Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 11:56 PM EDT

PDB ID	:	4V41
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:

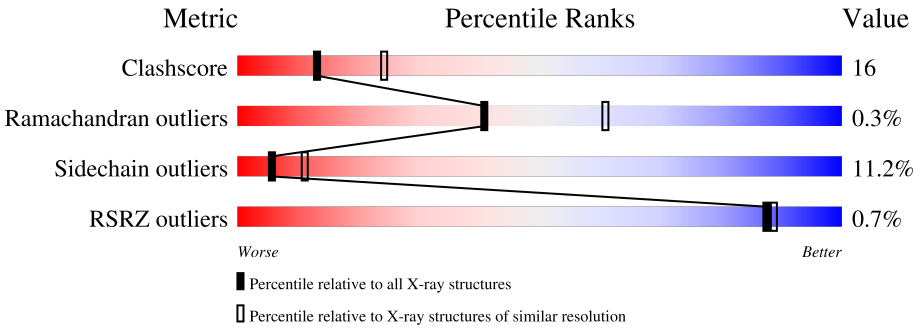
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	59% 30% 9% ·
1	B	1023	58% 31% 9% ·
1	C	1023	57% 31% 9% ·
1	D	1023	58% 30% 9% ·
1	E	1023	58% 30% 9% ·
1	F	1023	58% 31% 9% ·
1	G	1023	58% 31% 9% ·

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Mol	Chain	Length	Quality of chain
1	H	1023	58% 31% 9%
1	I	1023	58% 31% 9%
1	J	1023	58% 31% 9%
1	K	1023	% 58% 31% 9%
1	L	1023	58% 31% 9%
1	M	1023	2% 59% 30% 9%
1	N	1023	58% 30% 9%
1	O	1023	58% 31% 9%
1	P	1023	6% 58% 31% 9%

2 Entry composition (i)

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 (three-letter code: 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.

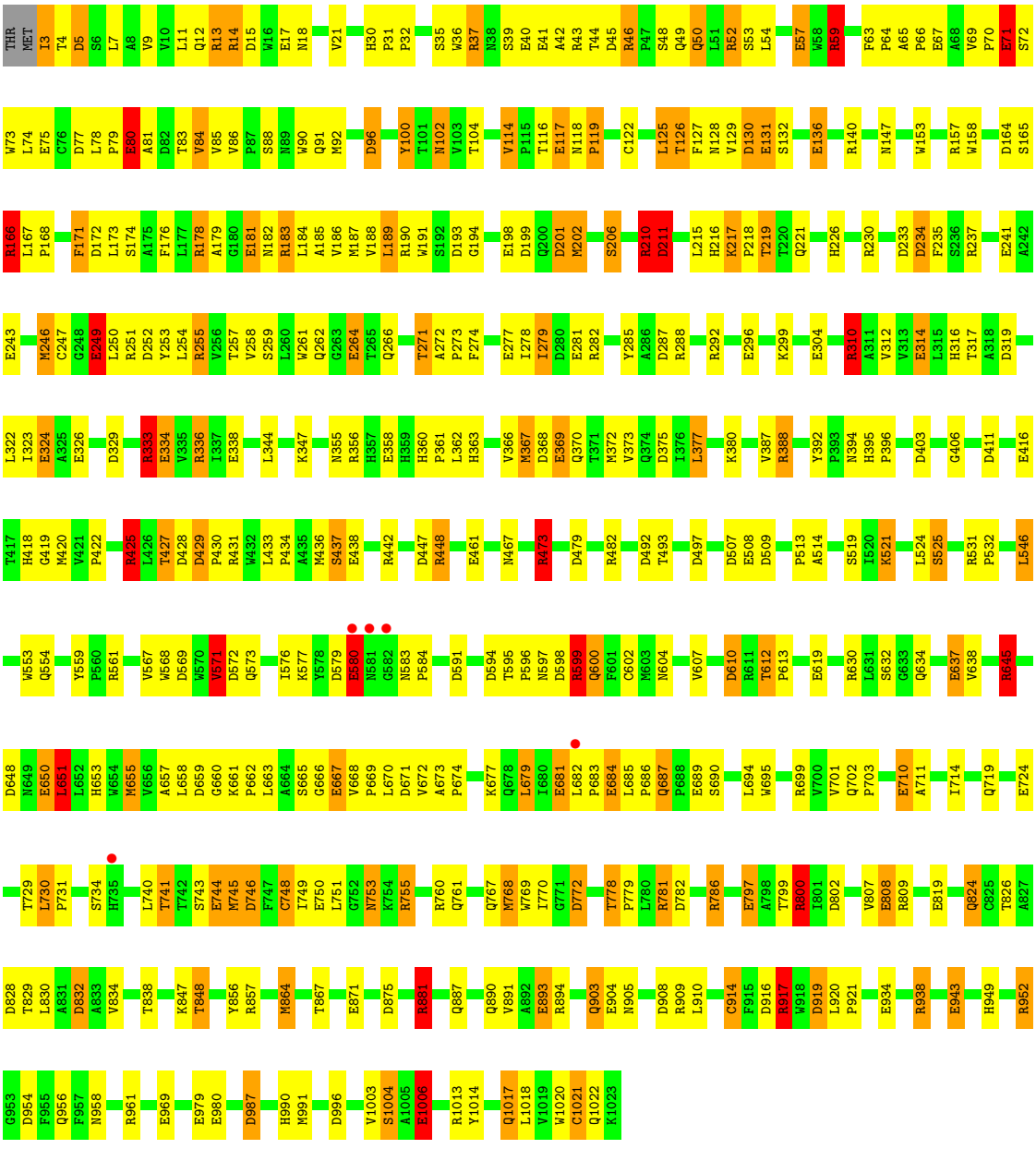
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	434	Total O 434 434	0	0
3	B	436	Total O 436 436	0	0
3	C	433	Total O 433 433	0	0
3	D	437	Total O 437 437	0	0
3	E	435	Total O 435 435	0	0
3	F	436	Total O 436 436	0	0
3	G	434	Total O 434 434	0	0
3	H	435	Total O 435 435	0	0
3	I	434	Total O 434 434	0	0
3	J	436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

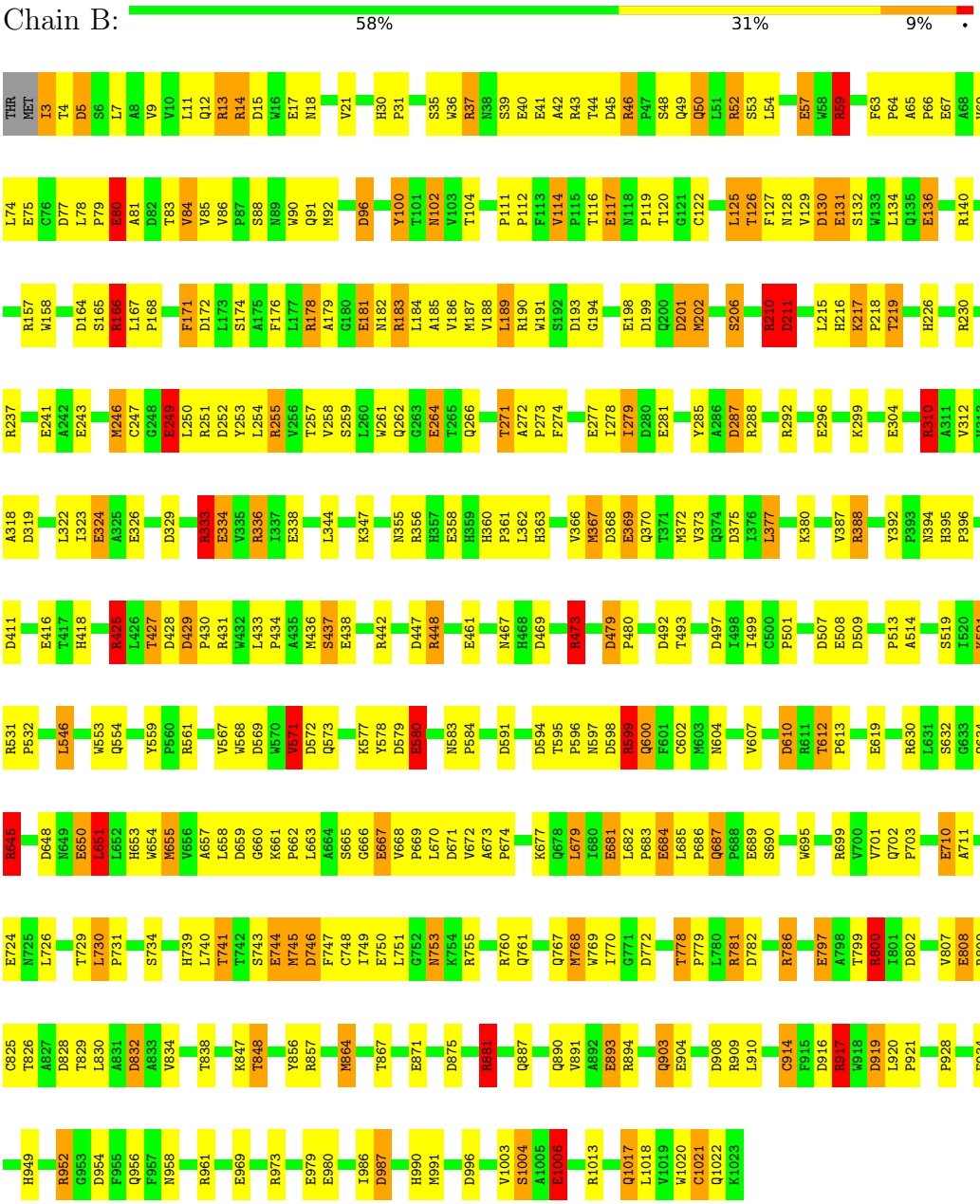
- Molecule 1: BETA-GALACTOSIDASE

Chain A:



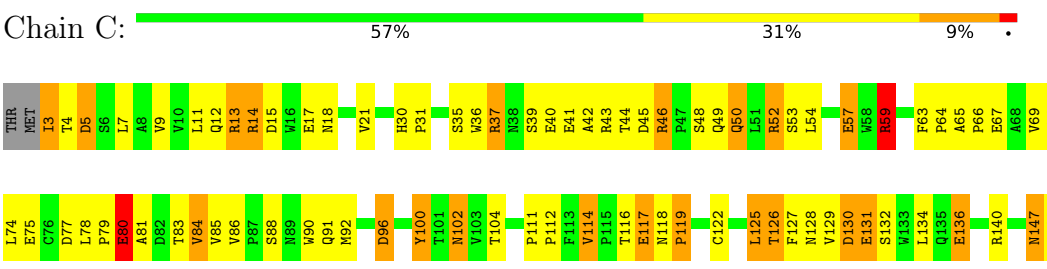
• Molecule 1: BETA-GALACTOSIDASE

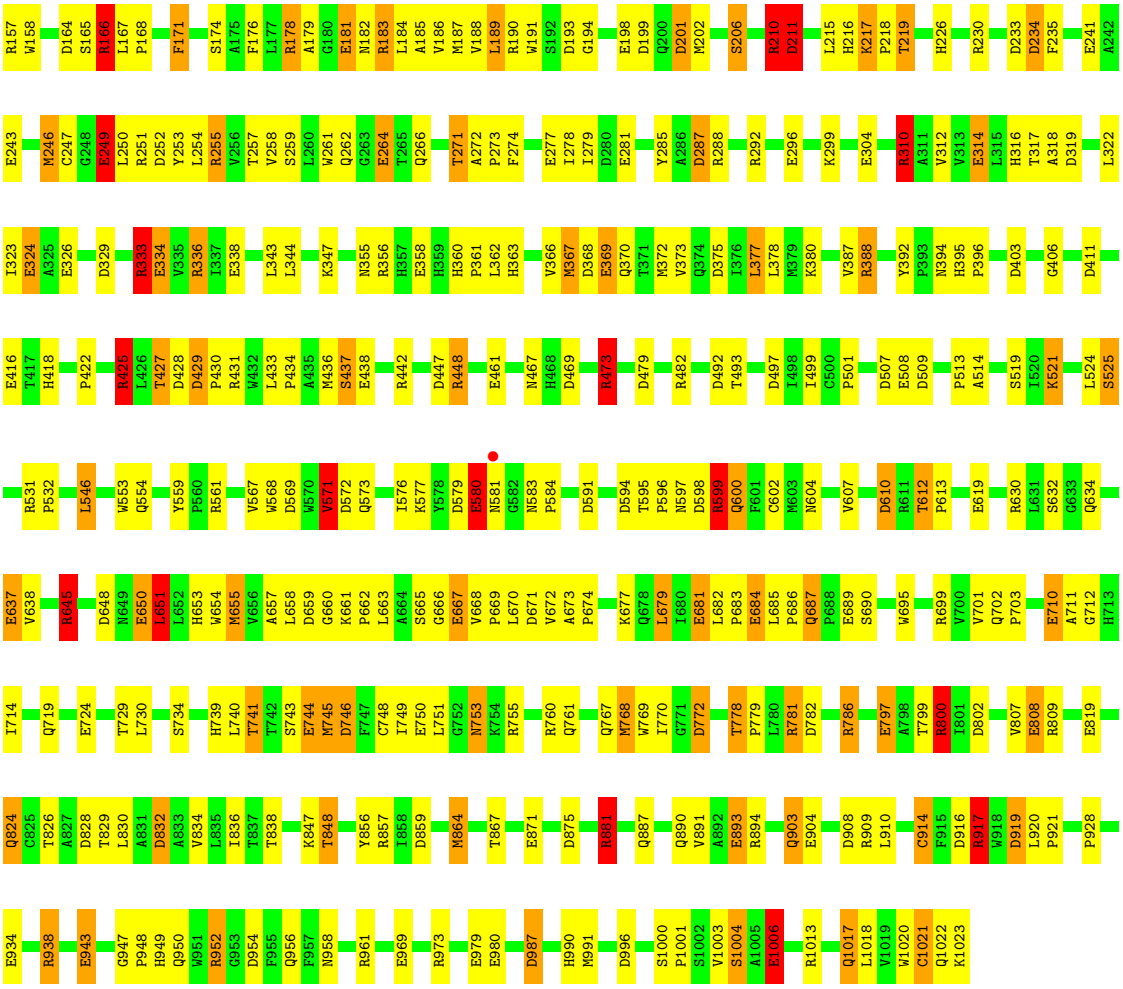
Chain B:



• Molecule 1: BETA-GALACTOSIDASE

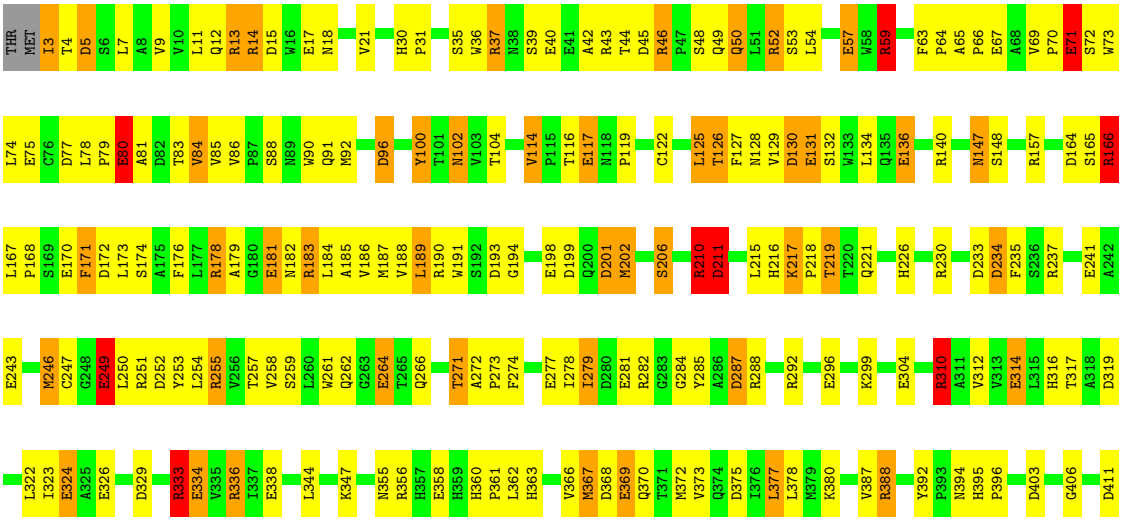
Chain C:

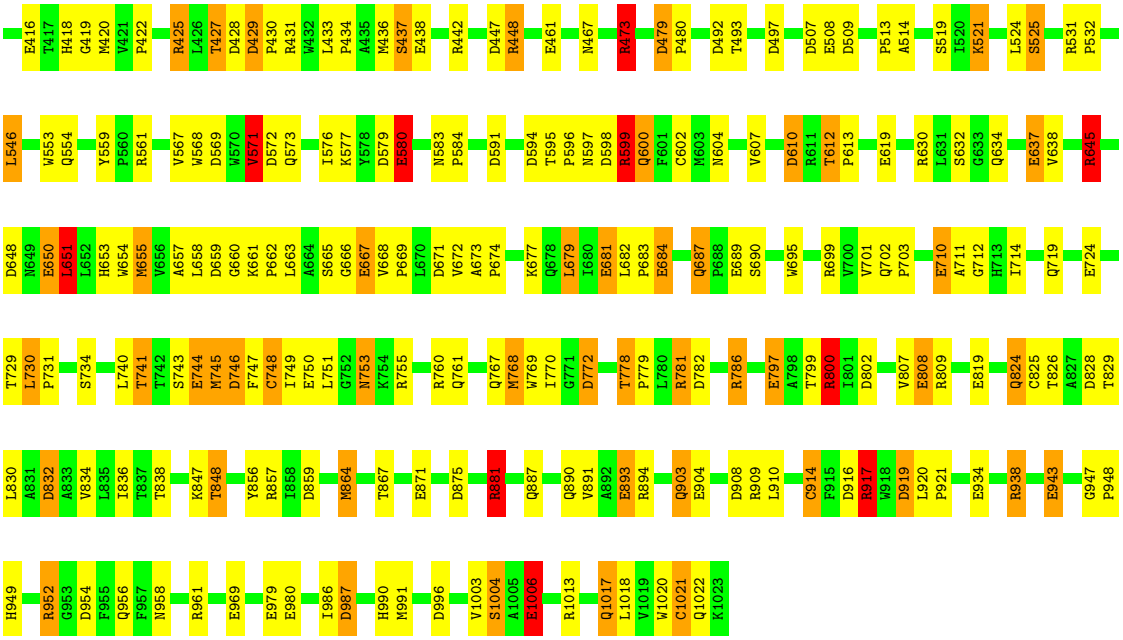




• Molecule 1: BETA-GALACTOSIDASE

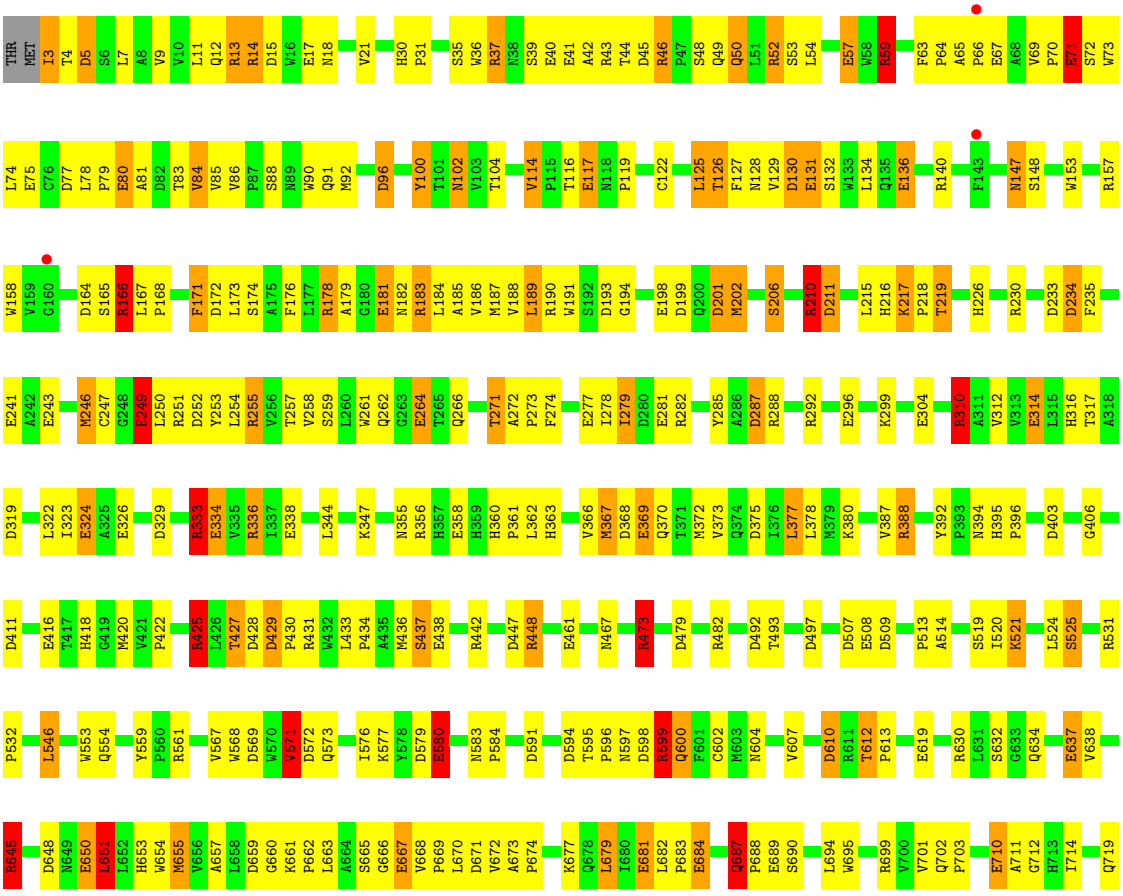
Chain D:

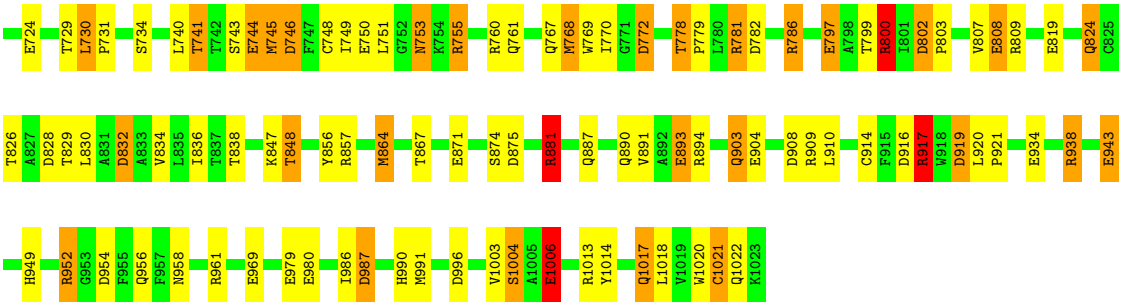




• Molecule 1: BETA-GALACTOSIDASE

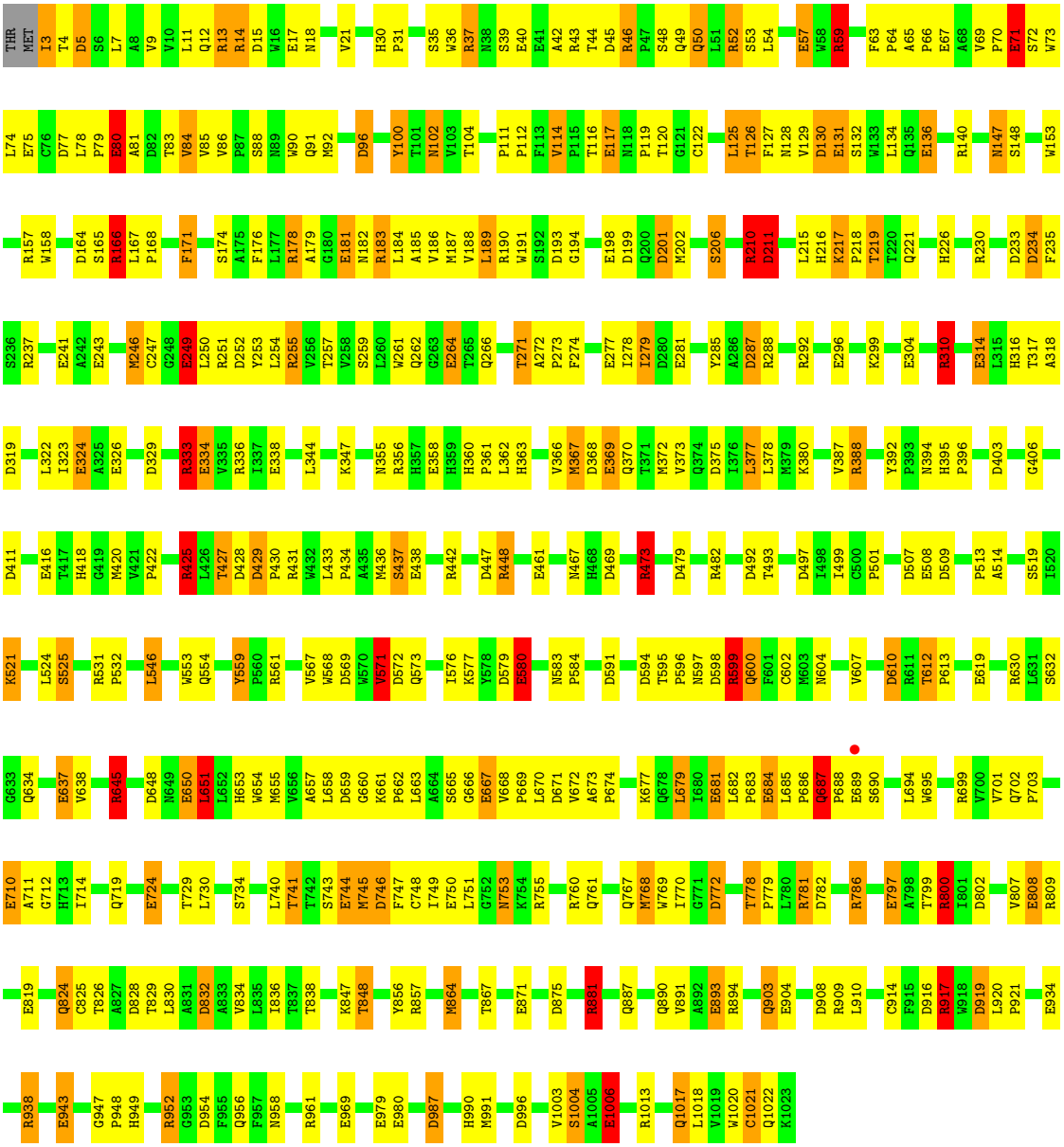
Chain E:





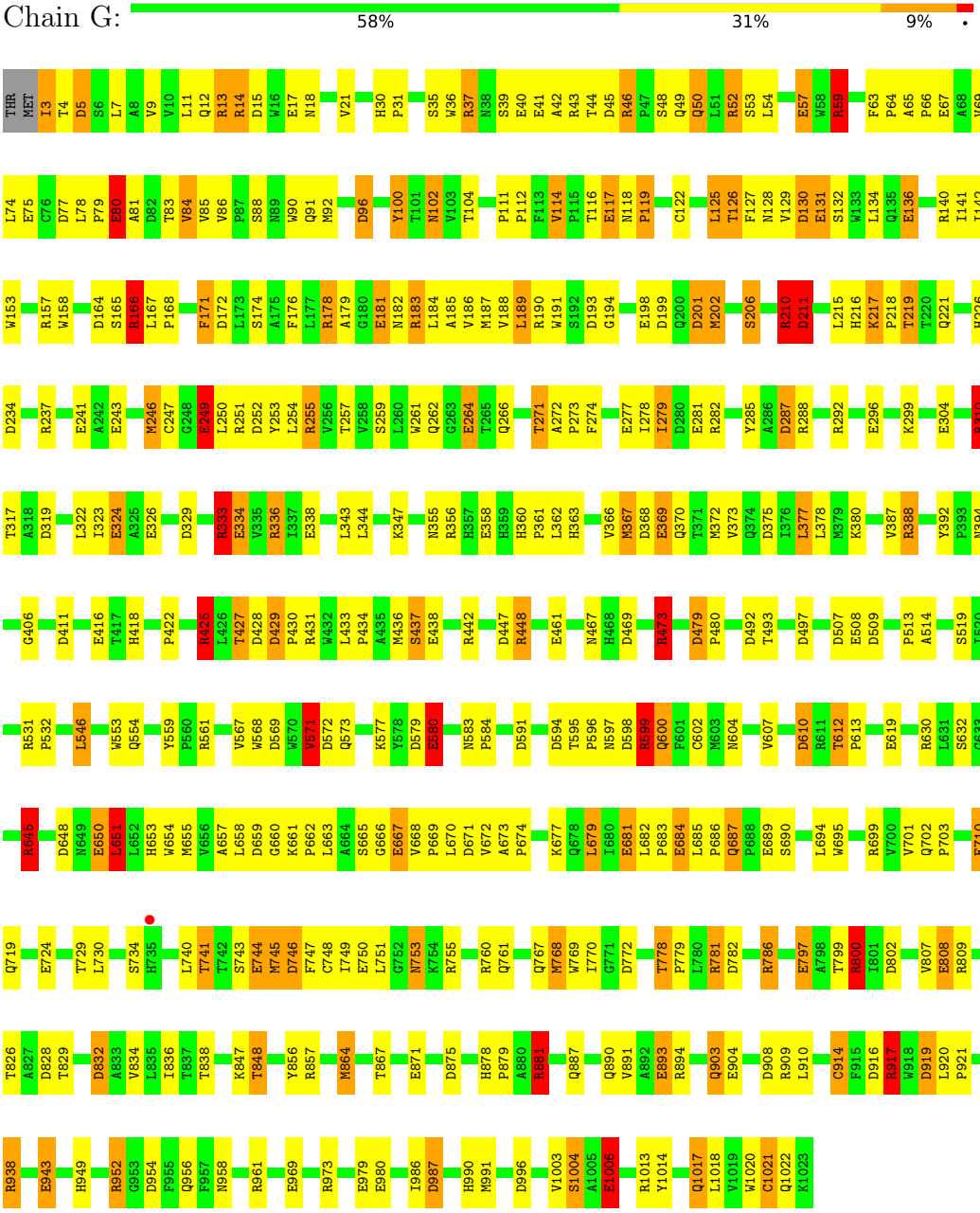
• Molecule 1: BETA-GALACTOSIDASE

Chain F:



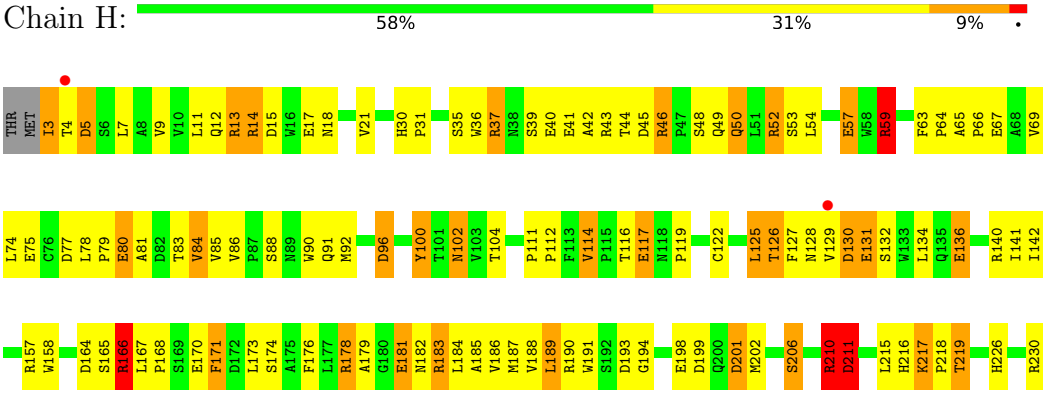
• Molecule 1: BETA-GALACTOSIDASE

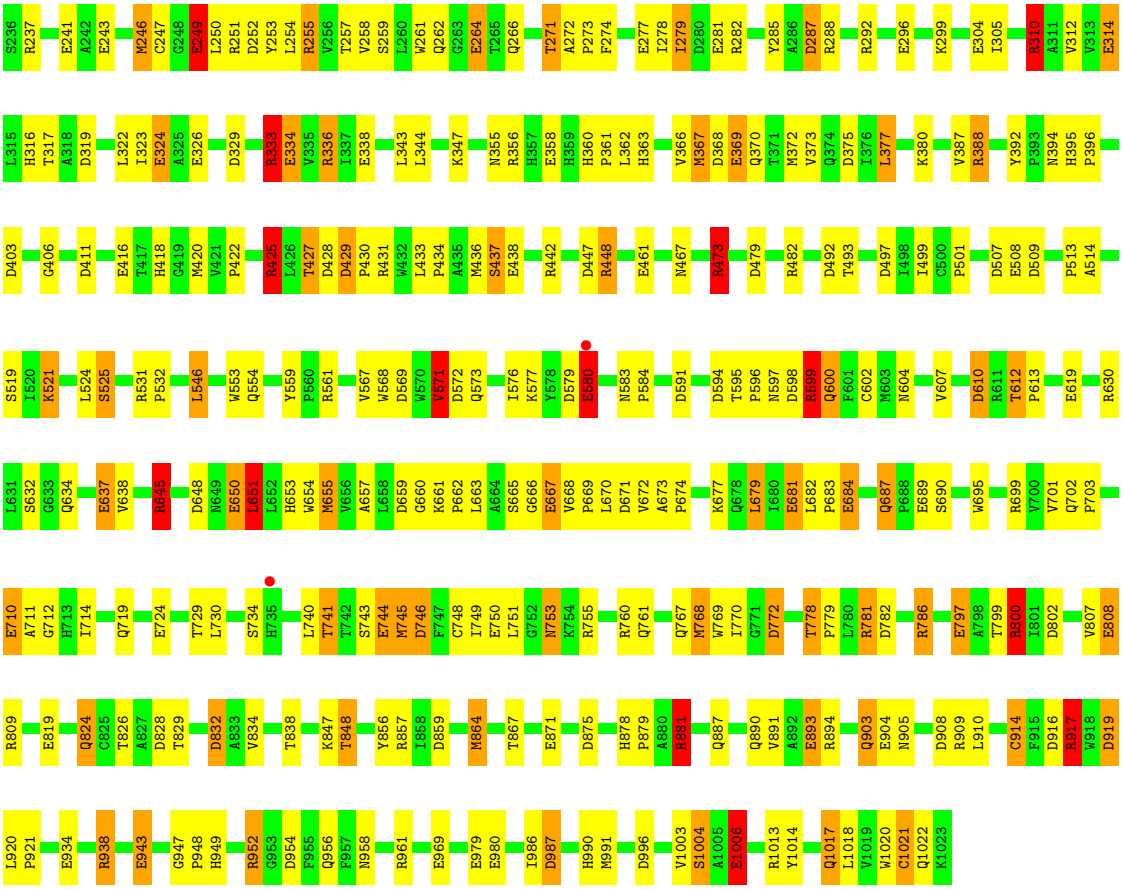
Chain G:



• Molecule 1: BETA-GALACTOSIDASE

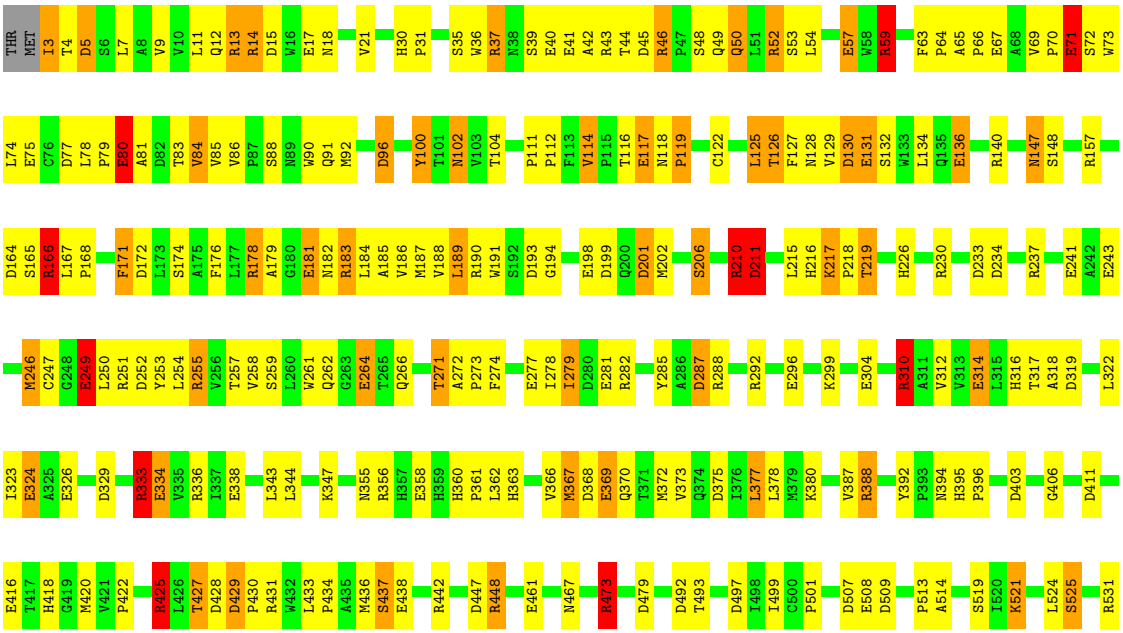
Chain H:

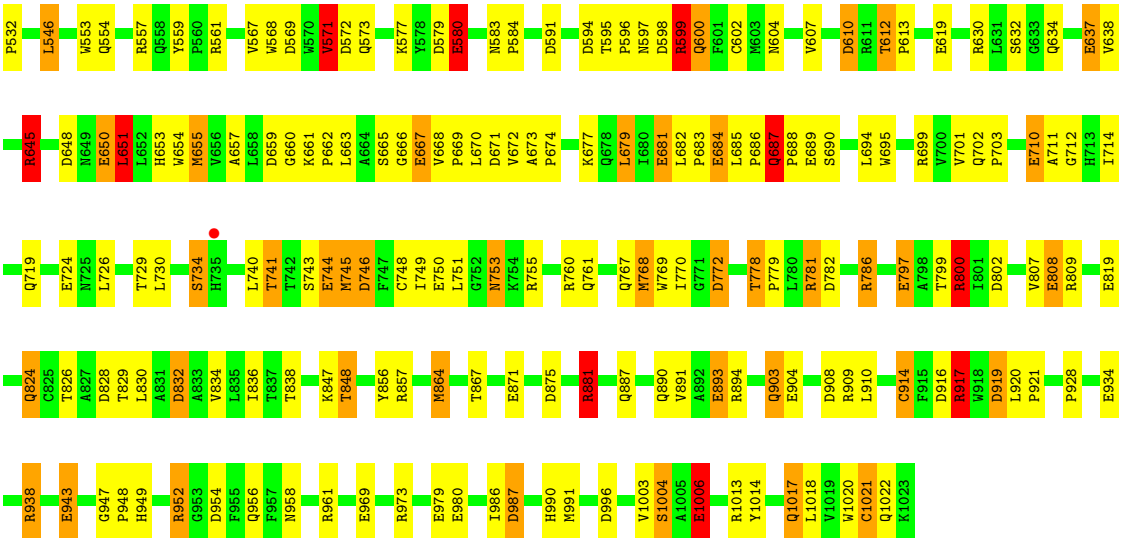




• Molecule 1: BETA-GALACTOSIDASE

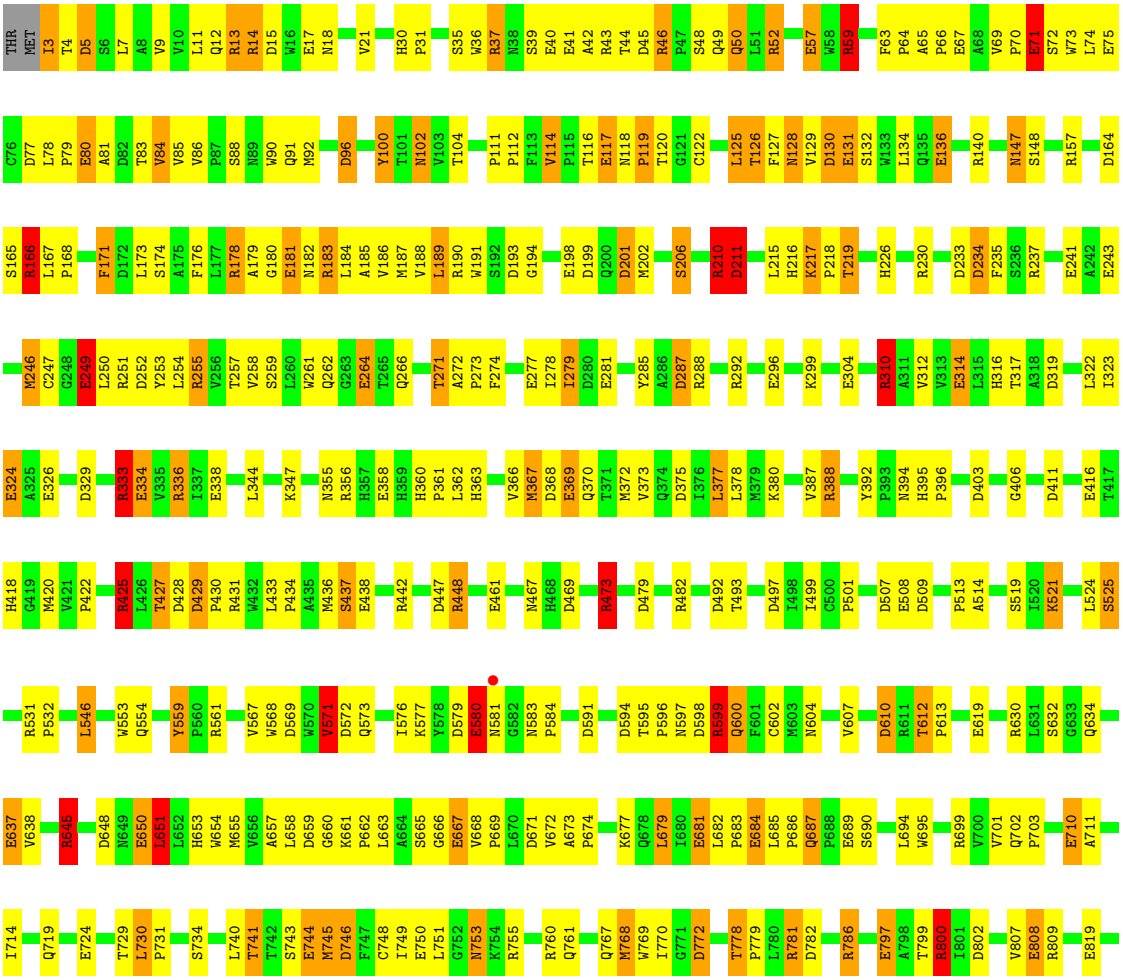
Chain I:

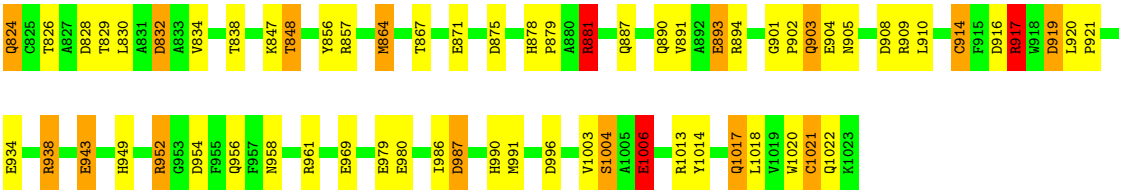




• Molecule 1: BETA-GALACTOSIDASE

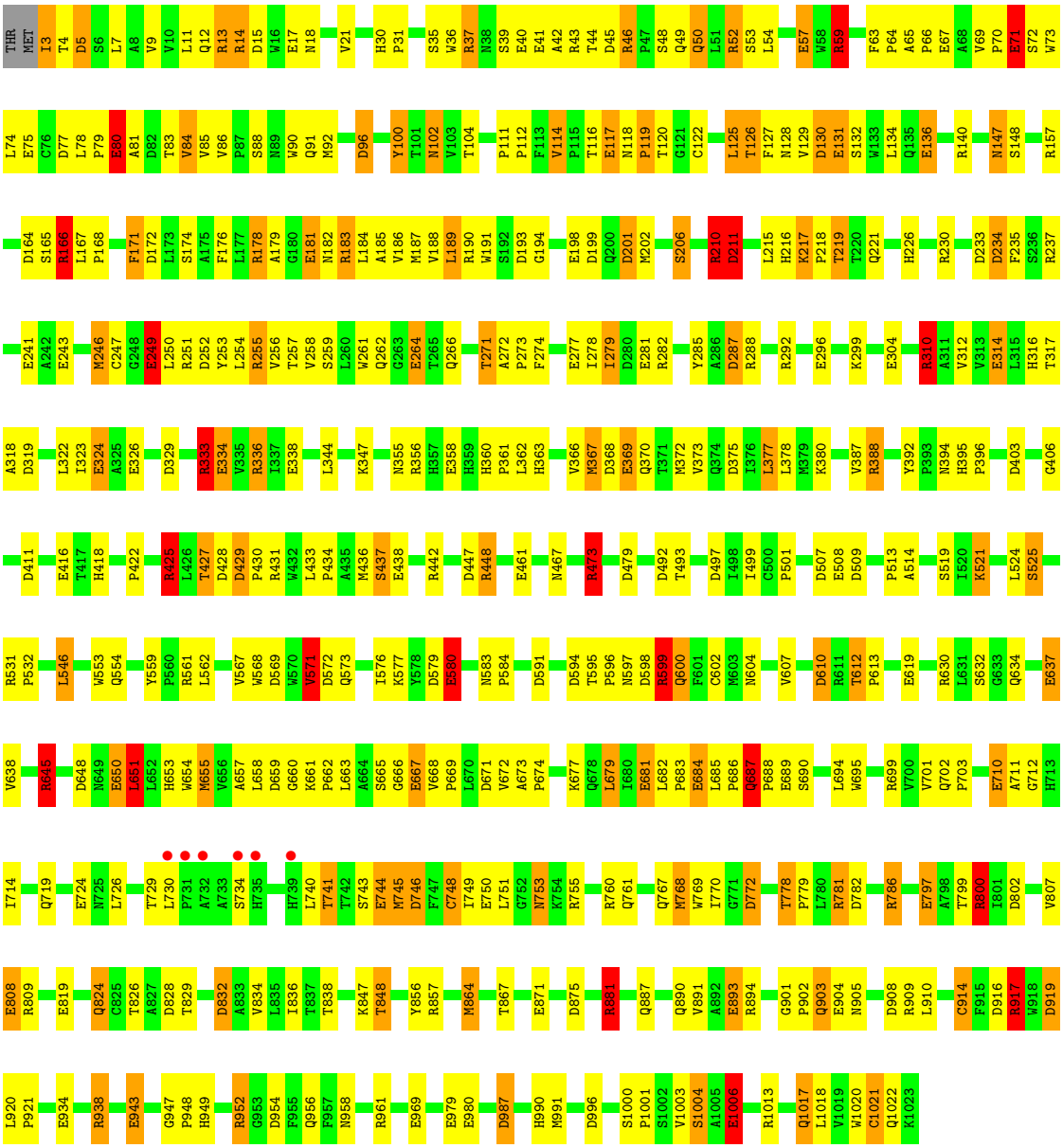
Chain J:





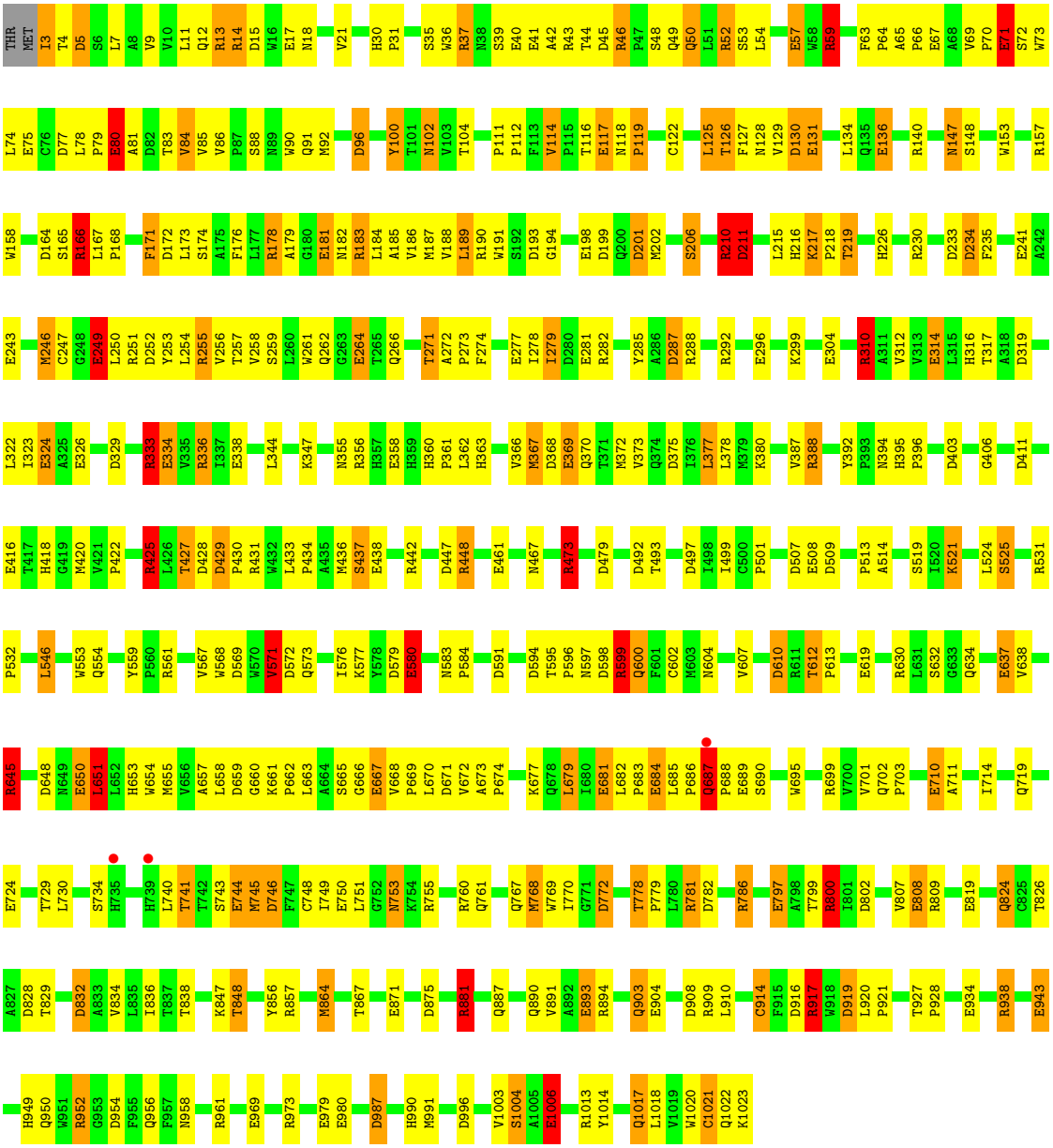
• Molecule 1: BETA-GALACTOSIDASE

Chain K:



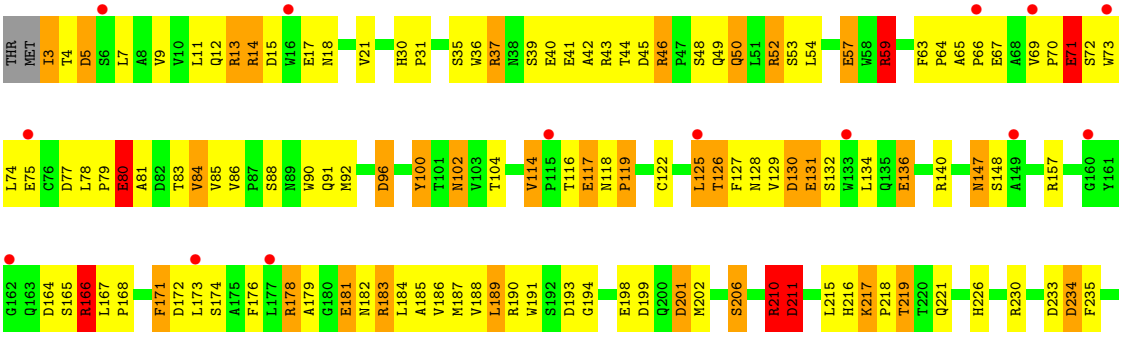
• Molecule 1: BETA-GALACTOSIDASE

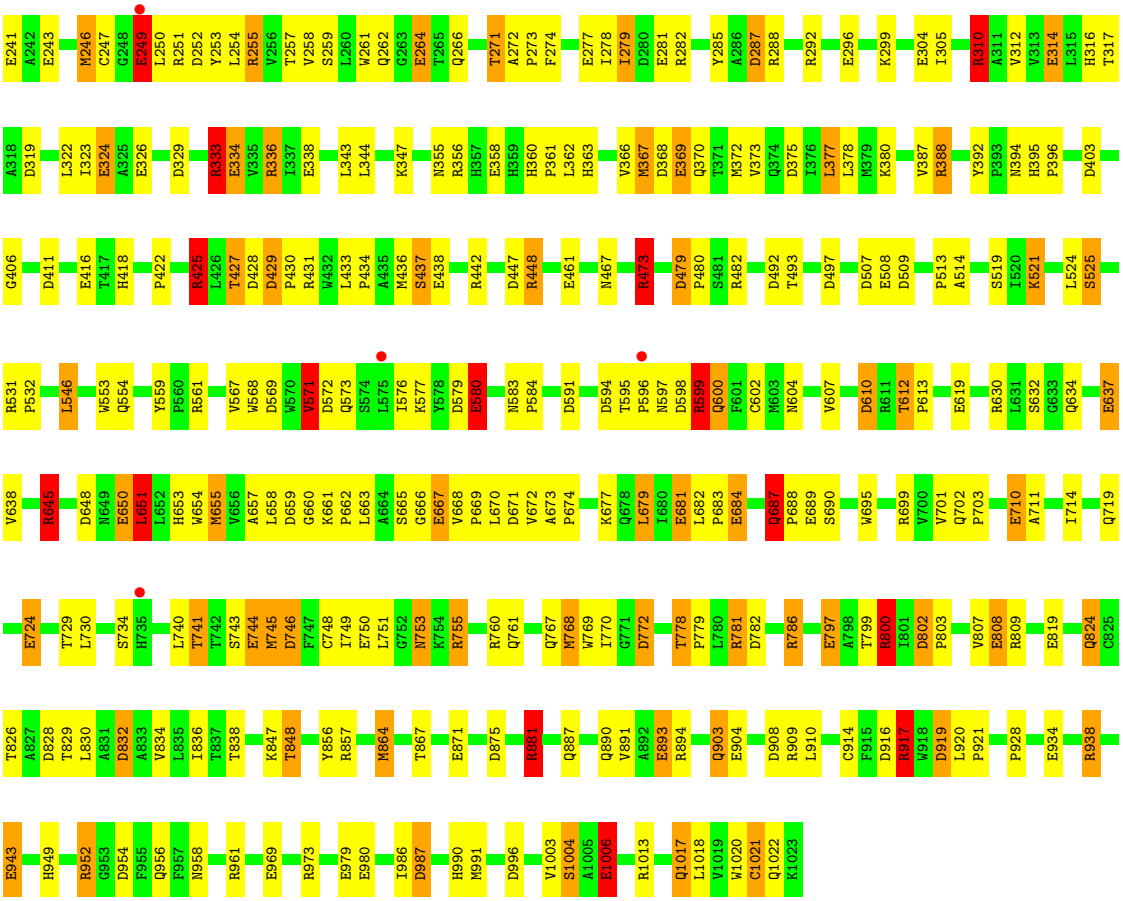
Chain L:



• Molecule 1: BETA-GALACTOSIDASE

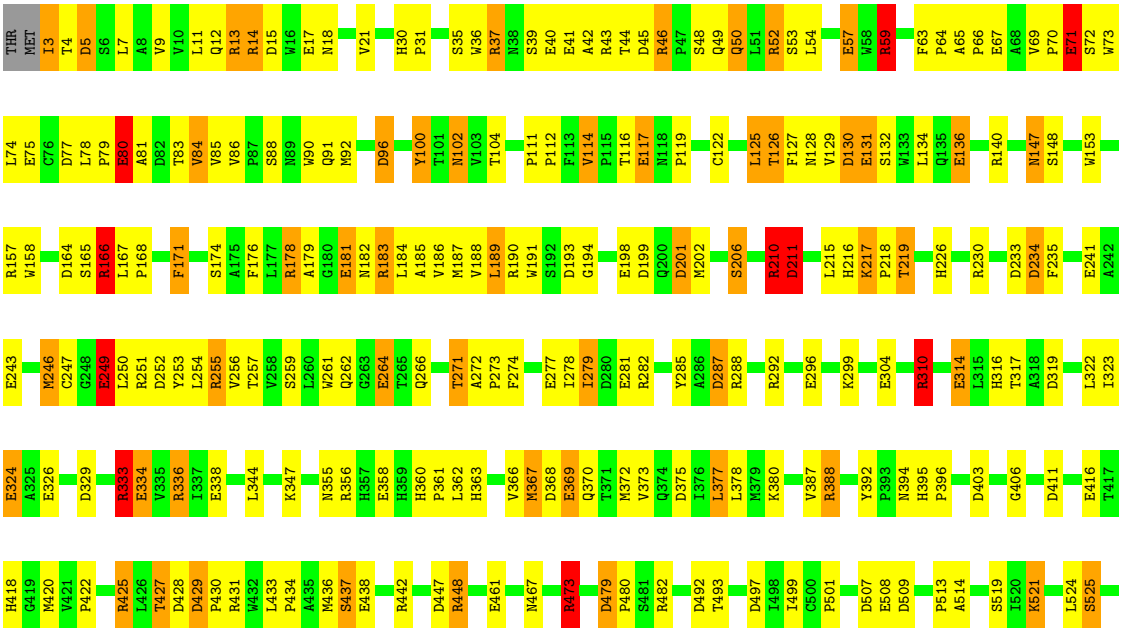
Chain M:

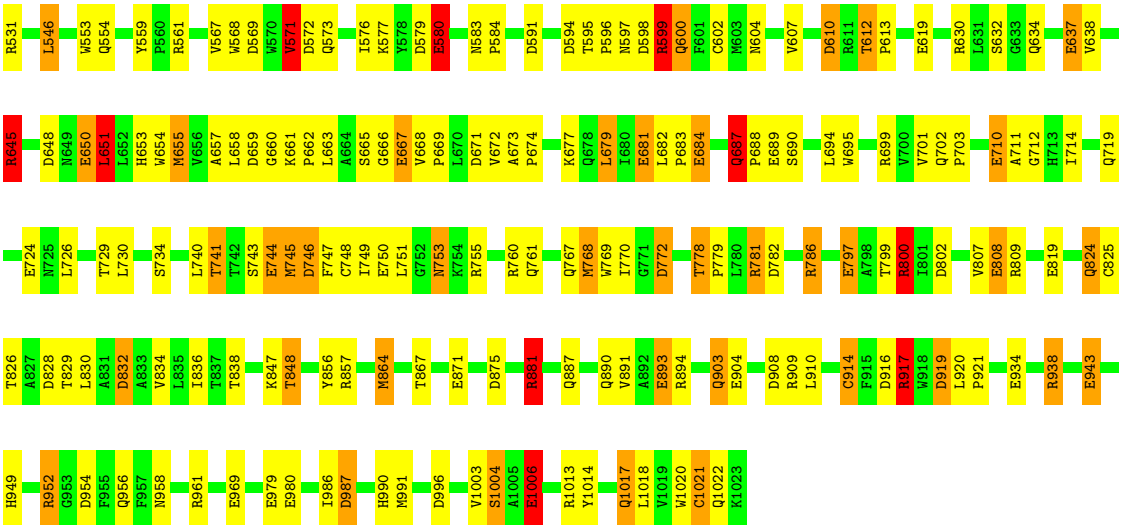




• Molecule 1: BETA-GALACTOSIDASE

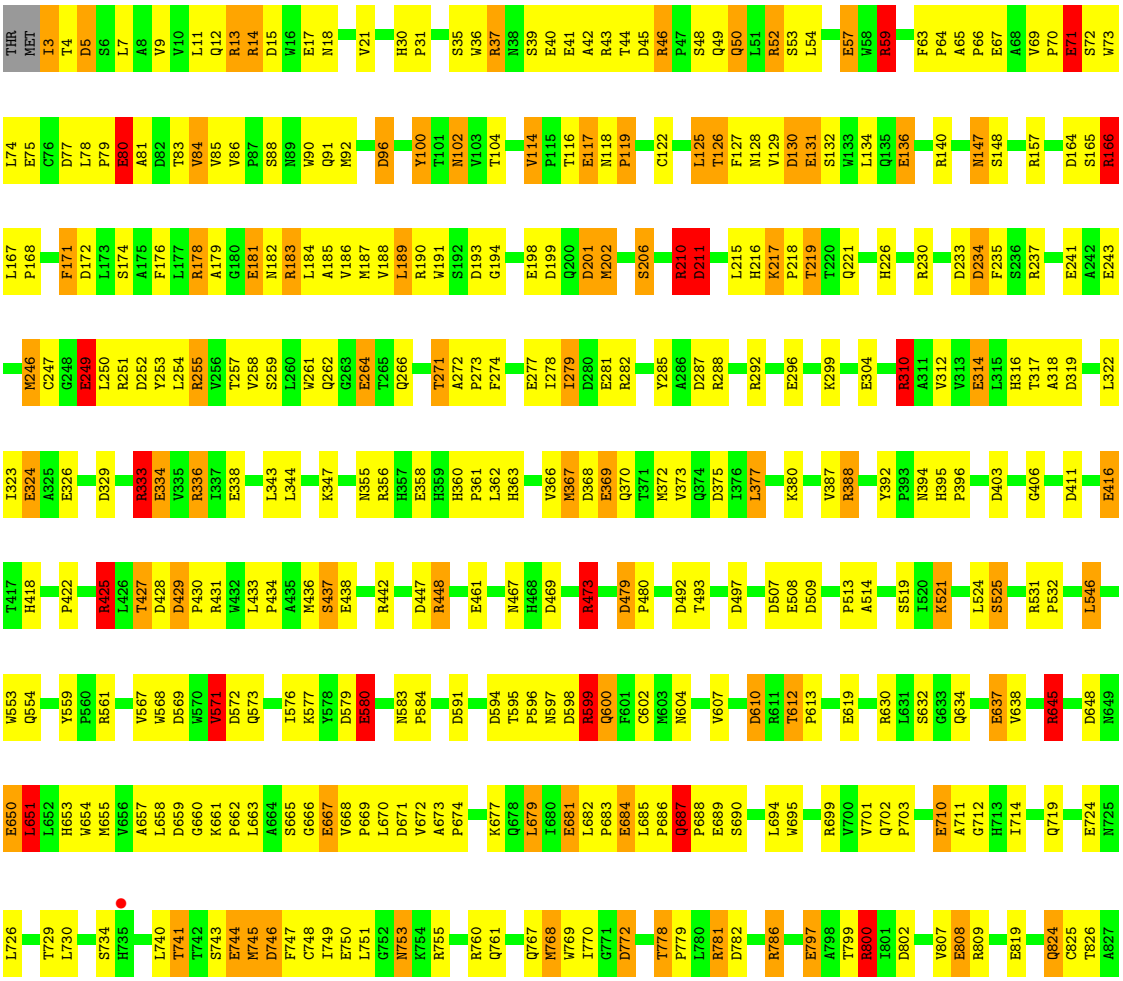
Chain N:

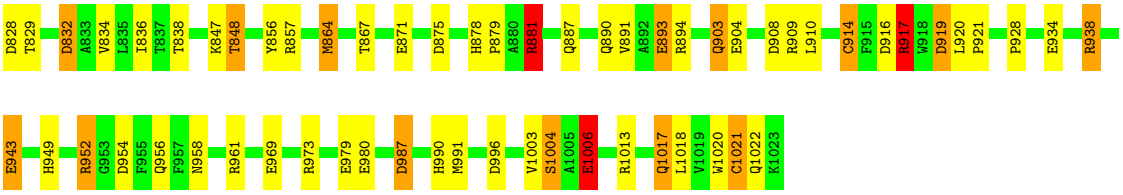




• Molecule 1: BETA-GALACTOSIDASE

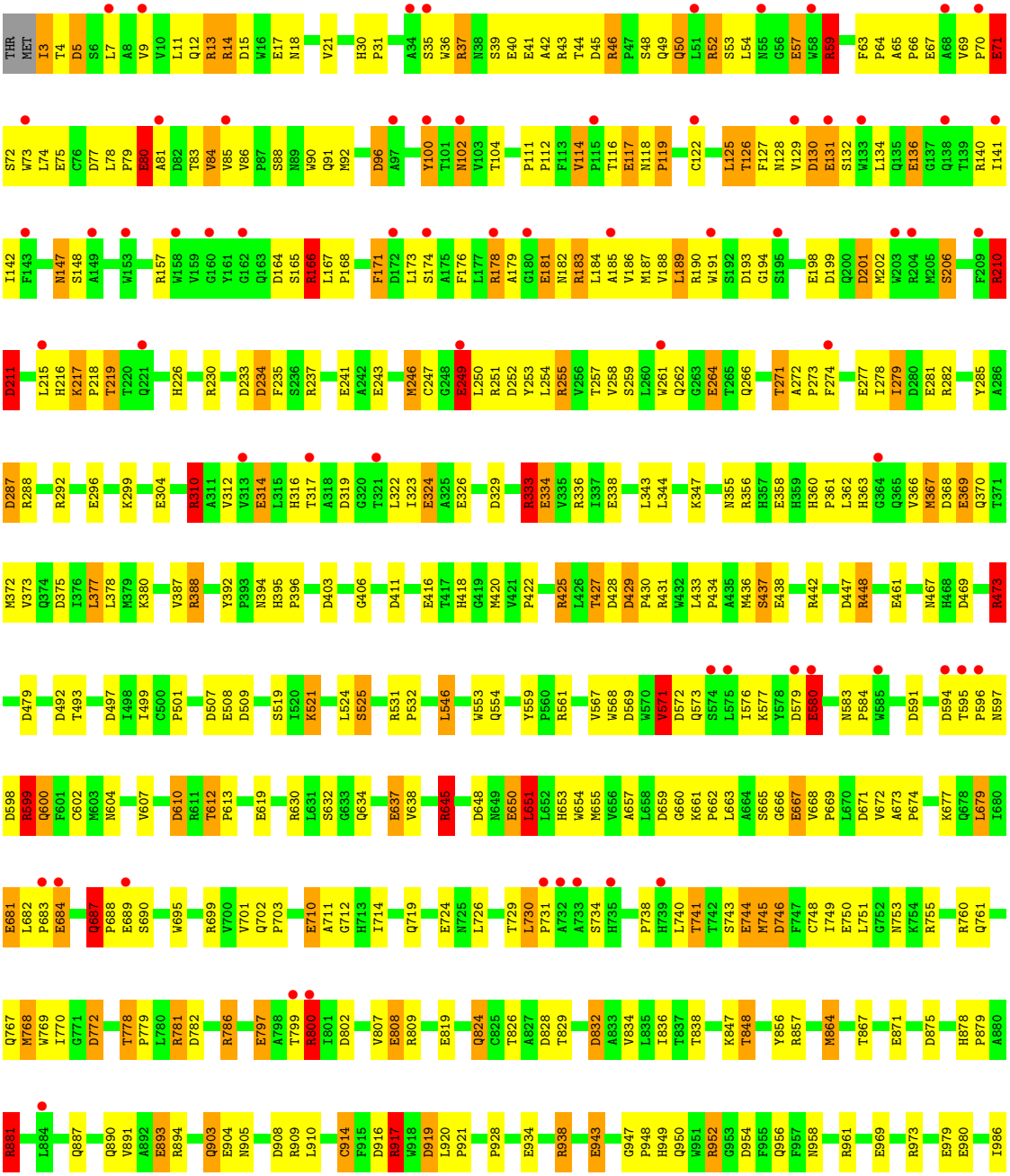
Chain O:

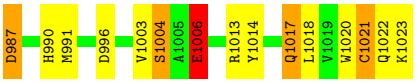




• Molecule 1: BETA-GALACTOSIDASE

Chain P:




D987
H990
M991
D996
V1003
S1004
A1005
E1006
R1013
Y1014
Q1017
L1018
V1019
W1020
C1021
Q1022
K1023

4 Data and refinement statistics (i)

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 92.62 – 2.00	Depositor EDS
% Data completeness (in resolution range)	71.0 ((Not available)-2.50) 39.3 (92.62-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.00Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.199 , 0.207 0.185 , (Not available)	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)	0.29 , 100.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.23	56/8472 (0.7%)	1.69	188/11553 (1.6%)
1	B	1.23	56/8472 (0.7%)	1.69	189/11553 (1.6%)
1	C	1.23	56/8472 (0.7%)	1.69	188/11553 (1.6%)
1	D	1.23	56/8472 (0.7%)	1.69	188/11553 (1.6%)
1	E	1.23	56/8472 (0.7%)	1.69	189/11553 (1.6%)
1	F	1.23	55/8472 (0.6%)	1.69	186/11553 (1.6%)
1	G	1.23	56/8472 (0.7%)	1.69	189/11553 (1.6%)
1	H	1.23	56/8472 (0.7%)	1.69	189/11553 (1.6%)
1	I	1.23	56/8472 (0.7%)	1.69	188/11553 (1.6%)
1	J	1.23	56/8472 (0.7%)	1.69	188/11553 (1.6%)
1	K	1.23	56/8472 (0.7%)	1.69	189/11553 (1.6%)
1	L	1.23	56/8472 (0.7%)	1.69	188/11553 (1.6%)
1	M	1.23	56/8472 (0.7%)	1.69	189/11553 (1.6%)
1	N	1.23	56/8472 (0.7%)	1.69	187/11553 (1.6%)
1	O	1.23	57/8472 (0.7%)	1.69	188/11553 (1.6%)
1	P	1.23	56/8472 (0.7%)	1.69	187/11553 (1.6%)
All	All	1.23	896/135552 (0.7%)	1.69	3010/184848 (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 (896) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	249	GLU	CD-OE2	12.04	1.38	1.25
1	O	249	GLU	CD-OE2	12.03	1.38	1.25
1	H	249	GLU	CD-OE2	12.01	1.38	1.25
1	J	249	GLU	CD-OE2	12.01	1.38	1.25
1	P	249	GLU	CD-OE2	12.01	1.38	1.25
1	I	249	GLU	CD-OE2	12.00	1.38	1.25
1	B	249	GLU	CD-OE2	11.99	1.38	1.25
1	F	249	GLU	CD-OE2	11.99	1.38	1.25
1	D	249	GLU	CD-OE2	11.98	1.38	1.25
1	A	249	GLU	CD-OE2	11.97	1.38	1.25
1	N	249	GLU	CD-OE2	11.96	1.38	1.25
1	K	249	GLU	CD-OE2	11.95	1.38	1.25
1	E	249	GLU	CD-OE2	11.93	1.38	1.25
1	M	249	GLU	CD-OE2	11.93	1.38	1.25
1	L	249	GLU	CD-OE2	11.92	1.38	1.25
1	G	249	GLU	CD-OE2	11.92	1.38	1.25
1	M	744	GLU	CD-OE2	11.53	1.38	1.25
1	L	744	GLU	CD-OE2	11.52	1.38	1.25
1	K	744	GLU	CD-OE2	11.50	1.38	1.25
1	H	744	GLU	CD-OE2	11.48	1.38	1.25
1	J	744	GLU	CD-OE2	11.47	1.38	1.25
1	C	744	GLU	CD-OE2	11.47	1.38	1.25
1	B	744	GLU	CD-OE2	11.46	1.38	1.25
1	G	744	GLU	CD-OE2	11.46	1.38	1.25
1	D	744	GLU	CD-OE2	11.45	1.38	1.25
1	A	744	GLU	CD-OE2	11.45	1.38	1.25
1	E	744	GLU	CD-OE2	11.45	1.38	1.25
1	P	744	GLU	CD-OE2	11.43	1.38	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	744	GLU	CD-OE2	11.43	1.38	1.25
1	O	744	GLU	CD-OE2	11.40	1.38	1.25
1	N	744	GLU	CD-OE2	11.38	1.38	1.25
1	I	744	GLU	CD-OE2	11.37	1.38	1.25
1	N	689	GLU	CD-OE2	10.61	1.37	1.25
1	F	689	GLU	CD-OE2	10.59	1.37	1.25
1	C	689	GLU	CD-OE2	10.58	1.37	1.25
1	B	689	GLU	CD-OE2	10.54	1.37	1.25
1	A	689	GLU	CD-OE2	10.53	1.37	1.25
1	P	689	GLU	CD-OE2	10.53	1.37	1.25
1	E	689	GLU	CD-OE2	10.52	1.37	1.25
1	D	689	GLU	CD-OE2	10.52	1.37	1.25
1	L	689	GLU	CD-OE2	10.51	1.37	1.25
1	J	689	GLU	CD-OE2	10.50	1.37	1.25
1	O	689	GLU	CD-OE2	10.50	1.37	1.25
1	M	689	GLU	CD-OE2	10.50	1.37	1.25
1	I	689	GLU	CD-OE2	10.49	1.37	1.25
1	H	689	GLU	CD-OE2	10.49	1.37	1.25
1	K	689	GLU	CD-OE2	10.49	1.37	1.25
1	G	689	GLU	CD-OE2	10.48	1.37	1.25
1	I	819	GLU	CD-OE2	10.44	1.37	1.25
1	G	819	GLU	CD-OE2	10.42	1.37	1.25
1	H	819	GLU	CD-OE2	10.41	1.37	1.25
1	M	819	GLU	CD-OE2	10.41	1.37	1.25
1	E	819	GLU	CD-OE2	10.41	1.37	1.25
1	C	819	GLU	CD-OE2	10.40	1.37	1.25
1	L	819	GLU	CD-OE2	10.39	1.37	1.25
1	O	819	GLU	CD-OE2	10.39	1.37	1.25
1	A	819	GLU	CD-OE2	10.39	1.37	1.25
1	K	819	GLU	CD-OE2	10.38	1.37	1.25
1	N	819	GLU	CD-OE2	10.38	1.37	1.25
1	D	819	GLU	CD-OE2	10.37	1.37	1.25
1	B	819	GLU	CD-OE2	10.37	1.37	1.25
1	F	819	GLU	CD-OE2	10.34	1.37	1.25
1	P	819	GLU	CD-OE2	10.33	1.37	1.25
1	J	819	GLU	CD-OE2	10.32	1.37	1.25
1	G	75	GLU	CD-OE2	10.18	1.36	1.25
1	L	75	GLU	CD-OE2	10.18	1.36	1.25
1	J	75	GLU	CD-OE2	10.18	1.36	1.25
1	O	75	GLU	CD-OE2	10.18	1.36	1.25
1	M	75	GLU	CD-OE2	10.17	1.36	1.25
1	I	75	GLU	CD-OE2	10.15	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	75	GLU	CD-OE2	10.15	1.36	1.25
1	C	75	GLU	CD-OE2	10.14	1.36	1.25
1	E	75	GLU	CD-OE2	10.14	1.36	1.25
1	A	75	GLU	CD-OE2	10.14	1.36	1.25
1	F	75	GLU	CD-OE2	10.14	1.36	1.25
1	N	75	GLU	CD-OE2	10.14	1.36	1.25
1	D	75	GLU	CD-OE2	10.14	1.36	1.25
1	H	75	GLU	CD-OE2	10.10	1.36	1.25
1	P	75	GLU	CD-OE2	10.10	1.36	1.25
1	K	75	GLU	CD-OE2	10.09	1.36	1.25
1	F	580	GLU	CD-OE2	9.81	1.36	1.25
1	D	580	GLU	CD-OE2	9.79	1.36	1.25
1	C	580	GLU	CD-OE2	9.78	1.36	1.25
1	I	580	GLU	CD-OE2	9.76	1.36	1.25
1	B	580	GLU	CD-OE2	9.75	1.36	1.25
1	M	580	GLU	CD-OE2	9.75	1.36	1.25
1	L	580	GLU	CD-OE2	9.74	1.36	1.25
1	E	580	GLU	CD-OE2	9.74	1.36	1.25
1	A	580	GLU	CD-OE2	9.73	1.36	1.25
1	N	580	GLU	CD-OE2	9.72	1.36	1.25
1	G	580	GLU	CD-OE2	9.72	1.36	1.25
1	O	580	GLU	CD-OE2	9.71	1.36	1.25
1	K	580	GLU	CD-OE2	9.71	1.36	1.25
1	H	580	GLU	CD-OE2	9.70	1.36	1.25
1	J	580	GLU	CD-OE2	9.70	1.36	1.25
1	P	580	GLU	CD-OE2	9.70	1.36	1.25
1	I	131	GLU	CD-OE2	9.58	1.36	1.25
1	C	131	GLU	CD-OE2	9.58	1.36	1.25
1	H	131	GLU	CD-OE2	9.57	1.36	1.25
1	E	131	GLU	CD-OE2	9.54	1.36	1.25
1	P	131	GLU	CD-OE2	9.54	1.36	1.25
1	G	131	GLU	CD-OE2	9.53	1.36	1.25
1	A	131	GLU	CD-OE2	9.52	1.36	1.25
1	F	131	GLU	CD-OE2	9.50	1.36	1.25
1	B	131	GLU	CD-OE2	9.50	1.36	1.25
1	J	131	GLU	CD-OE2	9.50	1.36	1.25
1	K	131	GLU	CD-OE2	9.50	1.36	1.25
1	D	131	GLU	CD-OE2	9.49	1.36	1.25
1	O	131	GLU	CD-OE2	9.48	1.36	1.25
1	M	131	GLU	CD-OE2	9.48	1.36	1.25
1	N	131	GLU	CD-OE2	9.47	1.36	1.25
1	L	131	GLU	CD-OE2	9.46	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	980	GLU	CD-OE2	9.37	1.35	1.25
1	G	980	GLU	CD-OE2	9.37	1.35	1.25
1	M	980	GLU	CD-OE2	9.36	1.35	1.25
1	B	980	GLU	CD-OE2	9.35	1.35	1.25
1	E	980	GLU	CD-OE2	9.32	1.35	1.25
1	D	980	GLU	CD-OE2	9.32	1.35	1.25
1	F	980	GLU	CD-OE2	9.31	1.35	1.25
1	A	980	GLU	CD-OE2	9.31	1.35	1.25
1	O	980	GLU	CD-OE2	9.29	1.35	1.25
1	H	980	GLU	CD-OE2	9.28	1.35	1.25
1	L	980	GLU	CD-OE2	9.27	1.35	1.25
1	I	980	GLU	CD-OE2	9.27	1.35	1.25
1	J	980	GLU	CD-OE2	9.27	1.35	1.25
1	D	684	GLU	CD-OE2	9.26	1.35	1.25
1	C	980	GLU	CD-OE2	9.25	1.35	1.25
1	K	980	GLU	CD-OE2	9.24	1.35	1.25
1	P	980	GLU	CD-OE2	9.22	1.35	1.25
1	G	684	GLU	CD-OE2	9.20	1.35	1.25
1	O	684	GLU	CD-OE2	9.20	1.35	1.25
1	K	684	GLU	CD-OE2	9.19	1.35	1.25
1	M	684	GLU	CD-OE2	9.19	1.35	1.25
1	P	684	GLU	CD-OE2	9.19	1.35	1.25
1	F	684	GLU	CD-OE2	9.19	1.35	1.25
1	A	684	GLU	CD-OE2	9.19	1.35	1.25
1	N	684	GLU	CD-OE2	9.18	1.35	1.25
1	L	684	GLU	CD-OE2	9.17	1.35	1.25
1	C	684	GLU	CD-OE2	9.16	1.35	1.25
1	B	684	GLU	CD-OE2	9.16	1.35	1.25
1	I	684	GLU	CD-OE2	9.15	1.35	1.25
1	H	684	GLU	CD-OE2	9.15	1.35	1.25
1	E	684	GLU	CD-OE2	9.13	1.35	1.25
1	J	684	GLU	CD-OE2	9.12	1.35	1.25
1	M	296	GLU	CD-OE2	9.06	1.35	1.25
1	N	296	GLU	CD-OE2	9.04	1.35	1.25
1	H	296	GLU	CD-OE2	9.03	1.35	1.25
1	O	296	GLU	CD-OE2	9.03	1.35	1.25
1	B	296	GLU	CD-OE2	9.02	1.35	1.25
1	G	296	GLU	CD-OE2	9.02	1.35	1.25
1	A	296	GLU	CD-OE2	9.02	1.35	1.25
1	E	296	GLU	CD-OE2	9.02	1.35	1.25
1	C	296	GLU	CD-OE2	9.02	1.35	1.25
1	F	296	GLU	CD-OE2	9.01	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	GLU	CD-OE2	9.01	1.35	1.25
1	L	296	GLU	CD-OE2	9.01	1.35	1.25
1	D	181	GLU	CD-OE2	9.00	1.35	1.25
1	J	296	GLU	CD-OE2	9.00	1.35	1.25
1	K	296	GLU	CD-OE2	9.00	1.35	1.25
1	I	296	GLU	CD-OE2	8.99	1.35	1.25
1	H	181	GLU	CD-OE2	8.99	1.35	1.25
1	D	296	GLU	CD-OE2	8.99	1.35	1.25
1	I	181	GLU	CD-OE2	8.98	1.35	1.25
1	N	181	GLU	CD-OE2	8.98	1.35	1.25
1	P	296	GLU	CD-OE2	8.98	1.35	1.25
1	J	181	GLU	CD-OE2	8.97	1.35	1.25
1	A	181	GLU	CD-OE2	8.96	1.35	1.25
1	K	181	GLU	CD-OE2	8.95	1.35	1.25
1	G	181	GLU	CD-OE2	8.94	1.35	1.25
1	B	181	GLU	CD-OE2	8.93	1.35	1.25
1	M	181	GLU	CD-OE2	8.93	1.35	1.25
1	O	181	GLU	CD-OE2	8.93	1.35	1.25
1	E	181	GLU	CD-OE2	8.92	1.35	1.25
1	F	181	GLU	CD-OE2	8.92	1.35	1.25
1	L	181	GLU	CD-OE2	8.92	1.35	1.25
1	G	136	GLU	CD-OE2	8.91	1.35	1.25
1	L	136	GLU	CD-OE2	8.90	1.35	1.25
1	O	136	GLU	CD-OE2	8.89	1.35	1.25
1	P	181	GLU	CD-OE2	8.88	1.35	1.25
1	K	136	GLU	CD-OE2	8.87	1.35	1.25
1	B	136	GLU	CD-OE2	8.85	1.35	1.25
1	E	136	GLU	CD-OE2	8.85	1.35	1.25
1	D	136	GLU	CD-OE2	8.85	1.35	1.25
1	F	136	GLU	CD-OE2	8.83	1.35	1.25
1	A	136	GLU	CD-OE2	8.83	1.35	1.25
1	C	136	GLU	CD-OE2	8.82	1.35	1.25
1	P	136	GLU	CD-OE2	8.81	1.35	1.25
1	J	136	GLU	CD-OE2	8.81	1.35	1.25
1	I	136	GLU	CD-OE2	8.80	1.35	1.25
1	H	136	GLU	CD-OE2	8.79	1.35	1.25
1	N	136	GLU	CD-OE2	8.78	1.35	1.25
1	E	710	GLU	CD-OE2	8.75	1.35	1.25
1	N	710	GLU	CD-OE2	8.74	1.35	1.25
1	M	136	GLU	CD-OE2	8.74	1.35	1.25
1	P	710	GLU	CD-OE2	8.73	1.35	1.25
1	F	710	GLU	CD-OE2	8.72	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	710	GLU	CD-OE2	8.71	1.35	1.25
1	O	710	GLU	CD-OE2	8.70	1.35	1.25
1	L	710	GLU	CD-OE2	8.70	1.35	1.25
1	J	710	GLU	CD-OE2	8.70	1.35	1.25
1	M	710	GLU	CD-OE2	8.70	1.35	1.25
1	G	710	GLU	CD-OE2	8.69	1.35	1.25
1	I	710	GLU	CD-OE2	8.69	1.35	1.25
1	A	710	GLU	CD-OE2	8.68	1.35	1.25
1	K	710	GLU	CD-OE2	8.66	1.35	1.25
1	D	710	GLU	CD-OE2	8.66	1.35	1.25
1	C	710	GLU	CD-OE2	8.65	1.35	1.25
1	B	710	GLU	CD-OE2	8.62	1.35	1.25
1	H	264	GLU	CD-OE2	8.60	1.35	1.25
1	N	264	GLU	CD-OE2	8.58	1.35	1.25
1	K	264	GLU	CD-OE2	8.57	1.35	1.25
1	G	264	GLU	CD-OE2	8.57	1.35	1.25
1	C	264	GLU	CD-OE2	8.57	1.35	1.25
1	O	264	GLU	CD-OE2	8.57	1.35	1.25
1	J	264	GLU	CD-OE2	8.56	1.35	1.25
1	D	264	GLU	CD-OE2	8.55	1.35	1.25
1	P	264	GLU	CD-OE2	8.54	1.35	1.25
1	M	264	GLU	CD-OE2	8.53	1.35	1.25
1	B	264	GLU	CD-OE2	8.52	1.35	1.25
1	A	264	GLU	CD-OE2	8.52	1.35	1.25
1	L	264	GLU	CD-OE2	8.51	1.35	1.25
1	I	264	GLU	CD-OE2	8.50	1.34	1.25
1	E	264	GLU	CD-OE2	8.50	1.34	1.25
1	F	264	GLU	CD-OE2	8.49	1.34	1.25
1	M	797	GLU	CD-OE2	8.44	1.34	1.25
1	J	797	GLU	CD-OE2	8.44	1.34	1.25
1	N	797	GLU	CD-OE2	8.42	1.34	1.25
1	C	277	GLU	CD-OE2	8.42	1.34	1.25
1	F	797	GLU	CD-OE2	8.41	1.34	1.25
1	G	797	GLU	CD-OE2	8.41	1.34	1.25
1	I	277	GLU	CD-OE2	8.41	1.34	1.25
1	A	797	GLU	CD-OE2	8.40	1.34	1.25
1	O	797	GLU	CD-OE2	8.40	1.34	1.25
1	H	797	GLU	CD-OE2	8.39	1.34	1.25
1	B	797	GLU	CD-OE2	8.39	1.34	1.25
1	I	797	GLU	CD-OE2	8.39	1.34	1.25
1	O	508	GLU	CD-OE2	8.39	1.34	1.25
1	P	797	GLU	CD-OE2	8.39	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	797	GLU	CD-OE2	8.38	1.34	1.25
1	E	797	GLU	CD-OE2	8.38	1.34	1.25
1	F	277	GLU	CD-OE2	8.36	1.34	1.25
1	A	277	GLU	CD-OE2	8.36	1.34	1.25
1	E	508	GLU	CD-OE2	8.36	1.34	1.25
1	M	277	GLU	CD-OE2	8.35	1.34	1.25
1	O	277	GLU	CD-OE2	8.35	1.34	1.25
1	L	797	GLU	CD-OE2	8.34	1.34	1.25
1	J	277	GLU	CD-OE2	8.34	1.34	1.25
1	C	508	GLU	CD-OE2	8.33	1.34	1.25
1	I	508	GLU	CD-OE2	8.33	1.34	1.25
1	D	797	GLU	CD-OE2	8.33	1.34	1.25
1	C	797	GLU	CD-OE2	8.33	1.34	1.25
1	E	277	GLU	CD-OE2	8.33	1.34	1.25
1	G	508	GLU	CD-OE2	8.33	1.34	1.25
1	H	508	GLU	CD-OE2	8.32	1.34	1.25
1	B	508	GLU	CD-OE2	8.32	1.34	1.25
1	D	508	GLU	CD-OE2	8.32	1.34	1.25
1	N	277	GLU	CD-OE2	8.32	1.34	1.25
1	D	277	GLU	CD-OE2	8.32	1.34	1.25
1	J	508	GLU	CD-OE2	8.32	1.34	1.25
1	M	508	GLU	CD-OE2	8.32	1.34	1.25
1	L	508	GLU	CD-OE2	8.31	1.34	1.25
1	P	277	GLU	CD-OE2	8.31	1.34	1.25
1	K	277	GLU	CD-OE2	8.31	1.34	1.25
1	G	277	GLU	CD-OE2	8.31	1.34	1.25
1	K	508	GLU	CD-OE2	8.30	1.34	1.25
1	F	508	GLU	CD-OE2	8.29	1.34	1.25
1	H	277	GLU	CD-OE2	8.30	1.34	1.25
1	L	277	GLU	CD-OE2	8.29	1.34	1.25
1	N	508	GLU	CD-OE2	8.29	1.34	1.25
1	B	277	GLU	CD-OE2	8.27	1.34	1.25
1	A	508	GLU	CD-OE2	8.26	1.34	1.25
1	P	508	GLU	CD-OE2	8.24	1.34	1.25
1	G	724	GLU	CD-OE2	8.02	1.34	1.25
1	I	724	GLU	CD-OE2	7.99	1.34	1.25
1	J	724	GLU	CD-OE2	7.98	1.34	1.25
1	K	724	GLU	CD-OE2	7.98	1.34	1.25
1	M	724	GLU	CD-OE2	7.98	1.34	1.25
1	E	724	GLU	CD-OE2	7.97	1.34	1.25
1	O	724	GLU	CD-OE2	7.96	1.34	1.25
1	C	724	GLU	CD-OE2	7.96	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	724	GLU	CD-OE2	7.95	1.34	1.25
1	A	724	GLU	CD-OE2	7.95	1.34	1.25
1	N	724	GLU	CD-OE2	7.94	1.34	1.25
1	D	893	GLU	CD-OE2	7.94	1.34	1.25
1	B	724	GLU	CD-OE2	7.93	1.34	1.25
1	L	724	GLU	CD-OE2	7.93	1.34	1.25
1	H	724	GLU	CD-OE2	7.92	1.34	1.25
1	P	724	GLU	CD-OE2	7.91	1.34	1.25
1	D	724	GLU	CD-OE2	7.91	1.34	1.25
1	C	893	GLU	CD-OE2	7.89	1.34	1.25
1	E	893	GLU	CD-OE2	7.88	1.34	1.25
1	I	893	GLU	CD-OE2	7.88	1.34	1.25
1	N	893	GLU	CD-OE2	7.88	1.34	1.25
1	J	893	GLU	CD-OE2	7.87	1.34	1.25
1	P	893	GLU	CD-OE2	7.87	1.34	1.25
1	G	893	GLU	CD-OE2	7.87	1.34	1.25
1	A	893	GLU	CD-OE2	7.83	1.34	1.25
1	B	893	GLU	CD-OE2	7.82	1.34	1.25
1	H	893	GLU	CD-OE2	7.82	1.34	1.25
1	F	893	GLU	CD-OE2	7.79	1.34	1.25
1	M	893	GLU	CD-OE2	7.78	1.34	1.25
1	K	893	GLU	CD-OE2	7.78	1.34	1.25
1	L	893	GLU	CD-OE2	7.77	1.34	1.25
1	O	893	GLU	CD-OE2	7.76	1.34	1.25
1	L	438	GLU	CD-OE2	7.58	1.33	1.25
1	O	438	GLU	CD-OE2	7.58	1.33	1.25
1	N	438	GLU	CD-OE2	7.55	1.33	1.25
1	H	438	GLU	CD-OE2	7.55	1.33	1.25
1	I	438	GLU	CD-OE2	7.54	1.33	1.25
1	J	438	GLU	CD-OE2	7.53	1.33	1.25
1	C	438	GLU	CD-OE2	7.53	1.33	1.25
1	A	438	GLU	CD-OE2	7.52	1.33	1.25
1	F	438	GLU	CD-OE2	7.51	1.33	1.25
1	E	438	GLU	CD-OE2	7.51	1.33	1.25
1	G	438	GLU	CD-OE2	7.51	1.33	1.25
1	D	438	GLU	CD-OE2	7.50	1.33	1.25
1	K	438	GLU	CD-OE2	7.49	1.33	1.25
1	M	438	GLU	CD-OE2	7.49	1.33	1.25
1	B	438	GLU	CD-OE2	7.48	1.33	1.25
1	O	80	GLU	CD-OE2	7.47	1.33	1.25
1	H	80	GLU	CD-OE2	7.46	1.33	1.25
1	K	40	GLU	CD-OE2	7.46	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	438	GLU	CD-OE2	7.46	1.33	1.25
1	I	40	GLU	CD-OE2	7.45	1.33	1.25
1	C	80	GLU	CD-OE2	7.45	1.33	1.25
1	J	80	GLU	CD-OE2	7.45	1.33	1.25
1	B	80	GLU	CD-OE2	7.45	1.33	1.25
1	M	80	GLU	CD-OE2	7.45	1.33	1.25
1	C	40	GLU	CD-OE2	7.44	1.33	1.25
1	D	40	GLU	CD-OE2	7.43	1.33	1.25
1	B	40	GLU	CD-OE2	7.42	1.33	1.25
1	E	80	GLU	CD-OE2	7.42	1.33	1.25
1	J	40	GLU	CD-OE2	7.42	1.33	1.25
1	A	80	GLU	CD-OE2	7.42	1.33	1.25
1	M	40	GLU	CD-OE2	7.42	1.33	1.25
1	F	40	GLU	CD-OE2	7.42	1.33	1.25
1	N	80	GLU	CD-OE2	7.42	1.33	1.25
1	I	80	GLU	CD-OE2	7.41	1.33	1.25
1	L	80	GLU	CD-OE2	7.40	1.33	1.25
1	P	40	GLU	CD-OE2	7.40	1.33	1.25
1	P	80	GLU	CD-OE2	7.40	1.33	1.25
1	A	40	GLU	CD-OE2	7.40	1.33	1.25
1	G	40	GLU	CD-OE2	7.39	1.33	1.25
1	H	40	GLU	CD-OE2	7.39	1.33	1.25
1	K	80	GLU	CD-OE2	7.39	1.33	1.25
1	N	40	GLU	CD-OE2	7.39	1.33	1.25
1	O	40	GLU	CD-OE2	7.39	1.33	1.25
1	L	40	GLU	CD-OE2	7.38	1.33	1.25
1	G	80	GLU	CD-OE2	7.36	1.33	1.25
1	E	40	GLU	CD-OE2	7.35	1.33	1.25
1	D	80	GLU	CD-OE2	7.35	1.33	1.25
1	B	808	GLU	CD-OE2	7.34	1.33	1.25
1	F	808	GLU	CD-OE2	7.33	1.33	1.25
1	F	80	GLU	CD-OE2	7.33	1.33	1.25
1	E	117	GLU	CD-OE2	7.32	1.33	1.25
1	D	117	GLU	CD-OE2	7.32	1.33	1.25
1	D	969	GLU	CD-OE2	7.32	1.33	1.25
1	C	969	GLU	CD-OE2	7.31	1.33	1.25
1	M	808	GLU	CD-OE2	7.31	1.33	1.25
1	I	969	GLU	CD-OE2	7.30	1.33	1.25
1	L	808	GLU	CD-OE2	7.30	1.33	1.25
1	P	969	GLU	CD-OE2	7.30	1.33	1.25
1	N	808	GLU	CD-OE2	7.29	1.33	1.25
1	J	808	GLU	CD-OE2	7.29	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	117	GLU	CD-OE2	7.28	1.33	1.25
1	G	969	GLU	CD-OE2	7.28	1.33	1.25
1	A	969	GLU	CD-OE2	7.28	1.33	1.25
1	J	117	GLU	CD-OE2	7.27	1.33	1.25
1	A	808	GLU	CD-OE2	7.27	1.33	1.25
1	K	969	GLU	CD-OE2	7.27	1.33	1.25
1	H	808	GLU	CD-OE2	7.27	1.33	1.25
1	O	808	GLU	CD-OE2	7.26	1.33	1.25
1	E	808	GLU	CD-OE2	7.26	1.33	1.25
1	J	969	GLU	CD-OE2	7.26	1.33	1.25
1	K	808	GLU	CD-OE2	7.26	1.33	1.25
1	L	969	GLU	CD-OE2	7.26	1.33	1.25
1	H	117	GLU	CD-OE2	7.25	1.33	1.25
1	O	969	GLU	CD-OE2	7.25	1.33	1.25
1	H	969	GLU	CD-OE2	7.25	1.33	1.25
1	M	969	GLU	CD-OE2	7.25	1.33	1.25
1	I	808	GLU	CD-OE2	7.25	1.33	1.25
1	N	969	GLU	CD-OE2	7.25	1.33	1.25
1	F	969	GLU	CD-OE2	7.24	1.33	1.25
1	B	969	GLU	CD-OE2	7.24	1.33	1.25
1	M	117	GLU	CD-OE2	7.23	1.33	1.25
1	D	808	GLU	CD-OE2	7.22	1.33	1.25
1	E	969	GLU	CD-OE2	7.22	1.33	1.25
1	I	117	GLU	CD-OE2	7.22	1.33	1.25
1	A	117	GLU	CD-OE2	7.22	1.33	1.25
1	N	117	GLU	CD-OE2	7.22	1.33	1.25
1	B	117	GLU	CD-OE2	7.22	1.33	1.25
1	C	117	GLU	CD-OE2	7.21	1.33	1.25
1	C	808	GLU	CD-OE2	7.21	1.33	1.25
1	K	117	GLU	CD-OE2	7.21	1.33	1.25
1	P	808	GLU	CD-OE2	7.20	1.33	1.25
1	G	808	GLU	CD-OE2	7.19	1.33	1.25
1	P	117	GLU	CD-OE2	7.19	1.33	1.25
1	O	117	GLU	CD-OE2	7.19	1.33	1.25
1	L	117	GLU	CD-OE2	7.18	1.33	1.25
1	G	117	GLU	CD-OE2	7.18	1.33	1.25
1	K	57	GLU	CD-OE2	7.16	1.33	1.25
1	D	57	GLU	CD-OE2	7.10	1.33	1.25
1	E	57	GLU	CD-OE2	7.10	1.33	1.25
1	I	57	GLU	CD-OE2	7.10	1.33	1.25
1	F	57	GLU	CD-OE2	7.10	1.33	1.25
1	G	57	GLU	CD-OE2	7.10	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	57	GLU	CD-OE2	7.09	1.33	1.25
1	M	57	GLU	CD-OE2	7.09	1.33	1.25
1	O	57	GLU	CD-OE2	7.09	1.33	1.25
1	J	57	GLU	CD-OE2	7.08	1.33	1.25
1	C	57	GLU	CD-OE2	7.08	1.33	1.25
1	N	57	GLU	CD-OE2	7.06	1.33	1.25
1	B	57	GLU	CD-OE2	7.06	1.33	1.25
1	L	57	GLU	CD-OE2	7.03	1.33	1.25
1	N	637	GLU	CD-OE2	7.01	1.33	1.25
1	H	57	GLU	CD-OE2	7.00	1.33	1.25
1	A	57	GLU	CD-OE2	7.00	1.33	1.25
1	H	637	GLU	CD-OE2	6.99	1.33	1.25
1	O	637	GLU	CD-OE2	6.99	1.33	1.25
1	F	637	GLU	CD-OE2	6.99	1.33	1.25
1	G	637	GLU	CD-OE2	6.98	1.33	1.25
1	I	637	GLU	CD-OE2	6.97	1.33	1.25
1	P	637	GLU	CD-OE2	6.97	1.33	1.25
1	M	637	GLU	CD-OE2	6.96	1.33	1.25
1	C	369	GLU	CD-OE2	6.95	1.33	1.25
1	A	637	GLU	CD-OE2	6.95	1.33	1.25
1	J	637	GLU	CD-OE2	6.95	1.33	1.25
1	B	314	GLU	CD-OE2	6.95	1.33	1.25
1	D	637	GLU	CD-OE2	6.95	1.33	1.25
1	G	314	GLU	CD-OE2	6.95	1.33	1.25
1	K	314	GLU	CD-OE2	6.94	1.33	1.25
1	B	637	GLU	CD-OE2	6.94	1.33	1.25
1	K	637	GLU	CD-OE2	6.94	1.33	1.25
1	C	637	GLU	CD-OE2	6.94	1.33	1.25
1	J	369	GLU	CD-OE2	6.94	1.33	1.25
1	L	637	GLU	CD-OE2	6.94	1.33	1.25
1	D	369	GLU	CD-OE2	6.93	1.33	1.25
1	E	369	GLU	CD-OE2	6.93	1.33	1.25
1	D	314	GLU	CD-OE2	6.92	1.33	1.25
1	F	369	GLU	CD-OE2	6.92	1.33	1.25
1	C	314	GLU	CD-OE2	6.92	1.33	1.25
1	I	314	GLU	CD-OE2	6.92	1.33	1.25
1	L	314	GLU	CD-OE2	6.92	1.33	1.25
1	O	369	GLU	CD-OE2	6.92	1.33	1.25
1	P	369	GLU	CD-OE2	6.92	1.33	1.25
1	A	314	GLU	CD-OE2	6.91	1.33	1.25
1	A	369	GLU	CD-OE2	6.91	1.33	1.25
1	E	637	GLU	CD-OE2	6.91	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	314	GLU	CD-OE2	6.91	1.33	1.25
1	H	369	GLU	CD-OE2	6.91	1.33	1.25
1	H	650	GLU	CD-OE2	6.90	1.33	1.25
1	N	369	GLU	CD-OE2	6.90	1.33	1.25
1	E	650	GLU	CD-OE2	6.90	1.33	1.25
1	O	314	GLU	CD-OE2	6.90	1.33	1.25
1	G	369	GLU	CD-OE2	6.90	1.33	1.25
1	I	369	GLU	CD-OE2	6.89	1.33	1.25
1	N	314	GLU	CD-OE2	6.89	1.33	1.25
1	P	314	GLU	CD-OE2	6.89	1.33	1.25
1	J	650	GLU	CD-OE2	6.89	1.33	1.25
1	D	650	GLU	CD-OE2	6.88	1.33	1.25
1	E	314	GLU	CD-OE2	6.88	1.33	1.25
1	P	650	GLU	CD-OE2	6.88	1.33	1.25
1	M	681	GLU	CD-OE2	6.88	1.33	1.25
1	C	650	GLU	CD-OE2	6.88	1.33	1.25
1	I	681	GLU	CD-OE2	6.88	1.33	1.25
1	P	681	GLU	CD-OE2	6.88	1.33	1.25
1	K	369	GLU	CD-OE2	6.87	1.33	1.25
1	M	369	GLU	CD-OE2	6.87	1.33	1.25
1	B	650	GLU	CD-OE2	6.87	1.33	1.25
1	C	681	GLU	CD-OE2	6.87	1.33	1.25
1	K	650	GLU	CD-OE2	6.86	1.33	1.25
1	M	314	GLU	CD-OE2	6.86	1.33	1.25
1	B	369	GLU	CD-OE2	6.86	1.33	1.25
1	L	369	GLU	CD-OE2	6.86	1.33	1.25
1	H	314	GLU	CD-OE2	6.85	1.33	1.25
1	J	314	GLU	CD-OE2	6.85	1.33	1.25
1	J	681	GLU	CD-OE2	6.85	1.33	1.25
1	O	681	GLU	CD-OE2	6.85	1.33	1.25
1	E	241	GLU	CD-OE2	6.85	1.33	1.25
1	E	681	GLU	CD-OE2	6.85	1.33	1.25
1	G	650	GLU	CD-OE2	6.85	1.33	1.25
1	F	650	GLU	CD-OE2	6.85	1.33	1.25
1	A	650	GLU	CD-OE2	6.84	1.33	1.25
1	N	650	GLU	CD-OE2	6.84	1.33	1.25
1	G	241	GLU	CD-OE2	6.84	1.33	1.25
1	N	681	GLU	CD-OE2	6.84	1.33	1.25
1	B	681	GLU	CD-OE2	6.84	1.33	1.25
1	G	681	GLU	CD-OE2	6.83	1.33	1.25
1	L	650	GLU	CD-OE2	6.83	1.33	1.25
1	O	650	GLU	CD-OE2	6.83	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	681	GLU	CD-OE2	6.83	1.33	1.25
1	M	650	GLU	CD-OE2	6.83	1.33	1.25
1	A	681	GLU	CD-OE2	6.82	1.33	1.25
1	I	650	GLU	CD-OE2	6.82	1.33	1.25
1	D	681	GLU	CD-OE2	6.81	1.33	1.25
1	O	241	GLU	CD-OE2	6.81	1.33	1.25
1	K	241	GLU	CD-OE2	6.80	1.33	1.25
1	H	241	GLU	CD-OE2	6.80	1.33	1.25
1	H	681	GLU	CD-OE2	6.80	1.33	1.25
1	L	241	GLU	CD-OE2	6.79	1.33	1.25
1	A	241	GLU	CD-OE2	6.79	1.33	1.25
1	I	241	GLU	CD-OE2	6.78	1.33	1.25
1	D	241	GLU	CD-OE2	6.78	1.33	1.25
1	F	241	GLU	CD-OE2	6.77	1.33	1.25
1	L	681	GLU	CD-OE2	6.77	1.33	1.25
1	B	67	GLU	CD-OE2	6.77	1.33	1.25
1	P	241	GLU	CD-OE2	6.77	1.33	1.25
1	K	681	GLU	CD-OE2	6.76	1.33	1.25
1	M	241	GLU	CD-OE2	6.75	1.33	1.25
1	M	67	GLU	CD-OE2	6.75	1.33	1.25
1	N	241	GLU	CD-OE2	6.73	1.33	1.25
1	P	67	GLU	CD-OE2	6.73	1.33	1.25
1	I	67	GLU	CD-OE2	6.73	1.33	1.25
1	J	241	GLU	CD-OE2	6.73	1.33	1.25
1	B	241	GLU	CD-OE2	6.73	1.33	1.25
1	E	67	GLU	CD-OE2	6.73	1.33	1.25
1	C	241	GLU	CD-OE2	6.72	1.33	1.25
1	G	67	GLU	CD-OE2	6.71	1.33	1.25
1	A	67	GLU	CD-OE2	6.71	1.33	1.25
1	F	67	GLU	CD-OE2	6.70	1.33	1.25
1	O	67	GLU	CD-OE2	6.69	1.33	1.25
1	C	67	GLU	CD-OE2	6.68	1.33	1.25
1	H	67	GLU	CD-OE2	6.68	1.32	1.25
1	L	67	GLU	CD-OE2	6.68	1.33	1.25
1	D	67	GLU	CD-OE2	6.67	1.32	1.25
1	N	67	GLU	CD-OE2	6.66	1.32	1.25
1	K	67	GLU	CD-OE2	6.66	1.32	1.25
1	J	67	GLU	CD-OE2	6.64	1.32	1.25
1	O	243	GLU	CD-OE2	6.62	1.32	1.25
1	P	243	GLU	CD-OE2	6.59	1.32	1.25
1	G	667	GLU	CD-OE2	6.58	1.32	1.25
1	K	667	GLU	CD-OE2	6.58	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	667	GLU	CD-OE2	6.58	1.32	1.25
1	N	243	GLU	CD-OE2	6.58	1.32	1.25
1	D	943	GLU	CD-OE2	6.58	1.32	1.25
1	M	243	GLU	CD-OE2	6.57	1.32	1.25
1	N	943	GLU	CD-OE2	6.56	1.32	1.25
1	A	667	GLU	CD-OE2	6.55	1.32	1.25
1	B	943	GLU	CD-OE2	6.55	1.32	1.25
1	K	943	GLU	CD-OE2	6.55	1.32	1.25
1	B	243	GLU	CD-OE2	6.55	1.32	1.25
1	F	667	GLU	CD-OE2	6.55	1.32	1.25
1	C	667	GLU	CD-OE2	6.54	1.32	1.25
1	A	243	GLU	CD-OE2	6.54	1.32	1.25
1	C	243	GLU	CD-OE2	6.54	1.32	1.25
1	I	243	GLU	CD-OE2	6.54	1.32	1.25
1	D	243	GLU	CD-OE2	6.52	1.32	1.25
1	J	243	GLU	CD-OE2	6.52	1.32	1.25
1	H	243	GLU	CD-OE2	6.51	1.32	1.25
1	K	243	GLU	CD-OE2	6.51	1.32	1.25
1	J	943	GLU	CD-OE2	6.51	1.32	1.25
1	P	667	GLU	CD-OE2	6.50	1.32	1.25
1	C	943	GLU	CD-OE2	6.50	1.32	1.25
1	O	943	GLU	CD-OE2	6.50	1.32	1.25
1	A	943	GLU	CD-OE2	6.50	1.32	1.25
1	H	667	GLU	CD-OE2	6.50	1.32	1.25
1	H	943	GLU	CD-OE2	6.50	1.32	1.25
1	L	243	GLU	CD-OE2	6.50	1.32	1.25
1	L	943	GLU	CD-OE2	6.50	1.32	1.25
1	F	943	GLU	CD-OE2	6.49	1.32	1.25
1	P	943	GLU	CD-OE2	6.49	1.32	1.25
1	J	667	GLU	CD-OE2	6.49	1.32	1.25
1	E	943	GLU	CD-OE2	6.49	1.32	1.25
1	M	667	GLU	CD-OE2	6.49	1.32	1.25
1	N	667	GLU	CD-OE2	6.49	1.32	1.25
1	M	943	GLU	CD-OE2	6.48	1.32	1.25
1	E	243	GLU	CD-OE2	6.48	1.32	1.25
1	F	243	GLU	CD-OE2	6.48	1.32	1.25
1	O	667	GLU	CD-OE2	6.47	1.32	1.25
1	D	667	GLU	CD-OE2	6.47	1.32	1.25
1	G	243	GLU	CD-OE2	6.46	1.32	1.25
1	B	667	GLU	CD-OE2	6.45	1.32	1.25
1	E	667	GLU	CD-OE2	6.45	1.32	1.25
1	I	943	GLU	CD-OE2	6.44	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	667	GLU	CD-OE2	6.43	1.32	1.25
1	G	943	GLU	CD-OE2	6.43	1.32	1.25
1	K	358	GLU	CD-OE2	6.42	1.32	1.25
1	C	358	GLU	CD-OE2	6.42	1.32	1.25
1	O	358	GLU	CD-OE2	6.40	1.32	1.25
1	B	358	GLU	CD-OE2	6.40	1.32	1.25
1	G	358	GLU	CD-OE2	6.39	1.32	1.25
1	J	358	GLU	CD-OE2	6.39	1.32	1.25
1	F	358	GLU	CD-OE2	6.39	1.32	1.25
1	N	358	GLU	CD-OE2	6.38	1.32	1.25
1	H	358	GLU	CD-OE2	6.37	1.32	1.25
1	L	358	GLU	CD-OE2	6.35	1.32	1.25
1	D	358	GLU	CD-OE2	6.35	1.32	1.25
1	A	358	GLU	CD-OE2	6.35	1.32	1.25
1	E	358	GLU	CD-OE2	6.35	1.32	1.25
1	I	358	GLU	CD-OE2	6.34	1.32	1.25
1	M	358	GLU	CD-OE2	6.34	1.32	1.25
1	P	358	GLU	CD-OE2	6.32	1.32	1.25
1	B	904	GLU	CD-OE2	6.09	1.32	1.25
1	F	904	GLU	CD-OE2	6.08	1.32	1.25
1	H	904	GLU	CD-OE2	6.08	1.32	1.25
1	E	904	GLU	CD-OE2	6.07	1.32	1.25
1	J	904	GLU	CD-OE2	6.07	1.32	1.25
1	K	904	GLU	CD-OE2	6.06	1.32	1.25
1	C	904	GLU	CD-OE2	6.05	1.32	1.25
1	N	904	GLU	CD-OE2	6.05	1.32	1.25
1	L	281	GLU	CD-OE2	6.05	1.32	1.25
1	I	281	GLU	CD-OE2	6.04	1.32	1.25
1	O	904	GLU	CD-OE2	6.04	1.32	1.25
1	G	281	GLU	CD-OE2	6.04	1.32	1.25
1	L	338	GLU	CD-OE2	6.04	1.32	1.25
1	I	904	GLU	CD-OE2	6.03	1.32	1.25
1	O	281	GLU	CD-OE2	6.03	1.32	1.25
1	C	338	GLU	CD-OE2	6.03	1.32	1.25
1	L	904	GLU	CD-OE2	6.03	1.32	1.25
1	E	281	GLU	CD-OE2	6.03	1.32	1.25
1	K	338	GLU	CD-OE2	6.03	1.32	1.25
1	M	904	GLU	CD-OE2	6.03	1.32	1.25
1	N	338	GLU	CD-OE2	6.03	1.32	1.25
1	D	281	GLU	CD-OE2	6.02	1.32	1.25
1	A	281	GLU	CD-OE2	6.02	1.32	1.25
1	P	904	GLU	CD-OE2	6.02	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	904	GLU	CD-OE2	6.01	1.32	1.25
1	H	281	GLU	CD-OE2	6.01	1.32	1.25
1	P	281	GLU	CD-OE2	6.01	1.32	1.25
1	C	281	GLU	CD-OE2	6.00	1.32	1.25
1	J	281	GLU	CD-OE2	6.00	1.32	1.25
1	E	1006	GLU	CD-OE2	6.00	1.32	1.25
1	B	338	GLU	CD-OE2	6.00	1.32	1.25
1	M	338	GLU	CD-OE2	5.99	1.32	1.25
1	F	338	GLU	CD-OE2	5.99	1.32	1.25
1	B	1006	GLU	CD-OE2	5.99	1.32	1.25
1	K	281	GLU	CD-OE2	5.98	1.32	1.25
1	F	281	GLU	CD-OE2	5.98	1.32	1.25
1	A	338	GLU	CD-OE2	5.97	1.32	1.25
1	A	904	GLU	CD-OE2	5.97	1.32	1.25
1	H	338	GLU	CD-OE2	5.97	1.32	1.25
1	O	338	GLU	CD-OE2	5.97	1.32	1.25
1	D	338	GLU	CD-OE2	5.97	1.32	1.25
1	G	904	GLU	CD-OE2	5.97	1.32	1.25
1	O	1006	GLU	CD-OE2	5.97	1.32	1.25
1	G	338	GLU	CD-OE2	5.97	1.32	1.25
1	M	281	GLU	CD-OE2	5.96	1.32	1.25
1	P	1006	GLU	CD-OE2	5.96	1.32	1.25
1	F	1006	GLU	CD-OE2	5.96	1.32	1.25
1	N	281	GLU	CD-OE2	5.96	1.32	1.25
1	B	281	GLU	CD-OE2	5.95	1.32	1.25
1	I	338	GLU	CD-OE2	5.95	1.32	1.25
1	P	338	GLU	CD-OE2	5.95	1.32	1.25
1	D	1006	GLU	CD-OE2	5.94	1.32	1.25
1	J	1006	GLU	CD-OE2	5.94	1.32	1.25
1	L	1006	GLU	CD-OE2	5.94	1.32	1.25
1	C	1006	GLU	CD-OE2	5.93	1.32	1.25
1	J	338	GLU	CD-OE2	5.93	1.32	1.25
1	N	1006	GLU	CD-OE2	5.93	1.32	1.25
1	A	1006	GLU	CD-OE2	5.92	1.32	1.25
1	I	1006	GLU	CD-OE2	5.92	1.32	1.25
1	E	338	GLU	CD-OE2	5.91	1.32	1.25
1	K	1006	GLU	CD-OE2	5.89	1.32	1.25
1	M	1006	GLU	CD-OE2	5.89	1.32	1.25
1	H	1006	GLU	CD-OE2	5.88	1.32	1.25
1	G	1006	GLU	CD-OE2	5.87	1.32	1.25
1	K	871	GLU	CD-OE2	5.87	1.32	1.25
1	N	871	GLU	CD-OE2	5.87	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	871	GLU	CD-OE2	5.86	1.32	1.25
1	I	871	GLU	CD-OE2	5.84	1.32	1.25
1	L	871	GLU	CD-OE2	5.84	1.32	1.25
1	J	871	GLU	CD-OE2	5.83	1.32	1.25
1	E	871	GLU	CD-OE2	5.83	1.32	1.25
1	G	871	GLU	CD-OE2	5.83	1.32	1.25
1	B	871	GLU	CD-OE2	5.83	1.32	1.25
1	A	871	GLU	CD-OE2	5.83	1.32	1.25
1	O	525	SER	CB-OG	5.82	1.49	1.42
1	P	871	GLU	CD-OE2	5.82	1.32	1.25
1	E	525	SER	CB-OG	5.81	1.49	1.42
1	D	871	GLU	CD-OE2	5.80	1.32	1.25
1	F	871	GLU	CD-OE2	5.80	1.32	1.25
1	H	525	SER	CB-OG	5.80	1.49	1.42
1	C	871	GLU	CD-OE2	5.80	1.32	1.25
1	N	525	SER	CB-OG	5.80	1.49	1.42
1	B	525	SER	CB-OG	5.79	1.49	1.42
1	C	525	SER	CB-OG	5.79	1.49	1.42
1	I	334	GLU	CD-OE2	5.78	1.32	1.25
1	K	525	SER	CB-OG	5.78	1.49	1.42
1	H	871	GLU	CD-OE2	5.78	1.32	1.25
1	M	871	GLU	CD-OE2	5.78	1.32	1.25
1	P	334	GLU	CD-OE2	5.78	1.32	1.25
1	L	525	SER	CB-OG	5.78	1.49	1.42
1	N	334	GLU	CD-OE2	5.76	1.31	1.25
1	G	334	GLU	CD-OE2	5.76	1.31	1.25
1	B	304	GLU	CD-OE1	-5.76	1.19	1.25
1	G	525	SER	CB-OG	5.76	1.49	1.42
1	B	334	GLU	CD-OE2	5.76	1.31	1.25
1	I	525	SER	CB-OG	5.76	1.49	1.42
1	L	334	GLU	CD-OE2	5.76	1.31	1.25
1	F	525	SER	CB-OG	5.75	1.49	1.42
1	J	334	GLU	CD-OE2	5.75	1.31	1.25
1	A	525	SER	CB-OG	5.74	1.49	1.42
1	D	334	GLU	CD-OE2	5.74	1.31	1.25
1	C	334	GLU	CD-OE2	5.74	1.31	1.25
1	D	525	SER	CB-OG	5.74	1.49	1.42
1	P	525	SER	CB-OG	5.73	1.49	1.42
1	J	525	SER	CB-OG	5.73	1.49	1.42
1	M	304	GLU	CD-OE1	-5.72	1.19	1.25
1	A	334	GLU	CD-OE2	5.72	1.31	1.25
1	F	334	GLU	CD-OE2	5.72	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	304	GLU	CD-OE1	-5.72	1.19	1.25
1	K	334	GLU	CD-OE2	5.71	1.31	1.25
1	M	525	SER	CB-OG	5.71	1.49	1.42
1	M	334	GLU	CD-OE2	5.71	1.31	1.25
1	P	304	GLU	CD-OE1	-5.70	1.19	1.25
1	E	334	GLU	CD-OE2	5.70	1.31	1.25
1	H	334	GLU	CD-OE2	5.70	1.31	1.25
1	A	304	GLU	CD-OE1	-5.69	1.19	1.25
1	C	304	GLU	CD-OE1	-5.68	1.19	1.25
1	O	334	GLU	CD-OE2	5.68	1.31	1.25
1	K	304	GLU	CD-OE1	-5.68	1.19	1.25
1	O	304	GLU	CD-OE1	-5.67	1.19	1.25
1	G	304	GLU	CD-OE1	-5.67	1.19	1.25
1	J	304	GLU	CD-OE1	-5.67	1.19	1.25
1	D	304	GLU	CD-OE1	-5.66	1.19	1.25
1	I	304	GLU	CD-OE1	-5.66	1.19	1.25
1	N	304	GLU	CD-OE1	-5.65	1.19	1.25
1	E	619	GLU	CD-OE2	5.64	1.31	1.25
1	F	304	GLU	CD-OE1	-5.63	1.19	1.25
1	F	461	GLU	CD-OE2	5.61	1.31	1.25
1	L	304	GLU	CD-OE1	-5.61	1.19	1.25
1	F	619	GLU	CD-OE2	5.61	1.31	1.25
1	H	304	GLU	CD-OE1	-5.60	1.19	1.25
1	C	461	GLU	CD-OE2	5.59	1.31	1.25
1	A	461	GLU	CD-OE2	5.58	1.31	1.25
1	G	619	GLU	CD-OE2	5.58	1.31	1.25
1	P	461	GLU	CD-OE2	5.58	1.31	1.25
1	C	619	GLU	CD-OE2	5.57	1.31	1.25
1	E	461	GLU	CD-OE2	5.57	1.31	1.25
1	G	461	GLU	CD-OE2	5.57	1.31	1.25
1	H	461	GLU	CD-OE2	5.57	1.31	1.25
1	J	619	GLU	CD-OE2	5.57	1.31	1.25
1	N	461	GLU	CD-OE2	5.56	1.31	1.25
1	I	619	GLU	CD-OE2	5.56	1.31	1.25
1	N	619	GLU	CD-OE2	5.56	1.31	1.25
1	O	619	GLU	CD-OE2	5.56	1.31	1.25
1	B	461	GLU	CD-OE2	5.56	1.31	1.25
1	I	461	GLU	CD-OE2	5.55	1.31	1.25
1	A	619	GLU	CD-OE2	5.55	1.31	1.25
1	M	461	GLU	CD-OE2	5.55	1.31	1.25
1	K	461	GLU	CD-OE2	5.54	1.31	1.25
1	L	461	GLU	CD-OE2	5.54	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	619	GLU	CD-OE2	5.54	1.31	1.25
1	K	619	GLU	CD-OE2	5.54	1.31	1.25
1	D	461	GLU	CD-OE2	5.53	1.31	1.25
1	D	619	GLU	CD-OE2	5.53	1.31	1.25
1	J	461	GLU	CD-OE2	5.53	1.31	1.25
1	M	619	GLU	CD-OE2	5.52	1.31	1.25
1	O	461	GLU	CD-OE2	5.52	1.31	1.25
1	B	619	GLU	CD-OE2	5.52	1.31	1.25
1	H	619	GLU	CD-OE2	5.51	1.31	1.25
1	P	619	GLU	CD-OE2	5.50	1.31	1.25
1	C	324	GLU	CD-OE2	5.49	1.31	1.25
1	G	324	GLU	CD-OE2	5.47	1.31	1.25
1	J	934	GLU	CD-OE2	5.47	1.31	1.25
1	P	324	GLU	CD-OE2	5.47	1.31	1.25
1	O	324	GLU	CD-OE2	5.46	1.31	1.25
1	K	934	GLU	CD-OE2	5.45	1.31	1.25
1	H	324	GLU	CD-OE2	5.45	1.31	1.25
1	A	934	GLU	CD-OE2	5.44	1.31	1.25
1	I	324	GLU	CD-OE2	5.44	1.31	1.25
1	N	324	GLU	CD-OE2	5.44	1.31	1.25
1	D	934	GLU	CD-OE2	5.44	1.31	1.25
1	A	324	GLU	CD-OE2	5.43	1.31	1.25
1	J	324	GLU	CD-OE2	5.42	1.31	1.25
1	F	324	GLU	CD-OE2	5.42	1.31	1.25
1	G	934	GLU	CD-OE2	5.41	1.31	1.25
1	D	324	GLU	CD-OE2	5.41	1.31	1.25
1	C	979	GLU	CD-OE2	5.41	1.31	1.25
1	N	979	GLU	CD-OE2	5.41	1.31	1.25
1	E	324	GLU	CD-OE2	5.40	1.31	1.25
1	E	934	GLU	CD-OE2	5.40	1.31	1.25
1	L	934	GLU	CD-OE2	5.40	1.31	1.25
1	B	934	GLU	CD-OE2	5.39	1.31	1.25
1	O	934	GLU	CD-OE2	5.39	1.31	1.25
1	K	324	GLU	CD-OE2	5.39	1.31	1.25
1	I	934	GLU	CD-OE2	5.39	1.31	1.25
1	I	979	GLU	CD-OE2	5.39	1.31	1.25
1	K	979	GLU	CD-OE2	5.38	1.31	1.25
1	B	324	GLU	CD-OE2	5.38	1.31	1.25
1	M	934	GLU	CD-OE2	5.38	1.31	1.25
1	L	324	GLU	CD-OE2	5.38	1.31	1.25
1	N	934	GLU	CD-OE2	5.37	1.31	1.25
1	M	324	GLU	CD-OE2	5.37	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	934	GLU	CD-OE2	5.35	1.31	1.25
1	P	934	GLU	CD-OE2	5.35	1.31	1.25
1	A	979	GLU	CD-OE2	5.35	1.31	1.25
1	O	979	GLU	CD-OE2	5.35	1.31	1.25
1	B	979	GLU	CD-OE2	5.35	1.31	1.25
1	M	979	GLU	CD-OE2	5.35	1.31	1.25
1	C	934	GLU	CD-OE2	5.34	1.31	1.25
1	F	934	GLU	CD-OE2	5.34	1.31	1.25
1	D	979	GLU	CD-OE2	5.34	1.31	1.25
1	P	979	GLU	CD-OE2	5.34	1.31	1.25
1	E	71	GLU	CD-OE2	5.34	1.31	1.25
1	H	979	GLU	CD-OE2	5.34	1.31	1.25
1	L	979	GLU	CD-OE2	5.33	1.31	1.25
1	G	979	GLU	CD-OE2	5.33	1.31	1.25
1	J	979	GLU	CD-OE2	5.33	1.31	1.25
1	B	71	GLU	CD-OE2	5.32	1.31	1.25
1	E	979	GLU	CD-OE2	5.32	1.31	1.25
1	A	71	GLU	CD-OE2	5.30	1.31	1.25
1	D	71	GLU	CD-OE2	5.29	1.31	1.25
1	C	71	GLU	CD-OE2	5.28	1.31	1.25
1	K	71	GLU	CD-OE2	5.28	1.31	1.25
1	F	979	GLU	CD-OE2	5.27	1.31	1.25
1	M	71	GLU	CD-OE2	5.25	1.31	1.25
1	I	71	GLU	CD-OE2	5.24	1.31	1.25
1	G	750	GLU	CD-OE2	5.22	1.31	1.25
1	G	71	GLU	CD-OE2	5.22	1.31	1.25
1	P	71	GLU	CD-OE2	5.22	1.31	1.25
1	H	71	GLU	CD-OE2	5.21	1.31	1.25
1	I	750	GLU	CD-OE2	5.21	1.31	1.25
1	F	71	GLU	CD-OE2	5.21	1.31	1.25
1	H	750	GLU	CD-OE2	5.20	1.31	1.25
1	L	71	GLU	CD-OE2	5.20	1.31	1.25
1	E	750	GLU	CD-OE2	5.20	1.31	1.25
1	L	750	GLU	CD-OE2	5.20	1.31	1.25
1	O	71	GLU	CD-OE2	5.20	1.31	1.25
1	J	71	GLU	CD-OE2	5.18	1.31	1.25
1	N	71	GLU	CD-OE2	5.18	1.31	1.25
1	F	750	GLU	CD-OE2	5.17	1.31	1.25
1	J	750	GLU	CD-OE2	5.17	1.31	1.25
1	P	750	GLU	CD-OE2	5.17	1.31	1.25
1	A	750	GLU	CD-OE2	5.17	1.31	1.25
1	K	750	GLU	CD-OE2	5.15	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	750	GLU	CD-OE2	5.15	1.31	1.25
1	M	750	GLU	CD-OE2	5.14	1.31	1.25
1	C	750	GLU	CD-OE2	5.13	1.31	1.25
1	B	750	GLU	CD-OE2	5.12	1.31	1.25
1	D	750	GLU	CD-OE2	5.12	1.31	1.25
1	B	17	GLU	CD-OE2	5.12	1.31	1.25
1	O	750	GLU	CD-OE2	5.12	1.31	1.25
1	C	800	ARG	NE-CZ	5.11	1.39	1.33
1	C	17	GLU	CD-OE2	5.11	1.31	1.25
1	B	800	ARG	NE-CZ	5.11	1.39	1.33
1	P	17	GLU	CD-OE2	5.11	1.31	1.25
1	A	800	ARG	CZ-NH1	5.10	1.39	1.33
1	K	800	ARG	CZ-NH1	5.10	1.39	1.33
1	O	800	ARG	NE-CZ	5.10	1.39	1.33
1	I	41	GLU	CD-OE2	5.10	1.31	1.25
1	J	17	GLU	CD-OE2	5.10	1.31	1.25
1	F	800	ARG	CZ-NH1	5.10	1.39	1.33
1	G	800	ARG	CZ-NH1	5.09	1.39	1.33
1	N	800	ARG	CZ-NH1	5.09	1.39	1.33
1	I	800	ARG	NE-CZ	5.09	1.39	1.33
1	N	17	GLU	CD-OE2	5.09	1.31	1.25
1	G	17	GLU	CD-OE2	5.09	1.31	1.25
1	I	17	GLU	CD-OE2	5.09	1.31	1.25
1	K	17	GLU	CD-OE2	5.09	1.31	1.25
1	F	17	GLU	CD-OE2	5.08	1.31	1.25
1	E	800	ARG	CZ-NH1	5.08	1.39	1.33
1	L	800	ARG	NE-CZ	5.08	1.39	1.33
1	H	17	GLU	CD-OE2	5.08	1.31	1.25
1	P	41	GLU	CD-OE2	5.08	1.31	1.25
1	P	800	ARG	CZ-NH1	5.08	1.39	1.33
1	D	17	GLU	CD-OE2	5.08	1.31	1.25
1	A	800	ARG	NE-CZ	5.08	1.39	1.33
1	E	17	GLU	CD-OE2	5.08	1.31	1.25
1	G	800	ARG	NE-CZ	5.07	1.39	1.33
1	A	17	GLU	CD-OE2	5.07	1.31	1.25
1	H	800	ARG	NE-CZ	5.07	1.39	1.33
1	N	800	ARG	NE-CZ	5.07	1.39	1.33
1	B	800	ARG	CZ-NH1	5.07	1.39	1.33
1	J	800	ARG	NE-CZ	5.07	1.39	1.33
1	L	17	GLU	CD-OE2	5.07	1.31	1.25
1	O	17	GLU	CD-OE2	5.07	1.31	1.25
1	C	800	ARG	CZ-NH1	5.06	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	41	GLU	CD-OE2	5.06	1.31	1.25
1	D	800	ARG	NE-CZ	5.06	1.39	1.33
1	M	17	GLU	CD-OE2	5.06	1.31	1.25
1	I	800	ARG	CZ-NH1	5.06	1.39	1.33
1	C	41	GLU	CD-OE2	5.06	1.31	1.25
1	B	41	GLU	CD-OE2	5.05	1.31	1.25
1	M	800	ARG	NE-CZ	5.05	1.39	1.33
1	E	41	GLU	CD-OE2	5.05	1.31	1.25
1	K	41	GLU	CD-OE2	5.05	1.31	1.25
1	M	800	ARG	CZ-NH1	5.05	1.39	1.33
1	P	800	ARG	NE-CZ	5.05	1.39	1.33
1	D	800	ARG	CZ-NH1	5.04	1.39	1.33
1	O	41	GLU	CD-OE2	5.04	1.31	1.25
1	O	800	ARG	CZ-NH1	5.04	1.39	1.33
1	J	800	ARG	CZ-NH1	5.04	1.39	1.33
1	L	41	GLU	CD-OE2	5.04	1.31	1.25
1	A	41	GLU	CD-OE2	5.03	1.31	1.25
1	F	800	ARG	NE-CZ	5.03	1.39	1.33
1	H	41	GLU	CD-OE2	5.03	1.31	1.25
1	N	41	GLU	CD-OE2	5.03	1.31	1.25
1	D	170	GLU	CD-OE2	5.02	1.31	1.25
1	H	170	GLU	CD-OE2	5.02	1.31	1.25
1	K	800	ARG	NE-CZ	5.02	1.39	1.33
1	L	800	ARG	CZ-NH1	5.01	1.39	1.33
1	G	41	GLU	CD-OE2	5.01	1.31	1.25
1	E	800	ARG	NE-CZ	5.01	1.39	1.33
1	O	416	GLU	CD-OE2	5.00	1.31	1.25
1	J	41	GLU	CD-OE2	5.00	1.31	1.25

All (3010) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	210	ARG	NE-CZ-NH1	18.08	129.34	120.30
1	L	210	ARG	NE-CZ-NH1	18.07	129.34	120.30
1	J	210	ARG	NE-CZ-NH1	18.07	129.33	120.30
1	M	210	ARG	NE-CZ-NH1	18.03	129.31	120.30
1	G	210	ARG	NE-CZ-NH1	18.01	129.30	120.30
1	P	210	ARG	NE-CZ-NH1	18.01	129.30	120.30
1	D	210	ARG	NE-CZ-NH1	18.00	129.30	120.30
1	A	210	ARG	NE-CZ-NH1	17.99	129.30	120.30
1	H	210	ARG	NE-CZ-NH1	17.98	129.29	120.30
1	C	210	ARG	NE-CZ-NH1	17.98	129.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	210	ARG	NE-CZ-NH1	17.98	129.29	120.30
1	F	210	ARG	NE-CZ-NH1	17.94	129.27	120.30
1	N	210	ARG	NE-CZ-NH1	17.92	129.26	120.30
1	K	210	ARG	NE-CZ-NH1	17.91	129.26	120.30
1	O	210	ARG	NE-CZ-NH1	17.91	129.25	120.30
1	B	210	ARG	NE-CZ-NH1	17.89	129.25	120.30
1	C	448	ARG	NE-CZ-NH2	-16.64	111.98	120.30
1	G	448	ARG	NE-CZ-NH2	-16.60	112.00	120.30
1	D	448	ARG	NE-CZ-NH2	-16.58	112.01	120.30
1	L	448	ARG	NE-CZ-NH2	-16.57	112.01	120.30
1	H	448	ARG	NE-CZ-NH2	-16.57	112.02	120.30
1	N	448	ARG	NE-CZ-NH2	-16.55	112.02	120.30
1	I	448	ARG	NE-CZ-NH2	-16.55	112.03	120.30
1	A	448	ARG	NE-CZ-NH2	-16.54	112.03	120.30
1	F	448	ARG	NE-CZ-NH2	-16.54	112.03	120.30
1	B	448	ARG	NE-CZ-NH2	-16.53	112.03	120.30
1	K	448	ARG	NE-CZ-NH2	-16.53	112.03	120.30
1	M	448	ARG	NE-CZ-NH2	-16.52	112.04	120.30
1	E	448	ARG	NE-CZ-NH2	-16.52	112.04	120.30
1	O	448	ARG	NE-CZ-NH2	-16.50	112.05	120.30
1	J	448	ARG	NE-CZ-NH2	-16.49	112.05	120.30
1	P	448	ARG	NE-CZ-NH2	-16.49	112.06	120.30
1	H	881	ARG	NE-CZ-NH2	-16.26	112.17	120.30
1	J	881	ARG	NE-CZ-NH2	-16.25	112.17	120.30
1	K	881	ARG	NE-CZ-NH2	-16.25	112.17	120.30
1	L	881	ARG	NE-CZ-NH2	-16.22	112.19	120.30
1	C	881	ARG	NE-CZ-NH2	-16.21	112.19	120.30
1	N	881	ARG	NE-CZ-NH2	-16.20	112.20	120.30
1	P	881	ARG	NE-CZ-NH2	-16.20	112.20	120.30
1	F	881	ARG	NE-CZ-NH2	-16.20	112.20	120.30
1	G	881	ARG	NE-CZ-NH2	-16.20	112.20	120.30
1	B	881	ARG	NE-CZ-NH2	-16.19	112.20	120.30
1	E	881	ARG	NE-CZ-NH2	-16.17	112.21	120.30
1	A	881	ARG	NE-CZ-NH2	-16.16	112.22	120.30
1	M	881	ARG	NE-CZ-NH2	-16.15	112.22	120.30
1	I	881	ARG	NE-CZ-NH2	-16.12	112.24	120.30
1	D	881	ARG	NE-CZ-NH2	-16.12	112.24	120.30
1	O	881	ARG	NE-CZ-NH2	-16.11	112.24	120.30
1	E	938	ARG	NE-CZ-NH2	-15.54	112.53	120.30
1	A	938	ARG	NE-CZ-NH2	-15.53	112.53	120.30
1	M	938	ARG	NE-CZ-NH2	-15.53	112.53	120.30
1	F	938	ARG	NE-CZ-NH2	-15.50	112.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	938	ARG	NE-CZ-NH2	-15.50	112.55	120.30
1	I	938	ARG	NE-CZ-NH2	-15.49	112.55	120.30
1	O	938	ARG	NE-CZ-NH2	-15.49	112.56	120.30
1	C	881	ARG	NE-CZ-NH1	15.48	128.04	120.30
1	J	938	ARG	NE-CZ-NH2	-15.46	112.57	120.30
1	G	881	ARG	NE-CZ-NH1	15.45	128.03	120.30
1	H	938	ARG	NE-CZ-NH2	-15.45	112.58	120.30
1	G	938	ARG	NE-CZ-NH2	-15.44	112.58	120.30
1	C	938	ARG	NE-CZ-NH2	-15.44	112.58	120.30
1	F	881	ARG	NE-CZ-NH1	15.44	128.02	120.30
1	N	881	ARG	NE-CZ-NH1	15.44	128.02	120.30
1	P	938	ARG	NE-CZ-NH2	-15.44	112.58	120.30
1	K	938	ARG	NE-CZ-NH2	-15.42	112.59	120.30
1	N	938	ARG	NE-CZ-NH2	-15.42	112.59	120.30
1	L	881	ARG	NE-CZ-NH1	15.40	128.00	120.30
1	B	881	ARG	NE-CZ-NH1	15.40	128.00	120.30
1	H	881	ARG	NE-CZ-NH1	15.39	128.00	120.30
1	M	881	ARG	NE-CZ-NH1	15.39	127.99	120.30
1	B	938	ARG	NE-CZ-NH2	-15.38	112.61	120.30
1	O	881	ARG	NE-CZ-NH1	15.38	127.99	120.30
1	J	881	ARG	NE-CZ-NH1	15.38	127.99	120.30
1	K	881	ARG	NE-CZ-NH1	15.35	127.98	120.30
1	A	881	ARG	NE-CZ-NH1	15.34	127.97	120.30
1	L	938	ARG	NE-CZ-NH2	-15.34	112.63	120.30
1	E	881	ARG	NE-CZ-NH1	15.33	127.96	120.30
1	P	881	ARG	NE-CZ-NH1	15.28	127.94	120.30
1	I	881	ARG	NE-CZ-NH1	15.24	127.92	120.30
1	D	881	ARG	NE-CZ-NH1	15.20	127.90	120.30
1	C	210	ARG	NE-CZ-NH2	-14.78	112.91	120.30
1	D	210	ARG	NE-CZ-NH2	-14.77	112.91	120.30
1	J	210	ARG	NE-CZ-NH2	-14.77	112.92	120.30
1	A	210	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	P	210	ARG	NE-CZ-NH2	-14.74	112.93	120.30
1	H	210	ARG	NE-CZ-NH2	-14.74	112.93	120.30
1	G	210	ARG	NE-CZ-NH2	-14.73	112.94	120.30
1	E	210	ARG	NE-CZ-NH2	-14.72	112.94	120.30
1	B	210	ARG	NE-CZ-NH2	-14.69	112.95	120.30
1	O	210	ARG	NE-CZ-NH2	-14.68	112.96	120.30
1	M	210	ARG	NE-CZ-NH2	-14.68	112.96	120.30
1	L	166	ARG	NE-CZ-NH1	14.68	127.64	120.30
1	L	210	ARG	NE-CZ-NH2	-14.68	112.96	120.30
1	O	166	ARG	NE-CZ-NH1	14.67	127.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	166	ARG	NE-CZ-NH1	14.66	127.63	120.30
1	N	210	ARG	NE-CZ-NH2	-14.66	112.97	120.30
1	I	210	ARG	NE-CZ-NH2	-14.65	112.98	120.30
1	K	210	ARG	NE-CZ-NH2	-14.62	112.99	120.30
1	D	166	ARG	NE-CZ-NH1	14.62	127.61	120.30
1	F	210	ARG	NE-CZ-NH2	-14.61	113.00	120.30
1	C	166	ARG	NE-CZ-NH1	14.60	127.60	120.30
1	E	166	ARG	NE-CZ-NH1	14.60	127.60	120.30
1	K	166	ARG	NE-CZ-NH1	14.60	127.60	120.30
1	J	166	ARG	NE-CZ-NH1	14.59	127.59	120.30
1	M	166	ARG	NE-CZ-NH1	14.59	127.59	120.30
1	A	166	ARG	NE-CZ-NH1	14.58	127.59	120.30
1	N	166	ARG	NE-CZ-NH1	14.58	127.59	120.30
1	G	166	ARG	NE-CZ-NH1	14.56	127.58	120.30
1	H	166	ARG	NE-CZ-NH1	14.56	127.58	120.30
1	F	166	ARG	NE-CZ-NH1	14.54	127.57	120.30
1	B	166	ARG	NE-CZ-NH1	14.53	127.56	120.30
1	P	166	ARG	NE-CZ-NH1	14.53	127.56	120.30
1	D	938	ARG	NE-CZ-NH1	13.60	127.10	120.30
1	E	938	ARG	NE-CZ-NH1	13.57	127.08	120.30
1	F	938	ARG	NE-CZ-NH1	13.55	127.08	120.30
1	B	938	ARG	NE-CZ-NH1	13.54	127.07	120.30
1	M	938	ARG	NE-CZ-NH1	13.53	127.07	120.30
1	I	938	ARG	NE-CZ-NH1	13.52	127.06	120.30
1	O	938	ARG	NE-CZ-NH1	13.51	127.06	120.30
1	H	938	ARG	NE-CZ-NH1	13.51	127.05	120.30
1	C	938	ARG	NE-CZ-NH1	13.51	127.05	120.30
1	P	938	ARG	NE-CZ-NH1	13.49	127.05	120.30
1	A	938	ARG	NE-CZ-NH1	13.49	127.04	120.30
1	K	938	ARG	NE-CZ-NH1	13.48	127.04	120.30
1	G	938	ARG	NE-CZ-NH1	13.46	127.03	120.30
1	N	938	ARG	NE-CZ-NH1	13.45	127.02	120.30
1	L	938	ARG	NE-CZ-NH1	13.44	127.02	120.30
1	J	938	ARG	NE-CZ-NH1	13.43	127.02	120.30
1	D	746	ASP	CB-CG-OD2	-12.36	107.17	118.30
1	E	746	ASP	CB-CG-OD2	-12.35	107.19	118.30
1	J	746	ASP	CB-CG-OD2	-12.34	107.19	118.30
1	L	746	ASP	CB-CG-OD2	-12.34	107.19	118.30
1	G	746	ASP	CB-CG-OD2	-12.33	107.20	118.30
1	I	746	ASP	CB-CG-OD2	-12.33	107.21	118.30
1	H	746	ASP	CB-CG-OD2	-12.32	107.21	118.30
1	M	746	ASP	CB-CG-OD2	-12.31	107.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	746	ASP	CB-CG-OD2	-12.31	107.22	118.30
1	N	746	ASP	CB-CG-OD2	-12.31	107.22	118.30
1	P	746	ASP	CB-CG-OD2	-12.31	107.22	118.30
1	A	746	ASP	CB-CG-OD2	-12.30	107.23	118.30
1	B	746	ASP	CB-CG-OD2	-12.29	107.24	118.30
1	K	746	ASP	CB-CG-OD2	-12.29	107.24	118.30
1	O	746	ASP	CB-CG-OD2	-12.28	107.25	118.30
1	F	746	ASP	CB-CG-OD2	-12.27	107.26	118.30
1	H	809	ARG	NE-CZ-NH1	11.03	125.81	120.30
1	N	809	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	A	809	ARG	NE-CZ-NH1	10.97	125.78	120.30
1	I	809	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	J	809	ARG	NE-CZ-NH1	10.95	125.78	120.30
1	P	809	ARG	NE-CZ-NH1	10.95	125.78	120.30
1	C	809	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	K	809	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	O	809	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	L	809	ARG	NE-CZ-NH1	10.93	125.77	120.30
1	D	809	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	F	809	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	M	809	ARG	NE-CZ-NH1	10.89	125.75	120.30
1	E	809	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	G	809	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	B	809	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	I	473	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	N	473	ARG	NE-CZ-NH1	10.05	125.33	120.30
1	D	473	ARG	NE-CZ-NH1	10.05	125.33	120.30
1	J	473	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	G	473	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	P	473	ARG	NE-CZ-NH1	10.03	125.31	120.30
1	A	473	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	B	473	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	M	473	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	E	473	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	L	473	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	H	473	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	D	645	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	H	645	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	M	645	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	C	473	ARG	NE-CZ-NH1	9.95	125.28	120.30
1	D	1018	LEU	CB-CA-C	-9.94	91.31	110.20
1	K	1018	LEU	CB-CA-C	-9.94	91.31	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1018	LEU	CB-CA-C	-9.93	91.33	110.20
1	C	1018	LEU	CB-CA-C	-9.93	91.34	110.20
1	L	1018	LEU	CB-CA-C	-9.93	91.34	110.20
1	A	1018	LEU	CB-CA-C	-9.92	91.35	110.20
1	F	1018	LEU	CB-CA-C	-9.92	91.35	110.20
1	O	1018	LEU	CB-CA-C	-9.92	91.35	110.20
1	P	1018	LEU	CB-CA-C	-9.92	91.35	110.20
1	B	1018	LEU	CB-CA-C	-9.92	91.35	110.20
1	H	1018	LEU	CB-CA-C	-9.92	91.35	110.20
1	M	1018	LEU	CB-CA-C	-9.92	91.35	110.20
1	F	473	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	G	1018	LEU	CB-CA-C	-9.92	91.36	110.20
1	O	473	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	I	1018	LEU	CB-CA-C	-9.91	91.37	110.20
1	K	473	ARG	NE-CZ-NH1	9.91	125.26	120.30
1	J	1018	LEU	CB-CA-C	-9.91	91.37	110.20
1	E	645	ARG	NE-CZ-NH1	9.89	125.25	120.30
1	N	1018	LEU	CB-CA-C	-9.89	91.41	110.20
1	G	645	ARG	NE-CZ-NH1	9.89	125.24	120.30
1	I	645	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	N	645	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	A	645	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	O	645	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	K	645	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	C	645	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	J	645	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	P	645	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	E	447	ASP	CB-CG-OD2	-9.80	109.48	118.30
1	L	645	ARG	NE-CZ-NH1	9.79	125.20	120.30
1	F	645	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	P	447	ASP	CB-CG-OD2	-9.78	109.50	118.30
1	G	447	ASP	CB-CG-OD2	-9.77	109.51	118.30
1	N	233	ASP	CB-CG-OD1	9.77	127.09	118.30
1	G	233	ASP	CB-CG-OD1	9.77	127.09	118.30
1	E	233	ASP	CB-CG-OD1	9.76	127.09	118.30
1	O	233	ASP	CB-CG-OD1	9.76	127.09	118.30
1	D	447	ASP	CB-CG-OD2	-9.76	109.52	118.30
1	J	447	ASP	CB-CG-OD2	-9.76	109.52	118.30
1	B	233	ASP	CB-CG-OD1	9.76	127.08	118.30
1	M	233	ASP	CB-CG-OD1	9.75	127.08	118.30
1	A	447	ASP	CB-CG-OD2	-9.75	109.53	118.30
1	F	233	ASP	CB-CG-OD1	9.75	127.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	233	ASP	CB-CG-OD1	9.75	127.07	118.30
1	B	645	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	M	447	ASP	CB-CG-OD2	-9.74	109.53	118.30
1	O	447	ASP	CB-CG-OD2	-9.74	109.53	118.30
1	C	233	ASP	CB-CG-OD1	9.73	127.06	118.30
1	L	447	ASP	CB-CG-OD2	-9.73	109.54	118.30
1	H	447	ASP	CB-CG-OD2	-9.73	109.54	118.30
1	N	447	ASP	CB-CG-OD2	-9.73	109.54	118.30
1	B	447	ASP	CB-CG-OD2	-9.73	109.54	118.30
1	F	447	ASP	CB-CG-OD2	-9.73	109.54	118.30
1	K	233	ASP	CB-CG-OD1	9.73	127.06	118.30
1	C	447	ASP	CB-CG-OD2	-9.73	109.55	118.30
1	J	233	ASP	CB-CG-OD1	9.73	127.06	118.30
1	D	781	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	H	233	ASP	CB-CG-OD1	9.72	127.05	118.30
1	I	447	ASP	CB-CG-OD2	-9.72	109.55	118.30
1	L	781	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	K	447	ASP	CB-CG-OD2	-9.72	109.55	118.30
1	P	781	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	G	781	ARG	NE-CZ-NH2	-9.71	115.44	120.30
1	P	233	ASP	CB-CG-OD1	9.71	127.04	118.30
1	B	781	ARG	NE-CZ-NH2	-9.71	115.45	120.30
1	D	233	ASP	CB-CG-OD1	9.71	127.03	118.30
1	I	233	ASP	CB-CG-OD1	9.71	127.03	118.30
1	A	233	ASP	CB-CG-OD1	9.68	127.01	118.30
1	E	431	ARG	NE-CZ-NH1	9.68	125.14	120.30
1	K	199	ASP	CB-CG-OD2	-9.68	109.59	118.30
1	K	431	ARG	NE-CZ-NH1	9.68	125.14	120.30
1	L	199	ASP	CB-CG-OD2	-9.67	109.59	118.30
1	P	199	ASP	CB-CG-OD2	-9.66	109.60	118.30
1	I	199	ASP	CB-CG-OD2	-9.65	109.61	118.30
1	J	199	ASP	CB-CG-OD2	-9.65	109.61	118.30
1	A	781	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	D	199	ASP	CB-CG-OD2	-9.64	109.62	118.30
1	D	431	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	A	199	ASP	CB-CG-OD2	-9.64	109.63	118.30
1	O	199	ASP	CB-CG-OD2	-9.64	109.63	118.30
1	C	781	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	K	781	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	H	199	ASP	CB-CG-OD2	-9.63	109.63	118.30
1	M	781	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	B	199	ASP	CB-CG-OD2	-9.62	109.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	199	ASP	CB-CG-OD2	-9.62	109.64	118.30
1	G	199	ASP	CB-CG-OD2	-9.62	109.64	118.30
1	N	199	ASP	CB-CG-OD2	-9.62	109.64	118.30
1	H	781	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	P	431	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	F	199	ASP	CB-CG-OD2	-9.61	109.65	118.30
1	M	199	ASP	CB-CG-OD2	-9.61	109.65	118.30
1	E	199	ASP	CB-CG-OD2	-9.61	109.65	118.30
1	J	431	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	I	431	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	F	781	ARG	NE-CZ-NH2	-9.59	115.51	120.30
1	I	781	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	F	431	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	M	431	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	N	781	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	A	431	ARG	NE-CZ-NH1	9.57	125.09	120.30
1	J	781	ARG	NE-CZ-NH2	-9.57	115.52	120.30
1	O	431	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	B	431	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	H	431	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	O	781	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	E	781	ARG	NE-CZ-NH2	-9.55	115.53	120.30
1	L	431	ARG	NE-CZ-NH1	9.53	125.07	120.30
1	N	431	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	C	431	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	G	431	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	M	809	ARG	NE-CZ-NH2	-9.49	115.55	120.30
1	K	13	ARG	NE-CZ-NH1	9.49	125.04	120.30
1	C	809	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	N	809	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	P	809	ARG	NE-CZ-NH2	-9.45	115.57	120.30
1	F	809	ARG	NE-CZ-NH2	-9.45	115.58	120.30
1	H	809	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	A	809	ARG	NE-CZ-NH2	-9.43	115.58	120.30
1	M	13	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	L	809	ARG	NE-CZ-NH2	-9.43	115.59	120.30
1	F	13	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	G	809	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	O	13	ARG	NE-CZ-NH1	9.41	125.01	120.30
1	O	809	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	I	13	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	I	809	ARG	NE-CZ-NH2	-9.41	115.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	13	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	J	809	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	H	13	ARG	NE-CZ-NH1	9.39	124.99	120.30
1	K	809	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	A	13	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	L	13	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	E	809	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	D	809	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	B	809	ARG	NE-CZ-NH2	-9.35	115.62	120.30
1	J	13	ARG	NE-CZ-NH1	9.35	124.98	120.30
1	G	13	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	B	13	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	N	13	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	C	13	ARG	NE-CZ-NH1	9.31	124.95	120.30
1	D	13	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	E	13	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	O	509	ASP	CB-CG-OD2	-9.19	110.03	118.30
1	H	509	ASP	CB-CG-OD2	-9.18	110.04	118.30
1	G	509	ASP	CB-CG-OD2	-9.17	110.05	118.30
1	P	509	ASP	CB-CG-OD2	-9.16	110.06	118.30
1	N	509	ASP	CB-CG-OD2	-9.15	110.07	118.30
1	B	509	ASP	CB-CG-OD2	-9.14	110.08	118.30
1	A	509	ASP	CB-CG-OD2	-9.13	110.08	118.30
1	K	509	ASP	CB-CG-OD2	-9.13	110.08	118.30
1	F	509	ASP	CB-CG-OD2	-9.13	110.08	118.30
1	L	509	ASP	CB-CG-OD2	-9.12	110.09	118.30
1	J	509	ASP	CB-CG-OD2	-9.12	110.09	118.30
1	M	509	ASP	CB-CG-OD2	-9.12	110.09	118.30
1	B	429	ASP	CB-CG-OD2	-9.12	110.09	118.30
1	J	429	ASP	CB-CG-OD2	-9.11	110.10	118.30
1	E	509	ASP	CB-CG-OD2	-9.11	110.10	118.30
1	O	429	ASP	CB-CG-OD2	-9.11	110.11	118.30
1	D	509	ASP	CB-CG-OD2	-9.10	110.11	118.30
1	N	429	ASP	CB-CG-OD2	-9.10	110.11	118.30
1	C	429	ASP	CB-CG-OD2	-9.10	110.11	118.30
1	C	509	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	I	509	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	A	429	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	F	429	ASP	CB-CG-OD2	-9.08	110.12	118.30
1	K	429	ASP	CB-CG-OD2	-9.08	110.12	118.30
1	D	429	ASP	CB-CG-OD2	-9.08	110.13	118.30
1	L	429	ASP	CB-CG-OD2	-9.07	110.13	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	429	ASP	CB-CG-OD2	-9.07	110.14	118.30
1	E	429	ASP	CB-CG-OD2	-9.07	110.14	118.30
1	I	429	ASP	CB-CG-OD2	-9.07	110.14	118.30
1	G	429	ASP	CB-CG-OD2	-9.05	110.16	118.30
1	H	429	ASP	CB-CG-OD2	-9.04	110.17	118.30
1	P	429	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	B	473	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	K	473	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	K	287	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	N	287	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	M	473	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	I	287	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	D	473	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	H	287	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	D	287	ASP	CB-CG-OD2	-8.87	110.32	118.30
1	C	287	ASP	CB-CG-OD2	-8.87	110.32	118.30
1	A	287	ASP	CB-CG-OD2	-8.86	110.33	118.30
1	A	473	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	J	287	ASP	CB-CG-OD2	-8.86	110.33	118.30
1	E	287	ASP	CB-CG-OD2	-8.85	110.33	118.30
1	C	473	ARG	NE-CZ-NH2	-8.85	115.87	120.30
1	I	473	ARG	NE-CZ-NH2	-8.85	115.87	120.30
1	B	287	ASP	CB-CG-OD2	-8.85	110.34	118.30
1	J	473	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	L	473	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	H	473	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	P	287	ASP	CB-CG-OD2	-8.84	110.34	118.30
1	L	287	ASP	CB-CG-OD2	-8.84	110.34	118.30
1	G	287	ASP	CB-CG-OD2	-8.84	110.35	118.30
1	O	473	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	F	287	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	O	287	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	P	473	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	M	287	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	G	473	ARG	NE-CZ-NH2	-8.81	115.90	120.30
1	E	473	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	N	473	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	F	52	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	K	210	ARG	CD-NE-CZ	8.72	135.81	123.60
1	L	210	ARG	CD-NE-CZ	8.72	135.81	123.60
1	I	210	ARG	CD-NE-CZ	8.72	135.80	123.60
1	H	210	ARG	CD-NE-CZ	8.71	135.80	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	210	ARG	CD-NE-CZ	8.71	135.79	123.60
1	N	210	ARG	CD-NE-CZ	8.71	135.79	123.60
1	C	210	ARG	CD-NE-CZ	8.70	135.78	123.60
1	F	210	ARG	CD-NE-CZ	8.70	135.78	123.60
1	F	473	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	A	210	ARG	CD-NE-CZ	8.70	135.78	123.60
1	B	210	ARG	CD-NE-CZ	8.70	135.77	123.60
1	O	52	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	P	210	ARG	CD-NE-CZ	8.70	135.77	123.60
1	D	210	ARG	CD-NE-CZ	8.69	135.77	123.60
1	G	210	ARG	CD-NE-CZ	8.69	135.76	123.60
1	E	210	ARG	CD-NE-CZ	8.68	135.76	123.60
1	J	210	ARG	CD-NE-CZ	8.68	135.75	123.60
1	M	210	ARG	CD-NE-CZ	8.68	135.76	123.60
1	I	52	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	B	52	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	N	52	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	P	52	ARG	NE-CZ-NH2	-8.63	115.99	120.30
1	E	52	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	H	52	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	D	52	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	J	52	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	A	52	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	B	448	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	K	368	ASP	CB-CG-OD2	-8.58	110.58	118.30
1	O	368	ASP	CB-CG-OD2	-8.58	110.58	118.30
1	G	52	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	E	368	ASP	CB-CG-OD2	-8.57	110.59	118.30
1	O	429	ASP	CB-CG-OD1	8.57	126.01	118.30
1	J	368	ASP	CB-CG-OD2	-8.56	110.59	118.30
1	L	52	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	M	368	ASP	CB-CG-OD2	-8.56	110.59	118.30
1	D	429	ASP	CB-CG-OD1	8.56	126.00	118.30
1	F	429	ASP	CB-CG-OD1	8.55	126.00	118.30
1	K	429	ASP	CB-CG-OD1	8.55	126.00	118.30
1	K	52	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	P	368	ASP	CB-CG-OD2	-8.55	110.61	118.30
1	C	368	ASP	CB-CG-OD2	-8.55	110.61	118.30
1	H	368	ASP	CB-CG-OD2	-8.54	110.61	118.30
1	M	429	ASP	CB-CG-OD1	8.55	125.99	118.30
1	N	429	ASP	CB-CG-OD1	8.55	125.99	118.30
1	J	429	ASP	CB-CG-OD1	8.54	125.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	448	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	C	52	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	L	368	ASP	CB-CG-OD2	-8.54	110.62	118.30
1	C	429	ASP	CB-CG-OD1	8.53	125.98	118.30
1	E	429	ASP	CB-CG-OD1	8.54	125.98	118.30
1	H	448	ARG	NE-CZ-NH1	8.53	124.57	120.30
1	A	368	ASP	CB-CG-OD2	-8.53	110.62	118.30
1	I	368	ASP	CB-CG-OD2	-8.53	110.62	118.30
1	A	429	ASP	CB-CG-OD1	8.53	125.97	118.30
1	I	429	ASP	CB-CG-OD1	8.53	125.97	118.30
1	G	448	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	B	368	ASP	CB-CG-OD2	-8.52	110.63	118.30
1	I	448	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	D	368	ASP	CB-CG-OD2	-8.52	110.64	118.30
1	F	368	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	K	448	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	P	448	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	D	448	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	G	429	ASP	CB-CG-OD1	8.51	125.96	118.30
1	H	429	ASP	CB-CG-OD1	8.51	125.96	118.30
1	M	52	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	B	429	ASP	CB-CG-OD1	8.51	125.95	118.30
1	G	368	ASP	CB-CG-OD2	-8.51	110.65	118.30
1	A	448	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	N	368	ASP	CB-CG-OD2	-8.50	110.65	118.30
1	P	571	VAL	CB-CA-C	-8.49	95.27	111.40
1	F	448	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	L	571	VAL	CB-CA-C	-8.49	95.27	111.40
1	O	448	ARG	NE-CZ-NH1	8.49	124.54	120.30
1	P	429	ASP	CB-CG-OD1	8.49	125.94	118.30
1	F	571	VAL	CB-CA-C	-8.48	95.28	111.40
1	E	448	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	E	571	VAL	CB-CA-C	-8.48	95.28	111.40
1	L	429	ASP	CB-CG-OD1	8.48	125.93	118.30
1	M	571	VAL	CB-CA-C	-8.48	95.29	111.40
1	C	571	VAL	CB-CA-C	-8.48	95.30	111.40
1	A	571	VAL	CB-CA-C	-8.47	95.30	111.40
1	C	448	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	O	571	VAL	CB-CA-C	-8.47	95.30	111.40
1	H	571	VAL	CB-CA-C	-8.47	95.31	111.40
1	J	448	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	K	571	VAL	CB-CA-C	-8.47	95.31	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	571	VAL	CB-CA-C	-8.47	95.31	111.40
1	L	448	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	I	571	VAL	CB-CA-C	-8.46	95.32	111.40
1	N	5	ASP	CB-CG-OD2	-8.46	110.68	118.30
1	B	571	VAL	CB-CA-C	-8.46	95.32	111.40
1	D	571	VAL	CB-CA-C	-8.46	95.32	111.40
1	N	571	VAL	CB-CA-C	-8.45	95.35	111.40
1	J	571	VAL	CB-CA-C	-8.45	95.35	111.40
1	M	448	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	F	5	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	F	13	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	K	5	ASP	CB-CG-OD2	-8.40	110.74	118.30
1	D	5	ASP	CB-CG-OD2	-8.39	110.75	118.30
1	O	5	ASP	CB-CG-OD2	-8.39	110.75	118.30
1	A	5	ASP	CB-CG-OD2	-8.38	110.76	118.30
1	I	13	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	P	5	ASP	CB-CG-OD2	-8.38	110.76	118.30
1	J	5	ASP	CB-CG-OD2	-8.37	110.77	118.30
1	B	5	ASP	CB-CG-OD2	-8.37	110.77	118.30
1	H	5	ASP	CB-CG-OD2	-8.36	110.77	118.30
1	M	13	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	G	5	ASP	CB-CG-OD2	-8.35	110.78	118.30
1	M	5	ASP	CB-CG-OD2	-8.35	110.78	118.30
1	G	13	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	L	5	ASP	CB-CG-OD2	-8.35	110.79	118.30
1	C	5	ASP	CB-CG-OD2	-8.33	110.80	118.30
1	E	13	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	G	428	ASP	CB-CG-OD2	-8.33	110.80	118.30
1	J	428	ASP	CB-CG-OD2	-8.33	110.80	118.30
1	J	13	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	I	5	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	E	5	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	N	428	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	A	13	ARG	NE-CZ-NH2	-8.29	116.15	120.30
1	H	13	ARG	NE-CZ-NH2	-8.29	116.15	120.30
1	B	13	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	K	428	ASP	CB-CG-OD2	-8.29	110.84	118.30
1	H	428	ASP	CB-CG-OD2	-8.28	110.84	118.30
1	L	428	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	E	428	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	C	428	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	K	13	ARG	NE-CZ-NH2	-8.28	116.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	13	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	A	428	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	B	428	ASP	CB-CG-OD2	-8.27	110.85	118.30
1	C	13	ARG	NE-CZ-NH2	-8.27	116.16	120.30
1	O	428	ASP	CB-CG-OD2	-8.27	110.85	118.30
1	M	428	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	P	428	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	D	13	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	F	428	ASP	CB-CG-OD2	-8.26	110.87	118.30
1	I	428	ASP	CB-CG-OD2	-8.25	110.88	118.30
1	L	13	ARG	NE-CZ-NH2	-8.25	116.18	120.30
1	P	13	ARG	NE-CZ-NH2	-8.25	116.18	120.30
1	D	428	ASP	CB-CG-OD2	-8.24	110.88	118.30
1	N	13	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	D	329	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	E	329	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	H	329	ASP	CB-CG-OD2	-8.15	110.97	118.30
1	L	329	ASP	CB-CG-OD2	-8.14	110.97	118.30
1	F	329	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	J	329	ASP	CB-CG-OD2	-8.12	110.99	118.30
1	A	329	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	N	329	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	B	329	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	P	329	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	K	329	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	G	329	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	M	329	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	I	329	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	C	329	ASP	CB-CG-OD2	-8.07	111.03	118.30
1	O	329	ASP	CB-CG-OD2	-8.07	111.04	118.30
1	E	130	ASP	CB-CG-OD1	7.96	125.46	118.30
1	G	130	ASP	CB-CG-OD1	7.94	125.44	118.30
1	A	130	ASP	CB-CG-OD1	7.93	125.44	118.30
1	M	130	ASP	CB-CG-OD1	7.93	125.44	118.30
1	H	130	ASP	CB-CG-OD1	7.91	125.42	118.30
1	B	130	ASP	CB-CG-OD1	7.91	125.42	118.30
1	D	130	ASP	CB-CG-OD1	7.90	125.41	118.30
1	N	130	ASP	CB-CG-OD1	7.90	125.41	118.30
1	I	130	ASP	CB-CG-OD1	7.89	125.40	118.30
1	H	916	ASP	CB-CG-OD1	7.89	125.40	118.30
1	L	916	ASP	CB-CG-OD1	7.88	125.39	118.30
1	O	130	ASP	CB-CG-OD1	7.88	125.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	130	ASP	CB-CG-OD1	7.88	125.39	118.30
1	P	130	ASP	CB-CG-OD1	7.88	125.39	118.30
1	C	130	ASP	CB-CG-OD1	7.87	125.39	118.30
1	F	916	ASP	CB-CG-OD1	7.87	125.38	118.30
1	M	916	ASP	CB-CG-OD1	7.87	125.38	118.30
1	N	916	ASP	CB-CG-OD1	7.87	125.38	118.30
1	K	916	ASP	CB-CG-OD1	7.86	125.38	118.30
1	C	916	ASP	CB-CG-OD1	7.86	125.37	118.30
1	D	916	ASP	CB-CG-OD1	7.86	125.37	118.30
1	L	130	ASP	CB-CG-OD1	7.85	125.37	118.30
1	P	916	ASP	CB-CG-OD1	7.84	125.36	118.30
1	A	916	ASP	CB-CG-OD1	7.84	125.36	118.30
1	O	916	ASP	CB-CG-OD1	7.84	125.36	118.30
1	B	916	ASP	CB-CG-OD1	7.84	125.35	118.30
1	G	916	ASP	CB-CG-OD1	7.84	125.35	118.30
1	K	130	ASP	CB-CG-OD1	7.83	125.35	118.30
1	J	130	ASP	CB-CG-OD1	7.83	125.34	118.30
1	O	659	ASP	CB-CG-OD2	-7.82	111.26	118.30
1	E	659	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	F	659	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	D	659	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	P	659	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	J	659	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	N	659	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	I	916	ASP	CB-CG-OD1	7.79	125.32	118.30
1	E	916	ASP	CB-CG-OD1	7.79	125.31	118.30
1	I	659	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	L	659	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	J	916	ASP	CB-CG-OD1	7.79	125.31	118.30
1	B	659	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	K	659	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	M	659	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	C	659	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	A	659	ASP	CB-CG-OD2	-7.76	111.31	118.30
1	H	659	ASP	CB-CG-OD2	-7.76	111.31	118.30
1	G	659	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	C	442	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	F	442	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	G	442	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	I	442	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	K	442	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	H	442	ARG	NE-CZ-NH2	-7.61	116.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	442	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	I	356	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	J	442	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	P	442	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	E	442	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	O	442	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	B	442	ARG	NE-CZ-NH2	-7.57	116.51	120.30
1	E	447	ASP	CB-CG-OD1	7.57	125.11	118.30
1	J	447	ASP	CB-CG-OD1	7.56	125.11	118.30
1	B	447	ASP	CB-CG-OD1	7.56	125.10	118.30
1	A	442	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	B	356	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	C	447	ASP	CB-CG-OD1	7.55	125.10	118.30
1	H	447	ASP	CB-CG-OD1	7.55	125.09	118.30
1	D	447	ASP	CB-CG-OD1	7.54	125.09	118.30
1	J	356	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	L	442	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	447	ASP	CB-CG-OD1	7.54	125.08	118.30
1	N	442	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	G	447	ASP	CB-CG-OD1	7.53	125.08	118.30
1	N	447	ASP	CB-CG-OD1	7.53	125.08	118.30
1	G	356	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	O	447	ASP	CB-CG-OD1	7.52	125.06	118.30
1	D	249	GLU	N-CA-CB	7.52	124.13	110.60
1	K	249	GLU	N-CA-CB	7.52	124.13	110.60
1	A	249	GLU	N-CA-CB	7.51	124.12	110.60
1	E	249	GLU	N-CA-CB	7.51	124.13	110.60
1	F	447	ASP	CB-CG-OD1	7.51	125.06	118.30
1	M	447	ASP	CB-CG-OD1	7.51	125.06	118.30
1	B	249	GLU	N-CA-CB	7.51	124.11	110.60
1	F	249	GLU	N-CA-CB	7.51	124.11	110.60
1	I	447	ASP	CB-CG-OD1	7.51	125.06	118.30
1	O	249	GLU	N-CA-CB	7.51	124.11	110.60
1	O	356	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	G	249	GLU	N-CA-CB	7.50	124.10	110.60
1	P	447	ASP	CB-CG-OD1	7.50	125.05	118.30
1	L	447	ASP	CB-CG-OD1	7.50	125.05	118.30
1	K	447	ASP	CB-CG-OD1	7.50	125.05	118.30
1	N	249	GLU	N-CA-CB	7.50	124.09	110.60
1	F	356	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	L	249	GLU	N-CA-CB	7.49	124.08	110.60
1	C	249	GLU	N-CA-CB	7.49	124.08	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	249	GLU	N-CA-CB	7.49	124.08	110.60
1	M	249	GLU	N-CA-CB	7.49	124.08	110.60
1	N	356	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	M	442	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	E	356	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	L	356	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	H	249	GLU	N-CA-CB	7.48	124.06	110.60
1	A	356	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	I	249	GLU	N-CA-CB	7.48	124.06	110.60
1	M	356	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	J	249	GLU	N-CA-CB	7.47	124.04	110.60
1	K	431	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	K	356	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	P	356	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	H	356	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	C	356	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	D	356	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	J	431	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	D	431	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	B	431	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	F	431	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	O	531	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	G	431	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	A	431	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	I	431	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	O	431	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	H	431	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	P	431	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	E	431	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	C	431	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	I	292	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	D	292	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	H	292	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	I	531	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	N	431	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	J	531	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	L	938	ARG	CD-NE-CZ	7.29	133.80	123.60
1	F	292	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	M	431	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	B	938	ARG	CD-NE-CZ	7.28	133.79	123.60
1	L	431	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	832	ASP	CB-CG-OD2	-7.28	111.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	938	ARG	CD-NE-CZ	7.28	133.79	123.60
1	P	531	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	C	292	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	N	938	ARG	CD-NE-CZ	7.27	133.78	123.60
1	A	938	ARG	CD-NE-CZ	7.26	133.77	123.60
1	C	938	ARG	CD-NE-CZ	7.26	133.77	123.60
1	L	531	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	D	531	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	G	938	ARG	CD-NE-CZ	7.26	133.76	123.60
1	M	531	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	N	292	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	292	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	531	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	M	832	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	C	531	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	A	292	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	K	292	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	E	292	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	J	938	ARG	CD-NE-CZ	7.25	133.75	123.60
1	P	938	ARG	CD-NE-CZ	7.25	133.75	123.60
1	E	531	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	O	938	ARG	CD-NE-CZ	7.25	133.75	123.60
1	G	832	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	A	531	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	E	938	ARG	CD-NE-CZ	7.24	133.74	123.60
1	M	292	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	F	832	ASP	CB-CG-OD2	-7.24	111.79	118.30
1	M	938	ARG	CD-NE-CZ	7.24	133.74	123.60
1	N	832	ASP	CB-CG-OD2	-7.24	111.79	118.30
1	D	938	ARG	CD-NE-CZ	7.23	133.72	123.60
1	F	531	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	H	938	ARG	CD-NE-CZ	7.23	133.72	123.60
1	I	938	ARG	CD-NE-CZ	7.23	133.73	123.60
1	K	832	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	P	52	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	F	938	ARG	CD-NE-CZ	7.23	133.72	123.60
1	M	233	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	P	832	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	C	832	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	H	832	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	J	832	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	L	832	ASP	CB-CG-OD2	-7.22	111.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	832	ASP	CB-CG-OD2	-7.22	111.81	118.30
1	G	233	ASP	CB-CG-OD2	-7.22	111.81	118.30
1	I	832	ASP	CB-CG-OD2	-7.22	111.81	118.30
1	O	292	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	O	832	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	J	292	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	L	292	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	H	199	ASP	CB-CG-OD1	7.20	124.78	118.30
1	G	531	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	L	233	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	I	233	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	D	52	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	D	832	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	E	233	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	P	292	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	E	832	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	J	233	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	K	199	ASP	CB-CG-OD1	7.18	124.76	118.30
1	F	52	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	O	233	ASP	CB-CG-OD2	-7.17	111.84	118.30
1	N	233	ASP	CB-CG-OD2	-7.17	111.84	118.30
1	H	52	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	I	199	ASP	CB-CG-OD1	7.17	124.75	118.30
1	N	531	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	H	531	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	P	233	ASP	CB-CG-OD2	-7.16	111.85	118.30
1	P	909	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	E	199	ASP	CB-CG-OD1	7.16	124.75	118.30
1	J	909	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	L	909	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	C	233	ASP	CB-CG-OD2	-7.15	111.86	118.30
1	G	292	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	D	233	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	M	199	ASP	CB-CG-OD1	7.15	124.73	118.30
1	F	233	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	I	52	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	D	199	ASP	CB-CG-OD1	7.14	124.73	118.30
1	K	193	ASP	CB-CG-OD1	7.14	124.73	118.30
1	B	199	ASP	CB-CG-OD1	7.14	124.73	118.30
1	B	233	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	M	52	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	O	52	ARG	NE-CZ-NH1	7.14	123.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	909	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	C	193	ASP	CB-CG-OD1	7.14	124.73	118.30
1	D	193	ASP	CB-CG-OD1	7.14	124.72	118.30
1	D	909	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	G	909	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	K	909	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	O	199	ASP	CB-CG-OD1	7.13	124.72	118.30
1	A	52	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	K	233	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	A	199	ASP	CB-CG-OD1	7.13	124.72	118.30
1	P	199	ASP	CB-CG-OD1	7.13	124.72	118.30
1	K	287	ASP	CB-CG-OD1	7.12	124.71	118.30
1	C	199	ASP	CB-CG-OD1	7.12	124.71	118.30
1	C	52	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	G	52	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	H	233	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	J	52	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	233	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	C	909	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	E	52	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	J	199	ASP	CB-CG-OD1	7.12	124.71	118.30
1	L	52	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	L	199	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	909	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	G	193	ASP	CB-CG-OD1	7.11	124.70	118.30
1	G	199	ASP	CB-CG-OD1	7.11	124.70	118.30
1	J	193	ASP	CB-CG-OD1	7.11	124.70	118.30
1	I	193	ASP	CB-CG-OD1	7.10	124.69	118.30
1	N	199	ASP	CB-CG-OD1	7.10	124.69	118.30
1	O	572	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	O	909	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	B	287	ASP	CB-CG-OD1	7.09	124.68	118.30
1	K	52	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	L	193	ASP	CB-CG-OD1	7.09	124.68	118.30
1	P	193	ASP	CB-CG-OD1	7.09	124.68	118.30
1	P	287	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	193	ASP	CB-CG-OD1	7.09	124.68	118.30
1	G	572	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	K	531	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	C	572	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	F	199	ASP	CB-CG-OD1	7.08	124.68	118.30
1	D	572	ASP	CB-CG-OD2	-7.08	111.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	287	ASP	CB-CG-OD1	7.08	124.67	118.30
1	I	287	ASP	CB-CG-OD1	7.08	124.67	118.30
1	O	193	ASP	CB-CG-OD1	7.08	124.67	118.30
1	M	572	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	N	193	ASP	CB-CG-OD1	7.08	124.67	118.30
1	N	52	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	C	287	ASP	CB-CG-OD1	7.08	124.67	118.30
1	H	572	ASP	CB-CG-OD2	-7.07	111.93	118.30
1	F	442	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	A	287	ASP	CB-CG-OD1	7.07	124.66	118.30
1	H	193	ASP	CB-CG-OD1	7.07	124.66	118.30
1	F	287	ASP	CB-CG-OD1	7.07	124.66	118.30
1	B	572	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	N	287	ASP	CB-CG-OD1	7.07	124.66	118.30
1	O	287	ASP	CB-CG-OD1	7.07	124.66	118.30
1	E	572	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	M	909	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	D	287	ASP	CB-CG-OD1	7.06	124.65	118.30
1	B	193	ASP	CB-CG-OD1	7.06	124.65	118.30
1	B	909	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	F	193	ASP	CB-CG-OD1	7.06	124.65	118.30
1	A	572	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	F	572	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	N	572	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	B	52	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	J	287	ASP	CB-CG-OD1	7.05	124.65	118.30
1	J	442	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	N	909	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	P	572	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	E	909	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	M	287	ASP	CB-CG-OD1	7.04	124.64	118.30
1	G	287	ASP	CB-CG-OD1	7.04	124.64	118.30
1	E	193	ASP	CB-CG-OD1	7.04	124.63	118.30
1	I	442	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	H	909	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	M	193	ASP	CB-CG-OD1	7.03	124.63	118.30
1	I	572	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	L	572	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	D	442	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	L	287	ASP	CB-CG-OD1	7.03	124.62	118.30
1	J	572	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	P	769	TRP	CB-CA-C	-7.02	96.36	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	769	TRP	CB-CA-C	-7.02	96.36	110.40
1	B	786	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	I	909	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	I	769	TRP	CB-CA-C	-7.01	96.37	110.40
1	A	769	TRP	CB-CA-C	-7.01	96.38	110.40
1	J	769	TRP	CB-CA-C	-7.01	96.38	110.40
1	K	572	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	B	442	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	H	442	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	O	769	TRP	CB-CA-C	-7.00	96.39	110.40
1	E	769	TRP	CB-CA-C	-7.00	96.40	110.40
1	G	769	TRP	CB-CA-C	-7.00	96.40	110.40
1	G	442	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	K	769	TRP	CB-CA-C	-7.00	96.40	110.40
1	P	786	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	D	769	TRP	CB-CA-C	-6.99	96.42	110.40
1	E	287	ASP	CB-CG-OD1	6.99	124.59	118.30
1	L	769	TRP	CB-CA-C	-6.99	96.41	110.40
1	N	769	TRP	CB-CA-C	-6.99	96.41	110.40
1	N	786	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	C	769	TRP	CB-CA-C	-6.99	96.42	110.40
1	F	769	TRP	CB-CA-C	-6.99	96.42	110.40
1	H	769	TRP	CB-CA-C	-6.99	96.42	110.40
1	M	769	TRP	CB-CA-C	-6.99	96.42	110.40
1	K	442	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	C	442	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	M	442	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	L	442	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	442	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	N	442	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	O	442	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	G	746	ASP	CB-CG-OD1	6.94	124.55	118.30
1	P	442	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	J	648	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	D	645	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	F	648	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	A	786	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	L	746	ASP	CB-CG-OD1	6.93	124.53	118.30
1	C	786	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	K	166	ARG	N-CA-CB	6.92	123.06	110.60
1	D	746	ASP	CB-CG-OD1	6.92	124.53	118.30
1	I	746	ASP	CB-CG-OD1	6.92	124.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	166	ARG	N-CA-CB	6.92	123.05	110.60
1	E	648	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	B	648	ASP	CB-CG-OD2	-6.92	112.08	118.30
1	I	786	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	J	166	ARG	N-CA-CB	6.91	123.05	110.60
1	K	746	ASP	CB-CG-OD1	6.91	124.52	118.30
1	N	746	ASP	CB-CG-OD1	6.91	124.52	118.30
1	C	166	ARG	N-CA-CB	6.91	123.04	110.60
1	G	166	ARG	N-CA-CB	6.91	123.04	110.60
1	L	648	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	L	166	ARG	N-CA-CB	6.91	123.04	110.60
1	N	166	ARG	N-CA-CB	6.91	123.03	110.60
1	E	442	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	E	746	ASP	CB-CG-OD1	6.91	124.52	118.30
1	N	1004	SER	N-CA-CB	6.91	120.86	110.50
1	A	648	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	L	1004	SER	N-CA-CB	6.90	120.86	110.50
1	I	166	ARG	N-CA-CB	6.90	123.03	110.60
1	O	166	ARG	N-CA-CB	6.90	123.03	110.60
1	A	166	ARG	N-CA-CB	6.90	123.02	110.60
1	H	746	ASP	CB-CG-OD1	6.90	124.51	118.30
1	P	166	ARG	N-CA-CB	6.90	123.02	110.60
1	C	561	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	E	687	GLN	C-N-CD	-6.90	105.42	120.60
1	E	786	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	I	648	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	J	786	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	O	648	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	C	687	GLN	C-N-CD	-6.90	105.43	120.60
1	K	561	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	746	ASP	CB-CG-OD1	6.89	124.50	118.30
1	D	687	GLN	C-N-CD	-6.89	105.43	120.60
1	C	1004	SER	N-CA-CB	6.89	120.84	110.50
1	F	561	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	M	687	GLN	C-N-CD	-6.89	105.44	120.60
1	M	786	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	B	166	ARG	N-CA-CB	6.89	123.00	110.60
1	F	1004	SER	N-CA-CB	6.89	120.84	110.50
1	M	645	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	M	746	ASP	CB-CG-OD1	6.89	124.50	118.30
1	F	746	ASP	CB-CG-OD1	6.89	124.50	118.30
1	P	687	GLN	C-N-CD	-6.89	105.45	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	645	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	C	648	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	C	746	ASP	CB-CG-OD1	6.89	124.50	118.30
1	F	687	GLN	C-N-CD	-6.89	105.45	120.60
1	G	687	GLN	C-N-CD	-6.89	105.45	120.60
1	H	166	ARG	N-CA-CB	6.89	123.00	110.60
1	H	1004	SER	N-CA-CB	6.89	120.83	110.50
1	P	648	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	P	746	ASP	CB-CG-OD1	6.89	124.50	118.30
1	H	648	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	M	648	ASP	CB-CG-OD2	-6.88	112.10	118.30
1	A	1004	SER	N-CA-CB	6.88	120.82	110.50
1	F	166	ARG	N-CA-CB	6.88	122.99	110.60
1	A	687	GLN	C-N-CD	-6.88	105.46	120.60
1	D	561	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	J	1004	SER	N-CA-CB	6.88	120.82	110.50
1	L	561	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	M	1004	SER	N-CA-CB	6.88	120.82	110.50
1	O	1004	SER	N-CA-CB	6.88	120.82	110.50
1	N	5	ASP	CB-CG-OD1	6.88	124.49	118.30
1	C	828	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	F	786	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	H	368	ASP	CB-CG-OD1	6.88	124.49	118.30
1	J	746	ASP	CB-CG-OD1	6.88	124.49	118.30
1	G	786	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	M	166	ARG	N-CA-CB	6.88	122.97	110.60
1	N	687	GLN	C-N-CD	-6.88	105.47	120.60
1	P	1004	SER	N-CA-CB	6.88	120.81	110.50
1	B	746	ASP	CB-CG-OD1	6.87	124.49	118.30
1	F	645	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	J	687	GLN	C-N-CD	-6.87	105.48	120.60
1	K	786	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	L	687	GLN	C-N-CD	-6.87	105.48	120.60
1	O	687	GLN	C-N-CD	-6.87	105.48	120.60
1	B	1004	SER	N-CA-CB	6.87	120.81	110.50
1	D	648	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	E	1004	SER	N-CA-CB	6.87	120.81	110.50
1	H	687	GLN	C-N-CD	-6.87	105.48	120.60
1	I	687	GLN	C-N-CD	-6.87	105.49	120.60
1	N	648	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	D	166	ARG	N-CA-CB	6.87	122.96	110.60
1	G	648	ASP	CB-CG-OD2	-6.87	112.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	746	ASP	CB-CG-OD1	6.87	124.48	118.30
1	O	786	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	D	786	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	K	1004	SER	N-CA-CB	6.86	120.80	110.50
1	B	687	GLN	C-N-CD	-6.86	105.50	120.60
1	I	1004	SER	N-CA-CB	6.86	120.79	110.50
1	O	5	ASP	CB-CG-OD1	6.86	124.48	118.30
1	D	1004	SER	N-CA-CB	6.86	120.79	110.50
1	G	1004	SER	N-CA-CB	6.86	120.79	110.50
1	K	687	GLN	C-N-CD	-6.86	105.51	120.60
1	B	5	ASP	CB-CG-OD1	6.86	124.47	118.30
1	K	648	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	A	561	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	F	5	ASP	CB-CG-OD1	6.85	124.47	118.30
1	I	828	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	H	786	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	M	368	ASP	CB-CG-OD1	6.85	124.46	118.30
1	A	5	ASP	CB-CG-OD1	6.85	124.46	118.30
1	C	368	ASP	CB-CG-OD1	6.84	124.46	118.30
1	E	561	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	K	5	ASP	CB-CG-OD1	6.84	124.46	118.30
1	L	786	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	N	828	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	G	5	ASP	CB-CG-OD1	6.84	124.45	118.30
1	H	329	ASP	CB-CG-OD1	6.84	124.46	118.30
1	L	5	ASP	CB-CG-OD1	6.84	124.46	118.30
1	H	5	ASP	CB-CG-OD1	6.84	124.45	118.30
1	G	561	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	H	645	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	H	828	ASP	CB-CG-OD2	-6.84	112.15	118.30
1	M	5	ASP	CB-CG-OD1	6.84	124.45	118.30
1	O	828	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	G	828	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	B	211	ASP	CB-CG-OD1	6.83	124.45	118.30
1	C	645	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	O	561	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	P	5	ASP	CB-CG-OD1	6.83	124.44	118.30
1	A	368	ASP	CB-CG-OD1	6.83	124.44	118.30
1	I	5	ASP	CB-CG-OD1	6.83	124.44	118.30
1	P	828	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	E	828	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	M	828	ASP	CB-CG-OD2	-6.82	112.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	5	ASP	CB-CG-OD1	6.82	124.44	118.30
1	L	368	ASP	CB-CG-OD1	6.82	124.44	118.30
1	N	561	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	O	645	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	J	329	ASP	CB-CG-OD1	6.82	124.44	118.30
1	D	5	ASP	CB-CG-OD1	6.82	124.44	118.30
1	F	828	ASP	CB-CG-OD2	-6.82	112.17	118.30
1	K	610	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	L	828	ASP	CB-CG-OD2	-6.82	112.17	118.30
1	O	492	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	D	368	ASP	CB-CG-OD1	6.81	124.43	118.30
1	O	610	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	I	561	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	A	828	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	F	368	ASP	CB-CG-OD1	6.81	124.43	118.30
1	E	5	ASP	CB-CG-OD1	6.81	124.42	118.30
1	L	329	ASP	CB-CG-OD1	6.80	124.42	118.30
1	L	610	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	P	211	ASP	CB-CG-OD1	6.80	124.42	118.30
1	P	645	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	J	561	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	E	645	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	H	610	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	K	329	ASP	CB-CG-OD1	6.80	124.42	118.30
1	M	610	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	N	329	ASP	CB-CG-OD1	6.80	124.42	118.30
1	D	45	ASP	CB-CG-OD1	6.80	124.42	118.30
1	G	610	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	J	828	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	B	368	ASP	CB-CG-OD1	6.80	124.42	118.30
1	F	329	ASP	CB-CG-OD1	6.80	124.42	118.30
1	H	561	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	L	645	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	B	645	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	E	329	ASP	CB-CG-OD1	6.79	124.42	118.30
1	P	329	ASP	CB-CG-OD1	6.79	124.42	118.30
1	C	610	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	G	368	ASP	CB-CG-OD1	6.79	124.41	118.30
1	P	368	ASP	CB-CG-OD1	6.79	124.42	118.30
1	P	561	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	D	211	ASP	CB-CG-OD1	6.79	124.41	118.30
1	I	610	ASP	CB-CG-OD2	-6.79	112.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	645	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	329	ASP	CB-CG-OD1	6.79	124.41	118.30
1	O	329	ASP	CB-CG-OD1	6.79	124.41	118.30
1	K	368	ASP	CB-CG-OD1	6.79	124.41	118.30
1	N	645	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	B	561	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	B	828	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	D	329	ASP	CB-CG-OD1	6.78	124.41	118.30
1	D	610	ASP	CB-CG-OD2	-6.78	112.19	118.30
1	I	368	ASP	CB-CG-OD1	6.78	124.40	118.30
1	J	211	ASP	CB-CG-OD1	6.78	124.41	118.30
1	O	368	ASP	CB-CG-OD1	6.78	124.41	118.30
1	P	610	ASP	CB-CG-OD2	-6.78	112.19	118.30
1	K	211	ASP	CB-CG-OD1	6.78	124.40	118.30
1	K	828	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	A	211	ASP	CB-CG-OD1	6.78	124.40	118.30
1	F	211	ASP	CB-CG-OD1	6.78	124.40	118.30
1	N	610	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	M	329	ASP	CB-CG-OD1	6.78	124.40	118.30
1	E	368	ASP	CB-CG-OD1	6.78	124.40	118.30
1	F	610	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	G	645	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	J	5	ASP	CB-CG-OD1	6.78	124.40	118.30
1	J	368	ASP	CB-CG-OD1	6.78	124.40	118.30
1	N	425	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	M	561	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	O	211	ASP	CB-CG-OD1	6.77	124.40	118.30
1	C	211	ASP	CB-CG-OD1	6.77	124.39	118.30
1	D	828	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	A	610	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	N	368	ASP	CB-CG-OD1	6.77	124.39	118.30
1	B	610	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	I	211	ASP	CB-CG-OD1	6.77	124.39	118.30
1	D	492	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	E	492	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	L	45	ASP	CB-CG-OD1	6.76	124.39	118.30
1	C	45	ASP	CB-CG-OD1	6.76	124.39	118.30
1	K	645	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	329	ASP	CB-CG-OD1	6.76	124.38	118.30
1	C	329	ASP	CB-CG-OD1	6.76	124.38	118.30
1	F	45	ASP	CB-CG-OD1	6.76	124.38	118.30
1	K	492	ASP	CB-CG-OD2	-6.76	112.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	211	ASP	CB-CG-OD1	6.76	124.38	118.30
1	G	329	ASP	CB-CG-OD1	6.76	124.38	118.30
1	L	492	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	N	492	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	G	211	ASP	CB-CG-OD1	6.76	124.38	118.30
1	J	610	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	C	492	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	E	211	ASP	CB-CG-OD1	6.75	124.37	118.30
1	P	492	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	A	492	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	E	59	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	E	610	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	O	45	ASP	CB-CG-OD1	6.74	124.36	118.30
1	H	211	ASP	CB-CG-OD1	6.74	124.36	118.30
1	I	45	ASP	CB-CG-OD1	6.74	124.36	118.30
1	I	329	ASP	CB-CG-OD1	6.74	124.36	118.30
1	N	45	ASP	CB-CG-OD1	6.73	124.36	118.30
1	D	411	ASP	CB-CG-OD1	6.73	124.36	118.30
1	M	211	ASP	CB-CG-OD1	6.73	124.36	118.30
1	A	45	ASP	CB-CG-OD1	6.73	124.36	118.30
1	B	45	ASP	CB-CG-OD1	6.73	124.36	118.30
1	G	45	ASP	CB-CG-OD1	6.73	124.36	118.30
1	G	492	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	J	645	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	J	492	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	B	492	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	E	45	ASP	CB-CG-OD1	6.72	124.35	118.30
1	F	492	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	M	492	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	I	492	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	K	45	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	425	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	P	45	ASP	CB-CG-OD1	6.70	124.33	118.30
1	E	425	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	H	45	ASP	CB-CG-OD1	6.70	124.33	118.30
1	M	425	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	M	45	ASP	CB-CG-OD1	6.70	124.33	118.30
1	J	45	ASP	CB-CG-OD1	6.70	124.33	118.30
1	L	211	ASP	CB-CG-OD1	6.70	124.33	118.30
1	L	425	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	H	425	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	H	492	ASP	CB-CG-OD2	-6.69	112.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	59	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	M	59	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	G	59	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	I	425	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	K	425	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	411	ASP	CB-CG-OD1	6.67	124.30	118.30
1	M	411	ASP	CB-CG-OD1	6.67	124.30	118.30
1	B	411	ASP	CB-CG-OD1	6.67	124.30	118.30
1	H	411	ASP	CB-CG-OD1	6.66	124.30	118.30
1	I	411	ASP	CB-CG-OD1	6.66	124.30	118.30
1	D	425	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	L	411	ASP	CB-CG-OD1	6.65	124.29	118.30
1	A	411	ASP	CB-CG-OD1	6.65	124.29	118.30
1	O	411	ASP	CB-CG-OD1	6.65	124.29	118.30
1	E	411	ASP	CB-CG-OD1	6.65	124.29	118.30
1	L	59	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	K	411	ASP	CB-CG-OD1	6.64	124.28	118.30
1	N	411	ASP	CB-CG-OD1	6.64	124.28	118.30
1	O	59	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	59	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	D	59	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	O	425	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	F	411	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	59	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	425	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	J	59	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	G	425	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	H	59	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	P	411	ASP	CB-CG-OD1	6.61	124.25	118.30
1	F	59	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	C	59	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	J	425	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	C	425	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	E	954	ASP	CB-CG-OD1	6.60	124.24	118.30
1	K	59	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	J	411	ASP	CB-CG-OD1	6.59	124.23	118.30
1	H	954	ASP	CB-CG-OD1	6.58	124.23	118.30
1	I	59	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	G	411	ASP	CB-CG-OD1	6.58	124.22	118.30
1	F	425	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	M	954	ASP	CB-CG-OD1	6.57	124.21	118.30
1	P	954	ASP	CB-CG-OD1	6.56	124.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	954	ASP	CB-CG-OD1	6.56	124.20	118.30
1	P	425	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	252	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	A	252	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	J	252	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	D	954	ASP	CB-CG-OD1	6.54	124.18	118.30
1	A	954	ASP	CB-CG-OD1	6.53	124.18	118.30
1	I	252	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	P	59	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	F	252	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	E	130	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	H	509	ASP	CB-CG-OD1	6.53	124.17	118.30
1	B	130	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	O	509	ASP	CB-CG-OD1	6.52	124.17	118.30
1	K	509	ASP	CB-CG-OD1	6.52	124.17	118.30
1	O	252	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	K	954	ASP	CB-CG-OD1	6.52	124.16	118.30
1	C	130	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	I	954	ASP	CB-CG-OD1	6.51	124.16	118.30
1	N	252	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	L	252	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	E	252	ASP	CB-CG-OD2	-6.50	112.44	118.30
1	B	954	ASP	CB-CG-OD1	6.50	124.15	118.30
1	L	509	ASP	CB-CG-OD1	6.50	124.15	118.30
1	M	130	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	O	130	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	F	954	ASP	CB-CG-OD1	6.50	124.15	118.30
1	J	509	ASP	CB-CG-OD1	6.50	124.15	118.30
1	D	130	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	G	130	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	D	252	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	N	509	ASP	CB-CG-OD1	6.50	124.15	118.30
1	P	252	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	K	252	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	E	367	MET	CG-SD-CE	-6.49	89.81	100.20
1	N	954	ASP	CB-CG-OD1	6.49	124.14	118.30
1	B	367	MET	CG-SD-CE	-6.49	89.81	100.20
1	F	367	MET	CG-SD-CE	-6.49	89.82	100.20
1	D	509	ASP	CB-CG-OD1	6.49	124.14	118.30
1	H	367	MET	CG-SD-CE	-6.49	89.82	100.20
1	I	509	ASP	CB-CG-OD1	6.49	124.14	118.30
1	J	130	ASP	CB-CG-OD2	-6.49	112.46	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	367	MET	CG-SD-CE	-6.49	89.82	100.20
1	F	130	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	J	954	ASP	CB-CG-OD1	6.48	124.13	118.30
1	C	509	ASP	CB-CG-OD1	6.48	124.13	118.30
1	D	367	MET	CG-SD-CE	-6.48	89.83	100.20
1	H	130	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	509	ASP	CB-CG-OD1	6.48	124.13	118.30
1	C	252	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	L	954	ASP	CB-CG-OD1	6.48	124.13	118.30
1	P	367	MET	CG-SD-CE	-6.48	89.84	100.20
1	G	252	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	M	252	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	367	MET	CG-SD-CE	-6.47	89.84	100.20
1	J	367	MET	CG-SD-CE	-6.47	89.84	100.20
1	O	367	MET	CG-SD-CE	-6.47	89.84	100.20
1	B	509	ASP	CB-CG-OD1	6.47	124.13	118.30
1	C	367	MET	CG-SD-CE	-6.47	89.84	100.20
1	H	252	ASP	CB-CG-OD2	-6.47	112.47	118.30
1	L	367	MET	CG-SD-CE	-6.47	89.84	100.20
1	C	954	ASP	CB-CG-OD1	6.47	124.12	118.30
1	F	509	ASP	CB-CG-OD1	6.47	124.12	118.30
1	L	130	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	M	509	ASP	CB-CG-OD1	6.47	124.12	118.30
1	N	367	MET	CG-SD-CE	-6.47	89.85	100.20
1	I	367	MET	CG-SD-CE	-6.47	89.85	100.20
1	G	509	ASP	CB-CG-OD1	6.47	124.12	118.30
1	N	130	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	P	130	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	A	130	ASP	CB-CG-OD2	-6.46	112.48	118.30
1	I	130	ASP	CB-CG-OD2	-6.46	112.48	118.30
1	G	367	MET	CG-SD-CE	-6.46	89.86	100.20
1	M	367	MET	CG-SD-CE	-6.46	89.86	100.20
1	K	130	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	P	509	ASP	CB-CG-OD1	6.45	124.10	118.30
1	O	954	ASP	CB-CG-OD1	6.44	124.10	118.30
1	E	509	ASP	CB-CG-OD1	6.43	124.09	118.30
1	D	15	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	K	15	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	J	15	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	D	938	ARG	N-CA-CB	6.38	122.09	110.60
1	N	938	ARG	N-CA-CB	6.38	122.08	110.60
1	L	15	ASP	CB-CG-OD2	-6.38	112.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	46	ARG	CA-CB-CG	-6.38	99.37	113.40
1	I	46	ARG	CA-CB-CG	-6.37	99.38	113.40
1	M	938	ARG	N-CA-CB	6.37	122.07	110.60
1	O	46	ARG	CA-CB-CG	-6.37	99.39	113.40
1	M	46	ARG	CA-CB-CG	-6.37	99.39	113.40
1	E	938	ARG	N-CA-CB	6.37	122.06	110.60
1	I	938	ARG	N-CA-CB	6.37	122.06	110.60
1	H	46	ARG	CA-CB-CG	-6.36	99.40	113.40
1	H	15	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	E	219	THR	CA-CB-CG2	-6.36	103.50	112.40
1	G	46	ARG	CA-CB-CG	-6.36	99.41	113.40
1	G	938	ARG	N-CA-CB	6.36	122.05	110.60
1	B	46	ARG	CA-CB-CG	-6.36	99.41	113.40
1	H	938	ARG	N-CA-CB	6.36	122.04	110.60
1	K	938	ARG	N-CA-CB	6.36	122.05	110.60
1	O	938	ARG	N-CA-CB	6.36	122.05	110.60
1	C	938	ARG	N-CA-CB	6.36	122.04	110.60
1	J	938	ARG	N-CA-CB	6.36	122.04	110.60
1	A	46	ARG	CA-CB-CG	-6.35	99.42	113.40
1	P	46	ARG	CA-CB-CG	-6.35	99.43	113.40
1	E	46	ARG	CA-CB-CG	-6.35	99.43	113.40
1	J	46	ARG	CA-CB-CG	-6.35	99.43	113.40
1	C	46	ARG	CA-CB-CG	-6.35	99.43	113.40
1	F	46	ARG	CA-CB-CG	-6.35	99.44	113.40
1	F	938	ARG	N-CA-CB	6.35	122.02	110.60
1	N	46	ARG	CA-CB-CG	-6.35	99.44	113.40
1	A	938	ARG	N-CA-CB	6.35	122.02	110.60
1	B	938	ARG	N-CA-CB	6.35	122.02	110.60
1	C	15	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	G	802	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	L	938	ARG	N-CA-CB	6.34	122.01	110.60
1	O	15	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	D	46	ARG	CA-CB-CG	-6.34	99.45	113.40
1	E	15	ASP	CB-CG-OD2	-6.34	112.60	118.30
1	P	938	ARG	N-CA-CB	6.34	122.00	110.60
1	F	15	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	J	219	THR	CA-CB-CG2	-6.33	103.54	112.40
1	K	219	THR	CA-CB-CG2	-6.33	103.54	112.40
1	A	15	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	I	591	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	K	46	ARG	CA-CB-CG	-6.33	99.48	113.40
1	P	15	ASP	CB-CG-OD2	-6.33	112.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	15	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	M	659	ASP	CB-CG-OD1	6.32	123.99	118.30
1	B	15	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	G	219	THR	CA-CB-CG2	-6.32	103.55	112.40
1	H	219	THR	CA-CB-CG2	-6.32	103.55	112.40
1	F	219	THR	CA-CB-CG2	-6.32	103.56	112.40
1	L	219	THR	CA-CB-CG2	-6.32	103.55	112.40
1	N	802	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	219	THR	CA-CB-CG2	-6.32	103.56	112.40
1	P	428	ASP	CB-CG-OD1	6.31	123.98	118.30
1	J	802	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	E	428	ASP	CB-CG-OD1	6.31	123.98	118.30
1	G	15	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	O	591	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	D	219	THR	CA-CB-CG2	-6.31	103.57	112.40
1	B	591	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	I	15	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	J	659	ASP	CB-CG-OD1	6.30	123.97	118.30
1	O	428	ASP	CB-CG-OD1	6.30	123.97	118.30
1	F	802	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	G	591	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	M	219	THR	CA-CB-CG2	-6.30	103.58	112.40
1	O	917	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	I	219	THR	CA-CB-CG2	-6.30	103.58	112.40
1	P	219	THR	CA-CB-CG2	-6.30	103.58	112.40
1	B	219	THR	CA-CB-CG2	-6.30	103.58	112.40
1	M	802	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	N	15	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	O	659	ASP	CB-CG-OD1	6.30	123.97	118.30
1	C	219	THR	CA-CB-CG2	-6.29	103.59	112.40
1	N	219	THR	CA-CB-CG2	-6.29	103.59	112.40
1	E	802	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	O	219	THR	CA-CB-CG2	-6.29	103.60	112.40
1	D	659	ASP	CB-CG-OD1	6.28	123.95	118.30
1	E	659	ASP	CB-CG-OD1	6.28	123.95	118.30
1	H	802	ASP	CB-CG-OD2	-6.28	112.64	118.30
1	A	802	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	G	917	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	M	591	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	P	659	ASP	CB-CG-OD1	6.28	123.95	118.30
1	P	802	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	F	659	ASP	CB-CG-OD1	6.28	123.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	802	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	J	428	ASP	CB-CG-OD1	6.28	123.95	118.30
1	K	428	ASP	CB-CG-OD1	6.28	123.95	118.30
1	K	591	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	H	591	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	K	802	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	N	428	ASP	CB-CG-OD1	6.27	123.94	118.30
1	O	802	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	A	591	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	D	428	ASP	CB-CG-OD1	6.27	123.94	118.30
1	G	428	ASP	CB-CG-OD1	6.27	123.94	118.30
1	K	659	ASP	CB-CG-OD1	6.27	123.94	118.30
1	I	659	ASP	CB-CG-OD1	6.27	123.94	118.30
1	C	802	ASP	CB-CG-OD2	-6.26	112.66	118.30
1	F	591	ASP	CB-CG-OD2	-6.26	112.66	118.30
1	A	428	ASP	CB-CG-OD1	6.26	123.94	118.30
1	L	428	ASP	CB-CG-OD1	6.26	123.94	118.30
1	L	802	ASP	CB-CG-OD2	-6.26	112.66	118.30
1	N	591	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	D	917	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	J	591	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	P	591	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	C	591	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	F	428	ASP	CB-CG-OD1	6.26	123.93	118.30
1	C	428	ASP	CB-CG-OD1	6.25	123.93	118.30
1	C	659	ASP	CB-CG-OD1	6.25	123.93	118.30
1	N	917	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	428	ASP	CB-CG-OD1	6.25	123.93	118.30
1	B	659	ASP	CB-CG-OD1	6.25	123.93	118.30
1	H	428	ASP	CB-CG-OD1	6.25	123.92	118.30
1	B	802	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	L	591	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	D	802	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	B	917	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	N	659	ASP	CB-CG-OD1	6.24	123.92	118.30
1	G	17	GLU	N-CA-CB	6.24	121.83	110.60
1	F	917	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	G	659	ASP	CB-CG-OD1	6.24	123.91	118.30
1	H	659	ASP	CB-CG-OD1	6.24	123.91	118.30
1	I	428	ASP	CB-CG-OD1	6.23	123.91	118.30
1	M	428	ASP	CB-CG-OD1	6.23	123.91	118.30
1	I	917	ARG	NE-CZ-NH2	-6.23	117.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	591	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	O	96	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	L	659	ASP	CB-CG-OD1	6.23	123.90	118.30
1	A	917	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	H	17	GLU	N-CA-CB	6.22	121.79	110.60
1	K	96	ASP	CB-CG-OD2	-6.22	112.71	118.30
1	A	659	ASP	CB-CG-OD1	6.21	123.89	118.30
1	D	17	GLU	N-CA-CB	6.21	121.78	110.60
1	K	17	GLU	N-CA-CB	6.21	121.78	110.60
1	E	917	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	F	17	GLU	N-CA-CB	6.21	121.78	110.60
1	B	17	GLU	N-CA-CB	6.21	121.78	110.60
1	E	591	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	O	17	GLU	N-CA-CB	6.21	121.77	110.60
1	P	17	GLU	N-CA-CB	6.21	121.77	110.60
1	M	17	GLU	N-CA-CB	6.21	121.77	110.60
1	A	17	GLU	N-CA-CB	6.20	121.77	110.60
1	J	17	GLU	N-CA-CB	6.20	121.77	110.60
1	L	96	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	P	96	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	L	17	GLU	N-CA-CB	6.20	121.76	110.60
1	N	17	GLU	N-CA-CB	6.20	121.76	110.60
1	J	917	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	C	17	GLU	N-CA-CB	6.20	121.75	110.60
1	H	96	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	H	917	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	I	17	GLU	N-CA-CB	6.19	121.75	110.60
1	B	96	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	G	96	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	D	96	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	E	17	GLU	N-CA-CB	6.18	121.72	110.60
1	A	96	ASP	CB-CG-OD2	-6.17	112.74	118.30
1	E	96	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	L	411	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	D	411	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	J	96	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	I	96	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	K	917	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	M	917	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	H	411	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	I	772	ASP	CB-CG-OD1	6.16	123.84	118.30
1	C	917	ARG	NE-CZ-NH2	-6.16	117.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	917	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	N	411	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	M	411	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	P	772	ASP	CB-CG-OD1	6.15	123.84	118.30
1	C	96	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	N	96	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	F	411	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	M	96	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	O	772	ASP	CB-CG-OD1	6.14	123.83	118.30
1	B	411	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	E	411	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	J	411	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	P	211	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	O	411	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	A	411	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	P	917	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	C	411	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	F	211	ASP	CB-CG-OD2	-6.13	112.79	118.30
1	N	772	ASP	CB-CG-OD1	6.13	123.81	118.30
1	M	772	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	772	ASP	CB-CG-OD1	6.12	123.80	118.30
1	F	772	ASP	CB-CG-OD1	6.12	123.80	118.30
1	I	411	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	F	96	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	J	772	ASP	CB-CG-OD1	6.11	123.80	118.30
1	C	211	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	C	772	ASP	CB-CG-OD1	6.11	123.80	118.30
1	O	211	ASP	CB-CG-OD2	-6.11	112.81	118.30
1	B	211	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	D	909	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	F	909	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	G	772	ASP	CB-CG-OD1	6.10	123.79	118.30
1	K	411	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	N	987	ASP	CB-CG-OD1	6.10	123.79	118.30
1	P	411	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	909	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	C	909	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	J	211	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	K	211	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	N	909	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	J	909	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	E	211	ASP	CB-CG-OD2	-6.09	112.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	909	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	211	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	K	909	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	G	211	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	E	772	ASP	CB-CG-OD1	6.08	123.77	118.30
1	H	211	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	H	772	ASP	CB-CG-OD1	6.07	123.77	118.30
1	E	987	ASP	CB-CG-OD1	6.07	123.76	118.30
1	D	211	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	F	179	ALA	N-CA-CB	6.07	118.60	110.10
1	G	411	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	A	987	ASP	CB-CG-OD1	6.07	123.76	118.30
1	M	987	ASP	CB-CG-OD1	6.07	123.76	118.30
1	I	909	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	K	772	ASP	CB-CG-OD1	6.07	123.76	118.30
1	J	987	ASP	CB-CG-OD1	6.06	123.76	118.30
1	C	292	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	D	772	ASP	CB-CG-OD1	6.06	123.76	118.30
1	O	987	ASP	CB-CG-OD1	6.06	123.75	118.30
1	H	292	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	G	909	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	I	292	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	K	987	ASP	CB-CG-OD1	6.05	123.75	118.30
1	M	179	ALA	N-CA-CB	6.05	118.58	110.10
1	O	1006	GLU	CG-CD-OE2	-6.05	106.19	118.30
1	B	772	ASP	CB-CG-OD1	6.05	123.75	118.30
1	J	179	ALA	N-CA-CB	6.05	118.57	110.10
1	O	179	ALA	N-CA-CB	6.05	118.57	110.10
1	D	987	ASP	CB-CG-OD1	6.05	123.74	118.30
1	N	211	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	G	292	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	L	987	ASP	CB-CG-OD1	6.05	123.74	118.30
1	C	987	ASP	CB-CG-OD1	6.05	123.74	118.30
1	E	1006	GLU	CG-CD-OE2	-6.05	106.21	118.30
1	G	179	ALA	N-CA-CB	6.05	118.56	110.10
1	J	1006	GLU	CG-CD-OE2	-6.05	106.20	118.30
1	K	179	ALA	N-CA-CB	6.05	118.56	110.10
1	P	987	ASP	CB-CG-OD1	6.05	123.74	118.30
1	B	1006	GLU	CG-CD-OE2	-6.04	106.21	118.30
1	B	987	ASP	CB-CG-OD1	6.04	123.74	118.30
1	K	1018	LEU	CB-CG-CD2	-6.04	100.73	111.00
1	L	211	ASP	CB-CG-OD2	-6.04	112.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	292	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	P	909	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	P	1006	GLU	CG-CD-OE2	-6.04	106.21	118.30
1	H	987	ASP	CB-CG-OD1	6.04	123.74	118.30
1	L	179	ALA	N-CA-CB	6.04	118.56	110.10
1	I	211	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	179	ALA	N-CA-CB	6.04	118.55	110.10
1	E	179	ALA	N-CA-CB	6.04	118.55	110.10
1	E	292	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	292	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	F	1006	GLU	CG-CD-OE2	-6.04	106.23	118.30
1	A	1006	GLU	CG-CD-OE2	-6.03	106.23	118.30
1	G	1018	LEU	CB-CG-CD2	-6.03	100.74	111.00
1	L	772	ASP	CB-CG-OD1	6.03	123.73	118.30
1	P	1018	LEU	CB-CG-CD2	-6.03	100.75	111.00
1	M	211	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	D	1006	GLU	CG-CD-OE2	-6.03	106.24	118.30
1	G	1006	GLU	CG-CD-OE2	-6.03	106.24	118.30
1	H	179	ALA	N-CA-CB	6.03	118.54	110.10
1	I	1006	GLU	CG-CD-OE2	-6.03	106.25	118.30
1	M	909	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	N	1006	GLU	CG-CD-OE2	-6.03	106.25	118.30
1	N	1018	LEU	CB-CG-CD2	-6.03	100.75	111.00
1	C	1006	GLU	CG-CD-OE2	-6.03	106.25	118.30
1	C	1018	LEU	CB-CG-CD2	-6.03	100.76	111.00
1	I	987	ASP	CB-CG-OD1	6.03	123.72	118.30
1	B	909	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	C	179	ALA	N-CA-CB	6.02	118.53	110.10
1	E	1018	LEU	CB-CG-CD2	-6.02	100.76	111.00
1	G	987	ASP	CB-CG-OD1	6.02	123.72	118.30
1	K	1006	GLU	CG-CD-OE2	-6.02	106.25	118.30
1	L	1018	LEU	CB-CG-CD2	-6.02	100.77	111.00
1	A	1018	LEU	CB-CG-CD2	-6.02	100.77	111.00
1	D	1018	LEU	CB-CG-CD2	-6.02	100.77	111.00
1	F	987	ASP	CB-CG-OD1	6.02	123.72	118.30
1	N	179	ALA	N-CA-CB	6.02	118.53	110.10
1	F	292	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	L	1006	GLU	CG-CD-OE2	-6.02	106.27	118.30
1	B	179	ALA	N-CA-CB	6.02	118.52	110.10
1	J	1018	LEU	CB-CG-CD2	-6.01	100.77	111.00
1	M	1018	LEU	CB-CG-CD2	-6.01	100.78	111.00
1	D	179	ALA	N-CA-CB	6.01	118.51	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1018	LEU	CB-CG-CD2	-6.01	100.78	111.00
1	H	1006	GLU	CG-CD-OE2	-6.01	106.28	118.30
1	O	1018	LEU	CB-CG-CD2	-6.01	100.78	111.00
1	I	1018	LEU	CB-CG-CD2	-6.01	100.79	111.00
1	K	292	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	M	1006	GLU	CG-CD-OE2	-6.01	106.29	118.30
1	M	292	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	I	179	ALA	N-CA-CB	6.00	118.50	110.10
1	B	1018	LEU	CB-CG-CD2	-6.00	100.80	111.00
1	H	1018	LEU	CB-CG-CD2	-6.00	100.80	111.00
1	P	179	ALA	N-CA-CB	5.99	118.49	110.10
1	L	800	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	O	333	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	J	292	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	D	919	ASP	CB-CG-OD1	5.98	123.68	118.30
1	E	909	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	J	919	ASP	CB-CG-OD1	5.97	123.67	118.30
1	E	648	ASP	CB-CG-OD1	5.97	123.67	118.30
1	D	292	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	N	333	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	M	1013	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	H	909	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	234	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	C	958	ASN	N-CA-CB	5.96	121.33	110.60
1	N	292	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	919	ASP	CB-CG-OD1	5.96	123.66	118.30
1	C	919	ASP	CB-CG-OD1	5.96	123.66	118.30
1	E	919	ASP	CB-CG-OD1	5.96	123.66	118.30
1	O	909	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	G	255	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	P	919	ASP	CB-CG-OD1	5.95	123.66	118.30
1	F	648	ASP	CB-CG-OD1	5.95	123.66	118.30
1	B	234	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	N	1013	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	O	255	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	E	958	ASN	N-CA-CB	5.95	121.30	110.60
1	I	919	ASP	CB-CG-OD1	5.95	123.65	118.30
1	F	919	ASP	CB-CG-OD1	5.95	123.65	118.30
1	I	255	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	I	800	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	K	919	ASP	CB-CG-OD1	5.95	123.65	118.30
1	G	1013	ARG	NE-CZ-NH2	-5.94	117.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	648	ASP	CB-CG-OD1	5.94	123.65	118.30
1	D	45	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	C	333	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	L	648	ASP	CB-CG-OD1	5.94	123.64	118.30
1	N	919	ASP	CB-CG-OD1	5.94	123.64	118.30
1	A	958	ASN	N-CA-CB	5.93	121.28	110.60
1	I	648	ASP	CB-CG-OD1	5.93	123.64	118.30
1	P	958	ASN	N-CA-CB	5.93	121.28	110.60
1	B	919	ASP	CB-CG-OD1	5.93	123.64	118.30
1	B	958	ASN	N-CA-CB	5.93	121.28	110.60
1	N	958	ASN	N-CA-CB	5.93	121.28	110.60
1	O	958	ASN	N-CA-CB	5.93	121.28	110.60
1	F	958	ASN	N-CA-CB	5.93	121.28	110.60
1	G	958	ASN	N-CA-CB	5.93	121.28	110.60
1	D	1013	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	L	919	ASP	CB-CG-OD1	5.93	123.64	118.30
1	M	333	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	J	648	ASP	CB-CG-OD1	5.93	123.64	118.30
1	M	919	ASP	CB-CG-OD1	5.93	123.63	118.30
1	G	45	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	H	958	ASN	N-CA-CB	5.92	121.26	110.60
1	F	234	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	O	234	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	F	45	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	L	958	ASN	N-CA-CB	5.92	121.26	110.60
1	H	919	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	648	ASP	CB-CG-OD1	5.92	123.63	118.30
1	E	1013	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	F	333	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	G	919	ASP	CB-CG-OD1	5.92	123.63	118.30
1	I	958	ASN	N-CA-CB	5.92	121.25	110.60
1	K	958	ASN	N-CA-CB	5.92	121.25	110.60
1	P	255	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	D	958	ASN	N-CA-CB	5.92	121.25	110.60
1	H	648	ASP	CB-CG-OD1	5.92	123.62	118.30
1	A	234	ASP	CB-CG-OD2	-5.92	112.98	118.30
1	J	45	ASP	CB-CG-OD2	-5.92	112.98	118.30
1	J	958	ASN	N-CA-CB	5.91	121.25	110.60
1	O	648	ASP	CB-CG-OD1	5.91	123.62	118.30
1	P	292	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	O	800	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	B	45	ASP	CB-CG-OD2	-5.91	112.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	648	ASP	CB-CG-OD1	5.91	123.62	118.30
1	K	234	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	L	255	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	K	648	ASP	CB-CG-OD1	5.91	123.62	118.30
1	B	292	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	648	ASP	CB-CG-OD1	5.90	123.61	118.30
1	M	958	ASN	N-CA-CB	5.90	121.22	110.60
1	F	255	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	J	255	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	K	800	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	L	45	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	O	45	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	C	800	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	G	234	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	N	648	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	255	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	E	45	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	45	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	P	234	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	D	648	ASP	CB-CG-OD1	5.89	123.60	118.30
1	C	45	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	H	800	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	1013	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	H	1013	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	P	45	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	P	333	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	P	648	ASP	CB-CG-OD1	5.88	123.59	118.30
1	H	234	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	L	234	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	P	800	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	G	648	ASP	CB-CG-OD1	5.88	123.59	118.30
1	K	333	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	N	234	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	B	800	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	D	800	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	L	1013	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	M	875	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	E	234	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	M	234	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	N	45	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	O	919	ASP	CB-CG-OD1	5.88	123.59	118.30
1	B	333	ARG	NE-CZ-NH1	5.88	123.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	559	TYR	CB-CG-CD1	5.88	124.53	121.00
1	K	45	ASP	CB-CG-OD2	-5.87	113.01	118.30
1	M	255	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	1013	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	D	255	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	I	45	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	J	234	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	333	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	J	800	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	D	333	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	H	333	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	D	234	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	C	1013	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	G	46	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	H	206	SER	N-CA-CB	5.86	119.29	110.50
1	M	45	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	O	292	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	F	1013	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	G	875	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	M	206	SER	N-CA-CB	5.85	119.27	110.50
1	L	333	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	E	333	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	N	206	SER	N-CA-CB	5.85	119.27	110.50
1	E	255	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	F	206	SER	N-CA-CB	5.84	119.27	110.50
1	B	206	SER	N-CA-CB	5.84	119.26	110.50
1	K	206	SER	N-CA-CB	5.84	119.26	110.50
1	N	800	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	C	206	SER	N-CA-CB	5.84	119.26	110.50
1	D	875	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	O	559	TYR	CB-CG-CD1	5.84	124.50	121.00
1	P	206	SER	N-CA-CB	5.84	119.26	110.50
1	E	875	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	G	800	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	I	234	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	I	333	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	J	206	SER	N-CA-CB	5.84	119.26	110.50
1	A	255	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	J	333	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	K	255	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	206	SER	N-CA-CB	5.83	119.25	110.50
1	L	875	ASP	CB-CG-OD2	-5.83	113.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	126	THR	CA-CB-CG2	-5.83	104.24	112.40
1	H	255	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	O	206	SER	N-CA-CB	5.83	119.24	110.50
1	F	800	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	H	45	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	A	875	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	C	255	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	K	1013	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	P	1013	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	E	800	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	L	559	TYR	CB-CG-CD1	5.82	124.50	121.00
1	B	387	VAL	CG1-CB-CG2	-5.82	101.58	110.90
1	F	875	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	P	875	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	D	46	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	D	206	SER	N-CA-CB	5.82	119.23	110.50
1	I	206	SER	N-CA-CB	5.82	119.22	110.50
1	M	800	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	H	126	THR	CA-CB-CG2	-5.81	104.26	112.40
1	L	206	SER	N-CA-CB	5.81	119.22	110.50
1	E	46	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	C	387	VAL	CG1-CB-CG2	-5.81	101.61	110.90
1	D	387	VAL	CG1-CB-CG2	-5.81	101.60	110.90
1	E	206	SER	N-CA-CB	5.81	119.22	110.50
1	G	206	SER	N-CA-CB	5.81	119.22	110.50
1	K	387	VAL	CG1-CB-CG2	-5.81	101.61	110.90
1	M	387	VAL	CG1-CB-CG2	-5.81	101.61	110.90
1	N	255	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	B	126	THR	CA-CB-CG2	-5.81	104.27	112.40
1	H	875	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	F	387	VAL	CG1-CB-CG2	-5.80	101.62	110.90
1	J	46	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	L	126	THR	CA-CB-CG2	-5.80	104.28	112.40
1	J	1013	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	O	1013	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	46	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	46	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	N	875	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	O	679	LEU	CA-CB-CG	-5.80	101.97	115.30
1	G	679	LEU	CA-CB-CG	-5.80	101.97	115.30
1	I	1013	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	M	126	THR	CA-CB-CG2	-5.80	104.28	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	679	LEU	CA-CB-CG	-5.80	101.97	115.30
1	B	679	LEU	CA-CB-CG	-5.79	101.97	115.30
1	B	875	ASP	CB-CG-OD2	-5.79	113.08	118.30
1	D	126	THR	CA-CB-CG2	-5.79	104.29	112.40
1	I	387	VAL	CG1-CB-CG2	-5.79	101.63	110.90
1	K	671	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	800	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	C	166	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	H	1006	GLU	CB-CA-C	-5.79	98.82	110.40
1	I	559	TYR	CB-CG-CD1	5.79	124.47	121.00
1	I	679	LEU	CA-CB-CG	-5.79	101.98	115.30
1	E	559	TYR	CB-CG-CD1	5.79	124.47	121.00
1	E	679	LEU	CA-CB-CG	-5.79	101.98	115.30
1	J	166	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	166	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	I	126	THR	CA-CB-CG2	-5.79	104.30	112.40
1	J	126	THR	CA-CB-CG2	-5.79	104.30	112.40
1	M	679	LEU	CA-CB-CG	-5.79	101.99	115.30
1	O	387	VAL	CG1-CB-CG2	-5.79	101.64	110.90
1	P	679	LEU	CA-CB-CG	-5.79	101.98	115.30
1	F	679	LEU	CA-CB-CG	-5.79	101.99	115.30
1	J	387	VAL	CG1-CB-CG2	-5.79	101.64	110.90
1	K	875	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	559	TYR	CB-CG-CD1	5.79	124.47	121.00
1	A	679	LEU	CA-CB-CG	-5.79	101.99	115.30
1	E	492	ASP	CB-CG-OD1	5.79	123.51	118.30
1	E	1006	GLU	CB-CA-C	-5.79	98.83	110.40
1	A	126	THR	CA-CB-CG2	-5.78	104.30	112.40
1	C	679	LEU	CA-CB-CG	-5.78	102.00	115.30
1	K	126	THR	CA-CB-CG2	-5.78	104.30	112.40
1	D	166	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	J	679	LEU	CA-CB-CG	-5.78	102.00	115.30
1	J	875	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	387	VAL	CG1-CB-CG2	-5.78	101.65	110.90
1	D	679	LEU	CA-CB-CG	-5.78	102.00	115.30
1	L	497	ASP	CB-CG-OD1	5.78	123.50	118.30
1	L	671	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	M	492	ASP	CB-CG-OD1	5.78	123.50	118.30
1	O	126	THR	CA-CB-CG2	-5.78	104.31	112.40
1	C	875	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	E	126	THR	CA-CB-CG2	-5.78	104.31	112.40
1	H	679	LEU	CA-CB-CG	-5.78	102.01	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	679	LEU	CA-CB-CG	-5.78	102.01	115.30
1	N	559	TYR	CB-CG-CD1	5.78	124.47	121.00
1	P	387	VAL	CG1-CB-CG2	-5.78	101.66	110.90
1	N	569	ASP	CB-CG-OD2	-5.77	113.10	118.30
1	O	875	ASP	CB-CG-OD2	-5.77	113.10	118.30
1	G	387	VAL	CG1-CB-CG2	-5.77	101.67	110.90
1	L	387	VAL	CG1-CB-CG2	-5.77	101.67	110.90
1	M	166	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	N	126	THR	CA-CB-CG2	-5.77	104.32	112.40
1	H	375	ASP	CB-CG-OD1	5.77	123.49	118.30
1	M	388	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	497	ASP	CB-CG-OD1	5.77	123.49	118.30
1	E	387	VAL	CG1-CB-CG2	-5.77	101.67	110.90
1	F	559	TYR	CB-CG-CD1	5.77	124.46	121.00
1	F	671	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	G	1006	GLU	CB-CA-C	-5.77	98.86	110.40
1	M	1006	GLU	CB-CA-C	-5.77	98.86	110.40
1	P	126	THR	CA-CB-CG2	-5.77	104.32	112.40
1	L	1006	GLU	CB-CA-C	-5.77	98.86	110.40
1	P	1006	GLU	CB-CA-C	-5.77	98.86	110.40
1	A	1006	GLU	CB-CA-C	-5.77	98.87	110.40
1	C	126	THR	CA-CB-CG2	-5.77	104.33	112.40
1	F	126	THR	CA-CB-CG2	-5.77	104.33	112.40
1	B	1006	GLU	CB-CA-C	-5.76	98.87	110.40
1	C	559	TYR	CB-CG-CD1	5.76	124.46	121.00
1	D	569	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	D	671	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	H	569	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	L	679	LEU	CA-CB-CG	-5.76	102.04	115.30
1	N	497	ASP	CB-CG-OD1	5.76	123.49	118.30
1	G	333	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	J	559	TYR	CB-CG-CD1	5.76	124.46	121.00
1	G	671	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	H	559	TYR	CB-CG-CD1	5.76	124.46	121.00
1	I	1006	GLU	CB-CA-C	-5.76	98.88	110.40
1	J	671	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	M	559	TYR	CB-CG-CD1	5.76	124.46	121.00
1	N	1006	GLU	CB-CA-C	-5.76	98.88	110.40
1	A	46	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	671	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	C	1006	GLU	CB-CA-C	-5.76	98.88	110.40
1	G	492	ASP	CB-CG-OD1	5.76	123.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	387	VAL	CG1-CB-CG2	-5.76	101.69	110.90
1	N	387	VAL	CG1-CB-CG2	-5.76	101.68	110.90
1	P	671	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	K	492	ASP	CB-CG-OD1	5.76	123.48	118.30
1	N	166	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	K	1006	GLU	CB-CA-C	-5.76	98.89	110.40
1	L	166	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	N	671	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	A	671	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	J	388	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	D	1006	GLU	CB-CA-C	-5.75	98.90	110.40
1	I	594	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	I	875	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	J	1006	GLU	CB-CA-C	-5.75	98.90	110.40
1	O	166	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	F	1006	GLU	CB-CA-C	-5.75	98.90	110.40
1	K	166	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	559	TYR	CB-CG-CD1	5.75	124.45	121.00
1	K	594	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	L	492	ASP	CB-CG-OD1	5.75	123.47	118.30
1	O	497	ASP	CB-CG-OD1	5.75	123.47	118.30
1	O	1006	GLU	CB-CA-C	-5.75	98.91	110.40
1	I	166	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	I	497	ASP	CB-CG-OD1	5.75	123.47	118.30
1	J	497	ASP	CB-CG-OD1	5.75	123.47	118.30
1	P	497	ASP	CB-CG-OD1	5.75	123.47	118.30
1	H	671	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	P	559	TYR	CB-CG-CD1	5.75	124.45	121.00
1	A	497	ASP	CB-CG-OD1	5.74	123.47	118.30
1	N	492	ASP	CB-CG-OD1	5.74	123.47	118.30
1	H	46	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	P	594	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	F	594	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	I	671	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	J	569	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	N	388	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	166	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	A	569	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	B	671	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	O	492	ASP	CB-CG-OD1	5.73	123.46	118.30
1	O	671	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	C	388	ARG	NE-CZ-NH1	5.73	123.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	492	ASP	CB-CG-OD1	5.73	123.46	118.30
1	M	671	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	K	388	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	O	594	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	E	497	ASP	CB-CG-OD1	5.73	123.45	118.30
1	F	46	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	H	166	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	L	569	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	M	497	ASP	CB-CG-OD1	5.73	123.45	118.30
1	P	46	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	492	ASP	CB-CG-OD1	5.73	123.45	118.30
1	C	497	ASP	CB-CG-OD1	5.73	123.45	118.30
1	K	559	TYR	CB-CG-CD1	5.73	124.44	121.00
1	A	594	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	D	497	ASP	CB-CG-OD1	5.72	123.45	118.30
1	H	594	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	I	46	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	I	388	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	K	569	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	H	388	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	O	388	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	O	610	ASP	CB-CG-OD1	5.72	123.45	118.30
1	E	594	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	F	497	ASP	CB-CG-OD1	5.72	123.45	118.30
1	G	559	TYR	CB-CG-CD1	5.72	124.43	121.00
1	H	492	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	375	ASP	CB-CG-OD1	5.72	123.45	118.30
1	G	497	ASP	CB-CG-OD1	5.72	123.45	118.30
1	H	186	VAL	CA-CB-CG1	-5.72	102.32	110.90
1	B	492	ASP	CB-CG-OD1	5.72	123.44	118.30
1	C	186	VAL	CA-CB-CG1	-5.72	102.32	110.90
1	C	569	ASP	CB-CG-OD2	-5.72	113.16	118.30
1	K	497	ASP	CB-CG-OD1	5.72	123.44	118.30
1	E	186	VAL	CA-CB-CG1	-5.71	102.33	110.90
1	I	492	ASP	CB-CG-OD1	5.71	123.44	118.30
1	I	772	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	M	375	ASP	CB-CG-OD1	5.71	123.44	118.30
1	P	569	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	N	186	VAL	CA-CB-CG1	-5.71	102.33	110.90
1	P	375	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	388	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	E	671	ASP	CB-CG-OD2	-5.71	113.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	186	VAL	CA-CB-CG1	-5.71	102.34	110.90
1	N	594	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	G	388	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	B	569	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	C	375	ASP	CB-CG-OD1	5.70	123.43	118.30
1	G	594	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	I	569	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	J	594	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	M	569	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	B	186	VAL	CA-CB-CG1	-5.70	102.35	110.90
1	F	166	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	J	553	TRP	CA-CB-CG	-5.70	102.87	113.70
1	K	186	VAL	CA-CB-CG1	-5.70	102.35	110.90
1	K	375	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	375	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	594	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	C	553	TRP	CA-CB-CG	-5.70	102.87	113.70
1	C	594	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	D	186	VAL	CA-CB-CG1	-5.70	102.35	110.90
1	E	166	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	F	569	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	N	46	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	553	TRP	CA-CB-CG	-5.70	102.88	113.70
1	C	492	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	388	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	H	497	ASP	CB-CG-OD1	5.70	123.43	118.30
1	I	186	VAL	CA-CB-CG1	-5.70	102.36	110.90
1	M	594	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	O	46	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	P	492	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	594	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	E	375	ASP	CB-CG-OD1	5.69	123.42	118.30
1	E	553	TRP	CA-CB-CG	-5.69	102.88	113.70
1	I	375	ASP	CB-CG-OD1	5.69	123.42	118.30
1	N	772	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	J	186	VAL	CA-CB-CG1	-5.69	102.36	110.90
1	A	186	VAL	CA-CB-CG1	-5.69	102.37	110.90
1	D	375	ASP	CB-CG-OD1	5.69	123.42	118.30
1	F	186	VAL	CA-CB-CG1	-5.69	102.37	110.90
1	F	375	ASP	CB-CG-OD1	5.69	123.42	118.30
1	F	772	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	N	610	ASP	CB-CG-OD1	5.69	123.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	772	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	M	46	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	O	375	ASP	CB-CG-OD1	5.69	123.42	118.30
1	G	569	ASP	CB-CG-OD2	-5.68	113.18	118.30
1	I	553	TRP	CA-CB-CG	-5.68	102.90	113.70
1	K	46	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	L	46	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	L	186	VAL	CA-CB-CG1	-5.68	102.37	110.90
1	L	375	ASP	CB-CG-OD1	5.68	123.42	118.30
1	L	610	ASP	CB-CG-OD1	5.68	123.42	118.30
1	M	186	VAL	CA-CB-CG1	-5.68	102.37	110.90
1	C	772	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	E	388	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	553	TRP	CA-CB-CG	-5.68	102.91	113.70
1	E	569	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	G	375	ASP	CB-CG-OD1	5.68	123.41	118.30
1	F	492	ASP	CB-CG-OD1	5.68	123.41	118.30
1	K	553	TRP	CA-CB-CG	-5.68	102.91	113.70
1	P	553	TRP	CA-CB-CG	-5.68	102.92	113.70
1	A	553	TRP	CA-CB-CG	-5.67	102.92	113.70
1	M	553	TRP	CA-CB-CG	-5.67	102.92	113.70
1	N	375	ASP	CB-CG-OD1	5.67	123.41	118.30
1	A	772	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	M	772	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	P	961	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	F	553	TRP	CA-CB-CG	-5.67	102.92	113.70
1	L	594	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	O	553	TRP	CA-CB-CG	-5.67	102.92	113.70
1	N	553	TRP	CA-CB-CG	-5.67	102.93	113.70
1	O	569	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	H	553	TRP	CA-CB-CG	-5.67	102.93	113.70
1	J	375	ASP	CB-CG-OD1	5.67	123.40	118.30
1	L	388	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	P	388	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	O	186	VAL	CA-CB-CG1	-5.67	102.40	110.90
1	P	186	VAL	CA-CB-CG1	-5.67	102.40	110.90
1	K	96	ASP	N-CA-CB	5.67	120.80	110.60
1	L	553	TRP	CA-CB-CG	-5.66	102.94	113.70
1	F	96	ASP	N-CA-CB	5.66	120.79	110.60
1	B	388	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	G	166	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	G	610	ASP	CB-CG-OD1	5.66	123.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	492	ASP	CB-CG-OD1	5.66	123.39	118.30
1	E	610	ASP	CB-CG-OD1	5.66	123.39	118.30
1	J	772	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	O	772	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	F	388	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	G	553	TRP	CA-CB-CG	-5.65	102.96	113.70
1	J	96	ASP	N-CA-CB	5.65	120.77	110.60
1	E	772	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	L	96	ASP	N-CA-CB	5.65	120.77	110.60
1	C	15	ASP	CB-CG-OD1	5.65	123.38	118.30
1	H	96	ASP	N-CA-CB	5.65	120.76	110.60
1	I	610	ASP	CB-CG-OD1	5.65	123.38	118.30
1	C	96	ASP	N-CA-CB	5.64	120.76	110.60
1	H	772	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	M	610	ASP	CB-CG-OD1	5.64	123.38	118.30
1	P	166	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	D	201	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	D	610	ASP	CB-CG-OD1	5.64	123.38	118.30
1	P	610	ASP	CB-CG-OD1	5.64	123.38	118.30
1	C	201	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	D	772	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	G	96	ASP	N-CA-CB	5.64	120.75	110.60
1	K	610	ASP	CB-CG-OD1	5.64	123.38	118.30
1	K	800	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	O	800	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	P	201	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	D	96	ASP	N-CA-CB	5.64	120.75	110.60
1	L	15	ASP	CB-CG-OD1	5.64	123.37	118.30
1	A	96	ASP	N-CA-CB	5.64	120.75	110.60
1	B	96	ASP	N-CA-CB	5.64	120.75	110.60
1	E	201	ASP	CB-CG-OD2	-5.64	113.23	118.30
1	H	961	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	P	980	GLU	C-N-CA	-5.64	110.46	122.30
1	B	772	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	I	800	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	L	772	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	P	96	ASP	N-CA-CB	5.63	120.74	110.60
1	A	610	ASP	CB-CG-OD1	5.63	123.37	118.30
1	C	610	ASP	CB-CG-OD1	5.63	123.37	118.30
1	F	610	ASP	CB-CG-OD1	5.63	123.37	118.30
1	G	961	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	J	610	ASP	CB-CG-OD1	5.63	123.37	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	772	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	M	96	ASP	N-CA-CB	5.63	120.74	110.60
1	N	961	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	G	15	ASP	CB-CG-OD1	5.63	123.37	118.30
1	E	96	ASP	N-CA-CB	5.63	120.73	110.60
1	G	772	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	K	201	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	B	610	ASP	CB-CG-OD1	5.63	123.36	118.30
1	E	800	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	H	610	ASP	CB-CG-OD1	5.63	123.36	118.30
1	N	96	ASP	N-CA-CB	5.63	120.73	110.60
1	O	980	GLU	C-N-CA	-5.63	110.48	122.30
1	E	15	ASP	CB-CG-OD1	5.62	123.36	118.30
1	I	96	ASP	N-CA-CB	5.62	120.73	110.60
1	I	980	GLU	C-N-CA	-5.62	110.49	122.30
1	H	980	GLU	C-N-CA	-5.62	110.50	122.30
1	J	980	GLU	C-N-CA	-5.62	110.49	122.30
1	O	96	ASP	N-CA-CB	5.62	120.72	110.60
1	F	201	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	K	980	GLU	C-N-CA	-5.62	110.50	122.30
1	N	980	GLU	C-N-CA	-5.62	110.50	122.30
1	E	980	GLU	C-N-CA	-5.62	110.51	122.30
1	M	980	GLU	C-N-CA	-5.62	110.51	122.30
1	A	980	GLU	C-N-CA	-5.61	110.51	122.30
1	D	800	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	I	201	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	P	800	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	L	980	GLU	C-N-CA	-5.61	110.52	122.30
1	N	425	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	B	980	GLU	C-N-CA	-5.61	110.53	122.30
1	C	980	GLU	C-N-CA	-5.61	110.53	122.30
1	F	980	GLU	C-N-CA	-5.61	110.53	122.30
1	G	980	GLU	C-N-CA	-5.61	110.53	122.30
1	H	15	ASP	CB-CG-OD1	5.61	123.34	118.30
1	A	201	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	D	980	GLU	C-N-CA	-5.60	110.53	122.30
1	J	599	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	L	201	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	L	800	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	O	961	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	H	201	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	N	201	ASP	CB-CG-OD2	-5.59	113.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	961	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	800	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	C	800	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	F	961	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	J	961	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	M	15	ASP	CB-CG-OD1	5.58	123.33	118.30
1	A	15	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	201	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	H	800	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	I	938	ARG	CG-CD-NE	-5.58	100.08	111.80
1	O	15	ASP	CB-CG-OD1	5.58	123.32	118.30
1	D	15	ASP	CB-CG-OD1	5.58	123.32	118.30
1	F	15	ASP	CB-CG-OD1	5.58	123.32	118.30
1	K	15	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	961	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	G	201	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	J	201	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	O	938	ARG	CG-CD-NE	-5.57	100.10	111.80
1	H	938	ARG	CG-CD-NE	-5.57	100.10	111.80
1	M	201	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	B	479	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	E	954	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	I	15	ASP	CB-CG-OD1	5.57	123.31	118.30
1	J	938	ARG	CG-CD-NE	-5.57	100.11	111.80
1	D	938	ARG	CG-CD-NE	-5.57	100.11	111.80
1	E	938	ARG	CG-CD-NE	-5.57	100.11	111.80
1	N	15	ASP	CB-CG-OD1	5.57	123.31	118.30
1	G	938	ARG	CG-CD-NE	-5.56	100.12	111.80
1	H	594	ASP	CB-CG-OD1	5.56	123.30	118.30
1	K	961	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	M	938	ARG	CG-CD-NE	-5.56	100.13	111.80
1	A	938	ARG	CG-CD-NE	-5.56	100.13	111.80
1	J	15	ASP	CB-CG-OD1	5.56	123.30	118.30
1	E	961	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	F	938	ARG	CG-CD-NE	-5.55	100.13	111.80
1	L	938	ARG	CG-CD-NE	-5.55	100.13	111.80
1	N	938	ARG	CG-CD-NE	-5.55	100.14	111.80
1	B	15	ASP	CB-CG-OD1	5.55	123.30	118.30
1	H	699[A]	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	H	699[B]	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	I	479	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	F	800	ARG	NE-CZ-NH1	5.55	123.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	938	ARG	CG-CD-NE	-5.55	100.15	111.80
1	K	699[A]	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	K	699[B]	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	P	599	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	P	938	ARG	CG-CD-NE	-5.55	100.15	111.80
1	D	425	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	599	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	C	699[A]	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	699[B]	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	938	ARG	CG-CD-NE	-5.54	100.16	111.80
1	I	599	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	J	425	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	M	800	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	N	800	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	O	201	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	B	938	ARG	CG-CD-NE	-5.54	100.17	111.80
1	K	594	ASP	CB-CG-OD1	5.54	123.28	118.30
1	G	599	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	H	599	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	J	800	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	M	961	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	D	271	THR	CA-CB-CG2	-5.53	104.66	112.40
1	H	954	ASP	CB-CG-OD2	-5.53	113.33	118.30
1	I	271	THR	CA-CB-CG2	-5.53	104.67	112.40
1	P	594	ASP	CB-CG-OD1	5.53	123.27	118.30
1	D	954	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	J	594	ASP	CB-CG-OD1	5.52	123.27	118.30
1	N	594	ASP	CB-CG-OD1	5.52	123.27	118.30
1	O	271	THR	CA-CB-CG2	-5.52	104.67	112.40
1	P	15	ASP	CB-CG-OD1	5.52	123.27	118.30
1	L	425	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	E	479	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	B	100	TYR	N-CA-CB	5.52	120.53	110.60
1	C	954	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	O	100	TYR	N-CA-CB	5.52	120.53	110.60
1	F	71	GLU	CB-CA-C	5.52	121.43	110.40
1	D	71	GLU	CB-CA-C	5.51	121.43	110.40
1	F	271	THR	CA-CB-CG2	-5.51	104.68	112.40
1	G	100	TYR	N-CA-CB	5.51	120.52	110.60
1	L	961	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	599	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	B	954	ASP	CB-CG-OD2	-5.51	113.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	699[A]	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	D	699[B]	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	F	594	ASP	CB-CG-OD1	5.51	123.26	118.30
1	H	425	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	H	100	TYR	N-CA-CB	5.51	120.52	110.60
1	J	100	TYR	N-CA-CB	5.51	120.52	110.60
1	A	425	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	C	479	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	D	100	TYR	N-CA-CB	5.51	120.52	110.60
1	F	479	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	I	594	ASP	CB-CG-OD1	5.51	123.26	118.30
1	K	954	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	C	828	ASP	CB-CG-OD1	5.51	123.26	118.30
1	G	71	GLU	CB-CA-C	5.51	121.42	110.40
1	G	425	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	A	479	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	699[A]	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	699[B]	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	D	828	ASP	CB-CG-OD1	5.51	123.26	118.30
1	K	425	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	O	71	GLU	CB-CA-C	5.51	121.41	110.40
1	I	100	TYR	N-CA-CB	5.50	120.51	110.60
1	L	599	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	A	100	TYR	N-CA-CB	5.50	120.51	110.60
1	E	100	TYR	N-CA-CB	5.50	120.51	110.60
1	G	800	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	H	271	THR	CA-CB-CG2	-5.50	104.70	112.40
1	J	71	GLU	CB-CA-C	5.50	121.40	110.40
1	L	71	GLU	CB-CA-C	5.50	121.40	110.40
1	L	100	TYR	N-CA-CB	5.50	120.50	110.60
1	N	100	TYR	N-CA-CB	5.50	120.50	110.60
1	E	699[A]	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	E	699[B]	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	H	479	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	271	THR	CA-CB-CG2	-5.50	104.70	112.40
1	B	271	THR	CA-CB-CG2	-5.50	104.70	112.40
1	C	100	TYR	N-CA-CB	5.50	120.50	110.60
1	E	271	THR	CA-CB-CG2	-5.50	104.70	112.40
1	H	92	MET	CG-SD-CE	-5.50	91.40	100.20
1	M	100	TYR	N-CA-CB	5.50	120.50	110.60
1	M	954	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	O	954	ASP	CB-CG-OD2	-5.50	113.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	71	GLU	CB-CA-C	5.50	121.39	110.40
1	F	100	TYR	N-CA-CB	5.50	120.49	110.60
1	P	479	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	C	71	GLU	CB-CA-C	5.50	121.39	110.40
1	E	71	GLU	CB-CA-C	5.50	121.39	110.40
1	G	594	ASP	CB-CG-OD1	5.50	123.25	118.30
1	L	594	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	954	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	D	599	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	G	954	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	N	954	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	594	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	479	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	G	479	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	I	699[A]	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	I	699[B]	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	M	271	THR	CA-CB-CG2	-5.49	104.71	112.40
1	K	71	GLU	CB-CA-C	5.49	121.38	110.40
1	K	479	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	P	699[A]	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	P	699[B]	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	K	100	TYR	N-CA-CB	5.49	120.48	110.60
1	L	271	THR	CA-CB-CG2	-5.49	104.72	112.40
1	C	961	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	D	961	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	H	71	GLU	CB-CA-C	5.49	121.37	110.40
1	J	271	THR	CA-CB-CG2	-5.49	104.72	112.40
1	L	828	ASP	CB-CG-OD1	5.49	123.24	118.30
1	M	71	GLU	CB-CA-C	5.49	121.37	110.40
1	N	271	THR	CA-CB-CG2	-5.49	104.72	112.40
1	N	479	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	P	71	GLU	CB-CA-C	5.49	121.37	110.40
1	A	594	ASP	CB-CG-OD1	5.48	123.24	118.30
1	J	954	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	K	271	THR	CA-CB-CG2	-5.48	104.72	112.40
1	N	92	MET	CG-SD-CE	-5.48	91.43	100.20
1	O	92	MET	CG-SD-CE	-5.48	91.43	100.20
1	G	271	THR	CA-CB-CG2	-5.48	104.73	112.40
1	G	832	ASP	CB-CG-OD1	5.48	123.23	118.30
1	I	71	GLU	CB-CA-C	5.48	121.36	110.40
1	I	92	MET	CG-SD-CE	-5.48	91.43	100.20
1	J	479	ASP	CB-CG-OD2	-5.48	113.37	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	594	ASP	CB-CG-OD1	5.48	123.23	118.30
1	P	100	TYR	N-CA-CB	5.48	120.47	110.60
1	F	92	MET	CG-SD-CE	-5.48	91.43	100.20
1	K	403	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	92	MET	CG-SD-CE	-5.48	91.44	100.20
1	D	92	MET	CG-SD-CE	-5.48	91.44	100.20
1	L	954	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	N	828	ASP	CB-CG-OD1	5.48	123.23	118.30
1	F	699[A]	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	F	699[B]	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	F	954	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	N	71	GLU	CB-CA-C	5.47	121.34	110.40
1	N	599	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	M	92	MET	CG-SD-CE	-5.47	91.45	100.20
1	O	403	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	B	961	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	L	92	MET	CG-SD-CE	-5.47	91.45	100.20
1	M	599	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	M	828	ASP	CB-CG-OD1	5.47	123.22	118.30
1	P	92	MET	CG-SD-CE	-5.47	91.45	100.20
1	B	71	GLU	CB-CA-C	5.47	121.33	110.40
1	B	92	MET	CG-SD-CE	-5.47	91.45	100.20
1	C	403	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	J	699[A]	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	J	699[B]	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	O	479	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	O	828	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C	271	THR	CA-CB-CG2	-5.47	104.75	112.40
1	F	599	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	G	699[A]	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	G	699[B]	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	G	828	ASP	CB-CG-OD1	5.47	123.22	118.30
1	J	92	MET	CG-SD-CE	-5.47	91.45	100.20
1	L	479	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	L	699[A]	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	L	699[B]	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	828	ASP	CB-CG-OD1	5.46	123.22	118.30
1	F	828	ASP	CB-CG-OD1	5.46	123.22	118.30
1	G	92	MET	CG-SD-CE	-5.46	91.46	100.20
1	P	271	THR	CA-CB-CG2	-5.46	104.75	112.40
1	E	92	MET	CG-SD-CE	-5.46	91.46	100.20
1	M	479	ASP	CB-CG-OD2	-5.46	113.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	92	MET	CG-SD-CE	-5.46	91.46	100.20
1	K	92	MET	CG-SD-CE	-5.46	91.46	100.20
1	D	594	ASP	CB-CG-OD1	5.46	123.21	118.30
1	H	828	ASP	CB-CG-OD1	5.46	123.21	118.30
1	I	954	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	B	403	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	E	599	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	C	425	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	M	425	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	N	699[A]	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	N	699[B]	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	P	954	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	832	ASP	CB-CG-OD1	5.45	123.21	118.30
1	D	178	ARG	NE-CZ-NH1	-5.45	117.57	120.30
1	I	828	ASP	CB-CG-OD1	5.45	123.21	118.30
1	P	828	ASP	CB-CG-OD1	5.45	123.21	118.30
1	M	699[A]	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	M	699[B]	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	N	832	ASP	CB-CG-OD1	5.45	123.20	118.30
1	K	832	ASP	CB-CG-OD1	5.45	123.20	118.30
1	E	425	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	E	594	ASP	CB-CG-OD1	5.44	123.20	118.30
1	O	425	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	P	178	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	M	594	ASP	CB-CG-OD1	5.44	123.19	118.30
1	N	403	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	P	425	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	800	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	M	77	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	599	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	J	828	ASP	CB-CG-OD1	5.43	123.19	118.30
1	G	403	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	P	403	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	B	425	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	O	599	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	C	594	ASP	CB-CG-OD1	5.42	123.18	118.30
1	H	403	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	I	425	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	L	403	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	403	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	F	832	ASP	CB-CG-OD1	5.42	123.17	118.30
1	E	996	ASP	CB-CG-OD2	-5.42	113.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	832	ASP	CB-CG-OD1	5.42	123.17	118.30
1	D	403	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	E	828	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	996	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	J	77	ASP	CB-CG-OD1	5.41	123.17	118.30
1	I	832	ASP	CB-CG-OD1	5.41	123.17	118.30
1	P	77	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	77	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	828	ASP	CB-CG-OD1	5.41	123.17	118.30
1	F	77	ASP	CB-CG-OD1	5.40	123.16	118.30
1	I	403	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	I	77	ASP	N-CA-CB	5.40	120.33	110.60
1	J	832	ASP	CB-CG-OD1	5.40	123.16	118.30
1	M	832	ASP	CB-CG-OD1	5.40	123.16	118.30
1	O	832	ASP	CB-CG-OD1	5.40	123.16	118.30
1	D	996	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	E	210	ARG	N-CA-CB	5.40	120.32	110.60
1	J	403	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	L	832	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	403	ASP	CB-CG-OD1	5.40	123.16	118.30
1	J	77	ASP	N-CA-CB	5.40	120.32	110.60
1	O	996	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	C	77	ASP	N-CA-CB	5.40	120.31	110.60
1	C	832	ASP	CB-CG-OD1	5.40	123.16	118.30
1	D	77	ASP	N-CA-CB	5.40	120.31	110.60
1	D	210	ARG	N-CA-CB	5.40	120.31	110.60
1	O	699[A]	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	O	699[B]	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	J	210	ARG	N-CA-CB	5.39	120.31	110.60
1	K	828	ASP	CB-CG-OD1	5.39	123.16	118.30
1	P	210	ARG	N-CA-CB	5.39	120.31	110.60
1	C	77	ASP	CB-CG-OD1	5.39	123.15	118.30
1	F	77	ASP	N-CA-CB	5.39	120.31	110.60
1	M	77	ASP	N-CA-CB	5.39	120.30	110.60
1	A	77	ASP	CB-CG-OD1	5.39	123.15	118.30
1	F	425	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	H	77	ASP	N-CA-CB	5.39	120.30	110.60
1	K	599	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	L	77	ASP	CB-CG-OD1	5.39	123.15	118.30
1	N	210	ARG	N-CA-CB	5.39	120.30	110.60
1	O	77	ASP	N-CA-CB	5.39	120.30	110.60
1	A	210	ARG	N-CA-CB	5.38	120.29	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	210	ARG	N-CA-CB	5.38	120.29	110.60
1	C	210	ARG	N-CA-CB	5.38	120.29	110.60
1	E	77	ASP	CB-CG-OD1	5.38	123.15	118.30
1	G	210	ARG	N-CA-CB	5.38	120.29	110.60
1	L	210	ARG	N-CA-CB	5.38	120.29	110.60
1	M	996	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	A	77	ASP	N-CA-CB	5.38	120.29	110.60
1	D	77	ASP	CB-CG-OD1	5.38	123.14	118.30
1	G	77	ASP	N-CA-CB	5.38	120.29	110.60
1	M	403	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	E	77	ASP	N-CA-CB	5.38	120.28	110.60
1	J	178	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	E	403	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	F	210	ARG	N-CA-CB	5.38	120.28	110.60
1	G	77	ASP	CB-CG-OD1	5.38	123.14	118.30
1	H	210	ARG	N-CA-CB	5.38	120.28	110.60
1	I	210	ARG	N-CA-CB	5.38	120.28	110.60
1	I	996	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	K	210	ARG	N-CA-CB	5.38	120.28	110.60
1	N	77	ASP	N-CA-CB	5.38	120.28	110.60
1	O	210	ARG	N-CA-CB	5.38	120.28	110.60
1	E	832	ASP	CB-CG-OD1	5.38	123.14	118.30
1	P	77	ASP	N-CA-CB	5.38	120.28	110.60
1	E	178	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	I	77	ASP	CB-CG-OD1	5.37	123.14	118.30
1	K	77	ASP	N-CA-CB	5.37	120.27	110.60
1	M	210	ARG	N-CA-CB	5.37	120.27	110.60
1	O	403	ASP	CB-CG-OD1	5.37	123.14	118.30
1	A	996	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	N	996	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	K	996	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	B	178	ARG	NE-CZ-NH1	-5.37	117.62	120.30
1	B	832	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	699[A]	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	699[B]	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	L	178	ARG	NE-CZ-NH1	-5.37	117.62	120.30
1	O	908	ASP	CB-CG-OD1	5.37	123.13	118.30
1	E	908	ASP	CB-CG-OD1	5.37	123.13	118.30
1	C	996	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	F	403	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	M	1013	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	77	ASP	N-CA-CB	5.36	120.25	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	832	ASP	CB-CG-OD1	5.36	123.12	118.30
1	G	178	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	H	996	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	O	77	ASP	CB-CG-OD1	5.36	123.12	118.30
1	P	996	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	K	864	MET	CG-SD-CE	-5.36	91.62	100.20
1	G	996	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	J	826	THR	CA-CB-CG2	-5.36	104.90	112.40
1	N	77	ASP	CB-CG-OD1	5.36	123.12	118.30
1	P	908	ASP	CB-CG-OD1	5.36	123.12	118.30
1	D	1018	LEU	CB-CG-CD1	-5.36	101.90	111.00
1	E	1018	LEU	CB-CG-CD1	-5.36	101.89	111.00
1	J	908	ASP	CB-CG-OD1	5.36	123.12	118.30
1	H	77	ASP	CB-CG-OD1	5.35	123.12	118.30
1	N	864	MET	CG-SD-CE	-5.35	91.63	100.20
1	L	77	ASP	N-CA-CB	5.35	120.23	110.60
1	M	864	MET	CG-SD-CE	-5.35	91.64	100.20
1	F	996	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	F	1018	LEU	CB-CG-CD1	-5.35	101.90	111.00
1	J	864	MET	CG-SD-CE	-5.35	91.64	100.20
1	C	864	MET	CG-SD-CE	-5.35	91.64	100.20
1	G	826	THR	CA-CB-CG2	-5.35	104.91	112.40
1	L	864	MET	CG-SD-CE	-5.35	91.64	100.20
1	H	864	MET	CG-SD-CE	-5.35	91.65	100.20
1	K	77	ASP	CB-CG-OD1	5.35	123.11	118.30
1	L	996	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	864	MET	CG-SD-CE	-5.34	91.65	100.20
1	D	864	MET	CG-SD-CE	-5.34	91.65	100.20
1	G	864	MET	CG-SD-CE	-5.34	91.65	100.20
1	I	178	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	N	403	ASP	CB-CG-OD1	5.34	123.11	118.30
1	D	826	THR	CA-CB-CG2	-5.34	104.92	112.40
1	H	1018	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	A	729	THR	CA-C-N	-5.34	105.45	117.20
1	D	908	ASP	CB-CG-OD1	5.34	123.11	118.30
1	G	1018	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	N	178	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	O	864	MET	CG-SD-CE	-5.34	91.66	100.20
1	P	826	THR	CA-CB-CG2	-5.34	104.92	112.40
1	P	864	MET	CG-SD-CE	-5.34	91.65	100.20
1	D	1013	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	J	996	ASP	CB-CG-OD2	-5.34	113.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	826	THR	CA-CB-CG2	-5.34	104.93	112.40
1	P	1018	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	A	908	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	1018	LEU	CB-CG-CD1	-5.34	101.93	111.00
1	G	183	ARG	CD-NE-CZ	-5.34	116.13	123.60
1	H	427	THR	CA-CB-CG2	-5.34	104.93	112.40
1	C	826	THR	CA-CB-CG2	-5.33	104.93	112.40
1	D	403	ASP	CB-CG-OD1	5.33	123.10	118.30
1	F	183	ARG	CD-NE-CZ	-5.33	116.13	123.60
1	N	826	THR	CA-CB-CG2	-5.33	104.93	112.40
1	P	729	THR	CA-C-N	-5.33	105.47	117.20
1	C	403	ASP	CB-CG-OD1	5.33	123.10	118.30
1	E	864	MET	CG-SD-CE	-5.33	91.67	100.20
1	B	695	TRP	CB-CA-C	-5.33	99.74	110.40
1	F	427	THR	CA-CB-CG2	-5.33	104.94	112.40
1	F	864	MET	CG-SD-CE	-5.33	91.67	100.20
1	H	826	THR	CA-CB-CG2	-5.33	104.94	112.40
1	H	832	ASP	CB-CG-OD1	5.33	123.10	118.30
1	I	427	THR	CA-CB-CG2	-5.33	104.94	112.40
1	I	864	MET	CG-SD-CE	-5.33	91.67	100.20
1	K	1018	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	O	826	THR	CA-CB-CG2	-5.33	104.94	112.40
1	O	1018	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	B	729	THR	CA-C-N	-5.33	105.48	117.20
1	D	729	THR	CA-C-N	-5.33	105.48	117.20
1	F	908	ASP	CB-CG-OD1	5.33	123.09	118.30
1	G	403	ASP	CB-CG-OD1	5.33	123.09	118.30
1	H	178	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	K	729	THR	CA-C-N	-5.33	105.49	117.20
1	N	1013	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	P	183	ARG	CD-NE-CZ	-5.33	116.14	123.60
1	C	729	THR	CA-C-N	-5.32	105.49	117.20
1	D	183	ARG	CD-NE-CZ	-5.32	116.15	123.60
1	I	1018	LEU	CB-CG-CD1	-5.32	101.95	111.00
1	J	1018	LEU	CB-CG-CD1	-5.32	101.95	111.00
1	P	403	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	1018	LEU	CB-CG-CD1	-5.32	101.95	111.00
1	B	864	MET	CG-SD-CE	-5.32	91.69	100.20
1	C	183	ARG	CD-NE-CZ	-5.32	116.15	123.60
1	H	729	THR	CA-C-N	-5.32	105.50	117.20
1	N	729	THR	CA-C-N	-5.32	105.49	117.20
1	B	183	ARG	CD-NE-CZ	-5.32	116.15	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	908	ASP	CB-CG-OD1	5.32	123.09	118.30
1	K	183	ARG	CD-NE-CZ	-5.32	116.15	123.60
1	M	183	ARG	CD-NE-CZ	-5.32	116.15	123.60
1	M	729	THR	CA-C-N	-5.32	105.50	117.20
1	A	178	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	J	427	THR	CA-CB-CG2	-5.32	104.95	112.40
1	K	908	ASP	CB-CG-OD1	5.32	123.09	118.30
1	L	403	ASP	CB-CG-OD1	5.32	123.08	118.30
1	L	729	THR	CA-C-N	-5.32	105.50	117.20
1	L	1018	LEU	CB-CG-CD1	-5.32	101.96	111.00
1	N	1018	LEU	CB-CG-CD1	-5.32	101.96	111.00
1	O	729	THR	CA-C-N	-5.32	105.50	117.20
1	C	427	THR	CA-CB-CG2	-5.32	104.96	112.40
1	O	695	TRP	CB-CA-C	-5.32	99.77	110.40
1	A	427	THR	CA-CB-CG2	-5.31	104.96	112.40
1	C	1018	LEU	CB-CG-CD1	-5.31	101.97	111.00
1	G	427	THR	CA-CB-CG2	-5.31	104.96	112.40
1	I	183	ARG	CD-NE-CZ	-5.31	116.16	123.60
1	J	729	THR	CA-C-N	-5.31	105.51	117.20
1	K	403	ASP	CB-CG-OD1	5.31	123.08	118.30
1	M	1018	LEU	CB-CG-CD1	-5.31	101.97	111.00
1	P	427	THR	CA-CB-CG2	-5.31	104.96	112.40
1	A	826	THR	CA-CB-CG2	-5.31	104.96	112.40
1	N	427	THR	CA-CB-CG2	-5.31	104.97	112.40
1	A	183	ARG	CD-NE-CZ	-5.31	116.17	123.60
1	B	826	THR	CA-CB-CG2	-5.31	104.97	112.40
1	C	104	THR	CA-CB-CG2	-5.31	104.97	112.40
1	G	729	THR	CA-C-N	-5.31	105.52	117.20
1	H	183	ARG	CD-NE-CZ	-5.31	116.17	123.60
1	I	729	THR	CA-C-N	-5.31	105.52	117.20
1	I	826	THR	CA-CB-CG2	-5.31	104.97	112.40
1	L	826	THR	CA-CB-CG2	-5.31	104.97	112.40
1	A	403	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	908	ASP	CB-CG-OD1	5.31	123.08	118.30
1	E	729	THR	CA-C-N	-5.31	105.53	117.20
1	P	104	THR	CA-CB-CG2	-5.31	104.97	112.40
1	D	695	TRP	CB-CA-C	-5.31	99.79	110.40
1	H	104	THR	CA-CB-CG2	-5.31	104.97	112.40
1	O	178	ARG	NE-CZ-NH1	-5.31	117.65	120.30
1	F	729	THR	CA-C-N	-5.30	105.53	117.20
1	N	908	ASP	CB-CG-OD1	5.30	123.07	118.30
1	E	183	ARG	CD-NE-CZ	-5.30	116.18	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	826	THR	CA-CB-CG2	-5.30	104.98	112.40
1	C	695	TRP	CB-CA-C	-5.30	99.80	110.40
1	M	427	THR	CA-CB-CG2	-5.30	104.98	112.40
1	A	695	TRP	CB-CA-C	-5.30	99.80	110.40
1	G	802	ASP	CB-CG-OD1	5.30	123.07	118.30
1	H	908	ASP	CB-CG-OD1	5.30	123.07	118.30
1	L	908	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	427	THR	CA-CB-CG2	-5.30	104.98	112.40
1	C	729	THR	N-CA-CB	5.30	120.37	110.30
1	J	695	TRP	CB-CA-C	-5.30	99.81	110.40
1	F	729	THR	N-CA-CB	5.30	120.36	110.30
1	H	695	TRP	CB-CA-C	-5.30	99.81	110.40
1	I	729	THR	N-CA-CB	5.30	120.36	110.30
1	N	729	THR	N-CA-CB	5.30	120.36	110.30
1	O	183	ARG	CD-NE-CZ	-5.30	116.18	123.60
1	G	695	TRP	CB-CA-C	-5.29	99.81	110.40
1	M	403	ASP	CB-CG-OD1	5.29	123.06	118.30
1	I	403	ASP	CB-CG-OD1	5.29	123.06	118.30
1	I	695	TRP	CB-CA-C	-5.29	99.81	110.40
1	L	427	THR	CA-CB-CG2	-5.29	104.99	112.40
1	M	695	TRP	CB-CA-C	-5.29	99.81	110.40
1	N	695	TRP	CB-CA-C	-5.29	99.81	110.40
1	O	427	THR	CA-CB-CG2	-5.29	104.99	112.40
1	B	104	THR	CA-CB-CG2	-5.29	104.99	112.40
1	F	826	THR	CA-CB-CG2	-5.29	104.99	112.40
1	K	802	ASP	CB-CG-OD1	5.29	123.06	118.30
1	K	178	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	K	695	TRP	CB-CA-C	-5.29	99.82	110.40
1	K	826	THR	CA-CB-CG2	-5.29	104.99	112.40
1	L	695	TRP	CB-CA-C	-5.29	99.82	110.40
1	M	908	ASP	CB-CG-OD1	5.29	123.06	118.30
1	O	104	THR	CA-CB-CG2	-5.29	104.99	112.40
1	B	729	THR	N-CA-CB	5.29	120.35	110.30
1	E	427	THR	CA-CB-CG2	-5.29	105.00	112.40
1	F	104	THR	CA-CB-CG2	-5.29	105.00	112.40
1	F	695	TRP	CB-CA-C	-5.29	99.82	110.40
1	H	403	ASP	CB-CG-OD1	5.29	123.06	118.30
1	M	729	THR	N-CA-CB	5.29	120.34	110.30
1	P	695	TRP	CB-CA-C	-5.29	99.83	110.40
1	A	104	THR	CA-CB-CG2	-5.29	105.00	112.40
1	B	84	VAL	N-CA-CB	-5.29	99.87	111.50
1	G	84	VAL	N-CA-CB	-5.29	99.87	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	427	THR	CA-CB-CG2	-5.28	105.00	112.40
1	L	802	ASP	CB-CG-OD1	5.28	123.06	118.30
1	J	183	ARG	CD-NE-CZ	-5.28	116.20	123.60
1	A	1013	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	D	427	THR	CA-CB-CG2	-5.28	105.01	112.40
1	J	729	THR	N-CA-CB	5.28	120.33	110.30
1	O	84	VAL	N-CA-CB	-5.28	99.89	111.50
1	B	114	VAL	N-CA-CB	-5.28	99.89	111.50
1	E	695	TRP	CB-CA-C	-5.28	99.85	110.40
1	F	84	VAL	N-CA-CB	-5.28	99.89	111.50
1	F	403	ASP	CB-CG-OD1	5.28	123.05	118.30
1	F	802	ASP	CB-CG-OD1	5.28	123.05	118.30
1	G	1013	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	J	104	THR	CA-CB-CG2	-5.28	105.01	112.40
1	L	729	THR	N-CA-CB	5.28	120.33	110.30
1	O	729	THR	N-CA-CB	5.28	120.33	110.30
1	P	729	THR	N-CA-CB	5.28	120.33	110.30
1	C	84	VAL	N-CA-CB	-5.28	99.89	111.50
1	G	729	THR	N-CA-CB	5.28	120.32	110.30
1	I	1013	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	H	114	VAL	N-CA-CB	-5.27	99.90	111.50
1	H	802	ASP	CB-CG-OD1	5.27	123.05	118.30
1	N	183	ARG	CD-NE-CZ	-5.27	116.22	123.60
1	P	114	VAL	N-CA-CB	-5.27	99.90	111.50
1	E	114	VAL	N-CA-CB	-5.27	99.90	111.50
1	K	84	VAL	N-CA-CB	-5.27	99.90	111.50
1	M	104	THR	CA-CB-CG2	-5.27	105.02	112.40
1	P	84	VAL	N-CA-CB	-5.27	99.90	111.50
1	D	729	THR	N-CA-CB	5.27	120.31	110.30
1	H	729	THR	N-CA-CB	5.27	120.31	110.30
1	B	908	ASP	CB-CG-OD1	5.27	123.04	118.30
1	K	729	THR	N-CA-CB	5.27	120.31	110.30
1	L	183	ARG	CD-NE-CZ	-5.27	116.22	123.60
1	M	178	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	N	104	THR	CA-CB-CG2	-5.27	105.02	112.40
1	A	84	VAL	N-CA-CB	-5.27	99.91	111.50
1	E	84	VAL	N-CA-CB	-5.27	99.91	111.50
1	E	104	THR	CA-CB-CG2	-5.27	105.03	112.40
1	E	729	THR	N-CA-CB	5.27	120.31	110.30
1	I	104	THR	CA-CB-CG2	-5.27	105.03	112.40
1	K	104	THR	CA-CB-CG2	-5.27	105.02	112.40
1	L	84	VAL	N-CA-CB	-5.27	99.91	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	114	VAL	N-CA-CB	-5.27	99.91	111.50
1	O	114	VAL	N-CA-CB	-5.27	99.91	111.50
1	E	403	ASP	CB-CG-OD1	5.26	123.04	118.30
1	J	403	ASP	CB-CG-OD1	5.26	123.04	118.30
1	D	84	VAL	N-CA-CB	-5.26	99.92	111.50
1	D	114	VAL	N-CA-CB	-5.26	99.92	111.50
1	J	114	VAL	N-CA-CB	-5.26	99.92	111.50
1	K	114	VAL	N-CA-CB	-5.26	99.92	111.50
1	B	1013	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	G	104	THR	CA-CB-CG2	-5.26	105.03	112.40
1	I	84	VAL	N-CA-CB	-5.26	99.92	111.50
1	L	104	THR	CA-CB-CG2	-5.26	105.03	112.40
1	M	84	VAL	N-CA-CB	-5.26	99.92	111.50
1	P	802	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	114	VAL	N-CA-CB	-5.26	99.93	111.50
1	B	782	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	802	ASP	CB-CG-OD1	5.26	123.03	118.30
1	D	104	THR	CA-CB-CG2	-5.26	105.04	112.40
1	H	84	VAL	N-CA-CB	-5.26	99.93	111.50
1	I	114	VAL	N-CA-CB	-5.26	99.93	111.50
1	N	84	VAL	N-CA-CB	-5.26	99.93	111.50
1	E	802	ASP	CB-CG-OD1	5.26	123.03	118.30
1	F	114	VAL	N-CA-CB	-5.26	99.94	111.50
1	E	1013	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	J	84	VAL	N-CA-CB	-5.25	99.94	111.50
1	O	1013	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	729	THR	N-CA-CB	5.25	120.28	110.30
1	A	802	ASP	CB-CG-OD1	5.25	123.03	118.30
1	G	114	VAL	N-CA-CB	-5.25	99.95	111.50
1	K	1013	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	D	802	ASP	CB-CG-OD1	5.25	123.02	118.30
1	C	114	VAL	N-CA-CB	-5.25	99.96	111.50
1	G	908	ASP	CB-CG-OD1	5.25	123.02	118.30
1	J	802	ASP	CB-CG-OD1	5.25	123.02	118.30
1	F	178	ARG	NE-CZ-NH1	-5.25	117.68	120.30
1	J	1013	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	L	114	VAL	N-CA-CB	-5.24	99.96	111.50
1	M	114	VAL	N-CA-CB	-5.24	99.97	111.50
1	L	761	GLN	CA-CB-CG	-5.24	101.87	113.40
1	H	761	GLN	CA-CB-CG	-5.24	101.88	113.40
1	N	802	ASP	CB-CG-OD1	5.24	123.02	118.30
1	O	802	ASP	CB-CG-OD1	5.24	123.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	178	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	P	761	GLN	CA-CB-CG	-5.23	101.89	113.40
1	C	761	GLN	CA-CB-CG	-5.23	101.89	113.40
1	O	761	GLN	CA-CB-CG	-5.23	101.89	113.40
1	P	1013	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	E	761	GLN	CA-CB-CG	-5.23	101.89	113.40
1	J	761	GLN	CA-CB-CG	-5.23	101.89	113.40
1	C	1013	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	I	761	GLN	CA-CB-CG	-5.23	101.90	113.40
1	P	782	ASP	CB-CG-OD1	5.23	123.00	118.30
1	G	761	GLN	CA-CB-CG	-5.23	101.90	113.40
1	A	761	GLN	CA-CB-CG	-5.22	101.91	113.40
1	E	782	ASP	CB-CG-OD1	5.22	123.00	118.30
1	K	761	GLN	CA-CB-CG	-5.22	101.91	113.40
1	B	761	GLN	CA-CB-CG	-5.22	101.92	113.40
1	D	761	GLN	CA-CB-CG	-5.22	101.92	113.40
1	M	802	ASP	CB-CG-OD1	5.22	123.00	118.30
1	E	651	LEU	CB-CA-C	-5.22	100.29	110.20
1	F	761	GLN	CA-CB-CG	-5.21	101.93	113.40
1	M	761	GLN	CA-CB-CG	-5.21	101.93	113.40
1	O	651	LEU	CB-CA-C	-5.21	100.30	110.20
1	I	802	ASP	CB-CG-OD1	5.21	122.99	118.30
1	N	761	GLN	CA-CB-CG	-5.21	101.93	113.40
1	C	651	LEU	CB-CA-C	-5.21	100.31	110.20
1	L	1013	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	L	745	MET	CB-CA-C	-5.21	99.99	110.40
1	F	651	LEU	CB-CA-C	-5.20	100.31	110.20
1	P	651	LEU	CB-CA-C	-5.20	100.31	110.20
1	D	651	LEU	CB-CA-C	-5.20	100.32	110.20
1	H	1013	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	O	782	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	802	ASP	CB-CG-OD1	5.20	122.98	118.30
1	F	745	MET	CB-CA-C	-5.20	100.00	110.40
1	K	745	MET	CB-CA-C	-5.20	100.00	110.40
1	K	651	LEU	CB-CA-C	-5.20	100.33	110.20
1	C	782	ASP	CB-CG-OD1	5.20	122.97	118.30
1	N	651	LEU	CB-CA-C	-5.20	100.33	110.20
1	I	782	ASP	CB-CG-OD1	5.19	122.97	118.30
1	J	651	LEU	CB-CA-C	-5.19	100.33	110.20
1	A	651	LEU	CB-CA-C	-5.19	100.33	110.20
1	H	651	LEU	CB-CA-C	-5.19	100.33	110.20
1	B	651	LEU	CB-CA-C	-5.19	100.34	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	651	LEU	CB-CA-C	-5.19	100.34	110.20
1	I	651	LEU	CB-CA-C	-5.19	100.34	110.20
1	J	745	MET	CB-CA-C	-5.19	100.02	110.40
1	H	745	MET	CB-CA-C	-5.19	100.03	110.40
1	M	745	MET	CB-CA-C	-5.19	100.03	110.40
1	A	782	ASP	CB-CG-OD1	5.19	122.97	118.30
1	P	745	MET	CB-CA-C	-5.18	100.03	110.40
1	J	782	ASP	CB-CG-OD1	5.18	122.96	118.30
1	L	651	LEU	CB-CA-C	-5.18	100.35	110.20
1	B	745	MET	CB-CA-C	-5.18	100.04	110.40
1	G	745	MET	CB-CA-C	-5.18	100.04	110.40
1	K	782	ASP	CB-CG-OD1	5.18	122.96	118.30
1	M	782	ASP	CB-CG-OD1	5.18	122.96	118.30
1	C	745	MET	CB-CA-C	-5.18	100.04	110.40
1	E	745	MET	CB-CA-C	-5.18	100.04	110.40
1	F	782	ASP	CB-CG-OD1	5.18	122.96	118.30
1	F	1013	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	745	MET	CB-CA-C	-5.18	100.05	110.40
1	D	745	MET	CB-CA-C	-5.18	100.05	110.40
1	M	651	LEU	CB-CA-C	-5.18	100.36	110.20
1	N	745	MET	CB-CA-C	-5.18	100.05	110.40
1	O	745	MET	CB-CA-C	-5.17	100.05	110.40
1	D	782	ASP	CB-CG-OD1	5.17	122.95	118.30
1	K	310	ARG	N-CA-CB	5.17	119.90	110.60
1	L	782	ASP	CB-CG-OD1	5.16	122.94	118.30
1	I	745	MET	CB-CA-C	-5.16	100.08	110.40
1	J	147	ASN	N-CA-CB	-5.16	101.32	110.60
1	M	147	ASN	N-CA-CB	-5.16	101.32	110.60
1	L	147	ASN	N-CA-CB	-5.16	101.32	110.60
1	O	310	ARG	N-CA-CB	5.16	119.88	110.60
1	D	310	ARG	N-CA-CB	5.15	119.88	110.60
1	G	147	ASN	N-CA-CB	-5.15	101.32	110.60
1	H	782	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	147	ASN	N-CA-CB	-5.15	101.33	110.60
1	B	310	ARG	N-CA-CB	5.15	119.87	110.60
1	I	147	ASN	N-CA-CB	-5.15	101.33	110.60
1	G	782	ASP	CB-CG-OD1	5.14	122.93	118.30
1	E	508	GLU	CA-CB-CG	5.14	124.71	113.40
1	H	508	GLU	CA-CB-CG	5.14	124.71	113.40
1	B	147	ASN	N-CA-CB	-5.14	101.35	110.60
1	K	508	GLU	CA-CB-CG	5.14	124.71	113.40
1	C	310	ARG	N-CA-CB	5.14	119.85	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	147	ASN	N-CA-CB	-5.14	101.35	110.60
1	C	508	GLU	CA-CB-CG	5.13	124.69	113.40
1	F	147	ASN	N-CA-CB	-5.13	101.36	110.60
1	N	310	ARG	N-CA-CB	5.13	119.84	110.60
1	N	508	GLU	CA-CB-CG	5.13	124.70	113.40
1	A	310	ARG	N-CA-CB	5.13	119.84	110.60
1	O	147	ASN	N-CA-CB	-5.13	101.36	110.60
1	I	524	LEU	CB-CA-C	-5.13	100.45	110.20
1	I	508	GLU	CA-CB-CG	5.13	124.69	113.40
1	A	508	GLU	CA-CB-CG	5.13	124.68	113.40
1	B	598	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	D	147	ASN	N-CA-CB	-5.13	101.37	110.60
1	K	147	ASN	N-CA-CB	-5.13	101.37	110.60
1	L	508	GLU	CA-CB-CG	5.13	124.68	113.40
1	L	848	THR	CA-CB-CG2	-5.13	105.22	112.40
1	B	508	GLU	CA-CB-CG	5.13	124.68	113.40
1	F	508	GLU	CA-CB-CG	5.13	124.68	113.40
1	H	147	ASN	N-CA-CB	-5.13	101.37	110.60
1	N	782	ASP	CB-CG-OD1	5.12	122.91	118.30
1	E	147	ASN	N-CA-CB	-5.12	101.38	110.60
1	E	310	ARG	N-CA-CB	5.12	119.82	110.60
1	G	310	ARG	N-CA-CB	5.12	119.82	110.60
1	H	310	ARG	N-CA-CB	5.12	119.82	110.60
1	O	848	THR	CA-CB-CG2	-5.12	105.23	112.40
1	P	147	ASN	N-CA-CB	-5.12	101.38	110.60
1	F	310	ARG	N-CA-CB	5.12	119.82	110.60
1	F	598	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	I	310	ARG	N-CA-CB	5.12	119.82	110.60
1	E	848	THR	CA-CB-CG2	-5.12	105.23	112.40
1	M	310	ARG	N-CA-CB	5.12	119.82	110.60
1	M	508	GLU	CA-CB-CG	5.12	124.66	113.40
1	P	310	ARG	N-CA-CB	5.12	119.82	110.60
1	H	524	LEU	CB-CA-C	-5.12	100.47	110.20
1	L	310	ARG	N-CA-CB	5.12	119.81	110.60
1	P	508	GLU	CA-CB-CG	5.12	124.66	113.40
1	B	524	LEU	CB-CA-C	-5.12	100.48	110.20
1	H	598	ASP	CB-CG-OD2	-5.12	113.70	118.30
1	J	508	GLU	CA-CB-CG	5.12	124.66	113.40
1	J	710	GLU	CB-CA-C	-5.12	100.17	110.40
1	O	508	GLU	CA-CB-CG	5.12	124.66	113.40
1	O	508	GLU	CB-CA-C	-5.12	100.17	110.40
1	O	524	LEU	CB-CA-C	-5.12	100.48	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	508	GLU	CB-CA-C	-5.11	100.17	110.40
1	F	524	LEU	CB-CA-C	-5.11	100.49	110.20
1	J	524	LEU	CB-CA-C	-5.11	100.48	110.20
1	K	598	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	N	147	ASN	N-CA-CB	-5.11	101.40	110.60
1	O	710	GLU	CB-CA-C	-5.11	100.17	110.40
1	P	524	LEU	CB-CA-C	-5.11	100.48	110.20
1	I	710	GLU	CB-CA-C	-5.11	100.17	110.40
1	M	524	LEU	CB-CA-C	-5.11	100.49	110.20
1	A	524	LEU	CB-CA-C	-5.11	100.49	110.20
1	D	710	GLU	CB-CA-C	-5.11	100.18	110.40
1	E	710	GLU	CB-CA-C	-5.11	100.18	110.40
1	J	310	ARG	N-CA-CB	5.11	119.80	110.60
1	K	226	HIS	CB-CA-C	-5.11	100.18	110.40
1	L	524	LEU	CB-CA-C	-5.11	100.49	110.20
1	O	226	HIS	CB-CA-C	-5.11	100.18	110.40
1	L	598	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	C	710	GLU	CB-CA-C	-5.11	100.19	110.40
1	D	508	GLU	CA-CB-CG	5.11	124.64	113.40
1	D	524	LEU	CB-CA-C	-5.11	100.50	110.20
1	I	508	GLU	CB-CA-C	-5.11	100.19	110.40
1	A	710	GLU	CB-CA-C	-5.11	100.19	110.40
1	B	710	GLU	CB-CA-C	-5.11	100.19	110.40
1	D	598	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	N	710	GLU	CB-CA-C	-5.11	100.19	110.40
1	P	710	GLU	CB-CA-C	-5.11	100.19	110.40
1	C	524	LEU	CB-CA-C	-5.10	100.50	110.20
1	D	226	HIS	CB-CA-C	-5.10	100.19	110.40
1	G	710	GLU	CB-CA-C	-5.10	100.19	110.40
1	N	226	HIS	CB-CA-C	-5.10	100.19	110.40
1	B	848	THR	CA-CB-CG2	-5.10	105.26	112.40
1	G	508	GLU	CA-CB-CG	5.10	124.63	113.40
1	K	848	THR	CA-CB-CG2	-5.10	105.26	112.40
1	M	710	GLU	CB-CA-C	-5.10	100.19	110.40
1	M	848	THR	CA-CB-CG2	-5.10	105.26	112.40
1	N	598	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	P	508	GLU	CB-CA-C	-5.10	100.19	110.40
1	A	508	GLU	CB-CA-C	-5.10	100.20	110.40
1	F	508	GLU	CB-CA-C	-5.10	100.20	110.40
1	F	710	GLU	CB-CA-C	-5.10	100.20	110.40
1	G	508	GLU	CB-CA-C	-5.10	100.20	110.40
1	K	524	LEU	CB-CA-C	-5.10	100.51	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	226	HIS	CB-CA-C	-5.10	100.20	110.40
1	G	524	LEU	CB-CA-C	-5.10	100.51	110.20
1	H	508	GLU	CB-CA-C	-5.10	100.20	110.40
1	H	1014	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	I	598	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	H	226	HIS	CB-CA-C	-5.10	100.20	110.40
1	J	336	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	J	508	GLU	CB-CA-C	-5.10	100.20	110.40
1	L	710	GLU	CB-CA-C	-5.10	100.20	110.40
1	M	508	GLU	CB-CA-C	-5.10	100.20	110.40
1	P	848	THR	CA-CB-CG2	-5.10	105.26	112.40
1	A	598	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	E	524	LEU	CB-CA-C	-5.09	100.52	110.20
1	I	226	HIS	CB-CA-C	-5.09	100.21	110.40
1	L	508	GLU	CB-CA-C	-5.09	100.21	110.40
1	N	508	GLU	CB-CA-C	-5.09	100.21	110.40
1	L	226	HIS	CB-CA-C	-5.09	100.21	110.40
1	A	226	HIS	CB-CA-C	-5.09	100.22	110.40
1	C	848	THR	CA-CB-CG2	-5.09	105.27	112.40
1	D	848	THR	CA-CB-CG2	-5.09	105.27	112.40
1	J	598	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	J	848	THR	CA-CB-CG2	-5.09	105.27	112.40
1	N	524	LEU	CB-CA-C	-5.09	100.53	110.20
1	B	226	HIS	CB-CA-C	-5.09	100.22	110.40
1	I	750	GLU	N-CA-CB	-5.09	101.44	110.60
1	M	226	HIS	CB-CA-C	-5.09	100.22	110.40
1	A	848	THR	CA-CB-CG2	-5.09	105.28	112.40
1	G	226	HIS	CB-CA-C	-5.09	100.22	110.40
1	E	508	GLU	CB-CA-C	-5.09	100.22	110.40
1	F	848	THR	CA-CB-CG2	-5.09	105.28	112.40
1	I	848	THR	CA-CB-CG2	-5.09	105.28	112.40
1	H	710	GLU	CB-CA-C	-5.08	100.23	110.40
1	K	508	GLU	CB-CA-C	-5.08	100.23	110.40
1	H	848	THR	CA-CB-CG2	-5.08	105.28	112.40
1	K	710	GLU	CB-CA-C	-5.08	100.23	110.40
1	B	508	GLU	CB-CA-C	-5.08	100.23	110.40
1	C	508	GLU	CB-CA-C	-5.08	100.24	110.40
1	E	612	THR	N-CA-CB	5.08	119.95	110.30
1	G	598	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	J	750	GLU	N-CA-CB	-5.08	101.45	110.60
1	N	612	THR	N-CA-CB	5.08	119.95	110.30
1	N	750	GLU	N-CA-CB	-5.08	101.45	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	612	THR	N-CA-CB	5.08	119.95	110.30
1	N	848	THR	CA-CB-CG2	-5.08	105.29	112.40
1	B	750	GLU	N-CA-CB	-5.08	101.46	110.60
1	C	598	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	F	226	HIS	CB-CA-C	-5.08	100.24	110.40
1	H	750	GLU	N-CA-CB	-5.08	101.46	110.60
1	M	750	GLU	N-CA-CB	-5.08	101.46	110.60
1	B	612	THR	N-CA-CB	5.08	119.95	110.30
1	E	226	HIS	CB-CA-C	-5.08	100.25	110.40
1	P	750	GLU	N-CA-CB	-5.08	101.46	110.60
1	M	598	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	E	598	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	G	750	GLU	N-CA-CB	-5.07	101.47	110.60
1	I	363	HIS	CA-CB-CG	-5.07	104.97	113.60
1	M	336	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	P	226	HIS	CB-CA-C	-5.07	100.26	110.40
1	E	750	GLU	N-CA-CB	-5.07	101.47	110.60
1	O	612	THR	N-CA-CB	5.07	119.93	110.30
1	I	612	THR	N-CA-CB	5.07	119.93	110.30
1	J	226	HIS	CB-CA-C	-5.07	100.27	110.40
1	K	750	GLU	N-CA-CB	-5.07	101.48	110.60
1	P	598	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	F	750	GLU	N-CA-CB	-5.07	101.48	110.60
1	G	363	HIS	CA-CB-CG	-5.07	104.99	113.60
1	L	750	GLU	N-CA-CB	-5.07	101.48	110.60
1	K	59	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	612	THR	N-CA-CB	5.06	119.92	110.30
1	A	750	GLU	N-CA-CB	-5.06	101.49	110.60
1	C	750	GLU	N-CA-CB	-5.06	101.49	110.60
1	F	363	HIS	CA-CB-CG	-5.06	104.99	113.60
1	H	612	THR	N-CA-CB	5.06	119.92	110.30
1	L	336	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	L	612	THR	N-CA-CB	5.06	119.92	110.30
1	N	336	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	O	750	GLU	N-CA-CB	-5.06	101.49	110.60
1	C	363	HIS	CA-CB-CG	-5.06	105.00	113.60
1	D	612	THR	N-CA-CB	5.06	119.91	110.30
1	G	848	THR	CA-CB-CG2	-5.06	105.32	112.40
1	M	612	THR	N-CA-CB	5.06	119.91	110.30
1	G	336	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	F	612	THR	N-CA-CB	5.05	119.90	110.30
1	A	363	HIS	CA-CB-CG	-5.05	105.01	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	363	HIS	CA-CB-CG	-5.05	105.01	113.60
1	G	612	THR	N-CA-CB	5.05	119.90	110.30
1	K	612	THR	N-CA-CB	5.05	119.90	110.30
1	C	612	THR	N-CA-CB	5.05	119.89	110.30
1	N	1014	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	E	336	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	G	172	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	H	363	HIS	CA-CB-CG	-5.05	105.02	113.60
1	P	363	HIS	CA-CB-CG	-5.05	105.02	113.60
1	M	59	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	N	363	HIS	CA-CB-CG	-5.04	105.02	113.60
1	O	172	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	D	750	GLU	N-CA-CB	-5.04	101.52	110.60
1	I	1014	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	J	363	HIS	CA-CB-CG	-5.04	105.03	113.60
1	J	612	THR	N-CA-CB	5.04	119.88	110.30
1	K	336	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	K	363	HIS	CA-CB-CG	-5.04	105.03	113.60
1	P	1014	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	H	336	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	L	363	HIS	CA-CB-CG	-5.04	105.03	113.60
1	O	598	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	E	172	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	O	363	HIS	CA-CB-CG	-5.04	105.03	113.60
1	M	363	HIS	CA-CB-CG	-5.04	105.04	113.60
1	C	336	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	K	172	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	B	120	THR	CA-CB-CG2	-5.03	105.36	112.40
1	B	172	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	O	336	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	H	859	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	E	363	HIS	CA-CB-CG	-5.02	105.06	113.60
1	D	172	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	G	1014	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	A	1014	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	M	343	LEU	CB-CA-C	-5.02	100.66	110.20
1	A	336	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	D	363	HIS	CA-CB-CG	-5.02	105.07	113.60
1	J	1014	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	A	172	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	O	343	LEU	CB-CA-C	-5.02	100.67	110.20
1	B	336	ARG	NE-CZ-NH1	5.01	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	336	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	I	172	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	E	59	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	G	343	LEU	CB-CA-C	-5.01	100.68	110.20
1	D	859	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	J	120	THR	CA-CB-CG2	-5.01	105.39	112.40
1	B	59	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	C	859	ASP	CB-CG-OD2	-5.01	113.80	118.30
1	E	1014	TYR	CB-CG-CD2	-5.00	118.00	121.00
1	I	343	LEU	CB-CA-C	-5.00	100.69	110.20
1	K	120	THR	CA-CB-CG2	-5.00	105.39	112.40
1	H	343	LEU	CB-CA-C	-5.00	100.69	110.20
1	L	1014	TYR	CB-CG-CD2	-5.00	118.00	121.00
1	C	343	LEU	CB-CA-C	-5.00	100.70	110.20
1	F	120	THR	CA-CB-CG2	-5.00	105.40	112.40
1	L	172	ASP	CB-CG-OD2	-5.00	113.80	118.30
1	M	172	ASP	CB-CG-OD2	-5.00	113.80	118.30
1	P	343	LEU	CB-CA-C	-5.00	100.70	110.20

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

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Mol	Chain	Res	Type	Atom
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8232	0	7817	270	3
1	B	8232	0	7817	267	4
1	C	8232	0	7817	262	1
1	D	8232	0	7817	275	0
1	E	8232	0	7817	266	0
1	F	8232	0	7817	269	0
1	G	8232	0	7817	267	0
1	H	8232	0	7817	261	0
1	I	8232	0	7817	269	1
1	J	8232	0	7817	274	0
1	K	8232	0	7817	277	0
1	L	8232	0	7817	264	0
1	M	8232	0	7817	271	0
1	N	8232	0	7817	269	0
1	O	8232	0	7817	271	0
1	P	8232	0	7817	269	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	4201	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 16.

All (4201) 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:L:427:THR:HA	1:L:436:MET:HE1	1.43	1.01
1:E:427:THR:HA	1:E:436:MET:HE1	1.41	1.00
1:M:427:THR:HA	1:M:436:MET:HE1	1.43	1.00
1:J:427:THR:HA	1:J:436:MET:HE1	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:THR:HA	1:C:436:MET:HE1	1.45	0.98
1:K:427:THR:HA	1:K:436:MET:HE1	1.47	0.97
1:I:427:THR:HA	1:I:436:MET:HE1	1.47	0.96
1:G:427:THR:HA	1:G:436:MET:HE1	1.47	0.96
1:P:427:THR:HA	1:P:436:MET:HE1	1.47	0.95
1:B:525:SER:HB3	3:B:3101:HOH:O	1.68	0.94
1:O:427:THR:HA	1:O:436:MET:HE1	1.50	0.93
1:D:427:THR:HA	1:D:436:MET:HE1	1.48	0.93
1:B:427:THR:HA	1:B:436:MET:HE1	1.50	0.93
1:A:427:THR:HA	1:A:436:MET:HE1	1.53	0.90
1:F:427:THR:HA	1:F:436:MET:HE1	1.53	0.90
1:N:427:THR:HA	1:N:436:MET:HE1	1.53	0.90
1:H:427:THR:HA	1:H:436:MET:CE	2.02	0.89
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:H:427:THR:HA	1:H:436:MET:HE1	1.53	0.89
1:A:427:THR:HA	1:A:436:MET:CE	2.02	0.88
1:K:427:THR:HA	1:K: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:O:427:THR:HA	1:O:436:MET:CE	2.02	0.87
1:N:595:THR:HG23	1:N:596:PRO:HA	1.57	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:427:THR:HA	1:P:436:MET:CE	2.02	0.87
1:P:595:THR:HG23	1:P:596:PRO:HA	1.57	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:C:595:THR:HG23	1:C:596:PRO:HA	1.57	0.86
1:K:595:THR:HG23	1:K:596:PRO:HA	1.57	0.86
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:434:PRO:HB3	1:C:434:PRO:HB3	1.58	0.83
1:H:525:SER:HB3	3:H:4178:HOH:O	1.77	0.83
1:A:282:ARG:HD3	1:D:420:MET:O	1.81	0.81
1:J:436:MET:CE	1:J:467:ASN:HD22	1.95	0.80
1:G:436:MET:CE	1:G:467:ASN:HD22	1.95	0.80
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
1:A:436:MET:CE	1:A:467:ASN:HD22	1.95	0.79
1:L:436:MET:CE	1:L: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: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: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: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:A:436:MET:HE1	1:A:467:ASN:HD22	1.49	0.77
1:H:316:HIS:HA	1:H:323:ILE:HD12	1.66	0.77
1:N:436:MET:HE1	1:N:467:ASN:HD22	1.49	0.77
1:F:436:MET:HE1	1:F:467:ASN:HD22	1.49	0.77
1:H:436:MET:HE1	1:H:467:ASN:HD22	1.49	0.77
1:B:316:HIS:HA	1:B:323:ILE:HD12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:745:MET:HE2	1:M:745:MET:HA	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:436:MET:HE1	1:O:467:ASN:HD22	1.52	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
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:I:745:MET:HE2	1:I:745:MET:HA	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:436:MET:HE1	1:B:467:ASN:HD22	1.52	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
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:K:436:MET:HE1	1:K:467:ASN:HD22	1.55	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:N:745:MET:HE2	1:N:745:MET:HA	1.72	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:F:745:MET:HE2	1:F:745:MET:HA	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:436:MET:HE1	1:D:467:ASN:HD22	1.53	0.71
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: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
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:G:436:MET:HE1	1:G:467:ASN:HD22	1.55	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:I:436:MET:HE1	1:I:467:ASN:HD22	1.55	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:C:436:MET:HE1	1:C:467:ASN:HD22	1.56	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:P:166:ARG:HG3	1:P:392:TYR:HB2	1.74	0.69
1:P:436:MET:HE1	1:P:467:ASN:HD22	1.55	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
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:C:579:ASP:OD1	1:C:583:ASN:HB2	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ARG:HG3	1:B:392:TYR:HB2	1.74	0.69
1:B:745:MET:HE2	1:B:745:MET:HA	1.73	0.69
1:F:579:ASP:OD1	1:F:583:ASN:HB2	1.92	0.69
1:A:579:ASP:OD1	1:A:583:ASN:HB2	1.92	0.69
1:E:856:TYR:HD2	1:E:864:MET:HE2	1.58	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:F:166:ARG:HG3	1:F:392:TYR:HB2	1.74	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
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: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:L:166:ARG:HG3	1:L:392:TYR:HB2	1.74	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:919:ASP:O	1:O:920:LEU:HD23	1.93	0.68
1:D:745:MET:HA	1:D:745:MET:HE2	1.74	0.68
1:H:919:ASP:O	1:H:920:LEU:HD23	1.94	0.68
1:J:436:MET:HE1	1:J:467:ASN:HD22	1.58	0.68
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.74	0.68
1:D:856:TYR:HD2	1:D:864:MET:HE2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:P:745:MET:HE2	1:P:745:MET:HA	1.75	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: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
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: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:745:MET:HA	1:L:745:MET:HE2	1.75	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:E:745:MET:HE2	1:E:745:MET:HA	1.76	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:N:43:ARG:HG2	1:N:43:ARG:HH11	1.59	0.67
1:O:920:LEU:HB3	1:O:921:PRO:HD2	1.76	0.67
1:K:920:LEU:HB3	1:K:921:PRO:HD2	1.76	0.67
1:M:425:ARG:HH22	1:P:287:ASP:CG	1.98	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:L:436:MET:HE1	1:L:467:ASN:HD22	1.59	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:J:745:MET:HE2	1:J:745:MET:HA	1.76	0.67
1:A:745:MET:HE2	1:A:745:MET:HA	1.76	0.67
1:A:856:TYR:HD2	1:A:864:MET:HE2	1.60	0.67
1:G:856:TYR:HD2	1:G:864:MET:HE2	1.59	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:O:745:MET:HA	1:O:745:MET:HE2	1.76	0.67
1:P:278:ILE:HD12	1:P:278:ILE:N	2.10	0.67
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:HD13	1:A:74:LEU:HD11	1.77	0.66
1:C:890:GLN:HG3	1:C:891:VAL:N	2.09	0.66
1:G:745:MET:HA	1:G:745:MET:HE2	1.76	0.66
1:H:745:MET:HE2	1:H:745:MET:HA	1.76	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:L:890:GLN:HG3	1:L:891:VAL:N	2.09	0.66
1:N:278:ILE:HD12	1:N:278:ILE:N	2.10	0.66
1:A:418:HIS:O	1:D:282:ARG:HD2	1.96	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: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: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: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:890:GLN:HG3	1:D:891:VAL:N	2.09	0.66
1:E:436:MET:HE3	1:E:467:ASN:HD22	1.60	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:745:MET:HE2	1:C:745:MET:HA	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:367:MET:HB3	1:B:372:MET:HE3	1.78	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:M:436:MET:HE1	1:M:467:ASN:HD22	1.59	0.65
1:M:436:MET:HE3	1:M:467:ASN:HD22	1.62	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:890:GLN:HG3	1:E:891:VAL:N	2.09	0.65
1:F:367:MET:HB3	1:F:372:MET:HE3	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:745:MET:HE2	1:K:745:MET:HA	1.76	0.65
1:L:7:LEU:N	1:L:71:GLU:OE2	2.30	0.65
1:O:254:LEU:C	1:O:255:ARG:HG2	2.17	0.65
1:E:254:LEU:C	1:E:255:ARG:HG2	2.17	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: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
1:D:367:MET:HB3	1:D:372:MET:HE3	1.77	0.65
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: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:G:254:LEU:C	1:G:255:ARG:HG2	2.17	0.65
1:J:43:ARG:HG2	1:J:43:ARG:NH1	2.11	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:A:425:ARG:HH22	1:D:287:ASP:CG	2.01	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:I:254:LEU:C	1:I:255:ARG:HG2	2.17	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:367:MET:HB3	1:I:372:MET:HE3	1.79	0.64
1:L:43:ARG:HG2	1:L:43:ARG:NH1	2.11	0.64
1:L:254:LEU:C	1:L:255:ARG:HG2	2.17	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:B:254:LEU:C	1:B:255:ARG:HG2	2.17	0.64
1:B:334:GLU:OE1	1:B:336:ARG:NH1	2.30	0.64
1:E:436:MET:HE1	1:E:467:ASN:HD22	1.61	0.64
1:F:254:LEU:C	1:F:255:ARG:HG2	2.17	0.64
1:G:917:ARG:NH2	1:G:943:GLU:OE1	2.30	0.64
1:H:254:LEU:C	1:H:255:ARG:HG2	2.17	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:P:254:LEU:C	1:P:255:ARG:HG2	2.17	0.64
1:D:254:LEU:C	1:D:255:ARG:HG2	2.17	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
1:O:334:GLU:OE1	1:O:336:ARG:NH1	2.30	0.64
1:O:856:TYR:HD2	1:O:864:MET:HE2	1.61	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:J:436:MET:HE3	1:J:467:ASN:HD22	1.63	0.64
1:N:287:ASP:CG	1:O:425:ARG:HH22	2.01	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:M:254:LEU:C	1:M:255:ARG:HG2	2.17	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:436:MET:HE3	1:L:467:ASN:HD22	1.62	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:917:ARG:NH2	1:M:943:GLU:OE1	2.30	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:L:367:MET:HB3	1:L:372:MET:HE3	1.79	0.63
1:C:367:MET:HB3	1:C:372:MET:HE3	1.79	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: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
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: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:254:LEU:C	1:K:255:ARG:HG2	2.17	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:A:681:GLU:HA	1:A:681:GLU:OE2	1.97	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:J:367:MET:HB3	1:J:372:MET:HE3	1.81	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:O:917:ARG:HH22	1:O:943:GLU:CD	2.02	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:LEU:C	1:C:255:ARG:HG2	2.17	0.63
1:E:681:GLU:HA	1:E:681:GLU:OE2	1.97	0.63
1:M:681:GLU:HA	1:M:681:GLU:OE2	1.97	0.63
1:A:254:LEU:C	1:A:255:ARG:HG2	2.17	0.63
1:J:254:LEU:C	1:J:255:ARG:HG2	2.17	0.63
1:L:681:GLU:OE2	1:L:681:GLU:HA	1.97	0.63
1:A:917:ARG:HH22	1:A:943:GLU:CD	2.02	0.63
1:F:681:GLU:HA	1:F:681:GLU:OE2	1.97	0.63
1:K:367:MET:HB3	1:K:372:MET:HE3	1.79	0.63
1:L:917:ARG:HH22	1:L:943:GLU:CD	2.02	0.63
1:N:254:LEU:C	1:N:255:ARG:HG2	2.17	0.63
1:E:66:PRO:HB3	1:E:187:MET:CE	2.29	0.63
1:E:367:MET:HB3	1:E:372:MET:HE3	1.79	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:I:917:ARG:HH22	1:I:943:GLU:CD	2.02	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:G:917:ARG:HH22	1:G:943:GLU:CD	2.02	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:K:917:ARG:HH22	1:K:943:GLU:CD	2.02	0.62
1:N:367:MET:HB3	1:N:372:MET:HE3	1.81	0.62
1:A:367:MET:HB3	1:A:372:MET:HE3	1.81	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:D:917:ARG:HH22	1:D:943:GLU:CD	2.02	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:M:917:ARG:HH22	1:M:943:GLU:CD	2.02	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: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:E:917:ARG:HH22	1:E:943:GLU:CD	2.02	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:66:PRO:HB3	1:L:187:MET:CE	2.29	0.62
1:M:367:MET:HB3	1:M:372:MET:HE3	1.79	0.62
1:A:66:PRO:HB3	1:A:187:MET:CE	2.29	0.62
1:H:917:ARG:HH22	1:H:943:GLU:CD	2.02	0.62
1:K:856:TYR:HD2	1:K:864:MET:HE2	1.63	0.62
1:B:917:ARG:HH22	1:B:943:GLU:CD	2.02	0.62
1:I:117:GLU:OE1	1:I:117:GLU:N	2.29	0.62
1:J:856:TYR:HD2	1:J:864:MET:HE2	1.63	0.62
1:N:30:HIS:ND1	1:N:31:PRO:O	2.30	0.62
1:C:917:ARG:HH22	1:C:943:GLU:CD	2.02	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:O:367:MET:HB3	1:O:372:MET:HE3	1.81	0.62
1:F:917:ARG:HH22	1:F:943:GLU:CD	2.02	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:J:917:ARG:HH22	1:J:943:GLU:CD	2.02	0.61
1:N:917:ARG:HH22	1:N:943:GLU:CD	2.02	0.61
1:P:66:PRO:HB3	1:P:187:MET:CE	2.29	0.61
1:P:917:ARG:HH22	1:P:943:GLU:CD	2.02	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:C:436:MET:HE3	1:C:467:ASN:HD22	1.64	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: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:I:436:MET:HE3	1:I:467:ASN:HD22	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:436:MET:HE3	1:G:467:ASN:HD22	1.66	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
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:427:THR:HA	1:H:436:MET:HE2	1.83	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:367:MET:HB3	1:P:372:MET:HE3	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:856:TYR:HD2	1:H:864:MET:HE2	1.66	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
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:G:367:MET:HB3	1:G:372:MET:HE3	1.82	0.60
1:H:322:LEU:HD23	1:H:324:GLU:N	2.17	0.60
1:H:367:MET:HB3	1:H:372:MET:HE3	1.81	0.60
1:I:178:ARG:NH1	1:I:181:GLU:O	2.35	0.60
1:K:436:MET:HE3	1:K:467:ASN:HD22	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:856:TYR:HD2	1:B:864:MET:HE2	1.67	0.59
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:F:427:THR:HA	1:F:436:MET:HE2	1.83	0.59
1:G:178:ARG:NH1	1:G:181:GLU:O	2.35	0.59
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:J:744:GLU:HB3	1:J:745:MET:HE3	1.84	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:HA	1:N:436:MET:HE2	1.83	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:P:436:MET:HE3	1:P:467:ASN:HD22	1.66	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:O:744:GLU:HB3	1:O:745:MET:HE3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LEU:HD23	1:A:324:GLU:N	2.17	0.59
1:B:744:GLU:HB3	1:B:745:MET:HE3	1.84	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
1:E:682:LEU:HD22	1:E:683:PRO:HD2	1.83	0.59
1:F:744:GLU:HB3	1:F:745:MET:HE3	1.84	0.59
1:G:360:HIS:CE1	1:G:362:LEU:HB2	2.37	0.59
1:G:744:GLU:HB3	1:G:745:MET:HE3	1.84	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:A:744:GLU:HB3	1:A:745:MET:HE3	1.84	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: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:744:GLU:HB3	1:N:745:MET:HE3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:744:GLU:HB3	1:D:745:MET:HE3	1.84	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:L:744:GLU:HB3	1:L:745:MET:HE3	1.84	0.59
1:M:894:ARG:NH1	1:M:919:ASP:OD2	2.36	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:K:744:GLU:HB3	1:K:745:MET:HE3	1.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:377:LEU:N	1:J:377:LEU:HD23	2.18	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:A:427:THR:HA	1:A:436:MET:HE2	1.83	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:H:744:GLU:HB3	1:H:745:MET:HE3	1.84	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: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: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: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:C:744:GLU:HB3	1:C:745:MET:HE3	1.84	0.58
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:724:GLU:O	1:N:847:LYS:NZ	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:856:TYR:HD2	1:C:864:MET:HE2	1.67	0.58
1:D:436:MET:HE3	1:D:467:ASN:HD22	1.67	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:P:744:GLU:HB3	1:P:745:MET:HE3	1.84	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: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:O:427:THR:HA	1:O:436:MET:HE2	1.86	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:E:744:GLU:HB3	1:E:745:MET:HE3	1.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:436:MET:HE3	1:B:467:ASN:HD22	1.69	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:I:744:GLU:HB3	1:I:745:MET:HE3	1.85	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: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:E:166:ARG:HG3	1:E:392:TYR:CB	2.34	0.57
1:G:377:LEU:N	1:G:377:LEU:HD23	2.18	0.57
1:M:744:GLU:HB3	1:M:745:MET:HE3	1.85	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: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:C:377:LEU:HD23	1:C:377:LEU:N	2.18	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:D:747:PHE:HE1	1:D:825:CYS:HG	1.51	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:668:VAL:HG13	1:N:669:PRO:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:E:856:TYR:CD2	1:E:864:MET:HE2	2.40	0.57
1:F:166:ARG:HG3	1:F:392:TYR:CB	2.34	0.57
1:J:597:ASN:HD22	1:J:599:ARG:H	1.52	0.57
1:C:30:HIS:ND1	1:C:31:PRO:O	2.30	0.57
1:E:249:GLU:OE1	1:E:251:ARG:NH1	2.34	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O:30:HIS:ND1	1:O:31:PRO:O	2.30	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
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: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:M:316:HIS:HD2	1:M:317:THR:O	1.89	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:I:63:PHE:CB	1:I:64:PRO:HD2	2.34	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:493:THR:HG23	3:M:4019:HOH:O	2.06	0.56
1:M:856:TYR:HD2	1:M:864:MET:HE2	1.69	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: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: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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:856:TYR:CD2	1:G:864:MET:HE2	2.41	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: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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:PRO:HG2	1:D:279:ILE:HD11	1.89	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:L:856:TYR:HD2	1:L:864:MET:HE2	1.71	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: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:G:894:ARG:HD3	1:G:919:ASP:OD2	2.06	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:A:856:TYR:CD2	1:A:864:MET:HE2	2.42	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:N:856:TYR:HD2	1:N:864:MET:HE2	1.72	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
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:P:427:THR:HA	1:P:436:MET:HE2	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:254:LEU:O	1:H:255:ARG:HG2	2.08	0.54
1:I:427:THR:HA	1:I:436:MET:HE2	1.89	0.54
1:M:167:LEU:HB3	1:M:168:PRO:HD2	1.90	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: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:254:LEU:O	1:K:255:ARG:HG2	2.08	0.54
1:K:651:LEU:HD12	1:K:668:VAL:O	2.07	0.54
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:C:50:GLN:O	1:C:215:LEU:HA	2.08	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: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:P:433:LEU:HB3	1:P:434:PRO:HD3	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:436:MET:HE3	1:H:467:ASN:HD22	1.72	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:K:427:THR:HA	1:K:436:MET:HE2	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:A:127:PHE:HE2	1:A:184:LEU:HG	1.73	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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:856:TYR:HD2	1:F:864:MET:HE2	1.73	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: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:436:MET:HE3	1:O:467:ASN:HD22	1.69	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:B:427:THR:HA	1:B:436:MET:HE2	1.86	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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:436:MET:HE3	1:A:467:ASN:HD22	1.72	0.53
1:E:127:PHE:HE2	1:E:184:LEU:HG	1.73	0.53
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:I:856:TYR:HD2	1:I:864:MET:HE2	1.73	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:B:745:MET:HA	1:B:745:MET:CE	2.39	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:J:745:MET:HA	1:J:745:MET:CE	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:H:745:MET:HA	1:H:745:MET:CE	2.39	0.53
1:I:125:LEU:HG	1:I:126:THR:N	2.23	0.53
1:J:703:PRO:O	1:J:711:ALA:HB1	2.09	0.53
1:L:37:ARG:NH2	1:L:218:PRO:HD3	2.23	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:P:745:MET:HA	1:P:745:MET:CE	2.39	0.53
1:A:322:LEU:HD23	1:A:323:ILE:N	2.23	0.53
1:A:745:MET:HA	1:A:745:MET:CE	2.39	0.53
1:B:651:LEU:CD1	1:B:669:PRO:HA	2.39	0.53
1:G:745:MET:HA	1:G:745:MET:CE	2.39	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: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:O:745:MET:HA	1:O:745:MET:CE	2.39	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:D:662:PRO:C	1:D:663:LEU:HD23	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:662:PRO:C	1:J:663:LEU:HD23	2.30	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: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
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:662:PRO:C	1:L:663:LEU:HD23	2.30	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:O:856:TYR:CD2	1:O:864:MET:HE2	2.43	0.52
1:P:278:ILE:H	1:P:278:ILE:CD1	2.22	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:E:662:PRO:C	1:E:663:LEU:HD23	2.30	0.52
1:F:436:MET:HE3	1:F:467:ASN:HD22	1.72	0.52
1:F:662:PRO:C	1:F:663:LEU:HD23	2.30	0.52
1:F:703:PRO:O	1:F:711:ALA:HB1	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:436:MET:HE3	1:N:467:ASN:HD22	1.72	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:C:7:LEU:HD13	1:C:74:LEU:CD1	2.39	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
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:I:434:PRO:HB3	1:L:434:PRO:HB3	1.90	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:N:662:PRO:C	1:N:663:LEU:HD23	2.30	0.52
1:P:662:PRO:C	1:P:663:LEU:HD23	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:745:MET:HA	1:K:745:MET:CE	2.39	0.52
1:L:251:ARG:HB3	1:L:253:TYR:CE2	2.45	0.52
1:O:127:PHE:HE2	1:O:184:LEU:HG	1.73	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:F:287:ASP:CG	1:G:425:ARG:HH22	2.12	0.52
1:G:651:LEU:CD1	1:G:669:PRO:HA	2.39	0.52
1:H:662:PRO:C	1:H:663:LEU:HD23	2.30	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:N:745:MET:HA	1:N:745:MET:CE	2.39	0.52
1:O:251:ARG:HB3	1:O:253:TYR:CE2	2.45	0.52
1:O:701:VAL:HG22	1:O:714:ILE:CD1	2.40	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:C:662:PRO:C	1:C:663:LEU:HD23	2.30	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: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:I:662:PRO:C	1:I:663:LEU:HD23	2.30	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:747:PHE:HE1	1:B:825:CYS:HG	1.58	0.52
1:B:881:ARG:HD3	1:B:987:ASP:OD1	2.10	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:251:ARG:HB3	1:G:253:TYR:CE2	2.45	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: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: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:745:MET:HA	1:E:745:MET:CE	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:662:PRO:C	1:G:663:LEU:HD23	2.30	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: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:J:856:TYR:CD2	1:J:864:MET:HE2	2.45	0.51
1:O:416:GLU:OE1	1:O:418:HIS:HB2	2.10	0.51
1:O:662:PRO:C	1:O:663:LEU:HD23	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:682:LEU:CD2	1:N:683:PRO:HD2	2.39	0.51
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:C:745:MET:HA	1:C:745:MET:CE	2.39	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:J:427:THR:HA	1:J:436:MET:HE2	1.92	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:O:69:VAL:HG13	1:O:70:PRO:HD2	1.91	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:B:662:PRO:C	1:B:663:LEU:HD23	2.30	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: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: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:M:662:PRO:C	1:M:663:LEU:HD23	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:767:GLN:HG3	1:P:768:MET:N	2.26	0.51
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:E:767:GLN:HG3	1:E:768:MET:N	2.26	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: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:662:PRO:C	1:K:663:LEU:HD23	2.30	0.51
1:K:1020:TRP:CD1	1:K:1021:CME:N	2.79	0.51
1:M:767:GLN:HG3	1:M:768:MET:N	2.26	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:767:GLN:HG3	1:J:768:MET:N	2.26	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: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:C:5:ASP:OD2	1:C:157:ARG:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:ARG:O	1:C:473:ARG:HD3	2.11	0.51
1:F:745:MET:HA	1:F:745:MET:CE	2.39	0.51
1:F:987:ASP:OD2	1:F:990:HIS:HD2	1.94	0.51
1:G:427:THR:HA	1:G:436:MET:HE2	1.89	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:L:745:MET:HA	1:L:745:MET:CE	2.39	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: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:682:LEU:CD2	1:P:683:PRO:HD2	2.39	0.51
1:A:662:PRO:C	1:A:663:LEU:HD23	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:427:THR:HA	1:D:436:MET:HE2	1.87	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:747:PHE:HE1	1:G:825:CYS:HG	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:741:THR:O	1:O:741:THR:HG22	2.12	0.50
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:O:747:PHE:HE1	1:O:825:CYS:HG	1.59	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:C:427:THR:HA	1:C:436:MET:HE2	1.90	0.50
1:D:573:GLN:HB2	1:D:602:CYS:O	2.12	0.50
1:D:856:TYR:CD2	1:D:864:MET:HE2	2.41	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:745:MET:HA	1:I:745:MET:CE	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:K:249:GLU:OE1	1:K:251:ARG:NH1	2.35	0.50
1:K:856:TYR:CD2	1:K:864:MET:HE2	2.45	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: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:287:ASP:CG	1:C:425:ARG:HH22	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:745:MET:HA	1:D:745:MET:CE	2.39	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:741:THR:O	1:I:741:THR:HG22	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:H:856:TYR:HD2	1:H:864:MET:CE	2.25	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:N:747:PHE:HE1	1:N:825:CYS:HG	1.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:856:TYR:CD2	1:H:864:MET:HE2	2.47	0.49
1:H:952:ARG:HD2	3:H:4432:HOH:O	2.11	0.49
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: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:O:856:TYR:HD2	1:O:864:MET:CE	2.25	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:O:952:ARG:HD2	3:O:3524:HOH:O	2.11	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:A:856:TYR:HD2	1:A:864:MET:CE	2.25	0.49
1:B:188:VAL:C	1:B:189:LEU:HD23	2.33	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:G:741:THR:O	1:G:741:THR:HG22	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:571:VAL:HG13	1:J:607:VAL:HG23	1.93	0.49
1:K:85:VAL:HG12	1:K:86:VAL:N	2.27	0.49
1:K:322:LEU:HD23	1:K:322:LEU:C	2.33	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
1:P:856:TYR:HD2	1:P:864:MET:CE	2.25	0.49
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:322:LEU:HD23	1:D:322:LEU:C	2.33	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:G:127:PHE:CE2	1:G:184:LEU:HG	2.47	0.49
1:I:322:LEU:HD23	1:I:322:LEU:C	2.33	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: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:188:VAL:C	1:N:189:LEU:HD23	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:322:LEU:HD23	1:F:322:LEU:C	2.33	0.49
1:F:856:TYR:HD2	1:F:864:MET:CE	2.25	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
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:322:LEU:HD23	1:A:322:LEU:C	2.33	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:C:856:TYR:HD2	1:C:864:MET:CE	2.25	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:N:856:TYR:HD2	1:N:864:MET:CE	2.25	0.49
1:P:800:ARG:HB3	1:P:800:ARG:CZ	2.43	0.49
1:P:856:TYR:HD2	1:P:864:MET:HE2	1.77	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:F:747:PHE:HE1	1:F:825:CYS:HG	1.59	0.49
1:G:65:ALA:HB1	1:G:66:PRO:HD2	1.95	0.49
1:G:188:VAL:C	1:G:189:LEU:HD23	2.33	0.49
1:G:433:LEU:O	1:G:437:SER:HB3	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:322:LEU:HD23	1:C:322:LEU:C	2.33	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: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:I:856:TYR:HD2	1:I:864:MET:CE	2.26	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
1:L:188:VAL:C	1:L:189:LEU:HD23	2.33	0.49
1:L:322:LEU:HD23	1:L:322:LEU:C	2.33	0.49
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:O:188:VAL:C	1:O:189:LEU:HD23	2.33	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:I:188:VAL:C	1:I:189:LEU:HD23	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:L:85:VAL:HG12	1:L:86:VAL:N	2.27	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:P:188:VAL:C	1:P:189:LEU:HD23	2.33	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
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:J:322:LEU:HD23	1:J:322:LEU:C	2.33	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:HG22	1:A:741:THR:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:429:ASP:OD1	1:J:430:PRO:HD2	2.13	0.48
1:M:856:TYR:HD2	1:M:864:MET:CE	2.25	0.48
1:N:322:LEU:HD23	1:N:322:LEU:C	2.33	0.48
1:O:322:LEU:HD23	1:O:322:LEU:C	2.33	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: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:322:LEU:HD23	1:G:322:LEU:C	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:188:VAL:C	1:J:189:LEU:HD23	2.33	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:N:85:VAL:HG12	1:N: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: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:322:LEU:HD23	1:E:322:LEU:C	2.33	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:188:VAL:C	1:K:189:LEU:HD23	2.33	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
1:M:73:TRP:CH2	1:M:185:ALA:HB1	2.49	0.48
1:M:322:LEU:HD23	1:M:322:LEU:C	2.33	0.48
1:N:73:TRP:CH2	1:N:185:ALA:HB1	2.49	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:B:322:LEU:HD23	1:B:322:LEU:C	2.33	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:429:ASP:OD1	1:E:430:PRO:HD2	2.13	0.48
1:F:188:VAL:C	1:F:189:LEU:HD23	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:856:TYR:HD2	1:B:864:MET:CE	2.25	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: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:G:856:TYR:HD2	1:G:864:MET:CE	2.26	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:L:856:TYR:HD2	1:L:864:MET:CE	2.26	0.48
1:M:9:VAL:O	1:M:12:GLN:HB3	2.13	0.48
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:322:LEU:HD23	1:P:322:LEU:C	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:188:VAL:C	1:A:189:LEU:HD23	2.33	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:H:188:VAL:C	1:H:189:LEU:HD23	2.33	0.48
1:H:322:LEU:HD23	1:H:322:LEU:C	2.33	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
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:C:188:VAL:C	1:C:189:LEU:HD23	2.33	0.47
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:K:910:LEU:C	1:K:910:LEU:HD12	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:261:TRP:CH2	1:M:266:GLN:HB2	2.49	0.47
1:M:745:MET:HA	1:M:745:MET:CE	2.39	0.47
1:N:217:LYS:HG2	1:N:218:PRO:HD2	1.96	0.47
1:P:595:THR:HG23	1:P:596:PRO:CA	2.35	0.47
1:A:3:ILE:HG13	1:A:4:THR:N	2.25	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:D:910:LEU:C	1:D:910:LEU:HD12	2.35	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:K:856:TYR:HD2	1:K:864:MET:CE	2.25	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: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:L:65:ALA:HB1	1:L:66:PRO:HD2	1.95	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:C:645:ARG:HH22	1:C:650:GLU:CD	2.18	0.47
1:D:9:VAL:O	1:D:12:GLN:HB3	2.13	0.47
1:E:910:LEU:C	1:E:910:LEU:HD12	2.35	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:F:645:ARG:HH22	1:F:650:GLU:CD	2.18	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:L:910:LEU:C	1:L:910:LEU:HD12	2.35	0.47
1:M:188:VAL:C	1:M:189:LEU:HD23	2.33	0.47
1:M:257:THR:OG1	1:M:316:HIS:HE1	1.98	0.47
1:C:429:ASP:OD1	1:C:430:PRO:HD2	2.13	0.47
1:E:188:VAL:C	1:E:189:LEU:HD23	2.33	0.47
1:E:645:ARG:HH22	1:E:650:GLU:CD	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3:ILE:HG13	1:J:4:THR:N	2.25	0.47
1:J:856:TYR:HD2	1:J:864:MET:CE	2.26	0.47
1:O:261:TRP:CH2	1:O:266:GLN:HB2	2.49	0.47
1:O:645:ARG:HH22	1:O:650:GLU:CD	2.18	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:P:910:LEU:C	1:P:910:LEU:HD12	2.35	0.47
1:A:419:GLY:C	1:D:282:ARG:HH11	2.16	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:H:73:TRP:CH2	1:H:185:ALA:HB1	2.49	0.47
1:H:910:LEU:C	1:H:910:LEU:HD12	2.35	0.47
1:I:287:ASP:OD2	1:L:425:ARG:NH2	2.47	0.47
1:O:910:LEU:C	1:O:910:LEU:HD12	2.35	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:A:910:LEU:C	1:A:910:LEU:HD12	2.35	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:B:645:ARG:HH22	1:B:650:GLU:CD	2.18	0.47
1:B:910:LEU:C	1:B:910:LEU:HD12	2.35	0.47
1:C:910:LEU:C	1:C:910:LEU:HD12	2.35	0.47
1:D:188:VAL:C	1:D:189:LEU:HD23	2.33	0.47
1:E:18:ASN:ND2	1:E:21:VAL:HG23	2.29	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:910:LEU:C	1:G:910:LEU:HD12	2.35	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:J:645:ARG:HH22	1:J:650:GLU:CD	2.18	0.47
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:M:35:SER:O	1:M:50:GLN:HG3	2.14	0.47
1:M:910:LEU:C	1:M:910:LEU:HD12	2.35	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:P:645:ARG:HH22	1:P:650:GLU:CD	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:217:LYS:HG2	1:G:218:PRO:HD2	1.96	0.47
1:H:645:ARG:HH22	1:H:650:GLU:CD	2.18	0.47
1:J:134:LEU:HD23	1:J:134:LEU:HA	1.68	0.47
1:K:645:ARG:HH22	1:K:650:GLU:CD	2.18	0.47
1:L:645:ARG:HH22	1:L:650:GLU:CD	2.18	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:202:MET:HB3	1:B:202:MET:HE3	1.82	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:856:TYR:CD2	1:C:864:MET:HE2	2.48	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:F:134:LEU:HA	1:F:134:LEU:HD23	1.68	0.47
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:I:7:LEU:HD12	1:I:74:LEU:HD11	1.97	0.47
1:I:287:ASP:CG	1:L:425:ARG:HH22	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:18:ASN:ND2	1:N:21:VAL:HG23	2.29	0.47
1:N:910:LEU:HD12	1:N:910:LEU:C	2.35	0.47
1:O:18:ASN:ND2	1:O:21:VAL:HG23	2.29	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:645:ARG:HH22	1:G:650:GLU:CD	2.18	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:910:LEU:C	1:J:910:LEU:HD12	2.35	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:N:645:ARG:HH22	1:N:650:GLU:CD	2.18	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:D:36:TRP:CE2	1:D:42:ALA:HA	2.50	0.46
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:I:91:GLN:HG3	1:I:96:ASP:OD1	2.16	0.46
1:I:645:ARG:HH22	1:I:650:GLU:CD	2.18	0.46
1:I:910:LEU:C	1:I:910:LEU:HD12	2.35	0.46
1:M:856:TYR:CD2	1:M:864:MET:HE2	2.50	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:645:ARG:HH22	1:D:650:GLU:CD	2.18	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: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: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:645:ARG:HH22	1:A:650:GLU:CD	2.18	0.46
1:A:658:LEU:N	1:A:661:LYS:O	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: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: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
1:I:595:THR:CG2	1:I:596:PRO:HA	2.37	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: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:F:910:LEU:HD12	1:F:910:LEU:C	2.35	0.46
1:G:612:THR:HB	1:G:613:PRO:HD2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:422:PRO:HG3	1:D:284:GLY:C	2.35	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:B:856:TYR:CD2	1:B:864:MET:HE2	2.48	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: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:427:THR:HA	1:L:436:MET:HE2	1.93	0.46
1:L:657:ALA:HA	1:L:661:LYS:O	2.16	0.46
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: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: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: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:J:287:ASP:CG	1:K:425:ARG:HH22	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:425:ARG:HH22	1:K:287:ASP:CG	2.19	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: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: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
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: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:E:767:GLN:CG	1:E:768:MET:N	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:701:VAL:HG12	1:P:702:GLN:N	2.31	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:D:701:VAL:HG12	1:D:702:GLN:N	2.31	0.46
1:E:85:VAL:CG1	1:E:86:VAL:N	2.79	0.46
1:E:655:MET:HE3	1:E:655:MET:HB2	1.73	0.46
1:E:701:VAL:HG12	1:E:702:GLN:N	2.31	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: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
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: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:M:701:VAL:HG12	1:M:702:GLN:N	2.31	0.46
1:N:3:ILE:HG13	1:N:4:THR:N	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:767:GLN:CG	1:M:768:MET:N	2.79	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:3:ILE:HG13	1:P:4:THR:N	2.25	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:202:MET:HB3	1:A:202:MET:HE3	1.84	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
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: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: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:91:GLN:HG3	1:K:96:ASP:OD1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:M:645:ARG:HH22	1:M:650:GLU:CD	2.18	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:C:767:GLN:CG	1:C:768:MET:N	2.79	0.45
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:433:LEU:N	1:D:434:PRO:CD	2.80	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:I:425:ARG:NH2	1:L:287:ASP:OD2	2.50	0.45
1:J:85:VAL:CG1	1:J:86:VAL:N	2.79	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:L:991:MET:HE2	1:L:1003:VAL:HG21	1.98	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:O:43:ARG:HH12	1:O:44:THR:CG2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:85:VAL:CG1	1:D:86:VAL:N	2.79	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: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:J:576:ILE:CG2	1:J:577:LYS:N	2.79	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:856:TYR:CD2	1:J:864:MET:CE	3.00	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:102:ASN:C	1:B:102:ASN:HD22	2.21	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:102:ASN:HD22	1:C:102:ASN:C	2.21	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
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:H:856:TYR:CD2	1:H:864:MET:CE	3.00	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:B:856:TYR:CD2	1:B:864:MET:CE	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:856:TYR:CD2	1:I:864:MET:CE	3.00	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:L:856:TYR:CD2	1:L:864:MET:HE2	2.51	0.45
1:M:13:ARG:O	1:M:14:ARG:HB2	2.17	0.45
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:M:856:TYR:CD2	1:M:864:MET:CE	3.00	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:P:856:TYR:CD2	1:P:864:MET:CE	3.00	0.45
1:B:43:ARG:HH12	1:B:44:THR:CG2	2.30	0.44
1:B:991:MET:HE2	1:B:1003:VAL:HG21	1.99	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:D:856:TYR:HD2	1:D:864:MET:CE	2.25	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:102:ASN:HD22	1:F:102:ASN:C	2.21	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: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:I:991:MET:HE2	1:I:1003:VAL:HG21	1.99	0.44
1:J:63:PHE:CB	1:J:64:PRO:HD2	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:13:ARG:O	1:K:14:ARG:HB2	2.17	0.44
1:K:85:VAL:CG1	1:K:86:VAL:N	2.79	0.44
1:K:102:ASN:HD22	1:K:102:ASN:C	2.21	0.44
1:K:991:MET:HE2	1:K:1003:VAL:HG21	2.00	0.44
1:L:43:ARG:HH12	1:L:44:THR:CG2	2.30	0.44
1:N:653[B]:HIS:CD2	1:N:667:GLU:HG2	2.51	0.44
1:O:433:LEU:N	1:O:434:PRO:CD	2.80	0.44
1:P:102:ASN:HD22	1:P:102:ASN:C	2.21	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: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: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:E:856:TYR:CD2	1:E:864:MET:CE	3.00	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
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: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:N:856:TYR:CD2	1:N:864:MET:HE2	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:102:ASN:C	1:D:102:ASN:HD22	2.21	0.44
1:E:102:ASN:C	1:E:102:ASN:HD22	2.21	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: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:G:856:TYR:CD2	1:G:864:MET:CE	3.00	0.44
1:G:991:MET:HE2	1:G:1003:VAL:HG21	1.99	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: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:856:TYR:CD2	1:K:864:MET:CE	3.00	0.44
1:M:102:ASN:C	1:M:102:ASN:HD22	2.21	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
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:O:991:MET:HE2	1:O:1003:VAL:HG21	1.99	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:E:567:VAL:HG12	1:E:568:TRP:N	2.32	0.44
1:E:778:THR:HG23	1:E:779:PRO:HD2	1.98	0.44
1:E:856:TYR:HD2	1:E:864:MET:CE	2.25	0.44
1:F:433:LEU:N	1:F:434:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:202:MET:HB3	1:G:202:MET:HE3	1.84	0.44
1:H:3:ILE:O	1:H:3:ILE:HD12	2.17	0.44
1:H:102:ASN:HD22	1:H:102:ASN:C	2.21	0.44
1:H:778:THR:HG23	1:H:779:PRO:HD2	1.98	0.44
1:I:102:ASN:C	1:I:102:ASN:HD22	2.21	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: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: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:O:202:MET:HB3	1:O:202:MET:HE3	1.84	0.44
1:P:91:GLN:HG3	1:P:96:ASP:OD1	2.16	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: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:102:ASN:C	1:G:102:ASN:HD22	2.21	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:L:856:TYR:CD2	1:L:864:MET:CE	3.00	0.44
1:M:658:LEU:N	1:M:661:LYS:O	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:F:856:TYR:CD2	1:F:864:MET:CE	3.00	0.44
1:H:7:LEU:O	1:H:11:LEU:HG	2.18	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: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
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:655:MET:HE3	1:A:655:MET:HB2	1.78	0.44
1:A:856:TYR:CD2	1:A:864:MET:CE	3.00	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: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:D:856:TYR:CD2	1:D:864:MET:CE	3.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:991:MET:HE2	1:J:1003:VAL:HG21	1.99	0.44
1:K:847:LYS:HG3	1:K:848:THR:N	2.32	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
1:P:857:ARG:HG2	1:P:857:ARG:HH11	1.83	0.44
1:B:3:ILE:HG13	1:B:4:THR:N	2.25	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: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: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: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: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:L:78:LEU:HB3	1:L:79:PRO:CD	2.43	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: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: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:C:856:TYR:CD2	1:C:864:MET:CE	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:599:ARG:HB2	1:E:600:GLN:OE1	2.18	0.44
1:F:856:TYR:CD2	1:F:864:MET:HE2	2.53	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
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: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:N	1:L:211:ASP:OD1	2.50	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:A:778:THR:HG23	1:A:779:PRO:HD2	1.98	0.43
1:D:3:ILE:HG13	1:D:4:THR:N	2.24	0.43
1:D:173:LEU:HD23	1:D:173:LEU:HA	1.85	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:I:111:PRO:HA	1:I:112:PRO:HA	1.65	0.43
1:I:322:LEU:CD2	1:I:324:GLU:N	2.80	0.43
1:J:7:LEU:O	1:J:11:LEU:HG	2.18	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:102:ASN:C	1:L:102:ASN:HD22	2.21	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: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:102:ASN:C	1:O:102:ASN:HD22	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:576:ILE:CG2	1:L:577:LYS:N	2.79	0.43
1:M:3:ILE:HG13	1:M:4:THR:N	2.25	0.43
1:M:991:MET:HE2	1:M:1003:VAL:HG21	1.99	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:102:ASN:C	1:A:102:ASN:HD22	2.21	0.43
1:A:857:ARG:HG2	1:A:857:ARG:HH11	1.83	0.43
1:A:991:MET:HE2	1:A:1003:VAL:HG21	2.00	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:G:127:PHE:CD2	1:G:127:PHE:N	2.87	0.43
1:H:947:GLY:HA3	1:H:948:PRO:HD2	1.82	0.43
1:J:127:PHE:CD2	1:J:127:PHE:N	2.87	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: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
1:M:857:ARG:HG2	1:M:857:ARG:HH11	1.83	0.43
1:N:102:ASN:HD22	1:N:102:ASN:C	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:LEU:HA	1:B:731:PRO:HD3	1.80	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:3:ILE:HG13	1:G:4:THR:N	2.25	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:H:655:MET:HE3	1:H:655:MET:HB2	1.73	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:425:ARG:HH22	1:L:287:ASP:CG	2.22	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: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:254:LEU:HD23	1:A:254:LEU:HA	1.71	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: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: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: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:567:VAL:HG12	1:A:568:TRP:N	2.32	0.43
1:D:778:THR:HB	1:D:887:GLN:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:567:VAL:HG12	1:H:568:TRP:N	2.32	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:N:7:LEU:O	1:N:11:LEU:HG	2.18	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:A:482:ARG:HH11	1:A:482:ARG:HD2	1.63	0.43
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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:F:991:MET:HE2	1:F:1003:VAL:HG21	2.00	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: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:N:134:LEU:HA	1:N:134:LEU:HD23	1.68	0.43
1:N:778:THR:HB	1:N:887:GLN:H	1.84	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:778:THR:HB	1:A:887:GLN:H	1.84	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: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:102:ASN:C	1:J:102:ASN:HD22	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:217:LYS:NZ	1:J:326:GLU:OE2	2.52	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
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:N:991:MET:HE2	1:N:1003:VAL:HG21	2.00	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: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: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: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: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: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
1:D:772:ASP:OD1	1:D:772:ASP:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:576:ILE:CG2	1:M:577:LYS:N	2.79	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:599:ARG:HD2	1:D:600:GLN:OE1	2.20	0.42
1:E:576:ILE:CG2	1:E:577:LYS:N	2.79	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: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:427:THR:HA	1:M:436:MET:HE2	1.93	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:O:576:ILE:CG2	1:O:577:LYS:N	2.79	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:202:MET:HB3	1:E:202:MET:HE3	1.90	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:667:GLU:C	1:F:668:VAL:HG23	2.40	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:667:GLU:C	1:M:668:VAL:HG23	2.40	0.42
1:N:667:GLU:C	1:N:668:VAL:HG23	2.40	0.42
1:O:667:GLU:C	1:O:668:VAL:HG23	2.40	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:OD2	1:H:425:ARG:NH2	2.53	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:211:ASP:OD1	1:F:211:ASP:N	2.50	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: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: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: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: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:513:PRO:O	1:G:514:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:667:GLU:C	1:J:668:VAL:HG23	2.40	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:B:234:ASP:O	1:B:235:PHE:HB2	2.20	0.42
1:B:655:MET:O	1:B:655:MET:HG3	2.20	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:D:667:GLU:C	1:D:668:VAL:HG23	2.40	0.42
1:E:599:ARG:HD2	1:E:600:GLN:OE1	2.20	0.42
1:E:991:MET:HE2	1:E:1003:VAL:HG21	2.01	0.42
1:H:482:ARG:HH11	1:H:482:ARG:HD2	1.63	0.42
1:H:667:GLU:C	1:H:668:VAL:HG23	2.40	0.42
1:I:856:TYR:CD2	1:I:864:MET:HE2	2.53	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:513:PRO:O	1:L:514:ALA:HB3	2.20	0.42
1:L:599:ARG:HD2	1:L:600:GLN:OE1	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:667:GLU:C	1:C:668:VAL:HG23	2.40	0.42
1:E:173:LEU:HD23	1:E:173:LEU:HA	1.85	0.42
1:E:667:GLU:C	1:E:668:VAL:HG23	2.40	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: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:K:655:MET:O	1:K:655:MET:HG3	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:53:SER:C	1:O:54:LEU:HD23	2.41	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: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: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:I:655:MET:HE3	1:I:655:MET:HB2	1.81	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
1:K:726:LEU:HA	1:K:726:LEU:HD23	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:667:GLU:C	1:A:668:VAL:HG23	2.40	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:667:GLU:C	1:I:668:VAL:HG23	2.40	0.41
1:I:726:LEU:HA	1:I:726:LEU:HD23	1.76	0.41
1:L:176:PHE:N	1:L:176:PHE:CD1	2.88	0.41
1:M:234:ASP:O	1:M:235:PHE:HB2	2.20	0.41
1:M:655:MET:O	1:M:655:MET:HG3	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:N:655:MET:O	1:N:655:MET:HG3	2.20	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:P:53:SER:C	1:P:54:LEU:HD23	2.41	0.41
1:A:69:VAL:CG1	1:A:70:PRO:HD2	2.50	0.41
1:A:513:PRO:O	1:A:514:ALA:HB3	2.20	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:53:SER:C	1:D:54:LEU:HD23	2.41	0.41
1:D:395:HIS:HA	1:D:396:PRO:HD3	1.69	0.41
1:F:947:GLY:HA3	1:F:948:PRO:HD2	1.82	0.41
1:J:4:THR:HA	1:J:9:VAL:HG11	2.02	0.41
1:J:694:LEU:HD12	1:J:694:LEU:HA	1.84	0.41
1:M:287:ASP:OD1	1:M:287:ASP:N	2.41	0.41
1:N:778:THR:HG22	1:N:779:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:4:THR:HA	1:O:9:VAL:HG11	2.01	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:53:SER:C	1:F:54:LEU:HD23	2.41	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:1017:GLN:HB3	3:I:4405:HOH:O	2.19	0.41
1:J:513:PRO:O	1:J:514:ALA:HB3	2.20	0.41
1:J:662:PRO:O	1:J:663:LEU:HD23	2.20	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:P:285:TYR:CB	1:P:288:ARG:HG3	2.42	0.41
1:P:667:GLU:C	1:P:668:VAL:HG23	2.40	0.41
1:A:418:HIS:O	1:D:282:ARG:CD	2.67	0.41
1:B:667:GLU:C	1:B:668:VAL:HG23	2.40	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:E:53:SER:C	1:E:54:LEU:HD23	2.41	0.41
1:E:130:ASP:OD1	1:E:131:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:702:GLN:HA	1:F:703:PRO:HD2	1.88	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:53:SER:C	1:I:54:LEU:HD23	2.41	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:K:667:GLU:C	1:K:668:VAL:HG23	2.40	0.41
1:L:4:THR:HA	1:L:9:VAL:HG11	2.01	0.41
1:L:53:SER:C	1:L:54:LEU:HD23	2.41	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:53:SER:C	1:N:54:LEU:HD23	2.41	0.41
1:N:668:VAL:HA	1:N:669:PRO:HD3	1.83	0.41
1:O:234:ASP:O	1:O:235:PHE:HB2	2.20	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:C:53:SER:C	1:C:54:LEU:HD23	2.41	0.41
1:C:991:MET:HE2	1:C:1003:VAL:HG21	2.01	0.41
1:D:258:VAL:HA	1:D:312:VAL:O	2.21	0.41
1:D:662:PRO:O	1:D:663:LEU:HD23	2.20	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:53:SER:C	1:G:54:LEU:HD23	2.41	0.41
1:G:661:LYS:HA	1:G:662:PRO:HD3	1.74	0.41
1:G:667:GLU:C	1:G:668:VAL:HG23	2.40	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:173:LEU:HD23	1:L:173:LEU:HA	1.86	0.41
1:M:53:SER:C	1:M:54:LEU:HD23	2.41	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: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:D:991:MET:HE2	1:D:1003:VAL:HG21	2.02	0.41
1:E:425:ARG:NH2	1:H:287:ASP:OD2	2.54	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:53:SER:C	1:H:54:LEU:HD23	2.41	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: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
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:654:TRP:CE2	1:O:666:GLY:HA3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:I:380:LYS:HE2	3:I:4074:HOH:O	2.19	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: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:P:991:MET:HE2	1:P:1003:VAL:HG21	2.01	0.41
1:A:53:SER:C	1:A:54:LEU:HD23	2.41	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:53:SER:C	1:B:54:LEU:HD23	2.41	0.41
1:B:272:ALA:HA	1:B:273:PRO:HD3	1.78	0.41
1:B:807:VAL:HG13	1:B:808:GLU:N	2.36	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: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:272:ALA:HA	1:G:273:PRO:HD3	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:991:MET:HE2	1:H:1003:VAL:HG21	2.02	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: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: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
1:O:36:TRP:CD2	1:O:42:ALA:HA	2.56	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: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: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:367:MET:HB3	1:A:372:MET:CE	2.50	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:69:VAL:CG1	1:C:70:PRO:HD2	2.51	0.41
1:C:654:TRP:CE2	1:C:666:GLY:HA3	2.56	0.41
1:C:655:MET:O	1:C:655:MET:HG3	2.20	0.41
1:D:69:VAL:CG1	1:D:70:PRO:HD2	2.51	0.41
1:D:202:MET:HB3	1:D:202:MET:HE3	1.87	0.41
1:D:748:CME:HE2	1:D:748:CME:HB3	1.15	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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:807:VAL:CG1	1:L:808:GLU:N	2.84	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:53:SER:C	1:K:54:LEU:HD23	2.41	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: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:253:TYR:O	1:F:318:ALA:N	2.54	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:367:MET:HB3	1:O:372:MET:CE	2.50	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: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: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: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: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:745:MET:CE	1:I:745:MET:CA	3.00	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:667:GLU:C	1:L:668:VAL:HG23	2.40	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:499:ILE:HG22	1:H:501:PRO:HD3	2.03	0.40
1:I:36:TRP:CD2	1:I:42:ALA:HA	2.56	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: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:D:745:MET:CE	1:D:745:MET:CA	3.00	0.40
1:E:395:HIS:HA	1:E:396:PRO:HD3	1.69	0.40
1:G:141:ILE:HG12	1:G:142:ILE:N	2.37	0.40
1:G:316:HIS:HA	1:G:323:ILE:HD13	2.01	0.40
1:G:928:PRO:HB2	1:G:973:ARG:HH11	1.86	0.40
1:H:63:PHE:N	1:H:63:PHE:CD1	2.90	0.40
1:H:141:ILE:HG12	1:H:142:ILE:N	2.37	0.40
1:I:63:PHE:CD1	1:I:63:PHE:N	2.90	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: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:K:745:MET:CE	1:K:745:MET:CA	3.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:141:ILE:HG12	1:P:142:ILE:N	2.37	0.40
1:P:807:VAL:HG13	1:P:808:GLU:N	2.36	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	41	61
1	B	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	41	61
1	C	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	41	61
1	D	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	41	61
1	E	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	41	61
1	F	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	41	61
1	G	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	41	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	41	61
1	I	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	41	61
1	J	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	41	61
1	K	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	41	61
1	L	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	41	61
1	M	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	41	61
1	N	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	41	61
1	O	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	41	61
1	P	1021/1023 (100%)	976 (96%)	42 (4%)	3 (0%)	41	61
All	All	16336/16368 (100%)	15616 (96%)	672 (4%)	48 (0%)	41	61

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
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

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Mol	Chain	Res	Type
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 (i)

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%)	776 (89%)	99 (11%)	6 11
1	B	875/872 (100%)	776 (89%)	99 (11%)	6 11
1	C	875/872 (100%)	776 (89%)	99 (11%)	6 11
1	D	875/872 (100%)	776 (89%)	99 (11%)	6 11
1	E	875/872 (100%)	776 (89%)	99 (11%)	6 11
1	F	875/872 (100%)	776 (89%)	99 (11%)	6 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	875/872 (100%)	776 (89%)	99 (11%)	6	11
1	H	875/872 (100%)	776 (89%)	99 (11%)	6	11
1	I	875/872 (100%)	776 (89%)	99 (11%)	6	11
1	J	875/872 (100%)	776 (89%)	99 (11%)	6	11
1	K	875/872 (100%)	776 (89%)	99 (11%)	6	11
1	L	875/872 (100%)	777 (89%)	98 (11%)	6	11
1	M	875/872 (100%)	776 (89%)	99 (11%)	6	11
1	N	875/872 (100%)	777 (89%)	98 (11%)	6	11
1	O	875/872 (100%)	776 (89%)	99 (11%)	6	11
1	P	875/872 (100%)	776 (89%)	99 (11%)	6	11
All	All	14000/13952 (100%)	12418 (89%)	1582 (11%)	6	11

All (1582) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	14	ARG
1	A	37	ARG
1	A	39	SER
1	A	46	ARG
1	A	48	SER
1	A	49	GLN
1	A	50	GLN
1	A	52	ARG
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	102	ASN
1	A	116	THR
1	A	125	LEU
1	A	128	ASN
1	A	132	SER
1	A	136	GLU
1	A	165	SER
1	A	166	ARG

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Mol	Chain	Res	Type
1	A	171	PHE
1	A	189	LEU
1	A	202	MET
1	A	210	ARG
1	A	211	ASP
1	A	217	LYS
1	A	219	THR
1	A	246	MET
1	A	247	CYS
1	A	249	GLU
1	A	250	LEU
1	A	259	SER
1	A	262	GLN
1	A	264	GLU
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
1	A	370	GLN
1	A	377	LEU
1	A	394	ASN
1	A	425	ARG
1	A	437	SER
1	A	448	ARG
1	A	473	ARG
1	A	519	SER
1	A	521	LYS
1	A	532	PRO
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	632	SER
1	A	645	ARG
1	A	651	LEU

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Mol	Chain	Res	Type
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	751	LEU
1	A	753	ASN
1	A	755	ARG
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	824	GLN
1	A	829	THR
1	A	832	ASP
1	A	881	ARG
1	A	893	GLU
1	A	903[A]	GLN
1	A	903[B]	GLN
1	A	917	ARG
1	A	938	ARG
1	A	952	ARG
1	A	956	GLN
1	A	1006	GLU
1	A	1017	GLN
1	B	3	ILE
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

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Mol	Chain	Res	Type
1	B	52	ARG
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	102	ASN
1	B	116	THR
1	B	125	LEU
1	B	128	ASN
1	B	132	SER
1	B	136	GLU
1	B	165	SER
1	B	166	ARG
1	B	171	PHE
1	B	189	LEU
1	B	202	MET
1	B	210	ARG
1	B	211	ASP
1	B	217	LYS
1	B	219	THR
1	B	246	MET
1	B	247	CYS
1	B	249	GLU
1	B	250	LEU
1	B	259	SER
1	B	262	GLN
1	B	264	GLU
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	394	ASN
1	B	425	ARG
1	B	437	SER

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Mol	Chain	Res	Type
1	B	448	ARG
1	B	473	ARG
1	B	519	SER
1	B	521	LYS
1	B	532	PRO
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	632	SER
1	B	645	ARG
1	B	651	LEU
1	B	655	MET
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	751	LEU
1	B	753	ASN
1	B	755	ARG
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	824	GLN
1	B	829	THR
1	B	832	ASP
1	B	881	ARG
1	B	893	GLU
1	B	903[A]	GLN

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Mol	Chain	Res	Type
1	B	903[B]	GLN
1	B	917	ARG
1	B	938	ARG
1	B	952	ARG
1	B	956	GLN
1	B	1006	GLU
1	B	1017	GLN
1	C	3	ILE
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	59	ARG
1	C	71	GLU
1	C	72	SER
1	C	80	GLU
1	C	84	VAL
1	C	90	TRP
1	C	102	ASN
1	C	116	THR
1	C	125	LEU
1	C	128	ASN
1	C	132	SER
1	C	136	GLU
1	C	165	SER
1	C	166	ARG
1	C	171	PHE
1	C	189	LEU
1	C	202	MET
1	C	210	ARG
1	C	211	ASP
1	C	217	LYS
1	C	219	THR
1	C	246	MET
1	C	247	CYS
1	C	249	GLU
1	C	250	LEU
1	C	259	SER

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Mol	Chain	Res	Type
1	C	262	GLN
1	C	264	GLU
1	C	279	ILE
1	C	299	LYS
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	394	ASN
1	C	425	ARG
1	C	437	SER
1	C	448	ARG
1	C	473	ARG
1	C	519	SER
1	C	521	LYS
1	C	532	PRO
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	632	SER
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

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Mol	Chain	Res	Type
1	C	751	LEU
1	C	753	ASN
1	C	755	ARG
1	C	768	MET
1	C	778	THR
1	C	781	ARG
1	C	797	GLU
1	C	799	THR
1	C	800	ARG
1	C	824	GLN
1	C	829	THR
1	C	832	ASP
1	C	881	ARG
1	C	893	GLU
1	C	903[A]	GLN
1	C	903[B]	GLN
1	C	917	ARG
1	C	938	ARG
1	C	952	ARG
1	C	956	GLN
1	C	1006	GLU
1	C	1017	GLN
1	D	3	ILE
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	59	ARG
1	D	71	GLU
1	D	72	SER
1	D	80	GLU
1	D	84	VAL
1	D	90	TRP
1	D	102	ASN
1	D	116	THR
1	D	125	LEU
1	D	128	ASN
1	D	132	SER

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Mol	Chain	Res	Type
1	D	136	GLU
1	D	165	SER
1	D	166	ARG
1	D	171	PHE
1	D	189	LEU
1	D	202	MET
1	D	210	ARG
1	D	211	ASP
1	D	217	LYS
1	D	219	THR
1	D	246	MET
1	D	247	CYS
1	D	249	GLU
1	D	250	LEU
1	D	259	SER
1	D	262	GLN
1	D	264	GLU
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	394	ASN
1	D	425	ARG
1	D	437	SER
1	D	448	ARG
1	D	473	ARG
1	D	519	SER
1	D	521	LYS
1	D	532	PRO
1	D	546	LEU
1	D	554	GLN
1	D	571	VAL
1	D	580	GLU
1	D	599	ARG
1	D	600	GLN
1	D	630	ARG

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Mol	Chain	Res	Type
1	D	632	SER
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	751	LEU
1	D	753	ASN
1	D	755	ARG
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	824	GLN
1	D	829	THR
1	D	832	ASP
1	D	881	ARG
1	D	893	GLU
1	D	903[A]	GLN
1	D	903[B]	GLN
1	D	917	ARG
1	D	938	ARG
1	D	952	ARG
1	D	956	GLN
1	D	1006	GLU
1	D	1017	GLN
1	E	3	ILE
1	E	14	ARG
1	E	37	ARG
1	E	39	SER
1	E	46	ARG

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Mol	Chain	Res	Type
1	E	48	SER
1	E	49	GLN
1	E	50	GLN
1	E	52	ARG
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	102	ASN
1	E	116	THR
1	E	125	LEU
1	E	128	ASN
1	E	132	SER
1	E	136	GLU
1	E	165	SER
1	E	166	ARG
1	E	171	PHE
1	E	189	LEU
1	E	202	MET
1	E	210	ARG
1	E	211	ASP
1	E	217	LYS
1	E	219	THR
1	E	246	MET
1	E	247	CYS
1	E	249	GLU
1	E	250	LEU
1	E	259	SER
1	E	262	GLN
1	E	264	GLU
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

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Mol	Chain	Res	Type
1	E	394	ASN
1	E	425	ARG
1	E	437	SER
1	E	448	ARG
1	E	473	ARG
1	E	519	SER
1	E	521	LYS
1	E	532	PRO
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	632	SER
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	751	LEU
1	E	753	ASN
1	E	755	ARG
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	824	GLN
1	E	829	THR
1	E	832	ASP

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Mol	Chain	Res	Type
1	E	881	ARG
1	E	893	GLU
1	E	903[A]	GLN
1	E	903[B]	GLN
1	E	917	ARG
1	E	938	ARG
1	E	952	ARG
1	E	956	GLN
1	E	1006	GLU
1	E	1017	GLN
1	F	3	ILE
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	59	ARG
1	F	71	GLU
1	F	72	SER
1	F	80	GLU
1	F	84	VAL
1	F	90	TRP
1	F	102	ASN
1	F	116	THR
1	F	125	LEU
1	F	128	ASN
1	F	132	SER
1	F	136	GLU
1	F	165	SER
1	F	166	ARG
1	F	171	PHE
1	F	189	LEU
1	F	202	MET
1	F	210	ARG
1	F	211	ASP
1	F	217	LYS
1	F	219	THR
1	F	246	MET
1	F	247	CYS

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Mol	Chain	Res	Type
1	F	249	GLU
1	F	250	LEU
1	F	259	SER
1	F	262	GLN
1	F	264	GLU
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	394	ASN
1	F	425	ARG
1	F	437	SER
1	F	448	ARG
1	F	473	ARG
1	F	519	SER
1	F	521	LYS
1	F	532	PRO
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	632	SER
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

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Mol	Chain	Res	Type
1	F	734	SER
1	F	741	THR
1	F	743	SER
1	F	751	LEU
1	F	753	ASN
1	F	755	ARG
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	824	GLN
1	F	829	THR
1	F	832	ASP
1	F	881	ARG
1	F	893	GLU
1	F	903[A]	GLN
1	F	903[B]	GLN
1	F	917	ARG
1	F	938	ARG
1	F	952	ARG
1	F	956	GLN
1	F	1006	GLU
1	F	1017	GLN
1	G	3	ILE
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	59	ARG
1	G	71	GLU
1	G	72	SER
1	G	80	GLU
1	G	84	VAL
1	G	90	TRP
1	G	102	ASN
1	G	116	THR

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Mol	Chain	Res	Type
1	G	125	LEU
1	G	128	ASN
1	G	132	SER
1	G	136	GLU
1	G	165	SER
1	G	166	ARG
1	G	171	PHE
1	G	189	LEU
1	G	202	MET
1	G	210	ARG
1	G	211	ASP
1	G	217	LYS
1	G	219	THR
1	G	246	MET
1	G	247	CYS
1	G	249	GLU
1	G	250	LEU
1	G	259	SER
1	G	262	GLN
1	G	264	GLU
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	394	ASN
1	G	425	ARG
1	G	437	SER
1	G	448	ARG
1	G	473	ARG
1	G	519	SER
1	G	521	LYS
1	G	532	PRO
1	G	546	LEU
1	G	554	GLN
1	G	571	VAL
1	G	580	GLU

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Mol	Chain	Res	Type
1	G	599	ARG
1	G	600	GLN
1	G	630	ARG
1	G	632	SER
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
1	G	719	GLN
1	G	730	LEU
1	G	734	SER
1	G	741	THR
1	G	743	SER
1	G	751	LEU
1	G	753	ASN
1	G	755	ARG
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	824	GLN
1	G	829	THR
1	G	832	ASP
1	G	881	ARG
1	G	893	GLU
1	G	903[A]	GLN
1	G	903[B]	GLN
1	G	917	ARG
1	G	938	ARG
1	G	952	ARG
1	G	956	GLN
1	G	1006	GLU
1	G	1017	GLN
1	H	3	ILE
1	H	14	ARG

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Mol	Chain	Res	Type
1	H	37	ARG
1	H	39	SER
1	H	46	ARG
1	H	48	SER
1	H	49	GLN
1	H	50	GLN
1	H	52	ARG
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	102	ASN
1	H	116	THR
1	H	125	LEU
1	H	128	ASN
1	H	132	SER
1	H	136	GLU
1	H	165	SER
1	H	166	ARG
1	H	171	PHE
1	H	189	LEU
1	H	202	MET
1	H	210	ARG
1	H	211	ASP
1	H	217	LYS
1	H	219	THR
1	H	246	MET
1	H	247	CYS
1	H	249	GLU
1	H	250	LEU
1	H	259	SER
1	H	262	GLN
1	H	264	GLU
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

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Mol	Chain	Res	Type
1	H	347	LYS
1	H	370	GLN
1	H	377	LEU
1	H	394	ASN
1	H	425	ARG
1	H	437	SER
1	H	448	ARG
1	H	473	ARG
1	H	519	SER
1	H	521	LYS
1	H	532	PRO
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	632	SER
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	751	LEU
1	H	753	ASN
1	H	755	ARG
1	H	768	MET
1	H	778	THR
1	H	781	ARG
1	H	797	GLU
1	H	799	THR
1	H	800	ARG

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Mol	Chain	Res	Type
1	H	824	GLN
1	H	829	THR
1	H	832	ASP
1	H	881	ARG
1	H	893	GLU
1	H	903[A]	GLN
1	H	903[B]	GLN
1	H	917	ARG
1	H	938	ARG
1	H	952	ARG
1	H	956	GLN
1	H	1006	GLU
1	H	1017	GLN
1	I	3	ILE
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	59	ARG
1	I	71	GLU
1	I	72	SER
1	I	80	GLU
1	I	84	VAL
1	I	90	TRP
1	I	102	ASN
1	I	116	THR
1	I	125	LEU
1	I	128	ASN
1	I	132	SER
1	I	136	GLU
1	I	165	SER
1	I	166	ARG
1	I	171	PHE
1	I	189	LEU
1	I	202	MET
1	I	210	ARG
1	I	211	ASP
1	I	217	LYS

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Mol	Chain	Res	Type
1	I	219	THR
1	I	246	MET
1	I	247	CYS
1	I	249	GLU
1	I	250	LEU
1	I	259	SER
1	I	262	GLN
1	I	264	GLU
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	394	ASN
1	I	425	ARG
1	I	437	SER
1	I	448	ARG
1	I	473	ARG
1	I	519	SER
1	I	521	LYS
1	I	532	PRO
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	632	SER
1	I	645	ARG
1	I	651	LEU
1	I	655	MET
1	I	665	SER
1	I	672	VAL
1	I	684	GLU
1	I	687	GLN
1	I	690	SER

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Mol	Chain	Res	Type
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	751	LEU
1	I	753	ASN
1	I	755	ARG
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	824	GLN
1	I	829	THR
1	I	832	ASP
1	I	881	ARG
1	I	893	GLU
1	I	903[A]	GLN
1	I	903[B]	GLN
1	I	917	ARG
1	I	938	ARG
1	I	952	ARG
1	I	956	GLN
1	I	1006	GLU
1	I	1017	GLN
1	J	3	ILE
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	59	ARG
1	J	71	GLU
1	J	72	SER
1	J	80	GLU
1	J	84	VAL

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Mol	Chain	Res	Type
1	J	90	TRP
1	J	102	ASN
1	J	116	THR
1	J	125	LEU
1	J	128	ASN
1	J	132	SER
1	J	136	GLU
1	J	165	SER
1	J	166	ARG
1	J	171	PHE
1	J	189	LEU
1	J	202	MET
1	J	210	ARG
1	J	211	ASP
1	J	217	LYS
1	J	219	THR
1	J	246	MET
1	J	247	CYS
1	J	249	GLU
1	J	250	LEU
1	J	259	SER
1	J	262	GLN
1	J	264	GLU
1	J	279	ILE
1	J	299	LYS
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	394	ASN
1	J	425	ARG
1	J	437	SER
1	J	448	ARG
1	J	473	ARG
1	J	519	SER
1	J	521	LYS
1	J	532	PRO
1	J	546	LEU

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Mol	Chain	Res	Type
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	632	SER
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	751	LEU
1	J	753	ASN
1	J	755	ARG
1	J	768	MET
1	J	778	THR
1	J	781	ARG
1	J	797	GLU
1	J	799	THR
1	J	800	ARG
1	J	824	GLN
1	J	829	THR
1	J	832	ASP
1	J	881	ARG
1	J	893	GLU
1	J	903[A]	GLN
1	J	903[B]	GLN
1	J	917	ARG
1	J	938	ARG
1	J	952	ARG
1	J	956	GLN
1	J	1006	GLU

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Mol	Chain	Res	Type
1	J	1017	GLN
1	K	3	ILE
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	59	ARG
1	K	71	GLU
1	K	72	SER
1	K	80	GLU
1	K	84	VAL
1	K	90	TRP
1	K	102	ASN
1	K	116	THR
1	K	125	LEU
1	K	128	ASN
1	K	132	SER
1	K	136	GLU
1	K	165	SER
1	K	166	ARG
1	K	171	PHE
1	K	189	LEU
1	K	202	MET
1	K	210	ARG
1	K	211	ASP
1	K	217	LYS
1	K	219	THR
1	K	246	MET
1	K	247	CYS
1	K	249	GLU
1	K	250	LEU
1	K	259	SER
1	K	262	GLN
1	K	264	GLU
1	K	279	ILE
1	K	299	LYS
1	K	310	ARG
1	K	314	GLU

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Mol	Chain	Res	Type
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	394	ASN
1	K	425	ARG
1	K	437	SER
1	K	448	ARG
1	K	473	ARG
1	K	519	SER
1	K	521	LYS
1	K	532	PRO
1	K	546	LEU
1	K	554	GLN
1	K	571	VAL
1	K	580	GLU
1	K	599	ARG
1	K	600	GLN
1	K	630	ARG
1	K	632	SER
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	751	LEU
1	K	753	ASN
1	K	755	ARG
1	K	768	MET
1	K	778	THR
1	K	781	ARG

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Mol	Chain	Res	Type
1	K	797	GLU
1	K	799	THR
1	K	800	ARG
1	K	824	GLN
1	K	829	THR
1	K	832	ASP
1	K	881	ARG
1	K	893	GLU
1	K	903[A]	GLN
1	K	903[B]	GLN
1	K	917	ARG
1	K	938	ARG
1	K	952	ARG
1	K	956	GLN
1	K	1006	GLU
1	K	1017	GLN
1	L	3	ILE
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	59	ARG
1	L	71	GLU
1	L	72	SER
1	L	80	GLU
1	L	84	VAL
1	L	90	TRP
1	L	102	ASN
1	L	116	THR
1	L	125	LEU
1	L	128	ASN
1	L	136	GLU
1	L	165	SER
1	L	166	ARG
1	L	171	PHE
1	L	189	LEU
1	L	202	MET
1	L	210	ARG

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Mol	Chain	Res	Type
1	L	211	ASP
1	L	217	LYS
1	L	219	THR
1	L	246	MET
1	L	247	CYS
1	L	249	GLU
1	L	250	LEU
1	L	259	SER
1	L	262	GLN
1	L	264	GLU
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	394	ASN
1	L	425	ARG
1	L	437	SER
1	L	448	ARG
1	L	473	ARG
1	L	519	SER
1	L	521	LYS
1	L	532	PRO
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	632	SER
1	L	645	ARG
1	L	651	LEU
1	L	655	MET
1	L	665	SER
1	L	672	VAL
1	L	684	GLU

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Mol	Chain	Res	Type
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	751	LEU
1	L	753	ASN
1	L	755	ARG
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	824	GLN
1	L	829	THR
1	L	832	ASP
1	L	881	ARG
1	L	893	GLU
1	L	903[A]	GLN
1	L	903[B]	GLN
1	L	917	ARG
1	L	938	ARG
1	L	952	ARG
1	L	956	GLN
1	L	1006	GLU
1	L	1017	GLN
1	M	3	ILE
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	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	102	ASN
1	M	116	THR
1	M	125	LEU
1	M	128	ASN
1	M	132	SER
1	M	136	GLU
1	M	165	SER
1	M	166	ARG
1	M	171	PHE
1	M	189	LEU
1	M	202	MET
1	M	210	ARG
1	M	211	ASP
1	M	217	LYS
1	M	219	THR
1	M	246	MET
1	M	247	CYS
1	M	249	GLU
1	M	250	LEU
1	M	259	SER
1	M	262	GLN
1	M	264	GLU
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	394	ASN
1	M	425	ARG
1	M	437	SER
1	M	448	ARG
1	M	473	ARG
1	M	519	SER
1	M	521	LYS

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Mol	Chain	Res	Type
1	M	532	PRO
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	632	SER
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	751	LEU
1	M	753	ASN
1	M	755	ARG
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	824	GLN
1	M	829	THR
1	M	832	ASP
1	M	881	ARG
1	M	893	GLU
1	M	903[A]	GLN
1	M	903[B]	GLN
1	M	917	ARG
1	M	938	ARG
1	M	952	ARG

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Mol	Chain	Res	Type
1	M	956	GLN
1	M	1006	GLU
1	M	1017	GLN
1	N	3	ILE
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	59	ARG
1	N	71	GLU
1	N	72	SER
1	N	80	GLU
1	N	84	VAL
1	N	90	TRP
1	N	102	ASN
1	N	116	THR
1	N	125	LEU
1	N	128	ASN
1	N	132	SER
1	N	136	GLU
1	N	165	SER
1	N	166	ARG
1	N	171	PHE
1	N	189	LEU
1	N	202	MET
1	N	210	ARG
1	N	211	ASP
1	N	217	LYS
1	N	219	THR
1	N	246	MET
1	N	247	CYS
1	N	249	GLU
1	N	250	LEU
1	N	259	SER
1	N	262	GLN
1	N	264	GLU
1	N	279	ILE
1	N	299	LYS

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Mol	Chain	Res	Type
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	394	ASN
1	N	425	ARG
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	632	SER
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
1	N	719	GLN
1	N	730	LEU
1	N	734	SER
1	N	741	THR
1	N	743	SER
1	N	751	LEU
1	N	753	ASN
1	N	755	ARG
1	N	768	MET
1	N	778	THR

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Mol	Chain	Res	Type
1	N	781	ARG
1	N	797	GLU
1	N	799	THR
1	N	800	ARG
1	N	824	GLN
1	N	829	THR
1	N	832	ASP
1	N	881	ARG
1	N	893	GLU
1	N	903[A]	GLN
1	N	903[B]	GLN
1	N	917	ARG
1	N	938	ARG
1	N	952	ARG
1	N	956	GLN
1	N	1006	GLU
1	N	1017	GLN
1	O	3	ILE
1	O	14	ARG
1	O	37	ARG
1	O	39	SER
1	O	46	ARG
1	O	48	SER
1	O	49	GLN
1	O	50	GLN
1	O	52	ARG
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	102	ASN
1	O	116	THR
1	O	125	LEU
1	O	128	ASN
1	O	132	SER
1	O	136	GLU
1	O	165	SER
1	O	166	ARG
1	O	171	PHE
1	O	189	LEU

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Mol	Chain	Res	Type
1	O	202	MET
1	O	210	ARG
1	O	211	ASP
1	O	217	LYS
1	O	219	THR
1	O	246	MET
1	O	247	CYS
1	O	249	GLU
1	O	250	LEU
1	O	259	SER
1	O	262	GLN
1	O	264	GLU
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
1	O	370	GLN
1	O	377	LEU
1	O	394	ASN
1	O	425	ARG
1	O	437	SER
1	O	448	ARG
1	O	473	ARG
1	O	519	SER
1	O	521	LYS
1	O	532	PRO
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	632	SER
1	O	645	ARG
1	O	651	LEU
1	O	655	MET
1	O	665	SER

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Mol	Chain	Res	Type
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	751	LEU
1	O	753	ASN
1	O	755	ARG
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	824	GLN
1	O	829	THR
1	O	832	ASP
1	O	881	ARG
1	O	893	GLU
1	O	903[A]	GLN
1	O	903[B]	GLN
1	O	917	ARG
1	O	938	ARG
1	O	952	ARG
1	O	956	GLN
1	O	1006	GLU
1	O	1017	GLN
1	P	3	ILE
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	59	ARG

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Mol	Chain	Res	Type
1	P	71	GLU
1	P	72	SER
1	P	80	GLU
1	P	84	VAL
1	P	90	TRP
1	P	102	ASN
1	P	116	THR
1	P	125	LEU
1	P	128	ASN
1	P	132	SER
1	P	136	GLU
1	P	165	SER
1	P	166	ARG
1	P	171	PHE
1	P	189	LEU
1	P	202	MET
1	P	210	ARG
1	P	211	ASP
1	P	217	LYS
1	P	219	THR
1	P	246	MET
1	P	247	CYS
1	P	249	GLU
1	P	250	LEU
1	P	259	SER
1	P	262	GLN
1	P	264	GLU
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	394	ASN
1	P	425	ARG
1	P	437	SER
1	P	448	ARG
1	P	473	ARG

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Mol	Chain	Res	Type
1	P	519	SER
1	P	521	LYS
1	P	532	PRO
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	632	SER
1	P	645	ARG
1	P	651	LEU
1	P	655	MET
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	751	LEU
1	P	753	ASN
1	P	755	ARG
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	824	GLN
1	P	829	THR
1	P	832	ASP
1	P	881	ARG
1	P	893	GLU
1	P	903[A]	GLN
1	P	903[B]	GLN
1	P	917	ARG

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Mol	Chain	Res	Type
1	P	938	ARG
1	P	952	ARG
1	P	956	GLN
1	P	1006	GLU
1	P	1017	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (234) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	128	ASN
1	A	226	HIS
1	A	316	HIS
1	A	467	ASN
1	A	597	ASN
1	A	604	ASN
1	A	624	GLN
1	A	761	GLN
1	A	817	GLN
1	A	824	GLN
1	A	949	HIS
1	A	990	HIS
1	A	1017	GLN
1	B	102	ASN
1	B	128	ASN
1	B	226	HIS
1	B	316	HIS
1	B	467	ASN
1	B	597	ASN
1	B	604	ASN
1	B	624	GLN
1	B	739	HIS
1	B	761	GLN
1	B	817	GLN
1	B	824	GLN
1	B	949	HIS
1	B	990	HIS
1	B	1017	GLN
1	C	102	ASN
1	C	128	ASN
1	C	226	HIS
1	C	316	HIS

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Mol	Chain	Res	Type
1	C	467	ASN
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	949	HIS
1	C	990	HIS
1	C	1017	GLN
1	D	102	ASN
1	D	128	ASN
1	D	226	HIS
1	D	316	HIS
1	D	467	ASN
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	949	HIS
1	D	990	HIS
1	D	1017	GLN
1	E	102	ASN
1	E	128	ASN
1	E	226	HIS
1	E	316	HIS
1	E	467	ASN
1	E	597	ASN
1	E	604	ASN
1	E	624	GLN
1	E	761	GLN
1	E	817	GLN
1	E	824	GLN
1	E	949	HIS
1	E	990	HIS
1	E	1017	GLN
1	F	102	ASN
1	F	128	ASN

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Mol	Chain	Res	Type
1	F	226	HIS
1	F	316	HIS
1	F	467	ASN
1	F	597	ASN
1	F	604	ASN
1	F	624	GLN
1	F	761	GLN
1	F	817	GLN
1	F	824	GLN
1	F	949	HIS
1	F	990	HIS
1	F	1017	GLN
1	G	102	ASN
1	G	128	ASN
1	G	226	HIS
1	G	316	HIS
1	G	467	ASN
1	G	597	ASN
1	G	604	ASN
1	G	624	GLN
1	G	739	HIS
1	G	761	GLN
1	G	817	GLN
1	G	824	GLN
1	G	949	HIS
1	G	990	HIS
1	G	1017	GLN
1	H	102	ASN
1	H	128	ASN
1	H	226	HIS
1	H	316	HIS
1	H	467	ASN
1	H	597	ASN
1	H	604	ASN
1	H	624	GLN
1	H	761	GLN
1	H	817	GLN
1	H	824	GLN
1	H	949	HIS
1	H	990	HIS
1	H	1017	GLN
1	I	102	ASN

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Mol	Chain	Res	Type
1	I	128	ASN
1	I	226	HIS
1	I	316	HIS
1	I	467	ASN
1	I	597	ASN
1	I	604	ASN
1	I	624	GLN
1	I	739	HIS
1	I	761	GLN
1	I	817	GLN
1	I	824	GLN
1	I	949	HIS
1	I	990	HIS
1	I	1017	GLN
1	J	102	ASN
1	J	128	ASN
1	J	226	HIS
1	J	316	HIS
1	J	467	ASN
1	J	597	ASN
1	J	604	ASN
1	J	624	GLN
1	J	739	HIS
1	J	761	GLN
1	J	817	GLN
1	J	824	GLN
1	J	949	HIS
1	J	990	HIS
1	J	1017	GLN
1	K	102	ASN
1	K	128	ASN
1	K	226	HIS
1	K	316	HIS
1	K	467	ASN
1	K	597	ASN
1	K	604	ASN
1	K	624	GLN
1	K	739	HIS
1	K	761	GLN
1	K	817	GLN
1	K	824	GLN
1	K	949	HIS

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Mol	Chain	Res	Type
1	K	990	HIS
1	K	1017	GLN
1	L	102	ASN
1	L	128	ASN
1	L	226	HIS
1	L	316	HIS
1	L	467	ASN
1	L	597	ASN
1	L	604	ASN
1	L	624	GLN
1	L	739	HIS
1	L	761	GLN
1	L	817	GLN
1	L	824	GLN
1	L	949	HIS
1	L	990	HIS
1	L	1017	GLN
1	M	102	ASN
1	M	128	ASN
1	M	226	HIS
1	M	316	HIS
1	M	467	ASN
1	M	597	ASN
1	M	604	ASN
1	M	624	GLN
1	M	739	HIS
1	M	761	GLN
1	M	817	GLN
1	M	824	GLN
1	M	949	HIS
1	M	990	HIS
1	M	1017	GLN
1	N	102	ASN
1	N	128	ASN
1	N	226	HIS
1	N	316	HIS
1	N	467	ASN
1	N	597	ASN
1	N	604	ASN
1	N	624	GLN
1	N	739	HIS
1	N	761	GLN

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Mol	Chain	Res	Type
1	N	817	GLN
1	N	824	GLN
1	N	949	HIS
1	N	990	HIS
1	N	1017	GLN
1	O	102	ASN
1	O	128	ASN
1	O	226	HIS
1	O	316	HIS
1	O	467	ASN
1	O	597	ASN
1	O	604	ASN
1	O	624	GLN
1	O	761	GLN
1	O	817	GLN
1	O	824	GLN
1	O	949	HIS
1	O	990	HIS
1	O	1017	GLN
1	P	102	ASN
1	P	128	ASN
1	P	226	HIS
1	P	316	HIS
1	P	467	ASN
1	P	597	ASN
1	P	604	ASN
1	P	624	GLN
1	P	761	GLN
1	P	817	GLN
1	P	824	GLN
1	P	949	HIS
1	P	990	HIS
1	P	1017	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CME	A	748	1	8,9,10	0.87	1 (12%)	5,9,11	0.95	0
1	CME	C	914	1	8,9,10	0.83	0	5,9,11	1.87	1 (20%)
1	CME	L	1021	1	8,9,10	1.26	0	5,9,11	3.68	1 (20%)
1	CME	L	914	1	8,9,10	0.83	0	5,9,11	1.87	1 (20%)
1	CME	B	748	1	8,9,10	0.88	1 (12%)	5,9,11	0.95	0
1	CME	D	1021	1	8,9,10	1.26	1 (12%)	5,9,11	3.69	1 (20%)
1	CME	G	914	1	8,9,10	0.83	0	5,9,11	1.87	1 (20%)
1	CME	H	914	1	8,9,10	0.83	0	5,9,11	1.87	1 (20%)
1	CME	I	748	1	8,9,10	0.87	1 (12%)	5,9,11	0.95	0
1	CME	K	914	1	8,9,10	0.84	0	5,9,11	1.87	1 (20%)
1	CME	N	914	1	8,9,10	0.83	0	5,9,11	1.87	1 (20%)
1	CME	E	1021	1	8,9,10	1.27	0	5,9,11	3.68	1 (20%)
1	CME	O	748	1	8,9,10	0.88	1 (12%)	5,9,11	0.96	0
1	CME	H	1021	1	8,9,10	1.27	1 (12%)	5,9,11	3.68	1 (20%)
1	CME	A	914	1	8,9,10	0.83	0	5,9,11	1.87	1 (20%)
1	CME	N	1021	1	8,9,10	1.27	1 (12%)	5,9,11	3.68	1 (20%)
1	CME	O	1021	1	8,9,10	1.27	1 (12%)	5,9,11	3.68	1 (20%)
1	CME	D	748	1	8,9,10	0.88	1 (12%)	5,9,11	0.95	0
1	CME	F	914	1	8,9,10	0.83	0	5,9,11	1.87	1 (20%)
1	CME	O	914	1	8,9,10	0.84	0	5,9,11	1.86	1 (20%)
1	CME	D	914	1	8,9,10	0.83	0	5,9,11	1.87	1 (20%)
1	CME	C	748	1	8,9,10	0.88	1 (12%)	5,9,11	0.95	0
1	CME	M	748	1	8,9,10	0.87	1 (12%)	5,9,11	0.95	0
1	CME	P	1021	1	8,9,10	1.27	0	5,9,11	3.69	1 (20%)
1	CME	I	914	1	8,9,10	0.83	0	5,9,11	1.87	1 (20%)
1	CME	B	914	1	8,9,10	0.83	0	5,9,11	1.87	1 (20%)
1	CME	H	748	1	8,9,10	0.88	1 (12%)	5,9,11	0.95	0
1	CME	A	1021	1	8,9,10	1.27	1 (12%)	5,9,11	3.68	1 (20%)
1	CME	F	1021	1	8,9,10	1.27	1 (12%)	5,9,11	3.68	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CME	P	914	1	8,9,10	0.83	0	5,9,11	1.86	1 (20%)
1	CME	P	748	1	8,9,10	0.87	1 (12%)	5,9,11	0.95	0
1	CME	J	1021	1	8,9,10	1.27	1 (12%)	5,9,11	3.68	1 (20%)
1	CME	J	914	1	8,9,10	0.84	0	5,9,11	1.87	1 (20%)
1	CME	G	1021	1	8,9,10	1.27	1 (12%)	5,9,11	3.68	1 (20%)
1	CME	I	1021	1	8,9,10	1.27	1 (12%)	5,9,11	3.68	1 (20%)
1	CME	F	748	1	8,9,10	0.88	1 (12%)	5,9,11	0.95	0
1	CME	K	1021	1	8,9,10	1.26	0	5,9,11	3.69	1 (20%)
1	CME	M	1021	1	8,9,10	1.28	1 (12%)	5,9,11	3.68	1 (20%)
1	CME	N	748	1	8,9,10	0.87	1 (12%)	5,9,11	0.95	0
1	CME	E	748	1	8,9,10	0.88	1 (12%)	5,9,11	0.95	0
1	CME	B	1021	1	8,9,10	1.27	1 (12%)	5,9,11	3.68	1 (20%)
1	CME	E	914	1	8,9,10	0.83	0	5,9,11	1.87	1 (20%)
1	CME	K	748	1	8,9,10	0.88	1 (12%)	5,9,11	0.95	0
1	CME	L	748	1	8,9,10	0.88	1 (12%)	5,9,11	0.95	0
1	CME	M	914	1	8,9,10	0.84	0	5,9,11	1.87	1 (20%)
1	CME	G	748	1	8,9,10	0.88	1 (12%)	5,9,11	0.95	0
1	CME	C	1021	1	8,9,10	1.27	1 (12%)	5,9,11	3.68	1 (20%)
1	CME	J	748	1	8,9,10	0.88	1 (12%)	5,9,11	0.95	0

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	748	1	-	3/5/8/10	-
1	CME	C	914	1	-	3/5/8/10	-
1	CME	L	1021	1	-	4/5/8/10	-
1	CME	L	914	1	-	3/5/8/10	-
1	CME	B	748	1	-	3/5/8/10	-
1	CME	D	1021	1	-	4/5/8/10	-
1	CME	G	914	1	-	3/5/8/10	-
1	CME	H	914	1	-	3/5/8/10	-
1	CME	I	748	1	-	3/5/8/10	-
1	CME	K	914	1	-	3/5/8/10	-

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	M	914	1	-	3/5/8/10	-
1	CME	G	748	1	-	3/5/8/10	-
1	CME	C	1021	1	-	4/5/8/10	-
1	CME	J	748	1	-	3/5/8/10	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	748	CME	CA-N	-2.35	1.41	1.48
1	H	748	CME	CA-N	-2.35	1.41	1.48
1	K	748	CME	CA-N	-2.35	1.41	1.48
1	F	748	CME	CA-N	-2.34	1.41	1.48
1	G	748	CME	CA-N	-2.34	1.41	1.48
1	L	748	CME	CA-N	-2.34	1.41	1.48
1	E	748	CME	CA-N	-2.34	1.41	1.48
1	O	748	CME	CA-N	-2.33	1.41	1.48
1	B	748	CME	CA-N	-2.33	1.41	1.48
1	A	748	CME	CA-N	-2.33	1.41	1.48
1	C	748	CME	CA-N	-2.33	1.41	1.48
1	D	748	CME	CA-N	-2.32	1.41	1.48
1	N	748	CME	CA-N	-2.32	1.41	1.48
1	M	748	CME	CA-N	-2.31	1.41	1.48
1	P	748	CME	CA-N	-2.31	1.41	1.48
1	I	748	CME	CA-N	-2.30	1.41	1.48
1	F	1021	CME	SD-SG	-2.01	1.88	2.03
1	N	1021	CME	SD-SG	-2.01	1.88	2.03
1	G	1021	CME	SD-SG	-2.01	1.88	2.03
1	O	1021	CME	SD-SG	-2.01	1.88	2.03
1	C	1021	CME	SD-SG	-2.01	1.88	2.03
1	A	1021	CME	SD-SG	-2.00	1.88	2.03
1	M	1021	CME	SD-SG	-2.00	1.88	2.03
1	J	1021	CME	SD-SG	-2.00	1.88	2.03
1	D	1021	CME	SD-SG	-2.00	1.88	2.03
1	H	1021	CME	SD-SG	-2.00	1.88	2.03
1	I	1021	CME	SD-SG	-2.00	1.88	2.03
1	B	1021	CME	SD-SG	-2.00	1.88	2.03

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1021	CME	CB-SG-SD	-8.01	83.06	103.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	1021	CME	CB-SG-SD	-8.01	83.07	103.82
1	P	1021	CME	CB-SG-SD	-8.00	83.08	103.82
1	N	1021	CME	CB-SG-SD	-8.00	83.09	103.82
1	I	1021	CME	CB-SG-SD	-8.00	83.10	103.82
1	L	1021	CME	CB-SG-SD	-8.00	83.10	103.82
1	E	1021	CME	CB-SG-SD	-8.00	83.11	103.82
1	A	1021	CME	CB-SG-SD	-8.00	83.11	103.82
1	F	1021	CME	CB-SG-SD	-7.99	83.11	103.82
1	J	1021	CME	CB-SG-SD	-7.99	83.11	103.82
1	H	1021	CME	CB-SG-SD	-7.99	83.11	103.82
1	G	1021	CME	CB-SG-SD	-7.99	83.11	103.82
1	B	1021	CME	CB-SG-SD	-7.99	83.11	103.82
1	M	1021	CME	CB-SG-SD	-7.99	83.12	103.82
1	C	1021	CME	CB-SG-SD	-7.99	83.12	103.82
1	O	1021	CME	CB-SG-SD	-7.98	83.15	103.82
1	C	914	CME	CB-SG-SD	-4.09	93.23	103.82
1	L	914	CME	CB-SG-SD	-4.09	93.24	103.82
1	B	914	CME	CB-SG-SD	-4.08	93.25	103.82
1	H	914	CME	CB-SG-SD	-4.08	93.26	103.82
1	E	914	CME	CB-SG-SD	-4.08	93.26	103.82
1	I	914	CME	CB-SG-SD	-4.08	93.26	103.82
1	M	914	CME	CB-SG-SD	-4.07	93.27	103.82
1	K	914	CME	CB-SG-SD	-4.07	93.27	103.82
1	J	914	CME	CB-SG-SD	-4.07	93.27	103.82
1	F	914	CME	CB-SG-SD	-4.07	93.27	103.82
1	N	914	CME	CB-SG-SD	-4.07	93.27	103.82
1	D	914	CME	CB-SG-SD	-4.07	93.28	103.82
1	G	914	CME	CB-SG-SD	-4.07	93.28	103.82
1	A	914	CME	CB-SG-SD	-4.07	93.28	103.82
1	O	914	CME	CB-SG-SD	-4.07	93.28	103.82
1	P	914	CME	CB-SG-SD	-4.06	93.29	103.82

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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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	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

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

There are no ring outliers.

32 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	748	CME	1	0
1	C	914	CME	1	0
1	L	1021	CME	3	0
1	L	914	CME	1	0
1	D	1021	CME	3	0
1	G	914	CME	1	0
1	H	914	CME	1	0
1	K	914	CME	1	0
1	N	914	CME	1	0

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

5.5 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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%)	-0.85	5 (0%) 91 91	3, 21, 66, 100	1 (0%)
1	B	1018/1023 (99%)	-0.91	0 100 100	3, 21, 66, 100	1 (0%)
1	C	1018/1023 (99%)	-0.79	1 (0%) 95 96	2, 19, 63, 98	1 (0%)
1	D	1018/1023 (99%)	-0.82	0 100 100	5, 24, 67, 100	1 (0%)
1	E	1018/1023 (99%)	-0.61	3 (0%) 94 94	15, 33, 74, 100	1 (0%)
1	F	1018/1023 (99%)	-0.85	1 (0%) 95 96	3, 21, 66, 100	1 (0%)
1	G	1018/1023 (99%)	-0.89	1 (0%) 95 96	7, 25, 68, 100	1 (0%)
1	H	1018/1023 (99%)	-0.64	4 (0%) 92 93	14, 33, 73, 100	1 (0%)
1	I	1018/1023 (99%)	-0.79	1 (0%) 95 96	10, 28, 70, 100	1 (0%)
1	J	1018/1023 (99%)	-0.81	1 (0%) 95 96	8, 26, 69, 100	1 (0%)
1	K	1018/1023 (99%)	-0.68	6 (0%) 89 90	17, 35, 76, 100	1 (0%)
1	L	1018/1023 (99%)	-0.62	3 (0%) 94 94	16, 34, 75, 100	1 (0%)
1	M	1018/1023 (99%)	-0.25	18 (1%) 68 71	22, 40, 79, 100	1 (0%)
1	N	1018/1023 (99%)	-0.74	0 100 100	11, 29, 71, 100	1 (0%)
1	O	1018/1023 (99%)	-0.81	1 (0%) 95 96	12, 30, 72, 100	1 (0%)
1	P	1018/1023 (99%)	0.26	66 (6%) 18 19	29, 47, 83, 100	1 (0%)
All	All	16288/16368 (99%)	-0.68	111 (0%) 87 89	2, 30, 72, 100	16 (0%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	735	HIS	5.3
1	P	739	HIS	5.2
1	P	313	VAL	5.2
1	P	70	PRO	5.0
1	O	735	HIS	4.8

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Mol	Chain	Res	Type	RSRZ
1	L	735	HIS	4.5
1	P	143	PHE	4.5
1	P	732	ALA	4.2
1	P	133	TRP	4.1
1	P	115	PRO	4.1
1	M	575	LEU	3.9
1	H	735	HIS	3.9
1	A	580	GLU	3.9
1	P	731	PRO	3.8
1	P	55	ASN	3.8
1	P	158	TRP	3.7
1	P	129	VAL	3.7
1	P	203	TRP	3.6
1	P	149	ALA	3.5
1	A	582	GLY	3.5
1	P	364	GLY	3.4
1	P	97	ALA	3.4
1	P	204	ARG	3.4
1	P	141	ILE	3.4
1	P	73	TRP	3.4
1	K	734	SER	3.3
1	P	735	HIS	3.3
1	P	34	ALA	3.3
1	L	739	HIS	3.3
1	P	81	ALA	3.2
1	P	595	THR	3.2
1	P	68	ALA	3.1
1	P	191	TRP	3.0
1	M	6	SER	3.0
1	M	66	PRO	3.0
1	P	799	THR	3.0
1	M	162	GLY	3.0
1	L	687	GLN	3.0
1	K	730	LEU	2.9
1	P	733	ALA	2.8
1	M	177	LEU	2.8
1	M	73	TRP	2.8
1	G	735	HIS	2.8
1	A	735	HIS	2.8
1	P	684	GLU	2.8
1	P	180	GLY	2.8
1	M	69	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	P	7	LEU	2.8
1	P	35	SER	2.7
1	P	209	PHE	2.7
1	P	9	VAL	2.7
1	M	75	GLU	2.7
1	M	149	ALA	2.7
1	P	317	THR	2.7
1	P	51	LEU	2.6
1	C	581	ASN	2.6
1	A	581	ASN	2.6
1	P	575	LEU	2.6
1	P	185	ALA	2.6
1	P	160	GLY	2.6
1	P	579	ASP	2.6
1	P	800	ARG	2.6
1	P	585	TRP	2.6
1	P	689	GLU	2.6
1	P	102	ASN	2.6
1	M	16	TRP	2.6
1	P	100	TYR	2.6
1	E	160	GLY	2.6
1	K	732	ALA	2.5
1	E	66	PRO	2.5
1	M	160	GLY	2.5
1	P	195	SER	2.5
1	J	581	ASN	2.5
1	M	735	HIS	2.4
1	P	174	SER	2.4
1	P	85	VAL	2.4
1	P	580	GLU	2.4
1	M	173	LEU	2.4
1	P	221	GLN	2.4
1	P	884	LEU	2.4
1	E	143	PHE	2.4
1	P	594	ASP	2.4
1	P	138	GLN	2.4
1	K	731	PRO	2.3
1	F	689	GLU	2.3
1	P	178	ARG	2.3
1	M	249	GLU	2.2
1	K	739	HIS	2.2
1	P	58	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	596	PRO	2.2
1	P	683	PRO	2.2
1	P	122	CYS	2.2
1	P	162	GLY	2.2
1	H	580	GLU	2.2
1	P	596	PRO	2.2
1	I	735	HIS	2.2
1	P	249	GLU	2.2
1	P	574	SER	2.2
1	H	4	THR	2.1
1	M	133	TRP	2.1
1	M	115	PRO	2.1
1	H	129	VAL	2.1
1	P	153	TRP	2.1
1	P	261	TRP	2.1
1	M	125	LEU	2.1
1	P	215	LEU	2.1
1	P	274	PHE	2.1
1	P	172	ASP	2.0
1	A	682	LEU	2.0
1	P	131	GLU	2.0
1	P	321	THR	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, 95^{th} 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	H	1021	10/11	0.89	0.14	13,36,100,100	0
1	CME	L	748	10/11	0.90	0.17	31,41,100,100	0
1	CME	K	748	10/11	0.91	0.15	32,42,100,100	0
1	CME	P	914	10/11	0.91	0.11	34,40,100,100	0
1	CME	P	1021	10/11	0.91	0.13	28,51,100,100	0
1	CME	M	1021	10/11	0.92	0.13	21,44,100,100	0
1	CME	N	1021	10/11	0.92	0.11	9,33,100,100	0
1	CME	O	748	10/11	0.92	0.12	27,37,100,100	0
1	CME	P	748	10/11	0.92	0.12	44,54,100,100	0
1	CME	E	1021	10/11	0.92	0.12	14,37,100,100	0
1	CME	C	748	10/11	0.92	0.12	16,26,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CME	F	1021	10/11	0.93	0.11	2,25,100,100	0
1	CME	H	748	10/11	0.93	0.13	29,39,100,100	0
1	CME	C	1021	10/11	0.93	0.11	1,23,97,97	0
1	CME	I	1021	10/11	0.93	0.13	9,32,100,100	0
1	CME	D	748	10/11	0.93	0.16	21,30,100,100	0
1	CME	B	748	10/11	0.93	0.08	18,28,99,99	0
1	CME	J	1021	10/11	0.94	0.10	7,30,100,100	0
1	CME	G	748	10/11	0.94	0.09	22,32,100,100	0
1	CME	D	1021	10/11	0.94	0.13	4,27,100,100	0
1	CME	M	914	10/11	0.95	0.13	27,33,100,100	0
1	CME	B	1021	10/11	0.95	0.08	2,25,99,99	0
1	CME	E	748	10/11	0.95	0.10	30,40,100,100	0
1	CME	A	1021	10/11	0.95	0.10	2,25,100,100	0
1	CME	O	1021	10/11	0.95	0.14	11,34,100,100	0
1	CME	K	914	10/11	0.95	0.09	22,28,100,100	0
1	CME	F	748	10/11	0.95	0.09	18,28,100,100	0
1	CME	L	1021	10/11	0.95	0.09	15,38,100,100	0
1	CME	H	914	10/11	0.96	0.11	19,25,100,100	0
1	CME	G	1021	10/11	0.96	0.09	6,29,100,100	0
1	CME	I	748	10/11	0.96	0.10	25,35,100,100	0
1	CME	K	1021	10/11	0.96	0.16	16,39,100,100	0
1	CME	O	914	10/11	0.96	0.08	17,23,100,100	0
1	CME	A	748	10/11	0.96	0.09	18,28,100,100	0
1	CME	L	914	10/11	0.96	0.09	21,27,100,100	0
1	CME	J	748	10/11	0.96	0.08	23,33,100,100	0
1	CME	M	748	10/11	0.96	0.10	37,47,100,100	0
1	CME	J	914	10/11	0.97	0.10	13,19,100,100	0
1	CME	E	914	10/11	0.97	0.12	20,26,100,100	0
1	CME	N	748	10/11	0.97	0.07	26,35,100,100	0
1	CME	N	914	10/11	0.97	0.08	16,22,100,100	0
1	CME	B	914	10/11	0.97	0.08	8,14,99,99	0
1	CME	D	914	10/11	0.97	0.10	10,16,100,100	0
1	CME	F	914	10/11	0.97	0.12	8,14,100,100	0
1	CME	C	914	10/11	0.97	0.10	6,12,97,97	0
1	CME	I	914	10/11	0.97	0.11	15,21,100,100	0
1	CME	A	914	10/11	0.97	0.10	8,14,100,100	0
1	CME	G	914	10/11	0.97	0.07	12,18,100,100	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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, 95^{th} 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
2	MG	P	3002	1/1	0.83	0.10	44,44,44,44	0
2	MG	L	3001	1/1	0.84	0.06	31,31,31,31	0
2	MG	I	3002	1/1	0.84	0.10	25,25,25,25	0
2	MG	P	3001	1/1	0.85	0.10	44,44,44,44	0
2	MG	E	3002	1/1	0.88	0.10	30,30,30,30	0
2	MG	F	3001	1/1	0.88	0.10	18,18,18,18	0
2	MG	M	3002	1/1	0.90	0.19	37,37,37,37	0
2	MG	M	3001	1/1	0.91	0.10	37,37,37,37	0
2	MG	A	3001	1/1	0.91	0.09	18,18,18,18	0
2	MG	N	3001	1/1	0.92	0.04	26,26,26,26	0
2	MG	D	3001	1/1	0.93	0.04	20,20,20,20	0
2	MG	J	3001	1/1	0.93	0.04	23,23,23,23	0
2	MG	K	3002	1/1	0.93	0.08	32,32,32,32	0
2	MG	N	3002	1/1	0.94	0.13	26,26,26,26	0
2	MG	H	3001	1/1	0.94	0.04	29,29,29,29	0
2	MG	C	3002	1/1	0.94	0.11	16,16,16,16	0
2	MG	I	3001	1/1	0.95	0.05	25,25,25,25	0
2	MG	G	3001	1/1	0.95	0.04	22,22,22,22	0
2	MG	F	3002	1/1	0.95	0.08	19,19,19,19	0
2	MG	J	3002	1/1	0.95	0.12	23,23,23,23	0
2	MG	K	3001	1/1	0.96	0.08	32,32,32,32	0
2	MG	O	3002	1/1	0.96	0.12	27,27,27,27	0
2	MG	G	3002	1/1	0.96	0.05	22,22,22,22	0
2	MG	D	3002	1/1	0.96	0.10	21,21,21,21	0
2	MG	E	3001	1/1	0.97	0.03	30,30,30,30	0
2	MG	C	3001	1/1	0.97	0.04	16,16,16,16	0
2	MG	A	3002	1/1	0.97	0.12	18,18,18,18	0
2	MG	B	3001	1/1	0.97	0.08	18,18,18,18	0
2	MG	L	3002	1/1	0.97	0.09	31,31,31,31	0
2	MG	B	3002	1/1	0.97	0.06	18,18,18,18	0
2	MG	O	3001	1/1	0.98	0.05	27,27,27,27	0
2	MG	H	3002	1/1	0.98	0.12	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.