:GLU:CD	2.18	0.52
1:N:251:ARG:HB3	1:N:253:TYR:CE2	2.45	0.52
1:P:210:ARG:HD3	3:P:3147:HOH:O	2.09	0.52
1:B:682:LEU:CD2	1:B:683:PRO:HD2	2.39	0.52
1:E:682:LEU:CD2	1:E:683:PRO:HD2	2.39	0.52
1:F:701:VAL:HG22	1:F:714:ILE:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:251:ARG:HB3	1:G:253:TYR:CE2	2.45	0.52
1:G:910:LEU:C	1:G:910:LEU:HD12	2.35	0.52
1:H:701:VAL:HG22	1:H:714:ILE:CD1	2.40	0.52
1:J:416:GLU:OE1	1:J:418:HIS:HB2	2.10	0.52
1:J:645:ARG:HH22	1:J:650:GLU:CD	2.18	0.52
1:M:251:ARG:HB3	1:M:253:TYR:CE2	2.45	0.52
1:M:881:ARG:HD3	1:M:987:ASP:OD1	2.10	0.52
1:M:910:LEU:C	1:M:910:LEU:HD12	2.35	0.52
1:O:210:ARG:HD3	3:O:3139:HOH:O	2.10	0.52
1:O:651:LEU:CD1	1:O:669:PRO:HA	2.39	0.52
1:O:682:LEU:CD2	1:O:683:PRO:HD2	2.39	0.52
1:A:69:VAL:HG13	1:A:70:PRO:HD2	1.91	0.51
1:A:416:GLU:OE1	1:A:418:HIS:HB2	2.10	0.51
1:D:673:ALA:HB1	1:D:674:PRO:HD2	1.91	0.51
1:D:701:VAL:HG22	1:D:714:ILE:CD1	2.40	0.51
1:E:251:ARG:HB3	1:E:253:TYR:CE2	2.45	0.51
1:E:651:LEU:CD1	1:E:669:PRO:HA	2.39	0.51
1:E:949:HIS:HD2	1:E:1020:TRP:HE1	1.53	0.51
1:G:210:ARG:HD3	3:G:3139:HOH:O	2.10	0.51
1:G:682:LEU:CD2	1:G:683:PRO:HD2	2.39	0.51
1:H:69:VAL:HG13	1:H:70:PRO:HD2	1.91	0.51
1:H:645:ARG:HH22	1:H:650:GLU:CD	2.18	0.51
1:I:251:ARG:HB3	1:I:253:TYR:CE2	2.45	0.51
1:J:595:THR:HG23	1:J:596:PRO:CA	2.35	0.51
1:J:701:VAL:HG22	1:J:714:ILE:CD1	2.40	0.51
1:K:645:ARG:HH22	1:K:650:GLU:CD	2.18	0.51
1:O:416:GLU:OE1	1:O:418:HIS:HB2	2.10	0.51
1:P:701:VAL:HG22	1:P:714:ILE:CD1	2.40	0.51
1:A:651:LEU:CD1	1:A:669:PRO:HA	2.39	0.51
1:B:416:GLU:OE1	1:B:418:HIS:HB2	2.10	0.51
1:C:69:VAL:HG13	1:C:70:PRO:HD2	1.91	0.51
1:C:251:ARG:HB3	1:C:253:TYR:CE2	2.45	0.51
1:F:194:GLY:O	1:F:198:GLU:HG3	2.10	0.51
1:F:416:GLU:OE1	1:F:418:HIS:HB2	2.10	0.51
1:F:682:LEU:CD2	1:F:683:PRO:HD2	2.39	0.51
1:I:37:ARG:NH2	1:I:218:PRO:HD3	2.24	0.51
1:I:287:ASP:CG	1:L:425:ARG:HH22	2.17	0.51
1:I:416:GLU:OE1	1:I:418:HIS:HB2	2.10	0.51
1:I:881:ARG:HD3	1:I:987:ASP:OD1	2.10	0.51
1:L:881:ARG:HD3	1:L:987:ASP:OD1	2.10	0.51
1:N:682:LEU:CD2	1:N:683:PRO:HD2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:701:VAL:HG22	1:N:714:ILE:CD1	2.40	0.51
1:O:43:ARG:HH11	1:O:43:ARG:CG	2.24	0.51
1:B:210:ARG:HD3	3:B:3140:HOH:O	2.09	0.51
1:C:43:ARG:HH11	1:C:43:ARG:CG	2.24	0.51
1:D:7:LEU:HD13	1:D:74:LEU:CD1	2.39	0.51
1:E:210:ARG:HD3	3:E:4035:HOH:O	2.10	0.51
1:E:473:ARG:O	1:E:473:ARG:HD3	2.11	0.51
1:F:473:ARG:O	1:F:473:ARG:HD3	2.11	0.51
1:F:651:LEU:CD1	1:F:669:PRO:HA	2.39	0.51
1:I:660:GLY:O	1:I:662:PRO:HD3	2.11	0.51
1:J:251:ARG:HB3	1:J:253:TYR:CE2	2.45	0.51
1:K:673:ALA:HB1	1:K:674:PRO:HD2	1.91	0.51
1:L:7:LEU:HD13	1:L:74:LEU:CD1	2.39	0.51
1:L:610:ASP:OD2	1:L:612:THR:HG23	2.11	0.51
1:L:701:VAL:HG22	1:L:714:ILE:CD1	2.40	0.51
1:M:660:GLY:O	1:M:662:PRO:HD3	2.11	0.51
1:N:210:ARG:HD3	3:N:3142:HOH:O	2.10	0.51
1:N:645:ARG:HH22	1:N:650:GLU:CD	2.18	0.51
1:O:69:VAL:HG13	1:O:70:PRO:HD2	1.91	0.51
1:P:427:THR:CA	1:P:436:MET:HE1	2.12	0.51
1:A:278:ILE:H	1:A:278:ILE:CD1	2.22	0.51
1:A:610:ASP:OD2	1:A:612:THR:HG23	2.11	0.51
1:C:881:ARG:HD3	1:C:987:ASP:OD1	2.10	0.51
1:G:69:VAL:HG13	1:G:70:PRO:HD2	1.91	0.51
1:G:416:GLU:OE1	1:G:418:HIS:HB2	2.10	0.51
1:G:645:ARG:HH22	1:G:650:GLU:CD	2.18	0.51
1:H:473:ARG:O	1:H:473:ARG:HD3	2.11	0.51
1:H:881:ARG:HD3	1:H:987:ASP:OD1	2.10	0.51
1:I:278:ILE:H	1:I:278:ILE:CD1	2.22	0.51
1:I:473:ARG:O	1:I:473:ARG:HD3	2.11	0.51
1:I:910:LEU:C	1:I:910:LEU:HD12	2.35	0.51
1:J:881:ARG:HD3	1:J:987:ASP:OD1	2.10	0.51
1:K:682:LEU:CD2	1:K:683:PRO:HD2	2.39	0.51
1:L:682:LEU:CD2	1:L:683:PRO:HD2	2.39	0.51
1:M:278:ILE:H	1:M:278:ILE:CD1	2.22	0.51
1:M:473:ARG:O	1:M:473:ARG:HD3	2.11	0.51
1:N:473:ARG:O	1:N:473:ARG:HD3	2.11	0.51
1:O:881:ARG:HD3	1:O:987:ASP:OD1	2.10	0.51
1:P:69:VAL:HG13	1:P:70:PRO:HD2	1.91	0.51
1:P:610:ASP:OD2	1:P:612:THR:HG23	2.11	0.51
1:P:767:GLN:HG3	1:P:768:MET:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:952:ARG:HD2	3:P:3534:HOH:O	2.11	0.51
1:A:194:GLY:O	1:A:198:GLU:HG3	2.10	0.51
1:C:767:GLN:HG3	1:C:768:MET:N	2.26	0.51
1:D:251:ARG:HB3	1:D:253:TYR:CE2	2.45	0.51
1:D:416:GLU:OE1	1:D:418:HIS:HB2	2.10	0.51
1:D:473:ARG:O	1:D:473:ARG:HD3	2.11	0.51
1:E:369:GLU:O	1:E:373:VAL:HG23	2.09	0.51
1:F:5:ASP:OD2	1:F:157:ARG:HA	2.11	0.51
1:G:278:ILE:H	1:G:278:ILE:CD1	2.22	0.51
1:G:881:ARG:HD3	1:G:987:ASP:OD1	2.11	0.51
1:H:949:HIS:HD2	1:H:1020:TRP:HE1	1.53	0.51
1:I:645:ARG:HH22	1:I:650:GLU:CD	2.18	0.51
1:J:194:GLY:O	1:J:198:GLU:HG3	2.10	0.51
1:K:194:GLY:O	1:K:198:GLU:HG3	2.10	0.51
1:K:416:GLU:OE1	1:K:418:HIS:HB2	2.10	0.51
1:K:660:GLY:O	1:K:662:PRO:HD3	2.11	0.51
1:K:1020:TRP:CD1	1:K:1021:CME:N	2.79	0.51
1:N:595:THR:HG23	1:N:596:PRO:CA	2.35	0.51
1:N:610:ASP:OD2	1:N:612:THR:HG23	2.11	0.51
1:P:7:LEU:HD13	1:P:74:LEU:CD1	2.39	0.51
1:P:473:ARG:O	1:P:473:ARG:HD3	2.11	0.51
1:A:881:ARG:HD3	1:A:987:ASP:OD1	2.10	0.51
1:C:952:ARG:HD2	3:C:4429:HOH:O	2.11	0.51
1:D:651:LEU:CD1	1:D:669:PRO:HA	2.39	0.51
1:E:278:ILE:H	1:E:278:ILE:CD1	2.22	0.51
1:J:422:PRO:HG2	1:K:279:ILE:CD1	2.41	0.51
1:J:660:GLY:O	1:J:662:PRO:HD3	2.11	0.51
1:J:1020:TRP:CD1	1:J:1021:CME:N	2.79	0.51
1:K:473:ARG:O	1:K:473:ARG:HD3	2.11	0.51
1:L:278:ILE:H	1:L:278:ILE:CD1	2.22	0.51
1:M:610:ASP:OD2	1:M:612:THR:HG23	2.11	0.51
1:N:43:ARG:HH11	1:N:43:ARG:CG	2.24	0.51
1:N:194:GLY:O	1:N:198:GLU:HG3	2.10	0.51
1:N:910:LEU:HD12	1:N:910:LEU:C	2.35	0.51
1:O:571:VAL:HG13	1:O:607:VAL:HG23	1.93	0.51
1:O:767:GLN:HG3	1:O:768:MET:N	2.26	0.51
1:A:210:ARG:HD3	3:A:4035:HOH:O	2.09	0.51
1:A:645:ARG:HH22	1:A:650:GLU:CD	2.18	0.51
1:C:5:ASP:OD2	1:C:157:ARG:HA	2.11	0.51
1:C:473:ARG:O	1:C:473:ARG:HD3	2.11	0.51
1:F:987:ASP:OD2	1:F:990:HIS:HD2	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:436:MET:HE3	1:G:467:ASN:ND2	2.13	0.51
1:G:767:GLN:HG3	1:G:768:MET:N	2.26	0.51
1:H:610:ASP:OD2	1:H:612:THR:HG23	2.11	0.51
1:K:952:ARG:HD2	3:K:4431:HOH:O	2.11	0.51
1:N:7:LEU:HD13	1:N:74:LEU:CD1	2.39	0.51
1:N:881:ARG:HD3	1:N:987:ASP:OD1	2.10	0.51
1:O:5:ASP:OD2	1:O:157:ARG:HA	2.11	0.51
1:O:610:ASP:OD2	1:O:612:THR:HG23	2.11	0.51
1:O:753:ASN:OD1	1:O:753:ASN:N	2.30	0.51
1:P:194:GLY:O	1:P:198:GLU:HG3	2.10	0.51
1:P:660:GLY:O	1:P:662:PRO:HD3	2.11	0.51
1:P:881:ARG:HD3	1:P:987:ASP:OD1	2.10	0.51
1:A:753:ASN:OD1	1:A:753:ASN:N	2.30	0.51
1:B:610:ASP:OD2	1:B:612:THR:HG23	2.11	0.51
1:E:194:GLY:O	1:E:198:GLU:HG3	2.10	0.51
1:E:595:THR:HG23	1:E:596:PRO:CA	2.35	0.51
1:E:610:ASP:OD2	1:E:612:THR:HG23	2.11	0.51
1:E:645:ARG:HH22	1:E:650:GLU:CD	2.18	0.51
1:F:910:LEU:HD12	1:F:910:LEU:C	2.35	0.51
1:G:5:ASP:OD2	1:G:157:ARG:HA	2.11	0.51
1:I:701:VAL:HG22	1:I:714:ILE:CD1	2.40	0.51
1:J:952:ARG:HD2	3:J:3529:HOH:O	2.11	0.51
1:L:416:GLU:OE1	1:L:418:HIS:HB2	2.10	0.51
1:M:701:VAL:HG22	1:M:714:ILE:CD1	2.40	0.51
1:M:987:ASP:OD2	1:M:990:HIS:HD2	1.94	0.51
1:N:987:ASP:OD2	1:N:990:HIS:HD2	1.94	0.51
1:P:645:ARG:HH22	1:P:650:GLU:CD	2.18	0.51
1:P:682:LEU:CD2	1:P:683:PRO:HD2	2.39	0.51
1:B:5:ASP:OD2	1:B:157:ARG:HA	2.11	0.51
1:B:571:VAL:HG13	1:B:607:VAL:HG23	1.93	0.51
1:B:767:GLN:HG3	1:B:768:MET:N	2.26	0.51
1:C:73:TRP:CZ2	1:C:185:ALA:HB1	2.46	0.51
1:C:571:VAL:HG13	1:C:607:VAL:HG23	1.93	0.51
1:G:571:VAL:HG13	1:G:607:VAL:HG23	1.93	0.51
1:H:261:TRP:CZ3	1:H:266:GLN:HB2	2.46	0.51
1:H:660:GLY:O	1:H:662:PRO:HD3	2.10	0.51
1:H:767:GLN:HG3	1:H:768:MET:N	2.26	0.51
1:I:210:ARG:HD3	3:I:4035:HOH:O	2.10	0.51
1:I:279:ILE:CD1	1:L:422:PRO:HG2	2.40	0.51
1:K:261:TRP:CZ3	1:K:266:GLN:HB2	2.46	0.51
1:K:610:ASP:OD2	1:K:612:THR:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:194:GLY:O	1:L:198:GLU:HG3	2.10	0.51
1:L:767:GLN:HG3	1:L:768:MET:N	2.26	0.51
1:M:210:ARG:HD3	3:M:4035:HOH:O	2.09	0.51
1:O:473:ARG:O	1:O:473:ARG:HD3	2.11	0.51
1:P:73:TRP:CZ2	1:P:185:ALA:HB1	2.46	0.51
1:A:261:TRP:CZ3	1:A:266:GLN:HB2	2.46	0.51
1:A:422:PRO:HG3	1:D:284:GLY:C	2.35	0.51
1:A:701:VAL:HG22	1:A:714:ILE:CD1	2.40	0.51
1:B:63:PHE:CB	1:B:64:PRO:HD2	2.34	0.51
1:B:73:TRP:CZ2	1:B:185:ALA:HB1	2.46	0.51
1:B:473:ARG:O	1:B:473:ARG:HD3	2.11	0.51
1:B:660:GLY:O	1:B:662:PRO:HD3	2.11	0.51
1:D:278:ILE:H	1:D:278:ILE:CD1	2.22	0.51
1:D:637:GLU:HA	1:D:679:LEU:HD23	1.93	0.51
1:D:660:GLY:O	1:D:662:PRO:HD3	2.11	0.51
1:F:610:ASP:OD2	1:F:612:THR:HG23	2.11	0.51
1:G:73:TRP:CZ2	1:G:185:ALA:HB1	2.46	0.51
1:G:660:GLY:O	1:G:662:PRO:HD3	2.11	0.51
1:J:7:LEU:HD13	1:J:74:LEU:CD1	2.39	0.51
1:J:287:ASP:CG	1:K:425:ARG:HH22	2.18	0.51
1:J:425:ARG:HH22	1:K:287:ASP:CG	2.19	0.51
1:K:573:GLN:HB2	1:K:602:CYS:O	2.11	0.51
1:L:43:ARG:HH11	1:L:43:ARG:CG	2.24	0.51
1:L:637:GLU:HA	1:L:679:LEU:HD23	1.93	0.51
1:L:741:THR:O	1:L:741:THR:HG22	2.11	0.51
1:N:637:GLU:HA	1:N:679:LEU:HD23	1.93	0.51
1:O:660:GLY:O	1:O:662:PRO:HD3	2.11	0.51
1:A:473:ARG:O	1:A:473:ARG:HD3	2.11	0.50
1:A:573:GLN:HB2	1:A:602:CYS:O	2.12	0.50
1:C:261:TRP:CZ3	1:C:266:GLN:HB2	2.46	0.50
1:D:767:GLN:HG3	1:D:768:MET:N	2.26	0.50
1:F:637:GLU:HA	1:F:679:LEU:HD23	1.94	0.50
1:F:881:ARG:HD3	1:F:987:ASP:OD1	2.10	0.50
1:G:952:ARG:HD2	3:G:3527:HOH:O	2.11	0.50
1:H:416:GLU:OE1	1:H:418:HIS:HB2	2.10	0.50
1:I:422:PRO:HG2	1:L:279:ILE:HD11	1.93	0.50
1:K:5:ASP:OD2	1:K:157:ARG:HA	2.11	0.50
1:K:73:TRP:CZ2	1:K:185:ALA:HB1	2.46	0.50
1:K:881:ARG:HD3	1:K:987:ASP:OD1	2.11	0.50
1:K:987:ASP:OD2	1:K:990:HIS:HD2	1.94	0.50
1:O:741:THR:O	1:O:741:THR:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HD13	1:B:74:LEU:CD1	2.39	0.50
1:B:85:VAL:HG12	1:B:86:VAL:N	2.26	0.50
1:B:261:TRP:CZ3	1:B:266:GLN:HB2	2.46	0.50
1:B:278:ILE:H	1:B:278:ILE:CD1	2.22	0.50
1:B:637:GLU:HA	1:B:679:LEU:HD23	1.93	0.50
1:C:637:GLU:HA	1:C:679:LEU:HD23	1.93	0.50
1:C:741:THR:O	1:C:741:THR:HG22	2.12	0.50
1:E:73:TRP:CZ2	1:E:185:ALA:HB1	2.46	0.50
1:F:69:VAL:HG13	1:F:70:PRO:HD2	1.91	0.50
1:G:7:LEU:HD13	1:G:74:LEU:CD1	2.39	0.50
1:G:194:GLY:O	1:G:198:GLU:HG3	2.10	0.50
1:G:595:THR:HG23	1:G:596:PRO:CA	2.35	0.50
1:H:278:ILE:H	1:H:278:ILE:CD1	2.22	0.50
1:K:767:GLN:HG3	1:K:768:MET:N	2.26	0.50
1:L:473:ARG:O	1:L:473:ARG:HD3	2.11	0.50
1:L:660:GLY:O	1:L:662:PRO:HD3	2.10	0.50
1:L:952:ARG:HD2	3:L:3532:HOH:O	2.11	0.50
1:M:595:THR:HG23	1:M:596:PRO:CA	2.35	0.50
1:M:1020:TRP:CD1	1:M:1021:CME:N	2.79	0.50
1:N:261:TRP:CZ3	1:N:266:GLN:HB2	2.46	0.50
1:O:261:TRP:CZ3	1:O:266:GLN:HB2	2.46	0.50
1:O:595:THR:CG2	1:O:596:PRO:HA	2.37	0.50
1:P:261:TRP:CZ3	1:P:266:GLN:HB2	2.46	0.50
1:P:573:GLN:HB2	1:P:602:CYS:O	2.11	0.50
1:C:194:GLY:O	1:C:198:GLU:HG3	2.10	0.50
1:D:573:GLN:HB2	1:D:602:CYS:O	2.12	0.50
1:E:741:THR:O	1:E:741:THR:HG22	2.12	0.50
1:E:952:ARG:HD2	3:E:4422:HOH:O	2.11	0.50
1:F:73:TRP:CZ2	1:F:185:ALA:HB1	2.46	0.50
1:F:595:THR:HG23	1:F:596:PRO:CA	2.35	0.50
1:H:571:VAL:HG13	1:H:607:VAL:HG23	1.93	0.50
1:I:987:ASP:OD2	1:I:990:HIS:HD2	1.94	0.50
1:K:278:ILE:H	1:K:278:ILE:CD1	2.22	0.50
1:L:380:LYS:HE3	1:L:406:GLY:O	2.12	0.50
1:L:571:VAL:HG13	1:L:607:VAL:HG23	1.93	0.50
1:M:63:PHE:CB	1:M:64:PRO:HD2	2.34	0.50
1:N:73:TRP:CZ2	1:N:185:ALA:HB1	2.46	0.50
1:O:194:GLY:O	1:O:198:GLU:HG3	2.10	0.50
1:P:1020:TRP:CD1	1:P:1021:CME:N	2.79	0.50
1:A:85:VAL:HG12	1:A:86:VAL:N	2.27	0.50
1:A:660:GLY:O	1:A:662:PRO:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:ARG:HD2	3:A:4429:HOH:O	2.11	0.50
1:B:987:ASP:OD2	1:B:990:HIS:HD2	1.94	0.50
1:C:610:ASP:OD2	1:C:612:THR:HG23	2.11	0.50
1:C:830:LEU:HD11	1:D:830:LEU:HD11	1.94	0.50
1:D:127:PHE:CE2	1:D:184:LEU:HG	2.47	0.50
1:D:571:VAL:HG13	1:D:607:VAL:HG23	1.93	0.50
1:D:610:ASP:OD2	1:D:612:THR:HG23	2.11	0.50
1:E:660:GLY:O	1:E:662:PRO:HD3	2.11	0.50
1:E:881:ARG:HD3	1:E:987:ASP:OD1	2.10	0.50
1:F:660:GLY:O	1:F:662:PRO:HD3	2.11	0.50
1:H:427:THR:CA	1:H:436:MET:HE1	2.12	0.50
1:H:573:GLN:HB2	1:H:602:CYS:O	2.12	0.50
1:I:637:GLU:HA	1:I:679:LEU:HD23	1.93	0.50
1:J:5:ASP:OD2	1:J:157:ARG:HA	2.11	0.50
1:J:610:ASP:OD2	1:J:612:THR:HG23	2.11	0.50
1:J:767:GLN:HG3	1:J:768:MET:N	2.26	0.50
1:K:249:GLU:OE1	1:K:251:ARG:NH1	2.35	0.50
1:L:261:TRP:CZ3	1:L:266:GLN:HB2	2.46	0.50
1:L:987:ASP:OD2	1:L:990:HIS:HD2	1.94	0.50
1:M:73:TRP:CZ2	1:M:185:ALA:HB1	2.46	0.50
1:M:741:THR:O	1:M:741:THR:HG22	2.12	0.50
1:M:767:GLN:HG3	1:M:768:MET:N	2.26	0.50
1:N:5:ASP:OD2	1:N:157:ARG:HA	2.11	0.50
1:N:69:VAL:HG13	1:N:70:PRO:HD2	1.91	0.50
1:N:952:ARG:HD2	3:N:3528:HOH:O	2.11	0.50
1:P:987:ASP:OD2	1:P:990:HIS:HD2	1.94	0.50
1:A:987:ASP:OD2	1:A:990:HIS:HD2	1.94	0.50
1:A:1004:SER:HB2	1:A:1006:GLU:OE2	2.12	0.50
1:B:380:LYS:HE3	1:B:406:GLY:O	2.12	0.50
1:C:85:VAL:HG12	1:C:86:VAL:N	2.27	0.50
1:E:571:VAL:HG13	1:E:607:VAL:HG23	1.93	0.50
1:F:261:TRP:CZ3	1:F:266:GLN:HB2	2.46	0.50
1:F:952:ARG:HD2	3:F:3528:HOH:O	2.11	0.50
1:F:1004:SER:HB2	1:F:1006:GLU:OE2	2.12	0.50
1:G:610:ASP:OD2	1:G:612:THR:HG23	2.11	0.50
1:G:637:GLU:HA	1:G:679:LEU:HD23	1.93	0.50
1:I:261:TRP:CZ3	1:I:266:GLN:HB2	2.46	0.50
1:I:380:LYS:HE3	1:I:406:GLY:O	2.12	0.50
1:N:127:PHE:CE2	1:N:184:LEU:HG	2.47	0.50
1:O:595:THR:HG23	1:O:596:PRO:CA	2.35	0.50
1:A:73:TRP:CZ2	1:A:185:ALA:HB1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1020:TRP:CD1	1:C:1021:CME:N	2.79	0.50
1:D:73:TRP:CZ2	1:D:185:ALA:HB1	2.46	0.50
1:D:741:THR:O	1:D:741:THR:HG22	2.11	0.50
1:E:127:PHE:CE2	1:E:184:LEU:HG	2.47	0.50
1:G:473:ARG:O	1:G:473:ARG:HD3	2.11	0.50
1:I:571:VAL:HG13	1:I:607:VAL:HG23	1.93	0.50
1:J:573:GLN:HB2	1:J:602:CYS:O	2.12	0.50
1:K:380:LYS:HE3	1:K:406:GLY:O	2.12	0.50
1:L:73:TRP:CZ2	1:L:185:ALA:HB1	2.46	0.50
1:M:645:ARG:HH22	1:M:650:GLU:CD	2.18	0.50
1:N:571:VAL:HG13	1:N:607:VAL:HG23	1.93	0.50
1:N:660:GLY:O	1:N:662:PRO:HD3	2.11	0.50
1:O:278:ILE:H	1:O:278:ILE:CD1	2.22	0.50
1:O:637:GLU:HA	1:O:679:LEU:HD23	1.94	0.50
1:O:987:ASP:OD2	1:O:990:HIS:HD2	1.94	0.50
1:O:1004:SER:HB2	1:O:1006:GLU:OE2	2.12	0.50
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.47	0.50
1:A:190:ARG:HG3	1:A:206:SER:OG	2.12	0.50
1:C:660:GLY:O	1:C:662:PRO:HD3	2.10	0.50
1:C:987:ASP:OD2	1:C:990:HIS:HD2	1.94	0.50
1:D:5:ASP:OD2	1:D:157:ARG:HA	2.11	0.50
1:D:261:TRP:CZ3	1:D:266:GLN:HB2	2.46	0.50
1:D:952:ARG:HD2	3:D:3534:HOH:O	2.11	0.50
1:D:1020:TRP:CD1	1:D:1021:CME:N	2.79	0.50
1:E:767:GLN:HG3	1:E:768:MET:N	2.26	0.50
1:F:380:LYS:HE3	1:F:406:GLY:O	2.12	0.50
1:F:571:VAL:HG13	1:F:607:VAL:HG23	1.93	0.50
1:G:573:GLN:HB2	1:G:602:CYS:O	2.12	0.50
1:G:987:ASP:OD2	1:G:990:HIS:HD2	1.94	0.50
1:H:73:TRP:CZ2	1:H:185:ALA:HB1	2.46	0.50
1:H:85:VAL:HG12	1:H:86:VAL:N	2.27	0.50
1:H:987:ASP:OD2	1:H:990:HIS:HD2	1.94	0.50
1:H:1004:SER:HB2	1:H:1006:GLU:OE2	2.12	0.50
1:H:1020:TRP:CD1	1:H:1021:CME:N	2.79	0.50
1:I:73:TRP:CZ2	1:I:185:ALA:HB1	2.46	0.50
1:J:73:TRP:CZ2	1:J:185:ALA:HB1	2.46	0.50
1:J:85:VAL:HG12	1:J:86:VAL:N	2.27	0.50
1:K:127:PHE:CE2	1:K:184:LEU:HG	2.47	0.50
1:K:595:THR:CG2	1:K:596:PRO:HA	2.37	0.50
1:L:903[A]:GLN:NE2	3:L:3424:HOH:O	2.45	0.50
1:N:380:LYS:HE3	1:N:406:GLY:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:571:VAL:HG13	1:P:607:VAL:HG23	1.93	0.50
1:A:767:GLN:HG3	1:A:768:MET:N	2.26	0.50
1:C:1004:SER:HB2	1:C:1006:GLU:OE2	2.12	0.50
1:E:5:ASP:OD2	1:E:157:ARG:HA	2.11	0.50
1:F:573:GLN:HB2	1:F:602:CYS:O	2.12	0.50
1:M:5:ASP:OD2	1:M:157:ARG:HA	2.11	0.50
1:P:5:ASP:OD2	1:P:157:ARG:HA	2.11	0.50
1:B:1020:TRP:CD1	1:B:1021:CME:N	2.79	0.50
1:D:194:GLY:O	1:D:198:GLU:HG3	2.10	0.50
1:E:85:VAL:HG12	1:E:86:VAL:N	2.27	0.50
1:E:261:TRP:CZ3	1:E:266:GLN:HB2	2.46	0.50
1:E:282:ARG:HD3	1:H:420:MET:O	2.12	0.50
1:E:1020:TRP:CD1	1:E:1021:CME:N	2.79	0.50
1:G:190:ARG:HG3	1:G:206:SER:OG	2.12	0.50
1:H:5:ASP:OD2	1:H:157:ARG:HA	2.11	0.50
1:H:355:ASN:OD1	1:H:388:ARG:HD3	2.12	0.50
1:H:380:LYS:HE3	1:H:406:GLY:O	2.12	0.50
1:J:127:PHE:CE2	1:J:184:LEU:HG	2.47	0.50
1:J:987:ASP:OD2	1:J:990:HIS:HD2	1.94	0.50
1:J:1004:SER:HB2	1:J:1006:GLU:OE2	2.12	0.50
1:L:595:THR:HG23	1:L:596:PRO:CA	2.35	0.50
1:M:261:TRP:CZ3	1:M:266:GLN:HB2	2.46	0.50
1:M:571:VAL:HG13	1:M:607:VAL:HG23	1.93	0.50
1:M:903[A]:GLN:NE2	3:M:4314:HOH:O	2.45	0.50
1:N:507:ASP:OD1	1:N:521:LYS:HE2	2.12	0.50
1:N:573:GLN:HB2	1:N:602:CYS:O	2.12	0.50
1:P:190:ARG:HG3	1:P:206:SER:OG	2.12	0.50
1:A:5:ASP:OD2	1:A:157:ARG:HA	2.11	0.49
1:A:571:VAL:HG13	1:A:607:VAL:HG23	1.93	0.49
1:B:507:ASP:OD1	1:B:521:LYS:HE2	2.12	0.49
1:C:903[A]:GLN:NE2	3:C:4315:HOH:O	2.45	0.49
1:D:507:ASP:OD1	1:D:521:LYS:HE2	2.12	0.49
1:D:881:ARG:HD3	1:D:987:ASP:OD1	2.10	0.49
1:D:987:ASP:OD2	1:D:990:HIS:HD2	1.94	0.49
1:D:1004:SER:HB2	1:D:1006:GLU:OE2	2.12	0.49
1:E:573:GLN:HB2	1:E:602:CYS:O	2.11	0.49
1:F:507:ASP:OD1	1:F:521:LYS:HE2	2.12	0.49
1:G:261:TRP:CZ3	1:G:266:GLN:HB2	2.46	0.49
1:G:380:LYS:HE3	1:G:406:GLY:O	2.12	0.49
1:H:127:PHE:CE2	1:H:184:LEU:HG	2.47	0.49
1:H:952:ARG:HD2	3:H:4432:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:5:ASP:OD2	1:I:157:ARG:HA	2.11	0.49
1:I:37:ARG:NH2	1:I:216:HIS:O	2.45	0.49
1:I:190:ARG:HG3	1:I:206:SER:OG	2.12	0.49
1:I:610:ASP:OD2	1:I:612:THR:HG23	2.11	0.49
1:K:37:ARG:NH2	1:K:216:HIS:O	2.45	0.49
1:K:190:ARG:HG3	1:K:206:SER:OG	2.12	0.49
1:L:190:ARG:HG3	1:L:206:SER:OG	2.12	0.49
1:M:102:ASN:C	1:M:102:ASN:HD22	2.21	0.49
1:M:127:PHE:CE2	1:M:184:LEU:HG	2.47	0.49
1:M:190:ARG:HG3	1:M:206:SER:OG	2.12	0.49
1:M:380:LYS:HE3	1:M:406:GLY:O	2.12	0.49
1:N:741:THR:O	1:N:741:THR:HG22	2.11	0.49
1:N:1004:SER:HB2	1:N:1006:GLU:OE2	2.12	0.49
1:N:1020:TRP:CD1	1:N:1021:CME:N	2.79	0.49
1:O:190:ARG:HG3	1:O:206:SER:OG	2.12	0.49
1:P:140:ARG:HB2	1:P:171:PHE:O	2.12	0.49
1:P:507:ASP:OD1	1:P:521:LYS:HE2	2.12	0.49
1:A:380:LYS:HE3	1:A:406:GLY:O	2.12	0.49
1:A:637:GLU:HA	1:A:679:LEU:HD23	1.93	0.49
1:B:573:GLN:HB2	1:B:602:CYS:O	2.12	0.49
1:C:102:ASN:HD22	1:C:102:ASN:C	2.21	0.49
1:C:507:ASP:OD1	1:C:521:LYS:HE2	2.12	0.49
1:E:380:LYS:HE3	1:E:406:GLY:O	2.12	0.49
1:E:595:THR:CG2	1:E:596:PRO:HA	2.37	0.49
1:G:1004:SER:HB2	1:G:1006:GLU:OE2	2.12	0.49
1:H:190:ARG:HG3	1:H:206:SER:OG	2.12	0.49
1:H:507:ASP:OD1	1:H:521:LYS:HE2	2.12	0.49
1:I:85:VAL:HG12	1:I:86:VAL:N	2.27	0.49
1:I:573:GLN:HB2	1:I:602:CYS:O	2.11	0.49
1:I:952:ARG:HD2	3:I:4420:HOH:O	2.11	0.49
1:J:140:ARG:HB2	1:J:171:PHE:O	2.13	0.49
1:J:473:ARG:O	1:J:473:ARG:HD3	2.11	0.49
1:K:43:ARG:HH11	1:K:43:ARG:CG	2.24	0.49
1:K:355:ASN:OD1	1:K:388:ARG:HD3	2.12	0.49
1:L:5:ASP:OD2	1:L:157:ARG:HA	2.11	0.49
1:L:37:ARG:NH2	1:L:216:HIS:O	2.46	0.49
1:L:573:GLN:HB2	1:L:602:CYS:O	2.12	0.49
1:M:85:VAL:HG12	1:M:86:VAL:N	2.27	0.49
1:M:573:GLN:HB2	1:M:602:CYS:O	2.12	0.49
1:O:73:TRP:CZ2	1:O:185:ALA:HB1	2.46	0.49
1:O:380:LYS:HE3	1:O:406:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:952:ARG:HD2	3:O:3524:HOH:O	2.11	0.49
1:B:102:ASN:C	1:B:102:ASN:HD22	2.21	0.49
1:B:1004:SER:HB2	1:B:1006:GLU:OE2	2.12	0.49
1:C:355:ASN:OD1	1:C:388:ARG:HD3	2.12	0.49
1:E:637:GLU:HA	1:E:679:LEU:HD23	1.93	0.49
1:F:127:PHE:CE2	1:F:184:LEU:HG	2.47	0.49
1:F:741:THR:O	1:F:741:THR:HG22	2.12	0.49
1:F:767:GLN:HG3	1:F:768:MET:N	2.26	0.49
1:F:1020:TRP:CD1	1:F:1021:CME:N	2.79	0.49
1:G:37:ARG:NH2	1:G:216:HIS:O	2.45	0.49
1:G:1020:TRP:CD1	1:G:1021:CME:N	2.79	0.49
1:I:127:PHE:CE2	1:I:184:LEU:HG	2.47	0.49
1:J:261:TRP:CZ3	1:J:266:GLN:HB2	2.46	0.49
1:L:355:ASN:OD1	1:L:388:ARG:HD3	2.12	0.49
1:M:37:ARG:NH2	1:M:216:HIS:O	2.45	0.49
1:M:952:ARG:HD2	3:M:4420:HOH:O	2.11	0.49
1:N:355:ASN:OD1	1:N:388:ARG:HD3	2.12	0.49
1:O:433:LEU:O	1:O:437:SER:HB3	2.13	0.49
1:O:507:ASP:OD1	1:O:521:LYS:HE2	2.12	0.49
1:O:1020:TRP:CD1	1:O:1021:CME:N	2.79	0.49
1:B:952:ARG:HD2	3:B:3528:HOH:O	2.11	0.49
1:C:37:ARG:NH2	1:C:216:HIS:O	2.46	0.49
1:C:573:GLN:HB2	1:C:602:CYS:O	2.11	0.49
1:E:1004:SER:HB2	1:E:1006:GLU:OE2	2.12	0.49
1:F:85:VAL:HG12	1:F:86:VAL:N	2.27	0.49
1:F:190:ARG:HG3	1:F:206:SER:OG	2.12	0.49
1:G:140:ARG:HB2	1:G:171:PHE:O	2.13	0.49
1:G:355:ASN:OD1	1:G:388:ARG:HD3	2.12	0.49
1:G:507:ASP:OD1	1:G:521:LYS:HE2	2.12	0.49
1:H:102:ASN:HD22	1:H:102:ASN:C	2.21	0.49
1:I:355:ASN:OD1	1:I:388:ARG:HD3	2.12	0.49
1:J:190:ARG:HG3	1:J:206:SER:OG	2.12	0.49
1:J:380:LYS:HE3	1:J:406:GLY:O	2.12	0.49
1:J:507:ASP:OD1	1:J:521:LYS:HE2	2.12	0.49
1:J:571:VAL:HG13	1:J:607:VAL:HG23	1.93	0.49
1:L:1020:TRP:CD1	1:L:1021:CME:N	2.79	0.49
1:M:279:ILE:CD1	1:P:422:PRO:HG2	2.42	0.49
1:M:433:LEU:O	1:M:437:SER:HB3	2.13	0.49
1:N:190:ARG:HG3	1:N:206:SER:OG	2.12	0.49
1:O:37:ARG:NH2	1:O:216:HIS:O	2.46	0.49
1:O:355:ASN:OD1	1:O:388:ARG:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ASN:OD1	1:A:388:ARG:HD3	2.12	0.49
1:A:433:LEU:O	1:A:437:SER:HB3	2.13	0.49
1:A:1020:TRP:CD1	1:A:1021:CME:N	2.79	0.49
1:B:37:ARG:NH2	1:B:216:HIS:O	2.46	0.49
1:B:140:ARG:HB2	1:B:171:PHE:O	2.12	0.49
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.12	0.49
1:B:741:THR:O	1:B:741:THR:HG22	2.11	0.49
1:D:433:LEU:O	1:D:437:SER:HB3	2.13	0.49
1:E:37:ARG:NH2	1:E:216:HIS:O	2.45	0.49
1:E:43:ARG:HH11	1:E:43:ARG:CG	2.24	0.49
1:E:190:ARG:HG3	1:E:206:SER:OG	2.12	0.49
1:E:903[A]:GLN:NE2	3:E:4314:HOH:O	2.45	0.49
1:F:37:ARG:NH2	1:F:216:HIS:O	2.46	0.49
1:F:102:ASN:HD22	1:F:102:ASN:C	2.21	0.49
1:G:127:PHE:CE2	1:G:184:LEU:HG	2.47	0.49
1:J:287:ASP:OD1	1:J:287:ASP:N	2.41	0.49
1:J:433:LEU:O	1:J:437:SER:HB3	2.13	0.49
1:J:903[A]:GLN:NE2	3:J:3421:HOH:O	2.45	0.49
1:K:102:ASN:HD22	1:K:102:ASN:C	2.21	0.49
1:K:433:LEU:O	1:K:437:SER:HB3	2.13	0.49
1:K:1004:SER:HB2	1:K:1006:GLU:OE2	2.12	0.49
1:L:507:ASP:OD1	1:L:521:LYS:HE2	2.12	0.49
1:M:140:ARG:HB2	1:M:171:PHE:O	2.13	0.49
1:N:37:ARG:NH2	1:N:216:HIS:O	2.46	0.49
1:N:278:ILE:H	1:N:278:ILE:CD1	2.22	0.49
1:O:127:PHE:CE2	1:O:184:LEU:HG	2.47	0.49
1:O:573:GLN:HB2	1:O:602:CYS:O	2.12	0.49
1:P:102:ASN:HD22	1:P:102:ASN:C	2.21	0.49
1:P:127:PHE:CE2	1:P:184:LEU:HG	2.47	0.49
1:B:433:LEU:O	1:B:437:SER:HB3	2.13	0.49
1:B:903[A]:GLN:NE2	3:B:3418:HOH:O	2.45	0.49
1:C:102:ASN:ND2	1:C:201:ASP:HB2	2.28	0.49
1:C:800:ARG:CZ	1:C:800:ARG:HB3	2.43	0.49
1:D:190:ARG:HG3	1:D:206:SER:OG	2.12	0.49
1:E:140:ARG:HB2	1:E:171:PHE:O	2.13	0.49
1:E:355:ASN:OD1	1:E:388:ARG:HD3	2.13	0.49
1:E:987:ASP:OD2	1:E:990:HIS:HD2	1.94	0.49
1:H:800:ARG:HB3	1:H:800:ARG:CZ	2.43	0.49
1:I:433:LEU:O	1:I:437:SER:HB3	2.13	0.49
1:J:741:THR:O	1:J:741:THR:HG22	2.12	0.49
1:K:507:ASP:OD1	1:K:521:LYS:HE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:767:GLN:HG3	1:N:768:MET:N	2.26	0.49
1:P:102:ASN:ND2	1:P:201:ASP:HB2	2.28	0.49
1:A:140:ARG:HB2	1:A:171:PHE:O	2.12	0.49
1:A:507:ASP:OD1	1:A:521:LYS:HE2	2.12	0.49
1:B:190:ARG:HG3	1:B:206:SER:OG	2.12	0.49
1:D:102:ASN:C	1:D:102:ASN:HD22	2.21	0.49
1:E:679:LEU:HD23	1:E:679:LEU:HA	1.40	0.49
1:F:800:ARG:CZ	1:F:800:ARG:HB3	2.43	0.49
1:H:102:ASN:ND2	1:H:201:ASP:HB2	2.28	0.49
1:I:767:GLN:HG3	1:I:768:MET:N	2.26	0.49
1:I:903[A]:GLN:NE2	3:I:4313:HOH:O	2.45	0.49
1:I:1020:TRP:CD1	1:I:1021:CME:N	2.79	0.49
1:K:571:VAL:HG13	1:K:607:VAL:HG23	1.93	0.49
1:L:140:ARG:HB2	1:L:171:PHE:O	2.13	0.49
1:P:800:ARG:HB3	1:P:800:ARG:CZ	2.43	0.49
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.47	0.49
1:C:380:LYS:HE3	1:C:406:GLY:O	2.12	0.49
1:D:380:LYS:HE3	1:D:406:GLY:O	2.12	0.49
1:G:65:ALA:HB1	1:G:66:PRO:HD2	1.95	0.49
1:G:433:LEU:O	1:G:437:SER:HB3	2.13	0.49
1:I:102:ASN:C	1:I:102:ASN:HD22	2.21	0.49
1:J:637:GLU:HA	1:J:679:LEU:HD23	1.93	0.49
1:L:102:ASN:ND2	1:L:201:ASP:HB2	2.28	0.49
1:L:127:PHE:CE2	1:L:184:LEU:HG	2.47	0.49
1:M:102:ASN:ND2	1:M:201:ASP:HB2	2.28	0.49
1:M:637:GLU:HA	1:M:679:LEU:HD23	1.93	0.49
1:N:57:GLU:HG2	1:N:83:THR:HG22	1.95	0.49
1:N:102:ASN:ND2	1:N:201:ASP:HB2	2.28	0.49
1:N:800:ARG:CZ	1:N:800:ARG:HB3	2.43	0.49
1:A:419:GLY:O	1:D:282:ARG:NH1	2.46	0.49
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.47	0.49
1:C:190:ARG:HG3	1:C:206:SER:OG	2.12	0.49
1:D:43:ARG:HH11	1:D:43:ARG:CG	2.24	0.49
1:E:102:ASN:ND2	1:E:201:ASP:HB2	2.28	0.49
1:F:102:ASN:ND2	1:F:201:ASP:HB2	2.28	0.49
1:G:102:ASN:C	1:G:102:ASN:HD22	2.21	0.49
1:H:140:ARG:HB2	1:H:171:PHE:O	2.13	0.49
1:H:741:THR:O	1:H:741:THR:HG22	2.12	0.49
1:I:102:ASN:ND2	1:I:201:ASP:HB2	2.28	0.49
1:K:595:THR:HG23	1:K:596:PRO:CA	2.35	0.49
1:K:637:GLU:HA	1:K:679:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:285:TYR:CB	1:M:288:ARG:HG3	2.42	0.49
1:M:1004:SER:HB2	1:M:1006:GLU:OE2	2.12	0.49
1:O:65:ALA:HB1	1:O:66:PRO:HD2	1.95	0.49
1:O:140:ARG:HB2	1:O:171:PHE:O	2.12	0.49
1:D:37:ARG:NH2	1:D:216:HIS:O	2.45	0.49
1:D:65:ALA:HB1	1:D:66:PRO:HD2	1.95	0.49
1:D:102:ASN:ND2	1:D:201:ASP:HB2	2.28	0.49
1:E:507:ASP:OD1	1:E:521:LYS:HE2	2.12	0.49
1:F:73:TRP:CZ2	1:F:122:CYS:HB3	2.48	0.49
1:F:903[A]:GLN:NE2	3:F:3420:HOH:O	2.45	0.49
1:G:85:VAL:HG12	1:G:86:VAL:N	2.27	0.49
1:J:355:ASN:OD1	1:J:388:ARG:HD3	2.12	0.49
1:K:102:ASN:ND2	1:K:201:ASP:HB2	2.28	0.49
1:L:1004:SER:HB2	1:L:1006:GLU:OE2	2.12	0.49
1:M:355:ASN:OD1	1:M:388:ARG:HD3	2.12	0.49
1:M:800:ARG:HB3	1:M:800:ARG:CZ	2.43	0.49
1:N:73:TRP:CZ2	1:N:122:CYS:HB3	2.48	0.49
1:P:380:LYS:HE3	1:P:406:GLY:O	2.12	0.49
1:P:429:ASP:OD1	1:P:430:PRO:HD2	2.13	0.49
1:P:1004:SER:HB2	1:P:1006:GLU:OE2	2.12	0.49
1:A:102:ASN:ND2	1:A:201:ASP:HB2	2.28	0.48
1:B:65:ALA:HB1	1:B:66:PRO:HD2	1.95	0.48
1:B:102:ASN:ND2	1:B:201:ASP:HB2	2.28	0.48
1:B:429:ASP:OD1	1:B:430:PRO:HD2	2.13	0.48
1:E:800:ARG:HB3	1:E:800:ARG:CZ	2.43	0.48
1:F:9:VAL:O	1:F:12:GLN:HB3	2.13	0.48
1:G:73:TRP:CZ2	1:G:122:CYS:HB3	2.48	0.48
1:G:903[A]:GLN:NE2	3:G:3418:HOH:O	2.45	0.48
1:I:800:ARG:HB3	1:I:800:ARG:CZ	2.43	0.48
1:I:949:HIS:HD2	1:I:1020:TRP:HE1	1.53	0.48
1:I:1004:SER:HB2	1:I:1006:GLU:OE2	2.12	0.48
1:J:37:ARG:NH2	1:J:216:HIS:O	2.45	0.48
1:J:102:ASN:C	1:J:102:ASN:HD22	2.21	0.48
1:J:285:TYR:CB	1:J:288:ARG:HG3	2.42	0.48
1:K:429:ASP:OD1	1:K:430:PRO:HD2	2.13	0.48
1:M:949:HIS:HD2	1:M:1020:TRP:HE1	1.53	0.48
1:P:85:VAL:HG12	1:P:86:VAL:N	2.27	0.48
1:B:73:TRP:CZ2	1:B:122:CYS:HB3	2.48	0.48
1:B:653[A]:HIS:HD2	1:B:666:GLY:O	1.97	0.48
1:D:134:LEU:HD23	1:D:134:LEU:HA	1.68	0.48
1:E:653[A]:HIS:HD2	1:E:666:GLY:O	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:653[A]:HIS:HD2	1:H:666:GLY:O	1.96	0.48
1:I:429:ASP:OD1	1:I:430:PRO:HD2	2.13	0.48
1:I:507:ASP:OD1	1:I:521:LYS:HE2	2.12	0.48
1:J:9:VAL:O	1:J:12:GLN:HB3	2.13	0.48
1:J:73:TRP:CZ2	1:J:122:CYS:HB3	2.48	0.48
1:L:9:VAL:O	1:L:12:GLN:HB3	2.13	0.48
1:L:73:TRP:CZ2	1:L:122:CYS:HB3	2.48	0.48
1:L:429:ASP:OD1	1:L:430:PRO:HD2	2.13	0.48
1:M:507:ASP:OD1	1:M:521:LYS:HE2	2.12	0.48
1:N:429:ASP:OD1	1:N:430:PRO:HD2	2.13	0.48
1:O:73:TRP:CZ2	1:O:122:CYS:HB3	2.48	0.48
1:O:85:VAL:HG12	1:O:86:VAL:N	2.27	0.48
1:P:57:GLU:HG2	1:P:83:THR:HG22	1.95	0.48
1:P:595:THR:CG2	1:P:596:PRO:HA	2.37	0.48
1:A:741:THR:O	1:A:741:THR:HG22	2.12	0.48
1:B:800:ARG:HB3	1:B:800:ARG:CZ	2.43	0.48
1:C:9:VAL:O	1:C:12:GLN:HB3	2.13	0.48
1:C:65:ALA:HB1	1:C:66:PRO:HD2	1.95	0.48
1:C:73:TRP:CZ2	1:C:122:CYS:HB3	2.48	0.48
1:C:433:LEU:O	1:C:437:SER:HB3	2.13	0.48
1:E:65:ALA:HB1	1:E:66:PRO:HD2	1.95	0.48
1:H:637:GLU:HA	1:H:679:LEU:HD23	1.93	0.48
1:J:469:ASP:HB3	1:K:473:ARG:HD2	1.94	0.48
1:K:65:ALA:HB1	1:K:66:PRO:HD2	1.95	0.48
1:L:800:ARG:HB3	1:L:800:ARG:CZ	2.43	0.48
1:M:653[A]:HIS:HD2	1:M:666:GLY:O	1.97	0.48
1:O:78:LEU:HB3	1:O:79:PRO:CD	2.43	0.48
1:O:429:ASP:OD1	1:O:430:PRO:HD2	2.13	0.48
1:O:903[A]:GLN:NE2	3:O:3418:HOH:O	2.45	0.48
1:P:637:GLU:HA	1:P:679:LEU:HD23	1.93	0.48
1:A:429:ASP:OD1	1:A:430:PRO:HD2	2.13	0.48
1:A:830:LEU:HD11	1:B:830:LEU:HD11	1.95	0.48
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.12	0.48
1:F:653[A]:HIS:HD2	1:F:666:GLY:O	1.97	0.48
1:H:9:VAL:O	1:H:12:GLN:HB3	2.13	0.48
1:H:78:LEU:HB3	1:H:79:PRO:CD	2.43	0.48
1:H:433:LEU:O	1:H:437:SER:HB3	2.13	0.48
1:I:73:TRP:CZ2	1:I:122:CYS:HB3	2.48	0.48
1:I:78:LEU:HB3	1:I:79:PRO:CD	2.43	0.48
1:I:287:ASP:OD1	1:I:287:ASP:N	2.41	0.48
1:J:73:TRP:CH2	1:J:185:ALA:HB1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:429:ASP:OD1	1:J:430:PRO:HD2	2.13	0.48
1:P:217:LYS:HG2	1:P:218:PRO:HD2	1.96	0.48
1:P:903[A]:GLN:NE2	3:P:3426:HOH:O	2.45	0.48
1:A:37:ARG:NH2	1:A:216:HIS:O	2.46	0.48
1:A:73:TRP:CZ2	1:A:122:CYS:HB3	2.48	0.48
1:A:102:ASN:C	1:A:102:ASN:HD22	2.21	0.48
1:B:9:VAL:O	1:B:12:GLN:HB3	2.14	0.48
1:C:35:SER:O	1:C:50:GLN:HG3	2.14	0.48
1:C:278:ILE:H	1:C:278:ILE:CD1	2.22	0.48
1:D:595:THR:CG2	1:D:596:PRO:HA	2.37	0.48
1:F:78:LEU:HB3	1:F:79:PRO:CD	2.43	0.48
1:F:420:MET:O	1:G:282:ARG:HD3	2.14	0.48
1:G:35:SER:O	1:G:50:GLN:HG3	2.14	0.48
1:G:741:THR:O	1:G:741:THR:HG22	2.12	0.48
1:H:217:LYS:HG2	1:H:218:PRO:HD2	1.96	0.48
1:I:35:SER:O	1:I:50:GLN:HG3	2.14	0.48
1:J:35:SER:O	1:J:50:GLN:HG3	2.14	0.48
1:J:65:ALA:HB1	1:J:66:PRO:HD2	1.95	0.48
1:J:278:ILE:H	1:J:278:ILE:CD1	2.22	0.48
1:J:800:ARG:HB3	1:J:800:ARG:CZ	2.43	0.48
1:K:903[A]:GLN:NE2	3:K:4315:HOH:O	2.45	0.48
1:L:85:VAL:HG12	1:L:86:VAL:N	2.27	0.48
1:N:433:LEU:O	1:N:437:SER:HB3	2.13	0.48
1:O:35:SER:O	1:O:50:GLN:HG3	2.14	0.48
1:O:724:GLU:O	1:P:847:LYS:NZ	2.27	0.48
1:O:800:ARG:HB3	1:O:800:ARG:CZ	2.43	0.48
1:P:9:VAL:O	1:P:12:GLN:HB3	2.14	0.48
1:P:355:ASN:OD1	1:P:388:ARG:HD3	2.12	0.48
1:A:217:LYS:HG2	1:A:218:PRO:HD2	1.96	0.48
1:A:903[A]:GLN:NE2	3:A:4315:HOH:O	2.45	0.48
1:E:73:TRP:CH2	1:E:185:ALA:HB1	2.49	0.48
1:E:433:LEU:O	1:E:437:SER:HB3	2.13	0.48
1:G:653[A]:HIS:HD2	1:G:666:GLY:O	1.97	0.48
1:H:35:SER:O	1:H:50:GLN:HG3	2.14	0.48
1:H:57:GLU:HG2	1:H:83:THR:HG22	1.95	0.48
1:H:261:TRP:CH2	1:H:266:GLN:HB2	2.49	0.48
1:I:73:TRP:CH2	1:I:185:ALA:HB1	2.49	0.48
1:K:73:TRP:CZ2	1:K:122:CYS:HB3	2.48	0.48
1:K:85:VAL:HG12	1:K:86:VAL:N	2.27	0.48
1:K:800:ARG:HB3	1:K:800:ARG:CZ	2.43	0.48
1:L:73:TRP:CH2	1:L:185:ALA:HB1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:102:ASN:C	1:L:102:ASN:HD22	2.21	0.48
1:M:73:TRP:CH2	1:M:185:ALA:HB1	2.49	0.48
1:N:73:TRP:CH2	1:N:185:ALA:HB1	2.49	0.48
1:N:102:ASN:HD22	1:N:102:ASN:C	2.21	0.48
1:O:9:VAL:O	1:O:12:GLN:HB3	2.13	0.48
1:A:9:VAL:O	1:A:12:GLN:HB3	2.13	0.48
1:A:595:THR:CG2	1:A:596:PRO:HA	2.37	0.48
1:C:140:ARG:HB2	1:C:171:PHE:O	2.12	0.48
1:C:581:ASN:O	1:J:581:ASN:O	2.30	0.48
1:D:903[A]:GLN:NE2	3:D:3427:HOH:O	2.45	0.48
1:E:102:ASN:C	1:E:102:ASN:HD22	2.21	0.48
1:E:429:ASP:OD1	1:E:430:PRO:HD2	2.13	0.48
1:G:800:ARG:HB3	1:G:800:ARG:CZ	2.43	0.48
1:I:140:ARG:HB2	1:I:171:PHE:O	2.13	0.48
1:I:147:ASN:HA	1:I:148:SER:HA	1.57	0.48
1:I:425:ARG:HH22	1:L:287:ASP:CG	2.22	0.48
1:K:73:TRP:CH2	1:K:185:ALA:HB1	2.49	0.48
1:K:261:TRP:CH2	1:K:266:GLN:HB2	2.49	0.48
1:L:433:LEU:O	1:L:437:SER:HB3	2.13	0.48
1:M:65:ALA:HB1	1:M:66:PRO:HD2	1.95	0.48
1:M:73:TRP:CZ2	1:M:122:CYS:HB3	2.48	0.48
1:N:78:LEU:HB3	1:N:79:PRO:CD	2.43	0.48
1:N:85:VAL:HG12	1:N:86:VAL:N	2.27	0.48
1:N:140:ARG:HB2	1:N:171:PHE:O	2.13	0.48
1:P:35:SER:O	1:P:50:GLN:HG3	2.14	0.48
1:P:73:TRP:CH2	1:P:185:ALA:HB1	2.49	0.48
1:P:261:TRP:CH2	1:P:266:GLN:HB2	2.49	0.48
1:P:741:THR:O	1:P:741:THR:HG22	2.12	0.48
1:B:57:GLU:HG2	1:B:83:THR:HG22	1.95	0.48
1:B:745:MET:HA	1:B:745:MET:CE	2.39	0.48
1:D:35:SER:O	1:D:50:GLN:HG3	2.14	0.48
1:D:73:TRP:CH2	1:D:185:ALA:HB1	2.49	0.48
1:D:85:VAL:HG12	1:D:86:VAL:N	2.27	0.48
1:D:800:ARG:HB3	1:D:800:ARG:CZ	2.43	0.48
1:E:246:MET:HE3	1:E:246:MET:C	2.39	0.48
1:G:80:GLU:H	1:G:80:GLU:HG3	1.29	0.48
1:G:102:ASN:ND2	1:G:201:ASP:HB2	2.28	0.48
1:G:429:ASP:OD1	1:G:430:PRO:HD2	2.13	0.48
1:K:140:ARG:HB2	1:K:171:PHE:O	2.13	0.48
1:K:741:THR:O	1:K:741:THR:HG22	2.12	0.48
1:M:9:VAL:O	1:M:12:GLN:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:429:ASP:OD1	1:M:430:PRO:HD2	2.13	0.48
1:N:147:ASN:HA	1:N:148:SER:HA	1.58	0.48
1:N:261:TRP:CH2	1:N:266:GLN:HB2	2.49	0.48
1:O:102:ASN:ND2	1:O:201:ASP:HB2	2.28	0.48
1:O:285:TYR:CB	1:O:288:ARG:HG3	2.42	0.48
1:P:433:LEU:O	1:P:437:SER:HB3	2.13	0.48
1:A:653[A]:HIS:HD2	1:A:666:GLY:O	1.97	0.48
1:A:744:GLU:HB3	1:A:745:MET:HE3	1.96	0.48
1:A:800:ARG:HB3	1:A:800:ARG:CZ	2.43	0.48
1:B:35:SER:O	1:B:50:GLN:HG3	2.14	0.48
1:C:80:GLU:H	1:C:80:GLU:HG3	1.29	0.48
1:C:595:THR:CG2	1:C:596:PRO:HA	2.37	0.48
1:D:140:ARG:HB2	1:D:171:PHE:O	2.13	0.48
1:D:217:LYS:HG2	1:D:218:PRO:HD2	1.96	0.48
1:E:9:VAL:O	1:E:12:GLN:HB3	2.13	0.48
1:E:78:LEU:HB3	1:E:79:PRO:CD	2.43	0.48
1:F:65:ALA:HB1	1:F:66:PRO:HD2	1.95	0.48
1:F:147:ASN:HA	1:F:148:SER:HA	1.57	0.48
1:F:261:TRP:CH2	1:F:266:GLN:HB2	2.49	0.48
1:F:355:ASN:OD1	1:F:388:ARG:HD3	2.12	0.48
1:G:285:TYR:CB	1:G:288:ARG:HG3	2.42	0.48
1:H:37:ARG:NH2	1:H:216:HIS:O	2.45	0.48
1:H:903[A]:GLN:NE2	3:H:4315:HOH:O	2.45	0.48
1:I:261:TRP:CH2	1:I:266:GLN:HB2	2.49	0.48
1:J:102:ASN:ND2	1:J:201:ASP:HB2	2.28	0.48
1:J:217:LYS:HG2	1:J:218:PRO:HD2	1.96	0.48
1:J:425:ARG:NH2	1:K:287:ASP:OD2	2.47	0.48
1:N:65:ALA:HB1	1:N:66:PRO:HD2	1.95	0.48
1:N:744:GLU:HB3	1:N:745:MET:HE3	1.96	0.48
1:O:744:GLU:HB3	1:O:745:MET:HE3	1.96	0.48
1:P:37:ARG:NH2	1:P:216:HIS:O	2.45	0.48
1:A:73:TRP:CH2	1:A:185:ALA:HB1	2.49	0.48
1:A:279:ILE:CD1	1:D:422:PRO:HG2	2.43	0.48
1:C:653[A]:HIS:HD2	1:C:666:GLY:O	1.97	0.48
1:E:73:TRP:CZ2	1:E:122:CYS:HB3	2.48	0.48
1:E:261:TRP:CH2	1:E:266:GLN:HB2	2.49	0.48
1:F:744:GLU:HB3	1:F:745:MET:HE3	1.96	0.48
1:G:744:GLU:HB3	1:G:745:MET:HE3	1.96	0.48
1:I:914:CME:HE2	1:I:914:CME:HB3	1.74	0.48
1:J:261:TRP:CH2	1:J:266:GLN:HB2	2.49	0.48
1:K:217:LYS:HG2	1:K:218:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:246:MET:HE3	1:K:246:MET:C	2.39	0.48
1:K:653[A]:HIS:HD2	1:K:666:GLY:O	1.97	0.48
1:N:35:SER:O	1:N:50:GLN:HG3	2.14	0.48
1:N:903[A]:GLN:NE2	3:N:3421:HOH:O	2.45	0.48
1:P:65:ALA:HB1	1:P:66:PRO:HD2	1.95	0.48
1:D:73:TRP:CZ2	1:D:122:CYS:HB3	2.48	0.47
1:D:261:TRP:CH2	1:D:266:GLN:HB2	2.49	0.47
1:E:279:ILE:HD11	1:H:422:PRO:HG2	1.95	0.47
1:F:35:SER:O	1:F:50:GLN:HG3	2.14	0.47
1:F:217:LYS:HG2	1:F:218:PRO:HD2	1.96	0.47
1:F:278:ILE:H	1:F:278:ILE:CD1	2.22	0.47
1:H:65:ALA:HB1	1:H:66:PRO:HD2	1.95	0.47
1:H:429:ASP:OD1	1:H:430:PRO:HD2	2.13	0.47
1:I:65:ALA:HB1	1:I:66:PRO:HD2	1.95	0.47
1:L:35:SER:O	1:L:50:GLN:HG3	2.14	0.47
1:L:217:LYS:HG2	1:L:218:PRO:HD2	1.96	0.47
1:M:246:MET:HE3	1:M:246:MET:C	2.39	0.47
1:M:261:TRP:CH2	1:M:266:GLN:HB2	2.49	0.47
1:N:217:LYS:HG2	1:N:218:PRO:HD2	1.96	0.47
1:O:102:ASN:C	1:O:102:ASN:HD22	2.21	0.47
1:P:595:THR:HG23	1:P:596:PRO:CA	2.35	0.47
1:A:35:SER:O	1:A:50:GLN:HG3	2.14	0.47
1:B:261:TRP:CH2	1:B:266:GLN:HB2	2.49	0.47
1:D:18:ASN:ND2	1:D:21:VAL:HG23	2.29	0.47
1:D:653[A]:HIS:HD2	1:D:666:GLY:O	1.96	0.47
1:G:57:GLU:HG2	1:G:83:THR:HG22	1.95	0.47
1:G:73:TRP:CH2	1:G:185:ALA:HB1	2.49	0.47
1:L:246:MET:C	1:L:246:MET:HE3	2.39	0.47
1:N:246:MET:C	1:N:246:MET:HE3	2.39	0.47
1:N:914:CME:HE2	1:N:914:CME:HB3	1.74	0.47
1:O:73:TRP:CH2	1:O:185:ALA:HB1	2.49	0.47
1:P:246:MET:HE3	1:P:246:MET:C	2.39	0.47
1:B:217:LYS:HG2	1:B:218:PRO:HD2	1.96	0.47
1:C:217:LYS:HG2	1:C:218:PRO:HD2	1.96	0.47
1:D:429:ASP:OD1	1:D:430:PRO:HD2	2.13	0.47
1:F:429:ASP:OD1	1:F:430:PRO:HD2	2.13	0.47
1:G:9:VAL:O	1:G:12:GLN:HB3	2.13	0.47
1:I:595:THR:HG23	1:I:596:PRO:CA	2.35	0.47
1:I:744:GLU:HB3	1:I:745:MET:HE3	1.96	0.47
1:J:744:GLU:HB3	1:J:745:MET:HE3	1.96	0.47
1:L:65:ALA:HB1	1:L:66:PRO:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:744:GLU:HB3	1:M:745:MET:HE3	1.96	0.47
1:N:653[A]:HIS:HD2	1:N:666:GLY:O	1.97	0.47
1:A:43:ARG:HH11	1:A:43:ARG:CG	2.24	0.47
1:C:73:TRP:CH2	1:C:185:ALA:HB1	2.49	0.47
1:D:9:VAL:O	1:D:12:GLN:HB3	2.13	0.47
1:F:254:LEU:HD23	1:F:254:LEU:HA	1.71	0.47
1:F:433:LEU:O	1:F:437:SER:HB3	2.13	0.47
1:G:257:THR:OG1	1:G:316:HIS:HE1	1.98	0.47
1:I:18:ASN:ND2	1:I:21:VAL:HG23	2.29	0.47
1:L:257:THR:OG1	1:L:316:HIS:HE1	1.98	0.47
1:L:653[A]:HIS:HD2	1:L:666:GLY:O	1.96	0.47
1:M:257:THR:OG1	1:M:316:HIS:HE1	1.98	0.47
1:A:246:MET:C	1:A:246:MET:HE3	2.39	0.47
1:C:429:ASP:OD1	1:C:430:PRO:HD2	2.13	0.47
1:O:261:TRP:CH2	1:O:266:GLN:HB2	2.49	0.47
1:P:18:ASN:ND2	1:P:21:VAL:HG23	2.29	0.47
1:P:254:LEU:HA	1:P:254:LEU:HD23	1.71	0.47
1:C:78:LEU:HB3	1:C:79:PRO:CD	2.43	0.47
1:F:73:TRP:CH2	1:F:185:ALA:HB1	2.49	0.47
1:F:246:MET:C	1:F:246:MET:HE3	2.39	0.47
1:H:73:TRP:CH2	1:H:185:ALA:HB1	2.49	0.47
1:H:744:GLU:HB3	1:H:745:MET:HE3	1.96	0.47
1:I:287:ASP:OD2	1:L:425:ARG:NH2	2.47	0.47
1:P:73:TRP:CZ2	1:P:122:CYS:HB3	2.48	0.47
1:P:257:THR:OG1	1:P:316:HIS:HE1	1.98	0.47
1:P:653[A]:HIS:HD2	1:P:666:GLY:O	1.96	0.47
1:A:261:TRP:CH2	1:A:266:GLN:HB2	2.49	0.47
1:B:43:ARG:HH11	1:B:43:ARG:CG	2.24	0.47
1:B:73:TRP:CH2	1:B:185:ALA:HB1	2.49	0.47
1:D:246:MET:C	1:D:246:MET:HE3	2.39	0.47
1:D:744:GLU:HB3	1:D:745:MET:HE3	1.96	0.47
1:E:18:ASN:ND2	1:E:21:VAL:HG23	2.29	0.47
1:E:744:GLU:HB3	1:E:745:MET:HE3	1.96	0.47
1:F:43:ARG:HH11	1:F:43:ARG:CG	2.24	0.47
1:F:595:THR:CG2	1:F:596:PRO:HA	2.37	0.47
1:G:237:ARG:HE	1:G:237:ARG:HB2	1.35	0.47
1:G:246:MET:C	1:G:246:MET:HE3	2.39	0.47
1:H:73:TRP:CZ2	1:H:122:CYS:HB3	2.48	0.47
1:I:9:VAL:O	1:I:12:GLN:HB3	2.13	0.47
1:I:741:THR:O	1:I:741:THR:HG22	2.12	0.47
1:J:246:MET:HE3	1:J:246:MET:C	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:653[A]:HIS:HD2	1:J:666:GLY:O	1.97	0.47
1:K:9:VAL:O	1:K:12:GLN:HB3	2.13	0.47
1:K:35:SER:O	1:K:50:GLN:HG3	2.14	0.47
1:K:744:GLU:HB3	1:K:745:MET:HE3	1.96	0.47
1:M:35:SER:O	1:M:50:GLN:HG3	2.14	0.47
1:N:9:VAL:O	1:N:12:GLN:HB3	2.13	0.47
1:O:653[A]:HIS:HD2	1:O:666:GLY:O	1.97	0.47
1:O:667:GLU:C	1:O:668:VAL:HG23	2.40	0.47
1:P:679:LEU:HD23	1:P:679:LEU:HA	1.40	0.47
1:A:18:ASN:ND2	1:A:21:VAL:HG23	2.29	0.47
1:A:679:LEU:HD23	1:A:679:LEU:HA	1.40	0.47
1:B:655:MET:HB2	1:B:655:MET:HE3	1.35	0.47
1:B:914:CME:HE2	1:B:914:CME:HB3	1.74	0.47
1:C:261:TRP:CH2	1:C:266:GLN:HB2	2.49	0.47
1:E:35:SER:O	1:E:50:GLN:HG3	2.14	0.47
1:F:140:ARG:HB2	1:F:171:PHE:O	2.13	0.47
1:F:257:THR:OG1	1:F:316:HIS:HE1	1.98	0.47
1:F:667:GLU:C	1:F:668:VAL:HG23	2.40	0.47
1:G:217:LYS:HG2	1:G:218:PRO:HD2	1.96	0.47
1:J:134:LEU:HD23	1:J:134:LEU:HA	1.68	0.47
1:N:667:GLU:C	1:N:668:VAL:HG23	2.40	0.47
1:O:362:LEU:HD23	1:O:362:LEU:HA	1.70	0.47
1:O:658:LEU:N	1:O:661:LYS:O	2.40	0.47
1:P:36:TRP:CE2	1:P:42:ALA:HA	2.50	0.47
1:A:183:ARG:HD3	1:A:183:ARG:HH11	1.62	0.47
1:B:18:ASN:ND2	1:B:21:VAL:HG23	2.29	0.47
1:B:257:THR:OG1	1:B:316:HIS:HE1	1.98	0.47
1:C:36:TRP:CE2	1:C:42:ALA:HA	2.50	0.47
1:C:667:GLU:C	1:C:668:VAL:HG23	2.40	0.47
1:F:18:ASN:ND2	1:F:21:VAL:HG23	2.29	0.47
1:G:261:TRP:CH2	1:G:266:GLN:HB2	2.49	0.47
1:H:18:ASN:ND2	1:H:21:VAL:HG23	2.29	0.47
1:I:257:THR:OG1	1:I:316:HIS:HE1	1.98	0.47
1:K:134:LEU:HD23	1:K:134:LEU:HA	1.68	0.47
1:M:78:LEU:HB3	1:M:79:PRO:CD	2.43	0.47
1:O:217:LYS:HG2	1:O:218:PRO:HD2	1.96	0.47
1:P:134:LEU:HA	1:P:134:LEU:HD23	1.68	0.47
1:P:744:GLU:HB3	1:P:745:MET:HE3	1.96	0.47
1:B:246:MET:HE3	1:B:246:MET:C	2.39	0.47
1:B:744:GLU:HB3	1:B:745:MET:HE3	1.96	0.47
1:F:134:LEU:HA	1:F:134:LEU:HD23	1.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:952:ARG:HH11	1:F:952:ARG:CG	2.28	0.47
1:G:18:ASN:ND2	1:G:21:VAL:HG23	2.29	0.47
1:H:43:ARG:HH11	1:H:43:ARG:CG	2.24	0.47
1:H:595:THR:HG23	1:H:596:PRO:CA	2.35	0.47
1:H:667:GLU:C	1:H:668:VAL:HG23	2.40	0.47
1:I:7:LEU:HD12	1:I:74:LEU:HD11	1.97	0.47
1:I:246:MET:C	1:I:246:MET:HE3	2.39	0.47
1:K:78:LEU:HB3	1:K:79:PRO:CD	2.43	0.47
1:K:668:VAL:CG1	1:K:669:PRO:HD2	2.45	0.47
1:K:949:HIS:HD2	1:K:1020:TRP:HE1	1.53	0.47
1:L:261:TRP:CH2	1:L:266:GLN:HB2	2.49	0.47
1:L:744:GLU:HB3	1:L:745:MET:HE3	1.96	0.47
1:M:667:GLU:C	1:M:668:VAL:HG23	2.40	0.47
1:N:18:ASN:ND2	1:N:21:VAL:HG23	2.29	0.47
1:O:18:ASN:ND2	1:O:21:VAL:HG23	2.29	0.47
1:O:745:MET:HA	1:O:745:MET:CE	2.39	0.47
1:A:65:ALA:HB1	1:A:66:PRO:HD2	1.95	0.46
1:A:914:CME:HE2	1:A:914:CME:HB3	1.74	0.46
1:B:612:THR:HB	1:B:613:PRO:HD2	1.98	0.46
1:C:18:ASN:ND2	1:C:21:VAL:HG23	2.29	0.46
1:C:429:ASP:HA	1:C:430:PRO:HD3	1.73	0.46
1:D:952:ARG:HH11	1:D:952:ARG:CG	2.28	0.46
1:E:830:LEU:HD11	1:F:830:LEU:HD11	1.97	0.46
1:F:668:VAL:CG1	1:F:669:PRO:HD2	2.45	0.46
1:G:745:MET:HA	1:G:745:MET:CE	2.39	0.46
1:G:753:ASN:OD1	1:G:753:ASN:N	2.30	0.46
1:I:378:LEU:HD23	1:I:378:LEU:HA	1.74	0.46
1:I:653[A]:HIS:HD2	1:I:666:GLY:O	1.97	0.46
1:J:429:ASP:HA	1:J:430:PRO:HD3	1.73	0.46
1:J:667:GLU:C	1:J:668:VAL:HG23	2.40	0.46
1:K:18:ASN:ND2	1:K:21:VAL:HG23	2.29	0.46
1:L:63:PHE:CB	1:L:64:PRO:HD2	2.34	0.46
1:L:134:LEU:HD23	1:L:134:LEU:HA	1.68	0.46
1:M:18:ASN:ND2	1:M:21:VAL:HG23	2.29	0.46
1:P:147:ASN:HA	1:P:148:SER:HA	1.57	0.46
1:A:36:TRP:CE2	1:A:42:ALA:HA	2.50	0.46
1:A:57:GLU:HG2	1:A:83:THR:HG22	1.95	0.46
1:A:100:TYR:CE1	1:A:602:CYS:HB3	2.51	0.46
1:C:246:MET:HE3	1:C:246:MET:C	2.39	0.46
1:C:744:GLU:HB3	1:C:745:MET:HE3	1.96	0.46
1:D:36:TRP:CE2	1:D:42:ALA:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:GLU:HG2	1:F:83:THR:HG22	1.95	0.46
1:G:91:GLN:HG3	1:G:96:ASP:OD1	2.15	0.46
1:H:100:TYR:CE1	1:H:602:CYS:HB3	2.51	0.46
1:H:114:VAL:HG22	1:H:191:TRP:HB3	1.98	0.46
1:H:246:MET:HE3	1:H:246:MET:C	2.39	0.46
1:I:91:GLN:HG3	1:I:96:ASP:OD1	2.16	0.46
1:N:91:GLN:HG3	1:N:96:ASP:OD1	2.16	0.46
1:O:7:LEU:HD12	1:O:74:LEU:HD11	1.97	0.46
1:O:53:SER:C	1:O:54:LEU:HD23	2.41	0.46
1:A:91:GLN:HG3	1:A:96:ASP:OD1	2.16	0.46
1:B:429:ASP:HA	1:B:430:PRO:HD3	1.73	0.46
1:B:753:ASN:OD1	1:B:753:ASN:N	2.30	0.46
1:C:668:VAL:CG1	1:C:669:PRO:HD2	2.45	0.46
1:D:57:GLU:HG2	1:D:83:THR:HG22	1.95	0.46
1:D:100:TYR:CE1	1:D:602:CYS:HB3	2.51	0.46
1:E:362:LEU:HD23	1:E:362:LEU:HA	1.70	0.46
1:G:36:TRP:CE2	1:G:42:ALA:HA	2.50	0.46
1:G:53:SER:C	1:G:54:LEU:HD23	2.41	0.46
1:I:36:TRP:CE2	1:I:42:ALA:HA	2.50	0.46
1:I:57:GLU:HG2	1:I:83:THR:HG22	1.95	0.46
1:J:257:THR:OG1	1:J:316:HIS:HE1	1.98	0.46
1:K:952:ARG:HH11	1:K:952:ARG:CG	2.28	0.46
1:L:18:ASN:ND2	1:L:21:VAL:HG23	2.29	0.46
1:L:36:TRP:CE2	1:L:42:ALA:HA	2.50	0.46
1:O:80:GLU:H	1:O:80:GLU:HG3	1.28	0.46
1:O:246:MET:C	1:O:246:MET:HE3	2.39	0.46
1:O:655:MET:HB2	1:O:655:MET:HE3	1.35	0.46
1:P:114:VAL:HG22	1:P:191:TRP:HB3	1.98	0.46
1:A:362:LEU:HA	1:A:362:LEU:HD23	1.70	0.46
1:A:658:LEU:N	1:A:661:LYS:O	2.40	0.46
1:A:667:GLU:C	1:A:668:VAL:HG23	2.40	0.46
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.16	0.46
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.51	0.46
1:C:952:ARG:HH11	1:C:952:ARG:CG	2.28	0.46
1:D:53:SER:C	1:D:54:LEU:HD23	2.41	0.46
1:D:91:GLN:HG3	1:D:96:ASP:OD1	2.16	0.46
1:E:257:THR:OG1	1:E:316:HIS:HE1	1.98	0.46
1:E:667:GLU:C	1:E:668:VAL:HG23	2.40	0.46
1:G:657:ALA:HA	1:G:661:LYS:O	2.16	0.46
1:I:43:ARG:HH11	1:I:43:ARG:CG	2.24	0.46
1:I:217:LYS:HG2	1:I:218:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:595:THR:CG2	1:I:596:PRO:HA	2.37	0.46
1:I:667:GLU:C	1:I:668:VAL:HG23	2.40	0.46
1:J:395:HIS:HA	1:J:396:PRO:HD3	1.69	0.46
1:K:3:ILE:HG13	1:K:4:THR:N	2.25	0.46
1:L:595:THR:CG2	1:L:596:PRO:HA	2.37	0.46
1:L:668:VAL:CG1	1:L:669:PRO:HD2	2.45	0.46
1:M:546:LEU:HA	3:M:4124:HOH:O	2.16	0.46
1:P:53:SER:C	1:P:54:LEU:HD23	2.41	0.46
1:A:114:VAL:HG22	1:A:191:TRP:HB3	1.98	0.46
1:A:657:ALA:HA	1:A:661:LYS:O	2.16	0.46
1:C:257:THR:OG1	1:C:316:HIS:HE1	1.98	0.46
1:D:78:LEU:HB3	1:D:79:PRO:CD	2.43	0.46
1:E:36:TRP:CE2	1:E:42:ALA:HA	2.50	0.46
1:E:272:ALA:HA	1:E:273:PRO:HD3	1.78	0.46
1:G:612:THR:HB	1:G:613:PRO:HD2	1.98	0.46
1:G:655:MET:HB2	1:G:655:MET:HE3	1.35	0.46
1:L:285:TYR:CB	1:L:288:ARG:HG3	2.42	0.46
1:L:612:THR:HB	1:L:613:PRO:HD2	1.98	0.46
1:M:43:ARG:HH11	1:M:43:ARG:CG	2.24	0.46
1:N:612:THR:HB	1:N:613:PRO:HD2	1.98	0.46
1:N:679:LEU:HD23	1:N:679:LEU:HA	1.40	0.46
1:O:36:TRP:CE2	1:O:42:ALA:HA	2.50	0.46
1:O:257:THR:OG1	1:O:316:HIS:HE1	1.98	0.46
1:O:668:VAL:CG1	1:O:669:PRO:HD2	2.45	0.46
1:P:772:ASP:OD1	1:P:772:ASP:N	2.48	0.46
1:P:952:ARG:HH11	1:P:952:ARG:CG	2.28	0.46
1:B:36:TRP:CE2	1:B:42:ALA:HA	2.50	0.46
1:B:579:ASP:HB2	1:B:580:GLU:OE2	2.16	0.46
1:D:657:ALA:HA	1:D:661:LYS:O	2.16	0.46
1:E:100:TYR:CE1	1:E:602:CYS:HB3	2.51	0.46
1:E:217:LYS:HG2	1:E:218:PRO:HD2	1.96	0.46
1:E:657:ALA:HA	1:E:661:LYS:O	2.16	0.46
1:F:36:TRP:CE2	1:F:42:ALA:HA	2.50	0.46
1:F:53:SER:C	1:F:54:LEU:HD23	2.41	0.46
1:F:612:THR:HB	1:F:613:PRO:HD2	1.98	0.46
1:H:254:LEU:HD23	1:H:254:LEU:HA	1.71	0.46
1:J:91:GLN:HG3	1:J:96:ASP:OD1	2.15	0.46
1:K:57:GLU:HG2	1:K:83:THR:HG22	1.95	0.46
1:K:114:VAL:HG22	1:K:191:TRP:HB3	1.98	0.46
1:L:53:SER:C	1:L:54:LEU:HD23	2.41	0.46
1:L:657:ALA:HA	1:L:661:LYS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:134:LEU:HA	1:M:134:LEU:HD23	1.68	0.46
1:O:657:ALA:HA	1:O:661:LYS:O	2.16	0.46
1:O:952:ARG:HH11	1:O:952:ARG:CG	2.28	0.46
1:A:668:VAL:CG1	1:A:669:PRO:HD2	2.45	0.46
1:B:657:ALA:HA	1:B:661:LYS:O	2.16	0.46
1:B:667:GLU:C	1:B:668:VAL:HG23	2.40	0.46
1:D:579:ASP:HB2	1:D:580:GLU:OE2	2.16	0.46
1:D:612:THR:HB	1:D:613:PRO:HD2	1.98	0.46
1:E:53:SER:C	1:E:54:LEU:HD23	2.41	0.46
1:F:469:ASP:HB3	1:G:473:ARG:HD2	1.97	0.46
1:F:920:LEU:HB3	1:F:921:PRO:CD	2.46	0.46
1:H:3:ILE:HG13	1:H:4:THR:N	2.25	0.46
1:H:91:GLN:HG3	1:H:96:ASP:OD1	2.16	0.46
1:H:657:ALA:HA	1:H:661:LYS:O	2.16	0.46
1:I:53:SER:C	1:I:54:LEU:HD23	2.41	0.46
1:I:579:ASP:HB2	1:I:580:GLU:OE2	2.16	0.46
1:I:612:THR:HB	1:I:613:PRO:HD2	1.98	0.46
1:I:767:GLN:CG	1:I:768:MET:N	2.79	0.46
1:J:100:TYR:CE1	1:J:602:CYS:HB3	2.51	0.46
1:J:147:ASN:HA	1:J:148:SER:HA	1.57	0.46
1:M:254:LEU:HA	1:M:254:LEU:HD23	1.71	0.46
1:N:36:TRP:CE2	1:N:42:ALA:HA	2.50	0.46
1:N:53:SER:C	1:N:54:LEU:HD23	2.41	0.46
1:O:237:ARG:HE	1:O:237:ARG:HB2	1.35	0.46
1:O:612:THR:HB	1:O:613:PRO:HD2	1.98	0.46
1:A:685:LEU:HA	1:A:686:PRO:HD3	1.83	0.46
1:B:114:VAL:HG22	1:B:191:TRP:HB3	1.98	0.46
1:B:279:ILE:HD11	1:C:422:PRO:HG2	1.96	0.46
1:C:100:TYR:CE1	1:C:602:CYS:HB3	2.51	0.46
1:C:118:ASN:HA	1:C:119:PRO:HD2	1.62	0.46
1:D:767:GLN:CG	1:D:768:MET:N	2.79	0.46
1:G:667:GLU:C	1:G:668:VAL:HG23	2.40	0.46
1:G:952:ARG:HH11	1:G:952:ARG:CG	2.28	0.46
1:H:285:TYR:CB	1:H:288:ARG:HG3	2.42	0.46
1:H:952:ARG:HH11	1:H:952:ARG:CG	2.28	0.46
1:J:18:ASN:ND2	1:J:21:VAL:HG23	2.29	0.46
1:J:78:LEU:HB3	1:J:79:PRO:CD	2.43	0.46
1:J:668:VAL:CG1	1:J:669:PRO:HD2	2.45	0.46
1:J:986:ILE:HD13	1:J:986:ILE:HG23	1.67	0.46
1:L:91:GLN:HG3	1:L:96:ASP:OD1	2.16	0.46
1:M:36:TRP:CE2	1:M:42:ALA:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:91:GLN:HG3	1:M:96:ASP:OD1	2.15	0.46
1:M:217:LYS:HG2	1:M:218:PRO:HD2	1.96	0.46
1:M:679:LEU:HD23	1:M:679:LEU:HA	1.40	0.46
1:N:257:THR:OG1	1:N:316:HIS:HE1	1.98	0.46
1:N:282:ARG:HD2	1:O:418:HIS:O	2.15	0.46
1:N:579:ASP:HB2	1:N:580:GLU:OE2	2.16	0.46
1:N:920:LEU:HB3	1:N:921:PRO:CD	2.46	0.46
1:P:118:ASN:HA	1:P:119:PRO:HD2	1.62	0.46
1:P:612:THR:HB	1:P:613:PRO:HD2	1.98	0.46
1:P:657:ALA:HA	1:P:661:LYS:O	2.16	0.46
1:B:111:PRO:HA	1:B:112:PRO:HA	1.66	0.46
1:B:668:VAL:CG1	1:B:669:PRO:HD2	2.45	0.46
1:C:53:SER:C	1:C:54:LEU:HD23	2.41	0.46
1:C:395:HIS:CG	1:C:396:PRO:HD2	2.51	0.46
1:D:658:LEU:N	1:D:661:LYS:O	2.40	0.46
1:E:668:VAL:CG1	1:E:669:PRO:HD2	2.45	0.46
1:G:254:LEU:HD23	1:G:254:LEU:HA	1.71	0.46
1:G:429:ASP:HA	1:G:430:PRO:HD3	1.74	0.46
1:G:579:ASP:HB2	1:G:580:GLU:OE2	2.16	0.46
1:H:237:ARG:HE	1:H:237:ARG:HB2	1.35	0.46
1:I:657:ALA:HA	1:I:661:LYS:O	2.16	0.46
1:K:42:ALA:O	1:K:310:ARG:NH1	2.49	0.46
1:K:546:LEU:HA	3:K:4124:HOH:O	2.16	0.46
1:K:701:VAL:HG12	1:K:702:GLN:N	2.31	0.46
1:L:7:LEU:HD12	1:L:74:LEU:HD11	1.97	0.46
1:L:42:ALA:O	1:L:310:ARG:NH1	2.49	0.46
1:M:85:VAL:CG1	1:M:86:VAL:N	2.79	0.46
1:O:57:GLU:HG2	1:O:83:THR:HG22	1.95	0.46
1:O:579:ASP:HB2	1:O:580:GLU:OE2	2.16	0.46
1:O:767:GLN:CG	1:O:768:MET:N	2.79	0.46
1:P:730:LEU:HA	1:P:731:PRO:HD3	1.80	0.46
1:A:395:HIS:HA	1:A:396:PRO:HD3	1.69	0.46
1:B:85:VAL:CG1	1:B:86:VAL:N	2.79	0.46
1:B:285:TYR:CB	1:B:288:ARG:HG3	2.42	0.46
1:C:57:GLU:HG2	1:C:83:THR:HG22	1.95	0.46
1:E:85:VAL:CG1	1:E:86:VAL:N	2.79	0.46
1:G:546:LEU:HA	3:G:3228:HOH:O	2.16	0.46
1:G:767:GLN:CG	1:G:768:MET:N	2.79	0.46
1:H:745:MET:HA	1:H:745:MET:CE	2.39	0.46
1:I:546:LEU:HA	3:I:4123:HOH:O	2.16	0.46
1:J:36:TRP:CE2	1:J:42:ALA:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:43:ARG:HH11	1:J:43:ARG:CG	2.24	0.46
1:J:546:LEU:HA	3:J:3231:HOH:O	2.16	0.46
1:J:579:ASP:HB2	1:J:580:GLU:OE2	2.16	0.46
1:J:701:VAL:HG12	1:J:702:GLN:N	2.31	0.46
1:K:100:TYR:CE1	1:K:602:CYS:HB3	2.51	0.46
1:K:667:GLU:C	1:K:668:VAL:HG23	2.40	0.46
1:K:767:GLN:CG	1:K:768:MET:N	2.79	0.46
1:M:653[B]:HIS:CD2	1:M:667:GLU:HG2	2.51	0.46
1:N:701:VAL:HG12	1:N:702:GLN:N	2.31	0.46
1:N:778:THR:HG23	1:N:779:PRO:HD2	1.98	0.46
1:O:546:LEU:HA	3:O:3228:HOH:O	2.16	0.46
1:O:920:LEU:HB3	1:O:921:PRO:CD	2.46	0.46
1:P:100:TYR:CE1	1:P:602:CYS:HB3	2.51	0.46
1:P:767:GLN:CG	1:P:768:MET:N	2.79	0.46
1:A:433:LEU:N	1:A:434:PRO:CD	2.80	0.45
1:A:612:THR:HB	1:A:613:PRO:HD2	1.98	0.45
1:B:395:HIS:HA	1:B:396:PRO:HD3	1.69	0.45
1:F:579:ASP:HB2	1:F:580:GLU:OE2	2.16	0.45
1:F:701:VAL:HG12	1:F:702:GLN:N	2.31	0.45
1:H:36:TRP:CE2	1:H:42:ALA:HA	2.50	0.45
1:H:579:ASP:HB2	1:H:580:GLU:OE2	2.16	0.45
1:H:595:THR:CG2	1:H:596:PRO:HA	2.37	0.45
1:I:653[B]:HIS:CD2	1:I:667:GLU:HG2	2.51	0.45
1:J:42:ALA:O	1:J:310:ARG:NH1	2.49	0.45
1:J:367:MET:HB3	1:J:372:MET:HE3	1.98	0.45
1:K:914:CME:HB3	1:K:914:CME:HE2	1.74	0.45
1:L:114:VAL:HG22	1:L:191:TRP:HB3	1.98	0.45
1:M:53:SER:C	1:M:54:LEU:HD23	2.41	0.45
1:M:595:THR:CG2	1:M:596:PRO:HA	2.37	0.45
1:M:687:GLN:HA	1:M:688:PRO:HD3	1.73	0.45
1:M:920:LEU:HB3	1:M:921:PRO:CD	2.46	0.45
1:O:118:ASN:HA	1:O:119:PRO:HD2	1.62	0.45
1:O:147:ASN:HA	1:O:148:SER:HA	1.57	0.45
1:P:395:HIS:CG	1:P:396:PRO:HD2	2.51	0.45
1:P:579:ASP:HB2	1:P:580:GLU:OE2	2.16	0.45
1:P:667:GLU:C	1:P:668:VAL:HG23	2.40	0.45
1:A:53:SER:C	1:A:54:LEU:HD23	2.41	0.45
1:B:53:SER:C	1:B:54:LEU:HD23	2.41	0.45
1:B:362:LEU:HA	1:B:362:LEU:HD23	1.70	0.45
1:C:7:LEU:HD12	1:C:74:LEU:HD11	1.97	0.45
1:C:653[B]:HIS:CD2	1:C:667:GLU:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:657:ALA:HA	1:C:661:LYS:O	2.16	0.45
1:C:679:LEU:HD23	1:C:679:LEU:HA	1.40	0.45
1:C:947:GLY:HA3	1:C:948:PRO:HD2	1.82	0.45
1:D:668:VAL:CG1	1:D:669:PRO:HD2	2.45	0.45
1:D:778:THR:HG23	1:D:779:PRO:HD2	1.98	0.45
1:E:43:ARG:NH1	1:E:44:THR:CG2	2.80	0.45
1:E:285:TYR:CB	1:E:288:ARG:HG3	2.42	0.45
1:E:653[B]:HIS:CD2	1:E:667:GLU:HG2	2.51	0.45
1:E:920:LEU:HB3	1:E:921:PRO:CD	2.46	0.45
1:F:395:HIS:CG	1:F:396:PRO:HD2	2.51	0.45
1:F:655:MET:HB2	1:F:655:MET:HE3	1.35	0.45
1:F:778:THR:HG23	1:F:779:PRO:HD2	1.98	0.45
1:G:100:TYR:CE1	1:G:602:CYS:HB3	2.51	0.45
1:G:118:ASN:HA	1:G:119:PRO:HD2	1.62	0.45
1:H:42:ALA:O	1:H:310:ARG:NH1	2.49	0.45
1:H:612:THR:HB	1:H:613:PRO:HD2	1.98	0.45
1:I:114:VAL:HG22	1:I:191:TRP:HB3	1.98	0.45
1:I:211:ASP:OD1	1:I:211:ASP:N	2.50	0.45
1:J:653[B]:HIS:CD2	1:J:667:GLU:HG2	2.51	0.45
1:J:878:HIS:HA	1:J:879:PRO:HD3	1.83	0.45
1:K:36:TRP:CE2	1:K:42:ALA:HA	2.50	0.45
1:K:433:LEU:N	1:K:434:PRO:CD	2.80	0.45
1:L:85:VAL:CG1	1:L:86:VAL:N	2.79	0.45
1:L:653[B]:HIS:CD2	1:L:667:GLU:HG2	2.51	0.45
1:L:767:GLN:CG	1:L:768:MET:N	2.79	0.45
1:M:114:VAL:HG22	1:M:191:TRP:HB3	1.98	0.45
1:M:668:VAL:CG1	1:M:669:PRO:HD2	2.45	0.45
1:O:395:HIS:CG	1:O:396:PRO:HD2	2.51	0.45
1:O:653[B]:HIS:CD2	1:O:667:GLU:HG2	2.51	0.45
1:P:13:ARG:O	1:P:14:ARG:HB2	2.17	0.45
1:P:986:ILE:HD13	1:P:986:ILE:HG23	1.67	0.45
1:A:579:ASP:HB2	1:A:580:GLU:OE2	2.16	0.45
1:B:129:VAL:CG2	1:B:182:ASN:ND2	2.80	0.45
1:B:425:ARG:NH2	1:C:287:ASP:OD2	2.50	0.45
1:B:778:THR:HG23	1:B:779:PRO:HD2	1.98	0.45
1:C:91:GLN:HG3	1:C:96:ASP:OD1	2.16	0.45
1:C:362:LEU:HD23	1:C:362:LEU:HA	1.70	0.45
1:C:579:ASP:HB2	1:C:580:GLU:OE2	2.16	0.45
1:C:701:VAL:HG12	1:C:702:GLN:N	2.31	0.45
1:D:129:VAL:CG2	1:D:182:ASN:ND2	2.80	0.45
1:D:257:THR:OG1	1:D:316:HIS:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:MET:HB3	1:D:372:MET:HE3	1.98	0.45
1:E:91:GLN:HG3	1:E:96:ASP:OD1	2.16	0.45
1:E:433:LEU:N	1:E:434:PRO:CD	2.80	0.45
1:E:612:THR:HA	1:E:613:PRO:HD3	1.59	0.45
1:E:767:GLN:CG	1:E:768:MET:N	2.79	0.45
1:F:100:TYR:CE1	1:F:602:CYS:HB3	2.51	0.45
1:F:653[B]:HIS:CD2	1:F:667:GLU:HG2	2.51	0.45
1:F:767:GLN:CG	1:F:768:MET:N	2.79	0.45
1:F:847:LYS:HG3	1:F:848:THR:N	2.32	0.45
1:G:395:HIS:CG	1:G:396:PRO:HD2	2.51	0.45
1:G:847:LYS:HG3	1:G:848:THR:N	2.32	0.45
1:H:257:THR:OG1	1:H:316:HIS:HE1	1.98	0.45
1:H:668:VAL:CG1	1:H:669:PRO:HD2	2.45	0.45
1:H:914:CME:HE2	1:H:914:CME:HB3	1.74	0.45
1:H:920:LEU:HB3	1:H:921:PRO:CD	2.46	0.45
1:I:100:TYR:CE1	1:I:602:CYS:HB3	2.51	0.45
1:J:43:ARG:NH1	1:J:44:THR:CG2	2.80	0.45
1:J:53:SER:C	1:J:54:LEU:HD23	2.41	0.45
1:J:129:VAL:CG2	1:J:182:ASN:ND2	2.80	0.45
1:J:211:ASP:OD1	1:J:211:ASP:N	2.50	0.45
1:J:322:LEU:CD2	1:J:324:GLU:N	2.80	0.45
1:J:778:THR:HG23	1:J:779:PRO:HD2	1.98	0.45
1:K:53:SER:C	1:K:54:LEU:HD23	2.41	0.45
1:K:91:GLN:HG3	1:K:96:ASP:OD1	2.15	0.45
1:K:254:LEU:HA	1:K:254:LEU:HD23	1.71	0.45
1:L:395:HIS:CG	1:L:396:PRO:HD2	2.51	0.45
1:L:579:ASP:HB2	1:L:580:GLU:OE2	2.16	0.45
1:L:667:GLU:C	1:L:668:VAL:HG23	2.40	0.45
1:L:914:CME:HE2	1:L:914:CME:HB3	1.74	0.45
1:M:43:ARG:NH1	1:M:44:THR:CG2	2.80	0.45
1:N:43:ARG:HH12	1:N:44:THR:CG2	2.30	0.45
1:N:114:VAL:HG22	1:N:191:TRP:HB3	1.98	0.45
1:N:395:HIS:CG	1:N:396:PRO:HD2	2.51	0.45
1:N:668:VAL:CG1	1:N:669:PRO:HD2	2.45	0.45
1:N:847:LYS:HG3	1:N:848:THR:N	2.32	0.45
1:O:100:TYR:CE1	1:O:602:CYS:HB3	2.51	0.45
1:P:42:ALA:O	1:P:310:ARG:NH1	2.49	0.45
1:A:85:VAL:CG1	1:A:86:VAL:N	2.79	0.45
1:A:211:ASP:OD1	1:A:211:ASP:N	2.50	0.45
1:A:367:MET:HB3	1:A:372:MET:HE3	1.98	0.45
1:C:767:GLN:CG	1:C:768:MET:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:778:THR:HG23	1:C:779:PRO:HD2	1.98	0.45
1:D:43:ARG:NH1	1:D:44:THR:CG2	2.80	0.45
1:D:211:ASP:OD1	1:D:211:ASP:N	2.50	0.45
1:D:667:GLU:C	1:D:668:VAL:HG23	2.40	0.45
1:E:687:GLN:HA	1:E:688:PRO:HD3	1.73	0.45
1:F:3:ILE:HD12	1:F:3:ILE:O	2.17	0.45
1:F:237:ARG:HE	1:F:237:ARG:HB2	1.35	0.45
1:F:657:ALA:HA	1:F:661:LYS:O	2.16	0.45
1:G:42:ALA:O	1:G:310:ARG:NH1	2.49	0.45
1:G:43:ARG:NH1	1:G:44:THR:CG2	2.80	0.45
1:H:43:ARG:NH1	1:H:44:THR:CG2	2.80	0.45
1:H:53:SER:C	1:H:54:LEU:HD23	2.41	0.45
1:H:85:VAL:CG1	1:H:86:VAL:N	2.79	0.45
1:H:653[B]:HIS:CD2	1:H:667:GLU:HG2	2.51	0.45
1:I:85:VAL:CG1	1:I:86:VAL:N	2.79	0.45
1:I:367:MET:HB3	1:I:372:MET:HE3	1.98	0.45
1:I:920:LEU:HB3	1:I:921:PRO:CD	2.46	0.45
1:J:433:LEU:N	1:J:434:PRO:CD	2.80	0.45
1:J:595:THR:CG2	1:J:596:PRO:HA	2.37	0.45
1:L:546:LEU:HA	3:L:3234:HOH:O	2.16	0.45
1:L:778:THR:HG23	1:L:779:PRO:HD2	1.98	0.45
1:M:657:ALA:HA	1:M:661:LYS:O	2.16	0.45
1:M:701:VAL:HG12	1:M:702:GLN:N	2.31	0.45
1:N:3:ILE:HD12	1:N:3:ILE:O	2.17	0.45
1:N:7:LEU:HD12	1:N:74:LEU:HD11	1.97	0.45
1:N:100:TYR:CE1	1:N:602:CYS:HB3	2.51	0.45
1:N:546:LEU:HA	3:N:3231:HOH:O	2.16	0.45
1:N:767:GLN:CG	1:N:768:MET:N	2.79	0.45
1:O:42:ALA:O	1:O:310:ARG:NH1	2.49	0.45
1:O:91:GLN:HG3	1:O:96:ASP:OD1	2.16	0.45
1:O:114:VAL:HG22	1:O:191:TRP:HB3	1.98	0.45
1:P:3:ILE:O	1:P:3:ILE:HD12	2.17	0.45
1:P:78:LEU:HB3	1:P:79:PRO:CD	2.43	0.45
1:P:546:LEU:HA	3:P:3236:HOH:O	2.16	0.45
1:P:668:VAL:CG1	1:P:669:PRO:HD2	2.45	0.45
1:A:653[B]:HIS:CD2	1:A:667:GLU:HG2	2.51	0.45
1:B:599:ARG:HB2	1:B:600:GLN:H	1.63	0.45
1:B:952:ARG:HH11	1:B:952:ARG:CG	2.28	0.45
1:D:147:ASN:HA	1:D:148:SER:HA	1.57	0.45
1:D:237:ARG:HE	1:D:237:ARG:HB2	1.35	0.45
1:D:278:ILE:N	1:D:278:ILE:CD1	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:LEU:N	1:D:434:PRO:CD	2.80	0.45
1:D:701:VAL:HG12	1:D:702:GLN:N	2.31	0.45
1:D:920:LEU:HB3	1:D:921:PRO:CD	2.46	0.45
1:D:947:GLY:HA3	1:D:948:PRO:HD2	1.82	0.45
1:F:7:LEU:HD12	1:F:74:LEU:HD11	1.97	0.45
1:F:114:VAL:HG22	1:F:191:TRP:HB3	1.98	0.45
1:F:279:ILE:HD12	1:F:279:ILE:HG21	1.77	0.45
1:G:114:VAL:HG22	1:G:191:TRP:HB3	1.98	0.45
1:G:778:THR:HG23	1:G:779:PRO:HD2	1.98	0.45
1:H:13:ARG:O	1:H:14:ARG:HB2	2.17	0.45
1:H:183:ARG:HD3	1:H:183:ARG:HH11	1.62	0.45
1:H:367:MET:HB3	1:H:372:MET:HE3	1.98	0.45
1:I:425:ARG:NH2	1:L:287:ASP:OD2	2.50	0.45
1:J:612:THR:HB	1:J:613:PRO:HD2	1.98	0.45
1:J:767:GLN:CG	1:J:768:MET:N	2.79	0.45
1:K:3:ILE:HD12	1:K:3:ILE:O	2.17	0.45
1:K:257:THR:OG1	1:K:316:HIS:HE1	1.98	0.45
1:K:395:HIS:CG	1:K:396:PRO:HD2	2.51	0.45
1:K:612:THR:HB	1:K:613:PRO:HD2	1.98	0.45
1:K:657:ALA:HA	1:K:661:LYS:O	2.16	0.45
1:L:100:TYR:CE1	1:L:602:CYS:HB3	2.51	0.45
1:M:42:ALA:O	1:M:310:ARG:NH1	2.49	0.45
1:M:80:GLU:H	1:M:80:GLU:HG3	1.29	0.45
1:M:433:LEU:N	1:M:434:PRO:CD	2.80	0.45
1:M:670:LEU:HD23	1:M:670:LEU:HA	1.75	0.45
1:M:847:LYS:HG3	1:M:848:THR:N	2.32	0.45
1:N:42:ALA:O	1:N:310:ARG:NH1	2.49	0.45
1:N:657:ALA:HA	1:N:661:LYS:O	2.16	0.45
1:N:745:MET:HA	1:N:745:MET:CE	2.39	0.45
1:O:43:ARG:HH12	1:O:44:THR:CG2	2.30	0.45
1:P:367:MET:HB3	1:P:372:MET:HE3	1.98	0.45
1:A:43:ARG:HH12	1:A:44:THR:CG2	2.30	0.45
1:A:237:ARG:HE	1:A:237:ARG:HB2	1.35	0.45
1:A:546:LEU:HA	3:A:4124:HOH:O	2.16	0.45
1:A:847:LYS:HG3	1:A:848:THR:N	2.32	0.45
1:B:847:LYS:HG3	1:B:848:THR:N	2.32	0.45
1:C:114:VAL:HG22	1:C:191:TRP:HB3	1.98	0.45
1:E:43:ARG:HH12	1:E:44:THR:CG2	2.30	0.45
1:E:114:VAL:HG22	1:E:191:TRP:HB3	1.98	0.45
1:E:395:HIS:CG	1:E:396:PRO:HD2	2.52	0.45
1:E:701:VAL:HG12	1:E:702:GLN:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:952:ARG:HH11	1:E:952:ARG:CG	2.28	0.45
1:F:42:ALA:O	1:F:310:ARG:NH1	2.49	0.45
1:G:134:LEU:HA	1:G:134:LEU:HD23	1.68	0.45
1:H:134:LEU:HA	1:H:134:LEU:HD23	1.68	0.45
1:H:395:HIS:CG	1:H:396:PRO:HD2	2.51	0.45
1:I:395:HIS:CG	1:I:396:PRO:HD2	2.51	0.45
1:I:701:VAL:HG12	1:I:702:GLN:N	2.31	0.45
1:J:13:ARG:O	1:J:14:ARG:HB2	2.17	0.45
1:J:395:HIS:CG	1:J:396:PRO:HD2	2.51	0.45
1:K:147:ASN:HA	1:K:148:SER:HA	1.57	0.45
1:K:395:HIS:HA	1:K:396:PRO:HD3	1.69	0.45
1:L:43:ARG:NH1	1:L:44:THR:CG2	2.80	0.45
1:M:3:ILE:O	1:M:3:ILE:HD12	2.17	0.45
1:M:418:HIS:O	1:P:282:ARG:HD2	2.17	0.45
1:M:579:ASP:HB2	1:M:580:GLU:OE2	2.16	0.45
1:M:767:GLN:CG	1:M:768:MET:N	2.79	0.45
1:O:134:LEU:HD23	1:O:134:LEU:HA	1.68	0.45
1:O:778:THR:HG23	1:O:779:PRO:HD2	1.98	0.45
1:P:111:PRO:HA	1:P:112:PRO:HA	1.66	0.45
1:P:183:ARG:HD3	1:P:183:ARG:HH11	1.62	0.45
1:A:7:LEU:HD12	1:A:74:LEU:HD11	1.97	0.45
1:A:42:ALA:O	1:A:310:ARG:NH1	2.49	0.45
1:A:701:VAL:HG12	1:A:702:GLN:N	2.31	0.45
1:B:211:ASP:OD1	1:B:211:ASP:N	2.50	0.45
1:B:701:VAL:HG12	1:B:702:GLN:N	2.31	0.45
1:C:285:TYR:CB	1:C:288:ARG:HG3	2.42	0.45
1:C:322:LEU:CD2	1:C:324:GLU:N	2.80	0.45
1:D:362:LEU:HD23	1:D:362:LEU:HA	1.70	0.45
1:D:395:HIS:CG	1:D:396:PRO:HD2	2.51	0.45
1:E:42:ALA:O	1:E:310:ARG:NH1	2.49	0.45
1:F:3:ILE:HG13	1:F:4:THR:N	2.25	0.45
1:F:91:GLN:HG3	1:F:96:ASP:OD1	2.15	0.45
1:F:679:LEU:HD23	1:F:679:LEU:HA	1.40	0.45
1:G:3:ILE:HD12	1:G:3:ILE:O	2.17	0.45
1:G:129:VAL:CG2	1:G:182:ASN:ND2	2.80	0.45
1:H:278:ILE:N	1:H:278:ILE:CD1	2.80	0.45
1:I:847:LYS:HG3	1:I:848:THR:N	2.32	0.45
1:K:63:PHE:CB	1:K:64:PRO:HD2	2.34	0.45
1:K:778:THR:HG23	1:K:779:PRO:HD2	1.98	0.45
1:L:129:VAL:CG2	1:L:182:ASN:ND2	2.80	0.45
1:L:687:GLN:HA	1:L:688:PRO:HD3	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:43:ARG:HH12	1:M:44:THR:CG2	2.30	0.45
1:M:479:ASP:HA	1:M:480:PRO:HD2	1.77	0.45
1:N:322:LEU:CD2	1:N:324:GLU:N	2.80	0.45
1:N:473:ARG:HD2	1:O:469:ASP:HB3	1.98	0.45
1:P:43:ARG:NH1	1:P:44:THR:CG2	2.80	0.45
1:P:85:VAL:CG1	1:P:86:VAL:N	2.79	0.45
1:P:278:ILE:N	1:P:278:ILE:CD1	2.80	0.45
1:P:947:GLY:HA3	1:P:948:PRO:HD2	1.82	0.45
1:C:42:ALA:O	1:C:310:ARG:NH1	2.49	0.45
1:C:546:LEU:HA	3:C:4124:HOH:O	2.16	0.45
1:C:920:LEU:HB3	1:C:921:PRO:CD	2.46	0.45
1:D:285:TYR:CB	1:D:288:ARG:HG3	2.42	0.45
1:D:847:LYS:HG3	1:D:848:THR:N	2.32	0.45
1:E:546:LEU:HA	3:E:4124:HOH:O	2.16	0.45
1:E:579:ASP:HB2	1:E:580:GLU:OE2	2.16	0.45
1:G:668:VAL:CG1	1:G:669:PRO:HD2	2.45	0.45
1:H:211:ASP:OD1	1:H:211:ASP:N	2.50	0.45
1:I:433:LEU:N	1:I:434:PRO:CD	2.80	0.45
1:J:114:VAL:HG22	1:J:191:TRP:HB3	1.98	0.45
1:J:254:LEU:HA	1:J:254:LEU:HD23	1.71	0.45
1:L:80:GLU:H	1:L:80:GLU:HG3	1.29	0.45
1:L:322:LEU:CD2	1:L:324:GLU:N	2.80	0.45
1:M:211:ASP:OD1	1:M:211:ASP:N	2.50	0.45
1:M:482:ARG:HH11	1:M:482:ARG:HD2	1.63	0.45
1:M:612:THR:HB	1:M:613:PRO:HD2	1.98	0.45
1:M:668:VAL:HA	1:M:669:PRO:HD3	1.83	0.45
1:M:778:THR:HG23	1:M:779:PRO:HD2	1.98	0.45
1:N:111:PRO:HA	1:N:112:PRO:HA	1.66	0.45
1:O:3:ILE:HD12	1:O:3:ILE:O	2.17	0.45
1:O:322:LEU:CD2	1:O:324:GLU:N	2.80	0.45
1:P:745:MET:HA	1:P:745:MET:CE	2.39	0.45
1:P:847:LYS:HG3	1:P:848:THR:N	2.32	0.45
1:A:395:HIS:CG	1:A:396:PRO:HD2	2.51	0.45
1:B:322:LEU:CD2	1:B:324:GLU:N	2.80	0.45
1:B:395:HIS:CG	1:B:396:PRO:HD2	2.51	0.45
1:B:433:LEU:N	1:B:434:PRO:CD	2.80	0.45
1:C:43:ARG:NH1	1:C:44:THR:CG2	2.80	0.45
1:C:246:MET:HG2	1:C:274:PHE:CE2	2.52	0.45
1:D:114:VAL:HG22	1:D:191:TRP:HB3	1.98	0.45
1:E:278:ILE:N	1:E:278:ILE:CD1	2.80	0.45
1:F:43:ARG:NH1	1:F:44:THR:CG2	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:ARG:HH12	1:F:44:THR:CG2	2.30	0.45
1:G:111:PRO:HA	1:G:112:PRO:HA	1.66	0.45
1:G:653[B]:HIS:CD2	1:G:667:GLU:HG2	2.51	0.45
1:G:701:VAL:HG12	1:G:702:GLN:N	2.31	0.45
1:H:546:LEU:HA	3:H:4124:HOH:O	2.16	0.45
1:I:254:LEU:HD23	1:I:254:LEU:HA	1.71	0.45
1:I:772:ASP:OD1	1:I:772:ASP:N	2.48	0.45
1:K:43:ARG:NH1	1:K:44:THR:CG2	2.80	0.45
1:K:43:ARG:HH12	1:K:44:THR:CG2	2.30	0.45
1:L:3:ILE:HD12	1:L:3:ILE:O	2.17	0.45
1:M:100:TYR:CE1	1:M:602:CYS:HB3	2.51	0.45
1:M:395:HIS:CG	1:M:396:PRO:HD2	2.51	0.45
1:M:867:THR:HG22	3:M:4298:HOH:O	2.17	0.45
1:N:43:ARG:NH1	1:N:44:THR:CG2	2.80	0.45
1:N:378:LEU:HD23	1:N:378:LEU:HA	1.74	0.45
1:O:211:ASP:OD1	1:O:211:ASP:N	2.50	0.45
1:O:246:MET:HG2	1:O:274:PHE:CE2	2.52	0.45
1:O:701:VAL:HG12	1:O:702:GLN:N	2.31	0.45
1:P:653[B]:HIS:CD2	1:P:667:GLU:HG2	2.51	0.45
1:P:778:THR:HG23	1:P:779:PRO:HD2	1.98	0.45
1:A:612:THR:HA	1:A:613:PRO:HD3	1.59	0.45
1:A:767:GLN:CG	1:A:768:MET:N	2.79	0.45
1:A:952:ARG:HH11	1:A:952:ARG:CG	2.28	0.45
1:B:78:LEU:HB3	1:B:79:PRO:CD	2.43	0.45
1:B:567:VAL:HG12	1:B:568:TRP:N	2.32	0.45
1:B:653[B]:HIS:CD2	1:B:667:GLU:HG2	2.51	0.45
1:B:767:GLN:CG	1:B:768:MET:N	2.79	0.45
1:C:3:ILE:HD12	1:C:3:ILE:O	2.17	0.45
1:D:42:ALA:O	1:D:310:ARG:NH1	2.49	0.45
1:D:80:GLU:H	1:D:80:GLU:HG3	1.29	0.45
1:E:867:THR:HG22	3:E:4298:HOH:O	2.17	0.45
1:F:378:LEU:HD23	1:F:378:LEU:HA	1.74	0.45
1:G:78:LEU:HB3	1:G:79:PRO:CD	2.43	0.45
1:H:433:LEU:N	1:H:434:PRO:CD	2.80	0.45
1:I:13:ARG:O	1:I:14:ARG:HB2	2.16	0.45
1:J:57:GLU:HG2	1:J:83:THR:HG22	1.95	0.45
1:J:679:LEU:HD23	1:J:679:LEU:HA	1.40	0.45
1:K:362:LEU:HD23	1:K:362:LEU:HA	1.70	0.45
1:K:579:ASP:HB2	1:K:580:GLU:OE2	2.16	0.45
1:K:653[B]:HIS:CD2	1:K:667:GLU:HG2	2.51	0.45
1:M:13:ARG:O	1:M:14:ARG:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:246:MET:HG2	1:M:274:PHE:CE2	2.52	0.45
1:M:322:LEU:CD2	1:M:324:GLU:N	2.80	0.45
1:N:612:THR:HA	1:N:613:PRO:HD3	1.59	0.45
1:P:129:VAL:CG2	1:P:182:ASN:ND2	2.80	0.45
1:B:43:ARG:HH12	1:B:44:THR:CG2	2.30	0.44
1:C:433:LEU:N	1:C:434:PRO:CD	2.80	0.44
1:C:612:THR:HB	1:C:613:PRO:HD2	1.98	0.44
1:D:546:LEU:HA	3:D:3237:HOH:O	2.16	0.44
1:E:3:ILE:O	1:E:3:ILE:HD12	2.17	0.44
1:E:246:MET:HG2	1:E:274:PHE:CE2	2.52	0.44
1:E:612:THR:HB	1:E:613:PRO:HD2	1.98	0.44
1:F:687:GLN:HA	1:F:688:PRO:HD3	1.73	0.44
1:G:362:LEU:HA	1:G:362:LEU:HD23	1.70	0.44
1:G:367:MET:HB3	1:G:372:MET:HE3	1.98	0.44
1:G:395:HIS:HA	1:G:396:PRO:HD3	1.69	0.44
1:G:694:LEU:HD12	1:G:694:LEU:HA	1.84	0.44
1:H:7:LEU:HD12	1:H:74:LEU:HD11	1.97	0.44
1:H:246:MET:HG2	1:H:274:PHE:CE2	2.52	0.44
1:I:43:ARG:HH12	1:I:44:THR:CG2	2.30	0.44
1:J:63:PHE:CB	1:J:64:PRO:HD2	2.34	0.44
1:J:246:MET:HG2	1:J:274:PHE:CE2	2.52	0.44
1:J:567:VAL:HG12	1:J:568:TRP:N	2.32	0.44
1:L:43:ARG:HH12	1:L:44:THR:CG2	2.30	0.44
1:M:367:MET:HB3	1:M:372:MET:HE3	1.98	0.44
1:N:653[B]:HIS:CD2	1:N:667:GLU:HG2	2.51	0.44
1:O:367:MET:HB3	1:O:372:MET:HE3	1.98	0.44
1:O:433:LEU:N	1:O:434:PRO:CD	2.80	0.44
1:P:701:VAL:HG12	1:P:702:GLN:N	2.31	0.44
1:A:246:MET:HG2	1:A:274:PHE:CE2	2.52	0.44
1:A:257:THR:OG1	1:A:316:HIS:HE1	1.98	0.44
1:B:13:ARG:O	1:B:14:ARG:HB2	2.17	0.44
1:B:42:ALA:O	1:B:310:ARG:NH1	2.49	0.44
1:B:367:MET:HB3	1:B:372:MET:HE3	1.98	0.44
1:B:595:THR:CG2	1:B:596:PRO:HA	2.37	0.44
1:C:85:VAL:CG1	1:C:86:VAL:N	2.79	0.44
1:C:367:MET:HB3	1:C:372:MET:HE3	1.98	0.44
1:D:3:ILE:HD12	1:D:3:ILE:O	2.17	0.44
1:E:730:LEU:HA	1:E:731:PRO:HD3	1.80	0.44
1:F:638:VAL:O	1:F:677:LYS:HA	2.18	0.44
1:G:43:ARG:HH11	1:G:43:ARG:CG	2.24	0.44
1:G:43:ARG:HH12	1:G:44:THR:CG2	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:VAL:CG1	1:G:86:VAL:N	2.79	0.44
1:G:246:MET:HG2	1:G:274:PHE:CE2	2.52	0.44
1:G:322:LEU:CD2	1:G:324:GLU:N	2.80	0.44
1:G:595:THR:CG2	1:G:596:PRO:HA	2.37	0.44
1:G:867:THR:HG22	3:G:3402:HOH:O	2.17	0.44
1:H:701:VAL:HG12	1:H:702:GLN:N	2.31	0.44
1:I:668:VAL:CG1	1:I:669:PRO:HD2	2.45	0.44
1:J:745:MET:HA	1:J:745:MET:CE	2.39	0.44
1:K:7:LEU:HD12	1:K:74:LEU:HD11	1.97	0.44
1:K:246:MET:HG2	1:K:274:PHE:CE2	2.52	0.44
1:L:272:ALA:HA	1:L:273:PRO:HD3	1.78	0.44
1:L:433:LEU:N	1:L:434:PRO:CD	2.80	0.44
1:N:85:VAL:CG1	1:N:86:VAL:N	2.79	0.44
1:P:43:ARG:HH12	1:P:44:THR:CG2	2.30	0.44
1:P:246:MET:HG2	1:P:274:PHE:CE2	2.52	0.44
1:P:914:CME:HB3	1:P:914:CME:HE2	1.74	0.44
1:A:3:ILE:HD12	1:A:3:ILE:O	2.17	0.44
1:A:80:GLU:H	1:A:80:GLU:HG3	1.29	0.44
1:A:670:LEU:HD23	1:A:670:LEU:HA	1.75	0.44
1:A:920:LEU:HB3	1:A:921:PRO:CD	2.46	0.44
1:B:3:ILE:HD12	1:B:3:ILE:O	2.17	0.44
1:B:546:LEU:HA	3:B:3228:HOH:O	2.16	0.44
1:B:638:VAL:O	1:B:677:LYS:HA	2.18	0.44
1:C:13:ARG:O	1:C:14:ARG:HB2	2.17	0.44
1:E:129:VAL:CG2	1:E:182:ASN:ND2	2.80	0.44
1:E:254:LEU:HA	1:E:254:LEU:HD23	1.71	0.44
1:E:322:LEU:CD2	1:E:324:GLU:N	2.80	0.44
1:F:129:VAL:CG2	1:F:182:ASN:ND2	2.80	0.44
1:F:367:MET:HB3	1:F:372:MET:HE3	1.98	0.44
1:F:567:VAL:HG12	1:F:568:TRP:N	2.32	0.44
1:G:433:LEU:N	1:G:434:PRO:CD	2.80	0.44
1:H:638:VAL:O	1:H:677:LYS:HA	2.18	0.44
1:H:767:GLN:CG	1:H:768:MET:N	2.79	0.44
1:I:367:MET:HB3	1:I:367:MET:HE3	1.77	0.44
1:I:778:THR:HG23	1:I:779:PRO:HD2	1.98	0.44
1:J:43:ARG:HH12	1:J:44:THR:CG2	2.30	0.44
1:K:129:VAL:CG2	1:K:182:ASN:ND2	2.80	0.44
1:K:745:MET:HA	1:K:745:MET:CE	2.39	0.44
1:M:986:ILE:HG23	1:M:986:ILE:HD13	1.67	0.44
1:N:433:LEU:N	1:N:434:PRO:CD	2.80	0.44
1:N:567:VAL:HG12	1:N:568:TRP:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:63:PHE:CB	1:O:64:PRO:HD2	2.34	0.44
1:O:85:VAL:CG1	1:O:86:VAL:N	2.80	0.44
1:O:694:LEU:HD12	1:O:694:LEU:HA	1.84	0.44
1:P:367:MET:HB3	1:P:367:MET:HE3	1.77	0.44
1:P:638:VAL:O	1:P:677:LYS:HA	2.18	0.44
1:P:702:GLN:O	1:P:712:GLY:N	2.47	0.44
1:B:43:ARG:NH1	1:B:44:THR:CG2	2.80	0.44
1:C:43:ARG:HH12	1:C:44:THR:CG2	2.30	0.44
1:C:129:VAL:CG2	1:C:182:ASN:ND2	2.80	0.44
1:C:847:LYS:HG3	1:C:848:THR:N	2.32	0.44
1:D:567:VAL:HG12	1:D:568:TRP:N	2.32	0.44
1:D:653[B]:HIS:CD2	1:D:667:GLU:HG2	2.51	0.44
1:D:655:MET:HE1	1:D:662:PRO:HB3	2.00	0.44
1:E:567:VAL:HG12	1:E:568:TRP:N	2.32	0.44
1:E:655:MET:HE1	1:E:662:PRO:HB3	2.00	0.44
1:E:778:THR:HG23	1:E:779:PRO:HD2	1.98	0.44
1:F:433:LEU:N	1:F:434:PRO:CD	2.80	0.44
1:F:658:LEU:N	1:F:661:LYS:O	2.40	0.44
1:G:7:LEU:O	1:G:11:LEU:HG	2.18	0.44
1:G:13:ARG:O	1:G:14:ARG:HB2	2.17	0.44
1:H:3:ILE:O	1:H:3:ILE:HD12	2.17	0.44
1:H:778:THR:HG23	1:H:779:PRO:HD2	1.98	0.44
1:I:638:VAL:O	1:I:677:LYS:HA	2.18	0.44
1:I:867:THR:HG22	3:I:4297:HOH:O	2.17	0.44
1:J:420:MET:O	1:K:282:ARG:HD3	2.18	0.44
1:K:367:MET:HB3	1:K:372:MET:HE3	1.98	0.44
1:M:221:GLN:H	1:M:221:GLN:HG2	1.63	0.44
1:M:567:VAL:HG12	1:M:568:TRP:N	2.32	0.44
1:M:655:MET:HE1	1:M:662:PRO:HB3	2.00	0.44
1:N:322:LEU:HD21	1:N:324:GLU:C	2.43	0.44
1:N:454:ILE:C	1:N:455:ILE:HG13	2.43	0.44
1:N:702:GLN:O	1:N:712:GLY:N	2.47	0.44
1:O:129:VAL:CG2	1:O:182:ASN:ND2	2.80	0.44
1:P:91:GLN:HG3	1:P:96:ASP:OD1	2.16	0.44
1:P:322:LEU:HD21	1:P:324:GLU:C	2.43	0.44
1:A:43:ARG:NH1	1:A:44:THR:CG2	2.80	0.44
1:A:867:THR:HG22	3:A:4299:HOH:O	2.17	0.44
1:B:7:LEU:O	1:B:11:LEU:HG	2.18	0.44
1:D:13:ARG:O	1:D:14:ARG:HB2	2.17	0.44
1:D:638:VAL:O	1:D:677:LYS:HA	2.18	0.44
1:E:367:MET:HB3	1:E:372:MET:HE3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:847:LYS:HG3	1:E:848:THR:N	2.32	0.44
1:F:111:PRO:HA	1:F:112:PRO:HA	1.66	0.44
1:G:183:ARG:HD3	1:G:183:ARG:HH11	1.62	0.44
1:G:599:ARG:HB2	1:G:600:GLN:H	1.64	0.44
1:G:638:VAL:O	1:G:677:LYS:HA	2.18	0.44
1:H:43:ARG:HH12	1:H:44:THR:CG2	2.30	0.44
1:H:772:ASP:OD1	1:H:772:ASP:N	2.48	0.44
1:H:847:LYS:HG3	1:H:848:THR:N	2.32	0.44
1:I:43:ARG:NH1	1:I:44:THR:CG2	2.80	0.44
1:J:638:VAL:O	1:J:677:LYS:HA	2.18	0.44
1:J:657:ALA:HA	1:J:661:LYS:O	2.16	0.44
1:K:285:TYR:CB	1:K:288:ARG:HG3	2.42	0.44
1:K:567:VAL:HG12	1:K:568:TRP:N	2.32	0.44
1:K:658:LEU:N	1:K:661:LYS:O	2.40	0.44
1:L:13:ARG:O	1:L:14:ARG:HB2	2.17	0.44
1:L:279:ILE:HD12	1:L:279:ILE:HG21	1.77	0.44
1:M:658:LEU:N	1:M:661:LYS:O	2.40	0.44
1:N:367:MET:HB3	1:N:372:MET:HE3	1.98	0.44
1:O:43:ARG:NH1	1:O:44:THR:CG2	2.80	0.44
1:O:847:LYS:HG3	1:O:848:THR:N	2.32	0.44
1:P:7:LEU:O	1:P:11:LEU:HG	2.18	0.44
1:P:80:GLU:H	1:P:80:GLU:HG3	1.29	0.44
1:A:129:VAL:CG2	1:A:182:ASN:ND2	2.80	0.44
1:B:479:ASP:HA	1:B:480:PRO:HD2	1.77	0.44
1:C:211:ASP:OD1	1:C:211:ASP:N	2.50	0.44
1:D:43:ARG:HH12	1:D:44:THR:CG2	2.30	0.44
1:D:322:LEU:HD21	1:D:324:GLU:C	2.43	0.44
1:D:702:GLN:O	1:D:712:GLY:N	2.47	0.44
1:F:322:LEU:CD2	1:F:324:GLU:N	2.80	0.44
1:F:367:MET:HB3	1:F:367:MET:HE3	1.77	0.44
1:F:454:ILE:C	1:F:455:ILE:HG13	2.43	0.44
1:F:546:LEU:HA	3:F:3230:HOH:O	2.16	0.44
1:F:685:LEU:HA	1:F:686:PRO:HD3	1.83	0.44
1:H:7:LEU:O	1:H:11:LEU:HG	2.18	0.44
1:H:322:LEU:HD21	1:H:324:GLU:C	2.43	0.44
1:I:7:LEU:O	1:I:11:LEU:HG	2.18	0.44
1:I:42:ALA:O	1:I:310:ARG:NH1	2.49	0.44
1:I:322:LEU:HD21	1:I:324:GLU:C	2.43	0.44
1:I:655:MET:HE1	1:I:662:PRO:HB3	2.00	0.44
1:J:111:PRO:HA	1:J:112:PRO:HA	1.65	0.44
1:K:7:LEU:O	1:K:11:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:322:LEU:CD2	1:K:324:GLU:N	2.80	0.44
1:K:702:GLN:O	1:K:712:GLY:N	2.47	0.44
1:K:867:THR:HG22	3:K:4299:HOH:O	2.17	0.44
1:L:701:VAL:HG12	1:L:702:GLN:N	2.31	0.44
1:M:638:VAL:O	1:M:677:LYS:HA	2.18	0.44
1:N:687:GLN:HA	1:N:688:PRO:HD3	1.73	0.44
1:O:567:VAL:HG12	1:O:568:TRP:N	2.32	0.44
1:P:322:LEU:CD2	1:P:324:GLU:N	2.80	0.44
1:P:433:LEU:N	1:P:434:PRO:CD	2.80	0.44
1:P:599:ARG:HB2	1:P:600:GLN:H	1.64	0.44
1:A:7:LEU:O	1:A:11:LEU:HG	2.18	0.44
1:A:13:ARG:O	1:A:14:ARG:HB2	2.17	0.44
1:A:856:TYR:CD2	1:A:864:MET:CE	3.00	0.44
1:B:202:MET:HE3	1:B:357:HIS:ND1	2.33	0.44
1:B:612:THR:HA	1:B:613:PRO:HD3	1.59	0.44
1:B:679:LEU:HD23	1:B:679:LEU:HA	1.40	0.44
1:C:111:PRO:HA	1:C:112:PRO:HA	1.66	0.44
1:C:454:ILE:C	1:C:455:ILE:HG13	2.43	0.44
1:D:322:LEU:CD2	1:D:324:GLU:N	2.80	0.44
1:D:378:LEU:HD23	1:D:378:LEU:HA	1.74	0.44
1:D:612:THR:HA	1:D:613:PRO:HD3	1.59	0.44
1:E:3:ILE:HG13	1:E:4:THR:N	2.25	0.44
1:E:147:ASN:HA	1:E:148:SER:HA	1.57	0.44
1:F:13:ARG:O	1:F:14:ARG:HB2	2.16	0.44
1:F:85:VAL:CG1	1:F:86:VAL:N	2.79	0.44
1:F:246:MET:HG2	1:F:274:PHE:CE2	2.52	0.44
1:F:856:TYR:CD2	1:F:864:MET:CE	3.00	0.44
1:G:202:MET:HE3	1:G:357:HIS:ND1	2.33	0.44
1:G:454:ILE:C	1:G:455:ILE:HG13	2.43	0.44
1:G:836:ILE:HG23	1:G:836:ILE:HD12	1.73	0.44
1:I:836:ILE:HG23	1:I:836:ILE:HD12	1.73	0.44
1:J:454:ILE:C	1:J:455:ILE:HG13	2.43	0.44
1:K:322:LEU:HD21	1:K:324:GLU:C	2.43	0.44
1:K:473:ARG:HD3	1:K:473:ARG:C	2.43	0.44
1:K:655:MET:HE1	1:K:662:PRO:HB3	2.00	0.44
1:L:322:LEU:HD21	1:L:324:GLU:C	2.43	0.44
1:N:254:LEU:HD23	1:N:254:LEU:HA	1.71	0.44
1:O:183:ARG:HD3	1:O:183:ARG:HH11	1.62	0.44
1:O:702:GLN:O	1:O:712:GLY:N	2.47	0.44
1:O:772:ASP:OD1	1:O:772:ASP:N	2.48	0.44
1:P:362:LEU:HA	1:P:362:LEU:HD23	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:454:ILE:C	1:P:455:ILE:HG13	2.43	0.44
1:P:857:ARG:HG2	1:P:857:ARG:HH11	1.83	0.44
1:B:278:ILE:N	1:B:278:ILE:CD1	2.80	0.44
1:C:638:VAL:O	1:C:677:LYS:HA	2.18	0.44
1:D:7:LEU:HD12	1:D:74:LEU:HD11	1.97	0.44
1:D:655:MET:HB2	1:D:655:MET:HE3	1.35	0.44
1:D:679:LEU:HD23	1:D:679:LEU:HA	1.40	0.44
1:D:867:THR:HG22	3:D:3411:HOH:O	2.17	0.44
1:D:914:CME:HE2	1:D:914:CME:HB3	1.74	0.44
1:E:322:LEU:HD21	1:E:324:GLU:C	2.43	0.44
1:F:285:TYR:CB	1:F:288:ARG:HG3	2.42	0.44
1:F:473:ARG:HD2	1:G:469:ASP:HB3	1.99	0.44
1:F:682:LEU:HD23	1:F:682:LEU:HA	1.85	0.44
1:G:655:MET:HE1	1:G:662:PRO:HB3	2.00	0.44
1:I:3:ILE:HD12	1:I:3:ILE:O	2.17	0.44
1:I:80:GLU:H	1:I:80:GLU:HG3	1.29	0.44
1:J:7:LEU:HD12	1:J:74:LEU:HD11	1.97	0.44
1:K:13:ARG:O	1:K:14:ARG:HB2	2.17	0.44
1:K:237:ARG:HE	1:K:237:ARG:HB2	1.35	0.44
1:K:599:ARG:HB2	1:K:600:GLN:H	1.64	0.44
1:K:847:LYS:HG3	1:K:848:THR:N	2.32	0.44
1:L:78:LEU:HB3	1:L:79:PRO:CD	2.43	0.44
1:L:202:MET:HE3	1:L:357:HIS:ND1	2.33	0.44
1:M:7:LEU:O	1:M:11:LEU:HG	2.18	0.44
1:N:479:ASP:HA	1:N:480:PRO:HD2	1.77	0.44
1:N:856:TYR:CD2	1:N:864:MET:CE	3.00	0.44
1:O:638:VAL:O	1:O:677:LYS:HA	2.18	0.44
1:O:655:MET:HE1	1:O:662:PRO:HB3	2.00	0.44
1:P:473:ARG:HD3	1:P:473:ARG:C	2.43	0.44
1:A:322:LEU:CD2	1:A:324:GLU:N	2.80	0.44
1:A:419:GLY:HA2	1:D:282:ARG:NH1	2.32	0.44
1:A:638:VAL:O	1:A:677:LYS:HA	2.18	0.44
1:B:322:LEU:HD21	1:B:324:GLU:C	2.43	0.44
1:B:867:THR:HG22	3:B:3402:HOH:O	2.17	0.44
1:C:7:LEU:O	1:C:11:LEU:HG	2.18	0.44
1:C:567:VAL:HG12	1:C:568:TRP:N	2.32	0.44
1:C:599:ARG:HB2	1:C:600:GLN:OE1	2.18	0.44
1:D:85:VAL:CG1	1:D:86:VAL:N	2.79	0.44
1:E:599:ARG:HB2	1:E:600:GLN:OE1	2.18	0.44
1:G:567:VAL:HG12	1:G:568:TRP:N	2.32	0.44
1:H:599:ARG:HB2	1:H:600:GLN:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:857:ARG:HG2	1:H:857:ARG:HH11	1.83	0.44
1:I:567:VAL:HG12	1:I:568:TRP:N	2.32	0.44
1:I:612:THR:HA	1:I:613:PRO:HD3	1.59	0.44
1:J:3:ILE:HD12	1:J:3:ILE:O	2.17	0.44
1:J:655:MET:HB2	1:J:655:MET:HE3	1.35	0.44
1:J:682:LEU:HD23	1:J:682:LEU:HA	1.85	0.44
1:K:638:VAL:O	1:K:677:LYS:HA	2.18	0.44
1:L:211:ASP:OD1	1:L:211:ASP:N	2.50	0.44
1:L:367:MET:HB3	1:L:372:MET:HE3	1.98	0.44
1:N:13:ARG:O	1:N:14:ARG:HB2	2.16	0.44
1:N:129:VAL:CG2	1:N:182:ASN:ND2	2.80	0.44
1:N:246:MET:HG2	1:N:274:PHE:CE2	2.52	0.44
1:O:454:ILE:C	1:O:455:ILE:HG13	2.43	0.44
1:A:473:ARG:HD3	1:A:473:ARG:C	2.43	0.43
1:A:778:THR:HG23	1:A:779:PRO:HD2	1.98	0.43
1:C:473:ARG:HD3	1:C:473:ARG:C	2.43	0.43
1:D:173:LEU:HD23	1:D:173:LEU:HA	1.85	0.43
1:D:202:MET:HE3	1:D:357:HIS:ND1	2.33	0.43
1:D:246:MET:HG2	1:D:274:PHE:CE2	2.52	0.43
1:D:599:ARG:HB2	1:D:600:GLN:OE1	2.18	0.43
1:F:322:LEU:HD21	1:F:324:GLU:C	2.43	0.43
1:I:111:PRO:HA	1:I:112:PRO:HA	1.65	0.43
1:I:202:MET:HE3	1:I:357:HIS:ND1	2.33	0.43
1:I:322:LEU:CD2	1:I:324:GLU:N	2.80	0.43
1:I:454:ILE:C	1:I:455:ILE:HG13	2.43	0.43
1:J:7:LEU:O	1:J:11:LEU:HG	2.18	0.43
1:J:322:LEU:HD21	1:J:324:GLU:C	2.43	0.43
1:J:378:LEU:HD23	1:J:378:LEU:HA	1.74	0.43
1:J:599:ARG:HB2	1:J:600:GLN:OE1	2.18	0.43
1:L:57:GLU:HG2	1:L:83:THR:HG22	1.95	0.43
1:L:567:VAL:HG12	1:L:568:TRP:N	2.32	0.43
1:M:772:ASP:OD1	1:M:772:ASP:N	2.48	0.43
1:N:202:MET:HE3	1:N:357:HIS:ND1	2.33	0.43
1:N:285:TYR:CB	1:N:288:ARG:HG3	2.42	0.43
1:N:658:LEU:N	1:N:661:LYS:O	2.40	0.43
1:N:836:ILE:HD12	1:N:836:ILE:HG23	1.73	0.43
1:O:202:MET:HE3	1:O:357:HIS:ND1	2.33	0.43
1:P:612:THR:HA	1:P:613:PRO:HD3	1.59	0.43
1:A:599:ARG:HB2	1:A:600:GLN:H	1.63	0.43
1:A:655:MET:HE1	1:A:662:PRO:HB3	2.00	0.43
1:B:454:ILE:C	1:B:455:ILE:HG13	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:LEU:HA	1:C:686:PRO:HD3	1.83	0.43
1:C:702:GLN:O	1:C:712:GLY:N	2.47	0.43
1:E:378:LEU:HA	1:E:378:LEU:HD23	1.74	0.43
1:E:482:ARG:HH11	1:E:482:ARG:HD2	1.63	0.43
1:G:986:ILE:HD13	1:G:986:ILE:HG23	1.67	0.43
1:H:322:LEU:CD2	1:H:324:GLU:N	2.80	0.43
1:I:857:ARG:HG2	1:I:857:ARG:HH11	1.83	0.43
1:J:278:ILE:N	1:J:278:ILE:CD1	2.80	0.43
1:J:867:THR:HG22	3:J:3405:HOH:O	2.18	0.43
1:K:378:LEU:HA	1:K:378:LEU:HD23	1.74	0.43
1:K:679:LEU:HD23	1:K:679:LEU:HA	1.40	0.43
1:L:127:PHE:CD2	1:L:127:PHE:N	2.87	0.43
1:L:246:MET:HG2	1:L:274:PHE:CE2	2.52	0.43
1:M:3:ILE:HG13	1:M:4:THR:N	2.25	0.43
1:N:857:ARG:HG2	1:N:857:ARG:HH11	1.83	0.43
1:O:856:TYR:CD2	1:O:864:MET:CE	3.00	0.43
1:P:567:VAL:HG12	1:P:568:TRP:N	2.32	0.43
1:P:599:ARG:HB2	1:P:600:GLN:OE1	2.18	0.43
1:P:687:GLN:HA	1:P:688:PRO:HD3	1.73	0.43
1:A:857:ARG:HG2	1:A:857:ARG:HH11	1.83	0.43
1:B:80:GLU:H	1:B:80:GLU:HG3	1.29	0.43
1:B:246:MET:HG2	1:B:274:PHE:CE2	2.52	0.43
1:C:576:ILE:CG2	1:C:577:LYS:N	2.79	0.43
1:D:221:GLN:H	1:D:221:GLN:HG2	1.63	0.43
1:D:576:ILE:CG2	1:D:577:LYS:N	2.79	0.43
1:E:638:VAL:O	1:E:677:LYS:HA	2.18	0.43
1:E:857:ARG:HG2	1:E:857:ARG:HH11	1.83	0.43
1:F:7:LEU:O	1:F:11:LEU:HG	2.18	0.43
1:F:202:MET:HE3	1:F:357:HIS:ND1	2.33	0.43
1:G:127:PHE:CD2	1:G:127:PHE:N	2.87	0.43
1:G:322:LEU:HD21	1:G:324:GLU:C	2.43	0.43
1:H:947:GLY:HA3	1:H:948:PRO:HD2	1.82	0.43
1:I:473:ARG:HD3	1:I:473:ARG:C	2.43	0.43
1:J:127:PHE:CD2	1:J:127:PHE:N	2.87	0.43
1:J:202:MET:HE3	1:J:357:HIS:ND1	2.33	0.43
1:J:847:LYS:HG3	1:J:848:THR:N	2.32	0.43
1:L:612:THR:HA	1:L:613:PRO:HD3	1.59	0.43
1:L:655:MET:HE1	1:L:662:PRO:HB3	2.00	0.43
1:L:847:LYS:HG3	1:L:848:THR:N	2.32	0.43
1:L:857:ARG:HG2	1:L:857:ARG:HH11	1.83	0.43
1:L:920:LEU:HB3	1:L:921:PRO:CD	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:857:ARG:HG2	1:M:857:ARG:HH11	1.83	0.43
1:N:638:VAL:O	1:N:677:LYS:HA	2.18	0.43
1:O:127:PHE:CD2	1:O:127:PHE:N	2.86	0.43
1:P:202:MET:HE3	1:P:357:HIS:ND1	2.33	0.43
1:A:127:PHE:CD2	1:A:127:PHE:N	2.87	0.43
1:A:599:ARG:HB2	1:A:600:GLN:OE1	2.18	0.43
1:B:183:ARG:HD3	1:B:183:ARG:HH11	1.62	0.43
1:B:599:ARG:HB2	1:B:600:GLN:OE1	2.18	0.43
1:B:730:LEU:HA	1:B:731:PRO:HD3	1.80	0.43
1:C:322:LEU:HD21	1:C:324:GLU:C	2.43	0.43
1:C:599:ARG:HB2	1:C:600:GLN:H	1.63	0.43
1:D:7:LEU:O	1:D:11:LEU:HG	2.18	0.43
1:F:279:ILE:HD11	1:G:422:PRO:HG2	2.01	0.43
1:F:867:THR:HG22	3:F:3404:HOH:O	2.17	0.43
1:G:670:LEU:HD23	1:G:670:LEU:HA	1.75	0.43
1:H:599:ARG:HB2	1:H:600:GLN:H	1.64	0.43
1:I:129:VAL:CG2	1:I:182:ASN:ND2	2.80	0.43
1:I:246:MET:HG2	1:I:274:PHE:CE2	2.52	0.43
1:I:947:GLY:HA3	1:I:948:PRO:HD2	1.82	0.43
1:J:914:CME:HE2	1:J:914:CME:HB3	1.74	0.43
1:J:952:ARG:HH11	1:J:952:ARG:CG	2.28	0.43
1:K:85:VAL:CG1	1:K:86:VAL:N	2.79	0.43
1:L:183:ARG:HD3	1:L:183:ARG:HH11	1.62	0.43
1:L:638:VAL:O	1:L:677:LYS:HA	2.18	0.43
1:M:279:ILE:HD12	1:M:279:ILE:HG21	1.77	0.43
1:N:772:ASP:OD1	1:N:772:ASP:N	2.48	0.43
1:O:7:LEU:O	1:O:11:LEU:HG	2.18	0.43
1:O:857:ARG:HG2	1:O:857:ARG:HH11	1.83	0.43
1:P:189:LEU:N	1:P:189:LEU:CD2	2.79	0.43
1:A:202:MET:HE3	1:A:357:HIS:ND1	2.33	0.43
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.71	0.43
1:A:282:ARG:HH11	1:D:419:GLY:C	2.27	0.43
1:C:655:MET:HE1	1:C:662:PRO:HB3	2.00	0.43
1:E:202:MET:HE3	1:E:357:HIS:ND1	2.33	0.43
1:F:473:ARG:HD3	1:F:473:ARG:C	2.43	0.43
1:F:694:LEU:HD12	1:F:694:LEU:HA	1.84	0.43
1:F:836:ILE:HD12	1:F:836:ILE:HG23	1.73	0.43
1:G:7:LEU:HD12	1:G:74:LEU:HD11	1.97	0.43
1:G:599:ARG:HB2	1:G:600:GLN:OE1	2.18	0.43
1:G:914:CME:HB3	1:G:914:CME:HE2	1.74	0.43
1:H:202:MET:HE3	1:H:357:HIS:ND1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:702:GLN:O	1:H:712:GLY:N	2.47	0.43
1:I:127:PHE:CD2	1:I:127:PHE:N	2.87	0.43
1:I:285:TYR:CB	1:I:288:ARG:HG3	2.42	0.43
1:I:685:LEU:HA	1:I:686:PRO:HD3	1.83	0.43
1:J:473:ARG:HD3	1:J:473:ARG:C	2.43	0.43
1:K:278:ILE:N	1:K:278:ILE:CD1	2.80	0.43
1:K:920:LEU:HB3	1:K:921:PRO:CD	2.46	0.43
1:M:856:TYR:CD2	1:M:864:MET:CE	3.00	0.43
1:N:279:ILE:CD1	1:O:422:PRO:CG	2.95	0.43
1:N:702:GLN:HA	1:N:703:PRO:HD2	1.88	0.43
1:N:986:ILE:HG21	1:N:986:ILE:HD12	1.75	0.43
1:O:599:ARG:HB2	1:O:600:GLN:OE1	2.18	0.43
1:P:867:THR:HG22	3:P:3410:HOH:O	2.17	0.43
1:A:322:LEU:HD21	1:A:324:GLU:C	2.43	0.43
1:D:778:THR:HB	1:D:887:GLN:H	1.84	0.43
1:E:13:ARG:O	1:E:14:ARG:HB2	2.17	0.43
1:E:702:GLN:O	1:E:712:GLY:N	2.47	0.43
1:F:80:GLU:H	1:F:80:GLU:HG3	1.28	0.43
1:F:183:ARG:HD3	1:F:183:ARG:HH11	1.62	0.43
1:F:670:LEU:HA	1:F:670:LEU:HD23	1.75	0.43
1:F:857:ARG:HG2	1:F:857:ARG:HH11	1.83	0.43
1:G:278:ILE:N	1:G:278:ILE:CD1	2.80	0.43
1:H:454:ILE:C	1:H:455:ILE:HG13	2.43	0.43
1:K:287:ASP:OD1	1:K:287:ASP:N	2.41	0.43
1:K:576:ILE:CG2	1:K:577:LYS:N	2.79	0.43
1:K:599:ARG:HB2	1:K:600:GLN:OE1	2.18	0.43
1:L:7:LEU:O	1:L:11:LEU:HG	2.18	0.43
1:L:658:LEU:N	1:L:661:LYS:O	2.40	0.43
1:M:129:VAL:CG2	1:M:182:ASN:ND2	2.80	0.43
1:M:183:ARG:HD3	1:M:183:ARG:HH11	1.62	0.43
1:M:429:ASP:HA	1:M:430:PRO:HD3	1.73	0.43
1:M:599:ARG:HB2	1:M:600:GLN:H	1.63	0.43
1:M:724:GLU:O	1:N:847:LYS:NZ	2.27	0.43
1:N:7:LEU:O	1:N:11:LEU:HG	2.18	0.43
1:N:473:ARG:HD3	1:N:473:ARG:C	2.43	0.43
1:N:1017:GLN:HB3	3:N:3513:HOH:O	2.19	0.43
1:O:685:LEU:HA	1:O:686:PRO:HD3	1.83	0.43
1:O:1017:GLN:HB3	3:O:3509:HOH:O	2.19	0.43
1:P:856:TYR:CD2	1:P:864:MET:CE	3.00	0.43
1:A:454:ILE:C	1:A:455:ILE:HG13	2.43	0.43
1:A:482:ARG:HH11	1:A:482:ARG:HD2	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HD12	1:B:74:LEU:HD11	1.97	0.43
1:B:1017:GLN:HB3	3:B:3513:HOH:O	2.19	0.43
1:D:454:ILE:C	1:D:455:ILE:HG13	2.43	0.43
1:D:473:ARG:HD3	1:D:473:ARG:C	2.43	0.43
1:E:57:GLU:HG2	1:E:83:THR:HG22	1.95	0.43
1:E:316:HIS:HA	1:E:323:ILE:HD13	2.01	0.43
1:E:454:ILE:C	1:E:455:ILE:HG13	2.43	0.43
1:E:702:GLN:HA	1:E:703:PRO:HD2	1.88	0.43
1:F:127:PHE:N	1:F:127:PHE:CD2	2.87	0.43
1:F:221:GLN:H	1:F:221:GLN:HG2	1.63	0.43
1:G:778:THR:HB	1:G:887:GLN:H	1.84	0.43
1:G:1017:GLN:HB3	3:G:3512:HOH:O	2.19	0.43
1:H:129:VAL:CG2	1:H:182:ASN:ND2	2.80	0.43
1:I:679:LEU:HD23	1:I:679:LEU:HA	1.40	0.43
1:I:702:GLN:O	1:I:712:GLY:N	2.47	0.43
1:J:85:VAL:CG1	1:J:86:VAL:N	2.79	0.43
1:K:454:ILE:C	1:K:455:ILE:HG13	2.43	0.43
1:K:1017:GLN:HB3	3:K:4414:HOH:O	2.19	0.43
1:L:3:ILE:HG13	1:L:4:THR:N	2.24	0.43
1:M:127:PHE:N	1:M:127:PHE:CD2	2.87	0.43
1:M:202:MET:HE3	1:M:357:HIS:ND1	2.33	0.43
1:M:454:ILE:C	1:M:455:ILE:HG13	2.43	0.43
1:N:599:ARG:HB2	1:N:600:GLN:OE1	2.18	0.43
1:O:778:THR:HB	1:O:887:GLN:H	1.84	0.43
1:O:867:THR:HG22	3:O:3402:HOH:O	2.17	0.43
1:P:237:ARG:HE	1:P:237:ARG:HB2	1.35	0.43
1:A:78:LEU:HB3	1:A:79:PRO:CD	2.43	0.43
1:B:279:ILE:HD11	1:C:422:PRO:HB2	2.01	0.43
1:B:986:ILE:HD13	1:B:986:ILE:HG23	1.67	0.43
1:C:202:MET:HE3	1:C:357:HIS:ND1	2.33	0.43
1:D:836:ILE:HD12	1:D:836:ILE:HG23	1.73	0.43
1:E:7:LEU:O	1:E:11:LEU:HG	2.18	0.43
1:E:127:PHE:N	1:E:127:PHE:CD2	2.87	0.43
1:E:772:ASP:OD1	1:E:772:ASP:N	2.48	0.43
1:G:612:THR:HA	1:G:613:PRO:HD3	1.59	0.43
1:H:867:THR:HG22	3:H:4299:HOH:O	2.17	0.43
1:I:856:TYR:CD2	1:I:864:MET:CE	3.00	0.43
1:L:147:ASN:HA	1:L:148:SER:HA	1.57	0.43
1:L:254:LEU:HD23	1:L:254:LEU:HA	1.71	0.43
1:L:278:ILE:N	1:L:278:ILE:CD1	2.80	0.43
1:L:679:LEU:HD23	1:L:679:LEU:HA	1.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:367:MET:HB3	1:M:367:MET:HE3	1.77	0.43
1:M:952:ARG:HH11	1:M:952:ARG:CG	2.28	0.43
1:N:279:ILE:HD11	1:O:422:PRO:HB2	1.99	0.43
1:O:13:ARG:O	1:O:14:ARG:HB2	2.17	0.43
1:A:221:GLN:H	1:A:221:GLN:HG2	1.63	0.43
1:B:655:MET:HE1	1:B:662:PRO:HB3	2.00	0.43
1:B:670:LEU:HD23	1:B:670:LEU:HA	1.75	0.43
1:C:1000:SER:HA	1:C:1001:PRO:HD3	1.88	0.43
1:G:682:LEU:HD23	1:G:682:LEU:HA	1.85	0.43
1:G:685:LEU:HA	1:G:686:PRO:HD3	1.83	0.43
1:G:857:ARG:HG2	1:G:857:ARG:HH11	1.83	0.43
1:H:473:ARG:HD3	1:H:473:ARG:C	2.43	0.43
1:H:655:MET:HE1	1:H:662:PRO:HB3	2.00	0.43
1:I:237:ARG:HE	1:I:237:ARG:HB2	1.35	0.43
1:J:118:ASN:HA	1:J:119:PRO:HD2	1.62	0.43
1:J:237:ARG:HE	1:J:237:ARG:HB2	1.35	0.43
1:K:778:THR:HB	1:K:887:GLN:H	1.84	0.43
1:K:857:ARG:HH11	1:K:857:ARG:HG2	1.83	0.43
1:L:454:ILE:C	1:L:455:ILE:HG13	2.43	0.43
1:N:134:LEU:HA	1:N:134:LEU:HD23	1.68	0.43
1:N:655:MET:HE1	1:N:662:PRO:HB3	2.00	0.43
1:N:778:THR:HB	1:N:887:GLN:H	1.84	0.43
1:P:655:MET:HE1	1:P:662:PRO:HB3	2.00	0.43
1:P:778:THR:HB	1:P:887:GLN:H	1.83	0.43
1:P:878:HIS:HA	1:P:879:PRO:HD3	1.83	0.43
1:A:567:VAL:HG12	1:A:568:TRP:N	2.32	0.43
1:A:778:THR:HB	1:A:887:GLN:H	1.84	0.43
1:B:473:ARG:HD3	1:B:473:ARG:C	2.43	0.43
1:B:778:THR:HB	1:B:887:GLN:H	1.84	0.43
1:C:127:PHE:N	1:C:127:PHE:CD2	2.86	0.43
1:D:1017:GLN:HB3	3:D:3519:HOH:O	2.19	0.43
1:F:599:ARG:HB2	1:F:600:GLN:OE1	2.19	0.43
1:F:655:MET:HE1	1:F:662:PRO:HB3	2.00	0.43
1:F:1017:GLN:HB3	3:F:3513:HOH:O	2.19	0.43
1:G:702:GLN:HA	1:G:703:PRO:HD2	1.88	0.43
1:H:778:THR:HB	1:H:887:GLN:H	1.84	0.43
1:J:217:LYS:NZ	1:J:326:GLU:OE2	2.52	0.43
1:J:655:MET:HE1	1:J:662:PRO:HB3	2.00	0.43
1:K:118:ASN:HA	1:K:119:PRO:HD2	1.62	0.43
1:L:836:ILE:HG23	1:L:836:ILE:HD12	1.73	0.43
1:L:867:THR:HG22	3:L:3408:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:599:ARG:HB2	1:M:600:GLN:OE1	2.18	0.43
1:N:127:PHE:N	1:N:127:PHE:CD2	2.87	0.43
1:N:694:LEU:HD12	1:N:694:LEU:HA	1.84	0.43
1:O:322:LEU:HD21	1:O:324:GLU:C	2.43	0.43
1:O:612:THR:HA	1:O:613:PRO:HD3	1.59	0.43
1:O:682:LEU:HD23	1:O:682:LEU:HA	1.85	0.43
1:B:857:ARG:HG2	1:B:857:ARG:HH11	1.83	0.42
1:C:134:LEU:HD23	1:C:134:LEU:HA	1.68	0.42
1:C:856:TYR:CD2	1:C:864:MET:CE	3.00	0.42
1:C:857:ARG:HH11	1:C:857:ARG:HG2	1.83	0.42
1:F:271:THR:HG22	1:F:272:ALA:N	2.34	0.42
1:H:189:LEU:N	1:H:189:LEU:CD2	2.79	0.42
1:I:395:HIS:HA	1:I:396:PRO:HD3	1.69	0.42
1:I:599:ARG:HB2	1:I:600:GLN:H	1.63	0.42
1:I:745:MET:HA	1:I:745:MET:CE	2.39	0.42
1:K:4:THR:HA	1:K:9:VAL:HG11	2.01	0.42
1:K:271:THR:HG22	1:K:272:ALA:N	2.35	0.42
1:M:217:LYS:NZ	1:M:326:GLU:OE2	2.52	0.42
1:O:702:GLN:HA	1:O:703:PRO:HD2	1.88	0.42
1:P:378:LEU:HD23	1:P:378:LEU:HA	1.74	0.42
1:A:217:LYS:NZ	1:A:326:GLU:OE2	2.52	0.42
1:A:380:LYS:HE2	3:A:4075:HOH:O	2.19	0.42
1:B:287:ASP:OD1	1:B:287:ASP:N	2.41	0.42
1:C:778:THR:HB	1:C:887:GLN:H	1.84	0.42
1:D:429:ASP:HA	1:D:430:PRO:HD3	1.73	0.42
1:E:217:LYS:NZ	1:E:326:GLU:OE2	2.52	0.42
1:G:378:LEU:HA	1:G:378:LEU:HD23	1.74	0.42
1:G:479:ASP:HA	1:G:480:PRO:HD2	1.77	0.42
1:H:217:LYS:NZ	1:H:326:GLU:OE2	2.52	0.42
1:H:271:THR:HG22	1:H:272:ALA:N	2.34	0.42
1:I:647:SER:HG	1:I:672:VAL:H	1.67	0.42
1:J:778:THR:HB	1:J:887:GLN:H	1.84	0.42
1:J:1017:GLN:HB3	3:J:3514:HOH:O	2.18	0.42
1:K:217:LYS:NZ	1:K:326:GLU:OE2	2.52	0.42
1:M:271:THR:HG22	1:M:272:ALA:N	2.34	0.42
1:M:322:LEU:HD21	1:M:324:GLU:C	2.43	0.42
1:N:867:THR:HG22	3:N:3405:HOH:O	2.17	0.42
1:P:316:HIS:HA	1:P:323:ILE:HD13	2.01	0.42
1:B:856:TYR:CD2	1:B:864:MET:CE	3.00	0.42
1:D:271:THR:HG22	1:D:272:ALA:N	2.34	0.42
1:D:702:GLN:HA	1:D:703:PRO:HD2	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:772:ASP:OD1	1:D:772:ASP:N	2.48	0.42
1:F:217:LYS:NZ	1:F:326:GLU:OE2	2.52	0.42
1:H:4:THR:HA	1:H:9:VAL:HG11	2.02	0.42
1:H:127:PHE:N	1:H:127:PHE:CD2	2.87	0.42
1:H:567:VAL:HG12	1:H:568:TRP:N	2.32	0.42
1:H:679:LEU:HD23	1:H:679:LEU:HA	1.40	0.42
1:I:118:ASN:HA	1:I:119:PRO:HD2	1.62	0.42
1:J:173:LEU:HD23	1:J:173:LEU:HA	1.85	0.42
1:J:271:THR:HG22	1:J:272:ALA:N	2.35	0.42
1:L:772:ASP:OD1	1:L:772:ASP:N	2.48	0.42
1:L:778:THR:HB	1:L:887:GLN:H	1.84	0.42
1:M:655:MET:HB2	1:M:655:MET:HE3	1.35	0.42
1:M:917:ARG:HD2	3:M:4341:HOH:O	2.19	0.42
1:N:80:GLU:H	1:N:80:GLU:HG3	1.29	0.42
1:N:422:PRO:HG2	1:O:279:ILE:CD1	2.49	0.42
1:P:4:THR:HA	1:P:9:VAL:HG11	2.02	0.42
1:P:127:PHE:N	1:P:127:PHE:CD2	2.87	0.42
1:P:576:ILE:CG2	1:P:577:LYS:N	2.79	0.42
1:A:130:ASP:OD1	1:A:131:GLU:N	2.53	0.42
1:A:173:LEU:HD23	1:A:173:LEU:HA	1.86	0.42
1:B:127:PHE:CD2	1:B:127:PHE:N	2.87	0.42
1:B:469:ASP:HB3	1:C:473:ARG:HD2	2.01	0.42
1:B:599:ARG:HD2	1:B:600:GLN:OE1	2.20	0.42
1:B:685:LEU:HA	1:B:686:PRO:HD3	1.83	0.42
1:C:4:THR:HA	1:C:9:VAL:HG11	2.01	0.42
1:C:254:LEU:HD23	1:C:254:LEU:HA	1.71	0.42
1:D:857:ARG:HG2	1:D:857:ARG:HH11	1.83	0.42
1:E:4:THR:HA	1:E:9:VAL:HG11	2.02	0.42
1:E:234:ASP:O	1:E:235:PHE:HB2	2.20	0.42
1:E:380:LYS:HE2	3:E:4075:HOH:O	2.19	0.42
1:E:655:MET:HB2	1:E:655:MET:HE3	1.35	0.42
1:F:278:ILE:N	1:F:278:ILE:CD1	2.80	0.42
1:F:778:THR:HB	1:F:887:GLN:H	1.84	0.42
1:H:380:LYS:HE2	3:H:4075:HOH:O	2.19	0.42
1:I:687:GLN:HA	1:I:688:PRO:HD3	1.73	0.42
1:K:80:GLU:H	1:K:80:GLU:HG3	1.29	0.42
1:K:111:PRO:HA	1:K:112:PRO:HA	1.66	0.42
1:L:429:ASP:HA	1:L:430:PRO:HD3	1.73	0.42
1:L:473:ARG:HD3	1:L:473:ARG:C	2.43	0.42
1:L:670:LEU:HD23	1:L:670:LEU:HA	1.75	0.42
1:M:380:LYS:HE2	3:M:4075:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:173:LEU:HD23	1:P:173:LEU:HA	1.85	0.42
1:P:380:LYS:HE2	3:P:3187:HOH:O	2.19	0.42
1:P:836:ILE:HG23	1:P:836:ILE:HD12	1.73	0.42
1:P:1017:GLN:HB3	3:P:3519:HOH:O	2.19	0.42
1:A:599:ARG:HD2	1:A:600:GLN:OE1	2.20	0.42
1:B:217:LYS:NZ	1:B:326:GLU:OE2	2.52	0.42
1:B:658:LEU:N	1:B:661:LYS:O	2.40	0.42
1:B:917:ARG:HD2	3:B:3446:HOH:O	2.19	0.42
1:B:920:LEU:HB3	1:B:921:PRO:CD	2.46	0.42
1:C:867:THR:HG22	3:C:4299:HOH:O	2.17	0.42
1:C:914:CME:HE2	1:C:914:CME:HB3	1.74	0.42
1:D:3:ILE:HG13	1:D:4:THR:N	2.24	0.42
1:D:599:ARG:HD2	1:D:600:GLN:OE1	2.20	0.42
1:E:367:MET:HB3	1:E:367:MET:HE3	1.77	0.42
1:E:425:ARG:HH22	1:H:287:ASP:CG	2.28	0.42
1:F:599:ARG:HD2	1:F:600:GLN:OE1	2.20	0.42
1:F:772:ASP:OD1	1:F:772:ASP:N	2.48	0.42
1:F:917:ARG:HD2	3:F:3447:HOH:O	2.19	0.42
1:G:176:PHE:CD1	1:G:176:PHE:N	2.88	0.42
1:G:473:ARG:HD3	1:G:473:ARG:C	2.43	0.42
1:H:856:TYR:CD2	1:H:864:MET:CE	3.00	0.42
1:J:857:ARG:HG2	1:J:857:ARG:HH11	1.83	0.42
1:K:127:PHE:N	1:K:127:PHE:CD2	2.87	0.42
1:K:562:LEU:HD23	1:K:562:LEU:HA	1.90	0.42
1:K:668:VAL:HA	1:K:669:PRO:HD3	1.83	0.42
1:L:1017:GLN:HB3	3:L:3517:HOH:O	2.19	0.42
1:M:4:THR:HA	1:M:9:VAL:HG11	2.02	0.42
1:M:599:ARG:HD2	1:M:600:GLN:OE1	2.20	0.42
1:N:380:LYS:HE2	3:N:3182:HOH:O	2.19	0.42
1:O:479:ASP:HA	1:O:480:PRO:HD2	1.77	0.42
1:P:130:ASP:OD1	1:P:131:GLU:N	2.53	0.42
1:B:237:ARG:HE	1:B:237:ARG:HB2	1.35	0.42
1:C:176:PHE:CD1	1:C:176:PHE:N	2.88	0.42
1:C:271:THR:HG22	1:C:272:ALA:N	2.35	0.42
1:C:670:LEU:HA	1:C:670:LEU:HD23	1.75	0.42
1:C:1017:GLN:HB3	3:C:4412:HOH:O	2.19	0.42
1:E:836:ILE:HD12	1:E:836:ILE:HG23	1.73	0.42
1:E:917:ARG:HD2	3:E:4342:HOH:O	2.19	0.42
1:F:702:GLN:O	1:F:712:GLY:N	2.47	0.42
1:H:111:PRO:HA	1:H:112:PRO:HA	1.66	0.42
1:H:173:LEU:HD23	1:H:173:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:599:ARG:HB2	1:I:600:GLN:OE1	2.18	0.42
1:J:176:PHE:CD1	1:J:176:PHE:N	2.88	0.42
1:J:482:ARG:HH11	1:J:482:ARG:HD2	1.63	0.42
1:K:130:ASP:OD1	1:K:131:GLU:N	2.53	0.42
1:K:856:TYR:CD2	1:K:864:MET:CE	3.00	0.42
1:L:130:ASP:OD1	1:L:131:GLU:N	2.53	0.42
1:L:217:LYS:NZ	1:L:326:GLU:OE2	2.52	0.42
1:L:599:ARG:HB2	1:L:600:GLN:OE1	2.18	0.42
1:M:130:ASP:OD1	1:M:131:GLU:N	2.53	0.42
1:M:176:PHE:N	1:M:176:PHE:CD1	2.88	0.42
1:P:920:LEU:HB3	1:P:921:PRO:CD	2.46	0.42
1:A:285:TYR:CB	1:A:288:ARG:HG3	2.42	0.42
1:C:147:ASN:HA	1:C:148:SER:HA	1.57	0.42
1:C:378:LEU:HA	1:C:378:LEU:HD23	1.74	0.42
1:C:380:LYS:HE2	3:C:4075:HOH:O	2.19	0.42
1:E:176:PHE:CD1	1:E:176:PHE:N	2.88	0.42
1:E:287:ASP:CG	1:H:425:ARG:HH22	2.27	0.42
1:E:287:ASP:OD2	1:H:425:ARG:NH2	2.53	0.42
1:E:367:MET:HB3	1:E:372:MET:CE	2.50	0.42
1:E:778:THR:HB	1:E:887:GLN:H	1.84	0.42
1:F:4:THR:HA	1:F:9:VAL:HG11	2.02	0.42
1:F:234:ASP:O	1:F:235:PHE:HB2	2.20	0.42
1:F:380:LYS:HE2	3:F:3181:HOH:O	2.19	0.42
1:G:147:ASN:HA	1:G:148:SER:HA	1.57	0.42
1:H:395:HIS:HA	1:H:396:PRO:HD3	1.69	0.42
1:I:272:ALA:HA	1:I:273:PRO:HD3	1.78	0.42
1:I:655:MET:HB2	1:I:655:MET:HE3	1.35	0.42
1:J:279:ILE:HD11	1:K:422:PRO:HG2	2.02	0.42
1:K:687:GLN:HA	1:K:688:PRO:HD3	1.73	0.42
1:L:378:LEU:HA	1:L:378:LEU:HD23	1.74	0.42
1:M:755:ARG:HH11	1:M:755:ARG:HD2	1.74	0.42
1:N:4:THR:HA	1:N:9:VAL:HG11	2.02	0.42
1:N:176:PHE:N	1:N:176:PHE:CD1	2.88	0.42
1:N:217:LYS:NZ	1:N:326:GLU:OE2	2.52	0.42
1:O:473:ARG:HD3	1:O:473:ARG:C	2.43	0.42
1:O:679:LEU:HD23	1:O:679:LEU:HA	1.40	0.42
1:A:176:PHE:N	1:A:176:PHE:CD1	2.88	0.42
1:A:755:ARG:HH11	1:A:755:ARG:HD2	1.74	0.42
1:B:176:PHE:CD1	1:B:176:PHE:N	2.88	0.42
1:B:726:LEU:HD23	1:B:726:LEU:HA	1.76	0.42
1:C:367:MET:HB3	1:C:372:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:772:ASP:OD1	1:C:772:ASP:N	2.48	0.42
1:D:127:PHE:CD2	1:D:127:PHE:N	2.87	0.42
1:D:367:MET:HB3	1:D:372:MET:CE	2.50	0.42
1:E:670:LEU:HA	1:E:670:LEU:HD23	1.75	0.42
1:E:1017:GLN:HB3	3:E:4407:HOH:O	2.19	0.42
1:G:130:ASP:OD1	1:G:131:GLU:N	2.53	0.42
1:G:878:HIS:HA	1:G:879:PRO:HD3	1.83	0.42
1:G:917:ARG:HD2	3:G:3446:HOH:O	2.19	0.42
1:I:668:VAL:HA	1:I:669:PRO:HD3	1.83	0.42
1:I:670:LEU:HA	1:I:670:LEU:HD23	1.75	0.42
1:I:778:THR:HB	1:I:887:GLN:H	1.84	0.42
1:I:917:ARG:HD2	3:I:4340:HOH:O	2.19	0.42
1:K:202:MET:HE3	1:K:357:HIS:ND1	2.33	0.42
1:L:856:TYR:CD2	1:L:864:MET:CE	3.00	0.42
1:M:7:LEU:HD12	1:M:74:LEU:HD11	1.97	0.42
1:M:778:THR:HG22	1:M:779:PRO:O	2.20	0.42
1:N:599:ARG:HD2	1:N:600:GLN:OE1	2.20	0.42
1:N:986:ILE:HG23	1:N:986:ILE:HD13	1.67	0.42
1:O:878:HIS:HA	1:O:879:PRO:HD3	1.83	0.42
1:O:917:ARG:HD2	3:O:3445:HOH:O	2.19	0.42
1:P:7:LEU:HD12	1:P:74:LEU:HD11	1.97	0.42
1:B:4:THR:HA	1:B:9:VAL:HG11	2.02	0.42
1:C:130:ASP:OD1	1:C:131:GLU:N	2.53	0.42
1:C:778:THR:HG22	1:C:779:PRO:O	2.20	0.42
1:D:4:THR:HA	1:D:9:VAL:HG11	2.01	0.42
1:D:217:LYS:NZ	1:D:326:GLU:OE2	2.52	0.42
1:E:599:ARG:HD2	1:E:600:GLN:OE1	2.20	0.42
1:F:367:MET:HB3	1:F:372:MET:CE	2.50	0.42
1:H:482:ARG:HH11	1:H:482:ARG:HD2	1.63	0.42
1:I:367:MET:HB3	1:I:372:MET:CE	2.50	0.42
1:J:362:LEU:HD23	1:J:362:LEU:HA	1.70	0.42
1:J:658:LEU:N	1:J:661:LYS:O	2.40	0.42
1:K:272:ALA:HA	1:K:273:PRO:HD3	1.78	0.42
1:K:513:PRO:O	1:K:514:ALA:HB3	2.20	0.42
1:K:778:THR:HG22	1:K:779:PRO:O	2.20	0.42
1:K:917:ARG:HD2	3:K:4343:HOH:O	2.19	0.42
1:L:599:ARG:HD2	1:L:600:GLN:OE1	2.20	0.42
1:M:367:MET:HB3	1:M:372:MET:CE	2.50	0.42
1:M:378:LEU:HA	1:M:378:LEU:HD23	1.74	0.42
1:M:395:HIS:HA	1:M:396:PRO:HD3	1.69	0.42
1:M:422:PRO:HB2	1:P:279:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:130:ASP:OD1	1:N:131:GLU:N	2.53	0.42
1:N:211:ASP:OD1	1:N:211:ASP:N	2.50	0.42
1:N:595:THR:CG2	1:N:596:PRO:HA	2.37	0.42
1:A:4:THR:HA	1:A:9:VAL:HG11	2.01	0.42
1:A:422:PRO:CG	1:D:279:ILE:CD1	2.97	0.42
1:B:513:PRO:O	1:B:514:ALA:HB3	2.20	0.42
1:E:173:LEU:HD23	1:E:173:LEU:HA	1.85	0.42
1:E:694:LEU:HD12	1:E:694:LEU:HA	1.84	0.42
1:F:176:PHE:CD1	1:F:176:PHE:N	2.88	0.42
1:F:576:ILE:CG2	1:F:577:LYS:N	2.79	0.42
1:F:745:MET:HA	1:F:745:MET:CE	2.39	0.42
1:G:211:ASP:OD1	1:G:211:ASP:N	2.50	0.42
1:G:599:ARG:HD2	1:G:600:GLN:OE1	2.20	0.42
1:H:130:ASP:OD1	1:H:131:GLU:N	2.53	0.42
1:H:513:PRO:O	1:H:514:ALA:HB3	2.20	0.42
1:H:917:ARG:HD2	3:H:4343:HOH:O	2.19	0.42
1:I:217:LYS:NZ	1:I:326:GLU:OE2	2.52	0.42
1:J:778:THR:HG22	1:J:779:PRO:O	2.20	0.42
1:K:221:GLN:H	1:K:221:GLN:HG2	1.62	0.42
1:K:234:ASP:O	1:K:235:PHE:HB2	2.20	0.42
1:K:316:HIS:HA	1:K:323:ILE:HD13	2.01	0.42
1:K:599:ARG:HD2	1:K:600:GLN:OE1	2.20	0.42
1:N:183:ARG:HD3	1:N:183:ARG:HH11	1.62	0.42
1:N:513:PRO:O	1:N:514:ALA:HB3	2.20	0.42
1:O:687:GLN:HA	1:O:688:PRO:HD3	1.73	0.42
1:P:279:ILE:HD12	1:P:279:ILE:HG21	1.77	0.42
1:P:702:GLN:HA	1:P:703:PRO:HD2	1.88	0.42
1:A:118:ASN:HA	1:A:119:PRO:HD2	1.62	0.41
1:A:367:MET:HB3	1:A:372:MET:CE	2.50	0.41
1:B:778:THR:HG22	1:B:779:PRO:O	2.20	0.41
1:C:217:LYS:NZ	1:C:326:GLU:OE2	2.52	0.41
1:C:599:ARG:HD2	1:C:600:GLN:OE1	2.20	0.41
1:D:917:ARG:HD2	3:D:3454:HOH:O	2.19	0.41
1:F:130:ASP:OD1	1:F:131:GLU:N	2.53	0.41
1:H:533:LEU:HD23	1:H:533:LEU:C	2.45	0.41
1:H:576:ILE:CG2	1:H:577:LYS:N	2.79	0.41
1:H:599:ARG:HD2	1:H:600:GLN:OE1	2.20	0.41
1:H:670:LEU:HA	1:H:670:LEU:HD23	1.75	0.41
1:I:422:PRO:HG2	1:L:279:ILE:CD1	2.50	0.41
1:J:599:ARG:HB2	1:J:600:GLN:H	1.64	0.41
1:K:176:PHE:N	1:K:176:PHE:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:726:LEU:HA	1:K:726:LEU:HD23	1.76	0.41
1:L:513:PRO:O	1:L:514:ALA:HB3	2.20	0.41
1:O:130:ASP:OD1	1:O:131:GLU:N	2.53	0.41
1:O:217:LYS:NZ	1:O:326:GLU:OE2	2.52	0.41
1:P:217:LYS:NZ	1:P:326:GLU:OE2	2.52	0.41
1:P:533:LEU:HD23	1:P:533:LEU:C	2.45	0.41
1:P:655:MET:HB2	1:P:655:MET:HE3	1.35	0.41
1:A:655:MET:HE3	1:A:655:MET:HB2	1.35	0.41
1:B:254:LEU:HA	1:B:254:LEU:HD23	1.71	0.41
1:B:271:THR:HG22	1:B:272:ALA:N	2.35	0.41
1:C:836:ILE:HD12	1:C:836:ILE:HG23	1.73	0.41
1:D:234:ASP:O	1:D:235:PHE:HB2	2.20	0.41
1:D:986:ILE:HD13	1:D:986:ILE:HG23	1.67	0.41
1:E:802:ASP:HA	1:E:803:PRO:HD3	1.83	0.41
1:F:74:LEU:HD23	1:F:74:LEU:HA	1.92	0.41
1:F:482:ARG:HH11	1:F:482:ARG:HD2	1.63	0.41
1:G:217:LYS:NZ	1:G:326:GLU:OE2	2.52	0.41
1:H:234:ASP:O	1:H:235:PHE:HB2	2.20	0.41
1:H:662:PRO:O	1:H:663:LEU:HD23	2.20	0.41
1:I:69:VAL:CG1	1:I:70:PRO:HD2	2.51	0.41
1:I:726:LEU:HA	1:I:726:LEU:HD23	1.76	0.41
1:K:367:MET:HB3	1:K:372:MET:CE	2.50	0.41
1:L:176:PHE:N	1:L:176:PHE:CD1	2.88	0.41
1:L:745:MET:HA	1:L:745:MET:CE	2.39	0.41
1:M:234:ASP:O	1:M:235:PHE:HB2	2.20	0.41
1:M:661:LYS:HA	1:M:662:PRO:HD3	1.74	0.41
1:M:662:PRO:O	1:M:663:LEU:HD23	2.20	0.41
1:M:1017:GLN:HB3	3:M:4405:HOH:O	2.19	0.41
1:N:576:ILE:CG2	1:N:577:LYS:N	2.79	0.41
1:O:599:ARG:HD2	1:O:600:GLN:OE1	2.20	0.41
1:O:836:ILE:HD12	1:O:836:ILE:HG23	1.73	0.41
1:A:69:VAL:CG1	1:A:70:PRO:HD2	2.50	0.41
1:A:772:ASP:OD1	1:A:772:ASP:N	2.48	0.41
1:A:917:ARG:HD2	3:A:4343:HOH:O	2.20	0.41
1:B:380:LYS:HE2	3:B:3180:HOH:O	2.19	0.41
1:D:395:HIS:HA	1:D:396:PRO:HD3	1.69	0.41
1:D:533:LEU:HD23	1:D:533:LEU:C	2.46	0.41
1:F:947:GLY:HA3	1:F:948:PRO:HD2	1.82	0.41
1:H:655:MET:HB2	1:H:655:MET:HE3	1.35	0.41
1:J:4:THR:HA	1:J:9:VAL:HG11	2.02	0.41
1:J:533:LEU:C	1:J:533:LEU:HD23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:694:LEU:HD12	1:J:694:LEU:HA	1.84	0.41
1:L:367:MET:HB3	1:L:372:MET:CE	2.50	0.41
1:L:533:LEU:HD23	1:L:533:LEU:C	2.45	0.41
1:M:287:ASP:OD1	1:M:287:ASP:N	2.41	0.41
1:M:473:ARG:HD3	1:M:473:ARG:C	2.43	0.41
1:N:367:MET:HB3	1:N:372:MET:CE	2.50	0.41
1:N:533:LEU:HD23	1:N:533:LEU:C	2.45	0.41
1:N:778:THR:HG22	1:N:779:PRO:O	2.20	0.41
1:O:4:THR:HA	1:O:9:VAL:HG11	2.01	0.41
1:O:533:LEU:HD23	1:O:533:LEU:C	2.45	0.41
1:O:914:CME:HE2	1:O:914:CME:HB3	1.74	0.41
1:P:599:ARG:HD2	1:P:600:GLN:OE1	2.20	0.41
1:A:576:ILE:CG2	1:A:577:LYS:N	2.79	0.41
1:B:134:LEU:HA	1:B:134:LEU:HD23	1.68	0.41
1:C:482:ARG:HH11	1:C:482:ARG:HD2	1.63	0.41
1:C:662:PRO:O	1:C:663:LEU:HD23	2.20	0.41
1:D:513:PRO:O	1:D:514:ALA:HB3	2.20	0.41
1:E:7:LEU:HD12	1:E:74:LEU:HD11	1.97	0.41
1:E:258:VAL:HA	1:E:312:VAL:O	2.21	0.41
1:F:533:LEU:HD23	1:F:533:LEU:C	2.45	0.41
1:F:778:THR:HG22	1:F:779:PRO:O	2.20	0.41
1:G:4:THR:HA	1:G:9:VAL:HG11	2.02	0.41
1:G:69:VAL:CG1	1:G:70:PRO:HD2	2.51	0.41
1:H:778:THR:HG22	1:H:779:PRO:O	2.20	0.41
1:I:4:THR:HA	1:I:9:VAL:HG11	2.01	0.41
1:I:183:ARG:HD3	1:I:183:ARG:HH11	1.62	0.41
1:I:533:LEU:HD23	1:I:533:LEU:C	2.45	0.41
1:I:1017:GLN:HB3	3:I:4405:HOH:O	2.19	0.41
1:J:730:LEU:HA	1:J:731:PRO:HD3	1.80	0.41
1:L:69:VAL:CG1	1:L:70:PRO:HD2	2.50	0.41
1:L:118:ASN:HA	1:L:119:PRO:HD2	1.62	0.41
1:L:258:VAL:HA	1:L:312:VAL:O	2.21	0.41
1:L:271:THR:HG22	1:L:272:ALA:N	2.35	0.41
1:L:380:LYS:HE2	3:L:3185:HOH:O	2.19	0.41
1:L:778:THR:HG22	1:L:779:PRO:O	2.20	0.41
1:M:118:ASN:HA	1:M:119:PRO:HD2	1.62	0.41
1:M:258:VAL:HA	1:M:312:VAL:O	2.21	0.41
1:M:513:PRO:O	1:M:514:ALA:HB3	2.20	0.41
1:M:836:ILE:HG23	1:M:836:ILE:HD12	1.73	0.41
1:M:1020:TRP:CD1	1:M:1020:TRP:C	2.99	0.41
1:P:285:TYR:CB	1:P:288:ARG:HG3	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:HIS:O	1:D:282:ARG:CD	2.67	0.41
1:C:234:ASP:O	1:C:235:PHE:HB2	2.20	0.41
1:C:258:VAL:HA	1:C:312:VAL:O	2.21	0.41
1:C:513:PRO:O	1:C:514:ALA:HB3	2.20	0.41
1:D:682:LEU:HD23	1:D:682:LEU:HA	1.85	0.41
1:D:856:TYR:CD2	1:D:864:MET:CE	3.00	0.41
1:E:130:ASP:OD1	1:E:131:GLU:N	2.53	0.41
1:E:271:THR:HG22	1:E:272:ALA:N	2.35	0.41
1:E:986:ILE:HG21	1:E:986:ILE:HD12	1.74	0.41
1:F:211:ASP:OD1	1:F:211:ASP:N	2.50	0.41
1:F:702:GLN:HA	1:F:703:PRO:HD2	1.88	0.41
1:H:367:MET:HB3	1:H:372:MET:CE	2.50	0.41
1:H:429:ASP:HA	1:H:430:PRO:HD3	1.73	0.41
1:H:702:GLN:HA	1:H:703:PRO:HD2	1.88	0.41
1:I:176:PHE:N	1:I:176:PHE:CD1	2.88	0.41
1:J:130:ASP:OD1	1:J:131:GLU:N	2.53	0.41
1:J:234:ASP:O	1:J:235:PHE:HB2	2.20	0.41
1:J:367:MET:HB3	1:J:372:MET:CE	2.50	0.41
1:K:429:ASP:HA	1:K:430:PRO:HD3	1.73	0.41
1:L:4:THR:HA	1:L:9:VAL:HG11	2.01	0.41
1:L:917:ARG:HD2	3:L:3452:HOH:O	2.19	0.41
1:M:69:VAL:CG1	1:M:70:PRO:HD2	2.50	0.41
1:M:473:ARG:HD2	1:P:469:ASP:HB3	2.02	0.41
1:M:778:THR:HB	1:M:887:GLN:H	1.84	0.41
1:M:807:VAL:HG13	1:M:808:GLU:N	2.36	0.41
1:N:3:ILE:HG13	1:N:4:THR:N	2.25	0.41
1:N:668:VAL:HA	1:N:669:PRO:HD3	1.83	0.41
1:O:651:LEU:HD13	1:O:651:LEU:HA	1.64	0.41
1:O:661:LYS:HA	1:O:662:PRO:HD3	1.74	0.41
1:O:726:LEU:HD23	1:O:726:LEU:HA	1.76	0.41
1:P:726:LEU:HD23	1:P:726:LEU:HA	1.76	0.41
1:A:271:THR:HG22	1:A:272:ALA:N	2.35	0.41
1:A:694:LEU:HD12	1:A:694:LEU:HA	1.84	0.41
1:B:130:ASP:OD1	1:B:131:GLU:N	2.53	0.41
1:B:654:TRP:CE2	1:B:666:GLY:HA3	2.56	0.41
1:D:258:VAL:HA	1:D:312:VAL:O	2.21	0.41
1:E:576:ILE:CG2	1:E:577:LYS:N	2.79	0.41
1:E:654:TRP:CE2	1:E:666:GLY:HA3	2.56	0.41
1:E:755:ARG:HH11	1:E:755:ARG:HD2	1.74	0.41
1:G:533:LEU:HD23	1:G:533:LEU:C	2.45	0.41
1:G:661:LYS:HA	1:G:662:PRO:HD3	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:807:VAL:HG13	1:G:808:GLU:N	2.36	0.41
1:H:986:ILE:HD13	1:H:986:ILE:HG23	1.67	0.41
1:I:271:THR:HG22	1:I:272:ALA:N	2.34	0.41
1:I:557:ARG:HH11	1:I:557:ARG:HD2	1.73	0.41
1:J:380:LYS:HE2	3:J:3182:HOH:O	2.19	0.41
1:K:380:LYS:HE2	3:K:4075:HOH:O	2.19	0.41
1:K:533:LEU:HD23	1:K:533:LEU:C	2.45	0.41
1:L:173:LEU:HD23	1:L:173:LEU:HA	1.86	0.41
1:M:682:LEU:HD23	1:M:682:LEU:HA	1.85	0.41
1:N:74:LEU:HD23	1:N:74:LEU:HA	1.92	0.41
1:N:271:THR:HG22	1:N:272:ALA:N	2.34	0.41
1:N:482:ARG:HH11	1:N:482:ARG:HD2	1.63	0.41
1:N:654:TRP:CE2	1:N:666:GLY:HA3	2.56	0.41
1:O:258:VAL:HA	1:O:312:VAL:O	2.21	0.41
1:O:271:THR:HG22	1:O:272:ALA:N	2.34	0.41
1:O:662:PRO:O	1:O:663:LEU:HD23	2.20	0.41
1:P:234:ASP:O	1:P:235:PHE:HB2	2.20	0.41
1:P:258:VAL:HA	1:P:312:VAL:O	2.21	0.41
1:P:654:TRP:CE2	1:P:666:GLY:HA3	2.56	0.41
1:A:234:ASP:O	1:A:235:PHE:HB2	2.20	0.41
1:A:730:LEU:HA	1:A:731:PRO:HD3	1.80	0.41
1:B:533:LEU:C	1:B:533:LEU:HD23	2.45	0.41
1:B:807:VAL:CG1	1:B:808:GLU:N	2.84	0.41
1:D:176:PHE:N	1:D:176:PHE:CD1	2.88	0.41
1:D:730:LEU:HA	1:D:731:PRO:HD3	1.80	0.41
1:D:807:VAL:HG13	1:D:808:GLU:N	2.36	0.41
1:E:425:ARG:NH2	1:H:287:ASP:OD2	2.54	0.41
1:E:473:ARG:HD3	1:E:473:ARG:C	2.43	0.41
1:E:599:ARG:HB2	1:E:600:GLN:H	1.63	0.41
1:F:422:PRO:HG2	1:G:279:ILE:CD1	2.50	0.41
1:G:271:THR:HG22	1:G:272:ALA:N	2.35	0.41
1:G:287:ASP:OD1	1:G:287:ASP:N	2.41	0.41
1:G:679:LEU:HD23	1:G:679:LEU:HA	1.40	0.41
1:H:69:VAL:CG1	1:H:70:PRO:HD2	2.51	0.41
1:H:258:VAL:HA	1:H:312:VAL:O	2.21	0.41
1:I:130:ASP:OD1	1:I:131:GLU:N	2.53	0.41
1:I:694:LEU:HD12	1:I:694:LEU:HA	1.84	0.41
1:J:90:TRP:HE1	1:J:96:ASP:CG	2.29	0.41
1:J:422:PRO:CG	1:K:279:ILE:CD1	2.98	0.41
1:K:499:ILE:HG22	1:K:501:PRO:HD3	2.03	0.41
1:K:1000:SER:HA	1:K:1001:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:367:MET:HB3	1:L:367:MET:HE3	1.77	0.41
1:M:57:GLU:HG2	1:M:83:THR:HG22	1.95	0.41
1:O:176:PHE:CD1	1:O:176:PHE:N	2.88	0.41
1:O:645:ARG:NH2	1:O:650:GLU:CD	2.79	0.41
1:O:654:TRP:CE2	1:O:666:GLY:HA3	2.56	0.41
1:P:69:VAL:CG1	1:P:70:PRO:HD2	2.51	0.41
1:A:258:VAL:HA	1:A:312:VAL:O	2.21	0.41
1:A:422:PRO:CG	1:D:279:ILE:HD13	2.50	0.41
1:B:147:ASN:HA	1:B:148:SER:HA	1.57	0.41
1:B:258:VAL:HA	1:B:312:VAL:O	2.21	0.41
1:B:662:PRO:O	1:B:663:LEU:HD23	2.20	0.41
1:C:36:TRP:CD2	1:C:42:ALA:HA	2.56	0.41
1:C:917:ARG:HD2	3:C:4343:HOH:O	2.19	0.41
1:D:90:TRP:HE1	1:D:96:ASP:CG	2.29	0.41
1:D:130:ASP:OD1	1:D:131:GLU:N	2.53	0.41
1:D:380:LYS:HE2	3:D:3188:HOH:O	2.19	0.41
1:D:807:VAL:CG1	1:D:808:GLU:N	2.84	0.41
1:E:745:MET:HA	1:E:745:MET:CE	2.39	0.41
1:G:645:ARG:NH2	1:G:650:GLU:CD	2.79	0.41
1:I:380:LYS:HE2	3:I:4074:HOH:O	2.19	0.41
1:I:925:MET:HE3	1:I:925:MET:HB3	1.98	0.41
1:J:612:THR:HA	1:J:613:PRO:HD3	1.59	0.41
1:J:917:ARG:HD2	3:J:3449:HOH:O	2.19	0.41
1:L:234:ASP:O	1:L:235:PHE:HB2	2.20	0.41
1:L:927:THR:HA	1:L:928:PRO:HD3	1.82	0.41
1:L:950:GLN:HB2	1:L:1023:LYS:HE2	2.03	0.41
1:L:952:ARG:HH11	1:L:952:ARG:CG	2.28	0.41
1:N:90:TRP:HE1	1:N:96:ASP:CG	2.29	0.41
1:N:367:MET:HB3	1:N:367:MET:HE3	1.77	0.41
1:N:807:VAL:CG1	1:N:808:GLU:N	2.84	0.41
1:N:917:ARG:HD2	3:N:3447:HOH:O	2.19	0.41
1:O:513:PRO:O	1:O:514:ALA:HB3	2.20	0.41
1:P:271:THR:HG22	1:P:272:ALA:N	2.35	0.41
1:P:917:ARG:HD2	3:P:3453:HOH:O	2.19	0.41
1:A:102:ASN:ND2	1:A:102:ASN:C	2.79	0.41
1:A:533:LEU:HD23	1:A:533:LEU:C	2.45	0.41
1:A:748:CME:HE2	1:A:748:CME:HB3	1.15	0.41
1:A:1017:GLN:HB3	3:A:4412:HOH:O	2.19	0.41
1:B:90:TRP:HE1	1:B:96:ASP:CG	2.29	0.41
1:B:234:ASP:O	1:B:235:PHE:HB2	2.20	0.41
1:B:272:ALA:HA	1:B:273:PRO:HD3	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:807:VAL:HG13	1:B:808:GLU:N	2.36	0.41
1:C:533:LEU:HD23	1:C:533:LEU:C	2.45	0.41
1:C:661:LYS:HA	1:C:662:PRO:HD3	1.74	0.41
1:D:63:PHE:CB	1:D:64:PRO:HD2	2.34	0.41
1:D:778:THR:HG22	1:D:779:PRO:O	2.20	0.41
1:E:90:TRP:HE1	1:E:96:ASP:CG	2.29	0.41
1:E:422:PRO:HG2	1:H:279:ILE:CD1	2.50	0.41
1:E:662:PRO:O	1:E:663:LEU:HD23	2.20	0.41
1:E:778:THR:HG22	1:E:779:PRO:O	2.20	0.41
1:F:36:TRP:CD2	1:F:42:ALA:HA	2.56	0.41
1:F:69:VAL:CG1	1:F:70:PRO:HD2	2.51	0.41
1:F:807:VAL:CG1	1:F:808:GLU:N	2.84	0.41
1:F:807:VAL:HG13	1:F:808:GLU:N	2.36	0.41
1:G:62:TRP:C	1:G:63:PHE:CD1	2.99	0.41
1:G:90:TRP:HE1	1:G:96:ASP:CG	2.29	0.41
1:G:102:ASN:C	1:G:102:ASN:ND2	2.79	0.41
1:G:272:ALA:HA	1:G:273:PRO:HD3	1.78	0.41
1:G:654:TRP:CE2	1:G:666:GLY:HA3	2.56	0.41
1:G:778:THR:HG22	1:G:779:PRO:O	2.20	0.41
1:H:62:TRP:C	1:H:63:PHE:CD1	2.99	0.41
1:H:305:ILE:HG21	1:H:305:ILE:HD13	1.84	0.41
1:H:654:TRP:CE2	1:H:666:GLY:HA3	2.56	0.41
1:H:1017:GLN:HB3	3:H:4415:HOH:O	2.19	0.41
1:I:258:VAL:HA	1:I:312:VAL:O	2.21	0.41
1:I:499:ILE:HG22	1:I:501:PRO:HD3	2.03	0.41
1:I:599:ARG:HD2	1:I:600:GLN:OE1	2.20	0.41
1:I:654:TRP:CE2	1:I:666:GLY:HA3	2.56	0.41
1:I:778:THR:HG22	1:I:779:PRO:O	2.20	0.41
1:I:986:ILE:HD13	1:I:986:ILE:HG23	1.67	0.41
1:J:69:VAL:CG1	1:J:70:PRO:HD2	2.51	0.41
1:J:367:MET:HB3	1:J:367:MET:HE3	1.77	0.41
1:J:499:ILE:HG22	1:J:501:PRO:HD3	2.03	0.41
1:J:668:VAL:HA	1:J:669:PRO:HD3	1.83	0.41
1:J:856:TYR:CD2	1:J:864:MET:CE	3.00	0.41
1:J:1017:GLN:HE21	1:J:1017:GLN:HB2	1.65	0.41
1:K:258:VAL:HA	1:K:312:VAL:O	2.21	0.41
1:K:662:PRO:O	1:K:663:LEU:HD23	2.20	0.41
1:K:836:ILE:HG23	1:K:836:ILE:HD12	1.73	0.41
1:M:36:TRP:CD2	1:M:42:ALA:HA	2.56	0.41
1:M:807:VAL:CG1	1:M:808:GLU:N	2.84	0.41
1:N:36:TRP:CD2	1:N:42:ALA:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:36:TRP:CD2	1:O:42:ALA:HA	2.56	0.41
1:O:62:TRP:C	1:O:63:PHE:CD1	2.99	0.41
1:O:69:VAL:CG1	1:O:70:PRO:HD2	2.51	0.41
1:O:221:GLN:H	1:O:221:GLN:HG2	1.63	0.41
1:O:367:MET:HB3	1:O:372:MET:CE	2.50	0.41
1:O:778:THR:HA	1:O:779:PRO:HD3	1.95	0.41
1:P:176:PHE:CD1	1:P:176:PHE:N	2.88	0.41
1:P:367:MET:HB3	1:P:372:MET:CE	2.50	0.41
1:P:395:HIS:HA	1:P:396:PRO:HD3	1.69	0.41
1:P:682:LEU:HD23	1:P:682:LEU:HA	1.85	0.41
1:P:714:ILE:HD13	1:P:714:ILE:HA	1.78	0.41
1:A:5:ASP:OD2	1:A:157:ARG:HG2	2.21	0.41
1:A:645:ARG:NH2	1:A:650:GLU:CD	2.79	0.41
1:B:153:TRP:CD1	1:B:158:TRP:HA	2.56	0.41
1:B:499:ILE:HG22	1:B:501:PRO:HD3	2.03	0.41
1:B:928:PRO:HB2	1:B:973:ARG:HH11	1.86	0.41
1:C:62:TRP:C	1:C:63:PHE:CD1	2.99	0.41
1:C:69:VAL:CG1	1:C:70:PRO:HD2	2.51	0.41
1:C:90:TRP:HE1	1:C:96:ASP:CG	2.29	0.41
1:C:102:ASN:C	1:C:102:ASN:ND2	2.79	0.41
1:C:645:ARG:NH2	1:C:650:GLU:CD	2.79	0.41
1:C:654:TRP:CE2	1:C:666:GLY:HA3	2.56	0.41
1:D:62:TRP:C	1:D:63:PHE:CD1	2.99	0.41
1:D:69:VAL:CG1	1:D:70:PRO:HD2	2.51	0.41
1:D:748:CME:HE2	1:D:748:CME:HB3	1.15	0.41
1:E:5:ASP:OD2	1:E:157:ARG:HG2	2.21	0.41
1:E:807:VAL:CG1	1:E:808:GLU:N	2.84	0.41
1:E:874:SER:HB3	1:F:724:GLU:OE1	2.21	0.41
1:F:425:ARG:HH22	1:G:287:ASP:CG	2.29	0.41
1:G:153:TRP:CD1	1:G:158:TRP:HA	2.56	0.41
1:G:221:GLN:H	1:G:221:GLN:HG2	1.63	0.41
1:G:856:TYR:CD2	1:G:864:MET:CE	3.00	0.41
1:H:36:TRP:CD2	1:H:42:ALA:HA	2.56	0.41
1:H:176:PHE:CD1	1:H:176:PHE:N	2.88	0.41
1:H:807:VAL:CG1	1:H:808:GLU:N	2.84	0.41
1:I:5:ASP:OD2	1:I:157:ARG:HG2	2.21	0.41
1:I:928:PRO:HB2	1:I:973:ARG:HH11	1.86	0.41
1:J:62:TRP:C	1:J:63:PHE:CD1	2.99	0.41
1:J:599:ARG:HD2	1:J:600:GLN:OE1	2.20	0.41
1:J:901:GLY:HA3	1:J:902:PRO:HA	1.89	0.41
1:J:905:ASN:HB2	1:J:910:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5:ASP:OD2	1:K:157:ARG:HG2	2.21	0.41
1:K:36:TRP:CD2	1:K:42:ALA:HA	2.56	0.41
1:K:654:TRP:CE2	1:K:666:GLY:HA3	2.56	0.41
1:K:905:ASN:HB2	1:K:910:LEU:HB3	2.03	0.41
1:L:62:TRP:C	1:L:63:PHE:CD1	2.99	0.41
1:L:807:VAL:CG1	1:L:808:GLU:N	2.84	0.41
1:M:90:TRP:HE1	1:M:96:ASP:CG	2.29	0.41
1:M:422:PRO:HG3	1:P:284:GLY:C	2.46	0.41
1:M:533:LEU:HD23	1:M:533:LEU:C	2.45	0.41
1:M:654:TRP:CE2	1:M:666:GLY:HA3	2.56	0.41
1:N:69:VAL:CG1	1:N:70:PRO:HD2	2.51	0.41
1:N:807:VAL:HG13	1:N:808:GLU:N	2.36	0.41
1:O:380:LYS:HE2	3:O:3179:HOH:O	2.19	0.41
1:O:778:THR:HG22	1:O:779:PRO:O	2.20	0.41
1:P:102:ASN:C	1:P:102:ASN:ND2	2.79	0.41
1:P:645:ARG:NH2	1:P:650:GLU:CD	2.79	0.41
1:P:662:PRO:O	1:P:663:LEU:HD23	2.20	0.41
1:P:807:VAL:CG1	1:P:808:GLU:N	2.84	0.41
1:A:282:ARG:HD2	1:D:418:HIS:O	2.21	0.40
1:A:807:VAL:CG1	1:A:808:GLU:N	2.84	0.40
1:A:807:VAL:HG13	1:A:808:GLU:N	2.36	0.40
1:A:905:ASN:HB2	1:A:910:LEU:HB3	2.03	0.40
1:B:645:ARG:NH2	1:B:650:GLU:CD	2.79	0.40
1:B:682:LEU:HD23	1:B:682:LEU:HA	1.85	0.40
1:C:153:TRP:CD1	1:C:158:TRP:HA	2.56	0.40
1:C:950:GLN:HB2	1:C:1023:LYS:HE2	2.03	0.40
1:D:102:ASN:C	1:D:102:ASN:ND2	2.79	0.40
1:D:599:ARG:HB2	1:D:600:GLN:H	1.64	0.40
1:D:654:TRP:CE2	1:D:666:GLY:HA3	2.56	0.40
1:D:745:MET:HA	1:D:745:MET:CE	2.39	0.40
1:E:520:ILE:HD13	1:E:520:ILE:HG21	1.79	0.40
1:E:807:VAL:HG13	1:E:808:GLU:N	2.36	0.40
1:F:5:ASP:OD2	1:F:157:ARG:HG2	2.21	0.40
1:F:662:PRO:O	1:F:663:LEU:HD23	2.20	0.40
1:G:380:LYS:HE2	3:G:3179:HOH:O	2.19	0.40
1:G:662:PRO:O	1:G:663:LEU:HD23	2.20	0.40
1:H:153:TRP:CD1	1:H:158:TRP:HA	2.56	0.40
1:H:905:ASN:HB2	1:H:910:LEU:HB3	2.04	0.40
1:I:134:LEU:HD23	1:I:134:LEU:HA	1.68	0.40
1:I:253:TYR:O	1:I:318:ALA:N	2.55	0.40
1:I:1020:TRP:CD1	1:I:1020:TRP:C	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:258:VAL:HA	1:J:312:VAL:O	2.21	0.40
1:J:422:PRO:CG	1:K:279:ILE:HD11	2.50	0.40
1:K:645:ARG:NH2	1:K:650:GLU:CD	2.79	0.40
1:K:685:LEU:HA	1:K:686:PRO:HD3	1.83	0.40
1:K:772:ASP:OD1	1:K:772:ASP:N	2.48	0.40
1:K:901:GLY:HA3	1:K:902:PRO:HA	1.89	0.40
1:L:499:ILE:HG22	1:L:501:PRO:HD3	2.03	0.40
1:L:654:TRP:CE2	1:L:666:GLY:HA3	2.56	0.40
1:M:173:LEU:HD23	1:M:173:LEU:HA	1.85	0.40
1:M:1017:GLN:HE21	1:M:1017:GLN:HB2	1.65	0.40
1:N:5:ASP:OD2	1:N:157:ARG:HG2	2.21	0.40
1:N:662:PRO:O	1:N:663:LEU:HD23	2.20	0.40
1:O:807:VAL:CG1	1:O:808:GLU:N	2.84	0.40
1:P:211:ASP:OD1	1:P:211:ASP:N	2.50	0.40
1:P:778:THR:HG22	1:P:779:PRO:O	2.20	0.40
1:A:513:PRO:O	1:A:514:ALA:HB3	2.20	0.40
1:B:63:PHE:CD1	1:B:63:PHE:N	2.90	0.40
1:B:253:TYR:O	1:B:318:ALA:N	2.54	0.40
1:D:479:ASP:HA	1:D:480:PRO:HD2	1.77	0.40
1:E:134:LEU:HA	1:E:134:LEU:HD23	1.68	0.40
1:E:429:ASP:HA	1:E:430:PRO:HD3	1.74	0.40
1:E:513:PRO:O	1:E:514:ALA:HB3	2.20	0.40
1:E:521:LYS:HB2	1:F:559:TYR:OH	2.21	0.40
1:E:661:LYS:HA	1:E:662:PRO:HD3	1.74	0.40
1:F:62:TRP:C	1:F:63:PHE:CD1	2.99	0.40
1:F:90:TRP:HE1	1:F:96:ASP:CG	2.29	0.40
1:F:253:TYR:O	1:F:318:ALA:N	2.54	0.40
1:G:3:ILE:HG13	1:G:4:THR:N	2.25	0.40
1:G:658:LEU:N	1:G:661:LYS:O	2.40	0.40
1:G:807:VAL:CG1	1:G:808:GLU:N	2.84	0.40
1:H:5:ASP:OD2	1:H:157:ARG:HG2	2.21	0.40
1:H:878:HIS:HA	1:H:879:PRO:HD3	1.83	0.40
1:J:63:PHE:CD1	1:J:63:PHE:N	2.90	0.40
1:J:316:HIS:HA	1:J:323:ILE:HD13	2.01	0.40
1:J:772:ASP:OD1	1:J:772:ASP:N	2.48	0.40
1:K:807:VAL:CG1	1:K:808:GLU:N	2.84	0.40
1:L:36:TRP:CD2	1:L:42:ALA:HA	2.56	0.40
1:L:256:VAL:HG12	1:L:257:THR:N	2.37	0.40
1:L:685:LEU:HA	1:L:686:PRO:HD3	1.83	0.40
1:L:928:PRO:HB2	1:L:973:ARG:HH11	1.86	0.40
1:M:62:TRP:C	1:M:63:PHE:CD1	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:74:LEU:HD23	1:M:74:LEU:HA	1.92	0.40
1:M:278:ILE:N	1:M:278:ILE:CD1	2.80	0.40
1:N:234:ASP:O	1:N:235:PHE:HB2	2.20	0.40
1:N:726:LEU:HA	1:N:726:LEU:HD23	1.76	0.40
1:O:3:ILE:HG13	1:O:4:THR:N	2.25	0.40
1:O:670:LEU:HA	1:O:670:LEU:HD23	1.75	0.40
1:O:928:PRO:HB2	1:O:973:ARG:HH11	1.86	0.40
1:P:499:ILE:HG22	1:P:501:PRO:HD3	2.03	0.40
1:A:778:THR:HG22	1:A:779:PRO:O	2.20	0.40
1:B:78:LEU:CB	1:B:79:PRO:CD	3.00	0.40
1:B:367:MET:HB3	1:B:372:MET:CE	2.50	0.40
1:B:702:GLN:HA	1:B:703:PRO:HD2	1.88	0.40
1:C:5:ASP:OD2	1:C:157:ARG:HG2	2.22	0.40
1:C:928:PRO:HB2	1:C:973:ARG:HH11	1.86	0.40
1:D:645:ARG:NH2	1:D:650:GLU:CD	2.79	0.40
1:D:1020:TRP:CD1	1:D:1020:TRP:C	2.99	0.40
1:E:36:TRP:CD2	1:E:42:ALA:HA	2.56	0.40
1:E:153:TRP:CD1	1:E:158:TRP:HA	2.56	0.40
1:E:856:TYR:CD2	1:E:864:MET:CE	3.00	0.40
1:F:78:LEU:CB	1:F:79:PRO:CD	3.00	0.40
1:F:612:THR:HA	1:F:613:PRO:HD3	1.59	0.40
1:G:5:ASP:OD2	1:G:157:ARG:HG2	2.21	0.40
1:H:645:ARG:NH2	1:H:650:GLU:CD	2.79	0.40
1:I:513:PRO:O	1:I:514:ALA:HB3	2.20	0.40
1:I:655:MET:O	1:I:655:MET:HG3	2.20	0.40
1:I:807:VAL:CG1	1:I:808:GLU:N	2.84	0.40
1:J:654:TRP:CE2	1:J:666:GLY:HA3	2.56	0.40
1:K:69:VAL:CG1	1:K:70:PRO:HD2	2.50	0.40
1:K:748:CME:HE2	1:K:748:CME:HB3	1.14	0.40
1:L:102:ASN:ND2	1:L:102:ASN:C	2.79	0.40
1:M:802:ASP:HA	1:M:803:PRO:HD3	1.83	0.40
1:M:928:PRO:HB2	1:M:973:ARG:HH11	1.86	0.40
1:N:153:TRP:CD1	1:N:158:TRP:HA	2.56	0.40
1:N:256:VAL:HG12	1:N:257:THR:N	2.37	0.40
1:O:5:ASP:OD2	1:O:157:ARG:HG2	2.21	0.40
1:P:905:ASN:HB2	1:P:910:LEU:HB3	2.03	0.40
1:A:31:PRO:CB	1:A:32:PRO:CD	3.00	0.40
1:A:62:TRP:C	1:A:63:PHE:CD1	2.99	0.40
1:A:153:TRP:CD1	1:A:158:TRP:HA	2.56	0.40
1:C:499:ILE:HG22	1:C:501:PRO:HD3	2.03	0.40
1:C:658:LEU:N	1:C:661:LYS:O	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:LEU:CB	1:D:79:PRO:CD	3.00	0.40
1:D:655:MET:O	1:D:655:MET:HG3	2.20	0.40
1:E:986:ILE:HG23	1:E:986:ILE:HD13	1.67	0.40
1:F:102:ASN:C	1:F:102:ASN:ND2	2.79	0.40
1:F:153:TRP:CD1	1:F:158:TRP:HA	2.56	0.40
1:F:425:ARG:NH2	1:G:287:ASP:OD2	2.55	0.40
1:F:499:ILE:HG22	1:F:501:PRO:HD3	2.03	0.40
1:F:513:PRO:O	1:F:514:ALA:HB3	2.20	0.40
1:F:654:TRP:CE2	1:F:666:GLY:HA3	2.56	0.40
1:F:1020:TRP:CD1	1:F:1020:TRP:C	2.99	0.40
1:G:367:MET:HB3	1:G:372:MET:CE	2.50	0.40
1:H:102:ASN:C	1:H:102:ASN:ND2	2.79	0.40
1:H:499:ILE:HG22	1:H:501:PRO:HD3	2.03	0.40
1:H:925:MET:HE3	1:H:925:MET:HB3	1.98	0.40
1:I:36:TRP:CD2	1:I:42:ALA:HA	2.56	0.40
1:I:102:ASN:C	1:I:102:ASN:ND2	2.79	0.40
1:I:189:LEU:N	1:I:189:LEU:CD2	2.79	0.40
1:J:36:TRP:CD2	1:J:42:ALA:HA	2.56	0.40
1:J:920:LEU:CB	1:J:921:PRO:CD	2.99	0.40
1:K:211:ASP:OD1	1:K:211:ASP:N	2.50	0.40
1:K:256:VAL:HG12	1:K:257:THR:N	2.37	0.40
1:K:714:ILE:HD13	1:K:714:ILE:HA	1.78	0.40
1:K:947:GLY:HA3	1:K:948:PRO:HD2	1.82	0.40
1:L:5:ASP:OD2	1:L:157:ARG:HG2	2.21	0.40
1:L:153:TRP:CD1	1:L:158:TRP:HA	2.56	0.40
1:M:147:ASN:HA	1:M:148:SER:HA	1.57	0.40
1:M:305:ILE:HD13	1:M:305:ILE:HG21	1.85	0.40
1:M:422:PRO:HG2	1:P:279:ILE:HD11	2.03	0.40
1:N:78:LEU:CB	1:N:79:PRO:CD	3.00	0.40
1:N:279:ILE:HD13	1:O:422:PRO:CG	2.52	0.40
1:N:499:ILE:HG22	1:N:501:PRO:HD3	2.03	0.40
1:P:36:TRP:CD2	1:P:42:ALA:HA	2.56	0.40
1:P:928:PRO:HB2	1:P:973:ARG:HH11	1.86	0.40
1:A:568:TRP:CD1	1:A:568:TRP:C	3.00	0.40
1:B:36:TRP:CD2	1:B:42:ALA:HA	2.56	0.40
1:C:253:TYR:O	1:C:318:ALA:N	2.55	0.40
1:C:807:VAL:HG13	1:C:808:GLU:N	2.36	0.40
1:D:74:LEU:HD23	1:D:74:LEU:HA	1.92	0.40
1:E:395:HIS:HA	1:E:396:PRO:HD3	1.69	0.40
1:E:533:LEU:C	1:E:533:LEU:HD23	2.45	0.40
1:G:316:HIS:HA	1:G:323:ILE:HD13	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:928:PRO:HB2	1:G:973:ARG:HH11	1.86	0.40
1:H:63:PHE:CD1	1:H:63:PHE:N	2.90	0.40
1:I:63:PHE:CD1	1:I:63:PHE:N	2.90	0.40
1:I:90:TRP:HE1	1:I:96:ASP:CG	2.29	0.40
1:I:521:LYS:HB2	1:J:559:TYR:OH	2.22	0.40
1:J:5:ASP:OD2	1:J:157:ARG:HG2	2.22	0.40
1:J:128:ASN:ND2	1:J:180:GLY:HA2	2.37	0.40
1:J:513:PRO:O	1:J:514:ALA:HB3	2.20	0.40
1:J:662:PRO:O	1:J:663:LEU:HD23	2.20	0.40
1:J:685:LEU:HA	1:J:686:PRO:HD3	1.83	0.40
1:J:807:VAL:CG1	1:J:808:GLU:N	2.84	0.40
1:K:253:TYR:O	1:K:318:ALA:N	2.55	0.40
1:K:694:LEU:HA	1:K:694:LEU:HD12	1.84	0.40
1:L:111:PRO:HA	1:L:112:PRO:HA	1.66	0.40
1:L:662:PRO:O	1:L:663:LEU:HD23	2.20	0.40
1:M:102:ASN:C	1:M:102:ASN:ND2	2.79	0.40
1:M:645:ARG:NH2	1:M:650:GLU:CD	2.79	0.40
1:N:1020:TRP:CD1	1:N:1020:TRP:C	2.99	0.40
1:O:234:ASP:O	1:O:235:PHE:HB2	2.20	0.40
1:O:253:TYR:O	1:O:318:ALA:N	2.55	0.40
1:O:254:LEU:HD23	1:O:254:LEU:HA	1.71	0.40
1:P:5:ASP:OD2	1:P:157:ARG:HG2	2.21	0.40
1:P:90:TRP:HE1	1:P:96:ASP:CG	2.29	0.40
1:P:950:GLN:HB2	1:P:1023:LYS:HE2	2.03	0.40

All (5) 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:CB[2_555]	1.77	0.43
1:A:580:GLU:O	1:B:578:TYR:CG[2_555]	1.85	0.35
1:A:580:GLU:O	1:B:578:TYR:CD1[2_555]	2.10	0.10
1:B:739:HIS:NE2	1:P:738:PRO:O[1_354]	2.10	0.10
1:C:739:HIS:ND1	1:I:734:SER:O[1_655]	2.15	0.05

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	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	B	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	C	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	D	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	E	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	F	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	G	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	H	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	I	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	J	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	K	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	L	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	M	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	N	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	O	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
1	P	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	36	55
All	All	16336/16368 (100%)	15616 (96%)	672 (4%)	48 (0%)	36	55

All (48) 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

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Mol	Chain	Res	Type
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	164	ASP
1	B	164	ASP
1	C	164	ASP
1	D	164	ASP
1	E	164	ASP
1	F	164	ASP
1	G	164	ASP
1	H	164	ASP
1	I	164	ASP
1	J	164	ASP
1	K	164	ASP
1	L	164	ASP
1	M	164	ASP
1	N	164	ASP
1	O	164	ASP
1	P	164	ASP
1	A	119	PRO
1	B	119	PRO
1	C	119	PRO
1	D	119	PRO
1	E	119	PRO
1	F	119	PRO
1	G	119	PRO
1	H	119	PRO
1	I	119	PRO
1	J	119	PRO
1	K	119	PRO
1	L	119	PRO
1	M	119	PRO
1	N	119	PRO
1	O	119	PRO
1	P	119	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	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	B	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	C	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	D	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	E	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	F	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	G	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	H	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	I	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	J	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	K	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	L	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	M	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	N	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	O	875/872 (100%)	767 (88%)	108 (12%)	4	10
1	P	875/872 (100%)	767 (88%)	108 (12%)	4	10
All	All	14000/13952 (100%)	12272 (88%)	1728 (12%)	4	10

All (1728) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	9	VAL
1	A	14	ARG
1	A	37	ARG
1	A	39	SER
1	A	46	ARG
1	A	48	SER
1	A	49	GLN

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Mol	Chain	Res	Type
1	A	50	GLN
1	A	52	ARG
1	A	57	GLU
1	A	59	ARG
1	A	71	GLU
1	A	72	SER
1	A	80	GLU
1	A	84	VAL
1	A	90	TRP
1	A	114	VAL
1	A	116	THR
1	A	125	LEU
1	A	128	ASN
1	A	131	GLU
1	A	136	GLU
1	A	165	SER
1	A	166	ARG
1	A	171	PHE
1	A	189	LEU
1	A	190	ARG
1	A	202	MET
1	A	210	ARG
1	A	211	ASP
1	A	217	LYS
1	A	219	THR
1	A	227	VAL
1	A	237	ARG
1	A	246	MET
1	A	247	CYS
1	A	249	GLU
1	A	250	LEU
1	A	251	ARG
1	A	259	SER
1	A	262	GLN
1	A	279	ILE
1	A	299	LYS
1	A	310	ARG
1	A	314	GLU
1	A	319	ASP
1	A	333	ARG
1	A	344	LEU
1	A	347	LYS

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Mol	Chain	Res	Type
1	A	370	GLN
1	A	377	LEU
1	A	380	LYS
1	A	437	SER
1	A	448	ARG
1	A	473	ARG
1	A	519	SER
1	A	521	LYS
1	A	546	LEU
1	A	554	GLN
1	A	571	VAL
1	A	580	GLU
1	A	599	ARG
1	A	600	GLN
1	A	630	ARG
1	A	645	ARG
1	A	651	LEU
1	A	655	MET
1	A	665	SER
1	A	672	VAL
1	A	684	GLU
1	A	687	GLN
1	A	690	SER
1	A	710	GLU
1	A	719	GLN
1	A	730	LEU
1	A	734	SER
1	A	741	THR
1	A	743	SER
1	A	749	ILE
1	A	751	LEU
1	A	753	ASN
1	A	755	ARG
1	A	761	GLN
1	A	768	MET
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	824	GLN

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Mol	Chain	Res	Type
1	A	829	THR
1	A	832	ASP
1	A	867	THR
1	A	881	ARG
1	A	893	GLU
1	A	894	ARG
1	A	903[A]	GLN
1	A	903[B]	GLN
1	A	938	ARG
1	A	952	ARG
1	A	956	GLN
1	A	965	GLN
1	A	986	ILE
1	A	1006	GLU
1	A	1017	GLN
1	A	1023	LYS
1	B	3	ILE
1	B	9	VAL
1	B	14	ARG
1	B	37	ARG
1	B	39	SER
1	B	46	ARG
1	B	48	SER
1	B	49	GLN
1	B	50	GLN
1	B	52	ARG
1	B	57	GLU
1	B	59	ARG
1	B	71	GLU
1	B	72	SER
1	B	80	GLU
1	B	84	VAL
1	B	90	TRP
1	B	114	VAL
1	B	116	THR
1	B	125	LEU
1	B	128	ASN
1	B	131	GLU
1	B	136	GLU
1	B	165	SER
1	B	166	ARG
1	B	171	PHE

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Mol	Chain	Res	Type
1	B	189	LEU
1	B	190	ARG
1	B	202	MET
1	B	210	ARG
1	B	211	ASP
1	B	217	LYS
1	B	219	THR
1	B	227	VAL
1	B	237	ARG
1	B	246	MET
1	B	247	CYS
1	B	249	GLU
1	B	250	LEU
1	B	251	ARG
1	B	259	SER
1	B	262	GLN
1	B	279	ILE
1	B	299	LYS
1	B	310	ARG
1	B	314	GLU
1	B	319	ASP
1	B	333	ARG
1	B	344	LEU
1	B	347	LYS
1	B	370	GLN
1	B	377	LEU
1	B	380	LYS
1	B	437	SER
1	B	448	ARG
1	B	473	ARG
1	B	519	SER
1	B	521	LYS
1	B	546	LEU
1	B	554	GLN
1	B	571	VAL
1	B	580	GLU
1	B	599	ARG
1	B	600	GLN
1	B	630	ARG
1	B	645	ARG
1	B	651	LEU
1	B	655	MET

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Mol	Chain	Res	Type
1	B	665	SER
1	B	672	VAL
1	B	684	GLU
1	B	687	GLN
1	B	690	SER
1	B	710	GLU
1	B	719	GLN
1	B	730	LEU
1	B	734	SER
1	B	741	THR
1	B	743	SER
1	B	749	ILE
1	B	751	LEU
1	B	753	ASN
1	B	755	ARG
1	B	761	GLN
1	B	768	MET
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	824	GLN
1	B	829	THR
1	B	832	ASP
1	B	867	THR
1	B	881	ARG
1	B	893	GLU
1	B	894	ARG
1	B	903[A]	GLN
1	B	903[B]	GLN
1	B	938	ARG
1	B	952	ARG
1	B	956	GLN
1	B	965	GLN
1	B	986	ILE
1	B	1006	GLU
1	B	1017	GLN
1	B	1023	LYS
1	C	3	ILE
1	C	9	VAL

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Mol	Chain	Res	Type
1	C	14	ARG
1	C	37	ARG
1	C	39	SER
1	C	46	ARG
1	C	48	SER
1	C	49	GLN
1	C	50	GLN
1	C	52	ARG
1	C	57	GLU
1	C	59	ARG
1	C	71	GLU
1	C	72	SER
1	C	80	GLU
1	C	84	VAL
1	C	90	TRP
1	C	114	VAL
1	C	116	THR
1	C	125	LEU
1	C	128	ASN
1	C	131	GLU
1	C	136	GLU
1	C	165	SER
1	C	166	ARG
1	C	171	PHE
1	C	189	LEU
1	C	190	ARG
1	C	202	MET
1	C	210	ARG
1	C	211	ASP
1	C	217	LYS
1	C	219	THR
1	C	227	VAL
1	C	237	ARG
1	C	246	MET
1	C	247	CYS
1	C	249	GLU
1	C	250	LEU
1	C	251	ARG
1	C	259	SER
1	C	262	GLN
1	C	279	ILE
1	C	299	LYS

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Mol	Chain	Res	Type
1	C	310	ARG
1	C	314	GLU
1	C	319	ASP
1	C	333	ARG
1	C	344	LEU
1	C	347	LYS
1	C	370	GLN
1	C	377	LEU
1	C	380	LYS
1	C	437	SER
1	C	448	ARG
1	C	473	ARG
1	C	519	SER
1	C	521	LYS
1	C	546	LEU
1	C	554	GLN
1	C	571	VAL
1	C	580	GLU
1	C	599	ARG
1	C	600	GLN
1	C	630	ARG
1	C	645	ARG
1	C	651	LEU
1	C	655	MET
1	C	665	SER
1	C	672	VAL
1	C	684	GLU
1	C	687	GLN
1	C	690	SER
1	C	710	GLU
1	C	719	GLN
1	C	730	LEU
1	C	734	SER
1	C	741	THR
1	C	743	SER
1	C	749	ILE
1	C	751	LEU
1	C	753	ASN
1	C	755	ARG
1	C	761	GLN
1	C	768	MET
1	C	778	THR

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Mol	Chain	Res	Type
1	C	781	ARG
1	C	797	GLU
1	C	799	THR
1	C	800	ARG
1	C	801	ILE
1	C	824	GLN
1	C	829	THR
1	C	832	ASP
1	C	867	THR
1	C	881	ARG
1	C	893	GLU
1	C	894	ARG
1	C	903[A]	GLN
1	C	903[B]	GLN
1	C	938	ARG
1	C	952	ARG
1	C	956	GLN
1	C	965	GLN
1	C	986	ILE
1	C	1006	GLU
1	C	1017	GLN
1	C	1023	LYS
1	D	3	ILE
1	D	9	VAL
1	D	14	ARG
1	D	37	ARG
1	D	39	SER
1	D	46	ARG
1	D	48	SER
1	D	49	GLN
1	D	50	GLN
1	D	52	ARG
1	D	57	GLU
1	D	59	ARG
1	D	71	GLU
1	D	72	SER
1	D	80	GLU
1	D	84	VAL
1	D	90	TRP
1	D	114	VAL
1	D	116	THR
1	D	125	LEU

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Mol	Chain	Res	Type
1	D	128	ASN
1	D	131	GLU
1	D	136	GLU
1	D	165	SER
1	D	166	ARG
1	D	171	PHE
1	D	189	LEU
1	D	190	ARG
1	D	202	MET
1	D	210	ARG
1	D	211	ASP
1	D	217	LYS
1	D	219	THR
1	D	227	VAL
1	D	237	ARG
1	D	246	MET
1	D	247	CYS
1	D	249	GLU
1	D	250	LEU
1	D	251	ARG
1	D	259	SER
1	D	262	GLN
1	D	279	ILE
1	D	299	LYS
1	D	310	ARG
1	D	314	GLU
1	D	319	ASP
1	D	333	ARG
1	D	344	LEU
1	D	347	LYS
1	D	370	GLN
1	D	377	LEU
1	D	380	LYS
1	D	437	SER
1	D	448	ARG
1	D	473	ARG
1	D	519	SER
1	D	521	LYS
1	D	546	LEU
1	D	554	GLN
1	D	571	VAL
1	D	580	GLU

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Mol	Chain	Res	Type
1	D	599	ARG
1	D	600	GLN
1	D	630	ARG
1	D	645	ARG
1	D	651	LEU
1	D	655	MET
1	D	665	SER
1	D	672	VAL
1	D	684	GLU
1	D	687	GLN
1	D	690	SER
1	D	710	GLU
1	D	719	GLN
1	D	730	LEU
1	D	734	SER
1	D	741	THR
1	D	743	SER
1	D	749	ILE
1	D	751	LEU
1	D	753	ASN
1	D	755	ARG
1	D	761	GLN
1	D	768	MET
1	D	778	THR
1	D	781	ARG
1	D	797	GLU
1	D	799	THR
1	D	800	ARG
1	D	801	ILE
1	D	824	GLN
1	D	829	THR
1	D	832	ASP
1	D	867	THR
1	D	881	ARG
1	D	893	GLU
1	D	894	ARG
1	D	903[A]	GLN
1	D	903[B]	GLN
1	D	938	ARG
1	D	952	ARG
1	D	956	GLN
1	D	965	GLN

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Mol	Chain	Res	Type
1	D	986	ILE
1	D	1006	GLU
1	D	1017	GLN
1	D	1023	LYS
1	E	3	ILE
1	E	9	VAL
1	E	14	ARG
1	E	37	ARG
1	E	39	SER
1	E	46	ARG
1	E	48	SER
1	E	49	GLN
1	E	50	GLN
1	E	52	ARG
1	E	57	GLU
1	E	59	ARG
1	E	71	GLU
1	E	72	SER
1	E	80	GLU
1	E	84	VAL
1	E	90	TRP
1	E	114	VAL
1	E	116	THR
1	E	125	LEU
1	E	128	ASN
1	E	131	GLU
1	E	136	GLU
1	E	165	SER
1	E	166	ARG
1	E	171	PHE
1	E	189	LEU
1	E	190	ARG
1	E	202	MET
1	E	210	ARG
1	E	211	ASP
1	E	217	LYS
1	E	219	THR
1	E	227	VAL
1	E	237	ARG
1	E	246	MET
1	E	247	CYS
1	E	249	GLU

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Mol	Chain	Res	Type
1	E	250	LEU
1	E	251	ARG
1	E	259	SER
1	E	262	GLN
1	E	279	ILE
1	E	299	LYS
1	E	310	ARG
1	E	314	GLU
1	E	319	ASP
1	E	333	ARG
1	E	344	LEU
1	E	347	LYS
1	E	370	GLN
1	E	377	LEU
1	E	380	LYS
1	E	437	SER
1	E	448	ARG
1	E	473	ARG
1	E	519	SER
1	E	521	LYS
1	E	546	LEU
1	E	554	GLN
1	E	571	VAL
1	E	580	GLU
1	E	599	ARG
1	E	600	GLN
1	E	630	ARG
1	E	645	ARG
1	E	651	LEU
1	E	655	MET
1	E	665	SER
1	E	672	VAL
1	E	684	GLU
1	E	687	GLN
1	E	690	SER
1	E	710	GLU
1	E	719	GLN
1	E	730	LEU
1	E	734	SER
1	E	741	THR
1	E	743	SER
1	E	749	ILE

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Mol	Chain	Res	Type
1	E	751	LEU
1	E	753	ASN
1	E	755	ARG
1	E	761	GLN
1	E	768	MET
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	824	GLN
1	E	829	THR
1	E	832	ASP
1	E	867	THR
1	E	881	ARG
1	E	893	GLU
1	E	894	ARG
1	E	903[A]	GLN
1	E	903[B]	GLN
1	E	938	ARG
1	E	952	ARG
1	E	956	GLN
1	E	965	GLN
1	E	986	ILE
1	E	1006	GLU
1	E	1017	GLN
1	E	1023	LYS
1	F	3	ILE
1	F	9	VAL
1	F	14	ARG
1	F	37	ARG
1	F	39	SER
1	F	46	ARG
1	F	48	SER
1	F	49	GLN
1	F	50	GLN
1	F	52	ARG
1	F	57	GLU
1	F	59	ARG
1	F	71	GLU
1	F	72	SER

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Mol	Chain	Res	Type
1	F	80	GLU
1	F	84	VAL
1	F	90	TRP
1	F	114	VAL
1	F	116	THR
1	F	125	LEU
1	F	128	ASN
1	F	131	GLU
1	F	136	GLU
1	F	165	SER
1	F	166	ARG
1	F	171	PHE
1	F	189	LEU
1	F	190	ARG
1	F	202	MET
1	F	210	ARG
1	F	211	ASP
1	F	217	LYS
1	F	219	THR
1	F	227	VAL
1	F	237	ARG
1	F	246	MET
1	F	247	CYS
1	F	249	GLU
1	F	250	LEU
1	F	251	ARG
1	F	259	SER
1	F	262	GLN
1	F	279	ILE
1	F	299	LYS
1	F	310	ARG
1	F	314	GLU
1	F	319	ASP
1	F	333	ARG
1	F	344	LEU
1	F	347	LYS
1	F	370	GLN
1	F	377	LEU
1	F	380	LYS
1	F	437	SER
1	F	448	ARG
1	F	473	ARG

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Mol	Chain	Res	Type
1	F	519	SER
1	F	521	LYS
1	F	546	LEU
1	F	554	GLN
1	F	571	VAL
1	F	580	GLU
1	F	599	ARG
1	F	600	GLN
1	F	630	ARG
1	F	645	ARG
1	F	651	LEU
1	F	655	MET
1	F	665	SER
1	F	672	VAL
1	F	684	GLU
1	F	687	GLN
1	F	690	SER
1	F	710	GLU
1	F	719	GLN
1	F	730	LEU
1	F	734	SER
1	F	741	THR
1	F	743	SER
1	F	749	ILE
1	F	751	LEU
1	F	753	ASN
1	F	755	ARG
1	F	761	GLN
1	F	768	MET
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	824	GLN
1	F	829	THR
1	F	832	ASP
1	F	867	THR
1	F	881	ARG
1	F	893	GLU
1	F	894	ARG

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Mol	Chain	Res	Type
1	F	903[A]	GLN
1	F	903[B]	GLN
1	F	938	ARG
1	F	952	ARG
1	F	956	GLN
1	F	965	GLN
1	F	986	ILE
1	F	1006	GLU
1	F	1017	GLN
1	F	1023	LYS
1	G	3	ILE
1	G	9	VAL
1	G	14	ARG
1	G	37	ARG
1	G	39	SER
1	G	46	ARG
1	G	48	SER
1	G	49	GLN
1	G	50	GLN
1	G	52	ARG
1	G	57	GLU
1	G	59	ARG
1	G	71	GLU
1	G	72	SER
1	G	80	GLU
1	G	84	VAL
1	G	90	TRP
1	G	114	VAL
1	G	116	THR
1	G	125	LEU
1	G	128	ASN
1	G	131	GLU
1	G	136	GLU
1	G	165	SER
1	G	166	ARG
1	G	171	PHE
1	G	189	LEU
1	G	190	ARG
1	G	202	MET
1	G	210	ARG
1	G	211	ASP
1	G	217	LYS

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Mol	Chain	Res	Type
1	G	219	THR
1	G	227	VAL
1	G	237	ARG
1	G	246	MET
1	G	247	CYS
1	G	249	GLU
1	G	250	LEU
1	G	251	ARG
1	G	259	SER
1	G	262	GLN
1	G	279	ILE
1	G	299	LYS
1	G	310	ARG
1	G	314	GLU
1	G	319	ASP
1	G	333	ARG
1	G	344	LEU
1	G	347	LYS
1	G	370	GLN
1	G	377	LEU
1	G	380	LYS
1	G	437	SER
1	G	448	ARG
1	G	473	ARG
1	G	519	SER
1	G	521	LYS
1	G	546	LEU
1	G	554	GLN
1	G	571	VAL
1	G	580	GLU
1	G	599	ARG
1	G	600	GLN
1	G	630	ARG
1	G	645	ARG
1	G	651	LEU
1	G	655	MET
1	G	665	SER
1	G	672	VAL
1	G	684	GLU
1	G	687	GLN
1	G	690	SER
1	G	710	GLU

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Mol	Chain	Res	Type
1	G	719	GLN
1	G	730	LEU
1	G	734	SER
1	G	741	THR
1	G	743	SER
1	G	749	ILE
1	G	751	LEU
1	G	753	ASN
1	G	755	ARG
1	G	761	GLN
1	G	768	MET
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	824	GLN
1	G	829	THR
1	G	832	ASP
1	G	867	THR
1	G	881	ARG
1	G	893	GLU
1	G	894	ARG
1	G	903[A]	GLN
1	G	903[B]	GLN
1	G	938	ARG
1	G	952	ARG
1	G	956	GLN
1	G	965	GLN
1	G	986	ILE
1	G	1006	GLU
1	G	1017	GLN
1	G	1023	LYS
1	H	3	ILE
1	H	9	VAL
1	H	14	ARG
1	H	37	ARG
1	H	39	SER
1	H	46	ARG
1	H	48	SER
1	H	49	GLN

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Mol	Chain	Res	Type
1	H	50	GLN
1	H	52	ARG
1	H	57	GLU
1	H	59	ARG
1	H	71	GLU
1	H	72	SER
1	H	80	GLU
1	H	84	VAL
1	H	90	TRP
1	H	114	VAL
1	H	116	THR
1	H	125	LEU
1	H	128	ASN
1	H	131	GLU
1	H	136	GLU
1	H	165	SER
1	H	166	ARG
1	H	171	PHE
1	H	189	LEU
1	H	190	ARG
1	H	202	MET
1	H	210	ARG
1	H	211	ASP
1	H	217	LYS
1	H	219	THR
1	H	227	VAL
1	H	237	ARG
1	H	246	MET
1	H	247	CYS
1	H	249	GLU
1	H	250	LEU
1	H	251	ARG
1	H	259	SER
1	H	262	GLN
1	H	279	ILE
1	H	299	LYS
1	H	310	ARG
1	H	314	GLU
1	H	319	ASP
1	H	333	ARG
1	H	344	LEU
1	H	347	LYS

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Mol	Chain	Res	Type
1	H	370	GLN
1	H	377	LEU
1	H	380	LYS
1	H	437	SER
1	H	448	ARG
1	H	473	ARG
1	H	519	SER
1	H	521	LYS
1	H	546	LEU
1	H	554	GLN
1	H	571	VAL
1	H	580	GLU
1	H	599	ARG
1	H	600	GLN
1	H	630	ARG
1	H	645	ARG
1	H	651	LEU
1	H	655	MET
1	H	665	SER
1	H	672	VAL
1	H	684	GLU
1	H	687	GLN
1	H	690	SER
1	H	710	GLU
1	H	719	GLN
1	H	730	LEU
1	H	734	SER
1	H	741	THR
1	H	743	SER
1	H	749	ILE
1	H	751	LEU
1	H	753	ASN
1	H	755	ARG
1	H	761	GLN
1	H	768	MET
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	824	GLN

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Mol	Chain	Res	Type
1	H	829	THR
1	H	832	ASP
1	H	867	THR
1	H	881	ARG
1	H	893	GLU
1	H	894	ARG
1	H	903[A]	GLN
1	H	903[B]	GLN
1	H	938	ARG
1	H	952	ARG
1	H	956	GLN
1	H	965	GLN
1	H	986	ILE
1	H	1006	GLU
1	H	1017	GLN
1	H	1023	LYS
1	I	3	ILE
1	I	9	VAL
1	I	14	ARG
1	I	37	ARG
1	I	39	SER
1	I	46	ARG
1	I	48	SER
1	I	49	GLN
1	I	50	GLN
1	I	52	ARG
1	I	57	GLU
1	I	59	ARG
1	I	71	GLU
1	I	72	SER
1	I	80	GLU
1	I	84	VAL
1	I	90	TRP
1	I	114	VAL
1	I	116	THR
1	I	125	LEU
1	I	128	ASN
1	I	131	GLU
1	I	136	GLU
1	I	165	SER
1	I	166	ARG
1	I	171	PHE

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Mol	Chain	Res	Type
1	I	189	LEU
1	I	190	ARG
1	I	202	MET
1	I	210	ARG
1	I	211	ASP
1	I	217	LYS
1	I	219	THR
1	I	227	VAL
1	I	237	ARG
1	I	246	MET
1	I	247	CYS
1	I	249	GLU
1	I	250	LEU
1	I	251	ARG
1	I	259	SER
1	I	262	GLN
1	I	279	ILE
1	I	299	LYS
1	I	310	ARG
1	I	314	GLU
1	I	319	ASP
1	I	333	ARG
1	I	344	LEU
1	I	347	LYS
1	I	370	GLN
1	I	377	LEU
1	I	380	LYS
1	I	437	SER
1	I	448	ARG
1	I	473	ARG
1	I	519	SER
1	I	521	LYS
1	I	546	LEU
1	I	554	GLN
1	I	571	VAL
1	I	580	GLU
1	I	599	ARG
1	I	600	GLN
1	I	630	ARG
1	I	645	ARG
1	I	651	LEU
1	I	655	MET

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Mol	Chain	Res	Type
1	I	665	SER
1	I	672	VAL
1	I	684	GLU
1	I	687	GLN
1	I	690	SER
1	I	710	GLU
1	I	719	GLN
1	I	730	LEU
1	I	734	SER
1	I	741	THR
1	I	743	SER
1	I	749	ILE
1	I	751	LEU
1	I	753	ASN
1	I	755	ARG
1	I	761	GLN
1	I	768	MET
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	824	GLN
1	I	829	THR
1	I	832	ASP
1	I	867	THR
1	I	881	ARG
1	I	893	GLU
1	I	894	ARG
1	I	903[A]	GLN
1	I	903[B]	GLN
1	I	938	ARG
1	I	952	ARG
1	I	956	GLN
1	I	965	GLN
1	I	986	ILE
1	I	1006	GLU
1	I	1017	GLN
1	I	1023	LYS
1	J	3	ILE
1	J	9	VAL

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Mol	Chain	Res	Type
1	J	14	ARG
1	J	37	ARG
1	J	39	SER
1	J	46	ARG
1	J	48	SER
1	J	49	GLN
1	J	50	GLN
1	J	52	ARG
1	J	57	GLU
1	J	59	ARG
1	J	71	GLU
1	J	72	SER
1	J	80	GLU
1	J	84	VAL
1	J	90	TRP
1	J	114	VAL
1	J	116	THR
1	J	125	LEU
1	J	128	ASN
1	J	131	GLU
1	J	136	GLU
1	J	165	SER
1	J	166	ARG
1	J	171	PHE
1	J	189	LEU
1	J	190	ARG
1	J	202	MET
1	J	210	ARG
1	J	211	ASP
1	J	217	LYS
1	J	219	THR
1	J	227	VAL
1	J	237	ARG
1	J	246	MET
1	J	247	CYS
1	J	249	GLU
1	J	250	LEU
1	J	251	ARG
1	J	259	SER
1	J	262	GLN
1	J	279	ILE
1	J	299	LYS

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Mol	Chain	Res	Type
1	J	310	ARG
1	J	314	GLU
1	J	319	ASP
1	J	333	ARG
1	J	344	LEU
1	J	347	LYS
1	J	370	GLN
1	J	377	LEU
1	J	380	LYS
1	J	437	SER
1	J	448	ARG
1	J	473	ARG
1	J	519	SER
1	J	521	LYS
1	J	546	LEU
1	J	554	GLN
1	J	571	VAL
1	J	580	GLU
1	J	599	ARG
1	J	600	GLN
1	J	630	ARG
1	J	645	ARG
1	J	651	LEU
1	J	655	MET
1	J	665	SER
1	J	672	VAL
1	J	684	GLU
1	J	687	GLN
1	J	690	SER
1	J	710	GLU
1	J	719	GLN
1	J	730	LEU
1	J	734	SER
1	J	741	THR
1	J	743	SER
1	J	749	ILE
1	J	751	LEU
1	J	753	ASN
1	J	755	ARG
1	J	761	GLN
1	J	768	MET
1	J	778	THR

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Mol	Chain	Res	Type
1	J	781	ARG
1	J	797	GLU
1	J	799	THR
1	J	800	ARG
1	J	801	ILE
1	J	824	GLN
1	J	829	THR
1	J	832	ASP
1	J	867	THR
1	J	881	ARG
1	J	893	GLU
1	J	894	ARG
1	J	903[A]	GLN
1	J	903[B]	GLN
1	J	938	ARG
1	J	952	ARG
1	J	956	GLN
1	J	965	GLN
1	J	986	ILE
1	J	1006	GLU
1	J	1017	GLN
1	J	1023	LYS
1	K	3	ILE
1	K	9	VAL
1	K	14	ARG
1	K	37	ARG
1	K	39	SER
1	K	46	ARG
1	K	48	SER
1	K	49	GLN
1	K	50	GLN
1	K	52	ARG
1	K	57	GLU
1	K	59	ARG
1	K	71	GLU
1	K	72	SER
1	K	80	GLU
1	K	84	VAL
1	K	90	TRP
1	K	114	VAL
1	K	116	THR
1	K	125	LEU

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Mol	Chain	Res	Type
1	K	128	ASN
1	K	131	GLU
1	K	136	GLU
1	K	165	SER
1	K	166	ARG
1	K	171	PHE
1	K	189	LEU
1	K	190	ARG
1	K	202	MET
1	K	210	ARG
1	K	211	ASP
1	K	217	LYS
1	K	219	THR
1	K	227	VAL
1	K	237	ARG
1	K	246	MET
1	K	247	CYS
1	K	249	GLU
1	K	250	LEU
1	K	251	ARG
1	K	259	SER
1	K	262	GLN
1	K	279	ILE
1	K	299	LYS
1	K	310	ARG
1	K	314	GLU
1	K	319	ASP
1	K	333	ARG
1	K	344	LEU
1	K	347	LYS
1	K	370	GLN
1	K	377	LEU
1	K	380	LYS
1	K	437	SER
1	K	448	ARG
1	K	473	ARG
1	K	519	SER
1	K	521	LYS
1	K	546	LEU
1	K	554	GLN
1	K	571	VAL
1	K	580	GLU

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Mol	Chain	Res	Type
1	K	599	ARG
1	K	600	GLN
1	K	630	ARG
1	K	645	ARG
1	K	651	LEU
1	K	655	MET
1	K	665	SER
1	K	672	VAL
1	K	684	GLU
1	K	687	GLN
1	K	690	SER
1	K	710	GLU
1	K	719	GLN
1	K	730	LEU
1	K	734	SER
1	K	741	THR
1	K	743	SER
1	K	749	ILE
1	K	751	LEU
1	K	753	ASN
1	K	755	ARG
1	K	761	GLN
1	K	768	MET
1	K	778	THR
1	K	781	ARG
1	K	797	GLU
1	K	799	THR
1	K	800	ARG
1	K	801	ILE
1	K	824	GLN
1	K	829	THR
1	K	832	ASP
1	K	867	THR
1	K	881	ARG
1	K	893	GLU
1	K	894	ARG
1	K	903[A]	GLN
1	K	903[B]	GLN
1	K	938	ARG
1	K	952	ARG
1	K	956	GLN
1	K	965	GLN

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Mol	Chain	Res	Type
1	K	986	ILE
1	K	1006	GLU
1	K	1017	GLN
1	K	1023	LYS
1	L	3	ILE
1	L	9	VAL
1	L	14	ARG
1	L	37	ARG
1	L	39	SER
1	L	46	ARG
1	L	48	SER
1	L	49	GLN
1	L	50	GLN
1	L	52	ARG
1	L	57	GLU
1	L	59	ARG
1	L	71	GLU
1	L	72	SER
1	L	80	GLU
1	L	84	VAL
1	L	90	TRP
1	L	114	VAL
1	L	116	THR
1	L	125	LEU
1	L	128	ASN
1	L	131	GLU
1	L	136	GLU
1	L	165	SER
1	L	166	ARG
1	L	171	PHE
1	L	189	LEU
1	L	190	ARG
1	L	202	MET
1	L	210	ARG
1	L	211	ASP
1	L	217	LYS
1	L	219	THR
1	L	227	VAL
1	L	237	ARG
1	L	246	MET
1	L	247	CYS
1	L	249	GLU

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Mol	Chain	Res	Type
1	L	250	LEU
1	L	251	ARG
1	L	259	SER
1	L	262	GLN
1	L	279	ILE
1	L	299	LYS
1	L	310	ARG
1	L	314	GLU
1	L	319	ASP
1	L	333	ARG
1	L	344	LEU
1	L	347	LYS
1	L	370	GLN
1	L	377	LEU
1	L	380	LYS
1	L	437	SER
1	L	448	ARG
1	L	473	ARG
1	L	519	SER
1	L	521	LYS
1	L	546	LEU
1	L	554	GLN
1	L	571	VAL
1	L	580	GLU
1	L	599	ARG
1	L	600	GLN
1	L	630	ARG
1	L	645	ARG
1	L	651	LEU
1	L	655	MET
1	L	665	SER
1	L	672	VAL
1	L	684	GLU
1	L	687	GLN
1	L	690	SER
1	L	710	GLU
1	L	719	GLN
1	L	730	LEU
1	L	734	SER
1	L	741	THR
1	L	743	SER
1	L	749	ILE

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Mol	Chain	Res	Type
1	L	751	LEU
1	L	753	ASN
1	L	755	ARG
1	L	761	GLN
1	L	768	MET
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	824	GLN
1	L	829	THR
1	L	832	ASP
1	L	867	THR
1	L	881	ARG
1	L	893	GLU
1	L	894	ARG
1	L	903[A]	GLN
1	L	903[B]	GLN
1	L	938	ARG
1	L	952	ARG
1	L	956	GLN
1	L	965	GLN
1	L	986	ILE
1	L	1006	GLU
1	L	1017	GLN
1	L	1023	LYS
1	M	3	ILE
1	M	9	VAL
1	M	14	ARG
1	M	37	ARG
1	M	39	SER
1	M	46	ARG
1	M	48	SER
1	M	49	GLN
1	M	50	GLN
1	M	52	ARG
1	M	57	GLU
1	M	59	ARG
1	M	71	GLU
1	M	72	SER

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Mol	Chain	Res	Type
1	M	80	GLU
1	M	84	VAL
1	M	90	TRP
1	M	114	VAL
1	M	116	THR
1	M	125	LEU
1	M	128	ASN
1	M	131	GLU
1	M	136	GLU
1	M	165	SER
1	M	166	ARG
1	M	171	PHE
1	M	189	LEU
1	M	190	ARG
1	M	202	MET
1	M	210	ARG
1	M	211	ASP
1	M	217	LYS
1	M	219	THR
1	M	227	VAL
1	M	237	ARG
1	M	246	MET
1	M	247	CYS
1	M	249	GLU
1	M	250	LEU
1	M	251	ARG
1	M	259	SER
1	M	262	GLN
1	M	279	ILE
1	M	299	LYS
1	M	310	ARG
1	M	314	GLU
1	M	319	ASP
1	M	333	ARG
1	M	344	LEU
1	M	347	LYS
1	M	370	GLN
1	M	377	LEU
1	M	380	LYS
1	M	437	SER
1	M	448	ARG
1	M	473	ARG

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Mol	Chain	Res	Type
1	M	519	SER
1	M	521	LYS
1	M	546	LEU
1	M	554	GLN
1	M	571	VAL
1	M	580	GLU
1	M	599	ARG
1	M	600	GLN
1	M	630	ARG
1	M	645	ARG
1	M	651	LEU
1	M	655	MET
1	M	665	SER
1	M	672	VAL
1	M	684	GLU
1	M	687	GLN
1	M	690	SER
1	M	710	GLU
1	M	719	GLN
1	M	730	LEU
1	M	734	SER
1	M	741	THR
1	M	743	SER
1	M	749	ILE
1	M	751	LEU
1	M	753	ASN
1	M	755	ARG
1	M	761	GLN
1	M	768	MET
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	824	GLN
1	M	829	THR
1	M	832	ASP
1	M	867	THR
1	M	881	ARG
1	M	893	GLU
1	M	894	ARG

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Mol	Chain	Res	Type
1	M	903[A]	GLN
1	M	903[B]	GLN
1	M	938	ARG
1	M	952	ARG
1	M	956	GLN
1	M	965	GLN
1	M	986	ILE
1	M	1006	GLU
1	M	1017	GLN
1	M	1023	LYS
1	N	3	ILE
1	N	9	VAL
1	N	14	ARG
1	N	37	ARG
1	N	39	SER
1	N	46	ARG
1	N	48	SER
1	N	49	GLN
1	N	50	GLN
1	N	52	ARG
1	N	57	GLU
1	N	59	ARG
1	N	71	GLU
1	N	72	SER
1	N	80	GLU
1	N	84	VAL
1	N	90	TRP
1	N	114	VAL
1	N	116	THR
1	N	125	LEU
1	N	128	ASN
1	N	131	GLU
1	N	136	GLU
1	N	165	SER
1	N	166	ARG
1	N	171	PHE
1	N	189	LEU
1	N	190	ARG
1	N	202	MET
1	N	210	ARG
1	N	211	ASP
1	N	217	LYS

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Mol	Chain	Res	Type
1	N	219	THR
1	N	227	VAL
1	N	237	ARG
1	N	246	MET
1	N	247	CYS
1	N	249	GLU
1	N	250	LEU
1	N	251	ARG
1	N	259	SER
1	N	262	GLN
1	N	279	ILE
1	N	299	LYS
1	N	310	ARG
1	N	314	GLU
1	N	319	ASP
1	N	333	ARG
1	N	344	LEU
1	N	347	LYS
1	N	370	GLN
1	N	377	LEU
1	N	380	LYS
1	N	437	SER
1	N	448	ARG
1	N	473	ARG
1	N	519	SER
1	N	521	LYS
1	N	546	LEU
1	N	554	GLN
1	N	571	VAL
1	N	580	GLU
1	N	599	ARG
1	N	600	GLN
1	N	630	ARG
1	N	645	ARG
1	N	651	LEU
1	N	655	MET
1	N	665	SER
1	N	672	VAL
1	N	684	GLU
1	N	687	GLN
1	N	690	SER
1	N	710	GLU

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Mol	Chain	Res	Type
1	N	719	GLN
1	N	730	LEU
1	N	734	SER
1	N	741	THR
1	N	743	SER
1	N	749	ILE
1	N	751	LEU
1	N	753	ASN
1	N	755	ARG
1	N	761	GLN
1	N	768	MET
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	824	GLN
1	N	829	THR
1	N	832	ASP
1	N	867	THR
1	N	881	ARG
1	N	893	GLU
1	N	894	ARG
1	N	903[A]	GLN
1	N	903[B]	GLN
1	N	938	ARG
1	N	952	ARG
1	N	956	GLN
1	N	965	GLN
1	N	986	ILE
1	N	1006	GLU
1	N	1017	GLN
1	N	1023	LYS
1	O	3	ILE
1	O	9	VAL
1	O	14	ARG
1	O	37	ARG
1	O	39	SER
1	O	46	ARG
1	O	48	SER
1	O	49	GLN

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Mol	Chain	Res	Type
1	O	50	GLN
1	O	52	ARG
1	O	57	GLU
1	O	59	ARG
1	O	71	GLU
1	O	72	SER
1	O	80	GLU
1	O	84	VAL
1	O	90	TRP
1	O	114	VAL
1	O	116	THR
1	O	125	LEU
1	O	128	ASN
1	O	131	GLU
1	O	136	GLU
1	O	165	SER
1	O	166	ARG
1	O	171	PHE
1	O	189	LEU
1	O	190	ARG
1	O	202	MET
1	O	210	ARG
1	O	211	ASP
1	O	217	LYS
1	O	219	THR
1	O	227	VAL
1	O	237	ARG
1	O	246	MET
1	O	247	CYS
1	O	249	GLU
1	O	250	LEU
1	O	251	ARG
1	O	259	SER
1	O	262	GLN
1	O	279	ILE
1	O	299	LYS
1	O	310	ARG
1	O	314	GLU
1	O	319	ASP
1	O	333	ARG
1	O	344	LEU
1	O	347	LYS

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Mol	Chain	Res	Type
1	O	370	GLN
1	O	377	LEU
1	O	380	LYS
1	O	437	SER
1	O	448	ARG
1	O	473	ARG
1	O	519	SER
1	O	521	LYS
1	O	546	LEU
1	O	554	GLN
1	O	571	VAL
1	O	580	GLU
1	O	599	ARG
1	O	600	GLN
1	O	630	ARG
1	O	645	ARG
1	O	651	LEU
1	O	655	MET
1	O	665	SER
1	O	672	VAL
1	O	684	GLU
1	O	687	GLN
1	O	690	SER
1	O	710	GLU
1	O	719	GLN
1	O	730	LEU
1	O	734	SER
1	O	741	THR
1	O	743	SER
1	O	749	ILE
1	O	751	LEU
1	O	753	ASN
1	O	755	ARG
1	O	761	GLN
1	O	768	MET
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	824	GLN

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Mol	Chain	Res	Type
1	O	829	THR
1	O	832	ASP
1	O	867	THR
1	O	881	ARG
1	O	893	GLU
1	O	894	ARG
1	O	903[A]	GLN
1	O	903[B]	GLN
1	O	938	ARG
1	O	952	ARG
1	O	956	GLN
1	O	965	GLN
1	O	986	ILE
1	O	1006	GLU
1	O	1017	GLN
1	O	1023	LYS
1	P	3	ILE
1	P	9	VAL
1	P	14	ARG
1	P	37	ARG
1	P	39	SER
1	P	46	ARG
1	P	48	SER
1	P	49	GLN
1	P	50	GLN
1	P	52	ARG
1	P	57	GLU
1	P	59	ARG
1	P	71	GLU
1	P	72	SER
1	P	80	GLU
1	P	84	VAL
1	P	90	TRP
1	P	114	VAL
1	P	116	THR
1	P	125	LEU
1	P	128	ASN
1	P	131	GLU
1	P	136	GLU
1	P	165	SER
1	P	166	ARG
1	P	171	PHE

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Mol	Chain	Res	Type
1	P	189	LEU
1	P	190	ARG
1	P	202	MET
1	P	210	ARG
1	P	211	ASP
1	P	217	LYS
1	P	219	THR
1	P	227	VAL
1	P	237	ARG
1	P	246	MET
1	P	247	CYS
1	P	249	GLU
1	P	250	LEU
1	P	251	ARG
1	P	259	SER
1	P	262	GLN
1	P	279	ILE
1	P	299	LYS
1	P	310	ARG
1	P	314	GLU
1	P	319	ASP
1	P	333	ARG
1	P	344	LEU
1	P	347	LYS
1	P	370	GLN
1	P	377	LEU
1	P	380	LYS
1	P	437	SER
1	P	448	ARG
1	P	473	ARG
1	P	519	SER
1	P	521	LYS
1	P	546	LEU
1	P	554	GLN
1	P	571	VAL
1	P	580	GLU
1	P	599	ARG
1	P	600	GLN
1	P	630	ARG
1	P	645	ARG
1	P	651	LEU
1	P	655	MET

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Mol	Chain	Res	Type
1	P	665	SER
1	P	672	VAL
1	P	684	GLU
1	P	687	GLN
1	P	690	SER
1	P	710	GLU
1	P	719	GLN
1	P	730	LEU
1	P	734	SER
1	P	741	THR
1	P	743	SER
1	P	749	ILE
1	P	751	LEU
1	P	753	ASN
1	P	755	ARG
1	P	761	GLN
1	P	768	MET
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	824	GLN
1	P	829	THR
1	P	832	ASP
1	P	867	THR
1	P	881	ARG
1	P	893	GLU
1	P	894	ARG
1	P	903[A]	GLN
1	P	903[B]	GLN
1	P	938	ARG
1	P	952	ARG
1	P	956	GLN
1	P	965	GLN
1	P	986	ILE
1	P	1006	GLU
1	P	1017	GLN
1	P	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (346) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	128	ASN
1	A	226	HIS
1	A	262	GLN
1	A	294	ASN
1	A	316	HIS
1	A	445	GLN
1	A	467	ASN
1	A	485	GLN
1	A	581	ASN
1	A	597	ASN
1	A	604	ASN
1	A	624	GLN
1	A	675	GLN
1	A	739	HIS
1	A	761	GLN
1	A	817	GLN
1	A	824	GLN
1	A	885	ASN
1	A	949	HIS
1	A	950	GLN
1	A	990	HIS
1	A	1017	GLN
1	B	102	ASN
1	B	128	ASN
1	B	226	HIS
1	B	262	GLN
1	B	294	ASN
1	B	316	HIS
1	B	445	GLN
1	B	467	ASN
1	B	485	GLN
1	B	581	ASN
1	B	597	ASN
1	B	604	ASN
1	B	624	GLN
1	B	675	GLN
1	B	739	HIS
1	B	761	GLN
1	B	817	GLN
1	B	824	GLN
1	B	949	HIS
1	B	950	GLN

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Mol	Chain	Res	Type
1	B	990	HIS
1	B	1017	GLN
1	C	102	ASN
1	C	128	ASN
1	C	226	HIS
1	C	262	GLN
1	C	294	ASN
1	C	316	HIS
1	C	363	HIS
1	C	445	GLN
1	C	467	ASN
1	C	485	GLN
1	C	597	ASN
1	C	604	ASN
1	C	624	GLN
1	C	739	HIS
1	C	761	GLN
1	C	817	GLN
1	C	824	GLN
1	C	885	ASN
1	C	949	HIS
1	C	950	GLN
1	C	990	HIS
1	C	1017	GLN
1	D	102	ASN
1	D	128	ASN
1	D	226	HIS
1	D	262	GLN
1	D	294	ASN
1	D	316	HIS
1	D	445	GLN
1	D	467	ASN
1	D	485	GLN
1	D	597	ASN
1	D	604	ASN
1	D	624	GLN
1	D	739	HIS
1	D	761	GLN
1	D	817	GLN
1	D	824	GLN
1	D	885	ASN
1	D	949	HIS

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Mol	Chain	Res	Type
1	D	950	GLN
1	D	990	HIS
1	D	1017	GLN
1	E	102	ASN
1	E	128	ASN
1	E	226	HIS
1	E	262	GLN
1	E	294	ASN
1	E	316	HIS
1	E	445	GLN
1	E	467	ASN
1	E	485	GLN
1	E	597	ASN
1	E	604	ASN
1	E	624	GLN
1	E	675	GLN
1	E	739	HIS
1	E	761	GLN
1	E	817	GLN
1	E	824	GLN
1	E	949	HIS
1	E	950	GLN
1	E	990	HIS
1	E	1017	GLN
1	F	102	ASN
1	F	128	ASN
1	F	226	HIS
1	F	262	GLN
1	F	294	ASN
1	F	316	HIS
1	F	363	HIS
1	F	445	GLN
1	F	467	ASN
1	F	485	GLN
1	F	597	ASN
1	F	604	ASN
1	F	624	GLN
1	F	675	GLN
1	F	739	HIS
1	F	761	GLN
1	F	817	GLN
1	F	824	GLN

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Mol	Chain	Res	Type
1	F	949	HIS
1	F	950	GLN
1	F	990	HIS
1	F	1017	GLN
1	G	102	ASN
1	G	128	ASN
1	G	226	HIS
1	G	262	GLN
1	G	294	ASN
1	G	316	HIS
1	G	445	GLN
1	G	467	ASN
1	G	485	GLN
1	G	581	ASN
1	G	597	ASN
1	G	604	ASN
1	G	624	GLN
1	G	739	HIS
1	G	761	GLN
1	G	775	GLN
1	G	817	GLN
1	G	824	GLN
1	G	949	HIS
1	G	950	GLN
1	G	990	HIS
1	G	1017	GLN
1	H	102	ASN
1	H	128	ASN
1	H	226	HIS
1	H	262	GLN
1	H	294	ASN
1	H	316	HIS
1	H	445	GLN
1	H	467	ASN
1	H	485	GLN
1	H	597	ASN
1	H	604	ASN
1	H	624	GLN
1	H	675	GLN
1	H	739	HIS
1	H	761	GLN
1	H	817	GLN

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Mol	Chain	Res	Type
1	H	824	GLN
1	H	949	HIS
1	H	950	GLN
1	H	990	HIS
1	H	1017	GLN
1	I	102	ASN
1	I	128	ASN
1	I	226	HIS
1	I	262	GLN
1	I	294	ASN
1	I	316	HIS
1	I	445	GLN
1	I	467	ASN
1	I	485	GLN
1	I	581	ASN
1	I	597	ASN
1	I	604	ASN
1	I	624	GLN
1	I	675	GLN
1	I	739	HIS
1	I	761	GLN
1	I	817	GLN
1	I	824	GLN
1	I	949	HIS
1	I	950	GLN
1	I	990	HIS
1	I	1017	GLN
1	J	102	ASN
1	J	128	ASN
1	J	226	HIS
1	J	262	GLN
1	J	294	ASN
1	J	316	HIS
1	J	445	GLN
1	J	467	ASN
1	J	485	GLN
1	J	597	ASN
1	J	604	ASN
1	J	624	GLN
1	J	675	GLN
1	J	739	HIS
1	J	761	GLN

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Mol	Chain	Res	Type
1	J	817	GLN
1	J	824	GLN
1	J	949	HIS
1	J	950	GLN
1	J	990	HIS
1	J	1017	GLN
1	K	102	ASN
1	K	128	ASN
1	K	226	HIS
1	K	262	GLN
1	K	294	ASN
1	K	316	HIS
1	K	363	HIS
1	K	445	GLN
1	K	467	ASN
1	K	485	GLN
1	K	597	ASN
1	K	604	ASN
1	K	624	GLN
1	K	675	GLN
1	K	739	HIS
1	K	761	GLN
1	K	817	GLN
1	K	824	GLN
1	K	949	HIS
1	K	950	GLN
1	K	990	HIS
1	K	1017	GLN
1	L	102	ASN
1	L	128	ASN
1	L	226	HIS
1	L	262	GLN
1	L	294	ASN
1	L	316	HIS
1	L	445	GLN
1	L	467	ASN
1	L	485	GLN
1	L	581	ASN
1	L	597	ASN
1	L	604	ASN
1	L	624	GLN
1	L	739	HIS

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Mol	Chain	Res	Type
1	L	761	GLN
1	L	817	GLN
1	L	824	GLN
1	L	949	HIS
1	L	950	GLN
1	L	990	HIS
1	L	1017	GLN
1	M	102	ASN
1	M	128	ASN
1	M	226	HIS
1	M	262	GLN
1	M	294	ASN
1	M	316	HIS
1	M	445	GLN
1	M	467	ASN
1	M	597	ASN
1	M	604	ASN
1	M	614	HIS
1	M	624	GLN
1	M	675	GLN
1	M	739	HIS
1	M	761	GLN
1	M	817	GLN
1	M	824	GLN
1	M	949	HIS
1	M	950	GLN
1	M	990	HIS
1	M	1017	GLN
1	N	102	ASN
1	N	128	ASN
1	N	226	HIS
1	N	262	GLN
1	N	294	ASN
1	N	316	HIS
1	N	363	HIS
1	N	445	GLN
1	N	467	ASN
1	N	485	GLN
1	N	581	ASN
1	N	597	ASN
1	N	604	ASN
1	N	624	GLN

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Mol	Chain	Res	Type
1	N	739	HIS
1	N	761	GLN
1	N	817	GLN
1	N	824	GLN
1	N	949	HIS
1	N	950	GLN
1	N	990	HIS
1	N	1017	GLN
1	O	102	ASN
1	O	128	ASN
1	O	226	HIS
1	O	262	GLN
1	O	294	ASN
1	O	316	HIS
1	O	363	HIS
1	O	445	GLN
1	O	467	ASN
1	O	485	GLN
1	O	581	ASN
1	O	597	ASN
1	O	604	ASN
1	O	624	GLN
1	O	675	GLN
1	O	739	HIS
1	O	761	GLN
1	O	817	GLN
1	O	824	GLN
1	O	949	HIS
1	O	950	GLN
1	O	990	HIS
1	O	1017	GLN
1	P	102	ASN
1	P	128	ASN
1	P	226	HIS
1	P	262	GLN
1	P	294	ASN
1	P	316	HIS
1	P	445	GLN
1	P	467	ASN
1	P	597	ASN
1	P	604	ASN
1	P	624	GLN

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Mol	Chain	Res	Type
1	P	675	GLN
1	P	739	HIS
1	P	761	GLN
1	P	817	GLN
1	P	824	GLN
1	P	949	HIS
1	P	950	GLN
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	A	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	C	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.98	0
1	CME	D	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.40	1 (16%)
1	CME	G	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	P	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	G	914	1	8,9,10	0.84	0	6,9,11	1.72	1 (16%)
1	CME	J	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	O	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	K	1021	1	8,9,10	1.29	1 (12%)	6,9,11	3.40	1 (16%)
1	CME	M	748	1	8,9,10	0.92	1 (12%)	6,9,11	0.99	0
1	CME	C	1021	1	8,9,10	1.31	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	G	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CME	J	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	D	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	F	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	H	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	F	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	N	748	1	8,9,10	0.92	1 (12%)	6,9,11	0.99	0
1	CME	C	914	1	8,9,10	0.84	0	6,9,11	1.72	1 (16%)
1	CME	I	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	J	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	O	1021	1	8,9,10	1.31	1 (12%)	6,9,11	3.38	1 (16%)
1	CME	A	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	O	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	P	914	1	8,9,10	0.84	0	6,9,11	1.72	1 (16%)
1	CME	H	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	B	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	I	748	1	8,9,10	0.92	1 (12%)	6,9,11	0.99	0
1	CME	N	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	H	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	A	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	B	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	B	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	F	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	L	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	L	914	1	8,9,10	0.85	0	6,9,11	1.73	1 (16%)
1	CME	I	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	E	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.99	0
1	CME	E	914	1	8,9,10	0.84	0	6,9,11	1.72	1 (16%)
1	CME	D	914	1	8,9,10	0.84	0	6,9,11	1.72	1 (16%)
1	CME	K	748	1	8,9,10	0.93	1 (12%)	6,9,11	0.98	0
1	CME	E	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	K	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)
1	CME	L	1021	1	8,9,10	1.30	1 (12%)	6,9,11	3.39	1 (16%)
1	CME	M	914	1	8,9,10	0.86	0	6,9,11	1.72	1 (16%)
1	CME	P	748	1	8,9,10	0.92	1 (12%)	6,9,11	0.99	0
1	CME	N	914	1	8,9,10	0.85	0	6,9,11	1.72	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CME	M	1021	1	8,9,10	1.31	1 (12%)	6,9,11	3.39	1 (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
1	CME	A	914	1	-	3/5/8/10	-
1	CME	C	748	1	-	3/5/8/10	-
1	CME	D	1021	1	-	4/5/8/10	-
1	CME	G	748	1	-	3/5/8/10	-
1	CME	P	1021	1	-	4/5/8/10	-
1	CME	G	914	1	-	3/5/8/10	-
1	CME	J	914	1	-	3/5/8/10	-
1	CME	O	748	1	-	3/5/8/10	-
1	CME	K	1021	1	-	4/5/8/10	-
1	CME	M	748	1	-	3/5/8/10	-
1	CME	C	1021	1	-	4/5/8/10	-
1	CME	G	1021	1	-	4/5/8/10	-
1	CME	J	748	1	-	3/5/8/10	-
1	CME	D	748	1	-	3/5/8/10	-
1	CME	F	748	1	-	3/5/8/10	-
1	CME	H	914	1	-	3/5/8/10	-
1	CME	F	914	1	-	3/5/8/10	-
1	CME	N	748	1	-	3/5/8/10	-
1	CME	C	914	1	-	3/5/8/10	-
1	CME	I	914	1	-	3/5/8/10	-
1	CME	J	1021	1	-	4/5/8/10	-
1	CME	O	1021	1	-	4/5/8/10	-
1	CME	A	748	1	-	3/5/8/10	-
1	CME	O	914	1	-	3/5/8/10	-
1	CME	P	914	1	-	3/5/8/10	-
1	CME	H	748	1	-	3/5/8/10	-
1	CME	B	1021	1	-	4/5/8/10	-
1	CME	I	748	1	-	3/5/8/10	-

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

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	748	CME	CA-N	-2.50	1.41	1.48
1	H	748	CME	CA-N	-2.50	1.41	1.48
1	K	748	CME	CA-N	-2.50	1.41	1.48
1	F	748	CME	CA-N	-2.49	1.41	1.48
1	G	748	CME	CA-N	-2.49	1.41	1.48
1	L	748	CME	CA-N	-2.49	1.41	1.48
1	E	748	CME	CA-N	-2.49	1.41	1.48
1	O	748	CME	CA-N	-2.48	1.41	1.48
1	B	748	CME	CA-N	-2.48	1.41	1.48
1	A	748	CME	CA-N	-2.48	1.41	1.48
1	C	748	CME	CA-N	-2.48	1.41	1.48
1	D	748	CME	CA-N	-2.48	1.41	1.48
1	N	748	CME	CA-N	-2.47	1.41	1.48
1	M	748	CME	CA-N	-2.46	1.41	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	748	CME	CA-N	-2.46	1.41	1.48
1	I	748	CME	CA-N	-2.45	1.41	1.48
1	F	1021	CME	SD-SG	-2.16	1.88	2.03
1	N	1021	CME	SD-SG	-2.16	1.88	2.03
1	G	1021	CME	SD-SG	-2.16	1.88	2.03
1	O	1021	CME	SD-SG	-2.16	1.88	2.03
1	C	1021	CME	SD-SG	-2.15	1.88	2.03
1	A	1021	CME	SD-SG	-2.15	1.88	2.03
1	M	1021	CME	SD-SG	-2.15	1.88	2.03
1	J	1021	CME	SD-SG	-2.15	1.88	2.03
1	D	1021	CME	SD-SG	-2.15	1.88	2.03
1	H	1021	CME	SD-SG	-2.15	1.88	2.03
1	I	1021	CME	SD-SG	-2.15	1.88	2.03
1	B	1021	CME	SD-SG	-2.15	1.88	2.03
1	P	1021	CME	SD-SG	-2.14	1.88	2.03
1	L	1021	CME	SD-SG	-2.14	1.88	2.03
1	E	1021	CME	SD-SG	-2.14	1.88	2.03
1	K	1021	CME	SD-SG	-2.14	1.88	2.03

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1021	CME	CB-SG-SD	-8.04	83.06	103.86
1	K	1021	CME	CB-SG-SD	-8.03	83.07	103.86
1	P	1021	CME	CB-SG-SD	-8.03	83.08	103.86
1	N	1021	CME	CB-SG-SD	-8.03	83.09	103.86
1	I	1021	CME	CB-SG-SD	-8.02	83.10	103.86
1	L	1021	CME	CB-SG-SD	-8.02	83.10	103.86
1	E	1021	CME	CB-SG-SD	-8.02	83.11	103.86
1	A	1021	CME	CB-SG-SD	-8.02	83.11	103.86
1	F	1021	CME	CB-SG-SD	-8.02	83.11	103.86
1	J	1021	CME	CB-SG-SD	-8.02	83.11	103.86
1	H	1021	CME	CB-SG-SD	-8.02	83.11	103.86
1	G	1021	CME	CB-SG-SD	-8.02	83.11	103.86
1	B	1021	CME	CB-SG-SD	-8.02	83.11	103.86
1	M	1021	CME	CB-SG-SD	-8.01	83.12	103.86
1	C	1021	CME	CB-SG-SD	-8.01	83.12	103.86
1	O	1021	CME	CB-SG-SD	-8.00	83.15	103.86
1	C	914	CME	CB-SG-SD	-4.11	93.23	103.86
1	L	914	CME	CB-SG-SD	-4.11	93.24	103.86
1	B	914	CME	CB-SG-SD	-4.10	93.25	103.86
1	H	914	CME	CB-SG-SD	-4.10	93.26	103.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	914	CME	CB-SG-SD	-4.10	93.26	103.86
1	I	914	CME	CB-SG-SD	-4.10	93.26	103.86
1	M	914	CME	CB-SG-SD	-4.09	93.27	103.86
1	K	914	CME	CB-SG-SD	-4.09	93.27	103.86
1	J	914	CME	CB-SG-SD	-4.09	93.27	103.86
1	F	914	CME	CB-SG-SD	-4.09	93.27	103.86
1	N	914	CME	CB-SG-SD	-4.09	93.27	103.86
1	D	914	CME	CB-SG-SD	-4.09	93.28	103.86
1	G	914	CME	CB-SG-SD	-4.09	93.28	103.86
1	A	914	CME	CB-SG-SD	-4.09	93.28	103.86
1	O	914	CME	CB-SG-SD	-4.09	93.28	103.86
1	P	914	CME	CB-SG-SD	-4.08	93.29	103.86

There are no chirality outliers.

All (160) torsion outliers are listed below:

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

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

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

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

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Mol	Chain	Res	Type	Atoms
1	L	1021	CME	CZ-CE-SD-SG
1	M	748	CME	CZ-CE-SD-SG
1	M	1021	CME	CZ-CE-SD-SG
1	N	748	CME	CZ-CE-SD-SG
1	N	1021	CME	CZ-CE-SD-SG
1	O	748	CME	CZ-CE-SD-SG
1	O	1021	CME	CZ-CE-SD-SG
1	P	748	CME	CZ-CE-SD-SG
1	P	1021	CME	CZ-CE-SD-SG

There are no ring outliers.

32 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	914	CME	1	0
1	D	1021	CME	3	0
1	P	1021	CME	3	0
1	G	914	CME	1	0
1	J	914	CME	1	0
1	K	1021	CME	3	0
1	C	1021	CME	3	0
1	G	1021	CME	3	0
1	D	748	CME	1	0
1	H	914	CME	1	0
1	C	914	CME	1	0
1	I	914	CME	1	0
1	J	1021	CME	3	0
1	O	1021	CME	3	0
1	A	748	CME	1	0
1	O	914	CME	1	0
1	P	914	CME	1	0
1	B	1021	CME	3	0
1	N	1021	CME	3	0
1	H	1021	CME	3	0
1	A	1021	CME	3	0
1	B	914	CME	1	0
1	F	1021	CME	3	0
1	L	914	CME	1	0
1	I	1021	CME	3	0
1	D	914	CME	1	0
1	K	748	CME	1	0
1	E	1021	CME	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	K	914	CME	1	0
1	L	1021	CME	3	0
1	N	914	CME	1	0
1	M	1021	CME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 32 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	1018/1023 (99%)	-0.13	37 (3%)	46	41	3, 21, 66, 100	6 (0%)
1	B	1018/1023 (99%)	-0.11	36 (3%)	47	42	3, 21, 66, 100	6 (0%)
1	C	1018/1023 (99%)	-0.08	32 (3%)	51	47	2, 19, 63, 98	6 (0%)
1	D	1018/1023 (99%)	0.04	38 (3%)	45	40	5, 23, 67, 100	6 (0%)
1	E	1018/1023 (99%)	0.46	53 (5%)	33	29	15, 33, 74, 100	6 (0%)
1	F	1018/1023 (99%)	-0.18	31 (3%)	52	48	3, 21, 66, 100	6 (0%)
1	G	1018/1023 (99%)	-0.09	24 (2%)	59	55	7, 25, 68, 100	6 (0%)
1	H	1018/1023 (99%)	0.25	36 (3%)	47	42	14, 32, 73, 100	6 (0%)
1	I	1018/1023 (99%)	0.06	24 (2%)	59	55	10, 28, 70, 100	6 (0%)
1	J	1018/1023 (99%)	-0.07	31 (3%)	52	48	8, 26, 69, 100	6 (0%)
1	K	1018/1023 (99%)	0.09	14 (1%)	73	70	17, 35, 76, 100	6 (0%)
1	L	1018/1023 (99%)	0.20	26 (2%)	57	52	16, 34, 75, 100	6 (0%)
1	M	1018/1023 (99%)	1.07	156 (15%)	5	4	22, 40, 79, 100	6 (0%)
1	N	1018/1023 (99%)	0.06	26 (2%)	57	52	11, 29, 71, 100	6 (0%)
1	O	1018/1023 (99%)	0.04	25 (2%)	58	54	12, 30, 72, 100	6 (0%)
1	P	1018/1023 (99%)	1.49	262 (25%)	1	1	29, 47, 83, 100	6 (0%)
All	All	16288/16368 (99%)	0.19	851 (5%)	33	29	2, 30, 72, 100	96 (0%)

All (851) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	582	GLY	8.3
1	D	734	SER	7.3
1	A	581	ASN	7.0
1	B	582	GLY	6.4
1	P	739	HIS	6.1

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Mol	Chain	Res	Type	RSRZ
1	P	684	GLU	6.0
1	I	734	SER	5.8
1	I	735	HIS	5.7
1	L	739	HIS	5.7
1	P	364	GLY	5.7
1	H	582	GLY	5.4
1	A	580	GLU	5.1
1	D	735	HIS	4.9
1	B	581	ASN	4.9
1	A	180	GLY	4.9
1	M	133	TRP	4.8
1	A	682	LEU	4.8
1	A	179	ALA	4.8
1	M	735	HIS	4.6
1	M	162	GLY	4.5
1	M	596	PRO	4.5
1	I	596	PRO	4.5
1	P	664	ALA	4.5
1	A	583	ASN	4.4
1	B	596	PRO	4.4
1	F	75	GLU	4.4
1	P	149	ALA	4.4
1	P	81	ALA	4.4
1	D	832	ASP	4.3
1	J	735	HIS	4.3
1	P	313	VAL	4.3
1	M	16	TRP	4.3
1	C	760	ARG	4.3
1	P	685	LEU	4.3
1	E	832	ASP	4.3
1	P	70	PRO	4.2
1	M	160	GLY	4.2
1	B	583	ASN	4.2
1	A	178	ARG	4.2
1	P	204	ARG	4.2
1	B	832	ASP	4.2
1	M	69	VAL	4.2
1	C	735	HIS	4.2
1	H	581	ASN	4.2
1	M	9	VAL	4.1
1	E	734	SER	4.1
1	J	832	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	582	GLY	4.1
1	M	736	ALA	4.1
1	M	123	TYR	4.1
1	I	832	ASP	4.0
1	M	575	LEU	4.0
1	P	143	PHE	4.0
1	D	689	GLU	4.0
1	A	135	GLN	4.0
1	H	832	ASP	4.0
1	M	734	SER	4.0
1	F	76	CYS	4.0
1	P	794	GLY	4.0
1	B	737	ILE	4.0
1	O	735	HIS	4.0
1	P	596	PRO	4.0
1	P	284	GLY	3.9
1	P	209	PHE	3.9
1	P	162	GLY	3.9
1	M	832	ASP	3.9
1	P	158	TRP	3.9
1	O	744	GLU	3.9
1	P	683	PRO	3.9
1	I	736	ALA	3.9
1	P	96	ASP	3.8
1	P	405	TYR	3.8
1	P	55	ASN	3.8
1	E	596	PRO	3.8
1	P	115	PRO	3.8
1	P	35	SER	3.8
1	G	829	THR	3.8
1	L	3	ILE	3.8
1	G	832	ASP	3.8
1	P	575	LEU	3.8
1	G	581	ASN	3.8
1	C	746	ASP	3.8
1	P	651	LEU	3.8
1	P	923	SER	3.7
1	C	739	HIS	3.7
1	M	173	LEU	3.7
1	P	195	SER	3.7
1	P	203	TRP	3.7
1	N	735	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	689	GLU	3.7
1	A	131	GLU	3.6
1	M	149	ALA	3.6
1	P	34	ALA	3.6
1	M	66	PRO	3.6
1	D	736	ALA	3.6
1	M	860	GLY	3.6
1	M	691	ALA	3.6
1	P	86	VAL	3.6
1	P	160	GLY	3.5
1	M	143	PHE	3.5
1	P	576	ILE	3.5
1	P	102	ASN	3.5
1	B	739	HIS	3.5
1	N	1023	LYS	3.5
1	M	595	THR	3.5
1	L	685	LEU	3.5
1	M	6	SER	3.5
1	B	798	ALA	3.5
1	P	261	TRP	3.5
1	O	128	ASN	3.5
1	P	699[A]	ARG	3.5
1	P	153	TRP	3.5
1	A	832	ASP	3.5
1	C	744	GLU	3.5
1	M	689	GLU	3.5
1	L	682	LEU	3.5
1	M	65	ALA	3.5
1	P	191	TRP	3.5
1	J	582	GLY	3.4
1	M	115	PRO	3.4
1	P	180	GLY	3.4
1	O	743	SER	3.4
1	M	203	TRP	3.4
1	F	832	ASP	3.4
1	H	682	LEU	3.4
1	M	161	TYR	3.4
1	P	73	TRP	3.4
1	P	701	VAL	3.4
1	E	3	ILE	3.4
1	K	735	HIS	3.4
1	P	634	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	M	116	THR	3.4
1	H	253	TYR	3.3
1	M	76	CYS	3.3
1	N	832	ASP	3.3
1	L	687	GLN	3.3
1	P	36	TRP	3.3
1	P	74	LEU	3.3
1	C	742	THR	3.3
1	J	739	HIS	3.3
1	M	36	TRP	3.3
1	P	111	PRO	3.3
1	P	679	LEU	3.3
1	B	829	THR	3.3
1	H	684	GLU	3.3
1	I	733	ALA	3.3
1	P	714	ILE	3.3
1	C	745	MET	3.3
1	M	15	ASP	3.3
1	P	129	VAL	3.3
1	P	698	VAL	3.3
1	P	133	TRP	3.3
1	P	654	TRP	3.3
1	P	689	GLU	3.3
1	P	311	ALA	3.3
1	P	274	PHE	3.3
1	P	594	ASP	3.3
1	F	80	GLU	3.3
1	E	160	GLY	3.3
1	G	737	ILE	3.3
1	K	798	ALA	3.3
1	M	690	SER	3.2
1	D	687	GLN	3.2
1	P	687	GLN	3.2
1	H	596	PRO	3.2
1	M	184	LEU	3.2
1	E	798	ALA	3.2
1	P	690	SER	3.2
1	K	596	PRO	3.2
1	P	173	LEU	3.2
1	E	143	PHE	3.2
1	P	663	LEU	3.2
1	C	734	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	747	PHE	3.2
1	F	734	SER	3.2
1	D	739	HIS	3.2
1	P	395	HIS	3.2
1	P	661	LYS	3.2
1	P	186	VAL	3.2
1	J	736	ALA	3.1
1	P	138	GLN	3.1
1	M	73	TRP	3.1
1	P	58	TRP	3.1
1	L	735	HIS	3.1
1	O	745	MET	3.1
1	D	760	ARG	3.1
1	F	744	GLU	3.1
1	H	580	GLU	3.1
1	J	319	ASP	3.1
1	M	189	LEU	3.1
1	M	730	LEU	3.1
1	A	737	ILE	3.1
1	M	13	ARG	3.1
1	L	634	GLN	3.1
1	G	596	PRO	3.1
1	C	253	TYR	3.1
1	P	4	THR	3.1
1	L	684	GLU	3.1
1	P	314	GLU	3.1
1	C	832	ASP	3.1
1	P	189	LEU	3.1
1	M	191	TRP	3.1
1	N	760	ARG	3.1
1	D	799	THR	3.0
1	J	733	ALA	3.0
1	P	100	TYR	3.0
1	G	580	GLU	3.0
1	A	134	LEU	3.0
1	P	51	LEU	3.0
1	N	319	ASP	3.0
1	P	48	SER	3.0
1	M	140	ARG	3.0
1	P	398	TRP	3.0
1	C	733	ALA	3.0
1	P	97	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	80	GLU	3.0
1	K	739	HIS	3.0
1	I	730	LEU	3.0
1	C	319	ASP	3.0
1	D	747	PHE	3.0
1	F	319	ASP	3.0
1	M	274	PHE	3.0
1	P	206	SER	3.0
1	H	583	ASN	3.0
1	M	114	VAL	3.0
1	M	158	TRP	3.0
1	M	186	VAL	3.0
1	F	179	ALA	3.0
1	P	362	LEU	3.0
1	C	39	SER	3.0
1	I	829	THR	3.0
1	J	742	THR	3.0
1	D	733	ALA	3.0
1	E	735	HIS	3.0
1	N	739	HIS	3.0
1	A	596	PRO	3.0
1	L	686	PRO	3.0
1	N	746	ASP	3.0
1	F	687	GLN	3.0
1	M	737	ILE	2.9
1	M	75	GLU	2.9
1	F	735	HIS	2.9
1	P	65	ALA	2.9
1	P	98	PRO	2.9
1	F	320	GLY	2.9
1	J	320	GLY	2.9
1	M	141	ILE	2.9
1	P	681	GLU	2.9
1	P	930	VAL	2.9
1	P	116	THR	2.9
1	D	798	ALA	2.9
1	E	66	PRO	2.9
1	J	596	PRO	2.9
1	P	686	PRO	2.9
1	M	60	PHE	2.9
1	L	750	GLU	2.9
1	L	596	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	1023	LYS	2.9
1	D	730	LEU	2.9
1	P	16	TRP	2.9
1	E	689	GLU	2.9
1	M	710	GLU	2.9
1	P	109	VAL	2.9
1	C	179	ALA	2.9
1	D	596	PRO	2.9
1	H	4	THR	2.9
1	P	63	PHE	2.9
1	J	743	SER	2.8
1	M	93	HIS	2.8
1	M	185	ALA	2.8
1	P	585	TRP	2.8
1	A	684	GLU	2.8
1	C	13	ARG	2.8
1	A	128	ASN	2.8
1	M	3	ILE	2.8
1	O	583	ASN	2.8
1	M	84	VAL	2.8
1	M	688	PRO	2.8
1	I	729	THR	2.8
1	B	833	ALA	2.8
1	C	831	ALA	2.8
1	E	65	ALA	2.8
1	P	179	ALA	2.8
1	P	652	LEU	2.8
1	P	633	GLY	2.8
1	F	581	ASN	2.8
1	J	734	SER	2.8
1	D	729	THR	2.8
1	J	831	ALA	2.8
1	O	742	THR	2.8
1	M	54	LEU	2.8
1	P	381	GLN	2.8
1	A	579	ASP	2.8
1	P	737	ILE	2.8
1	D	829	THR	2.8
1	M	152	LEU	2.8
1	M	177	LEU	2.8
1	M	729	THR	2.8
1	M	732	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	N	733	ALA	2.8
1	P	920	LEU	2.8
1	A	157	ARG	2.8
1	M	135	GLN	2.8
1	M	687	GLN	2.8
1	P	190	ARG	2.8
1	E	133	TRP	2.7
1	H	79	PRO	2.7
1	M	55	ASN	2.7
1	P	123	TYR	2.7
1	P	9	VAL	2.7
1	P	258	VAL	2.7
1	M	362	LEU	2.7
1	P	215	LEU	2.7
1	E	661	LYS	2.7
1	D	136	GLU	2.7
1	P	746	ASP	2.7
1	D	737	ILE	2.7
1	O	734	SER	2.7
1	P	929	TYR	2.7
1	A	661	LYS	2.7
1	E	179	ALA	2.7
1	M	246	MET	2.7
1	P	441	THR	2.7
1	P	733	ALA	2.7
1	M	63	PHE	2.7
1	P	141	ILE	2.7
1	P	279	ILE	2.7
1	M	325	ALA	2.7
1	N	798	ALA	2.7
1	P	829	THR	2.7
1	M	247	CYS	2.7
1	M	248	GLY	2.7
1	F	79	PRO	2.7
1	P	259	SER	2.7
1	P	751	LEU	2.7
1	P	105	TYR	2.7
1	M	739	HIS	2.7
1	P	666	GLY	2.6
1	M	70	PRO	2.6
1	M	190	ARG	2.6
1	P	59	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	P	92	MET	2.6
1	B	730	LEU	2.6
1	M	78	LEU	2.6
1	P	54	LEU	2.6
1	P	177	LEU	2.6
1	D	49	GLN	2.6
1	E	116	THR	2.6
1	G	253	TYR	2.6
1	H	977[A]	HIS	2.6
1	M	576	ILE	2.6
1	M	731	PRO	2.6
1	N	800	ARG	2.6
1	O	730	LEU	2.6
1	P	89	ASN	2.6
1	M	195	SER	2.6
1	N	734	SER	2.6
1	B	179	ALA	2.6
1	K	799	THR	2.6
1	J	253	TYR	2.6
1	E	73	TRP	2.6
1	P	447	ASP	2.6
1	D	3	ILE	2.6
1	J	760	ARG	2.6
1	P	52	ARG	2.6
1	M	134	LEU	2.6
1	P	7	LEU	2.6
1	P	297	ASN	2.6
1	A	634	GLN	2.6
1	P	50	GLN	2.6
1	C	798	ALA	2.6
1	F	742	THR	2.6
1	J	799	THR	2.6
1	E	191	TRP	2.6
1	P	62	TRP	2.6
1	L	180	GLY	2.6
1	M	45	ASP	2.6
1	N	745	MET	2.6
1	C	3	ILE	2.6
1	M	323	ILE	2.6
1	P	376	ILE	2.6
1	P	171	PHE	2.6
1	B	580	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	7	LEU	2.6
1	H	685	LEU	2.6
1	A	965	GLN	2.6
1	E	595	THR	2.6
1	E	729	THR	2.6
1	G	742	THR	2.6
1	H	735	HIS	2.6
1	P	216	HIS	2.6
1	P	140	ARG	2.5
1	J	746	ASP	2.5
1	D	75	GLU	2.5
1	C	12	GLN	2.5
1	G	735	HIS	2.5
1	P	413	ALA	2.5
1	N	829	THR	2.5
1	P	632	SER	2.5
1	B	13	ARG	2.5
1	P	205	MET	2.5
1	M	112	PRO	2.5
1	P	688	PRO	2.5
1	M	96	ASP	2.5
1	P	832	ASP	2.5
1	E	733	ALA	2.5
1	M	798	ALA	2.5
1	P	185	ALA	2.5
1	M	253	TYR	2.5
1	M	683	PRO	2.5
1	G	180	GLY	2.5
1	A	681	GLU	2.5
1	M	249	GLU	2.5
1	M	714	ILE	2.5
1	P	756	TRP	2.5
1	F	685	LEU	2.5
1	M	138	GLN	2.5
1	P	49	GLN	2.5
1	P	360	HIS	2.5
1	C	38	ASN	2.5
1	L	179	ALA	2.5
1	P	13	ARG	2.5
1	P	691	ALA	2.5
1	N	742	THR	2.5
1	C	76	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	731	PRO	2.5
1	B	578	TYR	2.5
1	I	737	ILE	2.5
1	I	49	GLN	2.5
1	P	225	PHE	2.5
1	P	601	PHE	2.5
1	M	52	ARG	2.5
1	P	449	ASN	2.5
1	E	97	ALA	2.5
1	O	733	ALA	2.5
1	O	736	ALA	2.5
1	A	799	THR	2.5
1	M	192	SER	2.5
1	M	427	THR	2.5
1	P	139	THR	2.5
1	P	218	PRO	2.4
1	B	181	GLU	2.4
1	D	744	GLU	2.4
1	F	180	GLY	2.4
1	K	136	GLU	2.4
1	P	184	LEU	2.4
1	H	127	PHE	2.4
1	E	140	ARG	2.4
1	F	760	ARG	2.4
1	C	581	ASN	2.4
1	G	583	ASN	2.4
1	H	128	ASN	2.4
1	M	289	VAL	2.4
1	P	668	VAL	2.4
1	M	833	ALA	2.4
1	O	179	ALA	2.4
1	P	325	ALA	2.4
1	A	729	THR	2.4
1	O	731	PRO	2.4
1	P	738	PRO	2.4
1	A	76	CYS	2.4
1	B	860	GLY	2.4
1	C	320	GLY	2.4
1	F	1023	LYS	2.4
1	I	1023	LYS	2.4
1	J	1023	LYS	2.4
1	M	180	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	130	ASP	2.4
1	M	772	ASP	2.4
1	P	653[A]	HIS	2.4
1	M	14	ARG	2.4
1	M	127	PHE	2.4
1	E	16	TRP	2.4
1	P	21	VAL	2.4
1	P	103	VAL	2.4
1	J	745	MET	2.4
1	E	833	ALA	2.4
1	M	179	ALA	2.4
1	M	733	ALA	2.4
1	N	736	ALA	2.4
1	O	798	ALA	2.4
1	A	132	SER	2.4
1	O	180	GLY	2.4
1	F	746	ASP	2.4
1	P	3	ILE	2.4
1	P	99	ILE	2.4
1	P	247	CYS	2.4
1	P	636	ILE	2.4
1	M	291	LEU	2.4
1	F	59	ARG	2.4
1	J	13	ARG	2.4
1	M	113	PHE	2.4
1	M	225	PHE	2.4
1	P	127	PHE	2.4
1	D	745	MET	2.4
1	E	158	TRP	2.4
1	P	723	ALA	2.4
1	H	799	THR	2.4
1	I	686	PRO	2.4
1	I	731	PRO	2.4
1	M	861	SER	2.4
1	H	180	GLY	2.4
1	D	46	ARG	2.4
1	M	125	LEU	2.4
1	M	315	LEU	2.4
1	N	237	ARG	2.4
1	E	60	PHE	2.4
1	P	202	MET	2.4
1	P	332	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	753	ASN	2.4
1	D	732	ALA	2.4
1	M	831	ALA	2.4
1	P	68	ALA	2.4
1	C	75	GLU	2.4
1	B	79	PRO	2.3
1	B	584	PRO	2.3
1	E	36	TRP	2.4
1	I	744	GLU	2.4
1	L	683	PRO	2.3
1	P	90	TRP	2.4
1	N	743	SER	2.3
1	C	582	GLY	2.3
1	B	178	ARG	2.3
1	D	685	LEU	2.3
1	E	737	ILE	2.3
1	M	46	ARG	2.3
1	M	363	HIS	2.3
1	N	685	LEU	2.3
1	P	890	GLN	2.3
1	L	247	CYS	2.3
1	P	367	MET	2.3
1	B	253	TYR	2.3
1	P	161	TYR	2.3
1	B	129	VAL	2.3
1	E	186	VAL	2.3
1	M	21	VAL	2.3
1	E	131	GLU	2.3
1	I	179	ALA	2.3
1	J	744	GLU	2.3
1	E	115	PRO	2.3
1	G	731	PRO	2.3
1	B	799	THR	2.3
1	O	741	THR	2.3
1	P	265	THR	2.3
1	P	799	THR	2.3
1	P	574	SER	2.3
1	A	735	HIS	2.3
1	G	135	GLN	2.3
1	M	977[A]	HIS	2.3
1	P	167	LEU	2.3
1	F	745	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	187	MET	2.3
1	D	661	LYS	2.3
1	P	895	VAL	2.3
1	M	136	GLU	2.3
1	B	731	PRO	2.3
1	E	34	ALA	2.3
1	G	179	ALA	2.3
1	K	733	ALA	2.3
1	K	595	THR	2.3
1	E	72	SER	2.3
1	B	735	HIS	2.3
1	E	687	GLN	2.3
1	J	39	SER	2.3
1	M	72	SER	2.3
1	P	56	GLY	2.3
1	P	665	SER	2.3
1	M	7	LEU	2.3
1	M	322	LEU	2.3
1	N	3	ILE	2.3
1	P	78	LEU	2.3
1	P	397	LEU	2.3
1	P	682	LEU	2.3
1	B	579	ASP	2.3
1	P	443	MET	2.3
1	B	744	GLU	2.3
1	N	825	CYS	2.3
1	P	85	VAL	2.3
1	A	798	ALA	2.3
1	J	581	ASN	2.3
1	M	87	PRO	2.3
1	M	827	ALA	2.3
1	P	798	ALA	2.3
1	P	210	ARG	2.3
1	D	741	THR	2.3
1	M	799	THR	2.3
1	P	741	THR	2.3
1	M	49	GLN	2.3
1	P	977[A]	HIS	2.3
1	H	737	ILE	2.3
1	M	433	LEU	2.3
1	P	323	ILE	2.3
1	P	749	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	918	TRP	2.3
1	M	164	ASP	2.3
1	M	594	ASP	2.3
1	P	217	LYS	2.3
1	E	9	VAL	2.3
1	H	683	PRO	2.3
1	O	596	PRO	2.3
1	P	32	PRO	2.3
1	M	472	TYR	2.3
1	M	725	ASN	2.2
1	M	753	ASN	2.2
1	P	46	ARG	2.3
1	P	928	PRO	2.3
1	B	128	ASN	2.2
1	D	68	ALA	2.2
1	I	831	ALA	2.2
1	P	736	ALA	2.2
1	C	49	GLN	2.2
1	D	752	GLY	2.2
1	D	860	GLY	2.2
1	P	316	HIS	2.2
1	E	685	LEU	2.2
1	I	3	ILE	2.2
1	P	187	MET	2.2
1	P	603	MET	2.2
1	H	681	GLU	2.2
1	P	249	GLU	2.2
1	E	59	ARG	2.2
1	M	795	VAL	2.2
1	P	703	PRO	2.2
1	P	800	ARG	2.2
1	P	894	ARG	2.2
1	D	831	ALA	2.2
1	K	179	ALA	2.2
1	B	76	CYS	2.2
1	F	253	TYR	2.2
1	L	578	TYR	2.2
1	P	196	TYR	2.2
1	D	116	THR	2.2
1	M	829	THR	2.2
1	P	735	HIS	2.2
1	L	1023	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	981	GLY	2.2
1	P	1023	LYS	2.2
1	K	734	SER	2.2
1	P	72	SER	2.2
1	B	746	ASP	2.2
1	G	828	ASP	2.2
1	O	772	ASP	2.2
1	M	33	PHE	2.2
1	E	64	PRO	2.2
1	B	736	ALA	2.2
1	H	149	ALA	2.2
1	P	753	ASN	2.2
1	A	49	GLN	2.2
1	M	742	THR	2.2
1	P	328	CYS	2.2
1	P	745	MET	2.2
1	P	39	SER	2.2
1	H	178	ARG	2.2
1	M	59	ARG	2.2
1	P	60	PHE	2.2
1	M	515	VAL	2.2
1	P	244	VAL	2.2
1	E	889	ALA	2.2
1	F	798	ALA	2.2
1	G	827	ALA	2.2
1	H	179	ALA	2.2
1	J	661	LYS	2.2
1	L	733	ALA	2.2
1	C	824	GLN	2.2
1	N	817	GLN	2.2
1	P	266	GLN	2.2
1	A	595	THR	2.2
1	E	100	TYR	2.2
1	M	139	THR	2.2
1	P	101	THR	2.2
1	P	635	THR	2.2
1	H	134	LEU	2.2
1	P	377	LEU	2.2
1	P	378	LEU	2.2
1	E	690	SER	2.2
1	G	734	SER	2.2
1	M	48	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	132	SER	2.2
1	P	715	SER	2.2
1	M	47	PRO	2.2
1	P	708	TRP	2.2
1	E	739	HIS	2.1
1	H	798	ALA	2.1
1	J	318	ALA	2.1
1	E	78	LEU	2.1
1	K	730	LEU	2.1
1	L	78	LEU	2.1
1	P	44	THR	2.1
1	P	260	LEU	2.1
1	P	970	THR	2.1
1	C	737	ILE	2.1
1	J	578	TYR	2.1
1	J	801	ILE	2.1
1	A	136	GLU	2.1
1	D	690	SER	2.1
1	H	800	ARG	2.1
1	P	296	GLU	2.1
1	P	390	SER	2.1
1	P	734	SER	2.1
1	H	686	PRO	2.1
1	M	79	PRO	2.1
1	M	150	PHE	2.1
1	M	188	VAL	2.1
1	P	359	HIS	2.1
1	H	135	GLN	2.1
1	A	833	ALA	2.1
1	H	185	ALA	2.1
1	L	736	ALA	2.1
1	M	34	ALA	2.1
1	P	609	ALA	2.1
1	B	595	THR	2.1
1	H	595	THR	2.1
1	O	670	LEU	2.1
1	P	11	LEU	2.1
1	P	263	GLY	2.1
1	P	406	GLY	2.1
1	B	3	ILE	2.1
1	I	253	TYR	2.1
1	J	80	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	178	ARG	2.1
1	P	285	TYR	2.1
1	I	594	ASP	2.1
1	I	690	SER	2.1
1	P	130	ASP	2.1
1	P	174	SER	2.1
1	P	671	ASP	2.1
1	K	731	PRO	2.1
1	P	47	PRO	2.1
1	P	298	PRO	2.1
1	M	216	HIS	2.1
1	M	655	MET	2.1
1	H	634	GLN	2.1
1	M	312	VAL	2.1
1	B	831	ALA	2.1
1	C	732	ALA	2.1
1	P	286	ALA	2.1
1	B	180	GLY	2.1
1	D	740	LEU	2.1
1	E	730	LEU	2.1
1	H	679	LEU	2.1
1	P	830	LEU	2.1
1	P	417	THR	2.1
1	P	778	THR	2.1
1	D	857	ARG	2.1
1	O	800	ARG	2.1
1	P	178	ARG	2.1
1	P	630	ARG	2.1
1	P	1013	ARG	2.1
1	G	3	ILE	2.1
1	P	750	GLU	2.1
1	M	100	TYR	2.1
1	B	773	LYS	2.1
1	G	746	ASP	2.1
1	M	661	LYS	2.1
1	J	825	CYS	2.1
1	L	76	CYS	2.1
1	L	734	SER	2.1
1	O	746	ASP	2.1
1	P	5	ASP	2.1
1	P	572	ASP	2.1
1	P	743	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	79	PRO	2.1
1	F	596	PRO	2.1
1	M	19	PRO	2.1
1	N	596	PRO	2.1
1	G	370	GLN	2.1
1	L	143	PHE	2.1
1	L	965	GLN	2.1
1	P	146	VAL	2.1
1	E	732	ALA	2.1
1	F	733	ALA	2.1
1	O	732	ALA	2.1
1	P	818	ALA	2.1
1	C	759	ASN	2.1
1	N	128	ASN	2.1
1	P	125	LEU	2.1
1	P	401	LEU	2.1
1	P	725	ASN	2.1
1	P	676	GLY	2.1
1	P	692	GLY	2.1
1	P	901	GLY	2.1
1	A	689	GLU	2.1
1	M	741	THR	2.1
1	N	265	THR	2.1
1	N	744	GLU	2.1
1	P	22	THR	2.1
1	P	595	THR	2.1
1	F	39	SER	2.1
1	A	686	PRO	2.1
1	P	655	MET	2.1
1	O	135	GLN	2.0
1	E	33	PHE	2.0
1	M	267	VAL	2.0
1	P	150	PHE	2.0
1	P	267	VAL	2.0
1	P	592	PHE	2.0
1	E	736	ALA	2.0
1	F	237	ARG	2.0
1	G	833	ALA	2.0
1	K	732	ALA	2.0
1	M	286	ALA	2.0
1	M	889	ALA	2.0
1	G	78	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	P	38	ASN	2.0
1	P	121	GLY	2.0
1	P	744	GLU	2.0
1	A	742	THR	2.0
1	E	141	ILE	2.0
1	E	829	THR	2.0
1	H	3	ILE	2.0
1	I	595	THR	2.0
1	M	220	THR	2.0
1	M	398	TRP	2.0
1	J	252	ASP	2.0
1	K	832	ASP	2.0
1	L	82	ASP	2.0
1	F	686	PRO	2.0
1	N	253	TYR	2.0
1	M	53	SER	2.0
1	P	768	MET	2.0
1	G	739	HIS	2.0
1	D	76	CYS	2.0
1	E	76	CYS	2.0
1	P	573	GLN	2.0
1	P	903[A]	GLN	2.0
1	E	171	PHE	2.0
1	P	237	ARG	2.0
1	A	736	ALA	2.0
1	H	733	ALA	2.0
1	L	97	ALA	2.0
1	P	61	ALA	2.0
1	P	327	ALA	2.0
1	P	631	LEU	2.0
1	P	889	ALA	2.0
1	P	892	ALA	2.0
1	F	136	GLU	2.0
1	H	744	GLU	2.0
1	O	136	GLU	2.0
1	F	582	GLY	2.0
1	M	414	ASN	2.0
1	P	752	GLY	2.0
1	O	3	ILE	2.0
1	P	305	ILE	2.0
1	I	133	TRP	2.0
1	M	90	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	585	TRP	2.0
1	M	5	ASP	2.0
1	F	743	SER	2.0
1	M	95	TYR	2.0
1	P	148	SER	2.0
1	P	974	HIS	2.0

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

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	748	10/11	0.83	0.17	44,54,100,100	0
1	CME	P	914	10/11	0.85	0.16	34,40,100,100	0
1	CME	C	748	10/11	0.88	0.16	16,26,97,97	0
1	CME	L	748	10/11	0.88	0.17	31,41,100,100	0
1	CME	H	748	10/11	0.89	0.15	29,39,100,100	0
1	CME	N	1021	10/11	0.90	0.14	9,33,100,100	0
1	CME	B	748	10/11	0.90	0.14	18,28,99,99	0
1	CME	M	1021	10/11	0.90	0.14	21,44,100,100	0
1	CME	P	1021	10/11	0.90	0.14	28,51,100,100	0
1	CME	F	1021	10/11	0.91	0.13	2,25,100,100	0
1	CME	I	1021	10/11	0.92	0.13	9,32,100,100	0
1	CME	J	1021	10/11	0.92	0.12	7,30,100,100	0
1	CME	O	1021	10/11	0.92	0.12	11,34,100,100	0
1	CME	K	748	10/11	0.92	0.13	32,42,100,100	0
1	CME	H	1021	10/11	0.92	0.13	13,36,100,100	0
1	CME	M	914	10/11	0.92	0.15	27,33,100,100	0
1	CME	L	1021	10/11	0.93	0.11	15,38,100,100	0
1	CME	E	1021	10/11	0.93	0.13	14,37,100,100	0
1	CME	C	1021	10/11	0.93	0.13	1,23,97,97	0
1	CME	J	748	10/11	0.93	0.11	23,33,100,100	0
1	CME	G	748	10/11	0.93	0.11	22,32,100,100	0
1	CME	G	1021	10/11	0.93	0.10	6,29,100,100	0
1	CME	K	1021	10/11	0.93	0.11	16,39,100,100	0
1	CME	D	748	10/11	0.93	0.15	21,30,100,100	0
1	CME	E	748	10/11	0.94	0.13	30,40,100,100	0
1	CME	A	1021	10/11	0.94	0.12	2,25,100,100	0
1	CME	O	748	10/11	0.94	0.13	27,37,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CME	F	748	10/11	0.94	0.12	18,28,100,100	0
1	CME	I	748	10/11	0.94	0.11	25,35,100,100	0
1	CME	A	748	10/11	0.94	0.12	18,28,100,100	0
1	CME	B	1021	10/11	0.94	0.11	2,25,99,99	0
1	CME	O	914	10/11	0.95	0.10	17,23,100,100	0
1	CME	D	1021	10/11	0.95	0.13	4,27,100,100	0
1	CME	N	748	10/11	0.95	0.10	26,35,100,100	0
1	CME	M	748	10/11	0.95	0.11	37,47,100,100	0
1	CME	H	914	10/11	0.95	0.12	19,25,100,100	0
1	CME	K	914	10/11	0.96	0.10	22,28,100,100	0
1	CME	G	914	10/11	0.96	0.10	12,18,100,100	0
1	CME	I	914	10/11	0.96	0.10	15,21,100,100	0
1	CME	L	914	10/11	0.96	0.10	21,27,100,100	0
1	CME	E	914	10/11	0.97	0.10	20,26,100,100	0
1	CME	A	914	10/11	0.97	0.10	8,14,100,100	0
1	CME	N	914	10/11	0.97	0.10	16,22,100,100	0
1	CME	J	914	10/11	0.97	0.10	13,19,100,100	0
1	CME	B	914	10/11	0.97	0.10	8,14,99,99	0
1	CME	C	914	10/11	0.98	0.09	6,12,97,97	0
1	CME	F	914	10/11	0.98	0.08	8,14,100,100	0
1	CME	D	914	10/11	0.98	0.09	10,16,100,100	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	MG	C	3002	1/1	0.89	0.09	16,16,16,16	0
2	MG	P	3002	1/1	0.91	0.07	44,44,44,44	0
2	MG	M	3002	1/1	0.92	0.14	37,37,37,37	0
2	MG	I	3001	1/1	0.93	0.07	25,25,25,25	0
2	MG	M	3001	1/1	0.93	0.12	37,37,37,37	0
2	MG	L	3002	1/1	0.94	0.07	31,31,31,31	0
2	MG	P	3001	1/1	0.94	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	E	3002	1/1	0.94	0.09	30,30,30,30	0
2	MG	D	3002	1/1	0.95	0.07	21,21,21,21	0
2	MG	I	3002	1/1	0.95	0.08	25,25,25,25	0
2	MG	L	3001	1/1	0.95	0.05	31,31,31,31	0
2	MG	H	3002	1/1	0.95	0.08	30,30,30,30	0
2	MG	B	3002	1/1	0.96	0.06	18,18,18,18	0
2	MG	K	3002	1/1	0.96	0.05	32,32,32,32	0
2	MG	J	3002	1/1	0.97	0.09	23,23,23,23	0
2	MG	A	3002	1/1	0.97	0.09	18,18,18,18	0
2	MG	F	3002	1/1	0.97	0.10	19,19,19,19	0
2	MG	G	3002	1/1	0.97	0.04	22,22,22,22	0
2	MG	A	3001	1/1	0.98	0.11	18,18,18,18	0
2	MG	B	3001	1/1	0.98	0.03	18,18,18,18	0
2	MG	N	3001	1/1	0.98	0.04	26,26,26,26	0
2	MG	N	3002	1/1	0.98	0.09	26,26,26,26	0
2	MG	H	3001	1/1	0.98	0.03	29,29,29,29	0
2	MG	J	3001	1/1	0.98	0.07	23,23,23,23	0
2	MG	E	3001	1/1	0.99	0.07	30,30,30,30	0
2	MG	D	3001	1/1	0.99	0.03	20,20,20,20	0
2	MG	K	3001	1/1	0.99	0.08	32,32,32,32	0
2	MG	F	3001	1/1	0.99	0.03	18,18,18,18	0
2	MG	O	3001	1/1	0.99	0.04	27,27,27,27	0
2	MG	O	3002	1/1	0.99	0.07	27,27,27,27	0
2	MG	C	3001	1/1	0.99	0.03	16,16,16,16	0
2	MG	G	3001	1/1	0.99	0.03	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.