



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 09:30 PM UTC

PDB ID : 5LDF / pdb_00005ldf
EMDB ID : EMD-4039
Title : Maltose binding protein genetically fused to dodecameric glutamine synthetase
Authors : Coscia, F.; Petosa, C.; Schoehn, G.
Deposited on : 2016-06-25
Resolution : 6.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

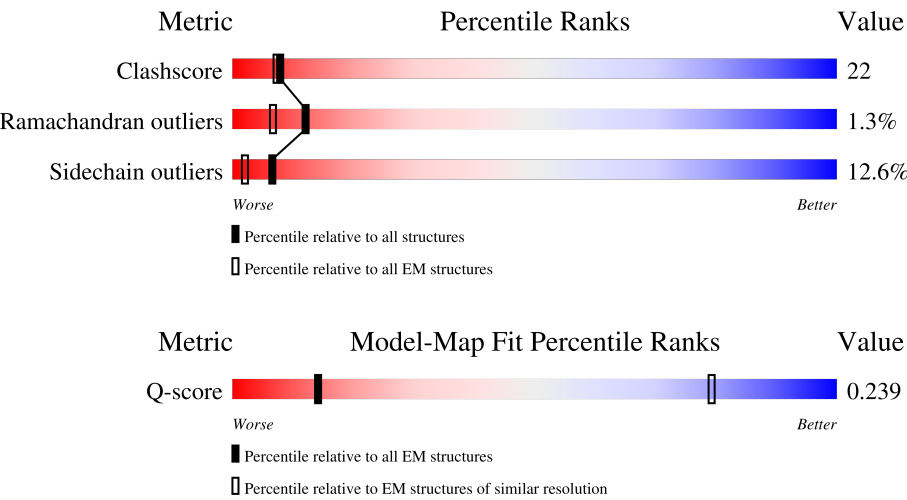
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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.



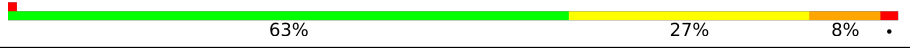
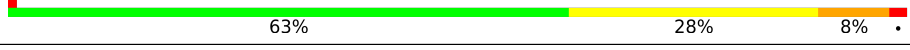
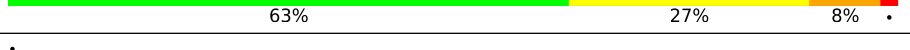
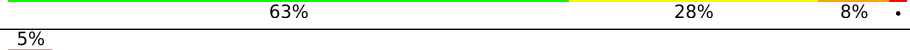
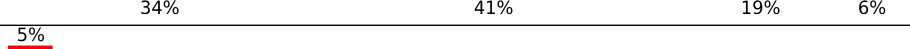
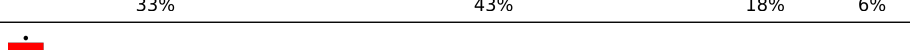
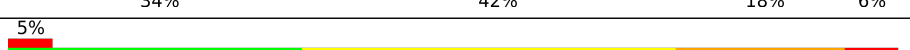
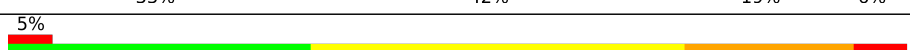
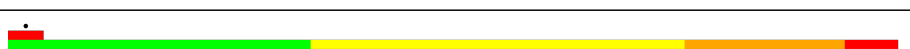
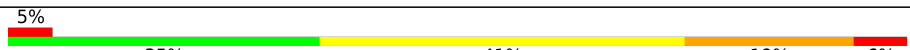
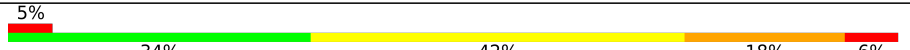
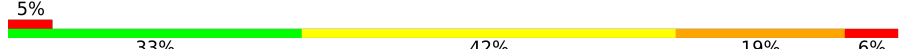
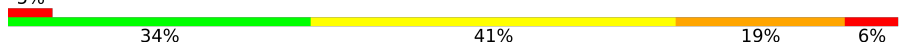
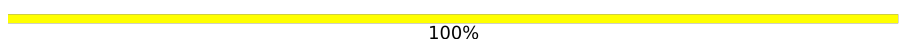
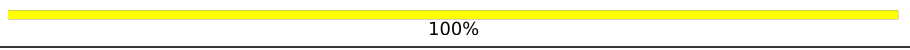
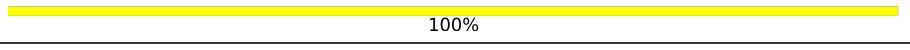
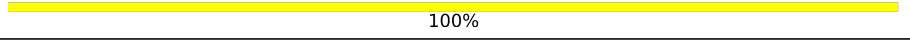
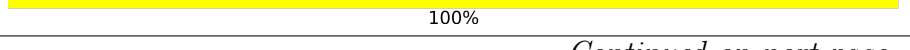
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	537 (5.70 - 6.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	466	
1	B	466	
1	C	466	
1	D	466	

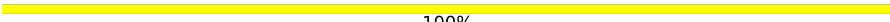
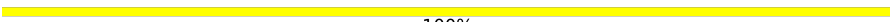
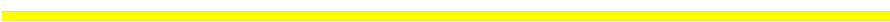
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Mol	Chain	Length	Quality of chain
1	E	466	
1	F	466	
1	G	466	
1	H	466	
1	I	466	
1	J	466	
1	K	466	
1	L	466	
2	M	370	
2	N	370	
2	O	370	
2	P	370	
2	Q	370	
2	R	370	
2	S	370	
2	T	370	
2	U	370	
2	V	370	
2	W	370	
2	X	370	
3	Y	2	
3	Z	2	
3	a	2	
3	b	2	
3	c	2	

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Mol	Chain	Length	Quality of chain
3	d	2	 100%
3	e	2	 100%
3	f	2	 100%
3	g	2	 100%
3	h	2	 100%
3	i	2	 100%
3	j	2	 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 78120 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Glutamine synthetase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	B	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	C	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	D	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	E	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	F	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	G	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	H	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	I	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	J	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	K	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		
1	L	466	Total	C	N	O	S	0	0
			3626	2295	622	689	20		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	391	PRO	ALA	conflict	UNP P0A1P7
B	391	PRO	ALA	conflict	UNP P0A1P7
C	391	PRO	ALA	conflict	UNP P0A1P7
D	391	PRO	ALA	conflict	UNP P0A1P7
E	391	PRO	ALA	conflict	UNP P0A1P7
F	391	PRO	ALA	conflict	UNP P0A1P7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	391	PRO	ALA	conflict	UNP P0A1P7
H	391	PRO	ALA	conflict	UNP P0A1P7
I	391	PRO	ALA	conflict	UNP P0A1P7
J	391	PRO	ALA	conflict	UNP P0A1P7
K	391	PRO	ALA	conflict	UNP P0A1P7
L	391	PRO	ALA	conflict	UNP P0A1P7

- Molecule 2 is a protein called Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	N	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	O	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	P	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	Q	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	R	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	S	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	T	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	U	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	V	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	W	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		
2	X	370	Total	C	N	O	S	0	0
			2861	1843	468	544	6		

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

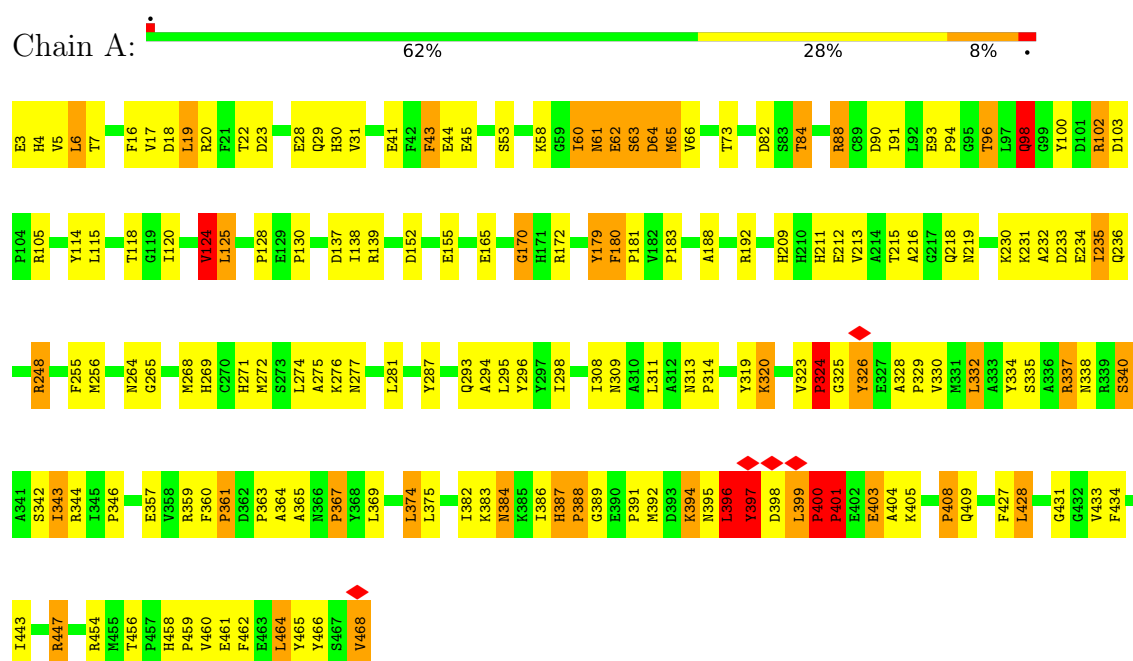


Mol	Chain	Residues	Atoms			AltConf	Trace
3	Y	2	Total	C	O	0	0
			23	12	11		
3	Z	2	Total	C	O	0	0
			23	12	11		
3	a	2	Total	C	O	0	0
			23	12	11		
3	b	2	Total	C	O	0	0
			23	12	11		
3	c	2	Total	C	O	0	0
			23	12	11		
3	d	2	Total	C	O	0	0
			23	12	11		
3	e	2	Total	C	O	0	0
			23	12	11		
3	f	2	Total	C	O	0	0
			23	12	11		
3	g	2	Total	C	O	0	0
			23	12	11		
3	h	2	Total	C	O	0	0
			23	12	11		
3	i	2	Total	C	O	0	0
			23	12	11		
3	j	2	Total	C	O	0	0
			23	12	11		

3 Residue-property plots

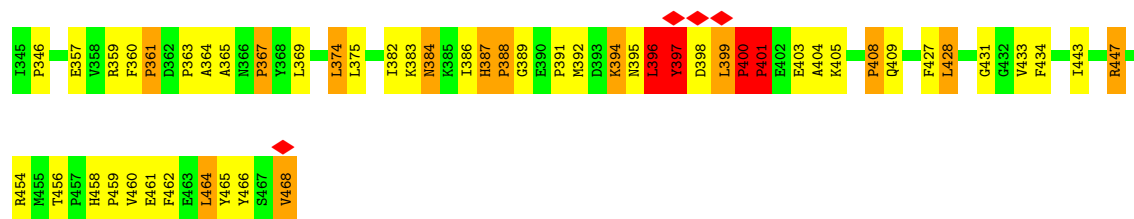
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Glutamine synthetase

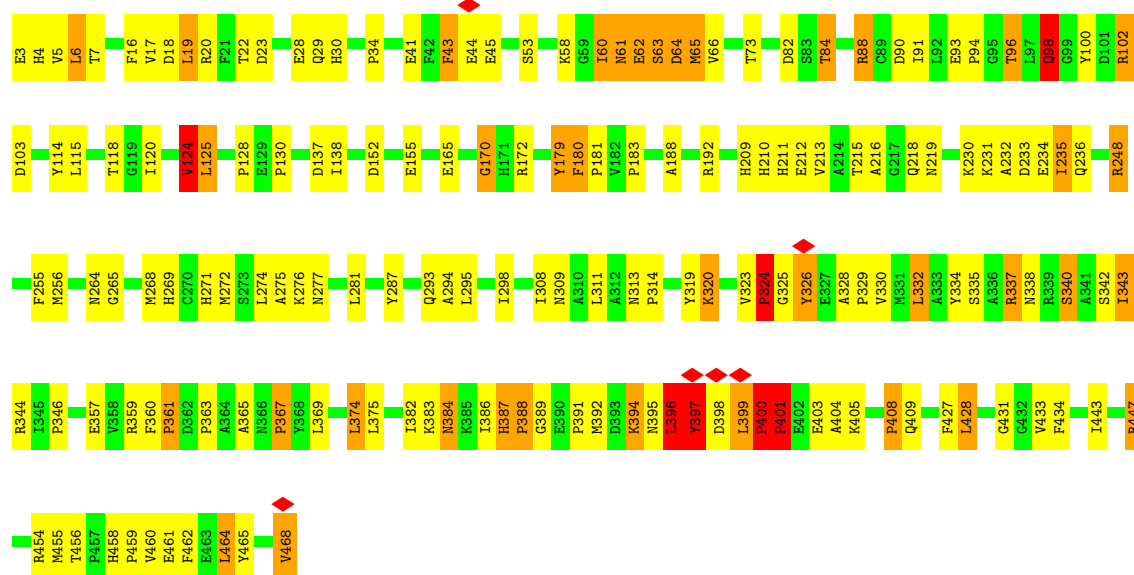


• Molecule 1: Glutamine synthetase

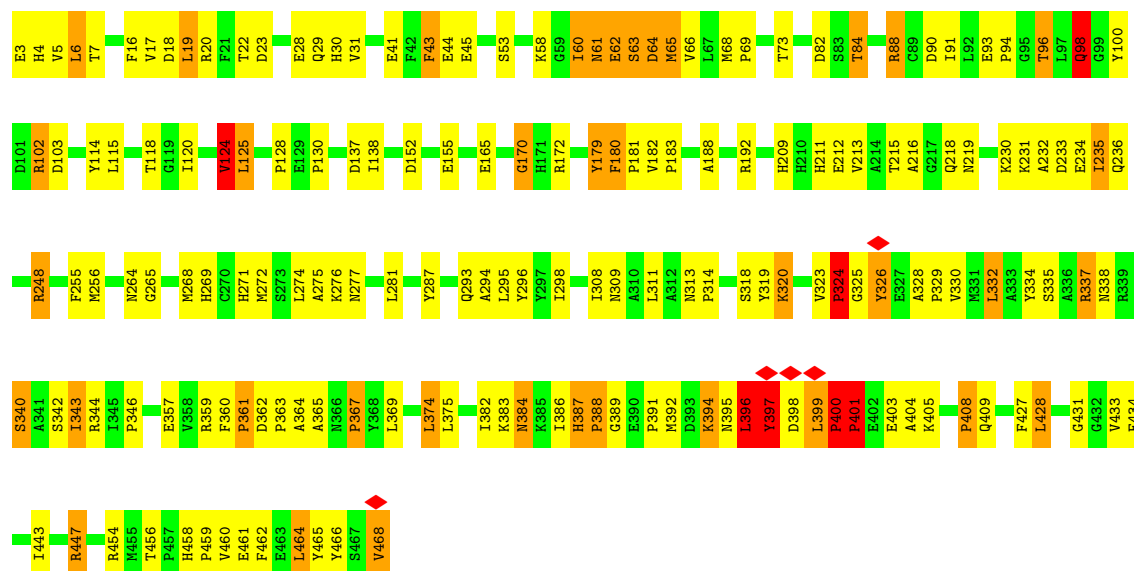




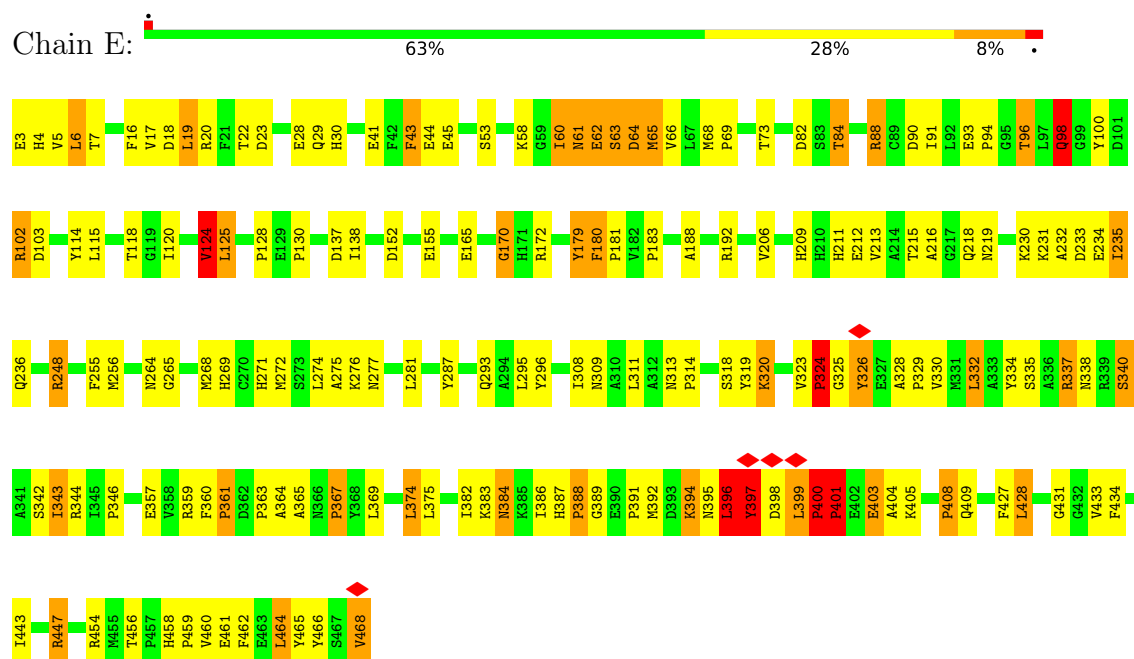
• Molecule 1: Glutamine synthetase



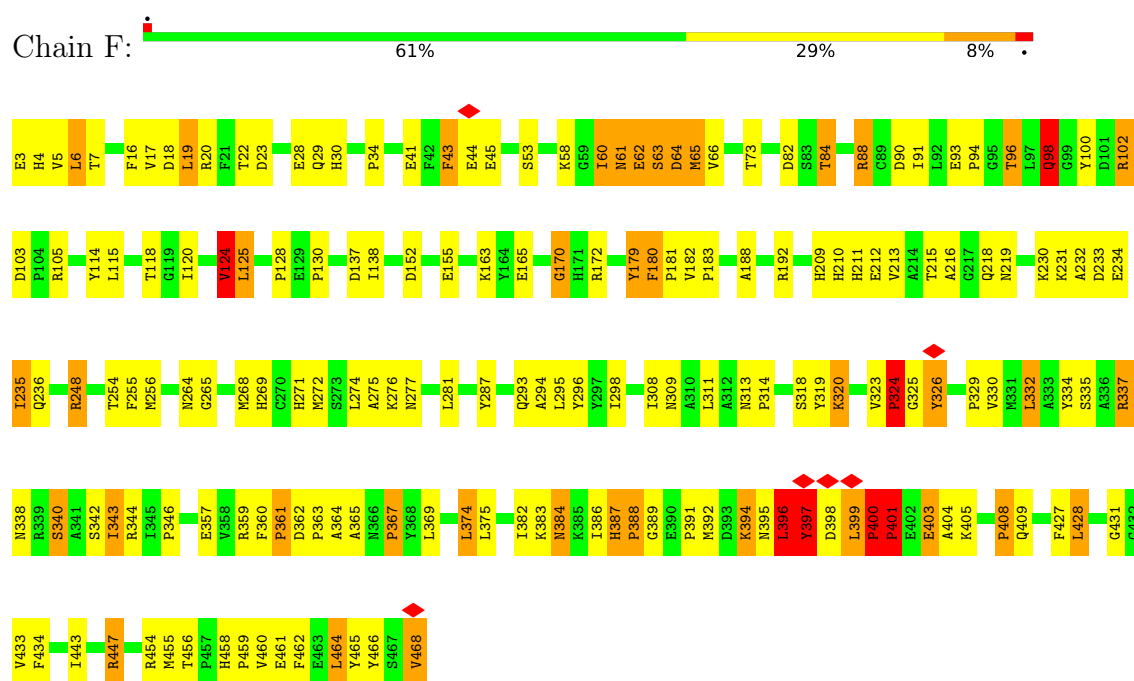
• Molecule 1: Glutamine synthetase



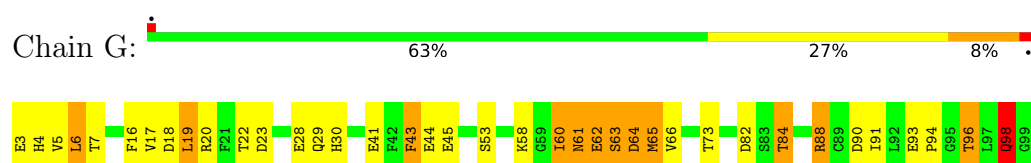
- Molecule 1: Glutamine synthetase

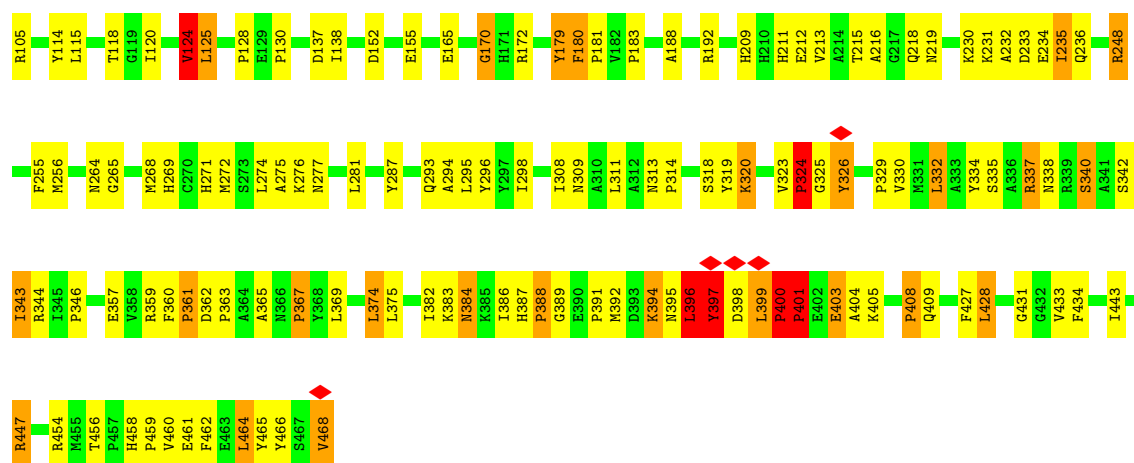


- Molecule 1: Glutamine synthetase

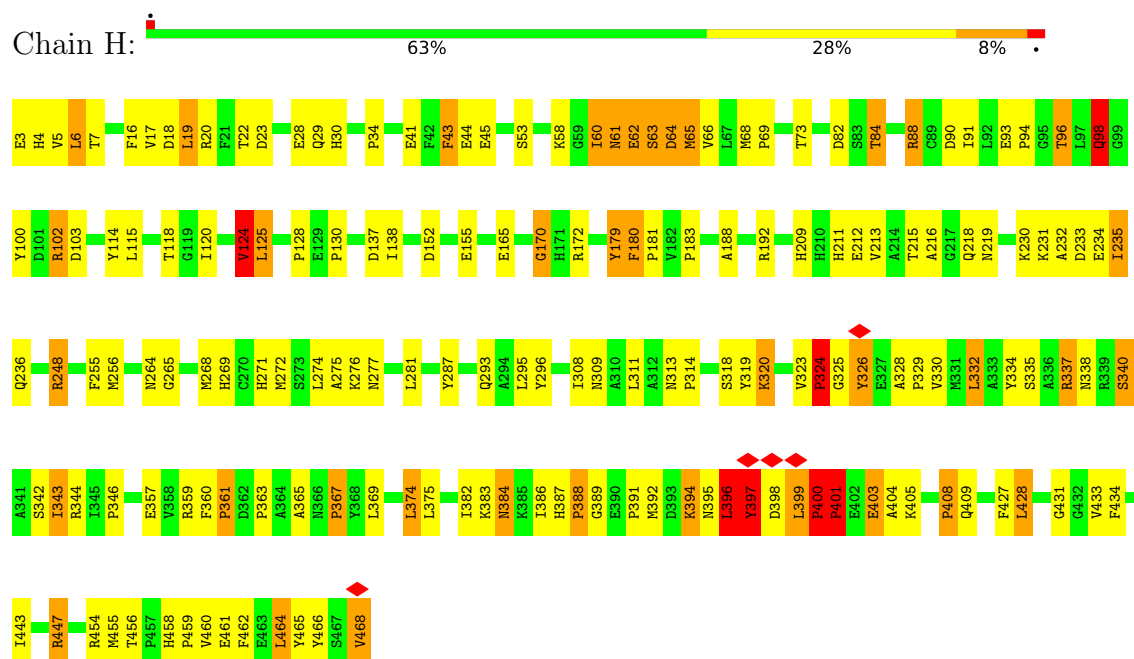


- Molecule 1: Glutamine synthetase

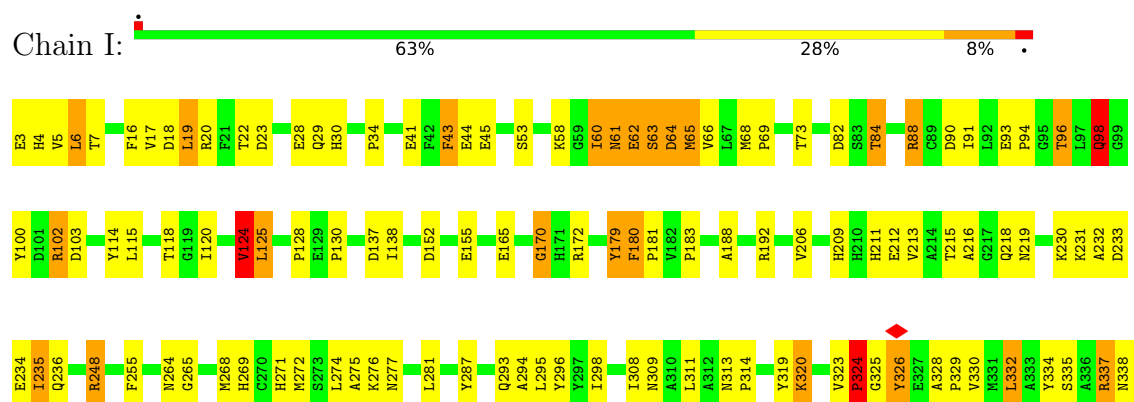




• Molecule 1: Glutamine synthetase



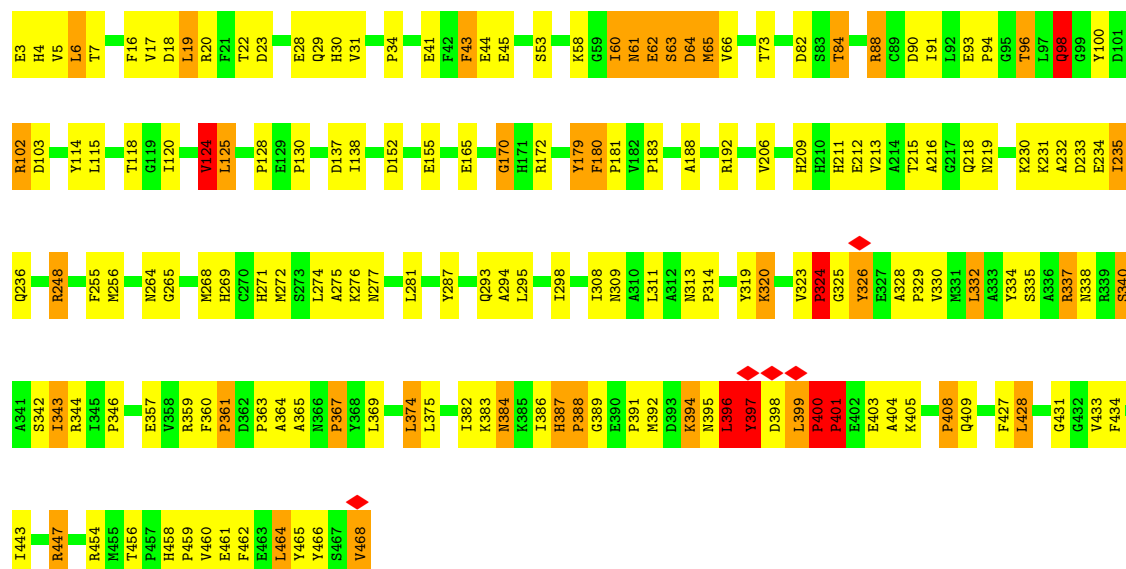
• Molecule 1: Glutamine synthetase





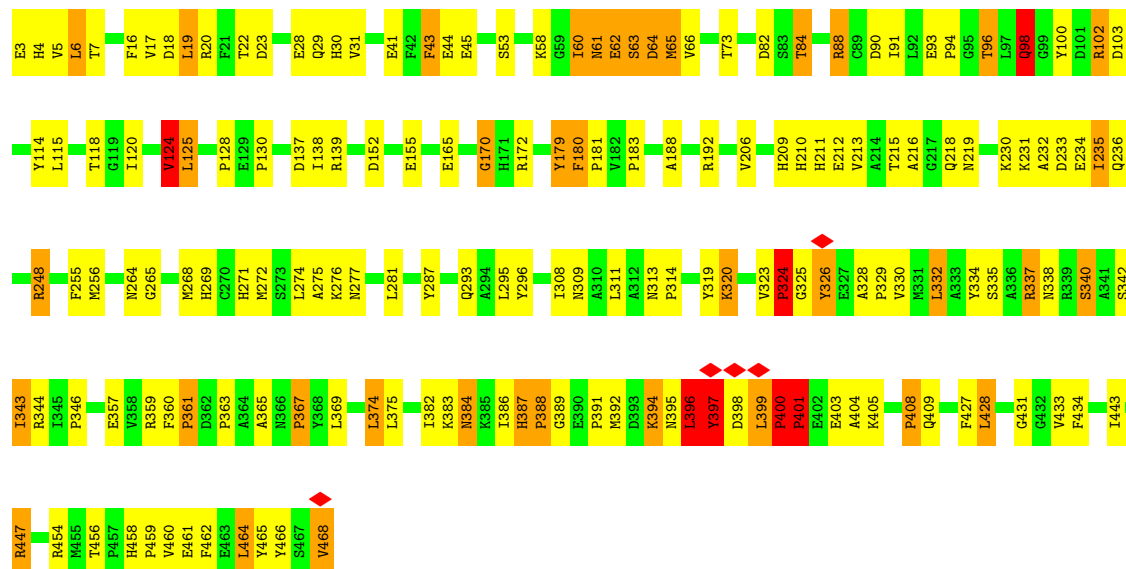
• Molecule 1: Glutamine synthetase

Chain J: 63% 28% 8%

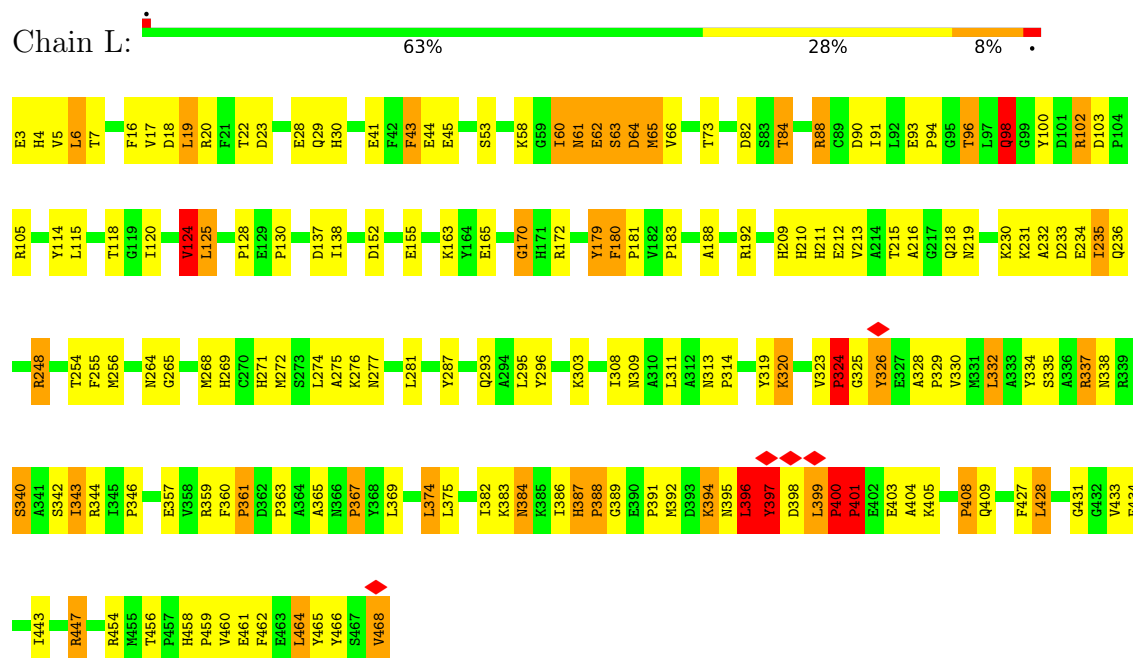


• Molecule 1: Glutamine synthetase

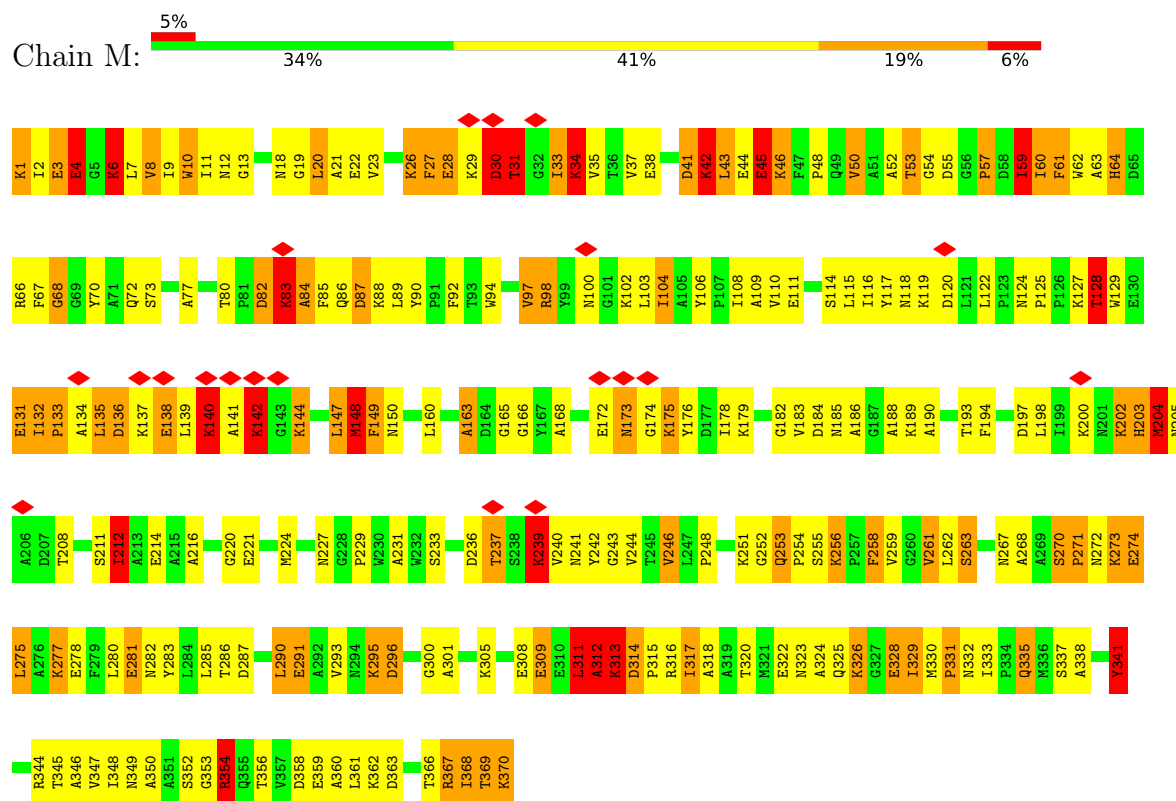
Chain K: 63% 27% 8%



• Molecule 1: Glutamine synthetase

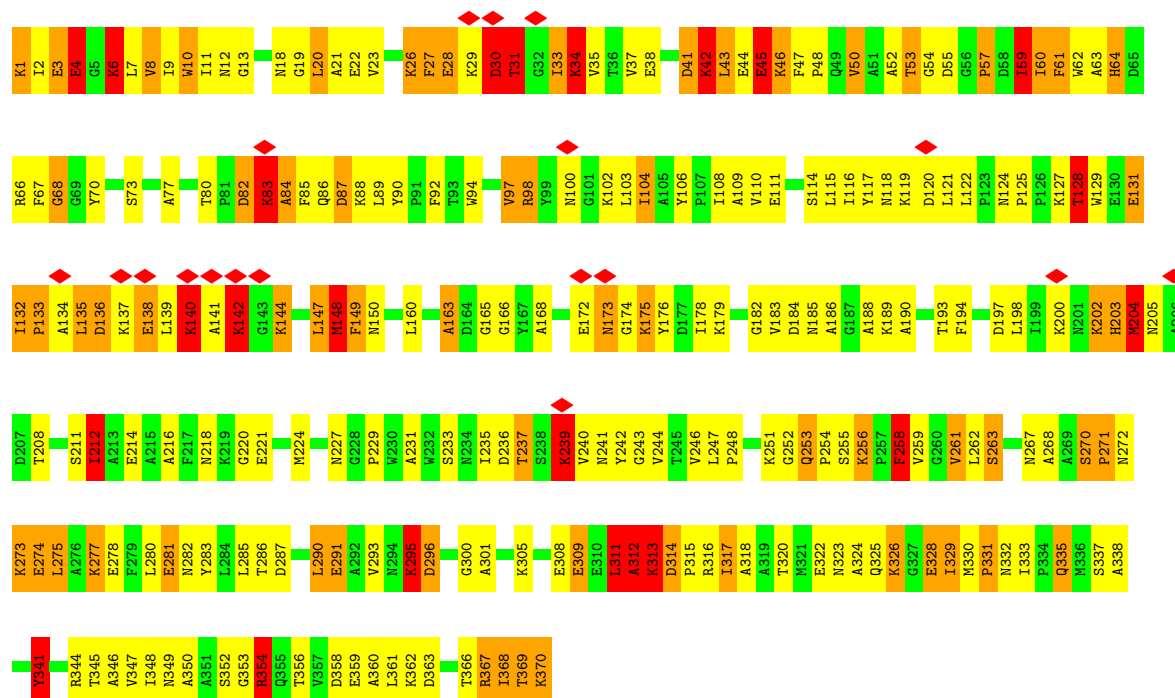


• Molecule 2: Maltose-binding periplasmic protein

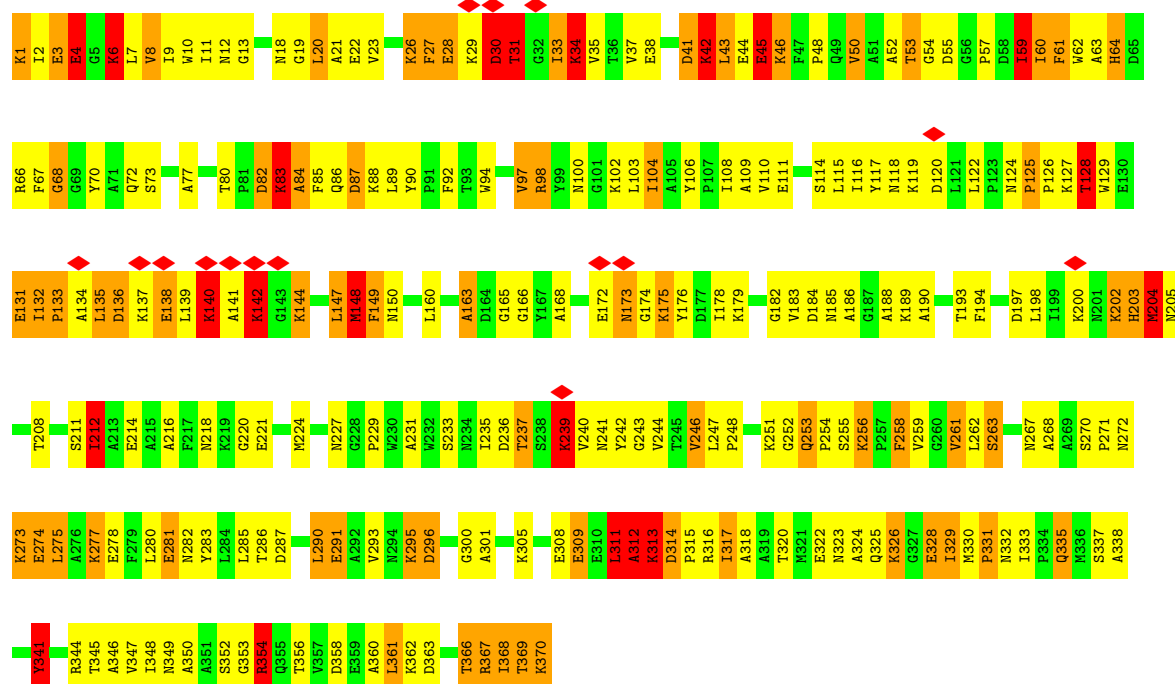


• Molecule 2: Maltose-binding periplasmic protein



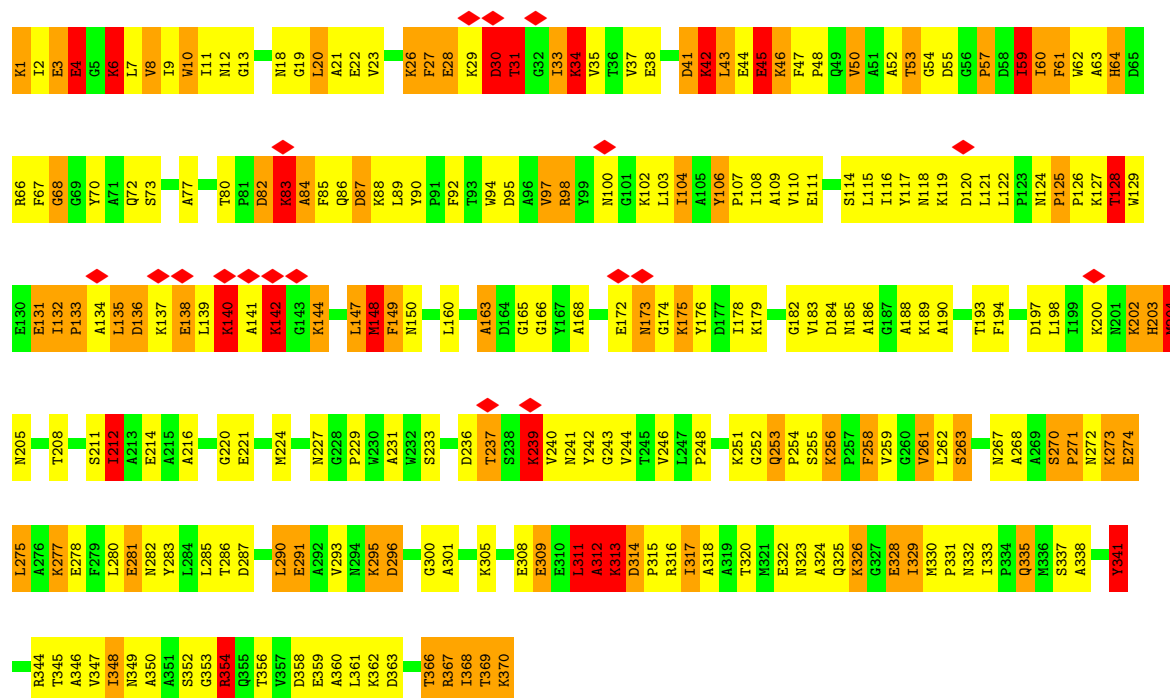


• Molecule 2: Maltose-binding periplasmic protein

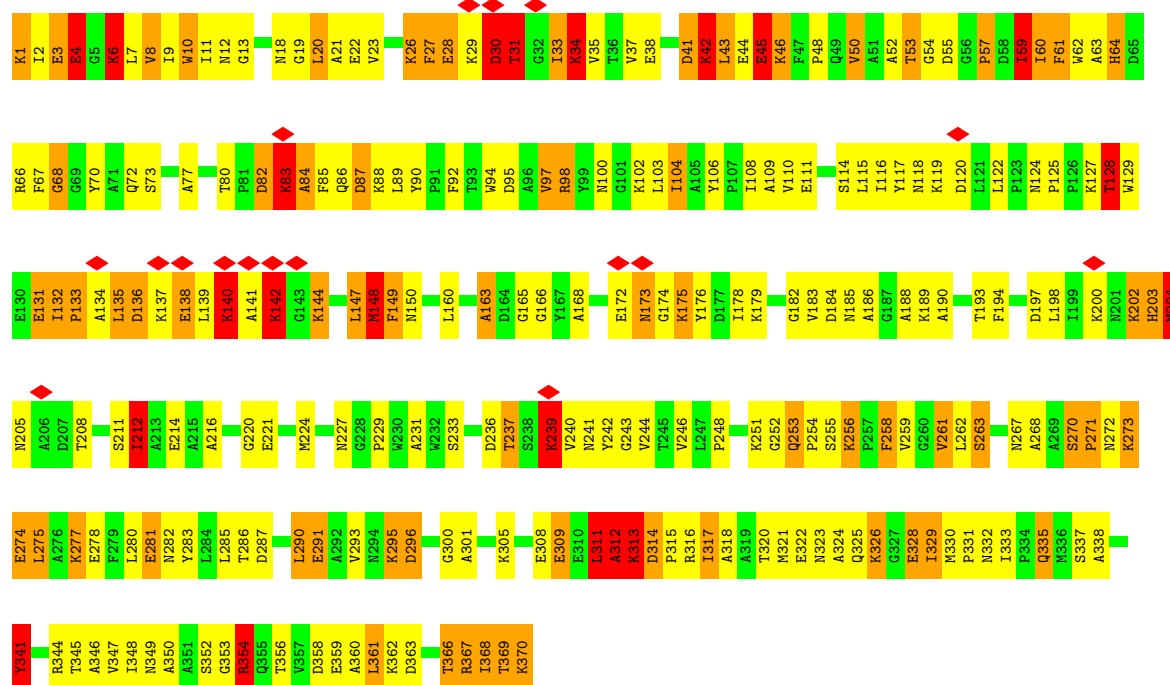


• Molecule 2: Maltose-binding periplasmic protein



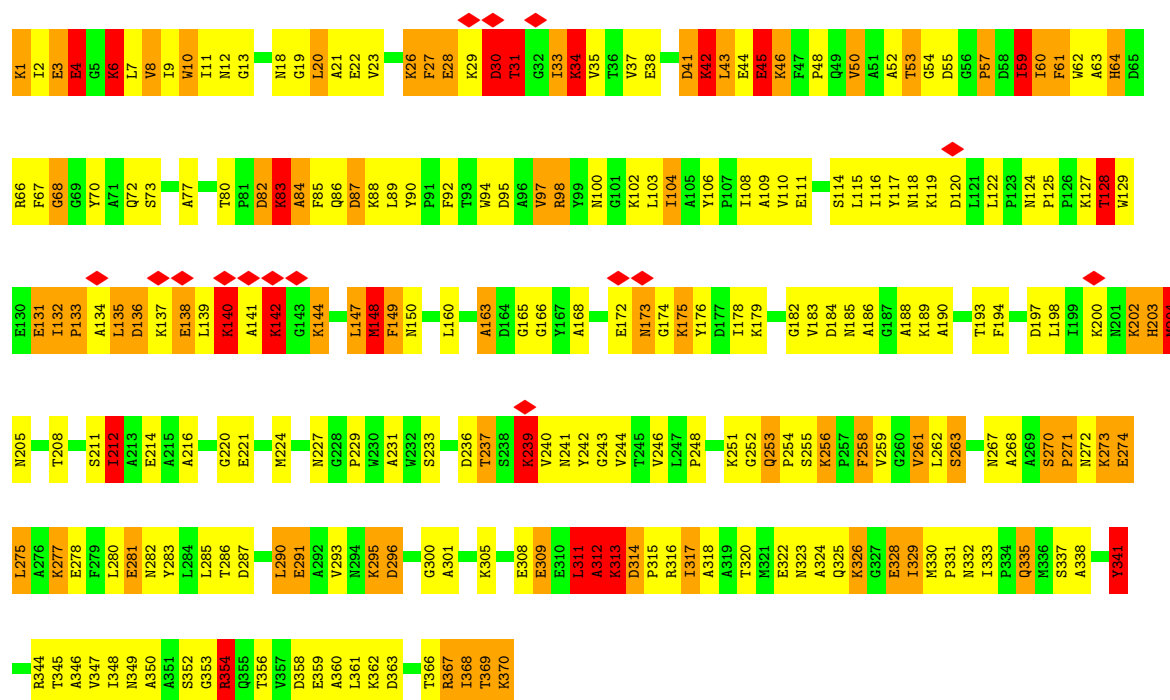


• Molecule 2: Maltose-binding periplasmic protein

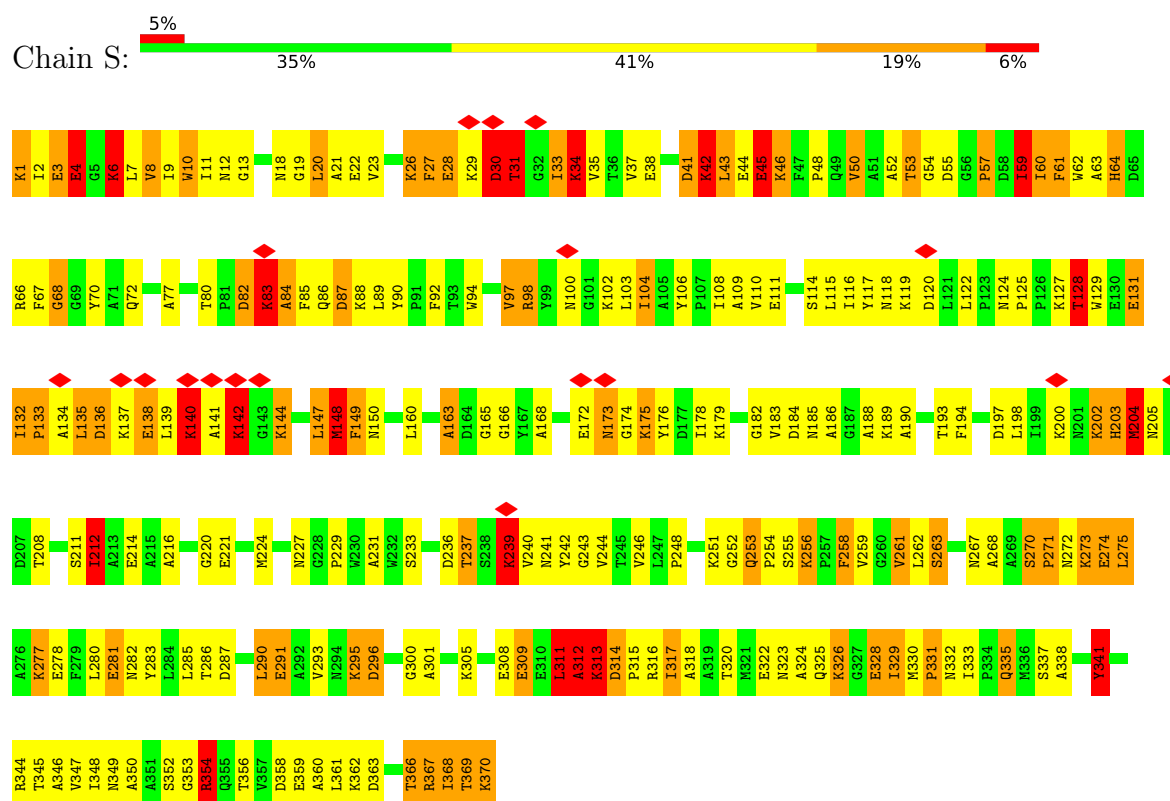


• Molecule 2: Maltose-binding periplasmic protein



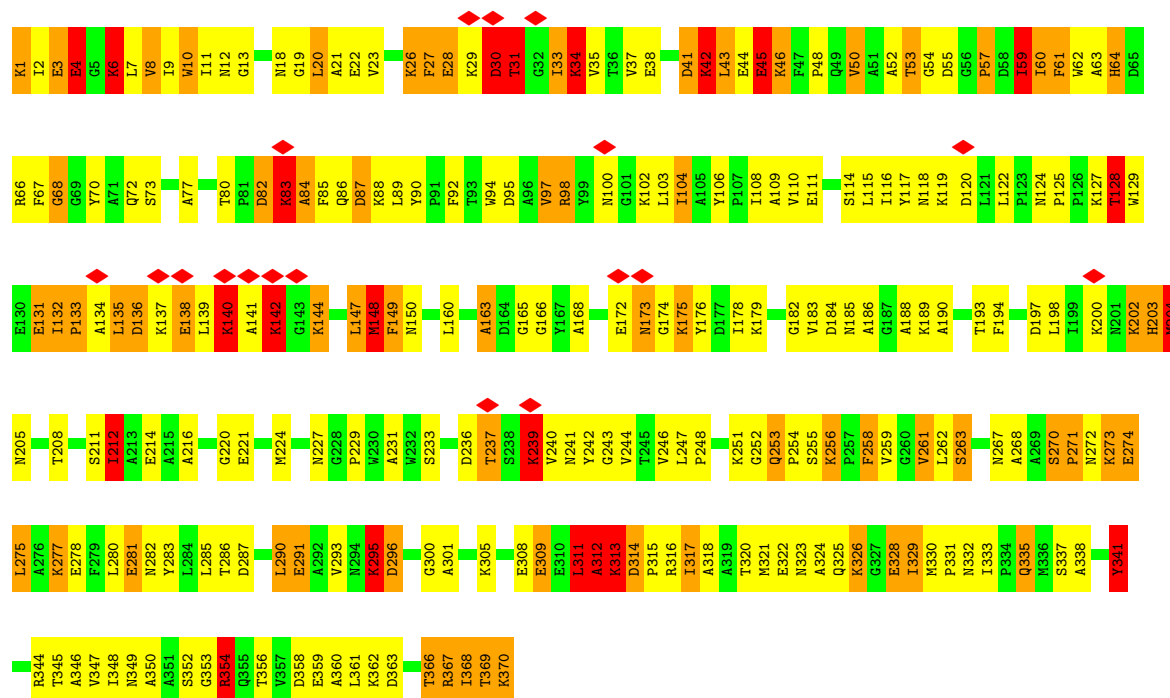


• Molecule 2: Maltose-binding periplasmic protein

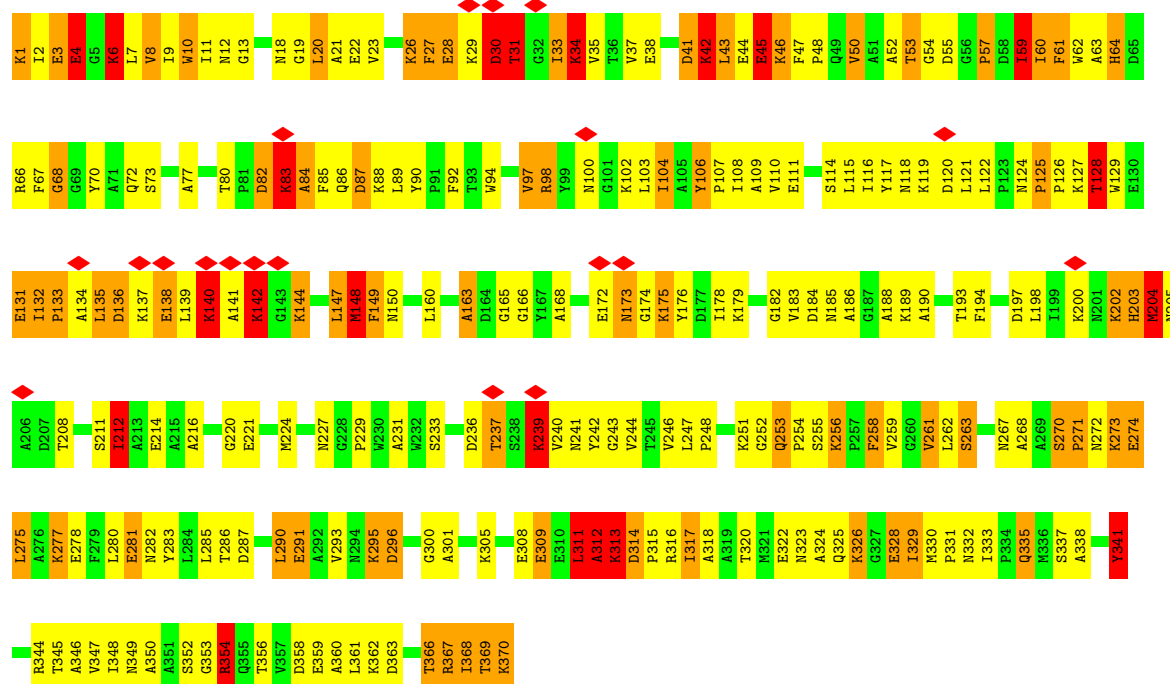


• Molecule 2: Maltose-binding periplasmic protein



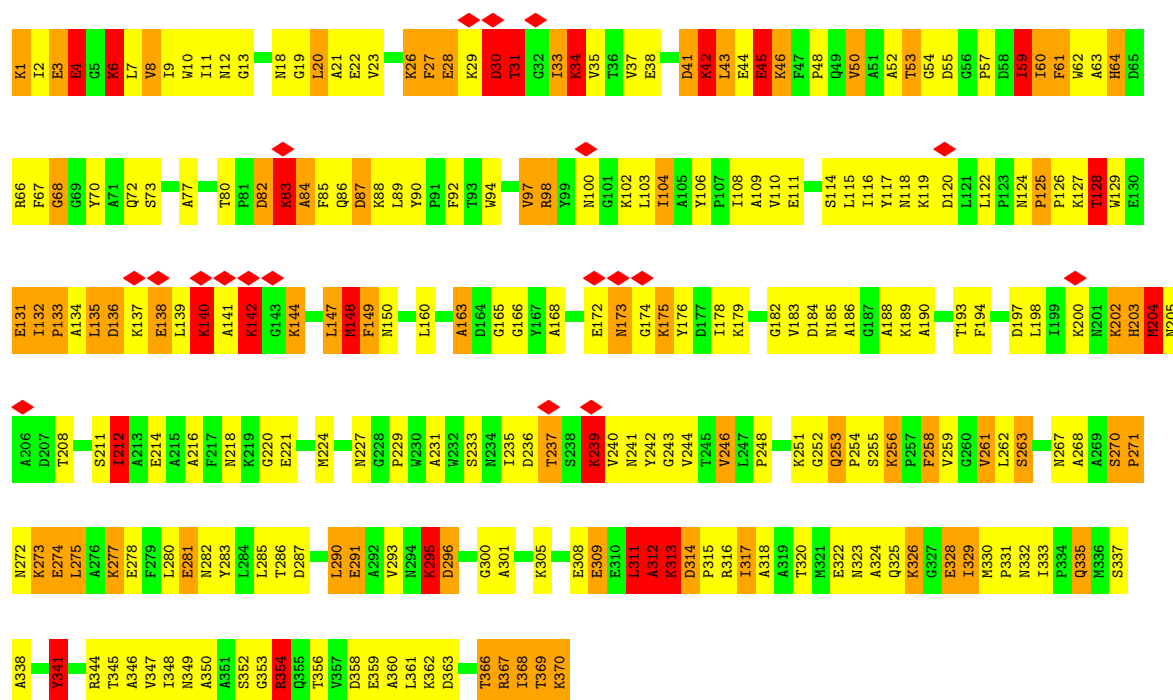


• Molecule 2: Maltose-binding periplasmic protein

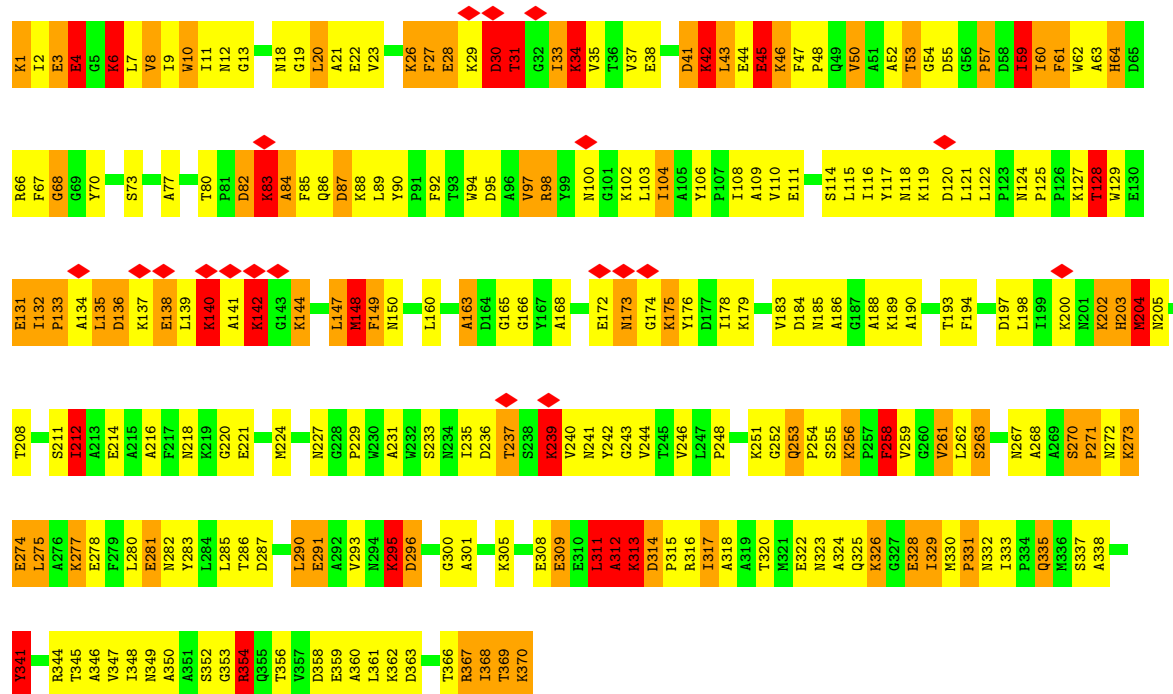


• Molecule 2: Maltose-binding periplasmic protein



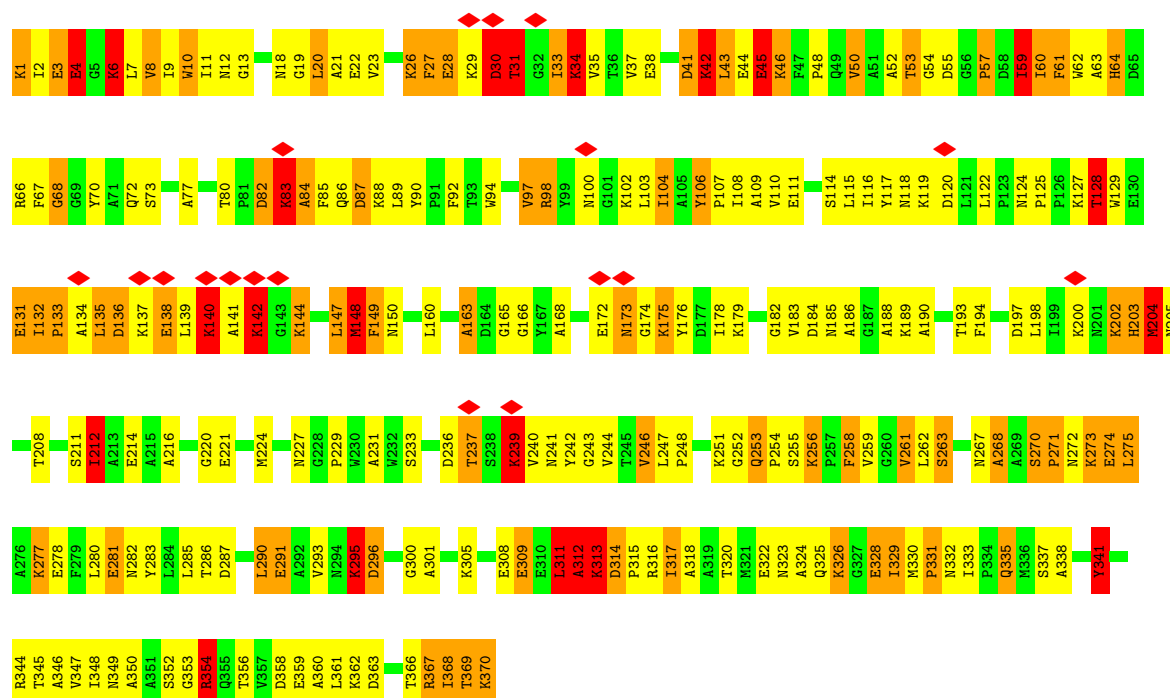


• Molecule 2: Maltose-binding periplasmic protein

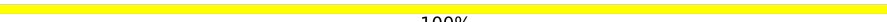


• Molecule 2: Maltose-binding periplasmic protein



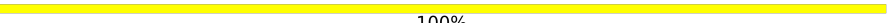


- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain Y:  100%

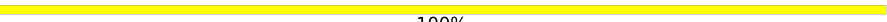
GLC1
GLC2

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain Z:  100%

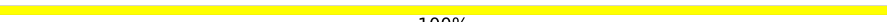
GLC1
GLC2

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain a:  100%

GLC1
GLC2

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain b:  100%

GLC1
GLC2

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain c:  100%

GLC1
GLC2

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain d:  100%

GLC1
GLC2

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain e:  100%

GLC1
GLC2

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain f:  100%

GLC1
GLC2

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain g:  100%

GLC1
GLC2

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain h:  100%

GLC1
GLC2

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain i:  100%

GLC1
GLC2

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain j:  100%

GLC1
GLC2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D6	Depositor
Number of particles used	13847	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.009	Depositor
Minimum map value	-0.003	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0015	Depositor
Map size ($\text{\AA}$)	326.2, 326.2, 326.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8155, 0.8155, 0.8155	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GLC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.66	0/3713	1.24	42/5028 (0.8%)
1	B	0.66	0/3713	1.24	41/5028 (0.8%)
1	C	0.66	0/3713	1.25	41/5028 (0.8%)
1	D	0.66	0/3713	1.25	41/5028 (0.8%)
1	E	0.66	0/3713	1.25	42/5028 (0.8%)
1	F	0.66	0/3713	1.25	42/5028 (0.8%)
1	G	0.66	0/3713	1.25	42/5028 (0.8%)
1	H	0.66	0/3713	1.25	42/5028 (0.8%)
1	I	0.66	0/3713	1.24	41/5028 (0.8%)
1	J	0.66	0/3713	1.24	41/5028 (0.8%)
1	K	0.66	0/3713	1.25	41/5028 (0.8%)
1	L	0.66	0/3713	1.25	41/5028 (0.8%)
2	M	1.95	52/2930 (1.8%)	2.90	307/3979 (7.7%)
2	N	1.95	52/2930 (1.8%)	2.90	310/3979 (7.8%)
2	O	1.95	52/2930 (1.8%)	2.90	306/3979 (7.7%)
2	P	1.95	52/2930 (1.8%)	2.90	310/3979 (7.8%)
2	Q	1.95	52/2930 (1.8%)	2.90	309/3979 (7.8%)
2	R	1.95	52/2930 (1.8%)	2.90	306/3979 (7.7%)
2	S	1.95	52/2930 (1.8%)	2.90	305/3979 (7.7%)
2	T	1.95	52/2930 (1.8%)	2.90	309/3979 (7.8%)
2	U	1.95	52/2930 (1.8%)	2.90	309/3979 (7.8%)
2	V	1.95	52/2930 (1.8%)	2.90	308/3979 (7.7%)
2	W	1.95	52/2930 (1.8%)	2.90	307/3979 (7.7%)
2	X	1.95	52/2930 (1.8%)	2.90	309/3979 (7.8%)
All	All	1.39	624/79716 (0.8%)	2.14	4192/108084 (3.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	2
2	N	0	2
2	O	0	2
2	P	0	2
2	Q	0	2
2	R	0	2
2	S	0	2
2	T	0	2
2	U	0	2
2	V	0	2
2	W	0	2
2	X	0	2
All	All	0	24

All (624) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	369	THR	C-N	25.18	1.68	1.33
2	O	369	THR	C-N	24.74	1.68	1.33
2	T	369	THR	C-N	24.74	1.68	1.33
2	P	369	THR	C-N	24.73	1.68	1.33
2	Q	369	THR	C-N	24.72	1.68	1.33
2	U	369	THR	C-N	24.70	1.68	1.33
2	V	369	THR	C-N	24.69	1.68	1.33
2	R	369	THR	C-N	24.67	1.67	1.33
2	S	369	THR	C-N	24.66	1.67	1.33
2	W	369	THR	C-N	24.65	1.67	1.33
2	N	369	THR	C-N	24.64	1.67	1.33
2	X	369	THR	C-N	24.63	1.67	1.33
2	U	370	LYS	C-O	12.65	1.48	1.23
2	V	370	LYS	C-O	12.65	1.48	1.23
2	R	370	LYS	C-O	12.64	1.48	1.23
2	N	370	LYS	C-O	12.63	1.48	1.23
2	W	370	LYS	C-O	12.63	1.48	1.23
2	M	370	LYS	C-O	12.61	1.48	1.23
2	X	370	LYS	C-O	12.61	1.48	1.23
2	T	370	LYS	C-O	12.60	1.48	1.23
2	S	370	LYS	C-O	12.60	1.48	1.23
2	P	370	LYS	C-O	12.59	1.48	1.23
2	Q	370	LYS	C-O	12.59	1.48	1.23
2	O	370	LYS	C-O	12.58	1.48	1.23
2	T	138	GLU	C-O	8.30	1.33	1.24
2	X	138	GLU	C-O	8.29	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	138	GLU	C-O	8.29	1.33	1.24
2	Q	138	GLU	C-O	8.27	1.33	1.24
2	V	138	GLU	C-O	8.27	1.33	1.24
2	N	138	GLU	C-O	8.26	1.33	1.24
2	S	138	GLU	C-O	8.25	1.33	1.24
2	U	138	GLU	C-O	8.25	1.33	1.24
2	O	138	GLU	C-O	8.24	1.33	1.24
2	R	138	GLU	C-O	8.22	1.33	1.24
2	M	138	GLU	C-O	8.20	1.33	1.24
2	W	138	GLU	C-O	8.19	1.33	1.24
2	W	149	PHE	N-CA	7.59	1.55	1.45
2	P	149	PHE	N-CA	7.59	1.55	1.45
2	R	149	PHE	N-CA	7.58	1.55	1.45
2	N	149	PHE	N-CA	7.58	1.55	1.45
2	O	149	PHE	N-CA	7.57	1.55	1.45
2	X	149	PHE	N-CA	7.54	1.55	1.45
2	S	149	PHE	N-CA	7.54	1.55	1.45
2	V	149	PHE	N-CA	7.53	1.55	1.45
2	M	149	PHE	N-CA	7.53	1.55	1.45
2	U	149	PHE	N-CA	7.50	1.55	1.45
2	Q	149	PHE	N-CA	7.49	1.55	1.45
2	T	149	PHE	N-CA	7.48	1.55	1.45
2	R	189	LYS	C-O	7.28	1.32	1.24
2	U	189	LYS	C-O	7.26	1.32	1.24
2	O	189	LYS	C-O	7.26	1.32	1.24
2	P	189	LYS	C-O	7.24	1.32	1.24
2	M	189	LYS	C-O	7.23	1.32	1.24
2	V	189	LYS	C-O	7.22	1.32	1.24
2	N	189	LYS	C-O	7.22	1.32	1.24
2	X	189	LYS	C-O	7.21	1.32	1.24
2	W	189	LYS	C-O	7.21	1.32	1.24
2	Q	189	LYS	C-O	7.20	1.32	1.24
2	S	189	LYS	C-O	7.17	1.32	1.24
2	T	189	LYS	C-O	7.14	1.32	1.24
2	W	212	ILE	C-N	7.11	1.43	1.33
2	R	212	ILE	C-N	7.10	1.43	1.33
2	N	212	ILE	C-N	7.08	1.42	1.33
2	X	212	ILE	C-N	7.07	1.42	1.33
2	U	212	ILE	C-N	7.06	1.42	1.33
2	M	212	ILE	C-N	6.91	1.43	1.33
2	Q	212	ILE	C-N	6.90	1.43	1.33
2	P	212	ILE	C-N	6.90	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	312	ALA	C-O	-6.89	1.16	1.23
2	O	212	ILE	C-N	6.88	1.43	1.33
2	N	312	ALA	C-O	-6.87	1.16	1.23
2	Q	312	ALA	C-O	-6.87	1.16	1.23
2	T	212	ILE	C-N	6.85	1.43	1.33
2	R	312	ALA	C-O	-6.85	1.16	1.23
2	V	212	ILE	C-N	6.85	1.43	1.33
2	S	312	ALA	C-O	-6.84	1.16	1.23
2	M	312	ALA	C-O	-6.84	1.16	1.23
2	U	312	ALA	C-O	-6.84	1.16	1.23
2	X	312	ALA	C-O	-6.84	1.16	1.23
2	V	312	ALA	C-O	-6.83	1.16	1.23
2	O	312	ALA	C-O	-6.82	1.16	1.23
2	P	312	ALA	C-O	-6.81	1.16	1.23
2	S	212	ILE	C-N	6.80	1.42	1.33
2	T	312	ALA	C-O	-6.80	1.16	1.23
2	R	55	ASP	N-CA	6.52	1.54	1.46
2	Q	55	ASP	N-CA	6.51	1.54	1.46
2	U	55	ASP	N-CA	6.51	1.54	1.46
2	V	55	ASP	N-CA	6.48	1.54	1.46
2	P	55	ASP	N-CA	6.48	1.54	1.46
2	X	55	ASP	N-CA	6.48	1.54	1.46
2	M	55	ASP	N-CA	6.47	1.54	1.46
2	S	55	ASP	N-CA	6.46	1.54	1.46
2	N	55	ASP	N-CA	6.46	1.54	1.46
2	T	55	ASP	N-CA	6.46	1.54	1.46
2	W	55	ASP	N-CA	6.43	1.54	1.46
2	O	55	ASP	N-CA	6.41	1.54	1.46
2	P	149	PHE	C-O	6.25	1.31	1.23
2	N	149	PHE	C-O	6.23	1.31	1.23
2	U	149	PHE	C-O	6.21	1.31	1.23
2	O	149	PHE	C-O	6.19	1.31	1.23
2	V	149	PHE	C-O	6.19	1.31	1.23
2	Q	149	PHE	C-O	6.18	1.31	1.23
2	T	149	PHE	C-O	6.17	1.31	1.23
2	M	149	PHE	C-O	6.16	1.31	1.23
2	X	149	PHE	C-O	6.16	1.31	1.23
2	W	149	PHE	C-O	6.15	1.31	1.23
2	R	149	PHE	C-O	6.14	1.31	1.23
2	S	149	PHE	C-O	6.13	1.31	1.23
2	U	248	PRO	C-O	6.11	1.30	1.23
2	W	248	PRO	C-O	6.09	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	248	PRO	C-O	6.08	1.30	1.23
2	M	262	LEU	CA-C	6.08	1.60	1.52
2	O	248	PRO	C-O	6.08	1.30	1.23
2	Q	262	LEU	CA-C	6.08	1.60	1.52
2	P	248	PRO	C-O	6.08	1.30	1.23
2	T	262	LEU	CA-C	6.08	1.60	1.52
2	X	262	LEU	CA-C	6.08	1.60	1.52
2	O	262	LEU	CA-C	6.07	1.60	1.52
2	T	248	PRO	C-O	6.07	1.30	1.23
2	S	248	PRO	C-O	6.06	1.30	1.23
2	S	262	LEU	CA-C	6.05	1.60	1.52
2	V	248	PRO	C-O	6.05	1.30	1.23
2	V	262	LEU	CA-C	6.05	1.60	1.52
2	Q	248	PRO	C-O	6.05	1.30	1.23
2	X	248	PRO	C-O	6.05	1.30	1.23
2	R	262	LEU	CA-C	6.05	1.60	1.52
2	W	262	LEU	CA-C	6.04	1.60	1.52
2	N	262	LEU	CA-C	6.04	1.60	1.52
2	U	262	LEU	CA-C	6.03	1.60	1.52
2	R	248	PRO	C-O	6.03	1.30	1.23
2	U	31	THR	CA-CB	6.03	1.63	1.53
2	M	248	PRO	C-O	6.02	1.30	1.23
2	S	31	THR	CA-CB	6.01	1.63	1.53
2	W	31	THR	CA-CB	6.00	1.63	1.53
2	N	31	THR	CA-CB	6.00	1.63	1.53
2	Q	31	THR	CA-CB	6.00	1.63	1.53
2	V	31	THR	CA-CB	6.00	1.63	1.53
2	R	31	THR	CA-CB	5.99	1.63	1.53
2	P	262	LEU	CA-C	5.98	1.60	1.52
2	M	31	THR	CA-CB	5.98	1.63	1.53
2	O	31	THR	CA-CB	5.98	1.63	1.53
2	P	31	THR	CA-CB	5.98	1.63	1.53
2	T	31	THR	CA-CB	5.97	1.63	1.53
2	X	31	THR	CA-CB	5.97	1.63	1.53
2	M	367	ARG	NE-CZ	5.91	1.39	1.33
2	U	147	LEU	CA-CB	5.91	1.64	1.53
2	Q	147	LEU	CA-CB	5.88	1.64	1.53
2	X	147	LEU	CA-CB	5.88	1.64	1.53
2	R	300	GLY	CA-C	5.88	1.60	1.51
2	N	300	GLY	CA-C	5.88	1.60	1.51
2	W	147	LEU	CA-CB	5.88	1.64	1.53
2	V	147	LEU	CA-CB	5.88	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	300	GLY	CA-C	5.88	1.60	1.51
2	R	147	LEU	CA-CB	5.88	1.63	1.53
2	T	367	ARG	NE-CZ	5.88	1.39	1.33
2	O	147	LEU	CA-CB	5.87	1.63	1.53
2	S	147	LEU	CA-CB	5.87	1.63	1.53
2	T	300	GLY	CA-C	5.87	1.60	1.51
2	V	300	GLY	CA-C	5.87	1.60	1.51
2	O	300	GLY	CA-C	5.86	1.60	1.51
2	P	147	LEU	CA-CB	5.86	1.63	1.53
2	P	300	GLY	CA-C	5.86	1.60	1.51
2	X	30	ASP	N-CA	5.86	1.53	1.46
2	Q	300	GLY	CA-C	5.86	1.60	1.51
2	P	296	ASP	C-O	5.86	1.31	1.24
2	Q	367	ARG	NE-CZ	5.86	1.39	1.33
2	T	97	VAL	C-N	-5.86	1.25	1.33
2	N	147	LEU	CA-CB	5.86	1.63	1.53
2	N	296	ASP	C-O	5.86	1.31	1.24
2	O	30	ASP	N-CA	5.85	1.53	1.46
2	T	147	LEU	CA-CB	5.84	1.63	1.53
2	W	367	ARG	NE-CZ	5.84	1.39	1.33
2	V	367	ARG	NE-CZ	5.84	1.39	1.33
2	M	147	LEU	CA-CB	5.83	1.63	1.53
2	U	300	GLY	CA-C	5.83	1.60	1.51
2	S	367	ARG	NE-CZ	5.83	1.39	1.33
2	W	300	GLY	CA-C	5.83	1.60	1.51
2	N	367	ARG	NE-CZ	5.83	1.39	1.33
2	W	30	ASP	N-CA	5.83	1.53	1.46
2	X	300	GLY	CA-C	5.83	1.60	1.51
2	P	367	ARG	NE-CZ	5.83	1.39	1.33
2	R	367	ARG	NE-CZ	5.83	1.39	1.33
2	V	30	ASP	N-CA	5.82	1.53	1.46
2	X	367	ARG	NE-CZ	5.82	1.39	1.33
2	S	30	ASP	N-CA	5.82	1.53	1.46
2	S	300	GLY	CA-C	5.82	1.60	1.51
2	X	97	VAL	C-N	-5.82	1.25	1.33
2	T	30	ASP	N-CA	5.82	1.53	1.46
2	W	97	VAL	C-N	-5.82	1.25	1.33
2	M	30	ASP	N-CA	5.82	1.53	1.46
2	P	30	ASP	N-CA	5.81	1.53	1.46
2	M	97	VAL	C-N	-5.81	1.25	1.33
2	U	296	ASP	C-O	5.81	1.31	1.24
2	N	30	ASP	N-CA	5.80	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	367	ARG	NE-CZ	5.80	1.39	1.33
2	O	296	ASP	C-O	5.80	1.31	1.24
2	R	296	ASP	C-O	5.80	1.31	1.24
2	Q	296	ASP	C-O	5.80	1.31	1.24
2	U	97	VAL	C-N	-5.80	1.25	1.33
2	R	30	ASP	N-CA	5.79	1.53	1.46
2	O	97	VAL	C-N	-5.79	1.25	1.33
2	V	97	VAL	C-N	-5.79	1.25	1.33
2	V	296	ASP	C-O	5.79	1.31	1.24
2	W	296	ASP	C-O	5.79	1.31	1.24
2	O	367	ARG	NE-CZ	5.78	1.39	1.33
2	P	97	VAL	C-N	-5.78	1.25	1.33
2	Q	30	ASP	N-CA	5.78	1.53	1.46
2	U	30	ASP	N-CA	5.78	1.53	1.46
2	P	312	ALA	C-N	-5.78	1.25	1.33
2	W	117	TYR	N-CA	5.78	1.53	1.45
2	N	117	TYR	N-CA	5.78	1.53	1.45
2	S	296	ASP	C-O	5.78	1.31	1.24
2	T	296	ASP	C-O	5.78	1.31	1.24
2	O	312	ALA	C-N	-5.77	1.25	1.33
2	T	261	VAL	CA-CB	5.77	1.60	1.53
2	T	312	ALA	C-N	-5.77	1.25	1.33
2	O	261	VAL	CA-CB	5.76	1.60	1.53
2	T	117	TYR	N-CA	5.76	1.53	1.45
2	U	261	VAL	CA-CB	5.76	1.60	1.53
2	V	261	VAL	CA-CB	5.76	1.60	1.53
2	N	97	VAL	C-N	-5.76	1.25	1.33
2	X	296	ASP	C-O	5.76	1.31	1.24
2	W	261	VAL	CA-CB	5.75	1.60	1.53
2	M	117	TYR	N-CA	5.75	1.53	1.45
2	S	111	GLU	N-CA	5.75	1.53	1.46
2	R	97	VAL	C-N	-5.75	1.25	1.33
2	S	117	TYR	N-CA	5.75	1.53	1.45
2	P	261	VAL	CA-CB	5.75	1.60	1.53
2	S	97	VAL	C-N	-5.75	1.25	1.33
2	W	368	ILE	CA-CB	5.75	1.61	1.54
2	O	368	ILE	CA-CB	5.74	1.61	1.54
2	P	117	TYR	N-CA	5.74	1.53	1.45
2	R	117	TYR	N-CA	5.74	1.53	1.45
2	X	117	TYR	N-CA	5.74	1.53	1.45
2	X	261	VAL	CA-CB	5.74	1.60	1.53
2	Q	261	VAL	CA-CB	5.74	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	296	ASP	C-O	5.74	1.31	1.24
2	U	117	TYR	N-CA	5.74	1.53	1.45
2	O	117	TYR	N-CA	5.74	1.53	1.45
2	V	117	TYR	N-CA	5.74	1.53	1.45
2	S	261	VAL	CA-CB	5.73	1.60	1.53
2	N	80	THR	CA-CB	5.73	1.60	1.53
2	N	312	ALA	C-N	-5.73	1.25	1.33
2	Q	97	VAL	C-N	-5.73	1.25	1.33
2	V	312	ALA	C-N	-5.73	1.25	1.33
2	R	261	VAL	CA-CB	5.73	1.60	1.53
2	Q	117	TYR	N-CA	5.72	1.53	1.45
2	R	312	ALA	C-N	-5.72	1.25	1.33
2	Q	312	ALA	C-N	-5.72	1.25	1.33
2	U	312	ALA	C-N	-5.72	1.25	1.33
2	S	80	THR	CA-CB	5.71	1.60	1.53
2	T	368	ILE	CA-CB	5.71	1.61	1.54
2	N	125	PRO	CA-CB	-5.71	1.49	1.54
2	X	312	ALA	C-N	-5.71	1.25	1.33
2	S	312	ALA	C-N	-5.71	1.25	1.33
2	T	80	THR	CA-CB	5.71	1.60	1.53
2	N	368	ILE	CA-CB	5.70	1.61	1.54
2	N	261	VAL	CA-CB	5.70	1.60	1.53
2	P	111	GLU	N-CA	5.70	1.52	1.46
2	P	125	PRO	CA-CB	-5.70	1.49	1.54
2	M	261	VAL	CA-CB	5.70	1.60	1.53
2	M	312	ALA	C-N	-5.70	1.25	1.33
2	N	111	GLU	N-CA	5.70	1.52	1.46
2	V	111	GLU	N-CA	5.70	1.52	1.46
2	Q	227	ASN	CA-C	5.69	1.59	1.52
2	U	111	GLU	N-CA	5.69	1.52	1.46
2	U	368	ILE	CA-CB	5.69	1.61	1.54
2	V	368	ILE	CA-CB	5.69	1.61	1.54
2	W	312	ALA	C-N	-5.69	1.25	1.33
2	O	111	GLU	N-CA	5.69	1.52	1.46
2	X	111	GLU	N-CA	5.68	1.52	1.46
2	P	368	ILE	CA-CB	5.68	1.61	1.54
2	M	368	ILE	CA-CB	5.68	1.61	1.54
2	U	220	GLY	C-O	5.68	1.31	1.24
2	W	227	ASN	CA-C	5.68	1.59	1.52
2	W	111	GLU	N-CA	5.68	1.52	1.46
2	U	227	ASN	CA-C	5.67	1.59	1.52
2	N	227	ASN	CA-C	5.67	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	227	ASN	CA-C	5.67	1.59	1.52
2	U	80	THR	CA-CB	5.66	1.60	1.53
2	V	227	ASN	CA-C	5.66	1.59	1.52
2	X	80	THR	CA-CB	5.66	1.60	1.53
2	S	368	ILE	CA-CB	5.66	1.61	1.54
2	T	220	GLY	C-O	5.66	1.31	1.24
2	U	125	PRO	CA-CB	-5.66	1.49	1.54
2	Q	80	THR	CA-CB	5.66	1.60	1.53
2	V	80	THR	CA-CB	5.66	1.60	1.53
2	V	125	PRO	CA-CB	-5.65	1.49	1.54
2	X	368	ILE	CA-CB	5.65	1.61	1.54
2	M	80	THR	CA-CB	5.65	1.60	1.53
2	P	80	THR	CA-CB	5.65	1.60	1.53
2	S	125	PRO	CA-CB	-5.65	1.49	1.54
2	M	111	GLU	N-CA	5.65	1.52	1.46
2	Q	111	GLU	N-CA	5.65	1.52	1.46
2	R	368	ILE	CA-CB	5.65	1.61	1.54
2	W	125	PRO	CA-CB	-5.65	1.49	1.54
2	P	220	GLY	C-O	5.65	1.31	1.24
2	T	111	GLU	N-CA	5.65	1.52	1.46
2	R	111	GLU	N-CA	5.65	1.52	1.46
2	S	315	PRO	C-N	-5.65	1.26	1.33
2	M	220	GLY	C-O	5.64	1.31	1.24
2	O	220	GLY	C-O	5.64	1.31	1.24
2	M	227	ASN	CA-C	5.64	1.59	1.52
2	P	227	ASN	CA-C	5.64	1.59	1.52
2	X	220	GLY	C-O	5.64	1.31	1.24
2	O	227	ASN	CA-C	5.64	1.59	1.52
2	R	227	ASN	CA-C	5.63	1.59	1.52
2	X	227	ASN	CA-C	5.63	1.59	1.52
2	Q	125	PRO	CA-CB	-5.63	1.49	1.54
2	R	80	THR	CA-CB	5.63	1.60	1.53
2	T	227	ASN	CA-C	5.63	1.59	1.52
2	P	194	PHE	C-N	-5.63	1.26	1.33
2	V	220	GLY	C-O	5.63	1.31	1.24
2	Q	368	ILE	CA-CB	5.62	1.61	1.54
2	O	125	PRO	CA-CB	-5.62	1.49	1.54
2	Q	220	GLY	C-O	5.62	1.31	1.24
2	O	315	PRO	C-N	-5.62	1.26	1.33
2	N	315	PRO	C-N	-5.62	1.26	1.33
2	W	220	GLY	C-O	5.61	1.31	1.24
2	M	315	PRO	C-N	-5.61	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	315	PRO	C-N	-5.61	1.26	1.33
2	R	125	PRO	CA-CB	-5.61	1.49	1.54
2	R	220	GLY	C-O	5.61	1.31	1.24
2	T	194	PHE	C-N	-5.61	1.26	1.33
2	W	315	PRO	C-N	-5.61	1.26	1.33
2	V	315	PRO	C-N	-5.60	1.26	1.33
2	W	80	THR	CA-CB	5.60	1.60	1.53
2	X	125	PRO	CA-CB	-5.60	1.49	1.54
2	Q	315	PRO	C-N	-5.59	1.26	1.33
2	O	80	THR	CA-CB	5.59	1.60	1.53
2	P	315	PRO	C-N	-5.59	1.26	1.33
2	O	194	PHE	C-N	-5.59	1.26	1.33
2	R	315	PRO	C-N	-5.59	1.26	1.33
2	S	345	THR	C-O	5.59	1.30	1.24
2	M	125	PRO	CA-CB	-5.58	1.49	1.54
2	M	194	PHE	C-N	-5.58	1.26	1.33
2	U	345	THR	C-O	5.58	1.30	1.24
2	V	345	THR	C-O	5.58	1.30	1.24
2	O	345	THR	C-O	5.58	1.30	1.24
2	S	194	PHE	C-N	-5.58	1.26	1.33
2	U	315	PRO	C-N	-5.58	1.26	1.33
2	O	224	MET	N-CA	5.57	1.53	1.45
2	S	220	GLY	C-O	5.57	1.31	1.24
2	W	194	PHE	C-N	-5.57	1.26	1.33
2	X	315	PRO	C-N	-5.56	1.26	1.33
2	R	194	PHE	C-N	-5.56	1.26	1.33
2	V	194	PHE	C-N	-5.56	1.26	1.33
2	R	345	THR	C-O	5.55	1.30	1.24
2	X	345	THR	C-O	5.55	1.30	1.24
2	N	194	PHE	C-N	-5.55	1.26	1.33
2	N	220	GLY	C-O	5.55	1.31	1.24
2	W	345	THR	C-O	5.55	1.30	1.24
2	T	125	PRO	CA-CB	-5.55	1.49	1.54
2	N	345	THR	C-O	5.54	1.30	1.24
2	M	345	THR	C-O	5.54	1.30	1.24
2	T	188	ALA	C-O	5.54	1.30	1.24
2	P	345	THR	C-O	5.53	1.30	1.24
2	T	345	THR	C-O	5.53	1.30	1.24
2	U	194	PHE	C-N	-5.53	1.26	1.33
2	Q	194	PHE	C-N	-5.52	1.26	1.33
2	Q	345	THR	C-O	5.52	1.30	1.24
2	R	188	ALA	C-O	5.52	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	224	MET	N-CA	5.52	1.52	1.45
2	N	188	ALA	C-O	5.52	1.30	1.24
2	X	194	PHE	C-N	-5.52	1.26	1.33
2	S	313	LYS	N-CA	-5.51	1.39	1.46
2	W	188	ALA	C-O	5.51	1.30	1.24
2	P	224	MET	N-CA	5.50	1.52	1.45
2	X	94	TRP	C-N	-5.50	1.26	1.34
2	R	224	MET	N-CA	5.49	1.52	1.45
2	W	224	MET	N-CA	5.49	1.52	1.45
2	M	188	ALA	C-O	5.49	1.30	1.24
2	U	224	MET	N-CA	5.49	1.52	1.45
2	V	224	MET	N-CA	5.49	1.52	1.45
2	N	94	TRP	C-N	-5.49	1.26	1.34
2	S	188	ALA	C-O	5.49	1.30	1.24
2	V	188	ALA	C-O	5.49	1.30	1.24
2	M	313	LYS	N-CA	-5.48	1.39	1.46
2	O	188	ALA	C-O	5.48	1.30	1.24
2	Q	313	LYS	N-CA	-5.48	1.39	1.46
2	M	224	MET	N-CA	5.47	1.52	1.45
2	O	94	TRP	C-N	-5.47	1.26	1.34
2	P	188	ALA	C-O	5.47	1.30	1.24
2	U	188	ALA	C-O	5.47	1.30	1.24
2	S	224	MET	N-CA	5.46	1.52	1.45
2	X	313	LYS	N-CA	-5.45	1.39	1.46
2	N	366	THR	CA-CB	5.45	1.61	1.53
2	W	313	LYS	N-CA	-5.45	1.39	1.46
2	Q	224	MET	N-CA	5.45	1.52	1.45
2	R	313	LYS	N-CA	-5.45	1.39	1.46
2	U	313	LYS	N-CA	-5.45	1.39	1.46
2	N	224	MET	N-CA	5.45	1.52	1.45
2	V	313	LYS	N-CA	-5.45	1.39	1.46
2	S	366	THR	CA-CB	5.45	1.61	1.53
2	S	94	TRP	C-N	-5.43	1.26	1.34
2	T	313	LYS	N-CA	-5.43	1.39	1.46
2	T	224	MET	N-CA	5.43	1.52	1.45
2	Q	366	THR	CA-CB	5.43	1.61	1.53
2	N	313	LYS	N-CA	-5.42	1.39	1.46
2	P	286	THR	CB-OG1	5.42	1.52	1.43
2	P	341	TYR	N-CA	5.42	1.53	1.46
2	X	188	ALA	C-O	5.42	1.30	1.24
2	V	94	TRP	C-N	-5.42	1.26	1.34
2	O	313	LYS	N-CA	-5.42	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	366	THR	CA-CB	5.41	1.61	1.53
2	Q	188	ALA	C-O	5.41	1.30	1.24
2	T	366	THR	CA-CB	5.41	1.61	1.53
2	V	366	THR	CA-CB	5.41	1.61	1.53
2	P	108	ILE	CA-CB	5.41	1.60	1.55
2	T	94	TRP	C-N	-5.41	1.26	1.34
2	W	94	TRP	C-N	-5.41	1.26	1.34
2	U	94	TRP	C-N	-5.41	1.26	1.34
2	U	286	THR	CB-OG1	5.41	1.52	1.43
2	R	366	THR	CA-CB	5.40	1.61	1.53
2	S	286	THR	CB-OG1	5.40	1.52	1.43
2	Q	341	TYR	N-CA	5.40	1.53	1.46
2	W	366	THR	CA-CB	5.40	1.61	1.53
2	M	366	THR	CA-CB	5.40	1.61	1.53
2	P	313	LYS	N-CA	-5.40	1.39	1.46
2	T	341	TYR	N-CA	5.40	1.53	1.46
2	Q	94	TRP	C-N	-5.40	1.26	1.34
2	N	286	THR	CB-OG1	5.40	1.52	1.43
2	Q	286	THR	CB-OG1	5.40	1.52	1.43
2	S	341	TYR	N-CA	5.40	1.52	1.46
2	T	252	GLY	C-O	5.39	1.31	1.24
2	U	341	TYR	N-CA	5.39	1.52	1.46
2	O	366	THR	CA-CB	5.39	1.61	1.53
2	P	94	TRP	C-N	-5.39	1.26	1.34
2	W	341	TYR	N-CA	5.39	1.52	1.46
2	X	366	THR	CA-CB	5.39	1.61	1.53
2	R	94	TRP	C-N	-5.38	1.26	1.34
2	R	108	ILE	CA-CB	5.38	1.60	1.55
2	R	252	GLY	C-O	5.38	1.31	1.24
2	M	108	ILE	CA-CB	5.38	1.60	1.55
2	P	366	THR	CA-CB	5.38	1.61	1.53
2	V	286	THR	CB-OG1	5.38	1.52	1.43
2	W	108	ILE	CA-CB	5.38	1.60	1.55
2	Q	311	LEU	C-N	5.38	1.41	1.34
2	U	183	VAL	N-CA	5.38	1.53	1.46
2	M	286	THR	CB-OG1	5.37	1.52	1.43
2	V	252	GLY	C-O	5.37	1.31	1.24
2	X	286	THR	CB-OG1	5.37	1.52	1.43
2	W	286	THR	CB-OG1	5.37	1.52	1.43
2	O	341	TYR	N-CA	5.37	1.52	1.46
2	X	252	GLY	C-O	5.37	1.31	1.24
2	V	341	TYR	N-CA	5.37	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	94	TRP	C-N	-5.36	1.26	1.34
2	O	286	THR	CB-OG1	5.36	1.52	1.43
2	U	252	GLY	C-O	5.36	1.31	1.24
2	R	286	THR	CB-OG1	5.36	1.52	1.43
2	S	108	ILE	CA-CB	5.36	1.60	1.55
2	M	341	TYR	N-CA	5.36	1.52	1.46
2	N	341	TYR	N-CA	5.36	1.52	1.46
2	T	183	VAL	N-CA	5.36	1.53	1.46
2	R	341	TYR	N-CA	5.36	1.52	1.46
2	U	108	ILE	CA-CB	5.36	1.60	1.55
2	V	108	ILE	CA-CB	5.35	1.60	1.55
2	M	252	GLY	C-O	5.35	1.31	1.24
2	O	108	ILE	CA-CB	5.35	1.60	1.55
2	O	311	LEU	C-N	5.35	1.41	1.34
2	O	252	GLY	C-O	5.35	1.31	1.24
2	N	108	ILE	CA-CB	5.35	1.60	1.55
2	W	252	GLY	C-O	5.35	1.31	1.24
2	N	252	GLY	C-O	5.34	1.31	1.24
2	T	286	THR	CB-OG1	5.34	1.52	1.43
2	U	311	LEU	C-N	5.34	1.41	1.34
2	M	311	LEU	C-N	5.33	1.41	1.34
2	P	252	GLY	C-O	5.33	1.31	1.24
2	Q	108	ILE	CA-CB	5.33	1.60	1.55
2	Q	252	GLY	C-O	5.33	1.31	1.24
2	Q	254	PRO	C-O	5.33	1.30	1.23
2	X	341	TYR	N-CA	5.33	1.52	1.46
2	R	254	PRO	C-O	5.33	1.30	1.23
2	V	183	VAL	N-CA	5.33	1.53	1.46
2	Q	183	VAL	N-CA	5.33	1.53	1.46
2	S	183	VAL	N-CA	5.33	1.53	1.46
2	S	252	GLY	C-O	5.33	1.31	1.24
2	W	311	LEU	C-N	5.33	1.41	1.34
2	X	108	ILE	CA-CB	5.33	1.60	1.55
2	P	183	VAL	N-CA	5.32	1.53	1.46
2	U	254	PRO	C-O	5.32	1.30	1.23
2	O	183	VAL	N-CA	5.32	1.53	1.46
2	R	311	LEU	C-N	5.32	1.41	1.34
2	V	311	LEU	C-N	5.32	1.41	1.34
2	Q	63	ALA	C-O	5.31	1.30	1.23
2	M	183	VAL	N-CA	5.31	1.53	1.46
2	X	183	VAL	N-CA	5.31	1.53	1.46
2	O	254	PRO	C-O	5.31	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	254	PRO	C-O	5.31	1.30	1.23
2	N	254	PRO	C-O	5.31	1.30	1.23
2	X	254	PRO	C-O	5.31	1.30	1.23
2	S	311	LEU	C-N	5.30	1.41	1.34
2	W	254	PRO	C-O	5.30	1.30	1.23
2	T	108	ILE	CA-CB	5.30	1.60	1.55
2	N	183	VAL	N-CA	5.30	1.53	1.46
2	O	63	ALA	C-O	5.30	1.30	1.23
2	P	311	LEU	C-N	5.30	1.41	1.34
2	X	311	LEU	C-N	5.29	1.41	1.34
2	S	254	PRO	C-O	5.29	1.30	1.23
2	N	311	LEU	C-N	5.29	1.41	1.34
2	T	311	LEU	C-N	5.29	1.41	1.34
2	W	183	VAL	N-CA	5.29	1.53	1.46
2	V	254	PRO	C-O	5.28	1.30	1.23
2	R	183	VAL	N-CA	5.28	1.53	1.46
2	O	3	GLU	C-O	5.27	1.30	1.24
2	Q	3	GLU	C-O	5.26	1.30	1.24
2	W	268	ALA	N-CA	5.25	1.52	1.46
2	T	63	ALA	C-O	5.25	1.30	1.23
2	U	3	GLU	C-O	5.25	1.30	1.24
2	W	3	GLU	C-O	5.25	1.30	1.24
2	P	63	ALA	C-O	5.25	1.30	1.23
2	U	63	ALA	C-O	5.24	1.30	1.23
2	T	268	ALA	N-CA	5.24	1.52	1.46
2	P	254	PRO	C-O	5.24	1.29	1.23
2	T	254	PRO	C-O	5.24	1.29	1.23
2	V	63	ALA	C-O	5.24	1.30	1.23
2	R	63	ALA	C-O	5.24	1.30	1.23
2	O	268	ALA	N-CA	5.24	1.52	1.46
2	P	3	GLU	C-O	5.24	1.30	1.24
2	V	3	GLU	C-O	5.24	1.30	1.24
2	N	3	GLU	C-O	5.23	1.30	1.24
2	N	268	ALA	N-CA	5.23	1.52	1.46
2	V	268	ALA	N-CA	5.23	1.52	1.46
2	P	268	ALA	N-CA	5.22	1.52	1.46
2	S	3	GLU	C-O	5.22	1.30	1.24
2	X	3	GLU	C-O	5.22	1.30	1.24
2	T	3	GLU	C-O	5.22	1.30	1.24
2	Q	132	ILE	CA-CB	5.21	1.60	1.54
2	R	132	ILE	CA-CB	5.21	1.60	1.54
2	S	268	ALA	N-CA	5.21	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	132	ILE	CA-CB	5.21	1.60	1.54
2	X	268	ALA	N-CA	5.21	1.52	1.46
2	R	268	ALA	N-CA	5.21	1.52	1.46
2	S	63	ALA	C-O	5.21	1.30	1.23
2	W	63	ALA	C-O	5.21	1.30	1.23
2	M	268	ALA	N-CA	5.20	1.52	1.46
2	R	3	GLU	C-O	5.20	1.30	1.24
2	X	63	ALA	C-O	5.19	1.30	1.23
2	M	63	ALA	C-O	5.19	1.30	1.23
2	O	117	TYR	C-O	5.19	1.30	1.23
2	N	117	TYR	C-O	5.19	1.30	1.23
2	N	63	ALA	C-O	5.18	1.30	1.23
2	U	268	ALA	N-CA	5.18	1.52	1.46
2	Q	268	ALA	N-CA	5.17	1.52	1.46
2	R	261	VAL	C-O	5.17	1.30	1.24
2	W	117	TYR	C-O	5.17	1.30	1.23
2	M	3	GLU	C-O	5.17	1.30	1.24
2	O	132	ILE	CA-CB	5.17	1.60	1.54
2	P	261	VAL	C-O	5.17	1.30	1.24
2	T	350	ALA	C-O	5.17	1.30	1.24
2	V	132	ILE	CA-CB	5.17	1.60	1.54
2	P	350	ALA	C-O	5.16	1.30	1.24
2	W	132	ILE	CA-CB	5.16	1.60	1.54
2	R	117	TYR	C-O	5.16	1.30	1.23
2	S	132	ILE	CA-CB	5.16	1.60	1.54
2	X	261	VAL	C-O	5.16	1.30	1.24
2	W	350	ALA	C-O	5.16	1.30	1.24
2	Q	117	TYR	C-O	5.15	1.30	1.23
2	P	117	TYR	C-O	5.15	1.30	1.23
2	P	132	ILE	CA-CB	5.15	1.60	1.54
2	U	132	ILE	CA-CB	5.15	1.60	1.54
2	U	61	PHE	CA-C	5.15	1.58	1.52
2	S	117	TYR	C-O	5.15	1.30	1.23
2	Q	261	VAL	C-O	5.14	1.30	1.24
2	N	132	ILE	CA-CB	5.14	1.60	1.54
2	T	117	TYR	C-O	5.14	1.30	1.23
2	S	61	PHE	CA-C	5.14	1.58	1.52
2	M	64	HIS	CD2-NE2	-5.13	1.32	1.37
2	T	61	PHE	CA-C	5.13	1.58	1.52
2	T	132	ILE	CA-CB	5.13	1.60	1.54
2	U	261	VAL	C-O	5.13	1.30	1.24
2	W	261	VAL	C-O	5.13	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	350	ALA	C-O	5.13	1.30	1.24
2	V	350	ALA	C-O	5.13	1.30	1.24
2	M	350	ALA	C-O	5.12	1.30	1.24
2	R	350	ALA	C-O	5.12	1.30	1.24
2	V	117	TYR	C-O	5.12	1.30	1.23
2	V	261	VAL	C-O	5.12	1.30	1.24
2	O	350	ALA	C-O	5.12	1.30	1.24
2	N	350	ALA	C-O	5.12	1.30	1.24
2	V	61	PHE	CA-C	5.12	1.58	1.52
2	Q	350	ALA	C-O	5.11	1.30	1.24
2	N	261	VAL	C-O	5.11	1.30	1.24
2	S	261	VAL	C-O	5.11	1.30	1.24
2	O	261	VAL	C-O	5.11	1.30	1.24
2	O	61	PHE	CA-C	5.10	1.58	1.52
2	R	64	HIS	CD2-NE2	-5.10	1.32	1.37
2	X	132	ILE	CA-CB	5.10	1.60	1.54
2	X	350	ALA	C-O	5.10	1.30	1.24
2	M	263	SER	C-N	5.10	1.40	1.33
2	U	350	ALA	C-O	5.10	1.30	1.24
2	M	261	VAL	C-O	5.09	1.30	1.24
2	N	64	HIS	CD2-NE2	-5.09	1.32	1.37
2	W	61	PHE	CA-C	5.09	1.58	1.52
2	M	61	PHE	CA-C	5.09	1.58	1.52
2	R	61	PHE	CA-C	5.09	1.58	1.52
2	T	64	HIS	CD2-NE2	-5.09	1.32	1.37
2	U	117	TYR	C-O	5.09	1.30	1.23
2	P	263	SER	C-N	5.09	1.40	1.33
2	Q	61	PHE	CA-C	5.09	1.58	1.52
2	U	64	HIS	CD2-NE2	-5.09	1.32	1.37
2	Q	64	HIS	CD2-NE2	-5.08	1.32	1.37
2	W	263	SER	C-N	5.08	1.40	1.33
2	X	64	HIS	CD2-NE2	-5.08	1.32	1.37
2	W	64	HIS	CD2-NE2	-5.07	1.32	1.37
2	X	117	TYR	C-O	5.07	1.30	1.23
2	X	263	SER	C-N	5.07	1.40	1.33
2	N	61	PHE	CA-C	5.07	1.58	1.52
2	O	64	HIS	CD2-NE2	-5.07	1.32	1.37
2	T	263	SER	C-N	5.07	1.40	1.33
2	V	64	HIS	CD2-NE2	-5.06	1.32	1.37
2	X	61	PHE	CA-C	5.06	1.58	1.52
2	M	117	TYR	C-O	5.05	1.30	1.23
2	R	263	SER	C-N	5.05	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	61	PHE	CA-C	5.05	1.58	1.52
2	T	261	VAL	C-O	5.05	1.30	1.24
2	V	263	SER	C-N	5.05	1.40	1.33
2	N	263	SER	C-N	5.04	1.40	1.33
2	Q	263	SER	C-N	5.04	1.40	1.33
2	S	64	HIS	CD2-NE2	-5.03	1.32	1.37
2	U	263	SER	C-N	5.03	1.40	1.33
2	S	263	SER	C-N	5.02	1.40	1.33
2	O	263	SER	C-N	5.02	1.40	1.33
2	P	64	HIS	CD2-NE2	-5.01	1.32	1.37

All (4192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	312	ALA	CA-C-N	26.00	171.19	121.54
2	X	312	ALA	C-N-CA	26.00	171.19	121.54
2	W	312	ALA	CA-C-N	25.98	171.16	121.54
2	W	312	ALA	C-N-CA	25.98	171.16	121.54
2	O	312	ALA	CA-C-N	25.98	171.15	121.54
2	O	312	ALA	C-N-CA	25.98	171.15	121.54
2	M	312	ALA	CA-C-N	25.97	171.15	121.54
2	M	312	ALA	C-N-CA	25.97	171.15	121.54
2	P	312	ALA	CA-C-N	25.97	171.13	121.54
2	P	312	ALA	C-N-CA	25.97	171.13	121.54
2	Q	312	ALA	CA-C-N	25.96	171.13	121.54
2	Q	312	ALA	C-N-CA	25.96	171.13	121.54
2	R	312	ALA	CA-C-N	25.96	171.13	121.54
2	R	312	ALA	C-N-CA	25.96	171.13	121.54
2	N	312	ALA	CA-C-N	25.96	171.12	121.54
2	N	312	ALA	C-N-CA	25.96	171.12	121.54
2	S	312	ALA	CA-C-N	25.96	171.12	121.54
2	S	312	ALA	C-N-CA	25.96	171.12	121.54
2	V	312	ALA	CA-C-N	25.96	171.12	121.54
2	V	312	ALA	C-N-CA	25.96	171.12	121.54
2	U	312	ALA	CA-C-N	25.95	171.10	121.54
2	U	312	ALA	C-N-CA	25.95	171.10	121.54
2	T	312	ALA	CA-C-N	25.95	171.09	121.54
2	T	312	ALA	C-N-CA	25.95	171.09	121.54
2	Q	30	ASP	CA-CB-CG	22.50	135.10	112.60
2	P	30	ASP	CA-CB-CG	22.48	135.08	112.60
2	U	30	ASP	CA-CB-CG	22.46	135.06	112.60
2	T	30	ASP	CA-CB-CG	22.45	135.05	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	30	ASP	CA-CB-CG	22.45	135.05	112.60
2	O	30	ASP	CA-CB-CG	22.45	135.05	112.60
2	N	30	ASP	CA-CB-CG	22.44	135.04	112.60
2	R	30	ASP	CA-CB-CG	22.44	135.04	112.60
2	W	30	ASP	CA-CB-CG	22.43	135.03	112.60
2	M	30	ASP	CA-CB-CG	22.43	135.03	112.60
2	X	30	ASP	CA-CB-CG	22.43	135.03	112.60
2	S	30	ASP	CA-CB-CG	22.42	135.02	112.60
2	P	354	ARG	NE-CZ-NH1	19.09	140.59	121.50
2	N	354	ARG	NE-CZ-NH1	19.08	140.58	121.50
2	S	354	ARG	NE-CZ-NH1	19.07	140.57	121.50
2	R	354	ARG	NE-CZ-NH1	19.06	140.56	121.50
2	X	354	ARG	NE-CZ-NH1	19.06	140.56	121.50
2	T	354	ARG	NE-CZ-NH1	19.06	140.56	121.50
2	M	354	ARG	NE-CZ-NH1	19.06	140.56	121.50
2	Q	354	ARG	NE-CZ-NH1	19.05	140.55	121.50
2	V	354	ARG	NE-CZ-NH1	19.05	140.55	121.50
2	W	354	ARG	NE-CZ-NH1	19.04	140.54	121.50
2	U	354	ARG	NE-CZ-NH1	19.02	140.52	121.50
2	O	354	ARG	NE-CZ-NH1	19.02	140.51	121.50
2	R	311	LEU	CA-C-N	-18.91	94.85	121.33
2	R	311	LEU	C-N-CA	-18.91	94.85	121.33
2	O	311	LEU	CA-C-N	-18.90	94.86	121.33
2	O	311	LEU	C-N-CA	-18.90	94.86	121.33
2	W	311	LEU	CA-C-N	-18.90	94.88	121.33
2	W	311	LEU	C-N-CA	-18.90	94.88	121.33
2	P	311	LEU	CA-C-N	-18.89	94.88	121.33
2	P	311	LEU	C-N-CA	-18.89	94.88	121.33
2	M	311	LEU	CA-C-N	-18.89	94.89	121.33
2	M	311	LEU	C-N-CA	-18.89	94.89	121.33
2	Q	311	LEU	CA-C-N	-18.88	94.89	121.33
2	Q	311	LEU	C-N-CA	-18.88	94.89	121.33
2	S	311	LEU	CA-C-N	-18.88	94.89	121.33
2	S	311	LEU	C-N-CA	-18.88	94.89	121.33
2	V	311	LEU	CA-C-N	-18.88	94.89	121.33
2	V	311	LEU	C-N-CA	-18.88	94.89	121.33
2	U	311	LEU	CA-C-N	-18.88	94.90	121.33
2	U	311	LEU	C-N-CA	-18.88	94.90	121.33
2	N	311	LEU	CA-C-N	-18.88	94.90	121.33
2	N	311	LEU	C-N-CA	-18.88	94.90	121.33
2	T	311	LEU	CA-C-N	-18.87	94.91	121.33
2	T	311	LEU	C-N-CA	-18.87	94.91	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	311	LEU	CA-C-N	-18.86	94.92	121.33
2	X	311	LEU	C-N-CA	-18.86	94.92	121.33
2	R	312	ALA	O-C-N	15.21	139.13	123.62
2	Q	312	ALA	O-C-N	15.20	139.13	123.62
2	N	312	ALA	O-C-N	15.19	139.12	123.62
2	T	312	ALA	O-C-N	15.18	139.10	123.62
2	V	312	ALA	O-C-N	15.18	139.10	123.62
2	X	312	ALA	O-C-N	15.18	139.10	123.62
2	O	312	ALA	O-C-N	15.17	139.09	123.62
2	W	312	ALA	O-C-N	15.17	139.09	123.62
2	P	312	ALA	O-C-N	15.16	139.09	123.62
2	S	312	ALA	O-C-N	15.16	139.08	123.62
2	U	312	ALA	O-C-N	15.16	139.08	123.62
2	M	312	ALA	O-C-N	15.15	139.07	123.62
2	N	124	ASN	CA-CB-CG	15.06	127.66	112.60
2	R	124	ASN	CA-CB-CG	15.05	127.65	112.60
2	O	124	ASN	CA-CB-CG	15.05	127.65	112.60
2	W	124	ASN	CA-CB-CG	15.04	127.64	112.60
2	T	124	ASN	CA-CB-CG	15.04	127.64	112.60
2	V	124	ASN	CA-CB-CG	15.04	127.64	112.60
2	P	124	ASN	CA-CB-CG	15.02	127.62	112.60
2	S	124	ASN	CA-CB-CG	15.01	127.61	112.60
2	X	124	ASN	CA-CB-CG	15.01	127.61	112.60
2	Q	124	ASN	CA-CB-CG	15.00	127.60	112.60
2	U	124	ASN	CA-CB-CG	15.00	127.60	112.60
2	M	124	ASN	CA-CB-CG	14.98	127.58	112.60
2	N	137	LYS	CA-CB-CG	13.37	140.84	114.10
2	X	137	LYS	CA-CB-CG	13.37	140.84	114.10
2	P	137	LYS	CA-CB-CG	13.36	140.82	114.10
2	Q	137	LYS	CA-CB-CG	13.36	140.81	114.10
2	O	137	LYS	CA-CB-CG	13.35	140.79	114.10
2	R	137	LYS	CA-CB-CG	13.35	140.79	114.10
2	T	137	LYS	CA-CB-CG	13.35	140.79	114.10
2	U	137	LYS	CA-CB-CG	13.35	140.79	114.10
2	V	137	LYS	CA-CB-CG	13.35	140.79	114.10
2	W	137	LYS	CA-CB-CG	13.34	140.79	114.10
2	M	137	LYS	CA-CB-CG	13.34	140.78	114.10
2	S	137	LYS	CA-CB-CG	13.34	140.77	114.10
2	S	369	THR	O-C-N	11.72	137.51	122.39
2	N	369	THR	O-C-N	11.69	137.47	122.39
2	X	369	THR	O-C-N	11.69	137.47	122.39
2	O	369	THR	O-C-N	11.67	137.45	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	369	THR	O-C-N	11.67	137.45	122.39
2	Q	369	THR	O-C-N	11.67	137.44	122.39
2	T	369	THR	O-C-N	11.67	137.44	122.39
2	R	369	THR	O-C-N	11.66	137.43	122.39
2	P	369	THR	O-C-N	11.65	137.42	122.39
2	U	369	THR	O-C-N	11.65	137.42	122.39
2	W	369	THR	O-C-N	11.65	137.42	122.39
2	M	369	THR	O-C-N	11.62	137.39	122.39
2	Q	136	ASP	O-C-N	11.21	134.00	122.12
2	T	136	ASP	O-C-N	11.20	134.00	122.12
2	O	136	ASP	O-C-N	11.19	133.99	122.12
2	M	236	ASP	O-C-N	11.19	133.98	122.12
2	N	236	ASP	O-C-N	11.19	133.98	122.12
2	R	136	ASP	O-C-N	11.18	133.97	122.12
2	X	136	ASP	O-C-N	11.17	133.96	122.12
2	S	236	ASP	O-C-N	11.17	133.96	122.12
2	M	136	ASP	O-C-N	11.17	133.96	122.12
2	N	136	ASP	O-C-N	11.17	133.96	122.12
2	W	236	ASP	O-C-N	11.17	133.96	122.12
2	W	136	ASP	O-C-N	11.16	133.96	122.12
2	U	236	ASP	O-C-N	11.16	133.95	122.12
2	V	136	ASP	O-C-N	11.16	133.95	122.12
2	X	236	ASP	O-C-N	11.16	133.95	122.12
2	S	136	ASP	O-C-N	11.16	133.95	122.12
2	U	136	ASP	O-C-N	11.15	133.94	122.12
2	R	236	ASP	O-C-N	11.15	133.94	122.12
2	O	236	ASP	O-C-N	11.15	133.94	122.12
2	T	236	ASP	O-C-N	11.14	133.93	122.12
2	V	236	ASP	O-C-N	11.14	133.93	122.12
2	P	236	ASP	O-C-N	11.13	133.92	122.12
2	Q	236	ASP	O-C-N	11.12	133.91	122.12
2	P	136	ASP	O-C-N	11.12	133.90	122.12
2	R	4	GLU	CA-C-N	11.08	143.13	121.41
2	R	4	GLU	C-N-CA	11.08	143.13	121.41
2	U	4	GLU	CA-C-N	11.07	143.12	121.41
2	U	4	GLU	C-N-CA	11.07	143.12	121.41
2	S	4	GLU	CA-C-N	11.07	143.11	121.41
2	S	4	GLU	C-N-CA	11.07	143.11	121.41
2	M	341	TYR	CA-CB-CG	11.07	133.82	113.90
2	R	341	TYR	CA-CB-CG	11.07	133.82	113.90
2	P	4	GLU	CA-C-N	11.06	143.10	121.41
2	P	4	GLU	C-N-CA	11.06	143.10	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	4	GLU	CA-C-N	11.06	143.09	121.41
2	Q	4	GLU	C-N-CA	11.06	143.09	121.41
2	V	4	GLU	CA-C-N	11.06	143.09	121.41
2	V	4	GLU	C-N-CA	11.06	143.09	121.41
2	O	341	TYR	CA-CB-CG	11.06	133.81	113.90
2	T	341	TYR	CA-CB-CG	11.06	133.81	113.90
2	N	341	TYR	CA-CB-CG	11.06	133.80	113.90
2	W	4	GLU	CA-C-N	11.06	143.08	121.41
2	W	4	GLU	C-N-CA	11.06	143.08	121.41
2	U	341	TYR	CA-CB-CG	11.05	133.80	113.90
2	X	4	GLU	CA-C-N	11.05	143.07	121.41
2	X	4	GLU	C-N-CA	11.05	143.07	121.41
2	Q	341	TYR	CA-CB-CG	11.05	133.79	113.90
2	S	341	TYR	CA-CB-CG	11.05	133.79	113.90
2	X	341	TYR	CA-CB-CG	11.05	133.79	113.90
2	T	4	GLU	CA-C-N	11.05	143.06	121.41
2	T	4	GLU	C-N-CA	11.05	143.06	121.41
2	V	341	TYR	CA-CB-CG	11.05	133.79	113.90
2	O	4	GLU	CA-C-N	11.04	143.06	121.41
2	O	4	GLU	C-N-CA	11.04	143.06	121.41
2	W	341	TYR	CA-CB-CG	11.04	133.78	113.90
2	N	4	GLU	CA-C-N	11.04	143.05	121.41
2	N	4	GLU	C-N-CA	11.04	143.05	121.41
2	P	341	TYR	CA-CB-CG	11.04	133.77	113.90
2	M	4	GLU	CA-C-N	11.03	143.03	121.41
2	M	4	GLU	C-N-CA	11.03	143.03	121.41
2	Q	59	ILE	CA-CB-CG2	10.96	129.14	110.50
2	R	59	ILE	CA-CB-CG2	10.95	129.12	110.50
2	N	59	ILE	CA-CB-CG2	10.95	129.12	110.50
2	W	59	ILE	CA-CB-CG2	10.95	129.12	110.50
2	M	59	ILE	CA-CB-CG2	10.94	129.10	110.50
2	P	59	ILE	CA-CB-CG2	10.94	129.10	110.50
2	V	59	ILE	CA-CB-CG2	10.94	129.10	110.50
2	S	59	ILE	CA-CB-CG2	10.94	129.09	110.50
2	O	59	ILE	CA-CB-CG2	10.93	129.09	110.50
2	X	59	ILE	CA-CB-CG2	10.93	129.09	110.50
2	T	59	ILE	CA-CB-CG2	10.93	129.08	110.50
2	U	59	ILE	CA-CB-CG2	10.93	129.07	110.50
2	X	55	ASP	CA-CB-CG	10.78	123.38	112.60
2	R	55	ASP	CA-CB-CG	10.71	123.31	112.60
2	U	55	ASP	CA-CB-CG	10.71	123.31	112.60
2	M	55	ASP	CA-CB-CG	10.71	123.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	55	ASP	CA-CB-CG	10.70	123.30	112.60
2	Q	55	ASP	CA-CB-CG	10.70	123.30	112.60
2	V	55	ASP	CA-CB-CG	10.70	123.30	112.60
2	W	55	ASP	CA-CB-CG	10.69	123.29	112.60
2	N	55	ASP	CA-CB-CG	10.69	123.28	112.60
2	T	55	ASP	CA-CB-CG	10.68	123.28	112.60
2	P	55	ASP	CA-CB-CG	10.67	123.27	112.60
2	S	354	ARG	NH1-CZ-NH2	-10.65	105.45	119.30
2	O	55	ASP	CA-CB-CG	10.65	123.25	112.60
2	Q	354	ARG	NH1-CZ-NH2	-10.64	105.47	119.30
2	N	354	ARG	NH1-CZ-NH2	-10.64	105.47	119.30
2	T	354	ARG	NH1-CZ-NH2	-10.63	105.48	119.30
2	V	354	ARG	NH1-CZ-NH2	-10.63	105.48	119.30
2	P	354	ARG	NH1-CZ-NH2	-10.63	105.48	119.30
2	W	354	ARG	NH1-CZ-NH2	-10.63	105.48	119.30
2	U	354	ARG	NH1-CZ-NH2	-10.62	105.49	119.30
2	X	354	ARG	NH1-CZ-NH2	-10.62	105.50	119.30
2	O	354	ARG	NH1-CZ-NH2	-10.61	105.50	119.30
2	M	354	ARG	NH1-CZ-NH2	-10.61	105.51	119.30
2	R	354	ARG	NH1-CZ-NH2	-10.61	105.51	119.30
2	R	134	ALA	CA-C-O	10.54	131.89	120.82
2	S	134	ALA	CA-C-O	10.52	131.87	120.82
2	O	134	ALA	CA-C-O	10.52	131.86	120.82
2	V	134	ALA	CA-C-O	10.51	131.85	120.82
2	P	134	ALA	CA-C-O	10.50	131.84	120.82
2	W	134	ALA	CA-C-O	10.50	131.85	120.82
2	Q	134	ALA	CA-C-O	10.49	131.83	120.82
2	T	134	ALA	CA-C-O	10.48	131.82	120.82
2	U	134	ALA	CA-C-O	10.47	131.82	120.82
2	M	134	ALA	CA-C-O	10.47	131.81	120.82
2	X	134	ALA	CA-C-O	10.46	131.81	120.82
2	N	134	ALA	CA-C-O	10.46	131.80	120.82
2	X	358	ASP	CA-CB-CG	10.41	123.02	112.60
2	U	358	ASP	CA-CB-CG	10.40	123.00	112.60
2	N	358	ASP	CA-CB-CG	10.40	123.00	112.60
2	P	358	ASP	CA-CB-CG	10.39	122.99	112.60
2	T	358	ASP	CA-CB-CG	10.38	122.98	112.60
2	V	358	ASP	CA-CB-CG	10.38	122.98	112.60
2	W	358	ASP	CA-CB-CG	10.37	122.97	112.60
2	Q	358	ASP	CA-CB-CG	10.36	122.96	112.60
2	S	358	ASP	CA-CB-CG	10.36	122.96	112.60
2	R	358	ASP	CA-CB-CG	10.34	122.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	358	ASP	CA-CB-CG	10.33	122.93	112.60
2	M	358	ASP	CA-CB-CG	10.32	122.92	112.60
2	U	35	VAL	CA-C-O	-10.01	109.86	120.57
2	T	347	VAL	O-C-N	9.84	131.97	121.83
2	W	347	VAL	O-C-N	9.83	131.95	121.83
2	O	347	VAL	O-C-N	9.81	131.94	121.83
2	M	347	VAL	O-C-N	9.81	131.93	121.83
2	P	347	VAL	O-C-N	9.79	131.92	121.83
2	S	347	VAL	O-C-N	9.80	131.92	121.83
2	U	347	VAL	O-C-N	9.80	131.92	121.83
2	V	347	VAL	O-C-N	9.79	131.91	121.83
2	N	347	VAL	O-C-N	9.77	131.89	121.83
2	Q	347	VAL	O-C-N	9.77	131.89	121.83
2	X	347	VAL	O-C-N	9.77	131.89	121.83
2	R	347	VAL	O-C-N	9.75	131.88	121.83
1	I	340	SER	N-CA-C	-9.71	101.94	113.88
1	H	340	SER	N-CA-C	-9.69	101.96	113.88
1	A	98	GLN	OE1-CD-NE2	-9.69	112.91	122.60
1	F	340	SER	N-CA-C	-9.69	101.96	113.88
1	B	340	SER	N-CA-C	-9.68	101.98	113.88
1	B	98	GLN	OE1-CD-NE2	-9.67	112.93	122.60
1	D	340	SER	N-CA-C	-9.67	101.99	113.88
1	L	98	GLN	OE1-CD-NE2	-9.67	112.93	122.60
1	C	340	SER	N-CA-C	-9.66	101.99	113.88
1	E	98	GLN	OE1-CD-NE2	-9.66	112.94	122.60
1	J	98	GLN	OE1-CD-NE2	-9.66	112.94	122.60
1	J	340	SER	N-CA-C	-9.66	102.00	113.88
1	D	98	GLN	OE1-CD-NE2	-9.65	112.94	122.60
1	L	340	SER	N-CA-C	-9.65	102.00	113.88
1	A	340	SER	N-CA-C	-9.65	102.01	113.88
1	G	98	GLN	OE1-CD-NE2	-9.64	112.96	122.60
1	K	98	GLN	OE1-CD-NE2	-9.64	112.96	122.60
1	K	340	SER	N-CA-C	-9.64	102.03	113.88
1	E	340	SER	N-CA-C	-9.63	102.03	113.88
1	I	98	GLN	OE1-CD-NE2	-9.63	112.97	122.60
1	C	98	GLN	OE1-CD-NE2	-9.62	112.98	122.60
1	F	98	GLN	OE1-CD-NE2	-9.61	112.99	122.60
1	G	340	SER	N-CA-C	-9.60	102.07	113.88
1	H	98	GLN	OE1-CD-NE2	-9.60	113.00	122.60
2	M	35	VAL	CA-C-O	-9.48	109.85	120.84
2	X	35	VAL	CA-C-O	-9.45	109.88	120.84
2	P	35	VAL	CA-C-O	-9.45	109.88	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	35	VAL	CA-C-O	-9.44	109.89	120.84
2	T	35	VAL	CA-C-O	-9.43	109.90	120.84
2	Q	35	VAL	CA-C-O	-9.43	109.90	120.84
2	S	35	VAL	CA-C-O	-9.43	109.91	120.84
2	O	35	VAL	CA-C-O	-9.42	109.92	120.84
2	N	35	VAL	CA-C-O	-9.41	109.92	120.84
2	R	35	VAL	CA-C-O	-9.40	109.93	120.84
2	W	35	VAL	CA-C-O	-9.39	109.94	120.84
2	O	316	ARG	CD-NE-CZ	9.32	137.45	124.40
2	M	316	ARG	CD-NE-CZ	9.31	137.43	124.40
2	R	316	ARG	CD-NE-CZ	9.30	137.42	124.40
2	X	316	ARG	CD-NE-CZ	9.30	137.42	124.40
2	P	272	ASN	CB-CG-ND2	9.30	130.35	116.40
2	U	272	ASN	CB-CG-ND2	9.29	130.34	116.40
2	Q	272	ASN	CB-CG-ND2	9.29	130.34	116.40
2	U	316	ARG	CD-NE-CZ	9.29	137.40	124.40
2	V	316	ARG	CD-NE-CZ	9.28	137.40	124.40
2	S	272	ASN	CB-CG-ND2	9.28	130.32	116.40
2	W	316	ARG	CD-NE-CZ	9.28	137.39	124.40
2	O	239	LYS	CB-CG-CD	9.28	132.64	111.30
2	N	316	ARG	CD-NE-CZ	9.28	137.39	124.40
2	S	239	LYS	CB-CG-CD	9.28	132.64	111.30
2	P	239	LYS	CB-CG-CD	9.28	132.64	111.30
2	S	316	ARG	CD-NE-CZ	9.28	137.39	124.40
2	M	272	ASN	CB-CG-ND2	9.28	130.31	116.40
2	R	239	LYS	CB-CG-CD	9.27	132.63	111.30
2	W	272	ASN	CB-CG-ND2	9.27	130.31	116.40
2	X	239	LYS	CB-CG-CD	9.27	132.63	111.30
1	D	400	PRO	CA-C-N	9.27	131.43	119.84
1	D	400	PRO	C-N-CA	9.27	131.43	119.84
2	Q	239	LYS	CB-CG-CD	9.27	132.62	111.30
2	T	316	ARG	CD-NE-CZ	9.27	137.38	124.40
2	V	272	ASN	CB-CG-ND2	9.27	130.30	116.40
2	N	239	LYS	CB-CG-CD	9.27	132.61	111.30
2	Q	316	ARG	CD-NE-CZ	9.27	137.37	124.40
2	R	272	ASN	CB-CG-ND2	9.27	130.30	116.40
2	T	239	LYS	CB-CG-CD	9.27	132.61	111.30
2	V	239	LYS	CB-CG-CD	9.27	132.62	111.30
2	T	272	ASN	CB-CG-ND2	9.27	130.30	116.40
1	J	400	PRO	CA-C-N	9.26	131.42	119.84
1	J	400	PRO	C-N-CA	9.26	131.42	119.84
2	M	239	LYS	CB-CG-CD	9.26	132.60	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	272	ASN	CB-CG-ND2	9.26	130.30	116.40
2	N	272	ASN	CB-CG-ND2	9.26	130.29	116.40
2	U	239	LYS	CB-CG-CD	9.26	132.60	111.30
1	G	400	PRO	CA-C-N	9.26	131.41	119.84
1	G	400	PRO	C-N-CA	9.26	131.41	119.84
2	O	272	ASN	CB-CG-ND2	9.26	130.28	116.40
2	W	239	LYS	CB-CG-CD	9.25	132.57	111.30
1	L	400	PRO	CA-C-N	9.25	131.40	119.84
1	L	400	PRO	C-N-CA	9.25	131.40	119.84
2	P	316	ARG	CD-NE-CZ	9.25	137.34	124.40
1	K	400	PRO	CA-C-N	9.24	131.39	119.84
1	K	400	PRO	C-N-CA	9.24	131.39	119.84
1	A	400	PRO	CA-C-N	9.24	131.39	119.84
1	A	400	PRO	C-N-CA	9.24	131.39	119.84
1	E	400	PRO	CA-C-N	9.24	131.39	119.84
1	E	400	PRO	C-N-CA	9.24	131.39	119.84
1	C	400	PRO	CA-C-N	9.23	131.38	119.84
1	C	400	PRO	C-N-CA	9.23	131.38	119.84
1	F	400	PRO	CA-C-N	9.23	131.38	119.84
1	F	400	PRO	C-N-CA	9.23	131.38	119.84
1	H	400	PRO	CA-C-N	9.23	131.38	119.84
1	H	400	PRO	C-N-CA	9.23	131.38	119.84
1	B	400	PRO	CA-C-N	9.22	131.37	119.84
1	B	400	PRO	C-N-CA	9.22	131.37	119.84
1	I	400	PRO	CA-C-N	9.21	131.35	119.84
1	I	400	PRO	C-N-CA	9.21	131.35	119.84
2	T	84	ALA	N-CA-CB	9.16	123.68	110.13
2	U	84	ALA	N-CA-CB	9.16	123.68	110.13
2	W	84	ALA	N-CA-CB	9.14	123.66	110.13
2	M	84	ALA	N-CA-CB	9.14	123.66	110.13
2	O	84	ALA	N-CA-CB	9.14	123.66	110.13
2	P	84	ALA	N-CA-CB	9.13	123.65	110.13
1	E	218	GLN	OE1-CD-NE2	-9.13	113.47	122.60
2	S	84	ALA	N-CA-CB	9.13	123.64	110.13
2	R	84	ALA	N-CA-CB	9.13	123.64	110.13
2	Q	84	ALA	N-CA-CB	9.12	123.63	110.13
2	V	84	ALA	N-CA-CB	9.12	123.63	110.13
2	X	84	ALA	N-CA-CB	9.12	123.63	110.13
2	N	84	ALA	N-CA-CB	9.11	123.61	110.13
1	D	218	GLN	OE1-CD-NE2	-9.09	113.51	122.60
1	B	218	GLN	OE1-CD-NE2	-9.09	113.51	122.60
1	K	218	GLN	OE1-CD-NE2	-9.07	113.53	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	GLN	OE1-CD-NE2	-9.06	113.54	122.60
1	H	218	GLN	OE1-CD-NE2	-9.05	113.55	122.60
1	C	218	GLN	OE1-CD-NE2	-9.05	113.55	122.60
1	F	218	GLN	OE1-CD-NE2	-9.05	113.55	122.60
1	J	218	GLN	OE1-CD-NE2	-9.03	113.57	122.60
1	I	218	GLN	OE1-CD-NE2	-9.01	113.59	122.60
1	L	218	GLN	OE1-CD-NE2	-9.01	113.59	122.60
1	G	218	GLN	OE1-CD-NE2	-8.97	113.63	122.60
2	P	86	GLN	CA-C-N	8.92	133.13	120.28
2	P	86	GLN	C-N-CA	8.92	133.13	120.28
2	Q	86	GLN	CA-C-N	8.91	133.12	120.28
2	Q	86	GLN	C-N-CA	8.91	133.12	120.28
2	S	86	GLN	CA-C-N	8.91	133.11	120.28
2	S	86	GLN	C-N-CA	8.91	133.11	120.28
2	R	86	GLN	CA-C-N	8.90	133.10	120.28
2	R	86	GLN	C-N-CA	8.90	133.10	120.28
2	X	86	GLN	CA-C-N	8.89	133.09	120.28
2	X	86	GLN	C-N-CA	8.89	133.09	120.28
2	N	86	GLN	CA-C-N	8.89	133.08	120.28
2	N	86	GLN	C-N-CA	8.89	133.08	120.28
2	T	86	GLN	CA-C-N	8.89	133.08	120.28
2	T	86	GLN	C-N-CA	8.89	133.08	120.28
2	W	86	GLN	CA-C-N	8.89	133.08	120.28
2	W	86	GLN	C-N-CA	8.89	133.08	120.28
2	M	278	GLU	CB-CG-CD	8.88	127.70	112.60
2	R	278	GLU	CB-CG-CD	8.88	127.70	112.60
2	V	86	GLN	CA-C-N	8.88	133.06	120.28
2	V	86	GLN	C-N-CA	8.88	133.06	120.28
2	U	278	GLU	CB-CG-CD	8.88	127.69	112.60
2	X	278	GLU	CB-CG-CD	8.87	127.68	112.60
2	S	278	GLU	CB-CG-CD	8.87	127.68	112.60
2	V	278	GLU	CB-CG-CD	8.87	127.67	112.60
2	N	278	GLU	CB-CG-CD	8.86	127.66	112.60
2	O	86	GLN	CA-C-N	8.86	133.04	120.28
2	O	86	GLN	C-N-CA	8.86	133.04	120.28
2	W	278	GLU	CB-CG-CD	8.86	127.67	112.60
2	M	86	GLN	CA-C-N	8.86	133.04	120.28
2	M	86	GLN	C-N-CA	8.86	133.04	120.28
2	U	86	GLN	CA-C-N	8.86	133.04	120.28
2	U	86	GLN	C-N-CA	8.86	133.04	120.28
2	P	278	GLU	CB-CG-CD	8.86	127.66	112.60
2	Q	278	GLU	CB-CG-CD	8.86	127.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	278	GLU	CB-CG-CD	8.86	127.66	112.60
2	O	278	GLU	CB-CG-CD	8.85	127.65	112.60
1	C	387	HIS	CA-C-N	8.76	129.63	119.47
1	C	387	HIS	C-N-CA	8.76	129.63	119.47
1	K	387	HIS	CA-C-N	8.72	129.59	119.47
1	K	387	HIS	C-N-CA	8.72	129.59	119.47
1	A	387	HIS	CA-C-N	8.71	129.57	119.47
1	A	387	HIS	C-N-CA	8.71	129.57	119.47
2	N	233	SER	CA-CB-OG	-8.71	93.68	111.10
1	I	387	HIS	CA-C-N	8.71	129.57	119.47
1	I	387	HIS	C-N-CA	8.71	129.57	119.47
2	O	233	SER	CA-CB-OG	-8.71	93.68	111.10
2	R	233	SER	CA-CB-OG	-8.70	93.71	111.10
1	G	387	HIS	CA-C-N	8.69	129.56	119.47
1	G	387	HIS	C-N-CA	8.69	129.56	119.47
2	X	233	SER	CA-CB-OG	-8.69	93.71	111.10
1	H	387	HIS	CA-C-N	8.69	129.55	119.47
1	H	387	HIS	C-N-CA	8.69	129.55	119.47
2	T	233	SER	CA-CB-OG	-8.69	93.72	111.10
1	L	387	HIS	CA-C-N	8.69	129.55	119.47
1	L	387	HIS	C-N-CA	8.69	129.55	119.47
2	U	233	SER	CA-CB-OG	-8.69	93.72	111.10
2	V	233	SER	CA-CB-OG	-8.69	93.72	111.10
2	M	233	SER	CA-CB-OG	-8.69	93.73	111.10
1	E	387	HIS	CA-C-N	8.68	129.54	119.47
1	E	387	HIS	C-N-CA	8.68	129.54	119.47
2	Q	233	SER	CA-CB-OG	-8.68	93.73	111.10
1	J	387	HIS	CA-C-N	8.68	129.54	119.47
1	J	387	HIS	C-N-CA	8.68	129.54	119.47
2	S	233	SER	CA-CB-OG	-8.68	93.74	111.10
2	M	335	GLN	CG-CD-NE2	8.67	129.41	116.40
1	B	387	HIS	CA-C-N	8.67	129.53	119.47
1	B	387	HIS	C-N-CA	8.67	129.53	119.47
1	D	61	ASN	CA-CB-CG	-8.67	103.93	112.60
1	D	387	HIS	CA-C-N	8.67	129.52	119.47
1	D	387	HIS	C-N-CA	8.67	129.52	119.47
1	G	61	ASN	CA-CB-CG	-8.67	103.93	112.60
2	O	335	GLN	CG-CD-NE2	8.67	129.40	116.40
2	W	233	SER	CA-CB-OG	-8.66	93.77	111.10
2	W	335	GLN	CG-CD-NE2	8.66	129.40	116.40
2	P	233	SER	CA-CB-OG	-8.66	93.78	111.10
2	S	335	GLN	CG-CD-NE2	8.66	129.39	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	274	GLU	CB-CG-CD	8.66	127.32	112.60
2	O	274	GLU	CB-CG-CD	8.66	127.32	112.60
2	T	335	GLN	CG-CD-NE2	8.66	129.39	116.40
1	E	61	ASN	CA-CB-CG	-8.66	103.94	112.60
1	F	387	HIS	CA-C-N	8.66	129.51	119.47
1	F	387	HIS	C-N-CA	8.66	129.51	119.47
2	U	335	GLN	CG-CD-NE2	8.66	129.39	116.40
2	Q	335	GLN	CG-CD-NE2	8.65	129.38	116.40
2	V	335	GLN	CG-CD-NE2	8.65	129.38	116.40
2	W	274	GLU	CB-CG-CD	8.65	127.30	112.60
2	P	335	GLN	CG-CD-NE2	8.65	129.37	116.40
2	T	274	GLU	CB-CG-CD	8.65	127.30	112.60
1	B	61	ASN	CA-CB-CG	-8.64	103.96	112.60
2	N	274	GLU	CB-CG-CD	8.64	127.29	112.60
2	N	335	GLN	CG-CD-NE2	8.64	129.36	116.40
2	S	274	GLU	CB-CG-CD	8.64	127.29	112.60
2	X	274	GLU	CB-CG-CD	8.64	127.29	112.60
2	V	274	GLU	CB-CG-CD	8.64	127.28	112.60
2	P	274	GLU	CB-CG-CD	8.64	127.28	112.60
2	R	335	GLN	CG-CD-NE2	8.63	129.35	116.40
2	U	274	GLU	CB-CG-CD	8.63	127.28	112.60
2	X	335	GLN	CG-CD-NE2	8.63	129.35	116.40
1	I	61	ASN	CA-CB-CG	-8.63	103.97	112.60
1	C	61	ASN	CA-CB-CG	-8.63	103.97	112.60
2	R	274	GLU	CB-CG-CD	8.62	127.26	112.60
2	Q	274	GLU	CB-CG-CD	8.62	127.25	112.60
1	H	61	ASN	CA-CB-CG	-8.61	103.99	112.60
1	J	61	ASN	CA-CB-CG	-8.60	104.00	112.60
1	K	61	ASN	CA-CB-CG	-8.60	104.00	112.60
1	A	61	ASN	CA-CB-CG	-8.60	104.00	112.60
1	F	61	ASN	CA-CB-CG	-8.59	104.01	112.60
1	L	61	ASN	CA-CB-CG	-8.59	104.01	112.60
2	W	50	VAL	CA-C-O	-8.55	111.23	120.47
2	N	42	LYS	CB-CA-C	-8.54	99.33	111.80
2	P	42	LYS	CB-CA-C	-8.54	99.33	111.80
2	W	42	LYS	CB-CA-C	-8.54	99.34	111.80
2	R	50	VAL	CA-C-O	-8.52	111.27	120.47
2	O	42	LYS	CB-CA-C	-8.52	99.36	111.80
2	X	42	LYS	CB-CA-C	-8.52	99.36	111.80
2	T	42	LYS	CB-CA-C	-8.52	99.36	111.80
2	M	42	LYS	CB-CA-C	-8.52	99.37	111.80
2	N	50	VAL	CA-C-O	-8.51	111.28	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	42	LYS	CB-CA-C	-8.51	99.38	111.80
2	S	50	VAL	CA-C-O	-8.50	111.29	120.47
2	O	50	VAL	CA-C-O	-8.50	111.29	120.47
2	U	42	LYS	CB-CA-C	-8.50	99.40	111.80
2	Q	50	VAL	CA-C-O	-8.49	111.30	120.47
2	R	42	LYS	CB-CA-C	-8.49	99.40	111.80
2	U	50	VAL	CA-C-O	-8.49	111.30	120.47
2	Q	42	LYS	CB-CA-C	-8.49	99.41	111.80
2	S	42	LYS	CB-CA-C	-8.49	99.40	111.80
2	T	50	VAL	CA-C-O	-8.49	111.30	120.47
2	V	50	VAL	CA-C-O	-8.48	111.31	120.47
2	P	50	VAL	CA-C-O	-8.47	111.32	120.47
2	M	50	VAL	CA-C-O	-8.46	111.33	120.47
2	X	50	VAL	CA-C-O	-8.44	111.36	120.47
2	Q	33	ILE	N-CA-CB	8.42	120.60	111.00
2	P	33	ILE	N-CA-CB	8.42	120.60	111.00
2	W	33	ILE	N-CA-CB	8.42	120.60	111.00
2	M	33	ILE	N-CA-CB	8.41	120.59	111.00
2	X	33	ILE	N-CA-CB	8.40	120.58	111.00
2	O	33	ILE	N-CA-CB	8.40	120.57	111.00
2	S	33	ILE	N-CA-CB	8.40	120.57	111.00
2	V	33	ILE	N-CA-CB	8.39	120.57	111.00
2	N	33	ILE	N-CA-CB	8.38	120.56	111.00
2	T	33	ILE	N-CA-CB	8.37	120.55	111.00
2	R	33	ILE	N-CA-CB	8.37	120.55	111.00
2	U	33	ILE	N-CA-CB	8.37	120.55	111.00
2	X	227	ASN	OD1-CG-ND2	-8.33	114.27	122.60
2	S	227	ASN	OD1-CG-ND2	-8.33	114.27	122.60
2	T	227	ASN	OD1-CG-ND2	-8.33	114.27	122.60
2	X	141	ALA	CA-C-O	8.33	129.62	119.38
2	R	227	ASN	OD1-CG-ND2	-8.32	114.28	122.60
2	N	141	ALA	CA-C-O	8.31	129.60	119.38
2	R	141	ALA	CA-C-O	8.31	129.60	119.38
2	S	141	ALA	CA-C-O	8.30	129.59	119.38
2	T	141	ALA	CA-C-O	8.30	129.59	119.38
2	P	141	ALA	CA-C-O	8.29	129.57	119.38
2	V	141	ALA	CA-C-O	8.29	129.57	119.38
2	M	227	ASN	OD1-CG-ND2	-8.28	114.32	122.60
2	Q	141	ALA	CA-C-O	8.28	129.56	119.38
2	Q	227	ASN	OD1-CG-ND2	-8.28	114.32	122.60
2	V	227	ASN	OD1-CG-ND2	-8.28	114.32	122.60
2	M	141	ALA	CA-C-O	8.28	129.56	119.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	227	ASN	OD1-CG-ND2	-8.28	114.32	122.60
2	N	227	ASN	OD1-CG-ND2	-8.27	114.33	122.60
2	O	227	ASN	OD1-CG-ND2	-8.27	114.33	122.60
2	U	141	ALA	CA-C-O	8.27	129.55	119.38
2	U	227	ASN	OD1-CG-ND2	-8.27	114.33	122.60
2	W	141	ALA	CA-C-O	8.27	129.55	119.38
2	P	227	ASN	OD1-CG-ND2	-8.26	114.34	122.60
2	O	141	ALA	CA-C-O	8.24	129.51	119.38
2	T	203	HIS	CA-CB-CG	-8.22	105.58	113.80
2	S	203	HIS	CA-CB-CG	-8.21	105.59	113.80
2	Q	203	HIS	CA-CB-CG	-8.20	105.60	113.80
2	R	203	HIS	CA-CB-CG	-8.20	105.60	113.80
2	U	203	HIS	CA-CB-CG	-8.19	105.61	113.80
2	O	203	HIS	CA-CB-CG	-8.18	105.62	113.80
2	V	203	HIS	CA-CB-CG	-8.18	105.62	113.80
2	P	203	HIS	CA-CB-CG	-8.18	105.62	113.80
2	M	203	HIS	CA-CB-CG	-8.18	105.62	113.80
2	Q	270	SER	CA-C-N	8.18	127.90	119.64
2	Q	270	SER	C-N-CA	8.18	127.90	119.64
2	X	203	HIS	CA-CB-CG	-8.16	105.64	113.80
2	N	203	HIS	CA-CB-CG	-8.15	105.65	113.80
2	X	270	SER	CA-C-N	8.15	127.87	119.64
2	X	270	SER	C-N-CA	8.15	127.87	119.64
2	M	270	SER	CA-C-N	8.14	127.87	119.64
2	M	270	SER	C-N-CA	8.14	127.87	119.64
2	W	203	HIS	CA-CB-CG	-8.14	105.66	113.80
2	W	270	SER	CA-C-N	8.14	127.86	119.64
2	W	270	SER	C-N-CA	8.14	127.86	119.64
2	N	270	SER	CA-C-N	8.13	127.85	119.64
2	N	270	SER	C-N-CA	8.13	127.85	119.64
2	P	270	SER	CA-C-N	8.13	127.85	119.64
2	P	270	SER	C-N-CA	8.13	127.85	119.64
2	V	270	SER	CA-C-N	8.12	127.84	119.64
2	V	270	SER	C-N-CA	8.12	127.84	119.64
2	O	278	GLU	CA-CB-CG	8.11	130.32	114.10
2	S	270	SER	CA-C-N	8.11	127.83	119.64
2	S	270	SER	C-N-CA	8.11	127.83	119.64
2	O	270	SER	CA-C-N	8.10	127.83	119.64
2	O	270	SER	C-N-CA	8.10	127.83	119.64
2	O	239	LYS	CG-CD-CE	8.10	129.94	111.30
2	P	278	GLU	CA-CB-CG	8.10	130.30	114.10
2	U	270	SER	CA-C-N	8.10	127.82	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	270	SER	C-N-CA	8.10	127.82	119.64
2	W	278	GLU	CA-CB-CG	8.10	130.30	114.10
2	T	270	SER	CA-C-N	8.10	127.82	119.64
2	T	270	SER	C-N-CA	8.10	127.82	119.64
2	N	68	GLY	O-C-N	-8.10	114.42	122.19
2	N	239	LYS	CG-CD-CE	8.10	129.92	111.30
2	S	68	GLY	O-C-N	-8.09	114.42	122.19
2	M	239	LYS	CG-CD-CE	8.09	129.91	111.30
2	Q	239	LYS	CG-CD-CE	8.09	129.91	111.30
2	M	278	GLU	CA-CB-CG	8.09	130.27	114.10
2	S	239	LYS	CG-CD-CE	8.09	129.90	111.30
2	T	278	GLU	CA-CB-CG	8.09	130.28	114.10
2	U	239	LYS	CG-CD-CE	8.09	129.90	111.30
2	R	239	LYS	CG-CD-CE	8.09	129.90	111.30
2	U	278	GLU	CA-CB-CG	8.09	130.27	114.10
2	V	278	GLU	CA-CB-CG	8.09	130.27	114.10
2	R	270	SER	CA-C-N	8.08	127.80	119.64
2	R	270	SER	C-N-CA	8.08	127.80	119.64
2	X	239	LYS	CG-CD-CE	8.08	129.89	111.30
2	X	278	GLU	CA-CB-CG	8.08	130.26	114.10
2	P	239	LYS	CG-CD-CE	8.08	129.89	111.30
2	N	278	GLU	CA-CB-CG	8.08	130.26	114.10
2	Q	278	GLU	CA-CB-CG	8.08	130.26	114.10
2	T	239	LYS	CG-CD-CE	8.08	129.88	111.30
2	V	239	LYS	CG-CD-CE	8.08	129.89	111.30
2	W	84	ALA	N-CA-C	-8.08	101.55	111.40
2	S	278	GLU	CA-CB-CG	8.07	130.25	114.10
2	R	278	GLU	CA-CB-CG	8.07	130.25	114.10
2	N	104	ILE	O-C-N	8.07	130.89	122.09
2	R	328	GLU	CA-CB-CG	8.07	130.24	114.10
2	W	239	LYS	CG-CD-CE	8.07	129.86	111.30
2	W	328	GLU	CA-CB-CG	8.07	130.23	114.10
2	M	68	GLY	O-C-N	-8.06	114.45	122.19
2	P	328	GLU	CA-CB-CG	8.06	130.23	114.10
2	S	104	ILE	O-C-N	8.06	130.88	122.09
2	T	68	GLY	O-C-N	-8.06	114.45	122.19
2	Q	328	GLU	CA-CB-CG	8.06	130.22	114.10
2	X	84	ALA	N-CA-C	-8.05	101.58	111.40
2	M	84	ALA	N-CA-C	-8.05	101.58	111.40
2	U	328	GLU	CA-CB-CG	8.05	130.20	114.10
2	U	84	ALA	N-CA-C	-8.05	101.58	111.40
2	V	328	GLU	CA-CB-CG	8.04	130.19	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	104	ILE	O-C-N	8.04	130.86	122.09
2	N	328	GLU	CA-CB-CG	8.04	130.18	114.10
2	Q	331	PRO	O-C-N	-8.04	113.18	122.91
2	S	328	GLU	CA-CB-CG	8.04	130.18	114.10
2	T	328	GLU	CA-CB-CG	8.04	130.18	114.10
2	U	104	ILE	O-C-N	8.04	130.85	122.09
2	X	328	GLU	CA-CB-CG	8.04	130.17	114.10
2	O	68	GLY	O-C-N	-8.03	114.48	122.19
2	O	331	PRO	O-C-N	-8.03	113.19	122.91
2	V	84	ALA	N-CA-C	-8.04	101.60	111.40
2	Q	84	ALA	N-CA-C	-8.03	101.60	111.40
2	M	328	GLU	CA-CB-CG	8.03	130.16	114.10
2	Q	104	ILE	O-C-N	8.03	130.84	122.09
2	R	84	ALA	N-CA-C	-8.03	101.60	111.40
2	V	104	ILE	O-C-N	8.03	130.84	122.09
1	K	213	VAL	N-CA-C	8.03	118.07	110.53
2	T	331	PRO	O-C-N	-8.03	113.20	122.91
2	N	84	ALA	N-CA-C	-8.02	101.61	111.40
2	O	84	ALA	N-CA-C	-8.02	101.61	111.40
2	O	328	GLU	CA-CB-CG	8.02	130.15	114.10
2	S	84	ALA	N-CA-C	-8.02	101.61	111.40
2	P	84	ALA	N-CA-C	-8.02	101.62	111.40
2	S	331	PRO	O-C-N	-8.02	113.21	122.91
2	P	331	PRO	O-C-N	-8.02	113.21	122.91
2	W	104	ILE	O-C-N	8.02	130.83	122.09
1	F	213	VAL	N-CA-C	8.01	118.06	110.53
2	X	331	PRO	O-C-N	-8.01	113.22	122.91
2	T	84	ALA	N-CA-C	-8.00	101.64	111.40
2	T	104	ILE	O-C-N	8.00	130.81	122.09
2	O	104	ILE	O-C-N	8.00	130.81	122.09
2	P	104	ILE	O-C-N	8.00	130.81	122.09
2	W	331	PRO	O-C-N	-8.00	113.23	122.91
2	M	104	ILE	O-C-N	8.00	130.81	122.09
2	Q	68	GLY	O-C-N	-8.00	114.42	122.17
2	X	68	GLY	O-C-N	-8.00	114.52	122.19
2	N	331	PRO	O-C-N	-7.99	113.24	122.91
2	V	331	PRO	O-C-N	-7.99	113.24	122.91
1	G	213	VAL	N-CA-C	7.99	118.04	110.53
2	W	68	GLY	O-C-N	-7.99	114.42	122.17
2	M	331	PRO	O-C-N	-7.98	113.25	122.91
2	R	104	ILE	O-C-N	7.98	130.79	122.09
2	R	331	PRO	O-C-N	-7.97	113.26	122.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	68	GLY	O-C-N	-7.97	114.44	122.17
2	U	331	PRO	O-C-N	-7.95	113.29	122.91
2	V	68	GLY	O-C-N	-7.95	114.46	122.17
2	U	68	GLY	O-C-N	-7.95	114.46	122.17
2	P	68	GLY	O-C-N	-7.91	114.50	122.17
2	P	272	ASN	CA-C-O	-7.90	109.22	119.80
2	N	272	ASN	CA-C-O	-7.89	109.22	119.80
2	O	272	ASN	CA-C-O	-7.89	109.22	119.80
2	W	272	ASN	CA-C-O	-7.89	109.23	119.80
2	R	272	ASN	CA-C-O	-7.88	109.24	119.80
2	M	272	ASN	CA-C-O	-7.87	109.26	119.80
2	V	272	ASN	CA-C-O	-7.87	109.26	119.80
2	N	27	PHE	N-CA-C	-7.86	100.72	112.04
2	Q	272	ASN	CA-C-O	-7.86	109.27	119.80
2	T	27	PHE	N-CA-C	-7.85	100.73	112.04
2	X	272	ASN	CA-C-O	-7.85	109.28	119.80
2	P	27	PHE	N-CA-C	-7.85	100.74	112.04
2	U	272	ASN	CA-C-O	-7.85	109.28	119.80
2	V	27	PHE	N-CA-C	-7.85	100.74	112.04
2	Q	27	PHE	N-CA-C	-7.84	100.75	112.04
2	S	272	ASN	CA-C-O	-7.84	109.30	119.80
2	T	272	ASN	CA-C-O	-7.84	109.30	119.80
2	W	27	PHE	N-CA-C	-7.84	100.75	112.04
2	R	27	PHE	N-CA-C	-7.83	100.76	112.04
2	U	27	PHE	N-CA-C	-7.83	100.76	112.04
2	M	27	PHE	N-CA-C	-7.83	100.77	112.04
2	O	27	PHE	N-CA-C	-7.83	100.77	112.04
2	S	27	PHE	N-CA-C	-7.81	100.79	112.04
2	X	27	PHE	N-CA-C	-7.81	100.79	112.04
2	W	18	ASN	OD1-CG-ND2	-7.79	114.81	122.60
1	B	397	TYR	CA-C-N	-7.78	112.26	123.00
1	B	397	TYR	C-N-CA	-7.78	112.26	123.00
2	T	18	ASN	OD1-CG-ND2	-7.78	114.82	122.60
1	G	397	TYR	CA-C-N	-7.77	112.28	123.00
1	G	397	TYR	C-N-CA	-7.77	112.28	123.00
2	M	18	ASN	OD1-CG-ND2	-7.77	114.83	122.60
2	U	18	ASN	OD1-CG-ND2	-7.77	114.83	122.60
1	F	397	TYR	CA-C-N	-7.76	112.28	123.00
1	F	397	TYR	C-N-CA	-7.76	112.28	123.00
2	Q	18	ASN	OD1-CG-ND2	-7.76	114.84	122.60
2	S	18	ASN	OD1-CG-ND2	-7.76	114.84	122.60
2	O	291	GLU	CA-C-O	-7.76	111.05	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	18	ASN	OD1-CG-ND2	-7.76	114.84	122.60
2	V	18	ASN	OD1-CG-ND2	-7.76	114.84	122.60
2	N	18	ASN	OD1-CG-ND2	-7.75	114.85	122.60
2	P	18	ASN	OD1-CG-ND2	-7.75	114.85	122.60
1	E	397	TYR	CA-C-N	-7.75	112.31	123.00
1	E	397	TYR	C-N-CA	-7.75	112.31	123.00
2	U	251	LYS	CG-CD-CE	7.75	129.12	111.30
2	T	251	LYS	CG-CD-CE	7.75	129.12	111.30
2	W	251	LYS	CG-CD-CE	7.75	129.12	111.30
2	O	18	ASN	OD1-CG-ND2	-7.75	114.86	122.60
1	H	397	TYR	CA-C-N	-7.74	112.31	123.00
1	H	397	TYR	C-N-CA	-7.74	112.31	123.00
1	K	397	TYR	CA-C-N	-7.74	112.31	123.00
1	K	397	TYR	C-N-CA	-7.74	112.31	123.00
2	O	251	LYS	CG-CD-CE	7.74	129.11	111.30
2	Q	251	LYS	CG-CD-CE	7.74	129.11	111.30
2	U	291	GLU	CA-C-O	-7.74	111.07	119.97
2	R	251	LYS	CG-CD-CE	7.74	129.10	111.30
2	V	251	LYS	CG-CD-CE	7.74	129.10	111.30
2	N	251	LYS	CG-CD-CE	7.74	129.09	111.30
2	P	251	LYS	CG-CD-CE	7.74	129.10	111.30
1	D	397	TYR	CA-C-N	-7.73	112.33	123.00
1	D	397	TYR	C-N-CA	-7.73	112.33	123.00
2	S	251	LYS	CG-CD-CE	7.73	129.09	111.30
1	A	397	TYR	CA-C-N	-7.73	112.33	123.00
1	A	397	TYR	C-N-CA	-7.73	112.33	123.00
2	Q	291	GLU	CA-C-O	-7.73	111.08	119.97
1	I	397	TYR	CA-C-N	-7.73	112.33	123.00
1	I	397	TYR	C-N-CA	-7.73	112.33	123.00
2	M	251	LYS	CG-CD-CE	7.73	129.07	111.30
2	P	291	GLU	CA-C-O	-7.72	111.09	119.97
2	X	251	LYS	CG-CD-CE	7.72	129.06	111.30
2	X	18	ASN	OD1-CG-ND2	-7.72	114.88	122.60
1	L	397	TYR	CA-C-N	-7.72	112.35	123.00
1	L	397	TYR	C-N-CA	-7.72	112.35	123.00
1	C	397	TYR	CA-C-N	-7.71	112.35	123.00
1	C	397	TYR	C-N-CA	-7.71	112.35	123.00
2	V	291	GLU	CA-C-O	-7.71	111.10	119.97
1	J	397	TYR	CA-C-N	-7.71	112.36	123.00
1	J	397	TYR	C-N-CA	-7.71	112.36	123.00
2	W	291	GLU	CA-C-O	-7.71	111.11	119.97
2	R	291	GLU	CA-C-O	-7.70	111.11	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	291	GLU	CA-C-O	-7.70	111.12	119.97
2	S	291	GLU	CA-C-O	-7.68	111.14	119.97
2	X	291	GLU	CA-C-O	-7.68	111.14	119.97
2	T	291	GLU	CA-C-O	-7.68	111.14	119.97
2	M	291	GLU	CA-C-O	-7.67	111.15	119.97
2	N	45	GLU	OE1-CD-OE2	7.67	141.30	122.90
2	Q	45	GLU	OE1-CD-OE2	7.66	141.29	122.90
2	R	45	GLU	OE1-CD-OE2	7.66	141.28	122.90
2	W	45	GLU	OE1-CD-OE2	7.66	141.28	122.90
2	T	45	GLU	OE1-CD-OE2	7.65	141.26	122.90
2	U	45	GLU	OE1-CD-OE2	7.65	141.26	122.90
2	V	45	GLU	OE1-CD-OE2	7.65	141.26	122.90
2	X	45	GLU	OE1-CD-OE2	7.65	141.26	122.90
2	P	45	GLU	OE1-CD-OE2	7.65	141.26	122.90
2	S	45	GLU	OE1-CD-OE2	7.65	141.26	122.90
2	O	45	GLU	OE1-CD-OE2	7.64	141.23	122.90
2	M	45	GLU	OE1-CD-OE2	7.63	141.20	122.90
2	W	185	ASN	CA-CB-CG	7.59	120.19	112.60
2	P	185	ASN	CA-CB-CG	7.59	120.19	112.60
2	S	185	ASN	CA-CB-CG	7.59	120.19	112.60
2	U	185	ASN	CA-CB-CG	7.58	120.19	112.60
2	R	185	ASN	CA-CB-CG	7.58	120.18	112.60
2	T	185	ASN	CA-CB-CG	7.58	120.18	112.60
2	Q	33	ILE	CA-C-O	-7.58	111.79	120.65
2	Q	185	ASN	CA-CB-CG	7.58	120.18	112.60
2	T	45	GLU	N-CA-CB	-7.57	98.84	110.42
2	U	45	GLU	N-CA-CB	-7.57	98.84	110.42
2	V	185	ASN	CA-CB-CG	7.57	120.17	112.60
2	X	84	ALA	O-C-N	7.57	131.33	122.17
2	N	185	ASN	CA-CB-CG	7.57	120.17	112.60
2	N	84	ALA	O-C-N	7.57	131.33	122.17
2	S	84	ALA	O-C-N	7.57	131.32	122.17
2	O	185	ASN	CA-CB-CG	7.56	120.16	112.60
2	U	84	ALA	O-C-N	7.56	131.32	122.17
2	W	45	GLU	N-CA-CB	-7.56	98.85	110.42
2	U	84	ALA	CA-C-O	-7.56	112.46	120.55
2	O	45	GLU	N-CA-CB	-7.56	98.86	110.42
2	S	84	ALA	CA-C-O	-7.56	112.46	120.55
2	X	84	ALA	CA-C-O	-7.56	112.47	120.55
2	M	45	GLU	N-CA-CB	-7.55	98.86	110.42
2	P	45	GLU	N-CA-CB	-7.55	98.87	110.42
2	Q	45	GLU	N-CA-CB	-7.55	98.86	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	185	ASN	CA-CB-CG	7.55	120.15	112.60
2	N	84	ALA	CA-C-O	-7.55	112.47	120.55
2	S	45	GLU	N-CA-CB	-7.55	98.87	110.42
2	R	45	GLU	N-CA-CB	-7.55	98.87	110.42
2	T	84	ALA	O-C-N	7.55	131.30	122.17
2	V	45	GLU	N-CA-CB	-7.55	98.87	110.42
2	P	84	ALA	O-C-N	7.54	131.30	122.17
2	T	33	ILE	CA-C-O	-7.54	111.82	120.65
2	N	45	GLU	N-CA-CB	-7.54	98.88	110.42
2	P	84	ALA	CA-C-O	-7.54	112.48	120.55
2	V	84	ALA	O-C-N	7.54	131.29	122.17
2	R	84	ALA	CA-C-O	-7.54	112.49	120.55
2	X	45	GLU	N-CA-CB	-7.54	98.89	110.42
2	M	84	ALA	CA-C-O	-7.53	112.49	120.55
2	O	84	ALA	O-C-N	7.53	131.29	122.17
2	S	33	ILE	CA-C-O	-7.53	111.84	120.65
2	X	185	ASN	CA-CB-CG	7.53	120.13	112.60
2	V	84	ALA	CA-C-O	-7.53	112.49	120.55
2	W	84	ALA	O-C-N	7.53	131.28	122.17
2	N	282	ASN	CA-C-O	-7.53	110.92	118.97
2	Q	84	ALA	O-C-N	7.53	131.28	122.17
2	M	84	ALA	O-C-N	7.53	131.28	122.17
2	W	33	ILE	CA-C-O	-7.53	111.84	120.65
2	R	84	ALA	O-C-N	7.52	131.27	122.17
2	V	33	ILE	CA-C-O	-7.52	111.85	120.65
2	W	282	ASN	CA-C-O	-7.52	110.92	118.97
2	T	282	ASN	CA-C-O	-7.52	110.93	118.97
2	M	282	ASN	CA-C-O	-7.51	110.93	118.97
2	R	33	ILE	CA-C-O	-7.51	111.86	120.65
2	Q	282	ASN	CA-C-O	-7.51	110.93	118.97
2	U	282	ASN	CA-C-O	-7.51	110.93	118.97
2	X	33	ILE	CA-C-O	-7.51	111.86	120.65
2	M	33	ILE	CA-C-O	-7.51	111.87	120.65
2	V	282	ASN	CA-C-O	-7.51	110.94	118.97
2	W	84	ALA	CA-C-O	-7.51	112.52	120.55
2	Q	84	ALA	CA-C-O	-7.50	112.52	120.55
2	O	33	ILE	CA-C-O	-7.50	111.87	120.65
2	O	84	ALA	CA-C-O	-7.50	112.52	120.55
2	R	282	ASN	CA-C-O	-7.50	110.94	118.97
2	N	33	ILE	CA-C-O	-7.50	111.88	120.65
2	T	84	ALA	CA-C-O	-7.50	112.53	120.55
2	P	33	ILE	CA-C-O	-7.50	111.88	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	282	ASN	CA-C-O	-7.49	110.95	118.97
2	O	282	ASN	CA-C-O	-7.49	110.96	118.97
2	S	282	ASN	CA-C-O	-7.48	110.97	118.97
2	U	33	ILE	CA-C-O	-7.47	111.91	120.65
2	X	282	ASN	CA-C-O	-7.46	110.98	118.97
2	S	109	ALA	CA-C-N	7.46	133.25	123.11
2	S	109	ALA	C-N-CA	7.46	133.25	123.11
2	W	109	ALA	CA-C-N	7.45	133.25	123.11
2	W	109	ALA	C-N-CA	7.45	133.25	123.11
2	X	109	ALA	CA-C-N	7.45	133.24	123.11
2	X	109	ALA	C-N-CA	7.45	133.24	123.11
2	N	109	ALA	CA-C-N	7.44	133.23	123.11
2	N	109	ALA	C-N-CA	7.44	133.23	123.11
2	U	109	ALA	CA-C-N	7.44	133.23	123.11
2	U	109	ALA	C-N-CA	7.44	133.23	123.11
2	Q	109	ALA	CA-C-N	7.43	133.21	123.11
2	Q	109	ALA	C-N-CA	7.43	133.21	123.11
2	V	109	ALA	CA-C-N	7.43	133.21	123.11
2	V	109	ALA	C-N-CA	7.43	133.21	123.11
2	R	109	ALA	CA-C-N	7.43	133.21	123.11
2	R	109	ALA	C-N-CA	7.43	133.21	123.11
2	T	38	GLU	O-C-N	7.42	133.06	123.11
2	T	109	ALA	CA-C-N	7.42	133.20	123.11
2	T	109	ALA	C-N-CA	7.42	133.20	123.11
2	M	109	ALA	CA-C-N	7.42	133.19	123.11
2	M	109	ALA	C-N-CA	7.42	133.19	123.11
2	S	29	LYS	N-CA-C	-7.41	103.70	112.89
2	P	109	ALA	CA-C-N	7.41	133.19	123.11
2	P	109	ALA	C-N-CA	7.41	133.19	123.11
2	S	38	GLU	O-C-N	7.41	133.03	123.11
2	W	38	GLU	O-C-N	7.41	133.03	123.11
2	N	29	LYS	N-CA-C	-7.40	103.71	112.89
2	Q	29	LYS	N-CA-C	-7.40	103.71	112.89
2	P	38	GLU	O-C-N	7.40	133.03	123.11
2	O	38	GLU	O-C-N	7.40	133.02	123.11
2	R	67	PHE	CA-C-O	-7.40	112.58	120.42
2	U	29	LYS	N-CA-C	-7.40	103.72	112.89
2	X	38	GLU	O-C-N	7.40	133.02	123.11
2	X	29	LYS	N-CA-C	-7.39	103.72	112.89
2	R	38	GLU	O-C-N	7.39	133.01	123.11
2	T	67	PHE	CA-C-O	-7.39	112.59	120.42
2	V	38	GLU	O-C-N	7.39	133.01	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	67	PHE	CA-C-O	-7.38	112.59	120.42
2	U	67	PHE	CA-C-O	-7.38	112.59	120.42
2	U	38	GLU	O-C-N	7.38	133.00	123.11
2	O	109	ALA	CA-C-N	7.38	133.15	123.11
2	O	109	ALA	C-N-CA	7.38	133.15	123.11
2	W	29	LYS	N-CA-C	-7.38	103.74	112.89
2	N	38	GLU	O-C-N	7.37	132.99	123.11
2	S	67	PHE	CA-C-O	-7.37	112.61	120.42
2	W	67	PHE	CA-C-O	-7.37	112.61	120.42
2	N	349	ASN	CA-CB-CG	7.37	119.97	112.60
2	V	29	LYS	N-CA-C	-7.37	103.75	112.89
2	R	29	LYS	N-CA-C	-7.37	103.75	112.89
2	V	67	PHE	CA-C-O	-7.37	112.61	120.42
2	N	97	VAL	O-C-N	7.37	131.78	122.57
2	Q	38	GLU	O-C-N	7.37	132.98	123.11
2	P	67	PHE	CA-C-O	-7.36	112.61	120.42
2	T	29	LYS	N-CA-C	-7.36	103.76	112.89
2	M	97	VAL	O-C-N	7.36	131.77	122.57
2	O	29	LYS	N-CA-C	-7.36	103.76	112.89
1	H	213	VAL	N-CA-C	7.36	118.15	110.72
2	N	67	PHE	CA-C-O	-7.36	112.62	120.42
2	P	29	LYS	N-CA-C	-7.35	103.77	112.89
2	Q	67	PHE	CA-C-O	-7.35	112.62	120.42
2	U	97	VAL	O-C-N	7.35	131.76	122.57
2	T	349	ASN	CA-CB-CG	7.35	119.95	112.60
2	O	67	PHE	CA-C-O	-7.35	112.63	120.42
2	Q	354	ARG	N-CA-CB	7.35	121.67	110.28
2	X	346	ALA	O-C-N	-7.35	114.45	122.09
2	M	38	GLU	O-C-N	7.35	132.95	123.11
2	M	349	ASN	CA-CB-CG	7.35	119.95	112.60
2	Q	346	ALA	O-C-N	-7.35	114.45	122.09
2	M	29	LYS	N-CA-C	-7.34	103.78	112.89
2	M	67	PHE	CA-C-O	-7.34	112.64	120.42
2	R	26	LYS	N-CA-C	-7.34	104.21	113.02
2	Q	97	VAL	O-C-N	7.34	131.75	122.57
2	R	97	VAL	O-C-N	7.34	131.74	122.57
2	U	349	ASN	CA-CB-CG	7.34	119.94	112.60
2	V	97	VAL	O-C-N	7.34	131.74	122.57
2	P	97	VAL	O-C-N	7.34	131.74	122.57
2	Q	26	LYS	N-CA-C	-7.34	104.22	113.02
2	R	354	ARG	N-CA-CB	7.34	121.65	110.28
2	P	26	LYS	N-CA-C	-7.34	104.22	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	354	ARG	N-CA-CB	7.34	121.65	110.28
2	U	26	LYS	N-CA-C	-7.33	104.22	113.02
2	M	26	LYS	N-CA-C	-7.33	104.22	113.02
2	T	97	VAL	O-C-N	7.33	131.73	122.57
2	M	346	ALA	O-C-N	-7.33	114.47	122.09
2	X	26	LYS	N-CA-C	-7.33	104.23	113.02
2	S	354	ARG	N-CA-CB	7.33	121.63	110.28
2	T	26	LYS	N-CA-C	-7.33	104.23	113.02
2	O	354	ARG	N-CA-CB	7.32	121.63	110.28
2	S	97	VAL	O-C-N	7.32	131.72	122.57
2	T	354	ARG	N-CA-CB	7.32	121.63	110.28
2	W	26	LYS	N-CA-C	-7.32	104.23	113.02
2	X	354	ARG	N-CA-CB	7.32	121.63	110.28
2	V	26	LYS	N-CA-C	-7.32	104.24	113.02
2	V	354	ARG	N-CA-CB	7.32	121.62	110.28
2	M	354	ARG	N-CA-CB	7.31	121.61	110.28
2	N	26	LYS	N-CA-C	-7.31	104.25	113.02
2	P	354	ARG	N-CA-CB	7.31	121.61	110.28
2	N	354	ARG	N-CA-CB	7.31	121.61	110.28
2	V	349	ASN	CA-CB-CG	7.31	119.91	112.60
1	L	213	VAL	N-CA-C	7.31	118.10	110.72
2	X	349	ASN	CA-CB-CG	7.31	119.91	112.60
2	Q	349	ASN	CA-CB-CG	7.31	119.91	112.60
2	R	346	ALA	O-C-N	-7.31	114.49	122.09
1	B	213	VAL	N-CA-C	7.30	118.10	110.72
2	N	346	ALA	O-C-N	-7.30	114.49	122.09
2	W	97	VAL	O-C-N	7.30	131.70	122.57
1	D	213	VAL	N-CA-C	7.30	118.09	110.72
2	R	349	ASN	CA-CB-CG	7.30	119.90	112.60
2	S	26	LYS	N-CA-C	-7.30	104.26	113.02
2	V	346	ALA	O-C-N	-7.30	114.50	122.09
2	O	97	VAL	O-C-N	7.30	131.69	122.57
2	U	354	ARG	N-CA-CB	7.30	121.59	110.28
2	P	349	ASN	CA-CB-CG	7.30	119.90	112.60
2	X	97	VAL	O-C-N	7.30	131.69	122.57
2	P	346	ALA	O-C-N	-7.29	114.50	122.09
2	T	346	ALA	O-C-N	-7.29	114.50	122.09
2	U	346	ALA	O-C-N	-7.29	114.50	122.09
2	O	26	LYS	N-CA-C	-7.29	104.28	113.02
2	Q	142	LYS	CA-CB-CG	7.29	128.67	114.10
2	S	346	ALA	O-C-N	-7.29	114.51	122.09
2	S	349	ASN	CA-CB-CG	7.29	119.89	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	349	ASN	CA-CB-CG	7.28	119.88	112.60
2	U	142	LYS	CA-CB-CG	7.28	128.67	114.10
2	M	142	LYS	CA-CB-CG	7.28	128.65	114.10
2	P	142	LYS	CA-CB-CG	7.28	128.65	114.10
2	W	349	ASN	CA-CB-CG	7.28	119.88	112.60
2	S	173	ASN	CA-CB-CG	7.27	119.87	112.60
1	J	213	VAL	N-CA-C	7.27	118.06	110.72
2	O	346	ALA	O-C-N	-7.27	114.53	122.09
2	U	173	ASN	CA-CB-CG	7.27	119.87	112.60
2	V	142	LYS	CA-CB-CG	7.27	128.63	114.10
2	W	346	ALA	O-C-N	-7.27	114.53	122.09
2	X	142	LYS	CA-CB-CG	7.27	128.63	114.10
1	H	401	PRO	CA-N-CD	-7.27	101.83	112.00
2	W	142	LYS	CA-CB-CG	7.26	128.63	114.10
2	P	173	ASN	CA-CB-CG	7.26	119.86	112.60
1	C	213	VAL	N-CA-C	7.26	118.05	110.72
2	R	142	LYS	CA-CB-CG	7.26	128.62	114.10
2	S	142	LYS	CA-CB-CG	7.26	128.62	114.10
1	E	213	VAL	N-CA-C	7.26	118.05	110.72
1	C	401	PRO	CA-N-CD	-7.26	101.84	112.00
1	D	401	PRO	CA-N-CD	-7.26	101.84	112.00
2	Q	173	ASN	CA-CB-CG	7.26	119.86	112.60
2	T	142	LYS	CA-CB-CG	7.26	128.61	114.10
2	W	173	ASN	CA-CB-CG	7.26	119.86	112.60
2	N	142	LYS	CA-CB-CG	7.25	128.60	114.10
2	O	173	ASN	CA-CB-CG	7.25	119.85	112.60
1	B	401	PRO	CA-N-CD	-7.25	101.85	112.00
1	A	401	PRO	CA-N-CD	-7.25	101.86	112.00
1	I	213	VAL	N-CA-C	7.25	118.04	110.72
2	O	142	LYS	CA-CB-CG	7.25	128.59	114.10
1	A	213	VAL	N-CA-C	7.25	118.04	110.72
1	J	401	PRO	CA-N-CD	-7.24	101.86	112.00
1	I	401	PRO	CA-N-CD	-7.24	101.86	112.00
2	N	173	ASN	CA-CB-CG	7.24	119.84	112.60
1	G	401	PRO	CA-N-CD	-7.24	101.87	112.00
1	K	401	PRO	CA-N-CD	-7.24	101.87	112.00
1	L	401	PRO	CA-N-CD	-7.24	101.87	112.00
1	E	401	PRO	CA-N-CD	-7.23	101.88	112.00
2	V	173	ASN	CA-CB-CG	7.23	119.83	112.60
2	R	173	ASN	CA-CB-CG	7.22	119.82	112.60
2	T	173	ASN	CA-CB-CG	7.20	119.80	112.60
1	F	401	PRO	CA-N-CD	-7.19	101.93	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	173	ASN	CA-CB-CG	7.19	119.79	112.60
2	X	173	ASN	CA-CB-CG	7.18	119.78	112.60
2	P	106	TYR	O-C-N	7.16	129.31	121.36
2	O	106	TYR	O-C-N	7.16	129.31	121.36
2	X	106	TYR	O-C-N	7.16	129.31	121.36
2	M	278	GLU	CA-C-N	7.16	130.20	120.54
2	M	278	GLU	C-N-CA	7.16	130.20	120.54
2	P	278	GLU	CA-C-N	7.16	130.20	120.54
2	P	278	GLU	C-N-CA	7.16	130.20	120.54
2	W	278	GLU	CA-C-N	7.16	130.20	120.54
2	W	278	GLU	C-N-CA	7.16	130.20	120.54
2	O	278	GLU	CA-C-N	7.15	130.19	120.54
2	O	278	GLU	C-N-CA	7.15	130.19	120.54
2	Q	128	THR	N-CA-CB	-7.14	98.34	111.13
2	R	278	GLU	CA-C-N	7.14	130.18	120.54
2	R	278	GLU	C-N-CA	7.14	130.18	120.54
2	S	128	THR	N-CA-CB	-7.14	98.35	111.13
2	M	106	TYR	O-C-N	7.14	129.28	121.36
2	S	106	TYR	O-C-N	7.14	129.28	121.36
2	V	278	GLU	CA-C-N	7.14	130.17	120.54
2	V	278	GLU	C-N-CA	7.14	130.17	120.54
2	N	278	GLU	CA-C-N	7.13	130.17	120.54
2	N	278	GLU	C-N-CA	7.13	130.17	120.54
2	V	106	TYR	O-C-N	7.13	129.28	121.36
2	W	106	TYR	O-C-N	7.13	129.28	121.36
2	R	128	THR	N-CA-CB	-7.13	98.36	111.13
1	F	66	VAL	N-CA-C	7.13	118.87	108.53
2	M	128	THR	N-CA-CB	-7.13	98.37	111.13
2	O	128	THR	N-CA-CB	-7.13	98.37	111.13
2	T	278	GLU	CA-C-N	7.13	130.16	120.54
2	T	278	GLU	C-N-CA	7.13	130.16	120.54
2	U	106	TYR	O-C-N	7.12	129.27	121.36
1	B	66	VAL	N-CA-C	7.12	118.86	108.53
1	K	66	VAL	N-CA-C	7.12	118.86	108.53
2	S	278	GLU	CA-C-N	7.12	130.16	120.54
2	S	278	GLU	C-N-CA	7.12	130.16	120.54
2	N	128	THR	N-CA-CB	-7.12	98.38	111.13
2	R	353	GLY	O-C-N	7.12	131.03	122.34
2	T	106	TYR	O-C-N	7.12	129.27	121.36
2	T	128	THR	N-CA-CB	-7.12	98.38	111.13
2	U	353	GLY	O-C-N	7.12	131.03	122.34
2	V	128	THR	N-CA-CB	-7.12	98.38	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	278	GLU	CA-C-N	7.12	130.15	120.54
2	Q	278	GLU	C-N-CA	7.12	130.15	120.54
2	W	128	THR	N-CA-CB	-7.12	98.39	111.13
1	L	66	VAL	N-CA-C	7.11	118.84	108.53
2	U	278	GLU	CA-C-N	7.11	130.14	120.54
2	U	278	GLU	C-N-CA	7.11	130.14	120.54
2	X	278	GLU	CA-C-N	7.11	130.14	120.54
2	X	278	GLU	C-N-CA	7.11	130.14	120.54
2	M	353	GLY	O-C-N	7.11	131.01	122.34
2	Q	106	TYR	O-C-N	7.11	129.25	121.36
2	X	128	THR	N-CA-CB	-7.11	98.41	111.13
1	E	66	VAL	N-CA-C	7.10	118.83	108.53
1	I	66	VAL	N-CA-C	7.10	118.83	108.53
1	J	66	VAL	N-CA-C	7.10	118.83	108.53
2	X	353	GLY	O-C-N	7.10	131.00	122.34
1	A	66	VAL	N-CA-C	7.10	118.82	108.53
2	P	128	THR	N-CA-CB	-7.10	98.42	111.13
2	U	128	THR	N-CA-CB	-7.10	98.43	111.13
1	G	66	VAL	N-CA-C	7.09	118.82	108.53
2	N	106	TYR	O-C-N	7.09	129.23	121.36
2	V	353	GLY	O-C-N	7.09	131.00	122.34
2	R	106	TYR	O-C-N	7.09	129.23	121.36
2	S	353	GLY	O-C-N	7.08	130.98	122.34
2	W	353	GLY	O-C-N	7.08	130.98	122.34
2	N	353	GLY	O-C-N	7.08	130.98	122.34
2	T	353	GLY	O-C-N	7.08	130.97	122.34
1	D	66	VAL	N-CA-C	7.07	118.79	108.53
2	O	353	GLY	O-C-N	7.07	130.97	122.34
2	P	353	GLY	O-C-N	7.07	130.97	122.34
1	H	66	VAL	N-CA-C	7.07	118.78	108.53
2	Q	262	LEU	O-C-N	7.06	131.71	122.95
2	Q	353	GLY	O-C-N	7.06	130.96	122.34
1	C	66	VAL	N-CA-C	7.06	118.77	108.53
2	S	30	ASP	CB-CA-C	7.06	122.78	110.64
2	T	262	LEU	O-C-N	7.06	131.70	122.95
1	F	387	HIS	O-C-N	7.05	128.90	121.42
2	X	30	ASP	CB-CA-C	7.04	122.76	110.64
2	O	262	LEU	O-C-N	7.04	131.68	122.95
1	B	387	HIS	O-C-N	7.03	128.88	121.42
2	N	30	ASP	CB-CA-C	7.03	122.74	110.64
2	S	262	LEU	O-C-N	7.03	131.67	122.95
2	U	30	ASP	CB-CA-C	7.03	122.73	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	30	ASP	CB-CA-C	7.03	122.73	110.64
2	R	262	LEU	O-C-N	7.03	131.66	122.95
2	V	30	ASP	CB-CA-C	7.03	122.73	110.64
2	W	30	ASP	CB-CA-C	7.02	122.72	110.64
2	T	30	ASP	CB-CA-C	7.02	122.72	110.64
2	M	30	ASP	CB-CA-C	7.02	122.71	110.64
2	R	30	ASP	CB-CA-C	7.01	122.70	110.64
2	P	30	ASP	CB-CA-C	7.01	122.70	110.64
2	V	262	LEU	O-C-N	7.01	131.64	122.95
2	Q	30	ASP	CB-CA-C	7.01	122.69	110.64
2	W	262	LEU	O-C-N	7.01	131.64	122.95
2	M	262	LEU	O-C-N	7.00	131.62	122.95
2	U	262	LEU	O-C-N	7.00	131.62	122.95
1	E	387	HIS	O-C-N	6.99	128.83	121.42
2	U	8	VAL	CB-CA-C	6.99	120.97	110.63
2	X	262	LEU	O-C-N	6.99	131.62	122.95
2	P	262	LEU	O-C-N	6.99	131.61	122.95
1	I	387	HIS	O-C-N	6.98	128.82	121.42
1	C	387	HIS	O-C-N	6.98	128.82	121.42
1	G	387	HIS	O-C-N	6.98	128.82	121.42
2	N	8	VAL	CB-CA-C	6.98	120.96	110.63
1	H	387	HIS	O-C-N	6.97	128.81	121.42
2	U	242	TYR	CA-C-N	-6.97	116.26	122.47
2	U	242	TYR	C-N-CA	-6.97	116.26	122.47
2	S	8	VAL	CB-CA-C	6.97	120.95	110.63
2	U	28	GLU	N-CA-C	6.97	119.91	111.82
2	W	28	GLU	N-CA-C	6.97	119.90	111.82
1	D	387	HIS	O-C-N	6.96	128.80	121.42
2	N	28	GLU	N-CA-C	6.96	119.89	111.82
1	L	387	HIS	O-C-N	6.96	128.80	121.42
2	N	262	LEU	O-C-N	6.96	131.58	122.95
2	V	8	VAL	CB-CA-C	6.96	120.93	110.63
2	Q	242	TYR	CA-C-N	-6.96	116.28	122.47
2	Q	242	TYR	C-N-CA	-6.96	116.28	122.47
1	K	387	HIS	O-C-N	6.95	128.79	121.42
1	J	387	HIS	O-C-N	6.95	128.79	121.42
2	T	8	VAL	CB-CA-C	6.95	120.92	110.63
2	O	28	GLU	N-CA-C	6.95	119.88	111.82
2	O	242	TYR	CA-C-N	-6.95	116.28	122.47
2	O	242	TYR	C-N-CA	-6.95	116.28	122.47
2	X	8	VAL	CB-CA-C	6.95	120.91	110.63
2	O	8	VAL	CB-CA-C	6.95	120.91	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	8	VAL	CB-CA-C	6.95	120.91	110.63
2	W	8	VAL	CB-CA-C	6.95	120.91	110.63
2	M	8	VAL	CB-CA-C	6.94	120.91	110.63
2	T	28	GLU	N-CA-C	6.94	119.87	111.82
1	A	387	HIS	O-C-N	6.94	128.78	121.42
2	R	8	VAL	CB-CA-C	6.94	120.90	110.63
2	Q	8	VAL	CB-CA-C	6.94	120.90	110.63
2	T	242	TYR	CA-C-N	-6.94	116.30	122.47
2	T	242	TYR	C-N-CA	-6.94	116.30	122.47
2	P	242	TYR	CA-C-N	-6.93	116.30	122.47
2	P	242	TYR	C-N-CA	-6.93	116.30	122.47
2	P	28	GLU	N-CA-C	6.93	119.86	111.82
2	Q	28	GLU	N-CA-C	6.93	119.86	111.82
2	X	28	GLU	N-CA-C	6.93	119.86	111.82
2	V	28	GLU	N-CA-C	6.93	119.86	111.82
2	R	28	GLU	N-CA-C	6.93	119.86	111.82
2	W	125	PRO	CB-CA-C	6.93	117.68	111.17
2	R	242	TYR	CA-C-N	-6.92	116.31	122.47
2	R	242	TYR	C-N-CA	-6.92	116.31	122.47
2	W	242	TYR	CA-C-N	-6.92	116.31	122.47
2	W	242	TYR	C-N-CA	-6.92	116.31	122.47
2	M	64	HIS	CA-CB-CG	-6.92	106.88	113.80
2	S	242	TYR	CA-C-N	-6.92	116.31	122.47
2	S	242	TYR	C-N-CA	-6.92	116.31	122.47
2	X	242	TYR	CA-C-N	-6.92	116.31	122.47
2	X	242	TYR	C-N-CA	-6.92	116.31	122.47
2	V	242	TYR	CA-C-N	-6.91	116.32	122.47
2	V	242	TYR	C-N-CA	-6.91	116.32	122.47
2	N	64	HIS	CA-CB-CG	-6.91	106.89	113.80
2	N	125	PRO	CB-CA-C	6.91	117.66	111.17
2	R	125	PRO	CB-CA-C	6.91	117.66	111.17
2	S	125	PRO	CB-CA-C	6.91	117.66	111.17
2	M	28	GLU	N-CA-C	6.90	119.83	111.82
2	O	125	PRO	CB-CA-C	6.90	117.66	111.17
2	O	64	HIS	CA-CB-CG	-6.90	106.90	113.80
2	V	125	PRO	CB-CA-C	6.90	117.65	111.17
2	M	208	THR	O-C-N	6.89	131.33	123.06
2	M	242	TYR	CA-C-N	-6.89	116.33	122.47
2	M	242	TYR	C-N-CA	-6.89	116.33	122.47
2	S	28	GLU	N-CA-C	6.89	119.82	111.82
2	M	125	PRO	CB-CA-C	6.89	117.65	111.17
2	N	242	TYR	CA-C-N	-6.89	116.34	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	242	TYR	C-N-CA	-6.89	116.34	122.47
2	Q	125	PRO	CB-CA-C	6.89	117.65	111.17
2	R	291	GLU	OE1-CD-OE2	6.89	139.44	122.90
2	X	64	HIS	CA-CB-CG	-6.89	106.91	113.80
2	X	125	PRO	CB-CA-C	6.89	117.64	111.17
2	P	125	PRO	CB-CA-C	6.89	117.64	111.17
2	X	291	GLU	OE1-CD-OE2	6.89	139.43	122.90
2	U	125	PRO	CB-CA-C	6.88	117.64	111.17
2	P	291	GLU	OE1-CD-OE2	6.88	139.41	122.90
2	R	64	HIS	CA-CB-CG	-6.88	106.92	113.80
2	T	64	HIS	CA-CB-CG	-6.88	106.92	113.80
2	U	64	HIS	CA-CB-CG	-6.88	106.92	113.80
2	N	291	GLU	OE1-CD-OE2	6.87	139.40	122.90
2	Q	208	THR	O-C-N	6.87	131.31	123.06
2	T	125	PRO	CB-CA-C	6.87	117.63	111.17
2	V	64	HIS	CA-CB-CG	-6.87	106.93	113.80
2	W	291	GLU	OE1-CD-OE2	6.87	139.39	122.90
2	P	64	HIS	CA-CB-CG	-6.87	106.93	113.80
2	Q	33	ILE	O-C-N	6.87	131.32	122.94
2	Q	133	PRO	O-C-N	6.87	129.93	122.17
2	S	291	GLU	OE1-CD-OE2	6.87	139.39	122.90
2	T	291	GLU	OE1-CD-OE2	6.87	139.38	122.90
2	M	291	GLU	OE1-CD-OE2	6.87	139.38	122.90
2	V	291	GLU	OE1-CD-OE2	6.87	139.38	122.90
2	O	208	THR	O-C-N	6.86	131.30	123.06
2	Q	64	HIS	CA-CB-CG	-6.86	106.94	113.80
2	P	120	ASP	CA-C-O	-6.86	111.69	119.79
2	U	208	THR	O-C-N	6.86	131.29	123.06
2	W	208	THR	O-C-N	6.86	131.29	123.06
2	W	64	HIS	CA-CB-CG	-6.86	106.94	113.80
2	Q	291	GLU	OE1-CD-OE2	6.86	139.36	122.90
2	U	291	GLU	OE1-CD-OE2	6.86	139.36	122.90
2	S	353	GLY	CA-C-O	-6.86	110.67	119.58
2	R	353	GLY	CA-C-O	-6.85	110.67	119.58
2	S	64	HIS	CA-CB-CG	-6.85	106.95	113.80
2	V	208	THR	O-C-N	6.85	131.28	123.06
2	P	55	ASP	CB-CA-C	6.85	124.05	110.42
2	X	120	ASP	CA-C-O	-6.85	111.71	119.79
2	U	353	GLY	CA-C-O	-6.85	110.68	119.58
2	X	208	THR	O-C-N	6.85	131.28	123.06
2	O	120	ASP	CA-C-O	-6.84	111.71	119.79
2	T	33	ILE	O-C-N	6.84	131.29	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	353	GLY	CA-C-O	-6.84	110.68	119.58
2	N	120	ASP	CA-C-O	-6.84	111.72	119.79
2	O	291	GLU	OE1-CD-OE2	6.84	139.32	122.90
2	T	55	ASP	CB-CA-C	6.84	124.03	110.42
2	W	55	ASP	CB-CA-C	6.84	124.02	110.42
2	W	120	ASP	CA-C-O	-6.84	111.72	119.79
2	N	33	ILE	O-C-N	6.83	131.28	122.94
2	T	120	ASP	CA-C-O	-6.83	111.72	119.79
2	V	353	GLY	CA-C-O	-6.83	110.69	119.58
2	P	208	THR	O-C-N	6.83	131.26	123.06
2	Q	55	ASP	CB-CA-C	6.83	124.02	110.42
2	R	55	ASP	CB-CA-C	6.83	124.02	110.42
2	S	120	ASP	CA-C-O	-6.83	111.73	119.79
2	W	33	ILE	O-C-N	6.83	131.28	122.94
2	M	55	ASP	CB-CA-C	6.83	124.01	110.42
2	X	133	PRO	O-C-N	6.83	129.89	122.17
2	X	353	GLY	CA-C-O	-6.83	110.70	119.58
2	M	353	GLY	CA-C-O	-6.83	110.70	119.58
2	R	120	ASP	CA-C-O	-6.83	111.73	119.79
2	S	208	THR	O-C-N	6.83	131.26	123.06
2	Q	353	GLY	CA-C-O	-6.83	110.70	119.58
2	R	33	ILE	O-C-N	6.83	131.27	122.94
2	S	33	ILE	O-C-N	6.83	131.27	122.94
2	T	133	PRO	O-C-N	6.83	129.89	122.17
2	U	55	ASP	CB-CA-C	6.83	124.01	110.42
2	V	120	ASP	CA-C-O	-6.83	111.73	119.79
2	M	133	PRO	O-C-N	6.83	129.88	122.17
2	N	55	ASP	CB-CA-C	6.83	124.00	110.42
2	Q	120	ASP	CA-C-O	-6.83	111.74	119.79
2	R	208	THR	O-C-N	6.83	131.25	123.06
2	T	208	THR	O-C-N	6.83	131.25	123.06
2	V	55	ASP	CB-CA-C	6.83	124.00	110.42
2	N	208	THR	O-C-N	6.82	131.25	123.06
2	O	353	GLY	CA-C-O	-6.82	110.71	119.58
2	P	353	GLY	CA-C-O	-6.82	110.71	119.58
2	V	33	ILE	O-C-N	6.82	131.26	122.94
2	W	133	PRO	O-C-N	6.82	129.88	122.17
2	M	120	ASP	CA-C-O	-6.82	111.74	119.79
2	O	133	PRO	O-C-N	6.82	129.88	122.17
2	M	293	VAL	CA-C-O	-6.81	113.49	121.05
2	T	353	GLY	CA-C-O	-6.81	110.72	119.58
2	V	133	PRO	O-C-N	6.81	129.87	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	55	ASP	CB-CA-C	6.81	123.97	110.42
2	N	133	PRO	O-C-N	6.81	129.86	122.17
2	N	353	GLY	CA-C-O	-6.81	110.73	119.58
2	P	133	PRO	O-C-N	6.81	129.87	122.17
2	S	55	ASP	CB-CA-C	6.81	123.97	110.42
2	P	33	ILE	O-C-N	6.81	131.25	122.94
2	M	33	ILE	O-C-N	6.80	131.24	122.94
2	O	94	TRP	CA-C-N	6.80	130.65	120.31
2	O	94	TRP	C-N-CA	6.80	130.65	120.31
2	U	120	ASP	CA-C-O	-6.80	111.76	119.79
2	X	55	ASP	CB-CA-C	6.80	123.95	110.42
2	Q	293	VAL	CA-C-O	-6.80	113.50	121.05
2	R	133	PRO	O-C-N	6.80	129.85	122.17
2	O	33	ILE	O-C-N	6.79	131.23	122.94
2	U	366	THR	CA-CB-OG1	-6.79	99.41	109.60
2	O	150	ASN	OD1-CG-ND2	-6.79	115.81	122.60
2	Q	94	TRP	CA-C-N	6.79	130.63	120.31
2	Q	94	TRP	C-N-CA	6.79	130.63	120.31
2	X	94	TRP	CA-C-N	6.79	130.63	120.31
2	X	94	TRP	C-N-CA	6.79	130.63	120.31
2	X	33	ILE	O-C-N	6.79	131.22	122.94
2	S	133	PRO	O-C-N	6.79	129.84	122.17
2	N	366	THR	CA-CB-OG1	-6.78	99.42	109.60
2	O	293	VAL	CA-C-O	-6.78	113.52	121.05
2	R	150	ASN	OD1-CG-ND2	-6.78	115.82	122.60
2	U	293	VAL	CA-C-O	-6.78	113.53	121.05
2	U	133	PRO	O-C-N	6.78	129.83	122.17
2	T	366	THR	CA-CB-OG1	-6.78	99.44	109.60
2	U	33	ILE	O-C-N	6.78	131.21	122.94
2	T	94	TRP	CA-C-N	6.77	130.60	120.31
2	T	94	TRP	C-N-CA	6.77	130.60	120.31
2	V	94	TRP	CA-C-N	6.77	130.60	120.31
2	V	94	TRP	C-N-CA	6.77	130.60	120.31
2	N	94	TRP	CA-C-N	6.77	130.60	120.31
2	N	94	TRP	C-N-CA	6.77	130.60	120.31
2	M	366	THR	CA-CB-OG1	-6.77	99.45	109.60
2	S	366	THR	CA-CB-OG1	-6.77	99.45	109.60
2	X	366	THR	CA-CB-OG1	-6.77	99.44	109.60
2	O	366	THR	CA-CB-OG1	-6.77	99.45	109.60
2	P	366	THR	CA-CB-OG1	-6.77	99.45	109.60
2	W	150	ASN	OD1-CG-ND2	-6.77	115.83	122.60
2	N	293	VAL	CA-C-O	-6.77	113.54	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	366	THR	CA-CB-OG1	-6.77	99.45	109.60
2	W	366	THR	CA-CB-OG1	-6.76	99.45	109.60
2	T	293	VAL	CA-C-O	-6.76	113.54	121.05
2	V	293	VAL	CA-C-O	-6.76	113.54	121.05
2	P	94	TRP	CA-C-N	6.76	130.59	120.31
2	P	94	TRP	C-N-CA	6.76	130.59	120.31
2	U	94	TRP	CA-C-N	6.76	130.59	120.31
2	U	94	TRP	C-N-CA	6.76	130.59	120.31
2	V	366	THR	CA-CB-OG1	-6.76	99.46	109.60
2	P	293	VAL	CA-C-O	-6.76	113.55	121.05
2	S	94	TRP	CA-C-N	6.76	130.59	120.31
2	S	94	TRP	C-N-CA	6.76	130.59	120.31
2	P	361	LEU	O-C-N	6.76	131.38	122.33
2	R	94	TRP	CA-C-N	6.76	130.58	120.31
2	R	94	TRP	C-N-CA	6.76	130.58	120.31
2	W	94	TRP	CA-C-N	6.75	130.58	120.31
2	W	94	TRP	C-N-CA	6.75	130.58	120.31
2	S	293	VAL	CA-C-O	-6.75	113.55	121.05
2	P	354	ARG	NE-CZ-NH2	-6.75	113.12	119.20
2	V	150	ASN	OD1-CG-ND2	-6.75	115.85	122.60
2	O	361	LEU	O-C-N	6.75	131.38	122.33
2	S	361	LEU	O-C-N	6.75	131.38	122.33
2	T	312	ALA	N-CA-C	6.75	118.67	107.20
2	Q	366	THR	CA-CB-OG1	-6.74	99.49	109.60
2	U	361	LEU	O-C-N	6.74	131.37	122.33
2	W	361	LEU	O-C-N	6.74	131.37	122.33
2	X	361	LEU	O-C-N	6.74	131.37	122.33
2	M	94	TRP	CA-C-N	6.74	130.56	120.31
2	M	94	TRP	C-N-CA	6.74	130.56	120.31
2	R	354	ARG	NE-CZ-NH2	-6.74	113.13	119.20
2	X	354	ARG	NE-CZ-NH2	-6.74	113.14	119.20
2	M	354	ARG	NE-CZ-NH2	-6.74	113.14	119.20
2	Q	150	ASN	OD1-CG-ND2	-6.74	115.86	122.60
2	V	361	LEU	O-C-N	6.74	131.36	122.33
2	M	361	LEU	O-C-N	6.73	131.35	122.33
2	T	361	LEU	O-C-N	6.73	131.35	122.33
2	U	150	ASN	OD1-CG-ND2	-6.73	115.87	122.60
2	W	293	VAL	CA-C-O	-6.73	113.58	121.05
2	N	150	ASN	OD1-CG-ND2	-6.73	115.87	122.60
2	V	312	ALA	N-CA-C	6.73	118.63	107.20
2	X	293	VAL	CA-C-O	-6.72	113.58	121.05
2	Q	290	LEU	O-C-N	6.72	129.24	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	293	VAL	CA-C-O	-6.72	113.59	121.05
2	R	361	LEU	O-C-N	6.72	131.34	122.33
2	S	312	ALA	N-CA-C	6.72	118.62	107.20
2	X	150	ASN	OD1-CG-ND2	-6.72	115.88	122.60
2	N	361	LEU	O-C-N	6.72	131.33	122.33
2	O	312	ALA	N-CA-C	6.72	118.62	107.20
2	X	312	ALA	N-CA-C	6.72	118.62	107.20
2	M	312	ALA	N-CA-C	6.71	118.61	107.20
2	N	354	ARG	NE-CZ-NH2	-6.71	113.16	119.20
2	T	150	ASN	OD1-CG-ND2	-6.71	115.89	122.60
2	U	312	ALA	N-CA-C	6.71	118.61	107.20
2	S	354	ARG	NE-CZ-NH2	-6.71	113.16	119.20
2	M	150	ASN	OD1-CG-ND2	-6.71	115.89	122.60
2	N	312	ALA	N-CA-C	6.71	118.61	107.20
2	X	128	THR	OG1-CB-CG2	6.71	122.72	109.30
2	P	150	ASN	OD1-CG-ND2	-6.71	115.89	122.60
2	Q	312	ALA	N-CA-C	6.71	118.60	107.20
2	W	354	ARG	NE-CZ-NH2	-6.71	113.17	119.20
2	P	312	ALA	N-CA-C	6.71	118.60	107.20
2	Q	361	LEU	O-C-N	6.70	131.31	122.33
2	T	354	ARG	NE-CZ-NH2	-6.70	113.17	119.20
2	W	312	ALA	N-CA-C	6.70	118.59	107.20
2	V	354	ARG	NE-CZ-NH2	-6.70	113.17	119.20
2	R	312	ALA	N-CA-C	6.70	118.58	107.20
2	S	150	ASN	OD1-CG-ND2	-6.70	115.90	122.60
2	Q	354	ARG	NE-CZ-NH2	-6.69	113.18	119.20
2	U	354	ARG	NE-CZ-NH2	-6.69	113.18	119.20
2	O	354	ARG	NE-CZ-NH2	-6.69	113.18	119.20
2	W	128	THR	OG1-CB-CG2	6.69	122.68	109.30
2	M	128	THR	OG1-CB-CG2	6.68	122.67	109.30
2	Q	128	THR	OG1-CB-CG2	6.68	122.67	109.30
2	U	128	THR	OG1-CB-CG2	6.68	122.66	109.30
2	P	128	THR	OG1-CB-CG2	6.68	122.66	109.30
2	T	128	THR	OG1-CB-CG2	6.68	122.66	109.30
2	V	128	THR	OG1-CB-CG2	6.68	122.66	109.30
2	M	290	LEU	O-C-N	6.67	129.19	122.12
2	O	128	THR	OG1-CB-CG2	6.67	122.65	109.30
2	N	128	THR	OG1-CB-CG2	6.67	122.64	109.30
2	P	290	LEU	O-C-N	6.67	129.19	122.12
2	S	128	THR	OG1-CB-CG2	6.67	122.64	109.30
2	V	290	LEU	O-C-N	6.67	129.19	122.12
2	T	290	LEU	O-C-N	6.67	129.19	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	290	LEU	O-C-N	6.66	129.18	122.12
2	R	290	LEU	O-C-N	6.66	129.17	122.12
2	R	128	THR	OG1-CB-CG2	6.65	122.61	109.30
2	W	290	LEU	O-C-N	6.65	129.17	122.12
2	S	290	LEU	O-C-N	6.64	129.16	122.12
2	N	290	LEU	O-C-N	6.64	129.16	122.12
2	O	290	LEU	O-C-N	6.63	129.15	122.12
2	P	341	TYR	CB-CA-C	6.63	122.12	110.85
2	T	341	TYR	CB-CA-C	6.62	122.11	110.85
2	W	341	TYR	CB-CA-C	6.62	122.10	110.85
2	U	341	TYR	CB-CA-C	6.62	122.10	110.85
2	V	341	TYR	CB-CA-C	6.61	122.09	110.85
2	Q	341	TYR	CB-CA-C	6.61	122.08	110.85
2	X	341	TYR	CB-CA-C	6.61	122.08	110.85
2	M	341	TYR	CB-CA-C	6.60	122.08	110.85
2	U	367	ARG	NE-CZ-NH2	6.60	125.14	119.20
2	N	341	TYR	CB-CA-C	6.60	122.07	110.85
2	Q	367	ARG	NE-CZ-NH2	6.60	125.14	119.20
2	R	367	ARG	NE-CZ-NH2	6.60	125.14	119.20
2	N	367	ARG	NE-CZ-NH2	6.60	125.14	119.20
2	S	341	TYR	CB-CA-C	6.60	122.06	110.85
2	O	341	TYR	CB-CA-C	6.59	122.06	110.85
1	E	64	ASP	N-CA-C	6.59	120.04	110.28
2	T	367	ARG	NE-CZ-NH2	6.59	125.13	119.20
2	O	367	ARG	NE-CZ-NH2	6.59	125.13	119.20
1	G	64	ASP	N-CA-C	6.59	120.03	110.28
1	K	64	ASP	N-CA-C	6.58	120.03	110.28
2	P	140	LYS	CA-C-N	6.58	131.71	120.72
2	P	140	LYS	C-N-CA	6.58	131.71	120.72
2	R	341	TYR	CB-CA-C	6.58	122.04	110.85
2	U	290	LEU	O-C-N	6.58	129.10	122.12
2	X	140	LYS	CA-C-N	6.58	131.70	120.72
2	X	140	LYS	C-N-CA	6.58	131.70	120.72
2	V	367	ARG	NE-CZ-NH2	6.57	125.12	119.20
2	W	367	ARG	NE-CZ-NH2	6.57	125.11	119.20
1	B	64	ASP	N-CA-C	6.57	120.00	110.28
1	D	63	SER	N-CA-C	6.57	118.99	111.11
1	L	64	ASP	N-CA-C	6.57	120.00	110.28
1	A	64	ASP	N-CA-C	6.56	119.99	110.28
2	P	367	ARG	NE-CZ-NH2	6.56	125.11	119.20
2	U	122	LEU	N-CA-CB	-6.56	102.90	111.23
2	X	367	ARG	NE-CZ-NH2	6.56	125.11	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	64	ASP	N-CA-C	6.56	119.99	110.28
2	M	140	LYS	CA-C-N	6.56	131.67	120.72
2	M	140	LYS	C-N-CA	6.56	131.67	120.72
1	B	98	GLN	CG-CD-NE2	6.56	126.23	116.40
1	D	64	ASP	N-CA-C	6.55	119.98	110.28
1	F	64	ASP	N-CA-C	6.55	119.98	110.28
1	H	64	ASP	N-CA-C	6.55	119.98	110.28
2	R	140	LYS	CA-C-N	6.55	131.67	120.72
2	R	140	LYS	C-N-CA	6.55	131.67	120.72
2	W	122	LEU	N-CA-CB	-6.55	102.91	111.23
2	X	204	MET	N-CA-CB	-6.55	100.72	111.66
2	O	140	LYS	CA-C-N	6.55	131.66	120.72
2	O	140	LYS	C-N-CA	6.55	131.66	120.72
2	W	86	GLN	CB-CG-CD	6.55	123.74	112.60
2	U	86	GLN	CB-CG-CD	6.55	123.73	112.60
1	C	64	ASP	N-CA-C	6.55	119.97	110.28
1	H	63	SER	N-CA-C	6.55	118.97	111.11
2	R	122	LEU	N-CA-CB	-6.55	102.92	111.23
1	A	98	GLN	CG-CD-NE2	6.54	126.22	116.40
2	M	204	MET	N-CA-CB	-6.54	100.73	111.66
1	I	64	ASP	N-CA-C	6.54	119.96	110.28
1	I	98	GLN	CG-CD-NE2	6.54	126.22	116.40
2	Q	140	LYS	CA-C-N	6.54	131.65	120.72
2	Q	140	LYS	C-N-CA	6.54	131.65	120.72
2	S	140	LYS	CA-C-N	6.54	131.65	120.72
2	S	140	LYS	C-N-CA	6.54	131.65	120.72
2	V	140	LYS	CA-C-N	6.54	131.65	120.72
2	V	140	LYS	C-N-CA	6.54	131.65	120.72
1	H	98	GLN	CG-CD-NE2	6.54	126.21	116.40
2	P	204	MET	N-CA-CB	-6.54	100.74	111.66
2	T	122	LEU	N-CA-CB	-6.54	102.92	111.23
2	V	122	LEU	N-CA-CB	-6.54	102.93	111.23
2	S	122	LEU	N-CA-CB	-6.54	102.93	111.23
2	W	204	MET	N-CA-CB	-6.54	100.74	111.66
2	M	122	LEU	N-CA-CB	-6.54	102.93	111.23
2	M	367	ARG	NE-CZ-NH2	6.54	125.08	119.20
2	N	122	LEU	N-CA-CB	-6.53	102.94	111.23
2	N	204	MET	N-CA-CB	-6.53	100.75	111.66
2	O	122	LEU	N-CA-CB	-6.53	102.94	111.23
2	Q	122	LEU	N-CA-CB	-6.53	102.94	111.23
2	S	204	MET	N-CA-CB	-6.53	100.75	111.66
1	L	98	GLN	CG-CD-NE2	6.53	126.19	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	140	LYS	CA-C-N	6.53	131.62	120.72
2	N	140	LYS	C-N-CA	6.53	131.62	120.72
2	X	122	LEU	N-CA-CB	-6.53	102.94	111.23
1	F	98	GLN	CG-CD-NE2	6.53	126.19	116.40
2	Q	204	MET	N-CA-CB	-6.53	100.76	111.66
2	V	204	MET	N-CA-CB	-6.53	100.76	111.66
1	G	98	GLN	CG-CD-NE2	6.53	126.19	116.40
2	P	86	GLN	CB-CG-CD	6.53	123.69	112.60
2	U	140	LYS	CA-C-N	6.53	131.62	120.72
2	U	140	LYS	C-N-CA	6.53	131.62	120.72
2	V	86	GLN	CB-CG-CD	6.53	123.69	112.60
2	W	140	LYS	CA-C-N	6.53	131.62	120.72
2	W	140	LYS	C-N-CA	6.53	131.62	120.72
2	M	86	GLN	CB-CG-CD	6.52	123.69	112.60
2	S	367	ARG	NE-CZ-NH2	6.52	125.07	119.20
2	U	204	MET	N-CA-CB	-6.52	100.77	111.66
1	K	63	SER	N-CA-C	6.52	118.94	111.11
2	Q	86	GLN	CB-CG-CD	6.52	123.69	112.60
2	X	86	GLN	CB-CG-CD	6.52	123.69	112.60
2	S	86	GLN	CB-CG-CD	6.52	123.69	112.60
2	P	122	LEU	N-CA-CB	-6.52	102.95	111.23
1	C	98	GLN	CG-CD-NE2	6.52	126.18	116.40
2	T	86	GLN	CB-CG-CD	6.52	123.68	112.60
2	T	140	LYS	CA-C-N	6.52	131.61	120.72
2	T	140	LYS	C-N-CA	6.52	131.61	120.72
2	T	204	MET	N-CA-CB	-6.52	100.78	111.66
1	K	98	GLN	CG-CD-NE2	6.52	126.17	116.40
1	D	98	GLN	CG-CD-NE2	6.51	126.17	116.40
2	N	86	GLN	CB-CG-CD	6.51	123.67	112.60
1	J	63	SER	N-CA-C	6.51	118.92	111.11
2	O	86	GLN	CB-CG-CD	6.51	123.67	112.60
2	U	285	LEU	O-C-N	-6.51	113.93	122.59
2	O	204	MET	N-CA-CB	-6.51	100.79	111.66
2	R	204	MET	N-CA-CB	-6.51	100.79	111.66
1	J	98	GLN	CG-CD-NE2	6.51	126.16	116.40
2	R	86	GLN	CB-CG-CD	6.51	123.66	112.60
1	L	63	SER	N-CA-C	6.50	118.92	111.11
1	C	63	SER	N-CA-C	6.50	118.92	111.11
1	E	98	GLN	CG-CD-NE2	6.50	126.16	116.40
1	G	63	SER	N-CA-C	6.50	118.91	111.11
2	O	285	LEU	O-C-N	-6.50	113.95	122.59
2	P	285	LEU	O-C-N	-6.50	113.94	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	63	SER	N-CA-C	6.49	118.90	111.11
2	X	285	LEU	O-C-N	-6.49	113.95	122.59
1	B	63	SER	N-CA-C	6.49	118.90	111.11
2	V	285	LEU	O-C-N	-6.49	113.96	122.59
1	E	63	SER	N-CA-C	6.49	118.89	111.11
1	A	63	SER	N-CA-C	6.49	118.89	111.11
2	M	285	LEU	O-C-N	-6.48	113.97	122.59
2	Q	253	GLN	CB-CG-CD	-6.48	101.58	112.60
2	T	285	LEU	O-C-N	-6.48	113.97	122.59
2	M	253	GLN	CB-CG-CD	-6.48	101.58	112.60
2	S	285	LEU	O-C-N	-6.48	113.98	122.59
2	T	305	LYS	CA-C-N	6.48	128.86	120.44
2	T	305	LYS	C-N-CA	6.48	128.86	120.44
2	R	27	PHE	CA-C-O	6.48	128.41	120.31
2	N	253	GLN	CB-CG-CD	-6.47	101.59	112.60
2	N	285	LEU	O-C-N	-6.47	113.98	122.59
2	P	186	ALA	CA-C-O	-6.47	113.69	120.55
2	R	285	LEU	O-C-N	-6.47	113.98	122.59
2	U	253	GLN	CB-CG-CD	-6.47	101.60	112.60
1	I	63	SER	N-CA-C	6.47	118.87	111.11
2	W	253	GLN	CB-CG-CD	-6.47	101.60	112.60
2	N	186	ALA	CA-C-O	-6.47	113.69	120.55
2	U	186	ALA	CA-C-O	-6.46	113.70	120.55
2	V	253	GLN	CB-CG-CD	-6.46	101.61	112.60
2	W	285	LEU	O-C-N	-6.46	113.99	122.59
2	O	27	PHE	CA-C-O	6.46	128.38	120.31
2	S	253	GLN	CB-CG-CD	-6.46	101.62	112.60
2	S	301	ALA	CA-C-O	-6.46	113.00	120.49
2	X	253	GLN	CB-CG-CD	-6.46	101.62	112.60
2	O	186	ALA	CA-C-O	-6.46	113.70	120.55
2	O	253	GLN	CB-CG-CD	-6.46	101.62	112.60
2	R	253	GLN	CB-CG-CD	-6.46	101.62	112.60
2	X	27	PHE	CA-C-O	6.46	128.38	120.31
2	Q	186	ALA	CA-C-O	-6.46	113.71	120.55
2	V	186	ALA	CA-C-O	-6.46	113.71	120.55
2	T	253	GLN	CB-CG-CD	-6.45	101.63	112.60
2	T	186	ALA	CA-C-O	-6.45	113.71	120.55
2	P	253	GLN	CB-CG-CD	-6.45	101.64	112.60
2	R	186	ALA	CA-C-O	-6.45	113.71	120.55
2	Q	285	LEU	O-C-N	-6.45	114.02	122.59
2	M	305	LYS	CA-C-N	6.44	128.82	120.44
2	M	305	LYS	C-N-CA	6.44	128.82	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	186	ALA	CA-C-O	-6.44	113.72	120.55
2	N	305	LYS	CA-C-N	6.44	128.82	120.44
2	N	305	LYS	C-N-CA	6.44	128.82	120.44
2	U	27	PHE	CA-C-O	6.44	128.36	120.31
2	U	305	LYS	CA-C-N	6.44	128.82	120.44
2	U	305	LYS	C-N-CA	6.44	128.82	120.44
2	X	301	ALA	CA-C-O	-6.44	113.02	120.49
2	Q	301	ALA	CA-C-O	-6.44	113.02	120.49
2	Q	305	LYS	CA-C-N	6.44	128.81	120.44
2	Q	305	LYS	C-N-CA	6.44	128.81	120.44
2	M	186	ALA	CA-C-O	-6.44	113.73	120.55
2	S	186	ALA	CA-C-O	-6.44	113.73	120.55
2	P	305	LYS	CA-C-N	6.43	128.81	120.44
2	P	305	LYS	C-N-CA	6.43	128.81	120.44
1	C	367	PRO	O-C-N	6.43	131.32	122.64
2	Q	27	PHE	CA-C-O	6.43	128.35	120.31
2	S	27	PHE	CA-C-O	6.43	128.35	120.31
2	T	27	PHE	CA-C-O	6.43	128.35	120.31
2	W	305	LYS	CA-C-N	6.43	128.80	120.44
2	W	305	LYS	C-N-CA	6.43	128.80	120.44
2	O	301	ALA	CA-C-O	-6.42	113.04	120.49
2	V	301	ALA	CA-C-O	-6.42	113.04	120.49
2	V	305	LYS	CA-C-N	6.42	128.79	120.44
2	V	305	LYS	C-N-CA	6.42	128.79	120.44
2	X	186	ALA	CA-C-O	-6.42	113.74	120.55
2	M	27	PHE	CA-C-O	6.42	128.34	120.31
2	O	305	LYS	CA-C-N	6.42	128.79	120.44
2	O	305	LYS	C-N-CA	6.42	128.79	120.44
2	V	27	PHE	CA-C-O	6.42	128.33	120.31
2	P	301	ALA	CA-C-O	-6.42	113.05	120.49
2	R	305	LYS	CA-C-N	6.42	128.78	120.44
2	R	305	LYS	C-N-CA	6.42	128.78	120.44
2	X	305	LYS	CA-C-N	6.41	128.77	120.44
2	X	305	LYS	C-N-CA	6.41	128.77	120.44
2	M	301	ALA	CA-C-O	-6.41	113.06	120.49
2	U	301	ALA	CA-C-O	-6.41	113.06	120.49
2	T	301	ALA	CA-C-O	-6.41	113.06	120.49
2	W	27	PHE	CA-C-O	6.41	128.32	120.31
1	J	367	PRO	O-C-N	6.40	131.28	122.64
2	N	301	ALA	CA-C-O	-6.40	113.07	120.49
2	R	301	ALA	CA-C-O	-6.40	113.07	120.49
2	W	301	ALA	CA-C-O	-6.40	113.07	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	27	PHE	CA-C-O	6.40	128.31	120.31
1	A	367	PRO	O-C-N	6.39	131.27	122.64
2	S	277	LYS	CB-CG-CD	6.39	126.01	111.30
2	U	277	LYS	CB-CG-CD	6.39	126.00	111.30
2	U	33	ILE	CB-CA-C	-6.39	103.23	110.96
2	X	165	GLY	CA-C-O	-6.39	109.46	120.57
1	H	367	PRO	O-C-N	6.38	131.26	122.64
2	M	277	LYS	CB-CG-CD	6.38	125.98	111.30
2	W	33	ILE	CB-CA-C	-6.38	103.24	110.96
2	M	274	GLU	CA-C-O	-6.38	113.66	120.42
2	P	277	LYS	CB-CG-CD	6.38	125.97	111.30
2	S	33	ILE	CB-CA-C	-6.38	103.24	110.96
2	M	165	GLY	CA-C-O	-6.38	109.48	120.57
2	U	165	GLY	CA-C-O	-6.38	109.47	120.57
2	O	33	ILE	CB-CA-C	-6.38	103.25	110.96
2	W	277	LYS	CB-CG-CD	6.38	125.96	111.30
2	V	277	LYS	CB-CG-CD	6.37	125.96	111.30
1	K	367	PRO	O-C-N	6.37	131.24	122.64
2	P	27	PHE	CA-C-O	6.37	128.28	120.31
2	S	305	LYS	CA-C-N	6.37	128.72	120.44
2	S	305	LYS	C-N-CA	6.37	128.72	120.44
2	X	277	LYS	CB-CG-CD	6.37	125.96	111.30
2	N	33	ILE	CB-CA-C	-6.37	103.25	110.96
2	R	165	GLY	CA-C-O	-6.37	109.49	120.57
2	P	165	GLY	CA-C-O	-6.37	109.49	120.57
1	F	367	PRO	O-C-N	6.37	131.24	122.64
2	Q	277	LYS	CB-CG-CD	6.37	125.94	111.30
2	V	33	ILE	CB-CA-C	-6.37	103.26	110.96
1	D	367	PRO	O-C-N	6.37	131.23	122.64
2	T	33	ILE	CB-CA-C	-6.37	103.26	110.96
2	T	277	LYS	CB-CG-CD	6.37	125.94	111.30
1	G	367	PRO	O-C-N	6.36	131.23	122.64
2	N	277	LYS	CB-CG-CD	6.36	125.94	111.30
2	R	277	LYS	CB-CG-CD	6.36	125.94	111.30
2	O	277	LYS	CB-CG-CD	6.36	125.93	111.30
2	S	100	ASN	OD1-CG-ND2	-6.36	116.24	122.60
2	S	165	GLY	CA-C-O	-6.36	109.51	120.57
1	L	367	PRO	O-C-N	6.36	131.22	122.64
2	N	7	LEU	O-C-N	-6.36	115.87	123.31
2	R	33	ILE	CB-CA-C	-6.36	103.27	110.96
2	V	165	GLY	CA-C-O	-6.36	109.51	120.57
2	O	165	GLY	CA-C-O	-6.36	109.51	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	53	THR	CA-CB-OG1	-6.35	100.07	109.60
2	Q	33	ILE	CB-CA-C	-6.35	103.27	110.96
2	T	165	GLY	CA-C-O	-6.35	109.52	120.57
2	X	274	GLU	CA-C-O	-6.35	113.69	120.42
2	M	33	ILE	CB-CA-C	-6.35	103.28	110.96
2	O	7	LEU	O-C-N	-6.35	115.88	123.31
2	W	165	GLY	CA-C-O	-6.35	109.52	120.57
1	I	367	PRO	O-C-N	6.35	131.21	122.64
2	N	165	GLY	CA-C-O	-6.35	109.53	120.57
2	Q	70	TYR	CA-C-N	6.35	128.69	120.44
2	Q	70	TYR	C-N-CA	6.35	128.69	120.44
2	U	53	THR	CA-CB-OG1	-6.35	100.08	109.60
2	P	33	ILE	CB-CA-C	-6.35	103.28	110.96
2	T	53	THR	CA-CB-OG1	-6.34	100.08	109.60
2	X	100	ASN	OD1-CG-ND2	-6.34	116.25	122.60
1	E	367	PRO	O-C-N	6.34	131.20	122.64
2	Q	165	GLY	CA-C-O	-6.34	109.53	120.57
2	X	33	ILE	CB-CA-C	-6.34	103.28	110.96
2	R	70	TYR	CA-C-N	6.34	128.68	120.44
2	R	70	TYR	C-N-CA	6.34	128.68	120.44
2	T	70	TYR	CA-C-N	6.34	128.69	120.44
2	T	70	TYR	C-N-CA	6.34	128.69	120.44
2	U	70	TYR	CA-C-N	6.34	128.69	120.44
2	U	70	TYR	C-N-CA	6.34	128.69	120.44
2	W	70	TYR	CA-C-N	6.34	128.68	120.44
2	W	70	TYR	C-N-CA	6.34	128.68	120.44
2	M	70	TYR	CA-C-N	6.34	128.68	120.44
2	M	70	TYR	C-N-CA	6.34	128.68	120.44
2	T	7	LEU	O-C-N	-6.34	115.89	123.31
2	X	7	LEU	O-C-N	-6.33	115.90	123.31
2	X	53	THR	CA-CB-OG1	-6.33	100.10	109.60
2	Q	274	GLU	CA-C-O	-6.33	113.71	120.42
2	T	100	ASN	OD1-CG-ND2	-6.33	116.27	122.60
2	X	70	TYR	CA-C-N	6.33	128.67	120.44
2	X	70	TYR	C-N-CA	6.33	128.67	120.44
2	M	7	LEU	O-C-N	-6.33	115.91	123.31
2	V	100	ASN	OD1-CG-ND2	-6.33	116.27	122.60
2	W	7	LEU	O-C-N	-6.33	115.91	123.31
2	O	29	LYS	CA-CB-CG	6.33	126.75	114.10
2	V	70	TYR	CA-C-N	6.33	128.66	120.44
2	V	70	TYR	C-N-CA	6.33	128.66	120.44
2	N	274	GLU	CA-C-O	-6.32	113.72	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	7	LEU	O-C-N	-6.32	115.91	123.31
2	W	100	ASN	OD1-CG-ND2	-6.32	116.28	122.60
2	Q	29	LYS	CA-CB-CG	6.32	126.74	114.10
2	N	100	ASN	OD1-CG-ND2	-6.32	116.28	122.60
2	S	274	GLU	CA-C-O	-6.32	113.72	120.42
2	O	53	THR	CA-CB-OG1	-6.32	100.12	109.60
2	P	274	GLU	CA-C-O	-6.32	113.72	120.42
2	V	53	THR	CA-CB-OG1	-6.32	100.12	109.60
2	P	100	ASN	OD1-CG-ND2	-6.32	116.28	122.60
2	Q	111	GLU	O-C-N	-6.32	115.83	123.29
2	T	29	LYS	CA-CB-CG	6.32	126.74	114.10
2	R	29	LYS	CA-CB-CG	6.32	126.73	114.10
2	R	274	GLU	CA-C-O	-6.32	113.73	120.42
2	U	100	ASN	OD1-CG-ND2	-6.32	116.28	122.60
2	V	274	GLU	CA-C-O	-6.32	113.73	120.42
2	W	274	GLU	CA-C-O	-6.32	113.72	120.42
1	B	367	PRO	O-C-N	6.31	131.16	122.64
2	Q	7	LEU	O-C-N	-6.31	115.92	123.31
2	R	100	ASN	OD1-CG-ND2	-6.31	116.29	122.60
2	S	29	LYS	CA-CB-CG	6.31	126.72	114.10
2	S	70	TYR	CA-C-N	6.31	128.65	120.44
2	S	70	TYR	C-N-CA	6.31	128.65	120.44
2	V	29	LYS	CA-CB-CG	6.31	126.73	114.10
2	N	103	LEU	CB-CA-C	6.31	120.15	109.80
2	U	29	LYS	CA-CB-CG	6.31	126.72	114.10
2	W	29	LYS	CA-CB-CG	6.31	126.72	114.10
2	W	53	THR	CA-CB-OG1	-6.31	100.13	109.60
2	X	111	GLU	O-C-N	-6.31	115.84	123.29
2	P	103	LEU	CB-CA-C	6.31	120.15	109.80
2	R	7	LEU	O-C-N	-6.31	115.93	123.31
2	W	103	LEU	CB-CA-C	6.31	120.15	109.80
2	M	111	GLU	O-C-N	-6.31	115.85	123.29
2	N	29	LYS	CA-CB-CG	6.31	126.72	114.10
2	N	53	THR	CA-CB-OG1	-6.31	100.14	109.60
2	O	70	TYR	CA-C-N	6.31	128.64	120.44
2	O	70	TYR	C-N-CA	6.31	128.64	120.44
2	P	29	LYS	CA-CB-CG	6.31	126.71	114.10
2	R	53	THR	CA-CB-OG1	-6.31	100.14	109.60
2	T	274	GLU	CA-C-O	-6.31	113.73	120.42
2	N	70	TYR	CA-C-N	6.30	128.64	120.44
2	N	70	TYR	C-N-CA	6.30	128.64	120.44
2	S	111	GLU	O-C-N	-6.30	115.85	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	103	LEU	CB-CA-C	6.30	120.14	109.80
2	P	70	TYR	CA-C-N	6.30	128.63	120.44
2	P	70	TYR	C-N-CA	6.30	128.63	120.44
2	Q	103	LEU	CB-CA-C	6.30	120.13	109.80
2	U	103	LEU	CB-CA-C	6.30	120.13	109.80
2	M	100	ASN	OD1-CG-ND2	-6.30	116.30	122.60
2	Q	100	ASN	OD1-CG-ND2	-6.30	116.30	122.60
2	T	111	GLU	O-C-N	-6.30	115.86	123.29
2	V	111	GLU	O-C-N	-6.30	115.86	123.29
2	W	111	GLU	O-C-N	-6.30	115.86	123.29
2	S	7	LEU	O-C-N	-6.30	115.94	123.31
2	P	53	THR	CA-CB-OG1	-6.30	100.16	109.60
2	S	103	LEU	CB-CA-C	6.30	120.13	109.80
2	U	7	LEU	O-C-N	-6.30	115.94	123.31
2	V	103	LEU	CB-CA-C	6.30	120.13	109.80
2	X	29	LYS	CA-CB-CG	6.30	126.69	114.10
2	P	7	LEU	O-C-N	-6.29	115.94	123.31
2	U	111	GLU	O-C-N	-6.29	115.86	123.29
2	M	103	LEU	CB-CA-C	6.29	120.12	109.80
2	P	111	GLU	O-C-N	-6.29	115.86	123.29
2	Q	53	THR	CA-CB-OG1	-6.29	100.16	109.60
2	M	29	LYS	CA-CB-CG	6.29	126.68	114.10
2	O	100	ASN	OD1-CG-ND2	-6.29	116.31	122.60
2	N	111	GLU	O-C-N	-6.29	115.87	123.29
2	O	274	GLU	CA-C-O	-6.29	113.76	120.42
2	T	103	LEU	CB-CA-C	6.29	120.11	109.80
2	O	103	LEU	CB-CA-C	6.28	120.10	109.80
2	R	103	LEU	CB-CA-C	6.28	120.11	109.80
2	S	53	THR	CA-CB-OG1	-6.28	100.18	109.60
2	U	274	GLU	CA-C-O	-6.28	113.76	120.42
2	P	320	THR	O-C-N	6.28	128.54	122.07
2	O	111	GLU	O-C-N	-6.28	115.89	123.29
1	F	408	PRO	CA-C-N	-6.27	112.06	122.21
1	F	408	PRO	C-N-CA	-6.27	112.06	122.21
2	M	320	THR	O-C-N	6.27	128.52	122.07
2	W	100	ASN	CB-CG-ND2	6.26	125.79	116.40
1	D	218	GLN	CG-CD-NE2	6.26	125.79	116.40
2	T	38	GLU	CA-C-O	-6.26	114.14	121.46
2	T	320	THR	O-C-N	6.26	128.52	122.07
2	X	333	ILE	CA-C-N	6.26	126.17	119.28
2	X	333	ILE	C-N-CA	6.26	126.17	119.28
2	P	333	ILE	CA-C-N	6.26	126.16	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	333	ILE	C-N-CA	6.26	126.16	119.28
2	S	320	THR	O-C-N	6.26	128.51	122.07
2	N	100	ASN	CB-CG-ND2	6.25	125.78	116.40
2	R	320	THR	O-C-N	6.25	128.51	122.07
2	X	100	ASN	CB-CG-ND2	6.25	125.78	116.40
2	O	333	ILE	CA-C-N	6.25	126.16	119.28
2	O	333	ILE	C-N-CA	6.25	126.16	119.28
1	E	188	ALA	N-CA-C	6.25	120.51	112.26
1	E	218	GLN	CG-CD-NE2	6.25	125.78	116.40
2	R	333	ILE	CA-C-N	6.25	126.16	119.28
2	R	333	ILE	C-N-CA	6.25	126.16	119.28
2	R	111	GLU	O-C-N	-6.25	115.92	123.29
1	I	408	PRO	CA-C-N	-6.24	112.10	122.21
1	I	408	PRO	C-N-CA	-6.24	112.10	122.21
2	S	333	ILE	CA-C-N	6.24	126.15	119.28
2	S	333	ILE	C-N-CA	6.24	126.15	119.28
2	U	100	ASN	CB-CG-ND2	6.24	125.76	116.40
2	V	100	ASN	CB-CG-ND2	6.24	125.76	116.40
2	T	37	VAL	CA-C-O	-6.24	113.79	120.59
1	D	188	ALA	N-CA-C	6.24	120.49	112.26
1	K	408	PRO	CA-C-N	-6.24	112.10	122.21
1	K	408	PRO	C-N-CA	-6.24	112.10	122.21
2	S	100	ASN	CB-CG-ND2	6.24	125.76	116.40
1	H	408	PRO	CA-C-N	-6.24	112.11	122.21
1	H	408	PRO	C-N-CA	-6.24	112.11	122.21
2	M	333	ILE	CA-C-N	6.24	126.14	119.28
2	M	333	ILE	C-N-CA	6.24	126.14	119.28
1	H	218	GLN	CG-CD-NE2	6.24	125.75	116.40
1	J	408	PRO	CA-C-N	-6.24	112.11	122.21
1	J	408	PRO	C-N-CA	-6.24	112.11	122.21
2	T	333	ILE	CA-C-N	6.24	126.14	119.28
2	T	333	ILE	C-N-CA	6.24	126.14	119.28
2	O	100	ASN	CB-CG-ND2	6.23	125.75	116.40
2	V	333	ILE	CA-C-N	6.23	126.14	119.28
2	V	333	ILE	C-N-CA	6.23	126.14	119.28
1	B	218	GLN	CG-CD-NE2	6.23	125.75	116.40
1	G	218	GLN	CG-CD-NE2	6.23	125.75	116.40
2	Q	333	ILE	CA-C-N	6.23	126.13	119.28
2	Q	333	ILE	C-N-CA	6.23	126.13	119.28
2	U	320	THR	O-C-N	6.23	128.49	122.07
2	O	37	VAL	CA-C-O	-6.23	113.80	120.59
2	P	100	ASN	CB-CG-ND2	6.23	125.74	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	100	ASN	CB-CG-ND2	6.23	125.74	116.40
2	Q	273	LYS	N-CA-C	6.23	118.07	111.28
2	Q	320	THR	O-C-N	6.23	128.49	122.07
2	T	100	ASN	CB-CG-ND2	6.23	125.74	116.40
2	V	320	THR	O-C-N	6.23	128.48	122.07
2	M	273	LYS	N-CA-C	6.23	118.07	111.28
2	N	320	THR	O-C-N	6.23	128.48	122.07
2	S	185	ASN	OD1-CG-ND2	-6.23	116.37	122.60
2	U	37	VAL	CA-C-O	-6.23	113.80	120.59
2	U	214	GLU	CA-C-O	-6.23	114.28	120.82
1	L	218	GLN	CG-CD-NE2	6.22	125.74	116.40
2	N	37	VAL	CA-C-O	-6.22	113.81	120.59
1	B	188	ALA	N-CA-C	6.22	120.47	112.26
2	X	273	LYS	N-CA-C	6.22	118.06	111.28
1	L	124	VAL	CB-CA-C	-6.22	101.36	110.81
2	N	193	THR	CA-CB-OG1	-6.22	100.27	109.60
2	W	193	THR	CA-CB-OG1	-6.22	100.27	109.60
2	U	333	ILE	CA-C-N	6.22	126.12	119.28
2	U	333	ILE	C-N-CA	6.22	126.12	119.28
2	X	37	VAL	CA-C-O	-6.22	113.81	120.59
1	L	188	ALA	N-CA-C	6.22	120.47	112.26
2	W	38	GLU	CA-C-O	-6.22	114.19	121.46
1	I	218	GLN	CG-CD-NE2	6.22	125.72	116.40
2	S	37	VAL	CA-C-O	-6.22	113.81	120.59
2	S	38	GLU	CA-C-O	-6.22	114.19	121.46
2	V	37	VAL	CA-C-O	-6.22	113.81	120.59
1	A	408	PRO	CA-C-N	-6.21	112.14	122.21
1	A	408	PRO	C-N-CA	-6.21	112.14	122.21
1	D	124	VAL	CB-CA-C	-6.21	101.36	110.81
1	E	408	PRO	CA-C-N	-6.21	112.14	122.21
1	E	408	PRO	C-N-CA	-6.21	112.14	122.21
2	M	100	ASN	CB-CG-ND2	6.21	125.72	116.40
2	P	273	LYS	N-CA-C	6.21	118.06	111.28
2	R	38	GLU	CA-C-O	-6.21	114.19	121.46
2	W	185	ASN	OD1-CG-ND2	-6.21	116.39	122.60
2	X	185	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	B	408	PRO	CA-C-N	-6.21	112.15	122.21
1	B	408	PRO	C-N-CA	-6.21	112.15	122.21
2	R	100	ASN	CB-CG-ND2	6.21	125.72	116.40
2	S	273	LYS	N-CA-C	6.21	118.05	111.28
2	T	273	LYS	N-CA-C	6.21	118.05	111.28
1	D	408	PRO	CA-C-N	-6.21	112.15	122.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	408	PRO	C-N-CA	-6.21	112.15	122.21
1	F	218	GLN	CG-CD-NE2	6.21	125.71	116.40
2	Q	37	VAL	CA-C-O	-6.21	113.82	120.59
2	Q	38	GLU	CA-C-O	-6.21	114.20	121.46
2	R	273	LYS	N-CA-C	6.21	118.05	111.28
2	T	185	ASN	OD1-CG-ND2	-6.21	116.39	122.60
2	T	214	GLU	CA-C-O	-6.21	114.30	120.82
1	A	218	GLN	CG-CD-NE2	6.21	125.71	116.40
1	C	218	GLN	CG-CD-NE2	6.21	125.71	116.40
1	G	408	PRO	CA-C-N	-6.21	112.15	122.21
1	G	408	PRO	C-N-CA	-6.21	112.15	122.21
2	M	193	THR	CA-CB-OG1	-6.21	100.29	109.60
2	N	214	GLU	CA-C-O	-6.21	114.30	120.82
2	N	273	LYS	N-CA-C	6.21	118.05	111.28
2	O	193	THR	CA-CB-OG1	-6.21	100.29	109.60
2	Q	185	ASN	OD1-CG-ND2	-6.21	116.39	122.60
2	U	193	THR	CA-CB-OG1	-6.21	100.29	109.60
1	J	218	GLN	CG-CD-NE2	6.20	125.70	116.40
2	O	185	ASN	OD1-CG-ND2	-6.20	116.40	122.60
2	P	37	VAL	CA-C-O	-6.20	113.83	120.59
2	P	193	THR	CA-CB-OG1	-6.20	100.30	109.60
2	V	38	GLU	CA-C-O	-6.20	114.20	121.46
2	W	320	THR	O-C-N	6.20	128.46	122.07
1	C	408	PRO	CA-C-N	-6.20	112.16	122.21
1	C	408	PRO	C-N-CA	-6.20	112.16	122.21
2	Q	193	THR	CA-CB-OG1	-6.20	100.30	109.60
2	O	273	LYS	N-CA-C	6.20	118.04	111.28
2	V	273	LYS	N-CA-C	6.20	118.04	111.28
2	X	38	GLU	CA-C-O	-6.20	114.20	121.46
1	J	188	ALA	N-CA-C	6.20	120.44	112.26
1	K	218	GLN	CG-CD-NE2	6.20	125.70	116.40
2	N	38	GLU	CA-C-O	-6.20	114.21	121.46
2	O	3	GLU	CB-CA-C	6.20	122.75	110.42
2	V	193	THR	CA-CB-OG1	-6.20	100.30	109.60
2	X	214	GLU	CA-C-O	-6.20	114.31	120.82
2	X	320	THR	O-C-N	6.20	128.45	122.07
2	W	3	GLU	CB-CA-C	6.20	122.75	110.42
2	W	214	GLU	CA-C-O	-6.20	114.31	120.82
2	S	193	THR	CA-CB-OG1	-6.20	100.31	109.60
2	V	3	GLU	CB-CA-C	6.20	122.75	110.42
2	V	185	ASN	OD1-CG-ND2	-6.20	116.41	122.60
1	G	188	ALA	N-CA-C	6.19	120.44	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	3	GLU	CB-CA-C	6.19	122.74	110.42
2	N	333	ILE	CA-C-N	6.19	126.09	119.28
2	N	333	ILE	C-N-CA	6.19	126.09	119.28
2	U	38	GLU	CA-C-O	-6.19	114.22	121.46
2	U	273	LYS	N-CA-C	6.19	118.03	111.28
1	F	124	VAL	CB-CA-C	-6.19	101.40	110.81
2	P	3	GLU	CB-CA-C	6.19	122.74	110.42
2	Q	341	TYR	CB-CG-CD1	6.19	130.09	120.80
2	S	3	GLU	CB-CA-C	6.19	122.74	110.42
1	I	124	VAL	CB-CA-C	-6.19	101.40	110.81
2	N	3	GLU	CB-CA-C	6.19	122.74	110.42
2	O	320	THR	O-C-N	6.19	128.44	122.07
2	P	341	TYR	CB-CG-CD1	6.19	130.08	120.80
2	Q	3	GLU	CB-CA-C	6.19	122.73	110.42
2	R	3	GLU	CB-CA-C	6.19	122.74	110.42
1	C	124	VAL	CB-CA-C	-6.19	101.41	110.81
1	J	124	VAL	CB-CA-C	-6.19	101.41	110.81
1	K	124	VAL	CB-CA-C	-6.19	101.41	110.81
2	W	333	ILE	CA-C-N	6.19	126.09	119.28
2	W	333	ILE	C-N-CA	6.19	126.09	119.28
2	O	38	GLU	CA-C-O	-6.19	114.22	121.46
2	R	37	VAL	CA-C-O	-6.19	113.85	120.59
2	R	214	GLU	CA-C-O	-6.19	114.33	120.82
2	U	41	ASP	CA-C-O	-6.19	114.82	121.56
1	C	188	ALA	N-CA-C	6.18	120.42	112.26
1	G	124	VAL	CB-CA-C	-6.18	101.41	110.81
1	H	124	VAL	CB-CA-C	-6.18	101.41	110.81
2	S	341	TYR	CB-CG-CD1	6.18	130.08	120.80
2	W	37	VAL	CA-C-O	-6.18	113.85	120.59
1	B	124	VAL	CB-CA-C	-6.18	101.41	110.81
2	M	37	VAL	CA-C-O	-6.18	113.85	120.59
2	T	3	GLU	CB-CA-C	6.18	122.72	110.42
2	W	41	ASP	CA-C-O	-6.18	114.82	121.56
2	O	214	GLU	CA-C-O	-6.18	114.33	120.82
2	P	38	GLU	CA-C-O	-6.18	114.23	121.46
2	V	214	GLU	CA-C-O	-6.18	114.33	120.82
1	L	408	PRO	CA-C-N	-6.18	112.20	122.21
1	L	408	PRO	C-N-CA	-6.18	112.20	122.21
2	R	193	THR	CA-CB-OG1	-6.18	100.33	109.60
2	U	3	GLU	CB-CA-C	6.18	122.72	110.42
2	W	341	TYR	CB-CG-CD1	6.18	130.07	120.80
2	X	193	THR	CA-CB-OG1	-6.18	100.33	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	214	GLU	CA-C-O	-6.18	114.33	120.82
2	T	341	TYR	CB-CG-CD1	6.18	130.07	120.80
2	X	41	ASP	CA-C-O	-6.18	114.83	121.56
2	M	38	GLU	CA-C-O	-6.18	114.23	121.46
2	O	341	TYR	CB-CG-CD1	6.18	130.06	120.80
2	T	193	THR	CA-CB-OG1	-6.18	100.33	109.60
1	A	124	VAL	CB-CA-C	-6.17	101.42	110.81
2	N	341	TYR	CB-CG-CD1	6.17	130.06	120.80
2	W	273	LYS	N-CA-C	6.17	118.01	111.28
2	X	3	GLU	CB-CA-C	6.17	122.71	110.42
2	S	21	ALA	CA-C-O	-6.17	114.01	120.55
1	K	188	ALA	N-CA-C	6.17	120.41	112.26
2	M	214	GLU	CA-C-O	-6.17	114.34	120.82
2	R	185	ASN	OD1-CG-ND2	-6.17	116.43	122.60
2	V	341	TYR	CB-CG-CD1	6.17	130.06	120.80
2	N	41	ASP	CA-C-O	-6.17	114.83	121.56
1	A	188	ALA	N-CA-C	6.17	120.40	112.26
1	E	124	VAL	CB-CA-C	-6.17	101.43	110.81
2	P	185	ASN	OD1-CG-ND2	-6.17	116.43	122.60
2	R	10	TRP	CB-CG-CD2	-6.17	118.17	126.80
2	M	185	ASN	OD1-CG-ND2	-6.16	116.44	122.60
2	M	341	TYR	CB-CG-CD1	6.16	130.05	120.80
2	P	88	LYS	CG-CD-CE	6.16	125.48	111.30
2	P	41	ASP	CA-C-O	-6.16	114.84	121.56
2	N	21	ALA	CA-C-O	-6.16	114.02	120.55
2	R	21	ALA	CA-C-O	-6.16	114.02	120.55
2	R	88	LYS	CG-CD-CE	6.16	125.47	111.30
2	S	41	ASP	CA-C-O	-6.16	114.84	121.56
2	S	88	LYS	CG-CD-CE	6.16	125.47	111.30
2	U	341	TYR	CB-CG-CD1	6.16	130.04	120.80
2	U	354	ARG	CA-CB-CG	6.16	126.42	114.10
1	H	188	ALA	N-CA-C	6.16	120.39	112.26
2	W	10	TRP	CB-CG-CD2	-6.16	118.18	126.80
2	N	88	LYS	CG-CD-CE	6.16	125.46	111.30
2	M	10	TRP	CB-CG-CD2	-6.16	118.18	126.80
2	N	185	ASN	OD1-CG-ND2	-6.16	116.44	122.60
2	R	341	TYR	CB-CG-CD1	6.16	130.03	120.80
2	U	185	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	F	188	ALA	N-CA-C	6.15	120.38	112.26
1	I	188	ALA	N-CA-C	6.15	120.38	112.26
2	O	88	LYS	CG-CD-CE	6.15	125.45	111.30
2	S	214	GLU	CA-C-O	-6.15	114.36	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	10	TRP	CB-CG-CD2	-6.15	118.19	126.80
2	U	10	TRP	CB-CG-CD2	-6.15	118.19	126.80
2	O	10	TRP	CB-CG-CD2	-6.15	118.19	126.80
2	W	88	LYS	CG-CD-CE	6.15	125.44	111.30
2	Q	214	GLU	CA-C-O	-6.15	114.37	120.82
2	V	88	LYS	CG-CD-CE	6.15	125.44	111.30
2	X	341	TYR	CB-CG-CD1	6.15	130.02	120.80
2	M	21	ALA	CA-C-O	-6.14	114.04	120.55
2	O	41	ASP	CA-C-O	-6.14	114.86	121.56
2	P	21	ALA	CA-C-O	-6.14	114.04	120.55
2	S	354	ARG	CA-CB-CG	6.14	126.39	114.10
2	T	21	ALA	CA-C-O	-6.14	114.04	120.55
2	U	88	LYS	CG-CD-CE	6.14	125.43	111.30
2	V	10	TRP	CB-CG-CD2	-6.14	118.20	126.80
2	M	88	LYS	CG-CD-CE	6.14	125.43	111.30
2	T	88	LYS	CG-CD-CE	6.14	125.43	111.30
2	V	21	ALA	CA-C-O	-6.14	114.04	120.55
2	W	21	ALA	CA-C-O	-6.14	114.04	120.55
2	Q	41	ASP	CA-C-O	-6.14	114.87	121.56
2	P	10	TRP	CB-CG-CD2	-6.14	118.20	126.80
2	Q	88	LYS	CG-CD-CE	6.14	125.42	111.30
2	T	41	ASP	CA-C-O	-6.14	114.87	121.56
2	U	21	ALA	CA-C-O	-6.14	114.04	120.55
2	P	354	ARG	CA-CB-CG	6.14	126.38	114.10
2	V	41	ASP	CA-C-O	-6.14	114.87	121.56
2	S	10	TRP	CB-CG-CD2	-6.14	118.21	126.80
2	X	88	LYS	CG-CD-CE	6.14	125.41	111.30
2	T	200	LYS	CB-CA-C	-6.13	100.56	110.74
2	M	354	ARG	CA-CB-CG	6.13	126.36	114.10
2	N	10	TRP	CB-CG-CD2	-6.13	118.22	126.80
2	Q	10	TRP	CB-CG-CD2	-6.13	118.22	126.80
2	V	354	ARG	CA-CB-CG	6.13	126.36	114.10
2	X	10	TRP	CB-CG-CD2	-6.13	118.22	126.80
2	W	200	LYS	CB-CA-C	-6.13	100.57	110.74
2	X	200	LYS	CB-CA-C	-6.12	100.57	110.74
2	Q	21	ALA	CA-C-O	-6.12	114.06	120.55
2	R	18	ASN	N-CA-C	-6.12	104.16	111.69
2	W	354	ARG	CA-CB-CG	6.12	126.34	114.10
2	X	21	ALA	CA-C-O	-6.12	114.06	120.55
2	X	354	ARG	CA-CB-CG	6.12	126.34	114.10
2	M	18	ASN	N-CA-C	-6.12	104.16	111.69
2	O	204	MET	CA-C-O	-6.12	114.72	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	354	ARG	CA-CB-CG	6.12	126.34	114.10
2	P	200	LYS	CB-CA-C	-6.12	100.58	110.74
2	Q	200	LYS	CB-CA-C	-6.12	100.58	110.74
2	U	18	ASN	N-CA-C	-6.12	104.16	111.69
2	R	200	LYS	CB-CA-C	-6.12	100.58	110.74
2	R	354	ARG	CA-CB-CG	6.12	126.33	114.10
2	N	354	ARG	CA-CB-CG	6.11	126.33	114.10
2	T	354	ARG	CA-CB-CG	6.11	126.33	114.10
2	O	21	ALA	CA-C-O	-6.11	114.07	120.55
2	V	200	LYS	CB-CA-C	-6.11	100.59	110.74
2	N	18	ASN	N-CA-C	-6.11	104.17	111.69
2	Q	204	MET	CA-C-O	-6.11	114.73	121.33
2	M	41	ASP	CA-C-O	-6.11	114.90	121.56
2	M	200	LYS	CB-CA-C	-6.11	100.60	110.74
2	N	200	LYS	CB-CA-C	-6.11	100.60	110.74
2	P	18	ASN	N-CA-C	-6.11	104.18	111.69
2	T	18	ASN	N-CA-C	-6.11	104.18	111.69
2	Q	354	ARG	CA-CB-CG	6.11	126.31	114.10
2	R	13	GLY	O-C-N	6.11	129.26	122.54
2	S	18	ASN	N-CA-C	-6.11	104.18	111.69
2	S	200	LYS	CB-CA-C	-6.10	100.61	110.74
2	S	204	MET	CA-C-O	-6.10	114.74	121.33
2	N	204	MET	CA-C-O	-6.10	114.74	121.33
2	S	13	GLY	O-C-N	6.10	129.25	122.54
2	U	200	LYS	CB-CA-C	-6.10	100.61	110.74
2	W	13	GLY	O-C-N	6.10	129.25	122.54
2	V	18	ASN	N-CA-C	-6.10	104.19	111.69
2	O	200	LYS	CB-CA-C	-6.10	100.62	110.74
2	P	13	GLY	O-C-N	6.09	129.24	122.54
2	W	18	ASN	N-CA-C	-6.09	104.20	111.69
2	O	13	GLY	O-C-N	6.09	129.24	122.54
2	T	204	MET	CA-C-O	-6.09	114.76	121.33
2	V	204	MET	CA-C-O	-6.08	114.76	121.33
2	W	204	MET	CA-C-O	-6.08	114.76	121.33
2	Q	18	ASN	N-CA-C	-6.08	104.21	111.69
2	T	13	GLY	O-C-N	6.08	129.23	122.54
2	X	18	ASN	N-CA-C	-6.08	104.21	111.69
2	N	13	GLY	O-C-N	6.08	129.23	122.54
2	X	13	GLY	O-C-N	6.08	129.23	122.54
2	R	41	ASP	CA-C-O	-6.08	114.94	121.56
2	O	18	ASN	N-CA-C	-6.08	104.22	111.69
2	M	175	LYS	CA-C-O	6.07	127.95	121.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	13	GLY	O-C-N	6.07	129.22	122.54
2	P	204	MET	CA-C-O	-6.07	114.78	121.33
2	R	204	MET	CA-C-O	-6.07	114.78	121.33
2	V	13	GLY	O-C-N	6.07	129.22	122.54
2	N	282	ASN	CB-CG-ND2	-6.07	107.30	116.40
2	U	13	GLY	O-C-N	6.07	129.22	122.54
2	Q	13	GLY	O-C-N	6.07	129.21	122.54
2	M	308	GLU	CA-C-O	6.06	126.95	120.10
2	U	204	MET	CA-C-O	-6.06	114.79	121.33
2	O	323	ASN	O-C-N	6.06	129.05	122.15
2	M	204	MET	CA-C-O	-6.05	114.79	121.33
2	P	175	LYS	CA-C-O	6.05	127.93	121.45
2	T	282	ASN	CB-CG-ND2	-6.05	107.32	116.40
2	R	282	ASN	CB-CG-ND2	-6.05	107.32	116.40
2	S	282	ASN	CB-CG-ND2	-6.05	107.32	116.40
2	N	175	LYS	CA-C-O	6.05	127.92	121.45
2	X	204	MET	CA-C-O	-6.05	114.79	121.33
2	T	11	ILE	CA-C-N	6.05	129.88	120.75
2	T	11	ILE	C-N-CA	6.05	129.88	120.75
2	W	282	ASN	CB-CG-ND2	-6.05	107.33	116.40
2	O	229	PRO	CA-C-N	6.05	128.99	120.28
2	O	229	PRO	C-N-CA	6.05	128.99	120.28
2	O	282	ASN	CB-CG-ND2	-6.05	107.33	116.40
2	Q	308	GLU	CA-C-O	6.05	126.93	120.10
2	T	175	LYS	CA-C-O	6.05	127.92	121.45
2	T	229	PRO	CA-C-N	6.05	128.99	120.28
2	T	229	PRO	C-N-CA	6.05	128.99	120.28
2	O	175	LYS	CA-C-O	6.04	127.92	121.45
2	Q	282	ASN	CB-CG-ND2	-6.04	107.33	116.40
2	W	323	ASN	O-C-N	6.04	129.04	122.15
2	S	229	PRO	CA-C-N	6.04	128.98	120.28
2	S	229	PRO	C-N-CA	6.04	128.98	120.28
2	U	323	ASN	O-C-N	6.04	129.04	122.15
2	V	282	ASN	CB-CG-ND2	-6.04	107.34	116.40
2	W	175	LYS	CA-C-O	6.04	127.91	121.45
2	P	308	GLU	CA-C-O	6.04	126.92	120.10
2	W	229	PRO	CA-C-N	6.04	128.98	120.28
2	W	229	PRO	C-N-CA	6.04	128.98	120.28
2	P	282	ASN	CB-CG-ND2	-6.04	107.34	116.40
2	Q	271	PRO	CA-C-O	6.04	126.89	118.86
2	M	11	ILE	CA-C-N	6.04	129.87	120.75
2	M	11	ILE	C-N-CA	6.04	129.87	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	175	LYS	CA-C-O	6.04	127.91	121.45
2	W	291	GLU	CA-C-N	6.04	128.37	120.28
2	W	291	GLU	C-N-CA	6.04	128.37	120.28
2	X	282	ASN	CB-CG-ND2	-6.04	107.35	116.40
2	N	11	ILE	CA-C-N	6.03	129.86	120.75
2	N	11	ILE	C-N-CA	6.03	129.86	120.75
2	U	229	PRO	CA-C-N	6.03	128.97	120.28
2	U	229	PRO	C-N-CA	6.03	128.97	120.28
2	V	175	LYS	CA-C-O	6.03	127.91	121.45
2	V	229	PRO	CA-C-N	6.03	128.97	120.28
2	V	229	PRO	C-N-CA	6.03	128.97	120.28
2	W	308	GLU	CA-C-O	6.03	126.92	120.10
2	X	114	SER	CA-C-O	-6.03	114.38	121.44
2	R	64	HIS	ND1-CE1-NE2	-6.03	102.37	108.40
2	U	308	GLU	CA-C-O	6.03	126.92	120.10
2	N	229	PRO	CA-C-N	6.03	128.96	120.28
2	N	229	PRO	C-N-CA	6.03	128.96	120.28
2	R	229	PRO	CA-C-N	6.03	128.96	120.28
2	R	229	PRO	C-N-CA	6.03	128.96	120.28
2	S	175	LYS	CA-C-O	6.03	127.90	121.45
2	M	114	SER	CA-C-O	-6.03	114.39	121.44
2	M	282	ASN	CB-CG-ND2	-6.03	107.36	116.40
2	S	308	GLU	CA-C-O	6.03	126.91	120.10
2	U	11	ILE	CA-C-N	6.03	129.85	120.75
2	U	11	ILE	C-N-CA	6.03	129.85	120.75
2	M	229	PRO	CA-C-N	6.02	128.95	120.28
2	M	229	PRO	C-N-CA	6.02	128.95	120.28
2	V	308	GLU	CA-C-O	6.02	126.91	120.10
2	P	11	ILE	CA-C-N	6.02	129.84	120.75
2	P	11	ILE	C-N-CA	6.02	129.84	120.75
2	S	323	ASN	O-C-N	6.02	129.01	122.15
2	V	11	ILE	CA-C-N	6.02	129.84	120.75
2	V	11	ILE	C-N-CA	6.02	129.84	120.75
2	V	323	ASN	O-C-N	6.02	129.01	122.15
2	X	175	LYS	CA-C-O	6.02	127.89	121.45
2	X	229	PRO	CA-C-N	6.02	128.95	120.28
2	X	229	PRO	C-N-CA	6.02	128.95	120.28
2	N	323	ASN	O-C-N	6.02	129.01	122.15
2	O	308	GLU	CA-C-O	6.02	126.90	120.10
2	P	229	PRO	CA-C-N	6.02	128.94	120.28
2	P	229	PRO	C-N-CA	6.02	128.94	120.28
2	U	282	ASN	CB-CG-ND2	-6.02	107.38	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	64	HIS	ND1-CE1-NE2	-6.01	102.39	108.40
2	Q	11	ILE	CA-C-N	6.01	129.83	120.75
2	Q	11	ILE	C-N-CA	6.01	129.83	120.75
2	R	11	ILE	CA-C-N	6.01	129.83	120.75
2	R	11	ILE	C-N-CA	6.01	129.83	120.75
2	S	11	ILE	CA-C-N	6.01	129.83	120.75
2	S	11	ILE	C-N-CA	6.01	129.83	120.75
2	T	308	GLU	CA-C-O	6.01	126.90	120.10
2	X	323	ASN	O-C-N	6.01	129.01	122.15
2	R	323	ASN	O-C-N	6.01	129.00	122.15
2	T	323	ASN	O-C-N	6.01	129.00	122.15
2	X	11	ILE	CA-C-N	6.01	129.83	120.75
2	X	11	ILE	C-N-CA	6.01	129.83	120.75
2	N	114	SER	CA-C-O	-6.01	114.41	121.44
2	Q	323	ASN	O-C-N	6.01	129.00	122.15
2	T	64	HIS	ND1-CE1-NE2	-6.01	102.39	108.40
2	N	308	GLU	CA-C-O	6.01	126.89	120.10
2	P	64	HIS	ND1-CE1-NE2	-6.01	102.39	108.40
2	P	323	ASN	O-C-N	6.01	129.00	122.15
2	U	64	HIS	ND1-CE1-NE2	-6.01	102.39	108.40
2	P	291	GLU	CA-C-N	6.00	128.32	120.28
2	P	291	GLU	C-N-CA	6.00	128.32	120.28
2	Q	229	PRO	CA-C-N	6.00	128.93	120.28
2	Q	229	PRO	C-N-CA	6.00	128.93	120.28
2	N	291	GLU	CA-C-N	6.00	128.32	120.28
2	N	291	GLU	C-N-CA	6.00	128.32	120.28
2	R	175	LYS	CA-C-O	6.00	127.87	121.45
2	V	64	HIS	ND1-CE1-NE2	-6.00	102.40	108.40
2	O	11	ILE	CA-C-N	6.00	129.80	120.75
2	O	11	ILE	C-N-CA	6.00	129.80	120.75
2	R	308	GLU	CA-C-O	5.99	126.87	120.10
2	R	271	PRO	CA-C-O	5.99	126.83	118.86
2	P	285	LEU	CA-C-O	5.99	129.08	120.51
2	U	114	SER	CA-C-O	-5.99	114.43	121.44
2	R	61	PHE	O-C-N	5.99	130.36	123.29
2	V	114	SER	CA-C-O	-5.99	114.43	121.44
2	X	131	GLU	CG-CD-OE1	5.99	132.18	118.40
2	X	285	LEU	CA-C-O	5.99	129.07	120.51
2	M	271	PRO	CA-C-O	5.99	126.82	118.86
2	Q	175	LYS	CA-C-O	5.99	127.86	121.45
2	S	291	GLU	CA-C-N	5.99	128.30	120.28
2	S	291	GLU	C-N-CA	5.99	128.30	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	271	PRO	CA-C-O	5.99	126.82	118.86
2	O	131	GLU	CG-CD-OE1	5.99	132.17	118.40
2	U	131	GLU	CG-CD-OE1	5.99	132.17	118.40
2	U	341	TYR	CB-CG-CD2	-5.99	111.82	120.80
2	W	64	HIS	ND1-CE1-NE2	-5.99	102.41	108.40
2	W	131	GLU	CG-CD-OE1	5.99	132.16	118.40
2	W	341	TYR	CB-CG-CD2	-5.99	111.82	120.80
2	X	308	GLU	CA-C-O	5.99	126.86	120.10
2	V	291	GLU	CA-C-N	5.98	128.30	120.28
2	V	291	GLU	C-N-CA	5.98	128.30	120.28
2	M	323	ASN	O-C-N	5.98	128.97	122.15
2	M	341	TYR	CB-CG-CD2	-5.98	111.83	120.80
2	N	285	LEU	CA-C-O	5.98	129.07	120.51
2	O	64	HIS	ND1-CE1-NE2	-5.98	102.42	108.40
2	Q	114	SER	CA-C-O	-5.98	114.44	121.44
2	Q	131	GLU	CG-CD-OE1	5.98	132.16	118.40
2	R	285	LEU	CA-C-O	5.98	129.06	120.51
2	U	360	ALA	O-C-N	5.98	128.46	122.12
2	X	64	HIS	ND1-CE1-NE2	-5.98	102.42	108.40
2	M	131	GLU	CG-CD-OE1	5.98	132.16	118.40
2	T	131	GLU	CG-CD-OE1	5.98	132.15	118.40
2	M	64	HIS	ND1-CE1-NE2	-5.98	102.42	108.40
2	O	291	GLU	CA-C-N	5.98	128.29	120.28
2	O	291	GLU	C-N-CA	5.98	128.29	120.28
2	T	271	PRO	CA-C-O	5.98	126.81	118.86
2	M	13	GLY	CA-C-O	-5.98	112.60	119.65
2	M	291	GLU	CA-C-N	5.98	128.29	120.28
2	M	291	GLU	C-N-CA	5.98	128.29	120.28
2	P	131	GLU	CG-CD-OE1	5.98	132.15	118.40
2	Q	64	HIS	ND1-CE1-NE2	-5.98	102.42	108.40
2	S	285	LEU	CA-C-O	5.98	129.06	120.51
2	T	291	GLU	CA-C-N	5.98	128.29	120.28
2	T	291	GLU	C-N-CA	5.98	128.29	120.28
2	V	285	LEU	CA-C-O	5.98	129.06	120.51
2	R	114	SER	CA-C-O	-5.98	114.45	121.44
2	S	64	HIS	ND1-CE1-NE2	-5.98	102.42	108.40
2	W	271	PRO	CA-C-O	5.98	126.81	118.86
2	U	61	PHE	O-C-N	5.97	130.34	123.29
2	V	131	GLU	CG-CD-OE1	5.97	132.14	118.40
2	W	11	ILE	CA-C-N	5.97	129.77	120.75
2	W	11	ILE	C-N-CA	5.97	129.77	120.75
2	X	271	PRO	CA-C-O	5.97	126.81	118.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	271	PRO	CA-C-O	5.97	126.80	118.86
2	O	285	LEU	CA-C-O	5.97	129.05	120.51
2	P	114	SER	CA-C-O	-5.97	114.45	121.44
2	P	271	PRO	CA-C-O	5.97	126.80	118.86
2	Q	341	TYR	CB-CG-CD2	-5.97	111.84	120.80
2	R	291	GLU	CA-C-N	5.97	128.28	120.28
2	R	291	GLU	C-N-CA	5.97	128.28	120.28
2	T	110	VAL	O-C-N	5.97	130.70	122.88
2	P	341	TYR	CB-CG-CD2	-5.97	111.85	120.80
2	R	131	GLU	CG-CD-OE1	5.97	132.13	118.40
2	R	341	TYR	CB-CG-CD2	-5.97	111.84	120.80
2	S	110	VAL	O-C-N	5.97	130.70	122.88
2	S	114	SER	CA-C-O	-5.97	114.46	121.44
2	V	341	TYR	CB-CG-CD2	-5.97	111.84	120.80
2	N	131	GLU	CG-CD-OE1	5.97	132.13	118.40
2	Q	291	GLU	CA-C-N	5.97	128.28	120.28
2	Q	291	GLU	C-N-CA	5.97	128.28	120.28
2	T	114	SER	CA-C-O	-5.97	114.46	121.44
2	T	341	TYR	CB-CG-CD2	-5.97	111.85	120.80
2	U	285	LEU	CA-C-O	5.97	129.04	120.51
2	X	291	GLU	CA-C-N	5.97	128.28	120.28
2	X	291	GLU	C-N-CA	5.97	128.28	120.28
2	O	341	TYR	CB-CG-CD2	-5.97	111.85	120.80
2	W	285	LEU	CA-C-O	5.97	129.04	120.51
2	N	61	PHE	O-C-N	5.96	130.33	123.29
2	N	271	PRO	CA-C-O	5.96	126.79	118.86
2	P	110	VAL	O-C-N	5.96	130.69	122.88
2	T	285	LEU	CA-C-O	5.96	129.04	120.51
2	U	291	GLU	CA-C-N	5.96	128.27	120.28
2	U	291	GLU	C-N-CA	5.96	128.27	120.28
2	N	341	TYR	CB-CG-CD2	-5.96	111.86	120.80
2	Q	285	LEU	CA-C-O	5.96	129.04	120.51
2	T	61	PHE	O-C-N	5.96	130.33	123.29
2	M	285	LEU	CA-C-O	5.96	129.03	120.51
2	S	271	PRO	CA-C-O	5.96	126.79	118.86
2	V	61	PHE	O-C-N	5.96	130.32	123.29
2	N	291	GLU	CG-CD-OE2	-5.96	104.69	118.40
2	R	168	ALA	CA-C-N	5.96	131.39	122.99
2	R	168	ALA	C-N-CA	5.96	131.39	122.99
2	S	291	GLU	CG-CD-OE2	-5.96	104.69	118.40
2	U	110	VAL	O-C-N	5.96	130.69	122.88
2	O	114	SER	CA-C-O	-5.96	114.47	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	110	VAL	O-C-N	5.96	130.68	122.88
2	R	291	GLU	CG-CD-OE2	-5.96	104.70	118.40
2	S	341	TYR	CB-CG-CD2	-5.96	111.87	120.80
2	T	291	GLU	CG-CD-OE2	-5.96	104.70	118.40
2	W	114	SER	CA-C-O	-5.96	114.47	121.44
2	M	110	VAL	O-C-N	5.95	130.68	122.88
2	S	131	GLU	CG-CD-OE1	5.95	132.09	118.40
2	X	291	GLU	CG-CD-OE2	-5.95	104.71	118.40
2	W	50	VAL	O-C-N	5.95	128.53	121.80
2	M	61	PHE	O-C-N	5.95	130.31	123.29
2	O	61	PHE	O-C-N	5.95	130.31	123.29
2	P	13	GLY	CA-C-O	-5.95	112.63	119.65
2	X	341	TYR	CB-CG-CD2	-5.95	111.87	120.80
2	P	291	GLU	CG-CD-OE2	-5.95	104.72	118.40
2	V	291	GLU	CG-CD-OE2	-5.95	104.72	118.40
2	X	13	GLY	CA-C-O	-5.95	112.63	119.65
2	U	271	PRO	CA-C-O	5.95	126.77	118.86
2	U	291	GLU	CG-CD-OE2	-5.95	104.72	118.40
2	W	291	GLU	CG-CD-OE2	-5.95	104.72	118.40
2	X	35	VAL	CA-C-N	5.95	131.38	123.05
2	X	35	VAL	C-N-CA	5.95	131.38	123.05
2	X	61	PHE	O-C-N	5.95	130.31	123.29
2	N	13	GLY	CA-C-O	-5.95	112.64	119.65
2	O	360	ALA	O-C-N	5.95	128.42	122.12
2	V	110	VAL	O-C-N	5.95	130.67	122.88
2	M	168	ALA	CA-C-N	5.94	131.37	122.99
2	M	168	ALA	C-N-CA	5.94	131.37	122.99
2	O	110	VAL	O-C-N	5.94	130.66	122.88
2	S	61	PHE	O-C-N	5.94	130.30	123.29
2	T	13	GLY	CA-C-O	-5.94	112.64	119.65
2	U	13	GLY	CA-C-O	-5.94	112.64	119.65
2	W	168	ALA	CA-C-N	5.94	131.37	122.99
2	W	168	ALA	C-N-CA	5.94	131.37	122.99
2	W	61	PHE	O-C-N	5.94	130.30	123.29
2	M	360	ALA	O-C-N	5.94	128.41	122.12
2	O	291	GLU	CG-CD-OE2	-5.94	104.75	118.40
2	Q	35	VAL	CA-C-N	5.94	131.36	123.05
2	Q	35	VAL	C-N-CA	5.94	131.36	123.05
2	R	315	PRO	CA-C-N	5.94	128.16	120.44
2	R	315	PRO	C-N-CA	5.94	128.16	120.44
2	X	168	ALA	CA-C-N	5.94	131.36	122.99
2	X	168	ALA	C-N-CA	5.94	131.36	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	110	VAL	O-C-N	5.93	130.66	122.88
2	O	50	VAL	O-C-N	5.93	128.50	121.80
2	Q	13	GLY	CA-C-O	-5.93	112.65	119.65
2	V	360	ALA	O-C-N	5.93	128.41	122.12
2	X	360	ALA	O-C-N	5.93	128.41	122.12
2	M	291	GLU	CG-CD-OE2	-5.93	104.75	118.40
2	W	315	PRO	CA-C-N	5.93	128.15	120.44
2	W	315	PRO	C-N-CA	5.93	128.15	120.44
2	N	315	PRO	CA-C-N	5.93	128.15	120.44
2	N	315	PRO	C-N-CA	5.93	128.15	120.44
2	Q	50	VAL	O-C-N	5.93	128.50	121.80
2	S	13	GLY	CA-C-O	-5.93	112.65	119.65
2	T	90	TYR	CA-C-O	5.93	125.32	119.75
2	V	13	GLY	CA-C-O	-5.93	112.65	119.65
2	V	168	ALA	CA-C-N	5.93	131.35	122.99
2	V	168	ALA	C-N-CA	5.93	131.35	122.99
2	O	13	GLY	CA-C-O	-5.93	112.66	119.65
2	Q	110	VAL	O-C-N	5.93	130.64	122.88
2	Q	291	GLU	CG-CD-OE2	-5.93	104.77	118.40
2	Q	360	ALA	O-C-N	5.93	128.40	122.12
2	W	13	GLY	CA-C-O	-5.93	112.66	119.65
2	M	35	VAL	CA-C-N	5.92	131.34	123.05
2	M	35	VAL	C-N-CA	5.92	131.34	123.05
2	U	35	VAL	CA-C-N	5.92	131.34	123.05
2	U	35	VAL	C-N-CA	5.92	131.34	123.05
2	U	168	ALA	CA-C-N	5.92	131.34	122.99
2	U	168	ALA	C-N-CA	5.92	131.34	122.99
2	W	35	VAL	CA-C-N	5.92	131.34	123.05
2	W	35	VAL	C-N-CA	5.92	131.34	123.05
2	Q	61	PHE	O-C-N	5.92	130.28	123.29
2	R	35	VAL	CA-C-N	5.92	131.34	123.05
2	R	35	VAL	C-N-CA	5.92	131.34	123.05
2	S	315	PRO	CA-C-N	5.92	128.14	120.44
2	S	315	PRO	C-N-CA	5.92	128.14	120.44
2	P	168	ALA	CA-C-N	5.92	131.34	122.99
2	P	168	ALA	C-N-CA	5.92	131.34	122.99
2	P	315	PRO	CA-C-N	5.92	128.13	120.44
2	P	315	PRO	C-N-CA	5.92	128.13	120.44
2	T	50	VAL	O-C-N	5.92	128.49	121.80
2	X	174	GLY	CA-C-N	-5.92	112.17	121.87
2	X	174	GLY	C-N-CA	-5.92	112.17	121.87
2	X	315	PRO	CA-C-N	5.92	128.13	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	315	PRO	C-N-CA	5.92	128.13	120.44
2	N	168	ALA	CA-C-N	5.92	131.33	122.99
2	N	168	ALA	C-N-CA	5.92	131.33	122.99
2	O	168	ALA	CA-C-N	5.92	131.33	122.99
2	O	168	ALA	C-N-CA	5.92	131.33	122.99
2	Q	117	TYR	O-C-N	5.92	130.84	123.15
2	T	168	ALA	CA-C-N	5.92	131.33	122.99
2	T	168	ALA	C-N-CA	5.92	131.33	122.99
2	W	174	GLY	CA-C-N	-5.92	112.17	121.87
2	W	174	GLY	C-N-CA	-5.92	112.17	121.87
2	M	117	TYR	O-C-N	5.91	130.84	123.15
2	P	117	TYR	O-C-N	5.91	130.84	123.15
2	R	13	GLY	CA-C-O	-5.91	112.67	119.65
2	R	50	VAL	O-C-N	5.91	128.48	121.80
2	T	315	PRO	CA-C-N	5.91	128.13	120.44
2	T	315	PRO	C-N-CA	5.91	128.13	120.44
2	U	50	VAL	O-C-N	5.91	128.48	121.80
2	M	174	GLY	CA-C-N	-5.91	112.17	121.87
2	M	174	GLY	C-N-CA	-5.91	112.17	121.87
2	M	315	PRO	CA-C-N	5.91	128.12	120.44
2	M	315	PRO	C-N-CA	5.91	128.12	120.44
2	P	360	ALA	O-C-N	5.91	128.39	122.12
2	R	110	VAL	O-C-N	5.91	130.62	122.88
2	T	117	TYR	O-C-N	5.91	130.83	123.15
2	P	61	PHE	O-C-N	5.91	130.26	123.29
2	S	50	VAL	O-C-N	5.91	128.48	121.80
2	U	117	TYR	O-C-N	5.91	130.83	123.15
2	V	315	PRO	CA-C-N	5.91	128.12	120.44
2	V	315	PRO	C-N-CA	5.91	128.12	120.44
2	T	174	GLY	CA-C-N	-5.91	112.18	121.87
2	T	174	GLY	C-N-CA	-5.91	112.18	121.87
2	O	90	TYR	CA-C-O	5.91	125.30	119.75
2	V	174	GLY	CA-C-N	-5.91	112.19	121.87
2	V	174	GLY	C-N-CA	-5.91	112.19	121.87
2	X	110	VAL	O-C-N	5.91	130.62	122.88
2	O	117	TYR	O-C-N	5.90	130.82	123.15
2	W	360	ALA	O-C-N	5.90	128.38	122.12
2	X	256	LYS	CA-CB-CG	5.90	125.91	114.10
2	R	256	LYS	CA-CB-CG	5.90	125.91	114.10
2	T	35	VAL	CA-C-N	5.90	131.31	123.05
2	T	35	VAL	C-N-CA	5.90	131.31	123.05
2	N	174	GLY	CA-C-N	-5.90	112.19	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	174	GLY	C-N-CA	-5.90	112.19	121.87
2	O	315	PRO	CA-C-N	5.90	128.11	120.44
2	O	315	PRO	C-N-CA	5.90	128.11	120.44
2	P	50	VAL	O-C-N	5.90	128.47	121.80
2	S	174	GLY	CA-C-N	-5.90	112.20	121.87
2	S	174	GLY	C-N-CA	-5.90	112.20	121.87
2	Q	315	PRO	CA-C-N	5.90	128.11	120.44
2	Q	315	PRO	C-N-CA	5.90	128.11	120.44
2	R	360	ALA	O-C-N	5.90	128.37	122.12
2	V	117	TYR	O-C-N	5.90	130.82	123.15
2	P	90	TYR	CA-C-O	5.90	125.29	119.75
2	P	174	GLY	CA-C-N	-5.90	112.20	121.87
2	P	174	GLY	C-N-CA	-5.90	112.20	121.87
2	V	35	VAL	CA-C-N	5.90	131.30	123.05
2	V	35	VAL	C-N-CA	5.90	131.30	123.05
2	V	50	VAL	O-C-N	5.90	128.46	121.80
2	M	90	TYR	CA-C-O	5.89	125.29	119.75
2	O	174	GLY	CA-C-N	-5.89	112.20	121.87
2	O	174	GLY	C-N-CA	-5.89	112.20	121.87
2	Q	174	GLY	CA-C-N	-5.89	112.20	121.87
2	Q	174	GLY	C-N-CA	-5.89	112.20	121.87
2	R	90	TYR	CA-C-O	5.89	125.29	119.75
2	S	360	ALA	O-C-N	5.89	128.37	122.12
2	N	50	VAL	O-C-N	5.89	128.46	121.80
2	Q	168	ALA	CA-C-N	5.89	131.30	122.99
2	Q	168	ALA	C-N-CA	5.89	131.30	122.99
2	O	256	LYS	CA-CB-CG	5.89	125.88	114.10
2	S	256	LYS	CA-CB-CG	5.89	125.88	114.10
2	V	90	TYR	CA-C-O	5.89	125.29	119.75
2	X	117	TYR	O-C-N	5.89	130.81	123.15
2	T	360	ALA	O-C-N	5.89	128.36	122.12
2	U	174	GLY	CA-C-N	-5.89	112.21	121.87
2	U	174	GLY	C-N-CA	-5.89	112.21	121.87
2	U	256	LYS	CA-CB-CG	5.89	125.88	114.10
2	O	35	VAL	CA-C-N	5.89	131.29	123.05
2	O	35	VAL	C-N-CA	5.89	131.29	123.05
2	Q	90	TYR	CA-C-O	5.89	125.28	119.75
2	S	90	TYR	CA-C-O	5.89	125.28	119.75
2	M	50	VAL	O-C-N	5.88	128.45	121.80
2	P	256	LYS	CA-CB-CG	5.88	125.87	114.10
2	S	168	ALA	CA-C-N	5.88	131.29	122.99
2	S	168	ALA	C-N-CA	5.88	131.29	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	256	LYS	CA-CB-CG	5.88	125.87	114.10
2	N	117	TYR	O-C-N	5.88	130.79	123.15
2	Q	94	TRP	O-C-N	-5.88	115.04	122.27
2	R	117	TYR	O-C-N	5.88	130.80	123.15
2	S	35	VAL	CA-C-N	5.88	131.28	123.05
2	S	35	VAL	C-N-CA	5.88	131.28	123.05
2	S	117	TYR	O-C-N	5.88	130.80	123.15
2	T	256	LYS	CA-CB-CG	5.88	125.86	114.10
2	U	315	PRO	CA-C-N	5.88	128.09	120.44
2	U	315	PRO	C-N-CA	5.88	128.09	120.44
2	N	314	ASP	CA-C-O	-5.88	113.67	119.49
2	T	314	ASP	CA-C-O	-5.88	113.67	119.49
2	M	256	LYS	CA-CB-CG	5.88	125.86	114.10
2	W	256	LYS	CA-CB-CG	5.88	125.85	114.10
2	N	360	ALA	O-C-N	5.88	128.35	122.12
2	Q	256	LYS	CA-CB-CG	5.88	125.85	114.10
2	R	174	GLY	CA-C-N	-5.87	112.24	121.87
2	R	174	GLY	C-N-CA	-5.87	112.24	121.87
2	M	314	ASP	CA-C-O	-5.87	113.68	119.49
2	N	35	VAL	CA-C-N	5.87	131.27	123.05
2	N	35	VAL	C-N-CA	5.87	131.27	123.05
2	P	118	ASN	CA-C-O	-5.87	114.30	120.58
2	S	43	LEU	O-C-N	5.87	129.49	122.27
2	W	117	TYR	O-C-N	5.87	130.78	123.15
2	X	50	VAL	O-C-N	5.87	128.43	121.80
2	N	256	LYS	CA-CB-CG	5.87	125.83	114.10
2	N	90	TYR	CA-C-O	5.87	125.26	119.75
2	O	314	ASP	CA-C-O	-5.87	113.68	119.49
2	M	118	ASN	CA-C-O	-5.86	114.31	120.58
2	O	94	TRP	O-C-N	-5.86	115.06	122.27
2	P	314	ASP	CA-C-O	-5.86	113.68	119.49
2	W	43	LEU	O-C-N	5.86	129.48	122.27
2	Q	43	LEU	O-C-N	5.86	129.48	122.27
2	X	90	TYR	CA-C-O	5.86	125.26	119.75
2	P	43	LEU	O-C-N	5.86	129.47	122.27
2	U	94	TRP	O-C-N	-5.86	115.07	122.27
2	M	94	TRP	O-C-N	-5.85	115.07	122.27
2	R	94	TRP	O-C-N	-5.85	115.07	122.27
2	T	94	TRP	O-C-N	-5.85	115.07	122.27
1	G	265	GLY	N-CA-C	-5.85	103.33	112.58
2	U	314	ASP	CA-C-O	-5.85	113.70	119.49
1	J	408	PRO	N-CA-C	5.85	120.79	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	90	TYR	CA-C-O	5.85	125.25	119.75
2	V	314	ASP	CA-C-O	-5.85	113.70	119.49
2	X	314	ASP	CA-C-O	-5.85	113.70	119.49
2	P	35	VAL	CA-C-N	5.85	131.24	123.05
2	P	35	VAL	C-N-CA	5.85	131.24	123.05
1	B	361	PRO	CB-CA-C	5.84	118.87	111.39
2	Q	314	ASP	CA-C-O	-5.84	113.70	119.49
2	V	43	LEU	O-C-N	5.84	129.46	122.27
2	V	94	TRP	O-C-N	-5.84	115.08	122.27
1	C	265	GLY	N-CA-C	-5.84	103.35	112.58
1	H	408	PRO	N-CA-C	5.84	120.78	111.26
2	W	118	ASN	CA-C-O	-5.84	114.33	120.58
2	R	43	LEU	O-C-N	5.84	129.45	122.27
2	W	90	TYR	CA-C-O	5.84	125.24	119.75
2	X	43	LEU	O-C-N	5.84	129.45	122.27
2	M	43	LEU	O-C-N	5.84	129.45	122.27
2	N	43	LEU	O-C-N	5.84	129.45	122.27
2	U	43	LEU	O-C-N	5.83	129.44	122.27
1	J	361	PRO	CB-CA-C	5.83	118.85	111.39
2	N	94	TRP	O-C-N	-5.83	115.10	122.27
2	W	94	TRP	O-C-N	-5.83	115.10	122.27
2	O	86	GLN	CG-CD-NE2	-5.83	107.66	116.40
2	P	94	TRP	O-C-N	-5.83	115.10	122.27
2	T	43	LEU	O-C-N	5.83	129.44	122.27
1	A	265	GLY	N-CA-C	-5.82	103.38	112.58
1	F	361	PRO	CB-CA-C	5.82	118.84	111.39
1	F	408	PRO	N-CA-C	5.82	120.75	111.26
2	V	118	ASN	CA-C-O	-5.82	114.35	120.58
1	G	361	PRO	CB-CA-C	5.82	118.84	111.39
2	O	243	GLY	N-CA-C	-5.82	101.44	111.57
2	S	314	ASP	CA-C-O	-5.82	113.73	119.49
1	E	361	PRO	CB-CA-C	5.82	118.84	111.39
2	N	118	ASN	CA-C-O	-5.82	114.36	120.58
2	O	43	LEU	O-C-N	5.82	129.43	122.27
2	T	243	GLY	N-CA-C	-5.82	101.45	111.57
1	L	265	GLY	N-CA-C	-5.82	103.39	112.58
2	P	86	GLN	CG-CD-NE2	-5.82	107.68	116.40
2	U	118	ASN	CA-C-O	-5.82	114.36	120.58
1	D	408	PRO	N-CA-C	5.81	120.74	111.26
1	L	408	PRO	N-CA-C	5.81	120.74	111.26
1	G	408	PRO	N-CA-C	5.81	120.73	111.26
2	W	86	GLN	CG-CD-NE2	-5.81	107.68	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	361	PRO	CB-CA-C	5.81	118.83	111.39
1	L	361	PRO	CB-CA-C	5.81	118.83	111.39
2	N	67	PHE	CA-C-N	5.81	126.43	119.98
2	N	67	PHE	C-N-CA	5.81	126.43	119.98
2	U	243	GLY	N-CA-C	-5.81	101.46	111.57
2	X	94	TRP	O-C-N	-5.81	115.12	122.27
1	K	408	PRO	N-CA-C	5.81	120.73	111.26
2	O	118	ASN	CA-C-O	-5.81	114.36	120.58
1	I	265	GLY	N-CA-C	-5.81	103.41	112.58
1	K	361	PRO	CB-CA-C	5.81	118.82	111.39
2	Q	118	ASN	CA-C-O	-5.81	114.37	120.58
2	S	67	PHE	CA-C-N	5.81	126.42	119.98
2	S	67	PHE	C-N-CA	5.81	126.42	119.98
2	S	94	TRP	O-C-N	-5.81	115.13	122.27
2	T	118	ASN	CA-C-O	-5.81	114.37	120.58
2	T	312	ALA	CA-C-O	-5.81	114.23	120.09
1	A	361	PRO	CB-CA-C	5.80	118.82	111.39
2	R	314	ASP	CA-C-O	-5.80	113.74	119.49
2	W	314	ASP	CA-C-O	-5.80	113.74	119.49
1	F	265	GLY	N-CA-C	-5.80	103.41	112.58
2	S	118	ASN	CA-C-O	-5.80	114.37	120.58
2	T	86	GLN	CG-CD-NE2	-5.80	107.70	116.40
1	K	265	GLY	N-CA-C	-5.80	103.41	112.58
2	Q	243	GLY	N-CA-C	-5.80	101.48	111.57
1	E	265	GLY	N-CA-C	-5.80	103.42	112.58
2	O	67	PHE	CA-C-N	5.80	126.42	119.98
2	O	67	PHE	C-N-CA	5.80	126.42	119.98
2	R	243	GLY	N-CA-C	-5.80	101.48	111.57
2	S	243	GLY	N-CA-C	-5.80	101.48	111.57
2	V	86	GLN	CG-CD-NE2	-5.80	107.70	116.40
2	M	86	GLN	CG-CD-NE2	-5.80	107.70	116.40
2	R	86	GLN	CG-CD-NE2	-5.80	107.70	116.40
2	V	243	GLY	N-CA-C	-5.80	101.48	111.57
1	C	408	PRO	N-CA-C	5.80	120.71	111.26
2	M	243	GLY	N-CA-C	-5.80	101.48	111.57
2	P	82	ASP	O-C-N	5.80	129.43	122.94
2	S	86	GLN	CG-CD-NE2	-5.80	107.70	116.40
1	B	408	PRO	N-CA-C	5.79	120.70	111.26
2	U	86	GLN	CG-CD-NE2	-5.79	107.71	116.40
2	W	243	GLY	N-CA-C	-5.79	101.49	111.57
2	P	243	GLY	N-CA-C	-5.79	101.49	111.57
2	Q	325	GLN	O-C-N	-5.79	115.44	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	86	GLN	CG-CD-NE2	-5.79	107.71	116.40
2	X	118	ASN	CA-C-O	-5.79	114.38	120.58
2	N	243	GLY	N-CA-C	-5.79	101.50	111.57
2	O	312	ALA	CA-C-O	-5.79	114.24	120.09
2	Q	135	LEU	CA-C-N	5.79	128.04	120.28
2	Q	135	LEU	C-N-CA	5.79	128.04	120.28
2	S	316	ARG	NE-CZ-NH1	5.79	127.29	121.50
2	X	135	LEU	CB-CA-C	5.79	120.40	110.79
2	T	67	PHE	CA-C-N	5.79	126.40	119.98
2	T	67	PHE	C-N-CA	5.79	126.40	119.98
1	H	265	GLY	N-CA-C	-5.79	103.44	112.58
2	U	135	LEU	CA-C-N	5.79	128.03	120.28
2	U	135	LEU	C-N-CA	5.79	128.03	120.28
1	D	265	GLY	N-CA-C	-5.78	103.44	112.58
2	Q	86	GLN	CG-CD-NE2	-5.78	107.72	116.40
1	B	265	GLY	N-CA-C	-5.78	103.44	112.58
2	O	135	LEU	CA-C-N	5.78	128.03	120.28
2	O	135	LEU	C-N-CA	5.78	128.03	120.28
2	Q	312	ALA	CA-C-O	-5.78	114.25	120.09
2	X	243	GLY	N-CA-C	-5.78	101.51	111.57
2	R	118	ASN	CA-C-O	-5.78	114.39	120.58
2	T	44	GLU	CA-C-O	5.78	126.49	119.38
2	V	312	ALA	CA-C-O	-5.78	114.25	120.09
2	N	86	GLN	CG-CD-NE2	-5.78	107.73	116.40
2	O	325	GLN	O-C-N	-5.78	115.46	122.22
1	I	361	PRO	CB-CA-C	5.78	118.78	111.39
1	I	408	PRO	N-CA-C	5.78	120.67	111.26
2	M	44	GLU	CA-C-O	5.78	126.48	119.38
2	O	44	GLU	CA-C-O	5.78	126.48	119.38
2	R	44	GLU	CA-C-O	5.78	126.48	119.38
2	T	135	LEU	CA-C-N	5.78	128.02	120.28
2	T	135	LEU	C-N-CA	5.78	128.02	120.28
2	R	275	LEU	CA-C-O	5.77	126.88	120.82
2	U	312	ALA	CA-C-O	-5.77	114.26	120.09
2	X	262	LEU	N-CA-CB	5.77	118.52	109.69
1	H	361	PRO	CB-CA-C	5.77	118.78	111.39
2	S	312	ALA	CA-C-O	-5.77	114.26	120.09
2	U	44	GLU	CA-C-O	5.77	126.48	119.38
2	W	53	THR	CA-CB-CG2	5.77	120.31	110.50
2	P	316	ARG	NE-CZ-NH1	5.77	127.27	121.50
2	X	53	THR	CA-CB-CG2	5.77	120.31	110.50
1	A	408	PRO	N-CA-C	5.77	120.67	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	361	PRO	CB-CA-C	5.77	118.78	111.39
1	J	265	GLY	N-CA-C	-5.77	103.46	112.58
2	N	366	THR	OG1-CB-CG2	5.77	120.84	109.30
2	M	22	GLU	CB-CG-CD	5.77	122.40	112.60
2	M	67	PHE	CA-C-N	5.77	126.38	119.98
2	M	67	PHE	C-N-CA	5.77	126.38	119.98
2	Q	316	ARG	NE-CZ-NH1	5.77	127.27	121.50
1	E	408	PRO	N-CA-C	5.77	120.66	111.26
2	N	262	LEU	N-CA-CB	5.77	118.51	109.69
2	N	44	GLU	CA-C-O	5.76	126.47	119.38
2	P	135	LEU	CA-C-N	5.76	128.00	120.28
2	P	135	LEU	C-N-CA	5.76	128.00	120.28
2	Q	22	GLU	CB-CG-CD	5.76	122.40	112.60
2	Q	135	LEU	CB-CA-C	5.76	120.36	110.79
2	R	312	ALA	CA-C-O	-5.76	114.27	120.09
2	V	135	LEU	CA-C-N	5.76	128.00	120.28
2	V	135	LEU	C-N-CA	5.76	128.00	120.28
2	N	325	GLN	O-C-N	-5.76	115.48	122.22
2	X	312	ALA	CA-C-O	-5.76	114.27	120.09
2	M	53	THR	CA-CB-CG2	5.76	120.30	110.50
2	Q	262	LEU	N-CA-CB	5.76	118.50	109.69
2	R	135	LEU	CA-C-N	5.76	128.00	120.28
2	R	135	LEU	C-N-CA	5.76	128.00	120.28
2	T	316	ARG	NE-CZ-NH1	5.76	127.26	121.50
1	H	359	ARG	N-CA-C	5.76	120.31	113.28
2	N	53	THR	CA-CB-CG2	5.76	120.29	110.50
2	N	324	ALA	CA-C-O	5.76	126.66	120.55
2	O	22	GLU	CB-CG-CD	5.76	122.39	112.60
2	O	82	ASP	O-C-N	5.76	129.39	122.94
2	P	325	GLN	O-C-N	-5.76	115.48	122.22
2	R	22	GLU	CB-CG-CD	5.76	122.39	112.60
2	S	22	GLU	CB-CG-CD	5.76	122.39	112.60
2	U	324	ALA	CA-C-O	5.76	126.66	120.55
2	X	82	ASP	O-C-N	5.76	129.39	122.94
2	O	262	LEU	N-CA-CB	5.76	118.50	109.69
2	P	312	ALA	CA-C-O	-5.76	114.28	120.09
2	R	135	LEU	CB-CA-C	5.76	120.35	110.79
2	S	135	LEU	CA-C-N	5.76	128.00	120.28
2	S	135	LEU	C-N-CA	5.76	128.00	120.28
2	O	366	THR	OG1-CB-CG2	5.76	120.81	109.30
2	P	53	THR	CA-CB-CG2	5.76	120.28	110.50
2	Q	44	GLU	CA-C-O	5.76	126.46	119.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	369	THR	CA-C-O	-5.75	112.47	119.43
2	U	135	LEU	CB-CA-C	5.75	120.34	110.79
2	W	44	GLU	CA-C-O	5.75	126.46	119.38
2	P	22	GLU	CB-CG-CD	5.75	122.38	112.60
2	R	53	THR	CA-CB-CG2	5.75	120.28	110.50
2	T	53	THR	CA-CB-CG2	5.75	120.28	110.50
2	V	44	GLU	CA-C-O	5.75	126.46	119.38
2	W	316	ARG	NE-CZ-NH1	5.75	127.25	121.50
2	W	325	GLN	O-C-N	-5.75	115.49	122.22
2	X	44	GLU	CA-C-O	5.75	126.46	119.38
2	M	135	LEU	CA-C-N	5.75	127.99	120.28
2	M	135	LEU	C-N-CA	5.75	127.99	120.28
2	V	53	THR	CA-CB-CG2	5.75	120.28	110.50
2	X	67	PHE	CA-C-N	5.75	126.36	119.98
2	X	67	PHE	C-N-CA	5.75	126.36	119.98
2	Q	53	THR	CA-CB-CG2	5.75	120.28	110.50
2	W	22	GLU	CB-CG-CD	5.75	122.38	112.60
2	M	135	LEU	CB-CA-C	5.75	120.33	110.79
2	M	325	GLN	O-C-N	-5.75	115.50	122.22
2	O	135	LEU	CB-CA-C	5.75	120.33	110.79
2	T	262	LEU	N-CA-CB	5.75	118.49	109.69
2	U	22	GLU	CB-CG-CD	5.75	122.37	112.60
2	U	82	ASP	O-C-N	5.75	129.38	122.94
2	V	22	GLU	CB-CG-CD	5.75	122.37	112.60
2	W	369	THR	CA-C-O	-5.75	112.47	119.43
2	M	366	THR	OG1-CB-CG2	5.75	120.79	109.30
2	S	44	GLU	CA-C-O	5.75	126.45	119.38
2	T	82	ASP	O-C-N	5.75	129.38	122.94
2	V	135	LEU	CB-CA-C	5.75	120.33	110.79
2	P	324	ALA	CA-C-O	5.75	126.64	120.55
2	W	135	LEU	CB-CA-C	5.75	120.33	110.79
2	W	312	ALA	CA-C-O	-5.75	114.29	120.09
1	C	359	ARG	N-CA-C	5.74	120.35	113.23
2	P	366	THR	OG1-CB-CG2	5.74	120.79	109.30
2	S	53	THR	CA-CB-CG2	5.74	120.26	110.50
2	T	135	LEU	CB-CA-C	5.74	120.33	110.79
2	U	53	THR	CA-CB-CG2	5.74	120.26	110.50
2	V	82	ASP	O-C-N	5.74	129.37	122.94
2	V	275	LEU	CA-C-O	5.74	126.85	120.82
2	V	366	THR	OG1-CB-CG2	5.74	120.79	109.30
2	N	22	GLU	CB-CG-CD	5.74	122.36	112.60
2	N	312	ALA	CA-C-O	-5.74	114.29	120.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	366	THR	OG1-CB-CG2	5.74	120.78	109.30
2	V	262	LEU	N-CA-CB	5.74	118.47	109.69
2	S	275	LEU	CA-C-O	5.74	126.85	120.82
2	T	22	GLU	CB-CG-CD	5.74	122.36	112.60
2	T	366	THR	OG1-CB-CG2	5.74	120.78	109.30
2	V	316	ARG	NE-CZ-NH1	5.74	127.24	121.50
2	X	135	LEU	CA-C-N	5.74	127.97	120.28
2	X	135	LEU	C-N-CA	5.74	127.97	120.28
2	X	369	THR	CA-C-O	-5.74	112.48	119.43
2	M	262	LEU	N-CA-CB	5.74	118.47	109.69
2	N	135	LEU	CA-C-N	5.74	127.97	120.28
2	N	135	LEU	C-N-CA	5.74	127.97	120.28
2	N	369	THR	CA-C-O	-5.74	112.49	119.43
2	O	275	LEU	CA-C-O	5.74	126.84	120.82
2	T	275	LEU	CA-C-O	5.74	126.84	120.82
2	U	366	THR	OG1-CB-CG2	5.74	120.78	109.30
2	V	325	GLN	O-C-N	-5.74	115.51	122.22
2	X	22	GLU	CB-CG-CD	5.74	122.36	112.60
2	O	53	THR	CA-CB-CG2	5.74	120.25	110.50
2	U	262	LEU	N-CA-CB	5.74	118.47	109.69
2	X	325	GLN	O-C-N	-5.74	115.51	122.22
2	N	275	LEU	CA-C-O	5.74	126.84	120.82
2	P	44	GLU	CA-C-O	5.74	126.43	119.38
2	R	82	ASP	O-C-N	5.74	129.36	122.94
2	S	135	LEU	CB-CA-C	5.74	120.31	110.79
2	N	316	ARG	NE-CZ-NH1	5.73	127.23	121.50
2	W	275	LEU	CA-C-O	5.73	126.84	120.82
2	X	366	THR	OG1-CB-CG2	5.73	120.77	109.30
2	P	135	LEU	CB-CA-C	5.73	120.31	110.79
2	P	275	LEU	CA-C-O	5.73	126.84	120.82
2	R	369	THR	CA-C-O	-5.73	112.49	119.43
2	S	262	LEU	N-CA-CB	5.73	118.46	109.69
2	W	324	ALA	CA-C-O	5.73	126.63	120.55
2	W	366	THR	OG1-CB-CG2	5.73	120.77	109.30
2	M	312	ALA	CA-C-O	-5.73	114.30	120.09
2	Q	324	ALA	CA-C-O	5.73	126.62	120.55
2	V	324	ALA	CA-C-O	5.73	126.62	120.55
2	Q	82	ASP	O-C-N	5.73	129.36	122.94
2	Q	366	THR	OG1-CB-CG2	5.73	120.76	109.30
2	X	275	LEU	CA-C-O	5.73	126.83	120.82
2	W	82	ASP	O-C-N	5.73	129.35	122.94
2	W	262	LEU	N-CA-CB	5.73	118.45	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	359	ARG	N-CA-C	5.72	120.33	113.23
2	S	82	ASP	O-C-N	5.72	129.35	122.94
2	W	135	LEU	CA-C-N	5.72	127.95	120.28
2	W	135	LEU	C-N-CA	5.72	127.95	120.28
2	R	262	LEU	N-CA-CB	5.72	118.44	109.69
2	R	316	ARG	NE-CZ-NH1	5.72	127.22	121.50
2	S	1	LYS	CA-C-N	5.72	132.27	121.97
2	S	1	LYS	C-N-CA	5.72	132.27	121.97
2	S	324	ALA	CA-C-O	5.72	126.62	120.55
2	U	316	ARG	NE-CZ-NH1	5.72	127.22	121.50
2	U	325	GLN	O-C-N	-5.72	115.53	122.22
2	N	82	ASP	O-C-N	5.72	129.35	122.94
2	P	262	LEU	N-CA-CB	5.72	118.44	109.69
2	S	366	THR	OG1-CB-CG2	5.72	120.73	109.30
2	U	1	LYS	CA-C-N	5.72	132.26	121.97
2	U	1	LYS	C-N-CA	5.72	132.26	121.97
2	N	135	LEU	CB-CA-C	5.71	120.28	110.79
2	S	325	GLN	O-C-N	-5.71	115.53	122.22
1	K	359	ARG	N-CA-C	5.71	120.31	113.23
2	M	275	LEU	CA-C-O	5.71	126.82	120.82
2	O	324	ALA	CA-C-O	5.71	126.60	120.55
2	Q	1	LYS	CA-C-N	5.71	132.25	121.97
2	Q	1	LYS	C-N-CA	5.71	132.25	121.97
2	Q	275	LEU	CA-C-O	5.71	126.82	120.82
2	R	325	GLN	O-C-N	-5.71	115.54	122.22
2	X	316	ARG	NE-CZ-NH1	5.71	127.21	121.50
2	N	129	TRP	CE2-CD2-CE3	5.71	124.51	118.80
1	E	359	ARG	N-CA-C	5.71	120.31	113.23
1	L	359	ARG	N-CA-C	5.71	120.31	113.23
2	V	369	THR	CA-C-O	-5.71	112.53	119.43
2	M	82	ASP	O-C-N	5.71	129.33	122.94
2	Q	67	PHE	CA-C-N	5.71	126.42	120.03
2	Q	67	PHE	C-N-CA	5.71	126.42	120.03
2	T	46	LYS	CA-C-O	-5.71	114.37	120.42
2	T	324	ALA	CA-C-O	5.71	126.60	120.55
2	M	97	VAL	CA-C-O	-5.70	113.65	120.78
2	P	144	LYS	CB-CG-CD	5.70	124.42	111.30
2	Q	46	LYS	CA-C-O	-5.70	114.38	120.42
2	T	129	TRP	CE2-CD2-CE3	5.70	124.50	118.80
1	J	359	ARG	N-CA-C	5.70	120.30	113.23
2	M	324	ALA	CA-C-O	5.70	126.59	120.55
2	N	144	LYS	CB-CG-CD	5.70	124.42	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	359	ARG	N-CA-C	5.70	120.30	113.23
2	T	97	VAL	CA-C-O	-5.70	113.65	120.78
2	U	275	LEU	CA-C-O	5.70	126.81	120.82
2	X	1	LYS	CA-C-N	5.70	132.23	121.97
2	X	1	LYS	C-N-CA	5.70	132.23	121.97
2	M	316	ARG	NE-CZ-NH1	5.70	127.20	121.50
2	R	1	LYS	CA-C-N	5.70	132.23	121.97
2	R	1	LYS	C-N-CA	5.70	132.23	121.97
2	T	325	GLN	O-C-N	-5.70	115.55	122.22
2	T	369	THR	CA-C-O	-5.70	112.54	119.43
1	G	359	ARG	N-CA-C	5.70	120.29	113.23
2	N	46	LYS	CA-C-O	-5.70	114.38	120.42
2	R	324	ALA	CA-C-O	5.70	126.59	120.55
2	V	1	LYS	CA-C-N	5.70	132.22	121.97
2	V	1	LYS	C-N-CA	5.70	132.22	121.97
2	S	367	ARG	CD-NE-CZ	-5.69	116.43	124.40
2	P	46	LYS	CA-C-O	-5.69	114.39	120.42
2	P	129	TRP	CE2-CD2-CE3	5.69	124.49	118.80
2	R	129	TRP	CE2-CD2-CE3	5.69	124.49	118.80
2	N	1	LYS	CA-C-N	5.69	132.21	121.97
2	N	1	LYS	C-N-CA	5.69	132.21	121.97
2	O	369	THR	CA-C-O	-5.69	112.55	119.43
2	P	367	ARG	CD-NE-CZ	-5.69	116.43	124.40
2	U	369	THR	CA-C-O	-5.69	112.55	119.43
2	M	369	THR	CA-C-O	-5.69	112.55	119.43
2	O	1	LYS	CA-C-N	5.69	132.21	121.97
2	O	1	LYS	C-N-CA	5.69	132.21	121.97
2	O	144	LYS	CB-CG-CD	5.69	124.38	111.30
2	P	1	LYS	CA-C-N	5.69	132.21	121.97
2	P	1	LYS	C-N-CA	5.69	132.21	121.97
2	Q	369	THR	CA-C-O	-5.69	112.55	119.43
2	R	144	LYS	CB-CG-CD	5.69	124.38	111.30
2	U	46	LYS	CA-C-O	-5.69	114.39	120.42
2	W	46	LYS	CA-C-O	-5.69	114.39	120.42
2	X	129	TRP	CE2-CD2-CE3	5.69	124.49	118.80
2	X	324	ALA	CA-C-O	5.69	126.58	120.55
2	R	67	PHE	CA-C-N	5.69	126.40	120.03
2	R	67	PHE	C-N-CA	5.69	126.40	120.03
2	M	1	LYS	CA-C-N	5.68	132.20	121.97
2	M	1	LYS	C-N-CA	5.68	132.20	121.97
2	M	46	LYS	CA-C-O	-5.68	114.40	120.42
2	S	46	LYS	CA-C-O	-5.68	114.40	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	1	LYS	CA-C-N	5.68	132.20	121.97
2	T	1	LYS	C-N-CA	5.68	132.20	121.97
2	V	46	LYS	CA-C-O	-5.68	114.40	120.42
2	W	97	VAL	CA-C-O	-5.68	113.68	120.78
2	Q	129	TRP	CE2-CD2-CE3	5.68	124.48	118.80
2	W	129	TRP	CE2-CD2-CE3	5.68	124.48	118.80
2	O	316	ARG	NE-CZ-NH1	5.68	127.18	121.50
1	D	359	ARG	N-CA-C	5.68	120.27	113.23
2	O	129	TRP	CE2-CD2-CE3	5.68	124.48	118.80
2	P	369	THR	CA-C-O	-5.68	112.56	119.43
2	S	144	LYS	CB-CG-CD	5.68	124.36	111.30
2	U	97	VAL	CA-C-O	-5.68	113.69	120.78
2	V	97	VAL	CA-C-O	-5.68	113.68	120.78
2	V	144	LYS	CB-CG-CD	5.68	124.36	111.30
2	M	144	LYS	CB-CG-CD	5.67	124.35	111.30
2	M	367	ARG	CD-NE-CZ	-5.67	116.45	124.40
2	W	1	LYS	CA-C-N	5.67	132.18	121.97
2	W	1	LYS	C-N-CA	5.67	132.18	121.97
1	A	359	ARG	N-CA-C	5.67	120.26	113.23
2	X	144	LYS	CB-CG-CD	5.67	124.34	111.30
2	Q	144	LYS	CB-CG-CD	5.67	124.34	111.30
2	V	67	PHE	CA-C-N	5.67	126.38	120.03
2	V	67	PHE	C-N-CA	5.67	126.38	120.03
2	X	97	VAL	CA-C-O	-5.67	113.69	120.78
2	P	97	VAL	CA-C-O	-5.67	113.69	120.78
2	R	46	LYS	CA-C-O	-5.67	114.41	120.42
2	U	144	LYS	CB-CG-CD	5.67	124.34	111.30
2	W	144	LYS	CB-CG-CD	5.67	124.34	111.30
2	M	129	TRP	CE2-CD2-CE3	5.67	124.47	118.80
2	T	144	LYS	CB-CG-CD	5.67	124.33	111.30
2	U	67	PHE	CA-C-N	5.67	126.38	120.03
2	U	67	PHE	C-N-CA	5.67	126.38	120.03
2	V	129	TRP	CE2-CD2-CE3	5.67	124.47	118.80
2	W	367	ARG	CD-NE-CZ	-5.67	116.47	124.40
2	O	367	ARG	CD-NE-CZ	-5.66	116.47	124.40
2	R	367	ARG	CD-NE-CZ	-5.66	116.47	124.40
2	U	129	TRP	CE2-CD2-CE3	5.66	124.46	118.80
2	P	67	PHE	CA-C-N	5.66	126.37	120.03
2	P	67	PHE	C-N-CA	5.66	126.37	120.03
2	V	367	ARG	CD-NE-CZ	-5.66	116.48	124.40
2	N	97	VAL	CA-C-O	-5.65	113.71	120.78
2	O	97	VAL	CA-C-O	-5.65	113.72	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	97	VAL	CA-C-O	-5.65	113.71	120.78
2	X	367	ARG	CD-NE-CZ	-5.65	116.48	124.40
2	Q	367	ARG	CD-NE-CZ	-5.65	116.49	124.40
2	R	97	VAL	CA-C-O	-5.65	113.72	120.78
2	T	367	ARG	CD-NE-CZ	-5.65	116.49	124.40
2	T	184	ASP	N-CA-CB	-5.65	101.88	111.20
2	Q	97	VAL	CA-C-O	-5.64	113.73	120.78
1	I	359	ARG	N-CA-C	5.64	120.22	113.23
2	Q	184	ASP	N-CA-CB	-5.64	101.89	111.20
2	X	46	LYS	CA-C-O	-5.64	114.44	120.42
2	P	184	ASP	N-CA-CB	-5.64	101.90	111.20
1	E	233	ASP	N-CA-C	-5.63	105.04	111.07
2	U	184	ASP	N-CA-CB	-5.63	101.91	111.20
2	U	367	ARG	CD-NE-CZ	-5.63	116.52	124.40
2	W	67	PHE	CA-C-N	5.63	126.34	120.03
2	W	67	PHE	C-N-CA	5.63	126.34	120.03
2	W	184	ASP	N-CA-CB	-5.63	101.91	111.20
2	M	184	ASP	N-CA-CB	-5.63	101.91	111.20
2	X	184	ASP	N-CA-CB	-5.63	101.91	111.20
2	S	184	ASP	N-CA-CB	-5.63	101.92	111.20
1	E	389	GLY	N-CA-C	-5.62	102.63	112.53
2	R	184	ASP	N-CA-CB	-5.62	101.92	111.20
2	V	184	ASP	N-CA-CB	-5.62	101.92	111.20
2	N	184	ASP	N-CA-CB	-5.62	101.92	111.20
2	O	184	ASP	N-CA-CB	-5.62	101.92	111.20
2	Q	312	ALA	CB-CA-C	5.62	118.40	111.43
1	J	462	PHE	CA-CB-CG	-5.62	108.18	113.80
2	S	129	TRP	CE2-CD2-CE3	5.62	124.42	118.80
1	A	389	GLY	N-CA-C	-5.62	102.65	112.53
1	H	462	PHE	CA-CB-CG	-5.62	108.18	113.80
2	R	312	ALA	CB-CA-C	5.62	118.39	111.43
2	S	312	ALA	CB-CA-C	5.62	118.39	111.43
2	X	312	ALA	CB-CA-C	5.62	118.39	111.43
1	G	233	ASP	N-CA-C	-5.61	105.06	111.07
1	L	233	ASP	N-CA-C	-5.61	105.06	111.07
2	N	367	ARG	CD-NE-CZ	-5.61	116.54	124.40
2	P	312	ALA	CB-CA-C	5.61	118.39	111.43
1	F	233	ASP	N-CA-C	-5.61	105.07	111.07
2	Q	104	ILE	CB-CA-C	-5.61	104.81	111.65
2	T	104	ILE	CB-CA-C	-5.61	104.81	111.65
1	A	462	PHE	CA-CB-CG	-5.61	108.19	113.80
1	L	389	GLY	N-CA-C	-5.61	102.67	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	104	ILE	CB-CA-C	-5.61	104.81	111.65
2	T	312	ALA	CB-CA-C	5.60	118.38	111.43
1	B	462	PHE	CA-CB-CG	-5.60	108.20	113.80
1	C	389	GLY	N-CA-C	-5.60	102.67	112.53
2	M	312	ALA	CB-CA-C	5.60	118.38	111.43
2	O	46	LYS	CA-C-O	-5.60	114.48	120.42
2	U	104	ILE	CB-CA-C	-5.60	104.81	111.65
1	H	389	GLY	N-CA-C	-5.60	102.68	112.53
2	U	20	LEU	CA-C-O	-5.60	114.94	120.82
1	G	462	PHE	CA-CB-CG	-5.60	108.20	113.80
2	R	20	LEU	CA-C-O	-5.60	114.94	120.82
2	R	104	ILE	CB-CA-C	-5.60	104.82	111.65
2	U	312	ALA	CB-CA-C	5.60	118.37	111.43
1	D	389	GLY	N-CA-C	-5.59	102.68	112.53
2	M	104	ILE	CB-CA-C	-5.59	104.83	111.65
2	W	20	LEU	CA-C-O	-5.59	114.95	120.82
1	A	233	ASP	N-CA-C	-5.59	105.09	111.07
1	B	233	ASP	N-CA-C	-5.59	105.09	111.07
2	W	312	ALA	CB-CA-C	5.59	118.36	111.43
1	F	389	GLY	N-CA-C	-5.59	102.69	112.53
1	G	389	GLY	N-CA-C	-5.59	102.70	112.53
1	I	389	GLY	N-CA-C	-5.59	102.69	112.53
2	M	20	LEU	CA-C-O	-5.59	114.95	120.82
1	J	389	GLY	N-CA-C	-5.59	102.70	112.53
2	V	312	ALA	CB-CA-C	5.58	118.36	111.43
2	P	20	LEU	CA-C-O	-5.58	114.96	120.82
1	J	233	ASP	N-CA-C	-5.58	105.10	111.07
2	N	20	LEU	CA-C-O	-5.58	114.96	120.82
2	N	312	ALA	CB-CA-C	5.58	118.35	111.43
2	V	104	ILE	CB-CA-C	-5.58	104.84	111.65
2	N	104	ILE	CB-CA-C	-5.58	104.85	111.65
1	D	462	PHE	CA-CB-CG	-5.58	108.22	113.80
2	W	104	ILE	CB-CA-C	-5.57	104.85	111.65
2	T	20	LEU	CA-C-O	-5.57	114.97	120.82
2	Q	20	LEU	CA-C-O	-5.57	114.97	120.82
1	K	389	GLY	N-CA-C	-5.57	102.73	112.53
1	B	389	GLY	N-CA-C	-5.57	102.73	112.53
1	K	233	ASP	N-CA-C	-5.57	105.11	111.07
2	O	312	ALA	CB-CA-C	5.57	118.33	111.43
2	V	20	LEU	CA-C-O	-5.57	114.97	120.82
2	S	20	LEU	CA-C-O	-5.56	114.98	120.82
1	D	233	ASP	N-CA-C	-5.56	105.12	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	104	ILE	CB-CA-C	-5.56	104.86	111.65
1	I	233	ASP	N-CA-C	-5.56	105.12	111.07
1	F	462	PHE	CA-CB-CG	-5.56	108.24	113.80
1	L	462	PHE	CA-CB-CG	-5.56	108.24	113.80
2	P	104	ILE	CB-CA-C	-5.56	104.87	111.65
2	X	104	ILE	CB-CA-C	-5.56	104.87	111.65
1	C	462	PHE	CA-CB-CG	-5.55	108.25	113.80
1	D	319	TYR	CA-CB-CG	-5.55	103.90	113.90
1	J	319	TYR	CA-CB-CG	-5.55	103.90	113.90
2	P	205	ASN	CA-C-N	5.55	129.49	120.60
2	P	205	ASN	C-N-CA	5.55	129.49	120.60
2	X	20	LEU	CA-C-O	-5.55	114.99	120.82
2	O	20	LEU	CA-C-O	-5.55	114.99	120.82
2	M	197	ASP	CA-CB-CG	5.55	118.15	112.60
2	N	205	ASN	CA-C-N	5.55	129.47	120.60
2	N	205	ASN	C-N-CA	5.55	129.47	120.60
1	C	233	ASP	N-CA-C	-5.54	105.14	111.07
1	E	462	PHE	CA-CB-CG	-5.54	108.25	113.80
1	F	319	TYR	CA-CB-CG	-5.54	103.92	113.90
1	H	233	ASP	N-CA-C	-5.54	105.14	111.07
2	Q	205	ASN	CA-C-N	5.54	129.47	120.60
2	Q	205	ASN	C-N-CA	5.54	129.47	120.60
2	Q	311	LEU	O-C-N	-5.54	114.91	122.33
2	S	60	ILE	CA-C-O	5.54	126.21	120.39
2	S	197	ASP	CA-CB-CG	5.54	118.14	112.60
2	O	197	ASP	CA-CB-CG	5.54	118.14	112.60
1	I	462	PHE	CA-CB-CG	-5.54	108.26	113.80
2	T	176	TYR	O-C-N	5.54	129.52	123.04
2	T	197	ASP	CA-CB-CG	5.54	118.14	112.60
2	W	205	ASN	CA-C-N	5.54	129.46	120.60
2	W	205	ASN	C-N-CA	5.54	129.46	120.60
2	P	208	THR	CA-CB-OG1	-5.54	101.30	109.60
1	A	319	TYR	CA-CB-CG	-5.54	103.94	113.90
1	H	319	TYR	CA-CB-CG	-5.54	103.94	113.90
2	R	205	ASN	CA-C-N	5.54	129.46	120.60
2	R	205	ASN	C-N-CA	5.54	129.46	120.60
1	K	319	TYR	CA-CB-CG	-5.53	103.94	113.90
2	M	311	LEU	O-C-N	-5.53	114.92	122.33
2	N	197	ASP	CA-CB-CG	5.53	118.13	112.60
2	O	205	ASN	CA-C-N	5.53	129.45	120.60
2	O	205	ASN	C-N-CA	5.53	129.45	120.60
2	X	197	ASP	CA-CB-CG	5.53	118.13	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	462	PHE	CA-CB-CG	-5.53	108.27	113.80
1	L	319	TYR	CA-CB-CG	-5.53	103.94	113.90
2	S	176	TYR	O-C-N	5.53	129.51	123.04
2	O	356	THR	N-CA-CB	5.53	118.86	110.45
2	U	205	ASN	CA-C-N	5.53	129.45	120.60
2	U	205	ASN	C-N-CA	5.53	129.45	120.60
2	O	311	LEU	O-C-N	-5.53	114.92	122.33
2	P	197	ASP	CA-CB-CG	5.53	118.13	112.60
1	C	319	TYR	CA-CB-CG	-5.53	103.95	113.90
2	U	311	LEU	O-C-N	-5.53	114.93	122.33
2	Q	208	THR	CA-CB-OG1	-5.52	101.31	109.60
2	M	205	ASN	CA-C-N	5.52	129.44	120.60
2	M	205	ASN	C-N-CA	5.52	129.44	120.60
2	N	311	LEU	O-C-N	-5.52	114.93	122.33
2	O	208	THR	CA-CB-OG1	-5.52	101.32	109.60
2	T	311	LEU	O-C-N	-5.52	114.93	122.33
2	V	197	ASP	CA-CB-CG	5.52	118.12	112.60
2	X	205	ASN	CA-C-N	5.52	129.44	120.60
2	X	205	ASN	C-N-CA	5.52	129.44	120.60
2	N	208	THR	CA-CB-OG1	-5.52	101.32	109.60
2	U	208	THR	CA-CB-OG1	-5.52	101.32	109.60
2	W	176	TYR	O-C-N	5.52	129.50	123.04
1	E	319	TYR	CA-CB-CG	-5.52	103.97	113.90
2	O	176	TYR	O-C-N	5.52	129.50	123.04
2	Q	305	LYS	N-CA-C	5.52	118.01	111.33
2	S	205	ASN	CA-C-N	5.52	129.43	120.60
2	S	205	ASN	C-N-CA	5.52	129.43	120.60
2	V	205	ASN	CA-C-N	5.52	129.43	120.60
2	V	205	ASN	C-N-CA	5.52	129.43	120.60
2	X	208	THR	CA-CB-OG1	-5.52	101.32	109.60
2	M	176	TYR	O-C-N	5.52	129.50	123.04
2	M	208	THR	CA-CB-OG1	-5.52	101.32	109.60
2	Q	356	THR	N-CA-CB	5.52	118.84	110.45
2	V	311	LEU	O-C-N	-5.52	114.94	122.33
2	X	147	LEU	N-CA-CB	-5.52	101.14	111.13
1	G	319	TYR	CA-CB-CG	-5.52	103.97	113.90
2	T	205	ASN	CA-C-N	5.52	129.43	120.60
2	T	205	ASN	C-N-CA	5.52	129.43	120.60
2	U	197	ASP	CA-CB-CG	5.52	118.12	112.60
1	B	319	TYR	CA-CB-CG	-5.51	103.97	113.90
2	N	176	TYR	O-C-N	5.51	129.49	123.04
2	N	356	THR	N-CA-CB	5.51	118.83	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	305	LYS	N-CA-C	5.51	118.00	111.33
2	V	208	THR	CA-CB-OG1	-5.51	101.33	109.60
1	I	319	TYR	CA-CB-CG	-5.51	103.98	113.90
2	Q	262	LEU	CA-C-O	-5.51	114.64	120.92
2	N	244	VAL	CA-C-O	-5.51	114.71	120.27
2	R	356	THR	N-CA-CB	5.51	118.83	110.45
2	S	244	VAL	CA-C-O	-5.51	114.70	120.27
2	X	311	LEU	O-C-N	-5.51	114.95	122.33
2	M	60	ILE	CA-C-O	5.51	126.17	120.39
2	V	176	TYR	O-C-N	5.51	129.48	123.04
2	X	356	THR	N-CA-CB	5.51	118.82	110.45
2	P	311	LEU	O-C-N	-5.51	114.95	122.33
2	R	208	THR	CA-CB-OG1	-5.51	101.34	109.60
2	R	311	LEU	O-C-N	-5.51	114.95	122.33
2	S	311	LEU	O-C-N	-5.51	114.95	122.33
2	Q	60	ILE	CA-C-O	5.50	126.17	120.39
2	Q	197	ASP	CA-CB-CG	5.50	118.11	112.60
2	W	311	LEU	O-C-N	-5.50	114.95	122.33
2	P	244	VAL	CA-C-O	-5.50	114.71	120.27
2	R	205	ASN	OD1-CG-ND2	5.50	128.10	122.60
2	S	208	THR	CA-CB-OG1	-5.50	101.34	109.60
2	W	208	THR	CA-CB-OG1	-5.50	101.34	109.60
2	R	147	LEU	N-CA-CB	-5.50	101.17	111.13
2	R	197	ASP	CA-CB-CG	5.50	118.10	112.60
2	V	356	THR	N-CA-CB	5.50	118.81	110.45
2	X	244	VAL	CA-C-O	-5.50	114.71	120.27
2	P	176	TYR	O-C-N	5.50	129.47	123.04
2	P	356	THR	N-CA-CB	5.50	118.81	110.45
2	R	176	TYR	O-C-N	5.50	129.47	123.04
2	T	205	ASN	OD1-CG-ND2	5.50	128.10	122.60
2	U	147	LEU	N-CA-CB	-5.50	101.18	111.13
2	N	205	ASN	OD1-CG-ND2	5.50	128.10	122.60
2	O	305	LYS	N-CA-C	5.50	117.98	111.33
2	S	205	ASN	OD1-CG-ND2	5.50	128.10	122.60
2	U	176	TYR	O-C-N	5.50	129.47	123.04
2	W	197	ASP	CA-CB-CG	5.50	118.10	112.60
2	V	305	LYS	N-CA-C	5.49	117.98	111.33
2	W	356	THR	N-CA-C	-5.49	103.14	110.55
2	M	356	THR	N-CA-C	-5.49	103.14	110.55
2	R	244	VAL	CA-C-O	-5.49	114.72	120.27
2	S	356	THR	N-CA-C	-5.49	103.14	110.55
2	U	356	THR	N-CA-CB	5.49	118.80	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	205	ASN	OD1-CG-ND2	5.49	128.09	122.60
2	X	176	TYR	O-C-N	5.49	129.47	123.04
2	O	205	ASN	OD1-CG-ND2	5.49	128.09	122.60
2	T	262	LEU	CA-C-O	-5.49	114.66	120.92
2	V	60	ILE	CA-C-O	5.49	126.15	120.39
2	W	244	VAL	CA-C-O	-5.49	114.73	120.27
2	X	305	LYS	N-CA-C	5.49	117.97	111.33
2	O	147	LEU	N-CA-CB	-5.49	101.20	111.13
2	O	262	LEU	CA-C-O	-5.49	114.67	120.92
2	M	356	THR	N-CA-CB	5.48	118.79	110.45
2	U	356	THR	N-CA-C	-5.48	103.15	110.55
2	N	60	ILE	CA-C-O	5.48	126.15	120.39
2	N	147	LEU	N-CA-CB	-5.48	101.20	111.13
2	Q	21	ALA	CA-C-N	5.48	128.17	120.28
2	Q	21	ALA	C-N-CA	5.48	128.17	120.28
2	V	147	LEU	N-CA-CB	-5.48	101.21	111.13
2	V	356	THR	N-CA-C	-5.48	103.15	110.55
2	W	356	THR	N-CA-CB	5.48	118.78	110.45
2	X	60	ILE	CA-C-O	5.48	126.15	120.39
2	P	147	LEU	N-CA-CB	-5.48	101.21	111.13
2	R	262	LEU	CA-C-O	-5.48	114.67	120.92
2	S	356	THR	N-CA-CB	5.48	118.78	110.45
2	W	305	LYS	N-CA-C	5.48	117.96	111.33
2	T	208	THR	CA-CB-OG1	-5.48	101.38	109.60
2	T	305	LYS	N-CA-C	5.48	117.96	111.33
2	N	142	LYS	N-CA-CB	-5.48	102.16	110.92
2	S	262	LEU	CA-C-O	-5.48	114.67	120.92
2	W	205	ASN	OD1-CG-ND2	5.48	128.08	122.60
2	W	281	GLU	N-CA-C	5.48	118.17	111.82
2	T	356	THR	N-CA-C	-5.48	103.16	110.55
2	M	305	LYS	N-CA-C	5.47	117.95	111.33
2	P	305	LYS	N-CA-C	5.47	117.95	111.33
2	R	356	THR	N-CA-C	-5.47	103.16	110.55
2	S	305	LYS	N-CA-C	5.47	117.95	111.33
2	N	305	LYS	N-CA-C	5.47	117.95	111.33
2	Q	356	THR	N-CA-C	-5.47	103.16	110.55
2	S	281	GLU	N-CA-C	5.47	118.17	111.82
2	U	28	GLU	CA-C-O	5.47	126.26	119.97
2	M	244	VAL	CA-C-O	-5.47	114.74	120.27
2	M	262	LEU	CA-C-O	-5.47	114.68	120.92
2	S	147	LEU	N-CA-CB	-5.47	101.23	111.13
2	U	68	GLY	CA-C-O	5.47	126.16	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	205	ASN	OD1-CG-ND2	5.47	128.07	122.60
2	Q	176	TYR	O-C-N	5.47	129.44	123.04
2	V	244	VAL	CA-C-O	-5.47	114.75	120.27
2	M	281	GLU	N-CA-C	5.47	118.16	111.82
2	T	356	THR	N-CA-CB	5.47	118.76	110.45
2	W	34	LYS	CA-C-O	5.47	127.21	120.92
2	N	356	THR	N-CA-C	-5.47	103.17	110.55
2	O	356	THR	N-CA-C	-5.47	103.17	110.55
2	Q	205	ASN	OD1-CG-ND2	5.47	128.07	122.60
2	Q	244	VAL	CA-C-O	-5.47	114.75	120.27
2	Q	281	GLU	N-CA-C	5.47	118.16	111.82
2	R	68	GLY	CA-C-O	5.47	126.16	120.80
2	T	142	LYS	N-CA-CB	-5.47	102.17	110.92
2	W	60	ILE	CA-C-O	5.47	126.13	120.39
2	W	68	GLY	CA-C-O	5.47	126.16	120.80
2	P	60	ILE	CA-C-O	5.46	126.13	120.39
2	Q	68	GLY	CA-C-O	5.46	126.16	120.80
2	Q	273	LYS	CB-CA-C	-5.46	101.72	110.79
2	R	21	ALA	CA-C-N	5.46	128.15	120.28
2	R	21	ALA	C-N-CA	5.46	128.15	120.28
2	U	293	VAL	CA-C-N	5.46	128.15	120.28
2	U	293	VAL	C-N-CA	5.46	128.15	120.28
2	M	147	LEU	N-CA-CB	-5.46	101.25	111.13
2	N	281	GLU	N-CA-C	5.46	118.16	111.82
2	P	262	LEU	CA-C-O	-5.46	114.69	120.92
2	P	293	VAL	CA-C-N	5.46	128.14	120.28
2	P	293	VAL	C-N-CA	5.46	128.14	120.28
2	Q	34	LYS	CA-C-O	5.46	127.20	120.92
2	T	147	LEU	N-CA-CB	-5.46	101.25	111.13
2	W	147	LEU	N-CA-CB	-5.46	101.24	111.13
2	Q	147	LEU	N-CA-CB	-5.46	101.25	111.13
2	V	262	LEU	CA-C-O	-5.46	114.70	120.92
2	M	205	ASN	OD1-CG-ND2	5.46	128.06	122.60
2	O	60	ILE	CA-C-O	5.46	126.12	120.39
2	O	281	GLU	N-CA-C	5.46	118.15	111.82
2	P	205	ASN	OD1-CG-ND2	5.46	128.06	122.60
2	T	281	GLU	N-CA-C	5.46	118.15	111.82
2	R	60	ILE	CA-C-O	5.46	126.12	120.39
2	T	293	VAL	CA-C-N	5.46	128.14	120.28
2	T	293	VAL	C-N-CA	5.46	128.14	120.28
2	T	244	VAL	CA-C-O	-5.46	114.76	120.27
2	U	205	ASN	OD1-CG-ND2	5.46	128.06	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	356	THR	N-CA-C	-5.46	103.19	110.55
2	N	262	LEU	CA-C-O	-5.45	114.70	120.92
2	R	305	LYS	N-CA-C	5.45	117.93	111.33
2	T	273	LYS	CB-CA-C	-5.45	101.74	110.79
2	X	273	LYS	CB-CA-C	-5.45	101.74	110.79
2	O	21	ALA	CA-C-N	5.45	128.13	120.28
2	O	21	ALA	C-N-CA	5.45	128.13	120.28
2	P	356	THR	N-CA-C	-5.45	103.19	110.55
2	Q	28	GLU	CA-C-O	5.45	126.24	119.97
2	T	60	ILE	CA-C-O	5.45	126.11	120.39
2	M	21	ALA	CA-C-N	5.45	128.13	120.28
2	M	21	ALA	C-N-CA	5.45	128.13	120.28
2	N	34	LYS	CA-C-O	5.45	127.19	120.92
2	U	273	LYS	CB-CA-C	-5.45	101.74	110.79
2	X	346	ALA	CA-C-O	5.45	126.73	120.90
2	O	255	SER	N-CA-C	-5.45	102.33	110.23
2	P	281	GLU	N-CA-C	5.45	118.14	111.82
2	U	60	ILE	CA-C-O	5.45	126.11	120.39
2	V	34	LYS	CA-C-O	5.45	127.19	120.92
2	V	68	GLY	CA-C-O	5.45	126.14	120.80
2	V	281	GLU	N-CA-C	5.45	118.14	111.82
2	M	28	GLU	CA-C-O	5.45	126.23	119.97
2	R	34	LYS	CA-C-O	5.45	127.18	120.92
2	U	142	LYS	N-CA-CB	-5.45	102.20	110.92
2	W	28	GLU	CA-C-O	5.45	126.23	119.97
2	O	244	VAL	CA-C-O	-5.45	114.77	120.27
2	P	211	SER	CA-CB-OG	-5.45	100.21	111.10
2	X	255	SER	N-CA-C	-5.45	102.33	110.23
2	X	262	LEU	CA-C-O	-5.45	114.71	120.92
2	N	28	GLU	CA-C-O	5.44	126.23	119.97
2	R	273	LYS	CB-CA-C	-5.44	101.76	110.79
2	U	21	ALA	CA-C-N	5.44	128.12	120.28
2	U	21	ALA	C-N-CA	5.44	128.12	120.28
2	N	273	LYS	CB-CA-C	-5.44	101.76	110.79
2	O	142	LYS	N-CA-CB	-5.44	102.22	110.92
2	R	142	LYS	N-CA-CB	-5.44	102.21	110.92
2	V	142	LYS	N-CA-CB	-5.44	102.22	110.92
2	M	211	SER	CA-CB-OG	-5.44	100.22	111.10
2	U	244	VAL	CA-C-O	-5.44	114.78	120.27
2	V	273	LYS	CB-CA-C	-5.44	101.76	110.79
2	X	34	LYS	CA-C-O	5.44	127.17	120.92
2	N	21	ALA	CA-C-N	5.44	128.11	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	21	ALA	C-N-CA	5.44	128.11	120.28
2	Q	211	SER	CA-CB-OG	-5.44	100.22	111.10
2	R	293	VAL	CA-C-N	5.44	128.11	120.28
2	R	293	VAL	C-N-CA	5.44	128.11	120.28
2	S	142	LYS	N-CA-CB	-5.44	102.22	110.92
2	S	293	VAL	CA-C-N	5.44	128.11	120.28
2	S	293	VAL	C-N-CA	5.44	128.11	120.28
2	V	293	VAL	CA-C-N	5.44	128.11	120.28
2	V	293	VAL	C-N-CA	5.44	128.11	120.28
2	W	273	LYS	CB-CA-C	-5.44	101.76	110.79
2	X	293	VAL	CA-C-N	5.44	128.11	120.28
2	X	293	VAL	C-N-CA	5.44	128.11	120.28
2	N	211	SER	CA-CB-OG	-5.43	100.23	111.10
2	P	34	LYS	CA-C-O	5.43	127.17	120.92
2	P	142	LYS	N-CA-CB	-5.43	102.22	110.92
2	U	262	LEU	CA-C-O	-5.43	114.72	120.92
2	V	21	ALA	CA-C-N	5.43	128.11	120.28
2	V	21	ALA	C-N-CA	5.43	128.11	120.28
2	V	211	SER	CA-CB-OG	-5.43	100.23	111.10
2	M	293	VAL	CA-C-N	5.43	128.10	120.28
2	M	293	VAL	C-N-CA	5.43	128.10	120.28
2	O	211	SER	CA-CB-OG	-5.43	100.23	111.10
2	O	273	LYS	CB-CA-C	-5.43	101.77	110.79
2	P	273	LYS	CB-CA-C	-5.43	101.77	110.79
2	R	211	SER	CA-CB-OG	-5.43	100.23	111.10
2	T	211	SER	CA-CB-OG	-5.43	100.24	111.10
2	W	211	SER	CA-CB-OG	-5.43	100.24	111.10
2	W	255	SER	N-CA-C	-5.43	102.35	110.23
2	Q	142	LYS	N-CA-CB	-5.43	102.23	110.92
2	X	142	LYS	N-CA-CB	-5.43	102.23	110.92
2	S	255	SER	N-CA-C	-5.43	102.36	110.23
2	T	34	LYS	CA-C-O	5.43	127.16	120.92
2	T	255	SER	N-CA-C	-5.43	102.36	110.23
2	W	262	LEU	CA-C-O	-5.43	114.73	120.92
2	R	281	GLU	N-CA-C	5.43	118.12	111.82
2	M	273	LYS	CB-CA-C	-5.43	101.78	110.79
2	O	293	VAL	CA-C-N	5.43	128.09	120.28
2	O	293	VAL	C-N-CA	5.43	128.09	120.28
2	P	28	GLU	CA-C-O	5.43	126.21	119.97
2	T	21	ALA	CA-C-N	5.43	128.09	120.28
2	T	21	ALA	C-N-CA	5.43	128.09	120.28
2	U	255	SER	N-CA-C	-5.43	102.36	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	28	GLU	CA-C-O	5.43	126.21	119.97
2	M	255	SER	N-CA-C	-5.42	102.37	110.23
2	P	68	GLY	CA-C-O	5.42	126.12	120.80
2	Q	293	VAL	CA-C-N	5.42	128.09	120.28
2	Q	293	VAL	C-N-CA	5.42	128.09	120.28
2	S	21	ALA	CA-C-N	5.42	128.09	120.28
2	S	21	ALA	C-N-CA	5.42	128.09	120.28
2	M	346	ALA	CA-C-O	5.42	126.70	120.90
2	N	293	VAL	CA-C-N	5.42	128.09	120.28
2	N	293	VAL	C-N-CA	5.42	128.09	120.28
2	S	273	LYS	CB-CA-C	-5.42	101.79	110.79
2	U	281	GLU	N-CA-C	5.42	118.11	111.82
2	X	281	GLU	N-CA-C	5.42	118.11	111.82
1	G	98	GLN	N-CA-C	5.42	118.02	111.40
2	N	255	SER	N-CA-C	-5.42	102.37	110.23
2	Q	346	ALA	CA-C-O	5.42	126.70	120.90
2	R	346	ALA	CA-C-O	5.42	126.70	120.90
2	S	211	SER	CA-CB-OG	-5.42	100.25	111.10
2	U	211	SER	CA-CB-OG	-5.42	100.25	111.10
2	V	255	SER	N-CA-C	-5.42	102.37	110.23
2	W	142	LYS	N-CA-CB	-5.42	102.25	110.92
2	O	28	GLU	CA-C-O	5.42	126.20	119.97
2	P	255	SER	N-CA-C	-5.42	102.37	110.23
2	T	28	GLU	CA-C-O	5.42	126.20	119.97
2	U	147	LEU	N-CA-C	5.42	118.02	108.75
2	V	28	GLU	CA-C-O	5.42	126.20	119.97
2	P	346	ALA	CA-C-O	5.42	126.70	120.90
2	M	34	LYS	CA-C-O	5.42	127.15	120.92
2	T	194	PHE	CA-C-O	-5.42	115.13	120.82
2	U	34	LYS	CA-C-O	5.42	127.15	120.92
2	V	346	ALA	CA-C-O	5.42	126.70	120.90
2	W	293	VAL	CA-C-N	5.42	128.08	120.28
2	W	293	VAL	C-N-CA	5.42	128.08	120.28
2	X	21	ALA	CA-C-N	5.42	128.08	120.28
2	X	21	ALA	C-N-CA	5.42	128.08	120.28
2	R	255	SER	N-CA-C	-5.42	102.38	110.23
2	T	346	ALA	CA-C-O	5.42	126.69	120.90
2	P	21	ALA	CA-C-N	5.41	128.08	120.28
2	P	21	ALA	C-N-CA	5.41	128.08	120.28
2	M	142	LYS	N-CA-CB	-5.41	102.26	110.92
2	P	194	PHE	CA-C-O	-5.41	115.14	120.82
2	X	211	SER	CA-CB-OG	-5.41	100.28	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	34	LYS	CA-C-O	5.41	127.14	120.92
2	X	147	LEU	N-CA-C	5.41	118.00	108.75
2	W	346	ALA	CA-C-O	5.41	126.69	120.90
2	W	21	ALA	CA-C-N	5.41	128.06	120.28
2	W	21	ALA	C-N-CA	5.41	128.06	120.28
2	Q	255	SER	N-CA-C	-5.40	102.39	110.23
2	S	34	LYS	CA-C-O	5.40	127.13	120.92
2	O	346	ALA	CA-C-O	5.40	126.68	120.90
2	Q	147	LEU	N-CA-C	5.39	117.98	108.75
2	Q	237	THR	O-C-N	5.39	128.53	122.22
2	R	237	THR	O-C-N	5.39	128.53	122.22
2	S	194	PHE	CA-C-O	-5.39	115.16	120.82
2	S	346	ALA	CA-C-O	5.39	126.67	120.90
2	S	28	GLU	CA-C-O	5.39	126.17	119.97
2	W	147	LEU	N-CA-C	5.39	117.97	108.75
2	O	147	LEU	N-CA-C	5.39	117.97	108.75
2	P	147	LEU	N-CA-C	5.39	117.97	108.75
2	S	237	THR	O-C-N	5.39	128.53	122.22
2	S	326	LYS	CA-CB-CG	-5.39	103.32	114.10
2	V	147	LEU	N-CA-C	5.39	117.96	108.75
2	S	147	LEU	N-CA-C	5.39	117.96	108.75
2	U	326	LYS	CA-CB-CG	-5.39	103.33	114.10
2	U	346	ALA	CA-C-O	5.39	126.66	120.90
2	W	59	ILE	CA-C-O	5.39	126.70	120.67
2	M	147	LEU	N-CA-C	5.38	117.96	108.75
2	N	147	LEU	N-CA-C	5.38	117.96	108.75
2	N	346	ALA	CA-C-O	5.38	126.66	120.90
2	W	326	LYS	CA-CB-CG	-5.38	103.33	114.10
2	S	59	ILE	CA-C-O	5.38	126.70	120.67
2	T	103	LEU	CA-C-O	-5.38	114.46	120.54
2	M	194	PHE	CA-C-O	-5.38	115.17	120.82
2	R	28	GLU	CA-C-O	5.38	126.16	119.97
2	T	326	LYS	CA-CB-CG	-5.38	103.34	114.10
2	R	147	LEU	N-CA-C	5.38	117.94	108.75
2	W	237	THR	O-C-N	5.38	128.51	122.22
2	V	326	LYS	CA-CB-CG	-5.38	103.35	114.10
2	M	326	LYS	CA-CB-CG	-5.37	103.35	114.10
2	R	326	LYS	CA-CB-CG	-5.37	103.35	114.10
2	P	326	LYS	CA-CB-CG	-5.37	103.36	114.10
2	Q	326	LYS	CA-CB-CG	-5.37	103.36	114.10
2	V	194	PHE	CA-C-O	-5.37	115.18	120.82
2	W	194	PHE	CA-C-O	-5.37	115.18	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	194	PHE	CA-C-O	-5.37	115.18	120.82
2	O	326	LYS	CA-CB-CG	-5.37	103.36	114.10
2	N	326	LYS	CA-CB-CG	-5.37	103.37	114.10
1	J	314	PRO	N-CA-C	5.37	120.26	114.68
2	N	237	THR	O-C-N	5.37	128.50	122.22
2	O	194	PHE	CA-C-O	-5.37	115.19	120.82
2	W	103	LEU	CA-C-O	-5.37	114.48	120.54
1	A	314	PRO	N-CA-C	5.36	120.26	114.68
2	X	103	LEU	CA-C-O	-5.36	114.48	120.54
2	X	326	LYS	CA-CB-CG	-5.36	103.38	114.10
2	M	237	THR	O-C-N	5.36	128.49	122.22
2	U	194	PHE	CA-C-O	-5.36	115.19	120.82
2	M	59	ILE	CA-C-O	5.36	126.67	120.67
2	O	237	THR	O-C-N	5.36	128.49	122.22
2	Q	194	PHE	CA-C-O	-5.36	115.20	120.82
2	T	147	LEU	N-CA-C	5.36	117.91	108.75
2	V	237	THR	O-C-N	5.36	128.49	122.22
2	O	59	ILE	CA-C-O	5.35	126.67	120.67
1	B	314	PRO	N-CA-C	5.35	120.25	114.68
2	X	194	PHE	CA-C-O	-5.35	115.20	120.82
1	E	98	GLN	N-CA-C	5.35	117.93	111.40
2	V	59	ILE	CA-C-O	5.35	126.66	120.67
1	G	314	PRO	N-CA-C	5.34	120.24	114.68
2	P	237	THR	O-C-N	5.34	128.47	122.22
2	Q	103	LEU	CA-C-O	-5.34	114.50	120.54
2	R	103	LEU	CA-C-O	-5.34	114.50	120.54
2	T	59	ILE	CA-C-O	5.34	126.66	120.67
2	V	103	LEU	CA-C-O	-5.34	114.50	120.54
2	N	344	ARG	O-C-N	5.34	127.57	122.07
2	Q	59	ILE	CA-C-O	5.34	126.65	120.67
2	U	103	LEU	CA-C-O	-5.34	114.50	120.54
2	P	103	LEU	CA-C-O	-5.34	114.51	120.54
2	X	59	ILE	CA-C-O	5.34	126.65	120.67
2	X	237	THR	O-C-N	5.34	128.47	122.22
2	T	237	THR	O-C-N	5.34	128.46	122.22
2	U	59	ILE	CA-C-O	5.33	126.64	120.67
2	U	237	THR	O-C-N	5.33	128.46	122.22
2	M	103	LEU	CA-C-O	-5.33	114.51	120.54
2	Q	344	ARG	O-C-N	5.33	127.56	122.07
2	S	316	ARG	NH1-CZ-NH2	-5.33	112.37	119.30
1	E	314	PRO	N-CA-C	5.33	120.22	114.68
2	M	166	GLY	N-CA-C	-5.33	106.47	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	59	ILE	CA-C-O	5.33	126.64	120.67
2	P	59	ILE	CA-C-O	5.33	126.64	120.67
2	U	190	ALA	CA-C-N	5.33	125.86	119.94
2	U	190	ALA	C-N-CA	5.33	125.86	119.94
2	W	344	ARG	O-C-N	5.33	127.56	122.07
2	R	316	ARG	NH1-CZ-NH2	-5.33	112.38	119.30
2	R	59	ILE	CA-C-O	5.33	126.64	120.67
2	R	194	PHE	CA-C-O	-5.33	115.23	120.82
2	Q	190	ALA	CA-C-N	5.32	125.85	119.94
2	Q	190	ALA	C-N-CA	5.32	125.85	119.94
2	S	103	LEU	CA-C-O	-5.32	114.52	120.54
2	S	344	ARG	O-C-N	5.32	127.55	122.07
2	X	316	ARG	NH1-CZ-NH2	-5.32	112.38	119.30
2	V	316	ARG	NH1-CZ-NH2	-5.32	112.38	119.30
2	P	316	ARG	NH1-CZ-NH2	-5.32	112.39	119.30
2	U	348	ILE	CB-CG1-CD1	-5.32	102.63	113.80
2	V	344	ARG	O-C-N	5.32	127.55	122.07
2	X	344	ARG	O-C-N	5.32	127.55	122.07
1	D	314	PRO	N-CA-C	5.32	120.21	114.68
2	N	103	LEU	CA-C-O	-5.32	114.53	120.54
2	O	190	ALA	CA-C-N	5.32	125.84	119.94
2	O	190	ALA	C-N-CA	5.32	125.84	119.94
2	Q	316	ARG	NH1-CZ-NH2	-5.32	112.39	119.30
2	T	190	ALA	CA-C-N	5.32	125.84	119.94
2	T	190	ALA	C-N-CA	5.32	125.84	119.94
2	T	348	ILE	CB-CG1-CD1	-5.32	102.64	113.80
2	M	316	ARG	NH1-CZ-NH2	-5.31	112.39	119.30
2	R	348	ILE	CB-CG1-CD1	-5.31	102.64	113.80
2	M	348	ILE	CB-CG1-CD1	-5.31	102.64	113.80
2	P	344	ARG	O-C-N	5.31	127.54	122.07
2	S	348	ILE	CB-CG1-CD1	-5.31	102.64	113.80
2	Q	348	ILE	CB-CG1-CD1	-5.31	102.65	113.80
2	T	344	ARG	O-C-N	5.31	127.54	122.07
2	U	344	ARG	O-C-N	5.31	127.54	122.07
2	P	348	ILE	CB-CG1-CD1	-5.31	102.65	113.80
2	Q	118	ASN	OD1-CG-ND2	5.31	127.91	122.60
2	U	316	ARG	NH1-CZ-NH2	-5.31	112.40	119.30
2	V	348	ILE	CB-CG1-CD1	-5.31	102.65	113.80
2	W	166	GLY	N-CA-C	-5.31	106.49	112.33
2	X	28	GLU	CG-CD-OE1	-5.31	106.19	118.40
2	X	348	ILE	CB-CG1-CD1	-5.31	102.65	113.80
1	B	43	PHE	N-CA-C	5.31	117.98	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	28	GLU	CG-CD-OE1	-5.31	106.19	118.40
2	R	344	ARG	O-C-N	5.31	127.54	122.07
1	I	314	PRO	N-CA-C	5.31	120.20	114.68
2	N	28	GLU	CG-CD-OE1	-5.31	106.20	118.40
2	N	316	ARG	NH1-CZ-NH2	-5.31	112.40	119.30
2	O	118	ASN	OD1-CG-ND2	5.31	127.91	122.60
2	Q	166	GLY	N-CA-C	-5.31	106.49	112.33
2	T	166	GLY	N-CA-C	-5.31	106.49	112.33
1	E	43	PHE	N-CA-C	5.30	117.97	111.82
2	T	316	ARG	NH1-CZ-NH2	-5.30	112.40	119.30
2	O	103	LEU	CA-C-O	-5.30	114.55	120.54
2	W	190	ALA	CA-C-N	5.30	125.83	119.94
2	W	190	ALA	C-N-CA	5.30	125.83	119.94
1	F	314	PRO	N-CA-C	5.30	120.19	114.68
1	G	20	ARG	N-CA-C	5.30	118.20	109.72
2	M	344	ARG	O-C-N	5.30	127.53	122.07
2	N	166	GLY	N-CA-C	-5.30	106.50	112.33
2	O	344	ARG	O-C-N	5.30	127.53	122.07
2	S	166	GLY	N-CA-C	-5.30	106.50	112.33
2	W	348	ILE	CB-CG1-CD1	-5.30	102.67	113.80
2	N	172	GLU	CG-CD-OE2	-5.30	106.21	118.40
2	T	28	GLU	CG-CD-OE1	-5.30	106.21	118.40
2	U	28	GLU	CG-CD-OE1	-5.30	106.21	118.40
2	V	28	GLU	CG-CD-OE1	-5.30	106.21	118.40
2	U	172	GLU	CG-CD-OE2	-5.30	106.21	118.40
2	R	118	ASN	OD1-CG-ND2	5.30	127.90	122.60
2	O	348	ILE	CB-CG1-CD1	-5.29	102.68	113.80
2	S	28	GLU	CG-CD-OE1	-5.29	106.22	118.40
2	V	166	GLY	N-CA-C	-5.29	106.51	112.33
1	B	20	ARG	N-CA-C	5.29	118.19	109.72
1	I	404	ALA	N-CA-C	-5.29	105.68	113.72
2	O	172	GLU	CG-CD-OE2	-5.29	106.23	118.40
2	P	172	GLU	CG-CD-OE2	-5.29	106.23	118.40
2	X	166	GLY	N-CA-C	-5.29	106.51	112.33
1	L	314	PRO	N-CA-C	5.29	120.18	114.68
2	N	348	ILE	CB-CG1-CD1	-5.29	102.69	113.80
2	W	316	ARG	NH1-CZ-NH2	-5.29	112.42	119.30
2	Q	172	GLU	CG-CD-OE2	-5.29	106.24	118.40
2	R	172	GLU	CG-CD-OE2	-5.29	106.24	118.40
2	X	114	SER	O-C-N	5.29	130.02	123.15
1	J	404	ALA	N-CA-C	-5.29	105.69	113.72
2	M	28	GLU	CG-CD-OE1	-5.29	106.24	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	148	MET	CG-SD-CE	-5.29	89.27	100.90
2	M	172	GLU	CG-CD-OE2	-5.29	106.25	118.40
2	N	190	ALA	CA-C-N	5.29	125.81	119.94
2	N	190	ALA	C-N-CA	5.29	125.81	119.94
2	P	28	GLU	CG-CD-OE1	-5.29	106.24	118.40
2	T	118	ASN	OD1-CG-ND2	5.29	127.89	122.60
2	T	148	MET	CG-SD-CE	-5.29	89.27	100.90
2	U	80	THR	CA-CB-OG1	-5.29	101.67	109.60
2	V	172	GLU	CG-CD-OE2	-5.29	106.24	118.40
2	V	190	ALA	CA-C-N	5.29	125.81	119.94
2	V	190	ALA	C-N-CA	5.29	125.81	119.94
2	W	28	GLU	CG-CD-OE1	-5.29	106.24	118.40
2	O	28	GLU	CG-CD-OE1	-5.28	106.25	118.40
2	U	166	GLY	N-CA-C	-5.28	106.52	112.33
1	H	314	PRO	N-CA-C	5.28	120.17	114.68
2	R	148	MET	CG-SD-CE	-5.28	89.28	100.90
2	R	166	GLY	N-CA-C	-5.28	106.52	112.33
2	T	80	THR	CA-CB-OG1	-5.28	101.68	109.60
2	P	148	MET	CG-SD-CE	-5.28	89.28	100.90
2	V	148	MET	CG-SD-CE	-5.28	89.28	100.90
2	W	80	THR	CA-CB-OG1	-5.28	101.68	109.60
2	X	148	MET	CG-SD-CE	-5.28	89.28	100.90
1	B	404	ALA	N-CA-C	-5.28	105.70	113.72
1	L	404	ALA	N-CA-C	-5.28	105.70	113.72
1	C	404	ALA	N-CA-C	-5.28	105.70	113.72
1	H	20	ARG	N-CA-C	5.28	118.16	109.72
1	K	314	PRO	N-CA-C	5.28	120.17	114.68
2	M	80	THR	CA-CB-OG1	-5.28	101.68	109.60
2	N	148	MET	CG-SD-CE	-5.28	89.29	100.90
2	O	166	GLY	N-CA-C	-5.28	106.52	112.33
2	Q	28	GLU	CG-CD-OE1	-5.28	106.26	118.40
2	T	172	GLU	CG-CD-OE2	-5.28	106.26	118.40
2	V	118	ASN	OD1-CG-ND2	5.28	127.88	122.60
2	S	172	GLU	CG-CD-OE2	-5.28	106.27	118.40
2	W	148	MET	CG-SD-CE	-5.28	89.29	100.90
1	D	404	ALA	N-CA-C	-5.27	105.70	113.72
2	X	80	THR	CA-CB-OG1	-5.27	101.69	109.60
1	D	330	VAL	N-CA-C	5.27	119.70	113.22
2	R	190	ALA	CA-C-N	5.27	125.79	119.94
2	R	190	ALA	C-N-CA	5.27	125.79	119.94
2	S	118	ASN	OD1-CG-ND2	5.27	127.87	122.60
2	S	148	MET	CG-SD-CE	-5.27	89.30	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	190	ALA	CA-C-N	5.27	125.79	119.94
2	S	190	ALA	C-N-CA	5.27	125.79	119.94
2	X	190	ALA	CA-C-N	5.27	125.79	119.94
2	X	190	ALA	C-N-CA	5.27	125.79	119.94
1	C	20	ARG	N-CA-C	5.27	118.15	109.72
1	D	20	ARG	N-CA-C	5.27	118.15	109.72
2	O	148	MET	CG-SD-CE	-5.27	89.31	100.90
2	P	166	GLY	N-CA-C	-5.27	106.53	112.33
2	Q	148	MET	CG-SD-CE	-5.27	89.31	100.90
2	W	118	ASN	OD1-CG-ND2	5.27	127.87	122.60
2	W	172	GLU	CG-CD-OE2	-5.27	106.28	118.40
2	X	172	GLU	CG-CD-OE2	-5.27	106.28	118.40
2	X	231	ALA	N-CA-CB	-5.27	101.56	110.41
2	R	80	THR	CA-CB-OG1	-5.27	101.70	109.60
2	S	231	ALA	N-CA-CB	-5.27	101.56	110.41
2	V	80	THR	CA-CB-OG1	-5.27	101.70	109.60
2	X	118	ASN	OD1-CG-ND2	5.27	127.87	122.60
2	M	114	SER	O-C-N	5.27	130.00	123.15
1	A	404	ALA	N-CA-C	-5.26	105.72	113.72
1	H	404	ALA	N-CA-C	-5.26	105.72	113.72
2	N	80	THR	CA-CB-OG1	-5.26	101.70	109.60
2	O	316	ARG	NH1-CZ-NH2	-5.26	112.46	119.30
2	Q	80	THR	CA-CB-OG1	-5.26	101.70	109.60
2	M	190	ALA	CA-C-N	5.26	125.78	119.94
2	M	190	ALA	C-N-CA	5.26	125.78	119.94
2	U	148	MET	CG-SD-CE	-5.26	89.33	100.90
1	E	330	VAL	N-CA-C	5.26	119.69	113.22
1	G	404	ALA	N-CA-C	-5.26	105.73	113.72
1	L	43	PHE	N-CA-C	5.26	117.92	111.82
2	N	118	ASN	OD1-CG-ND2	5.26	127.86	122.60
1	K	404	ALA	N-CA-C	-5.26	105.73	113.72
2	P	190	ALA	CA-C-N	5.26	125.77	119.94
2	P	190	ALA	C-N-CA	5.26	125.77	119.94
2	N	114	SER	O-C-N	5.25	129.98	123.15
2	O	80	THR	CA-CB-OG1	-5.25	101.72	109.60
2	P	114	SER	O-C-N	5.25	129.98	123.15
2	W	119	LYS	O-C-N	5.25	129.22	122.39
2	S	80	THR	CA-CB-OG1	-5.25	101.72	109.60
2	V	114	SER	O-C-N	5.25	129.98	123.15
2	W	114	SER	O-C-N	5.25	129.98	123.15
1	C	314	PRO	N-CA-C	5.25	120.14	114.68
1	F	330	VAL	N-CA-C	5.25	119.68	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	231	ALA	N-CA-CB	-5.25	101.59	110.41
1	I	330	VAL	N-CA-C	5.25	119.68	113.22
2	N	231	ALA	N-CA-CB	-5.25	101.59	110.41
2	O	231	ALA	N-CA-CB	-5.25	101.59	110.41
2	P	231	ALA	N-CA-CB	-5.25	101.59	110.41
2	T	68	GLY	CA-C-O	5.25	126.16	120.75
1	A	20	ARG	N-CA-C	5.25	118.11	109.72
1	E	404	ALA	N-CA-C	-5.25	105.75	113.72
1	F	404	ALA	N-CA-C	-5.25	105.75	113.72
2	T	231	ALA	N-CA-CB	-5.25	101.59	110.41
2	U	231	ALA	N-CA-CB	-5.25	101.60	110.41
2	V	231	ALA	N-CA-CB	-5.25	101.60	110.41
1	K	20	ARG	N-CA-C	5.25	118.11	109.72
2	M	267	ASN	O-C-N	5.25	129.45	122.95
2	U	267	ASN	O-C-N	5.25	129.45	122.95
1	L	20	ARG	N-CA-C	5.24	118.11	109.72
2	P	80	THR	CA-CB-OG1	-5.24	101.73	109.60
2	P	118	ASN	OD1-CG-ND2	5.24	127.84	122.60
2	Q	231	ALA	N-CA-CB	-5.24	101.60	110.41
2	S	114	SER	O-C-N	5.24	129.97	123.15
2	U	118	ASN	OD1-CG-ND2	5.24	127.84	122.60
2	M	231	ALA	N-CA-CB	-5.24	101.61	110.41
2	N	267	ASN	O-C-N	5.24	129.45	122.95
2	S	68	GLY	CA-C-O	5.24	126.15	120.75
2	W	267	ASN	O-C-N	5.24	129.45	122.95
1	C	43	PHE	N-CA-C	5.24	117.90	111.82
1	I	20	ARG	N-CA-C	5.24	118.10	109.72
2	M	118	ASN	OD1-CG-ND2	5.24	127.84	122.60
2	O	119	LYS	O-C-N	5.24	129.20	122.39
2	R	267	ASN	O-C-N	5.24	129.45	122.95
2	U	114	SER	O-C-N	5.24	129.96	123.15
2	U	119	LYS	O-C-N	5.24	129.20	122.39
2	T	114	SER	O-C-N	5.24	129.96	123.15
2	R	119	LYS	O-C-N	5.24	129.20	122.39
1	I	98	GLN	N-CA-C	5.23	117.99	111.24
1	G	43	PHE	N-CA-C	5.23	117.89	111.82
2	N	119	LYS	O-C-N	5.23	129.19	122.39
2	Q	114	SER	O-C-N	5.23	129.95	123.15
2	R	114	SER	O-C-N	5.23	129.95	123.15
2	T	267	ASN	O-C-N	5.23	129.44	122.95
2	R	231	ALA	N-CA-CB	-5.23	101.62	110.41
1	C	330	VAL	N-CA-C	5.23	119.65	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	267	ASN	O-C-N	5.23	129.43	122.95
2	N	68	GLY	CA-C-O	5.23	126.13	120.75
2	O	114	SER	O-C-N	5.23	129.95	123.15
2	Q	119	LYS	O-C-N	5.23	129.19	122.39
1	H	43	PHE	N-CA-C	5.22	117.88	111.82
2	Q	142	LYS	CA-C-N	5.22	132.62	121.18
2	Q	142	LYS	C-N-CA	5.22	132.62	121.18
2	S	267	ASN	O-C-N	5.22	129.43	122.95
1	A	43	PHE	N-CA-C	5.22	117.88	111.82
2	P	124	ASN	CB-CG-ND2	-5.22	108.57	116.40
1	D	98	GLN	N-CA-C	5.22	117.97	111.24
1	H	98	GLN	N-CA-C	5.22	117.97	111.24
1	J	20	ARG	N-CA-C	5.22	118.07	109.72
2	O	267	ASN	O-C-N	5.22	129.42	122.95
2	X	277	LYS	O-C-N	-5.22	116.59	122.12
2	P	119	LYS	O-C-N	5.22	129.17	122.39
2	X	119	LYS	O-C-N	5.22	129.17	122.39
1	D	43	PHE	N-CA-C	5.21	117.87	111.82
1	K	98	GLN	N-CA-C	5.21	117.97	111.24
1	L	330	VAL	N-CA-C	5.21	119.63	113.22
2	P	267	ASN	O-C-N	5.21	129.42	122.95
2	M	281	GLU	CB-CG-CD	-5.21	103.74	112.60
2	Q	314	ASP	CA-CB-CG	5.21	117.81	112.60
1	F	43	PHE	N-CA-C	5.21	117.86	111.82
1	J	43	PHE	N-CA-C	5.21	117.87	111.82
2	X	28	GLU	CG-CD-OE2	5.21	130.39	118.40
2	Q	124	ASN	CB-CG-ND2	-5.21	108.58	116.40
2	R	142	LYS	CA-C-N	5.21	132.59	121.18
2	R	142	LYS	C-N-CA	5.21	132.59	121.18
2	S	119	LYS	O-C-N	5.21	129.16	122.39
1	E	20	ARG	N-CA-C	5.21	118.05	109.72
2	M	142	LYS	CA-C-N	5.21	132.58	121.18
2	M	142	LYS	C-N-CA	5.21	132.58	121.18
2	N	28	GLU	CG-CD-OE2	5.21	130.38	118.40
2	U	142	LYS	CA-C-N	5.21	132.58	121.18
2	U	142	LYS	C-N-CA	5.21	132.58	121.18
2	V	119	LYS	O-C-N	5.21	129.16	122.39
2	W	314	ASP	CA-CB-CG	5.21	117.81	112.60
2	Q	277	LYS	O-C-N	-5.21	116.60	122.12
2	R	277	LYS	O-C-N	-5.21	116.60	122.12
2	S	277	LYS	O-C-N	-5.21	116.60	122.12
1	F	20	ARG	N-CA-C	5.20	118.05	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	98	GLN	N-CA-C	5.20	117.95	111.24
1	K	330	VAL	N-CA-C	5.20	119.62	113.22
2	N	281	GLU	CB-CG-CD	-5.20	103.75	112.60
2	P	142	LYS	CA-C-N	5.20	132.57	121.18
2	P	142	LYS	C-N-CA	5.20	132.57	121.18
1	B	98	GLN	N-CA-C	5.20	117.95	111.24
2	M	68	GLY	CA-C-O	5.20	126.11	120.75
2	M	124	ASN	CB-CG-ND2	-5.20	108.60	116.40
2	X	68	GLY	CA-C-O	5.20	126.11	120.75
1	L	98	GLN	N-CA-C	5.20	117.95	111.24
2	Q	28	GLU	CG-CD-OE2	5.20	130.36	118.40
2	T	124	ASN	CB-CG-ND2	-5.20	108.60	116.40
2	X	124	ASN	CB-CG-ND2	-5.20	108.60	116.40
2	X	281	GLU	CB-CG-CD	-5.20	103.76	112.60
1	J	330	VAL	N-CA-C	5.20	119.61	113.22
2	N	124	ASN	CB-CG-ND2	-5.20	108.60	116.40
2	O	68	GLY	CA-C-O	5.20	126.10	120.75
2	R	28	GLU	CG-CD-OE2	5.20	130.36	118.40
2	T	119	LYS	O-C-N	5.20	129.15	122.39
2	T	142	LYS	CA-C-N	5.20	132.56	121.18
2	T	142	LYS	C-N-CA	5.20	132.56	121.18
1	K	43	PHE	N-CA-C	5.20	117.85	111.82
2	O	281	GLU	CB-CG-CD	-5.20	103.77	112.60
2	T	281	GLU	CB-CG-CD	-5.20	103.77	112.60
2	T	314	ASP	CA-CB-CG	5.20	117.80	112.60
2	W	124	ASN	CB-CG-ND2	-5.20	108.61	116.40
2	T	28	GLU	CG-CD-OE2	5.19	130.35	118.40
2	W	142	LYS	CA-C-N	5.19	132.56	121.18
2	W	142	LYS	C-N-CA	5.19	132.56	121.18
1	B	330	VAL	N-CA-C	5.19	119.61	113.22
2	O	12	ASN	CA-C-O	5.19	127.05	121.55
2	P	28	GLU	CG-CD-OE2	5.19	130.34	118.40
2	P	258	PHE	N-CA-C	-5.19	101.50	109.76
2	P	281	GLU	CB-CG-CD	-5.19	103.77	112.60
2	V	142	LYS	CA-C-N	5.19	132.55	121.18
2	V	142	LYS	C-N-CA	5.19	132.55	121.18
2	X	267	ASN	O-C-N	5.19	129.39	122.95
2	X	314	ASP	CA-CB-CG	5.19	117.79	112.60
1	G	330	VAL	N-CA-C	5.19	119.61	113.22
2	V	28	GLU	CG-CD-OE2	5.19	130.34	118.40
2	V	281	GLU	CB-CG-CD	-5.19	103.78	112.60
2	V	314	ASP	CA-CB-CG	5.19	117.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	28	GLU	CG-CD-OE2	5.19	130.34	118.40
2	M	119	LYS	O-C-N	5.19	129.13	122.39
2	M	258	PHE	N-CA-C	-5.19	101.51	109.76
2	O	142	LYS	CA-C-N	5.19	132.54	121.18
2	O	142	LYS	C-N-CA	5.19	132.54	121.18
2	P	314	ASP	CA-CB-CG	5.19	117.79	112.60
2	R	281	GLU	CB-CG-CD	-5.19	103.78	112.60
2	S	124	ASN	CB-CG-ND2	-5.19	108.62	116.40
2	S	314	ASP	CA-CB-CG	5.19	117.79	112.60
1	A	330	VAL	N-CA-C	5.19	119.60	113.22
1	I	43	PHE	N-CA-C	5.19	117.84	111.82
2	M	28	GLU	CG-CD-OE2	5.19	130.33	118.40
2	U	124	ASN	CB-CG-ND2	-5.19	108.62	116.40
2	V	124	ASN	CB-CG-ND2	-5.19	108.62	116.40
2	X	142	LYS	CA-C-N	5.19	132.54	121.18
2	X	142	LYS	C-N-CA	5.19	132.54	121.18
2	R	258	PHE	N-CA-C	-5.18	101.52	109.76
2	S	281	GLU	CB-CG-CD	-5.18	103.78	112.60
2	O	28	GLU	CG-CD-OE2	5.18	130.32	118.40
2	Q	267	ASN	O-C-N	5.18	129.38	122.95
2	U	28	GLU	CG-CD-OE2	5.18	130.32	118.40
2	X	258	PHE	N-CA-C	-5.18	101.52	109.76
2	R	314	ASP	CA-CB-CG	5.18	117.78	112.60
1	J	98	GLN	N-CA-C	5.18	117.92	111.24
2	Q	281	GLU	CB-CG-CD	-5.18	103.80	112.60
2	S	142	LYS	CA-C-N	5.18	132.52	121.18
2	S	142	LYS	C-N-CA	5.18	132.52	121.18
2	U	258	PHE	N-CA-C	-5.18	101.52	109.76
2	W	258	PHE	N-CA-C	-5.18	101.53	109.76
1	H	330	VAL	N-CA-C	5.18	119.59	113.22
2	N	314	ASP	CA-CB-CG	5.18	117.78	112.60
2	O	102	LYS	CB-CA-C	-5.18	100.66	109.51
2	U	314	ASP	CA-CB-CG	5.18	117.78	112.60
2	X	259	VAL	O-C-N	-5.18	117.44	122.93
2	M	314	ASP	CA-CB-CG	5.17	117.77	112.60
2	N	142	LYS	CA-C-N	5.17	132.51	121.18
2	N	142	LYS	C-N-CA	5.17	132.51	121.18
2	R	12	ASN	CA-C-O	5.17	127.03	121.55
2	S	258	PHE	N-CA-C	-5.17	101.53	109.76
2	R	59	ILE	CB-CA-C	5.17	118.47	110.50
2	T	12	ASN	CA-C-O	5.17	127.03	121.55
2	W	198	LEU	O-C-N	5.17	127.60	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	281	GLU	CB-CG-CD	-5.17	103.81	112.60
1	K	388	PRO	CA-N-CD	-5.17	104.76	112.00
2	M	277	LYS	O-C-N	-5.17	116.64	122.12
2	Q	258	PHE	N-CA-C	-5.17	101.54	109.76
2	S	12	ASN	CA-C-O	5.17	127.03	121.55
2	T	258	PHE	N-CA-C	-5.17	101.54	109.76
2	T	259	VAL	O-C-N	-5.17	117.45	122.93
2	V	258	PHE	N-CA-C	-5.17	101.54	109.76
1	A	98	GLN	N-CA-C	5.17	117.91	111.24
1	L	388	PRO	CA-N-CD	-5.17	104.77	112.00
2	S	28	GLU	CG-CD-OE2	5.17	130.28	118.40
2	U	281	GLU	CB-CG-CD	-5.17	103.82	112.60
2	V	277	LYS	O-C-N	-5.17	116.64	122.12
2	M	59	ILE	CB-CA-C	5.16	118.45	110.50
2	M	198	LEU	O-C-N	5.16	127.59	122.12
2	N	277	LYS	O-C-N	-5.16	116.65	122.12
2	O	314	ASP	CA-CB-CG	5.16	117.76	112.60
2	R	124	ASN	CB-CG-ND2	-5.16	108.66	116.40
2	U	259	VAL	O-C-N	-5.16	117.46	122.93
2	P	259	VAL	O-C-N	-5.16	117.46	122.93
2	S	102	LYS	CB-CA-C	-5.16	100.69	109.51
2	R	242	TYR	N-CA-C	5.16	118.15	109.95
1	B	388	PRO	CA-N-CD	-5.16	104.78	112.00
2	N	12	ASN	CA-C-O	5.16	127.02	121.55
2	O	124	ASN	CB-CG-ND2	-5.16	108.67	116.40
2	O	277	LYS	O-C-N	-5.16	116.66	122.12
2	T	277	LYS	O-C-N	-5.16	116.66	122.12
1	E	388	PRO	CA-N-CD	-5.15	104.79	112.00
2	N	258	PHE	N-CA-C	-5.15	101.57	109.76
2	V	102	LYS	CB-CA-C	-5.15	100.70	109.51
1	F	388	PRO	CA-N-CD	-5.15	104.80	112.00
2	X	102	LYS	CB-CA-C	-5.15	100.71	109.51
1	C	98	GLN	N-CA-C	5.14	117.88	111.24
2	O	259	VAL	O-C-N	-5.14	117.48	122.93
2	Q	12	ASN	CA-C-O	5.14	127.00	121.55
2	T	175	LYS	CB-CA-C	5.14	122.77	111.09
2	M	12	ASN	CA-C-O	5.14	127.00	121.55
2	O	258	PHE	N-CA-C	-5.14	101.58	109.76
2	P	59	ILE	CB-CA-C	5.14	118.42	110.50
2	P	175	LYS	CB-CA-C	5.14	122.76	111.09
2	T	102	LYS	CB-CA-C	-5.14	100.72	109.51
2	U	102	LYS	CB-CA-C	-5.14	100.72	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	277	LYS	O-C-N	-5.14	116.67	122.12
2	V	259	VAL	O-C-N	-5.14	117.48	122.93
1	H	388	PRO	CA-N-CD	-5.14	104.80	112.00
1	I	388	PRO	CA-N-CD	-5.14	104.81	112.00
2	M	242	TYR	N-CA-C	5.14	118.12	109.95
2	N	242	TYR	N-CA-C	5.14	118.12	109.95
2	Q	175	LYS	CB-CA-C	5.14	122.76	111.09
2	V	12	ASN	CA-C-O	5.14	127.00	121.55
2	W	59	ILE	CB-CA-C	5.14	118.42	110.50
2	W	102	LYS	CB-CA-C	-5.14	100.72	109.51
1	J	388	PRO	CA-N-CD	-5.14	104.81	112.00
2	M	102	LYS	CB-CA-C	-5.14	100.72	109.51
2	P	12	ASN	CA-C-O	5.14	127.00	121.55
2	S	175	LYS	CB-CA-C	5.14	122.75	111.09
2	V	175	LYS	CB-CA-C	5.14	122.75	111.09
2	W	259	VAL	O-C-N	-5.14	117.48	122.93
1	J	90	ASP	N-CA-C	-5.14	102.18	110.14
2	Q	259	VAL	O-C-N	-5.14	117.49	122.93
2	T	242	TYR	N-CA-C	5.14	118.12	109.95
2	V	59	ILE	CB-CA-C	5.14	118.41	110.50
2	X	175	LYS	CB-CA-C	5.14	122.75	111.09
2	N	59	ILE	CB-CA-C	5.13	118.41	110.50
2	O	59	ILE	CB-CA-C	5.13	118.41	110.50
2	R	175	LYS	CB-CA-C	5.13	122.74	111.09
2	U	242	TYR	N-CA-C	5.13	118.11	109.95
2	X	198	LEU	O-C-N	5.13	127.56	122.12
2	M	175	LYS	CB-CA-C	5.13	122.74	111.09
2	Q	3	GLU	O-C-N	-5.13	115.76	122.59
2	R	102	LYS	CB-CA-C	-5.13	100.73	109.51
2	U	59	ILE	CB-CA-C	5.13	118.41	110.50
2	U	175	LYS	CB-CA-C	5.13	122.74	111.09
1	I	287	TYR	N-CA-C	5.13	117.91	110.42
2	M	287	ASP	CA-CB-CG	5.13	117.73	112.60
2	N	175	LYS	CB-CA-C	5.13	122.74	111.09
2	O	242	TYR	N-CA-C	5.13	118.11	109.95
1	F	287	TYR	N-CA-C	5.13	117.91	110.42
2	Q	102	LYS	CB-CA-C	-5.13	100.74	109.51
2	S	198	LEU	O-C-N	5.13	127.56	122.12
2	X	59	ILE	CB-CA-C	5.13	118.40	110.50
1	I	93	GLU	N-CA-C	-5.13	103.32	109.83
2	N	102	LYS	CB-CA-C	-5.13	100.74	109.51
2	N	198	LEU	O-C-N	5.13	127.56	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	3	GLU	O-C-N	-5.13	115.77	122.59
1	A	388	PRO	CA-N-CD	-5.13	104.82	112.00
1	C	388	PRO	CA-N-CD	-5.13	104.82	112.00
1	E	287	TYR	N-CA-C	5.13	117.90	110.42
1	I	90	ASP	N-CA-C	-5.13	102.19	110.14
2	O	198	LEU	O-C-N	5.13	127.55	122.12
2	V	242	TYR	N-CA-C	5.13	118.10	109.95
2	W	242	TYR	N-CA-C	5.13	118.10	109.95
2	O	175	LYS	CB-CA-C	5.12	122.72	111.09
2	Q	242	TYR	N-CA-C	5.12	118.10	109.95
2	R	259	VAL	O-C-N	-5.12	117.50	122.93
1	B	90	ASP	N-CA-C	-5.12	102.20	110.14
1	G	287	TYR	N-CA-C	5.12	117.90	110.42
2	V	198	LEU	O-C-N	5.12	127.55	122.12
2	W	277	LYS	O-C-N	-5.12	116.69	122.12
1	E	90	ASP	N-CA-C	-5.12	102.21	110.14
1	G	388	PRO	CA-N-CD	-5.12	104.83	112.00
2	O	57	PRO	O-C-N	-5.12	116.90	123.14
2	P	102	LYS	CB-CA-C	-5.12	100.76	109.51
2	P	135	LEU	N-CA-CB	-5.12	102.60	110.12
2	P	198	LEU	O-C-N	5.12	127.55	122.12
2	S	59	ILE	CB-CA-C	5.12	118.38	110.50
2	T	59	ILE	CB-CA-C	5.12	118.38	110.50
2	T	198	LEU	O-C-N	5.12	127.55	122.12
2	W	12	ASN	CA-C-O	5.12	126.97	121.55
2	X	242	TYR	N-CA-C	5.12	118.09	109.95
2	X	287	ASP	CA-CB-CG	5.12	117.72	112.60
2	M	352	SER	CA-C-N	5.12	130.93	120.80
2	M	352	SER	C-N-CA	5.12	130.93	120.80
2	R	22	GLU	CA-C-O	5.12	125.88	120.10
2	S	259	VAL	O-C-N	-5.12	117.51	122.93
2	T	135	LEU	N-CA-CB	-5.12	102.60	110.12
1	K	287	TYR	N-CA-C	5.12	117.89	110.42
2	Q	59	ILE	CB-CA-C	5.12	118.38	110.50
2	V	3	GLU	O-C-N	-5.12	115.79	122.59
1	C	93	GLU	N-CA-C	-5.11	103.34	109.83
1	F	93	GLU	N-CA-C	-5.11	103.33	109.83
1	H	90	ASP	N-CA-C	-5.11	102.22	110.14
1	K	90	ASP	N-CA-C	-5.11	102.21	110.14
2	S	287	ASP	CA-CB-CG	5.11	117.71	112.60
2	S	352	SER	CA-C-N	5.11	130.93	120.80
2	S	352	SER	C-N-CA	5.11	130.93	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	175	LYS	CB-CA-C	5.11	122.70	111.09
1	D	388	PRO	CA-N-CD	-5.11	104.84	112.00
2	P	3	GLU	O-C-N	-5.11	115.79	122.59
2	R	3	GLU	O-C-N	-5.11	115.79	122.59
2	S	242	TYR	N-CA-C	5.11	118.08	109.95
2	O	116	ILE	CA-C-N	-5.11	114.57	122.59
2	O	116	ILE	C-N-CA	-5.11	114.57	122.59
2	P	242	TYR	N-CA-C	5.11	118.08	109.95
1	B	287	TYR	N-CA-C	5.11	117.88	110.42
1	G	90	ASP	N-CA-C	-5.11	102.22	110.14
1	L	287	TYR	N-CA-C	5.11	117.88	110.42
2	U	12	ASN	CA-C-O	5.11	126.96	121.55
2	M	116	ILE	CA-C-N	-5.11	114.58	122.59
2	M	116	ILE	C-N-CA	-5.11	114.58	122.59
2	M	22	GLU	CA-C-O	5.10	125.87	120.10
2	R	57	PRO	O-C-N	-5.10	116.91	123.14
2	R	116	ILE	CA-C-N	-5.10	114.58	122.59
2	R	116	ILE	C-N-CA	-5.10	114.58	122.59
2	W	22	GLU	CA-C-O	5.10	125.87	120.10
2	M	135	LEU	N-CA-CB	-5.10	102.62	110.12
2	P	277	LYS	O-C-N	-5.10	116.71	122.12
2	T	57	PRO	O-C-N	-5.10	116.92	123.14
1	C	90	ASP	N-CA-C	-5.10	102.23	110.14
2	U	22	GLU	CA-C-O	5.10	125.86	120.10
2	U	318	ALA	CA-C-O	5.10	125.96	120.55
2	V	287	ASP	CA-CB-CG	5.10	117.70	112.60
1	F	90	ASP	N-CA-C	-5.10	102.24	110.14
1	J	287	TYR	N-CA-C	5.10	117.86	110.42
2	M	3	GLU	O-C-N	-5.10	115.81	122.59
2	N	135	LEU	N-CA-CB	-5.10	102.62	110.12
2	Q	198	LEU	O-C-N	5.10	127.53	122.12
2	S	3	GLU	O-C-N	-5.10	115.81	122.59
2	S	135	LEU	N-CA-CB	-5.10	102.62	110.12
2	T	22	GLU	CA-C-O	5.10	125.86	120.10
2	U	316	ARG	O-C-N	5.10	127.32	122.07
1	A	90	ASP	N-CA-C	-5.10	102.24	110.14
1	D	90	ASP	N-CA-C	-5.10	102.24	110.14
2	N	259	VAL	O-C-N	-5.10	117.53	122.93
2	T	352	SER	CA-C-N	5.10	130.89	120.80
2	T	352	SER	C-N-CA	5.10	130.89	120.80
2	U	352	SER	CA-C-N	5.10	130.89	120.80
2	U	352	SER	C-N-CA	5.10	130.89	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	135	LEU	N-CA-CB	-5.10	102.63	110.12
2	V	352	SER	CA-C-N	5.10	130.89	120.80
2	V	352	SER	C-N-CA	5.10	130.89	120.80
2	X	116	ILE	CA-C-N	-5.10	114.59	122.59
2	X	116	ILE	C-N-CA	-5.10	114.59	122.59
1	L	90	ASP	N-CA-C	-5.10	102.24	110.14
2	U	3	GLU	O-C-N	-5.10	115.81	122.59
2	P	116	ILE	CA-C-N	-5.09	114.59	122.59
2	P	116	ILE	C-N-CA	-5.09	114.59	122.59
2	P	314	ASP	O-C-N	5.09	125.92	121.18
2	R	287	ASP	CA-CB-CG	5.09	117.69	112.60
2	T	287	ASP	CA-CB-CG	5.09	117.69	112.60
2	U	57	PRO	O-C-N	-5.09	116.93	123.14
2	X	3	GLU	O-C-N	-5.09	115.81	122.59
1	G	93	GLU	N-CA-C	-5.09	103.36	109.83
2	X	135	LEU	N-CA-CB	-5.09	102.63	110.12
1	E	93	GLU	N-CA-C	-5.09	103.36	109.83
1	H	93	GLU	N-CA-C	-5.09	103.36	109.83
1	J	93	GLU	N-CA-C	-5.09	103.36	109.83
2	M	259	VAL	O-C-N	-5.09	117.53	122.93
2	N	116	ILE	CA-C-N	-5.09	114.60	122.59
2	N	116	ILE	C-N-CA	-5.09	114.60	122.59
2	N	287	ASP	CA-CB-CG	5.09	117.69	112.60
2	P	287	ASP	CA-CB-CG	5.09	117.69	112.60
2	Q	135	LEU	N-CA-CB	-5.09	102.64	110.12
2	U	287	ASP	CA-CB-CG	5.09	117.69	112.60
2	W	135	LEU	N-CA-CB	-5.09	102.64	110.12
2	X	12	ASN	CA-C-O	5.09	126.95	121.55
2	U	116	ILE	CA-C-N	-5.09	114.60	122.59
2	U	116	ILE	C-N-CA	-5.09	114.60	122.59
2	V	116	ILE	CA-C-N	-5.09	114.60	122.59
2	V	116	ILE	C-N-CA	-5.09	114.60	122.59
2	X	352	SER	CA-C-N	5.09	130.88	120.80
2	X	352	SER	C-N-CA	5.09	130.88	120.80
2	Q	352	SER	CA-C-N	5.09	130.87	120.80
2	Q	352	SER	C-N-CA	5.09	130.87	120.80
2	U	135	LEU	N-CA-CB	-5.09	102.64	110.12
2	V	22	GLU	CA-C-O	5.09	125.85	120.10
2	N	352	SER	CA-C-N	5.09	130.87	120.80
2	N	352	SER	C-N-CA	5.09	130.87	120.80
2	O	22	GLU	CA-C-O	5.09	125.85	120.10
2	S	53	THR	N-CA-CB	5.09	118.29	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	92	PHE	N-CA-C	-5.09	106.17	112.38
2	V	57	PRO	O-C-N	-5.09	116.93	123.14
2	W	116	ILE	CA-C-N	-5.09	114.60	122.59
2	W	116	ILE	C-N-CA	-5.09	114.60	122.59
1	A	287	TYR	N-CA-C	5.08	117.84	110.42
1	D	287	TYR	N-CA-C	5.08	117.84	110.42
2	Q	287	ASP	CA-CB-CG	5.08	117.68	112.60
2	R	135	LEU	N-CA-CB	-5.08	102.65	110.12
2	S	57	PRO	O-C-N	-5.08	116.94	123.14
2	T	3	GLU	O-C-N	-5.08	115.83	122.59
2	W	3	GLU	O-C-N	-5.08	115.83	122.59
2	X	22	GLU	CA-C-O	5.08	125.84	120.10
1	K	93	GLU	N-CA-C	-5.08	103.38	109.83
2	P	352	SER	CA-C-N	5.08	130.86	120.80
2	P	352	SER	C-N-CA	5.08	130.86	120.80
2	R	300	GLY	N-CA-C	-5.08	101.14	113.18
2	R	352	SER	CA-C-N	5.08	130.86	120.80
2	R	352	SER	C-N-CA	5.08	130.86	120.80
2	S	300	GLY	N-CA-C	-5.08	101.14	113.18
1	A	93	GLU	N-CA-C	-5.08	103.38	109.83
2	P	22	GLU	CA-C-O	5.08	125.84	120.10
2	S	116	ILE	CA-C-N	-5.08	114.61	122.59
2	S	116	ILE	C-N-CA	-5.08	114.61	122.59
2	N	3	GLU	O-C-N	-5.08	115.84	122.59
2	O	135	LEU	N-CA-CB	-5.08	102.65	110.12
2	O	287	ASP	CA-CB-CG	5.08	117.68	112.60
2	O	316	ARG	O-C-N	5.08	127.30	122.07
2	O	352	SER	CA-C-N	5.08	130.86	120.80
2	O	352	SER	C-N-CA	5.08	130.86	120.80
2	Q	57	PRO	O-C-N	-5.08	116.94	123.14
2	U	198	LEU	O-C-N	5.08	127.50	122.12
2	W	57	PRO	O-C-N	-5.08	116.95	123.14
2	N	6	LYS	CA-C-N	5.08	130.56	122.74
2	N	6	LYS	C-N-CA	5.08	130.56	122.74
2	R	318	ALA	CA-C-O	5.08	125.93	120.55
2	T	324	ALA	CA-C-N	5.08	127.59	120.28
2	T	324	ALA	C-N-CA	5.08	127.59	120.28
1	H	287	TYR	N-CA-C	5.07	117.83	110.42
2	M	314	ASP	O-C-N	5.07	125.90	121.18
2	M	344	ARG	NE-CZ-NH2	5.07	123.77	119.20
2	N	57	PRO	O-C-N	-5.07	116.95	123.14
2	Q	324	ALA	CA-C-N	5.07	127.59	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	324	ALA	C-N-CA	5.07	127.59	120.28
2	S	22	GLU	CA-C-O	5.07	125.83	120.10
2	U	300	GLY	N-CA-C	-5.07	101.16	113.18
2	W	287	ASP	CA-CB-CG	5.07	117.67	112.60
2	X	57	PRO	O-C-N	-5.07	116.95	123.14
2	X	98	ARG	CA-CB-CG	5.07	124.25	114.10
2	T	116	ILE	CA-C-N	-5.07	114.63	122.59
2	T	116	ILE	C-N-CA	-5.07	114.63	122.59
2	W	352	SER	CA-C-N	5.07	130.84	120.80
2	W	352	SER	C-N-CA	5.07	130.84	120.80
1	B	93	GLU	N-CA-C	-5.07	103.39	109.83
2	N	314	ASP	O-C-N	5.07	125.90	121.18
2	U	53	THR	N-CA-CB	5.07	118.27	110.46
2	Q	116	ILE	CA-C-N	-5.07	114.63	122.59
2	Q	116	ILE	C-N-CA	-5.07	114.63	122.59
2	Q	300	GLY	N-CA-C	-5.07	101.17	113.18
2	R	316	ARG	O-C-N	5.07	127.29	122.07
1	D	93	GLU	N-CA-C	-5.07	103.39	109.83
1	E	403	GLU	N-CA-C	-5.07	107.60	112.97
1	L	93	GLU	N-CA-C	-5.07	103.39	109.83
2	M	300	GLY	N-CA-C	-5.07	101.17	113.18
2	N	182	GLY	O-C-N	5.07	129.29	122.70
2	T	300	GLY	N-CA-C	-5.07	101.17	113.18
2	V	316	ARG	O-C-N	5.07	127.29	122.07
2	W	300	GLY	N-CA-C	-5.07	101.17	113.18
1	C	287	TYR	N-CA-C	5.07	117.82	110.42
2	N	22	GLU	CA-C-O	5.07	125.83	120.10
2	P	6	LYS	CA-C-N	5.07	130.54	122.74
2	P	6	LYS	C-N-CA	5.07	130.54	122.74
2	P	57	PRO	O-C-N	-5.07	116.96	123.14
2	R	198	LEU	O-C-N	5.07	127.49	122.12
2	V	300	GLY	N-CA-C	-5.07	101.17	113.18
2	M	53	THR	N-CA-CB	5.06	118.26	110.46
2	Q	316	ARG	O-C-N	5.06	127.29	122.07
2	T	92	PHE	N-CA-C	-5.06	106.20	112.38
2	P	182	GLY	O-C-N	5.06	129.28	122.70
2	M	324	ALA	CA-C-N	5.06	127.57	120.28
2	M	324	ALA	C-N-CA	5.06	127.57	120.28
2	Q	53	THR	N-CA-CB	5.06	118.25	110.46
2	X	92	PHE	N-CA-C	-5.06	106.20	112.38
2	X	300	GLY	N-CA-C	-5.06	101.19	113.18
2	N	300	GLY	N-CA-C	-5.06	101.19	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	53	THR	N-CA-CB	5.06	118.25	110.46
2	M	98	ARG	CA-CB-CG	5.06	124.22	114.10
2	M	163	ALA	N-CA-C	5.06	117.18	111.11
2	N	53	THR	N-CA-CB	5.06	118.25	110.46
2	O	53	THR	N-CA-CB	5.06	118.25	110.46
2	O	318	ALA	CA-C-O	5.06	125.91	120.55
2	O	324	ALA	CA-C-N	5.06	127.56	120.28
2	O	324	ALA	C-N-CA	5.06	127.56	120.28
2	P	300	GLY	N-CA-C	-5.06	101.20	113.18
2	X	318	ALA	CA-C-O	5.06	125.91	120.55
2	R	53	THR	N-CA-CB	5.06	118.25	110.46
2	M	57	PRO	O-C-N	-5.05	116.97	123.14
2	M	316	ARG	O-C-N	5.05	127.28	122.07
2	N	318	ALA	CA-C-O	5.05	125.91	120.55
2	O	6	LYS	CA-C-N	5.05	130.53	122.74
2	O	6	LYS	C-N-CA	5.05	130.53	122.74
2	U	163	ALA	N-CA-C	5.05	117.18	111.11
2	V	318	ALA	CA-C-O	5.05	125.91	120.55
2	W	6	LYS	CA-C-N	5.05	130.52	122.74
2	W	6	LYS	C-N-CA	5.05	130.52	122.74
2	X	6	LYS	CA-C-N	5.05	130.53	122.74
2	X	6	LYS	C-N-CA	5.05	130.53	122.74
2	X	182	GLY	O-C-N	5.05	129.27	122.70
2	M	318	ALA	CA-C-O	5.05	125.91	120.55
2	N	324	ALA	CA-C-N	5.05	127.56	120.28
2	N	324	ALA	C-N-CA	5.05	127.56	120.28
2	W	324	ALA	CA-C-N	5.05	127.56	120.28
2	W	324	ALA	C-N-CA	5.05	127.56	120.28
2	X	314	ASP	O-C-N	5.05	125.88	121.18
2	N	239	LYS	CD-CE-NZ	5.05	128.06	111.90
2	O	73	SER	CA-C-N	5.05	131.37	121.06
2	O	73	SER	C-N-CA	5.05	131.37	121.06
2	R	92	PHE	N-CA-C	-5.05	106.22	112.38
2	R	98	ARG	CA-CB-CG	5.05	124.20	114.10
2	T	6	LYS	CA-C-N	5.05	130.52	122.74
2	T	6	LYS	C-N-CA	5.05	130.52	122.74
2	W	318	ALA	CA-C-O	5.05	125.91	120.55
2	O	300	GLY	N-CA-C	-5.05	101.21	113.18
2	P	163	ALA	N-CA-C	5.05	117.17	111.11
2	T	53	THR	N-CA-CB	5.05	118.24	110.46
2	U	314	ASP	O-C-N	5.05	125.88	121.18
2	U	324	ALA	CA-C-N	5.05	127.55	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	324	ALA	C-N-CA	5.05	127.55	120.28
2	V	53	THR	N-CA-CB	5.05	118.24	110.46
2	W	92	PHE	N-CA-C	-5.05	106.22	112.38
2	X	316	ARG	O-C-N	5.05	127.27	122.07
2	O	92	PHE	N-CA-C	-5.05	106.22	112.38
2	O	163	ALA	N-CA-C	5.05	117.17	111.11
2	Q	92	PHE	N-CA-C	-5.05	106.22	112.38
2	Q	267	ASN	CA-CB-CG	5.05	117.65	112.60
2	R	163	ALA	N-CA-C	5.05	117.17	111.11
2	T	318	ALA	CA-C-O	5.05	125.90	120.55
2	U	92	PHE	N-CA-C	-5.05	106.22	112.38
2	U	98	ARG	CA-CB-CG	5.05	124.19	114.10
2	V	6	LYS	CA-C-N	5.05	130.51	122.74
2	V	6	LYS	C-N-CA	5.05	130.51	122.74
2	V	98	ARG	CA-CB-CG	5.05	124.19	114.10
2	W	98	ARG	CA-CB-CG	5.05	124.19	114.10
2	T	316	ARG	O-C-N	5.04	127.27	122.07
2	V	324	ALA	CA-C-N	5.04	127.54	120.28
2	V	324	ALA	C-N-CA	5.04	127.54	120.28
2	O	98	ARG	CA-CB-CG	5.04	124.19	114.10
2	P	316	ARG	O-C-N	5.04	127.26	122.07
2	R	6	LYS	CA-C-N	5.04	130.51	122.74
2	R	6	LYS	C-N-CA	5.04	130.51	122.74
2	S	6	LYS	CA-C-N	5.04	130.51	122.74
2	S	6	LYS	C-N-CA	5.04	130.51	122.74
2	U	6	LYS	CA-C-O	-5.04	115.64	121.49
2	O	182	GLY	O-C-N	5.04	129.25	122.70
2	P	267	ASN	CA-CB-CG	5.04	117.64	112.60
2	Q	314	ASP	O-C-N	5.04	125.87	121.18
2	V	92	PHE	N-CA-C	-5.04	106.23	112.38
2	U	6	LYS	CA-C-N	5.04	130.50	122.74
2	U	6	LYS	C-N-CA	5.04	130.50	122.74
2	X	359	GLU	CB-CA-C	-5.04	102.97	110.88
2	N	316	ARG	O-C-N	5.04	127.26	122.07
2	Q	22	GLU	CA-C-O	5.04	125.79	120.10
2	S	316	ARG	O-C-N	5.04	127.26	122.07
2	T	98	ARG	CA-CB-CG	5.04	124.18	114.10
2	W	163	ALA	N-CA-C	5.04	117.16	111.11
2	X	324	ALA	CA-C-N	5.04	127.54	120.28
2	X	324	ALA	C-N-CA	5.04	127.54	120.28
2	P	92	PHE	N-CA-C	-5.04	106.23	112.38
2	M	6	LYS	CA-C-N	5.04	130.50	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	6	LYS	C-N-CA	5.04	130.50	122.74
2	N	295	LYS	CA-CB-CG	5.04	124.17	114.10
2	P	324	ALA	CA-C-N	5.04	127.53	120.28
2	P	324	ALA	C-N-CA	5.04	127.53	120.28
2	T	247	LEU	CA-C-O	5.04	126.38	120.69
2	U	73	SER	CA-C-N	5.04	131.33	121.06
2	U	73	SER	C-N-CA	5.04	131.33	121.06
2	U	239	LYS	CD-CE-NZ	5.04	128.02	111.90
2	V	163	ALA	N-CA-C	5.04	117.15	111.11
2	N	73	SER	CA-C-N	5.03	131.33	121.06
2	N	73	SER	C-N-CA	5.03	131.33	121.06
2	N	98	ARG	CA-CB-CG	5.03	124.17	114.10
2	P	98	ARG	CA-CB-CG	5.03	124.17	114.10
2	Q	6	LYS	CA-C-N	5.03	130.49	122.74
2	Q	6	LYS	C-N-CA	5.03	130.49	122.74
2	Q	98	ARG	CA-CB-CG	5.03	124.17	114.10
2	M	92	PHE	N-CA-C	-5.03	106.24	112.38
2	R	239	LYS	CD-CE-NZ	5.03	128.00	111.90
2	T	314	ASP	O-C-N	5.03	125.86	121.18
2	V	182	GLY	O-C-N	5.03	129.24	122.70
2	X	239	LYS	CD-CE-NZ	5.03	128.00	111.90
2	N	92	PHE	N-CA-C	-5.03	106.24	112.38
2	O	239	LYS	CD-CE-NZ	5.03	128.00	111.90
2	P	239	LYS	CD-CE-NZ	5.03	128.00	111.90
2	P	251	LYS	N-CA-C	-5.03	105.80	112.24
2	S	324	ALA	CA-C-N	5.03	127.52	120.28
2	S	324	ALA	C-N-CA	5.03	127.52	120.28
2	U	359	GLU	CB-CA-C	-5.03	102.98	110.88
2	V	239	LYS	CD-CE-NZ	5.03	128.00	111.90
2	W	359	GLU	CB-CA-C	-5.03	102.98	110.88
2	T	163	ALA	N-CA-C	5.03	117.14	111.11
2	T	182	GLY	O-C-N	5.03	129.24	122.70
2	T	239	LYS	CD-CE-NZ	5.03	127.99	111.90
2	U	247	LEU	CA-C-O	5.03	126.37	120.69
2	Q	251	LYS	N-CA-C	-5.03	105.80	112.24
2	S	239	LYS	CD-CE-NZ	5.03	127.99	111.90
2	U	182	GLY	O-C-N	5.03	129.24	122.70
2	V	314	ASP	O-C-N	5.03	125.86	121.18
2	M	239	LYS	CD-CE-NZ	5.03	127.98	111.90
2	N	163	ALA	N-CA-C	5.03	117.14	111.11
2	Q	239	LYS	CD-CE-NZ	5.03	127.98	111.90
2	R	73	SER	CA-C-N	5.03	131.31	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	73	SER	C-N-CA	5.03	131.31	121.06
2	T	359	GLU	CB-CA-C	-5.03	102.99	110.88
2	X	53	THR	N-CA-CB	5.03	118.20	110.46
2	R	324	ALA	CA-C-N	5.02	127.52	120.28
2	R	324	ALA	C-N-CA	5.02	127.52	120.28
2	S	182	GLY	O-C-N	5.02	129.23	122.70
2	S	359	GLU	CB-CA-C	-5.02	102.99	110.88
2	O	314	ASP	O-C-N	5.02	125.85	121.18
2	Q	73	SER	CA-C-N	5.02	131.31	121.06
2	Q	73	SER	C-N-CA	5.02	131.31	121.06
2	S	251	LYS	N-CA-C	-5.02	105.81	112.24
2	X	163	ALA	N-CA-C	5.02	117.14	111.11
2	P	318	ALA	CA-C-O	5.02	125.87	120.55
2	P	359	GLU	CB-CA-C	-5.02	103.00	110.88
2	U	267	ASN	CA-CB-CG	5.02	117.62	112.60
2	W	73	SER	CA-C-N	5.02	131.30	121.06
2	W	73	SER	C-N-CA	5.02	131.30	121.06
2	N	359	GLU	CB-CA-C	-5.02	103.00	110.88
2	Q	163	ALA	N-CA-C	5.02	117.13	111.11
2	S	98	ARG	CA-CB-CG	5.02	124.14	114.10
2	S	163	ALA	N-CA-C	5.02	117.13	111.11
2	V	73	SER	CA-C-N	5.02	131.30	121.06
2	V	73	SER	C-N-CA	5.02	131.30	121.06
2	V	359	GLU	CB-CA-C	-5.02	103.00	110.88
2	W	53	THR	N-CA-CB	5.02	118.19	110.46
2	N	247	LEU	CA-C-O	5.02	126.36	120.69
2	Q	182	GLY	O-C-N	5.02	129.22	122.70
2	Q	318	ALA	CA-C-O	5.02	125.87	120.55
2	W	239	LYS	CD-CE-NZ	5.02	127.95	111.90
1	G	403	GLU	N-CA-C	-5.02	107.65	112.97
2	M	73	SER	CA-C-N	5.02	131.29	121.06
2	M	73	SER	C-N-CA	5.02	131.29	121.06
2	O	247	LEU	CA-C-O	5.02	126.36	120.69
2	P	95	ASP	CA-CB-CG	5.02	117.62	112.60
2	T	95	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	403	GLU	N-CA-C	-5.01	107.66	112.97
2	M	6	LYS	CA-C-O	-5.01	115.67	121.49
2	M	182	GLY	O-C-N	5.01	129.22	122.70
2	N	267	ASN	CA-CB-CG	5.01	117.61	112.60
2	O	344	ARG	NE-CZ-NH2	5.01	123.71	119.20
2	P	344	ARG	NE-CZ-NH2	5.01	123.71	119.20
2	R	12	ASN	CA-CB-CG	-5.01	107.58	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	182	GLY	O-C-N	5.01	129.22	122.70
2	X	73	SER	CA-C-N	5.01	131.29	121.06
2	X	73	SER	C-N-CA	5.01	131.29	121.06
2	M	359	GLU	CB-CA-C	-5.01	103.01	110.88
2	S	314	ASP	O-C-N	5.01	125.84	121.18
2	T	344	ARG	NE-CZ-NH2	5.01	123.71	119.20
2	W	267	ASN	CA-CB-CG	5.01	117.61	112.60
2	X	6	LYS	CA-C-O	-5.01	115.68	121.49
1	H	403	GLU	N-CA-C	-5.01	107.66	112.97
2	Q	6	LYS	CA-C-O	-5.01	115.68	121.49
2	R	359	GLU	CB-CA-C	-5.01	103.01	110.88
2	X	247	LEU	CA-C-O	5.01	126.35	120.69
2	X	267	ASN	CA-CB-CG	5.01	117.61	112.60
2	P	73	SER	CA-C-N	5.01	131.28	121.06
2	P	73	SER	C-N-CA	5.01	131.28	121.06
2	Q	95	ASP	CA-CB-CG	5.01	117.61	112.60
2	R	95	ASP	CA-CB-CG	5.01	117.61	112.60
2	T	295	LYS	CA-CB-CG	5.01	124.12	114.10
2	W	12	ASN	CA-CB-CG	-5.01	107.59	112.60
1	F	403	GLU	N-CA-C	-5.01	107.66	112.97
2	M	270	SER	CB-CA-C	-5.01	101.81	108.87
2	O	6	LYS	CA-C-O	-5.01	115.68	121.49
2	Q	359	GLU	CB-CA-C	-5.01	103.02	110.88
2	S	267	ASN	CA-CB-CG	5.01	117.61	112.60
2	S	318	ALA	CA-C-O	5.01	125.86	120.55
2	W	316	ARG	O-C-N	5.01	127.23	122.07
2	V	267	ASN	CA-CB-CG	5.00	117.61	112.60
2	W	95	ASP	CA-CB-CG	5.00	117.61	112.60
2	X	344	ARG	NE-CZ-NH2	5.00	123.70	119.20
2	N	6	LYS	CA-C-O	-5.00	115.69	121.49
2	N	59	ILE	CA-C-N	5.00	129.69	123.14
2	N	59	ILE	C-N-CA	5.00	129.69	123.14
2	P	6	LYS	CA-C-O	-5.00	115.69	121.49
2	P	270	SER	CB-CA-C	-5.00	101.81	108.87
2	Q	270	SER	CB-CA-C	-5.00	101.82	108.87
2	R	267	ASN	CA-CB-CG	5.00	117.60	112.60
2	S	6	LYS	CA-C-O	-5.00	115.69	121.49
2	U	270	SER	CB-CA-C	-5.00	101.81	108.87
2	U	344	ARG	NE-CZ-NH2	5.00	123.70	119.20
2	V	344	ARG	NE-CZ-NH2	5.00	123.70	119.20
2	W	344	ARG	NE-CZ-NH2	5.00	123.70	119.20
2	T	73	SER	CA-C-N	5.00	131.26	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	73	SER	C-N-CA	5.00	131.26	121.06
2	T	270	SER	CB-CA-C	-5.00	101.82	108.87
2	V	270	SER	CB-CA-C	-5.00	101.82	108.87
2	V	295	LYS	CA-CB-CG	5.00	124.10	114.10
2	W	295	LYS	CA-CB-CG	5.00	124.10	114.10
2	X	295	LYS	CA-CB-CG	5.00	124.10	114.10

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	312	ALA	Peptide
2	M	354	ARG	Sidechain
2	N	312	ALA	Peptide
2	N	354	ARG	Sidechain
2	O	312	ALA	Peptide
2	O	354	ARG	Sidechain
2	P	312	ALA	Peptide
2	P	354	ARG	Sidechain
2	Q	312	ALA	Peptide
2	Q	354	ARG	Sidechain
2	R	312	ALA	Peptide
2	R	354	ARG	Sidechain
2	S	312	ALA	Peptide
2	S	354	ARG	Sidechain
2	T	312	ALA	Peptide
2	T	354	ARG	Sidechain
2	U	312	ALA	Peptide
2	U	354	ARG	Sidechain
2	V	312	ALA	Peptide
2	V	354	ARG	Sidechain
2	W	312	ALA	Peptide
2	W	354	ARG	Sidechain
2	X	312	ALA	Peptide
2	X	354	ARG	Sidechain

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3626	0	3531	193	0
1	B	3626	0	3531	188	0
1	C	3626	0	3531	189	0
1	D	3626	0	3531	198	0
1	E	3626	0	3531	187	0
1	F	3626	0	3531	196	0
1	G	3626	0	3531	192	0
1	H	3626	0	3531	193	0
1	I	3626	0	3531	193	0
1	J	3626	0	3531	195	0
1	K	3626	0	3531	189	0
1	L	3626	0	3531	193	0
2	M	2861	0	2827	151	0
2	N	2861	0	2827	158	0
2	O	2861	0	2827	156	0
2	P	2861	0	2827	162	0
2	Q	2861	0	2827	155	0
2	R	2861	0	2827	153	0
2	S	2861	0	2827	156	0
2	T	2861	0	2827	154	0
2	U	2861	0	2827	160	0
2	V	2861	0	2827	157	0
2	W	2861	0	2827	158	0
2	X	2861	0	2827	152	0
3	Y	23	0	20	0	0
3	Z	23	0	20	0	0
3	a	23	0	20	0	0
3	b	23	0	20	0	0
3	c	23	0	20	0	0
3	d	23	0	20	0	0
3	e	23	0	20	0	0
3	f	23	0	20	0	0
3	g	23	0	20	0	0
3	h	23	0	20	0	0
3	i	23	0	20	0	0
3	j	23	0	20	0	0
All	All	78120	0	76536	3464	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (3464) 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:K:43:PHE:HB3	2:W:370:LYS:CE	1.36	1.55
1:B:43:PHE:HB3	2:N:370:LYS:CE	1.36	1.55
1:L:43:PHE:HB3	2:X:370:LYS:CE	1.36	1.54
1:A:43:PHE:HB3	2:M:370:LYS:CE	1.36	1.54
2:P:369:THR:C	2:P:370:LYS:N	1.68	1.52
2:U:369:THR:C	2:U:370:LYS:N	1.67	1.52
2:Q:369:THR:C	2:Q:370:LYS:N	1.68	1.51
1:E:43:PHE:HB3	2:Q:370:LYS:CE	1.36	1.51
2:T:369:THR:C	2:T:370:LYS:N	1.68	1.51
1:J:43:PHE:HB3	2:V:370:LYS:CE	1.36	1.51
1:C:43:PHE:HB3	2:O:370:LYS:CE	1.36	1.51
2:O:369:THR:C	2:O:370:LYS:N	1.68	1.51
1:H:43:PHE:HB3	2:T:370:LYS:CE	1.36	1.50
1:D:43:PHE:HB3	2:P:370:LYS:CE	1.36	1.50
2:V:369:THR:C	2:V:370:LYS:N	1.67	1.50
1:I:43:PHE:HB3	2:U:370:LYS:CE	1.36	1.50
1:G:43:PHE:HB3	2:S:370:LYS:CE	1.36	1.49
2:N:369:THR:C	2:N:370:LYS:N	1.67	1.49
2:W:369:THR:C	2:W:370:LYS:N	1.67	1.49
2:S:369:THR:C	2:S:370:LYS:N	1.67	1.48
1:F:43:PHE:HB3	2:R:370:LYS:CE	1.36	1.48
2:R:369:THR:C	2:R:370:LYS:N	1.67	1.47
1:B:4:HIS:C	2:N:179:LYS:HZ3	1.21	1.47
1:C:4:HIS:C	2:O:179:LYS:HZ3	1.20	1.47
1:D:43:PHE:CB	2:P:370:LYS:HE2	1.44	1.47
1:L:4:HIS:C	2:X:179:LYS:HZ3	1.22	1.47
2:X:369:THR:C	2:X:370:LYS:N	1.67	1.47
1:I:43:PHE:CB	2:U:370:LYS:HE2	1.45	1.47
1:J:4:HIS:C	2:V:179:LYS:HZ3	1.20	1.47
1:K:4:HIS:C	2:W:179:LYS:HZ3	1.21	1.47
1:A:4:HIS:C	2:M:179:LYS:HZ3	1.23	1.46
1:C:43:PHE:CB	2:O:370:LYS:HE2	1.45	1.46
1:H:4:HIS:C	2:T:179:LYS:HZ3	1.20	1.46
1:J:43:PHE:CB	2:V:370:LYS:HE2	1.45	1.46
2:M:369:THR:C	2:M:370:LYS:N	1.68	1.46
1:E:4:HIS:C	2:Q:179:LYS:HZ3	1.20	1.45
1:E:43:PHE:CB	2:Q:370:LYS:HE2	1.44	1.45
1:H:43:PHE:CB	2:T:370:LYS:HE2	1.44	1.45
1:G:4:HIS:C	2:S:179:LYS:HZ3	1.21	1.44
1:F:4:HIS:C	2:R:179:LYS:HZ3	1.21	1.44
1:B:43:PHE:CB	2:N:370:LYS:HE2	1.44	1.44
1:K:43:PHE:CB	2:W:370:LYS:HE2	1.44	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PHE:CB	2:M:370:LYS:HE2	1.44	1.44
1:G:43:PHE:CB	2:S:370:LYS:HE2	1.45	1.44
1:L:43:PHE:CB	2:X:370:LYS:HE2	1.45	1.43
1:F:43:PHE:CB	2:R:370:LYS:HE2	1.44	1.43
1:D:4:HIS:C	2:P:179:LYS:HZ3	1.20	1.42
1:I:4:HIS:C	2:U:179:LYS:HZ3	1.20	1.42
1:A:337:ARG:HB2	1:B:61:ASN:O	1.36	1.25
1:I:61:ASN:O	1:J:337:ARG:HB2	1.30	1.24
1:F:5:VAL:N	2:R:179:LYS:NZ	1.87	1.23
1:G:5:VAL:N	2:S:179:LYS:NZ	1.87	1.23
1:A:5:VAL:N	2:M:179:LYS:NZ	1.87	1.23
1:B:5:VAL:N	2:N:179:LYS:NZ	1.87	1.23
1:E:4:HIS:CD2	2:Q:178:ILE:HG13	1.74	1.23
1:F:4:HIS:CD2	2:R:178:ILE:HG13	1.74	1.23
1:G:4:HIS:CD2	2:S:178:ILE:HG13	1.74	1.23
1:H:4:HIS:CD2	2:T:178:ILE:HG13	1.74	1.23
1:H:5:VAL:N	2:T:179:LYS:NZ	1.87	1.23
1:L:5:VAL:N	2:X:179:LYS:NZ	1.87	1.23
2:R:239:LYS:O	2:R:239:LYS:HE3	1.39	1.23
1:K:5:VAL:N	2:W:179:LYS:NZ	1.87	1.22
2:M:239:LYS:O	2:M:239:LYS:HE3	1.39	1.22
2:S:239:LYS:O	2:S:239:LYS:HE3	1.39	1.22
1:E:5:VAL:N	2:Q:179:LYS:NZ	1.87	1.22
2:X:239:LYS:O	2:X:239:LYS:HE3	1.39	1.22
1:A:4:HIS:CD2	2:M:178:ILE:HG13	1.74	1.22
1:C:5:VAL:N	2:O:179:LYS:NZ	1.87	1.22
1:I:4:HIS:CD2	2:U:178:ILE:HG13	1.74	1.22
1:D:4:HIS:CD2	2:P:178:ILE:HG13	1.74	1.21
1:J:5:VAL:N	2:V:179:LYS:NZ	1.87	1.21
1:L:4:HIS:CD2	2:X:178:ILE:HG13	1.74	1.21
1:D:5:VAL:N	2:P:179:LYS:NZ	1.87	1.21
1:G:61:ASN:O	1:H:337:ARG:HB2	1.35	1.21
1:K:4:HIS:CD2	2:W:178:ILE:HG13	1.74	1.21
2:W:239:LYS:O	2:W:239:LYS:HE3	1.39	1.21
1:B:4:HIS:CD2	2:N:178:ILE:HG13	1.74	1.21
1:C:4:HIS:CD2	2:O:178:ILE:HG13	1.74	1.21
1:I:5:VAL:N	2:U:179:LYS:NZ	1.87	1.21
1:J:4:HIS:CD2	2:V:178:ILE:HG13	1.74	1.21
2:N:239:LYS:HE3	2:N:239:LYS:O	1.39	1.21
2:T:239:LYS:O	2:T:239:LYS:HE3	1.39	1.21
1:B:4:HIS:C	2:N:179:LYS:NZ	1.99	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:HIS:C	2:R:179:LYS:NZ	1.99	1.20
1:K:4:HIS:C	2:W:179:LYS:NZ	1.99	1.20
2:Q:239:LYS:HE3	2:Q:239:LYS:O	1.39	1.20
1:G:4:HIS:C	2:S:179:LYS:NZ	1.99	1.20
1:J:61:ASN:O	1:K:337:ARG:HB2	1.42	1.20
1:A:4:HIS:C	2:M:179:LYS:NZ	1.99	1.19
1:C:337:ARG:HB2	1:D:61:ASN:O	1.37	1.19
1:L:4:HIS:C	2:X:179:LYS:NZ	1.99	1.19
1:H:4:HIS:C	2:T:179:LYS:NZ	1.99	1.19
1:E:4:HIS:C	2:Q:179:LYS:NZ	1.99	1.19
1:J:4:HIS:C	2:V:179:LYS:NZ	1.99	1.19
1:C:4:HIS:C	2:O:179:LYS:NZ	1.99	1.18
1:I:4:HIS:C	2:U:179:LYS:NZ	1.99	1.18
1:D:4:HIS:C	2:P:179:LYS:NZ	1.99	1.18
2:U:239:LYS:O	2:U:239:LYS:HE3	1.39	1.18
2:O:239:LYS:O	2:O:239:LYS:HE3	1.39	1.18
2:P:239:LYS:O	2:P:239:LYS:HE3	1.39	1.17
2:V:239:LYS:HE3	2:V:239:LYS:O	1.39	1.17
2:S:311:LEU:O	2:S:312:ALA:HB2	1.34	1.16
1:E:360:PHE:CD2	1:E:361:PRO:HD3	1.81	1.15
1:F:360:PHE:CD2	1:F:361:PRO:HD3	1.81	1.15
2:R:311:LEU:O	2:R:312:ALA:HB2	1.34	1.15
1:G:360:PHE:CD2	1:G:361:PRO:HD3	1.81	1.15
1:H:360:PHE:CD2	1:H:361:PRO:HD3	1.81	1.15
1:C:360:PHE:CD2	1:C:361:PRO:HD3	1.81	1.14
1:J:360:PHE:CD2	1:J:361:PRO:HD3	1.81	1.14
2:M:311:LEU:O	2:M:312:ALA:HB2	1.34	1.14
2:T:311:LEU:O	2:T:312:ALA:HB2	1.34	1.14
1:G:337:ARG:HB2	1:L:61:ASN:O	1.46	1.14
1:A:360:PHE:CD2	1:A:361:PRO:HD3	1.81	1.14
1:D:360:PHE:CD2	1:D:361:PRO:HD3	1.81	1.14
1:I:360:PHE:CD2	1:I:361:PRO:HD3	1.81	1.14
1:K:360:PHE:CD2	1:K:361:PRO:HD3	1.81	1.14
1:L:360:PHE:CD2	1:L:361:PRO:HD3	1.81	1.14
1:B:360:PHE:CD2	1:B:361:PRO:HD3	1.81	1.13
2:Q:311:LEU:O	2:Q:312:ALA:HB2	1.34	1.13
2:X:311:LEU:O	2:X:312:ALA:HB2	1.34	1.13
1:A:399:LEU:N	1:A:401:PRO:HG2	1.64	1.13
1:G:399:LEU:N	1:G:401:PRO:HG2	1.64	1.13
1:L:399:LEU:N	1:L:401:PRO:HG2	1.64	1.13
1:B:4:HIS:HD2	2:N:178:ILE:HG13	1.00	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:399:LEU:N	1:F:401:PRO:HG2	1.64	1.12
1:K:4:HIS:HD2	2:W:178:ILE:HG13	1.00	1.12
2:N:311:LEU:O	2:N:312:ALA:HB2	1.34	1.12
2:W:31:THR:HG23	2:W:33:ILE:H	1.09	1.12
2:N:31:THR:HG23	2:N:33:ILE:H	1.09	1.12
2:P:311:LEU:O	2:P:312:ALA:HB2	1.34	1.12
2:U:311:LEU:O	2:U:312:ALA:HB2	1.34	1.11
2:O:311:LEU:O	2:O:312:ALA:HB2	1.34	1.11
2:W:311:LEU:O	2:W:312:ALA:HB2	1.34	1.11
1:D:399:LEU:N	1:D:401:PRO:HG2	1.64	1.11
1:E:399:LEU:N	1:E:401:PRO:HG2	1.64	1.11
1:H:399:LEU:N	1:H:401:PRO:HG2	1.64	1.11
1:I:399:LEU:N	1:I:401:PRO:HG2	1.64	1.11
1:B:399:LEU:N	1:B:401:PRO:HG2	1.64	1.10
1:J:399:LEU:N	1:J:401:PRO:HG2	1.64	1.10
2:V:31:THR:HG23	2:V:33:ILE:H	1.09	1.10
2:V:311:LEU:O	2:V:312:ALA:HB2	1.34	1.10
2:X:31:THR:HG23	2:X:33:ILE:H	1.09	1.10
1:A:60:ILE:HD13	1:A:60:ILE:H	1.08	1.10
1:C:399:LEU:N	1:C:401:PRO:HG2	1.64	1.10
1:J:4:HIS:HD2	2:V:178:ILE:HG13	1.00	1.10
1:K:399:LEU:N	1:K:401:PRO:HG2	1.64	1.10
2:M:31:THR:HG23	2:M:33:ILE:H	1.09	1.10
1:C:4:HIS:HD2	2:O:178:ILE:HG13	1.00	1.10
1:A:4:HIS:HD2	2:M:178:ILE:HG13	1.00	1.10
1:L:60:ILE:HD13	1:L:60:ILE:H	1.08	1.10
1:L:4:HIS:HD2	2:X:178:ILE:HG13	1.00	1.09
2:Q:31:THR:HG23	2:Q:33:ILE:H	1.09	1.09
2:O:31:THR:HG23	2:O:33:ILE:H	1.09	1.09
2:T:31:THR:HG23	2:T:33:ILE:H	1.08	1.09
1:F:399:LEU:H	1:F:401:PRO:HG2	0.95	1.09
1:K:60:ILE:HD13	1:K:60:ILE:H	1.08	1.09
2:S:31:THR:HG23	2:S:33:ILE:H	1.08	1.09
1:B:60:ILE:H	1:B:60:ILE:HD13	1.08	1.09
2:P:31:THR:HG23	2:P:33:ILE:H	1.09	1.09
1:B:400:PRO:HB3	1:B:405:LYS:HE3	1.35	1.08
1:K:400:PRO:HB3	1:K:405:LYS:HE3	1.35	1.08
2:R:31:THR:HG23	2:R:33:ILE:H	1.09	1.08
1:F:60:ILE:HD13	1:F:60:ILE:H	1.08	1.08
1:J:60:ILE:H	1:J:60:ILE:HD13	1.08	1.08
1:A:399:LEU:H	1:A:401:PRO:HG2	0.95	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:399:LEU:H	1:G:401:PRO:HG2	0.95	1.08
1:E:60:ILE:HD13	1:E:60:ILE:H	1.08	1.08
1:J:400:PRO:HB3	1:J:405:LYS:HE3	1.35	1.08
1:L:399:LEU:H	1:L:401:PRO:HG2	0.95	1.08
2:U:31:THR:HG23	2:U:33:ILE:H	1.09	1.08
1:L:400:PRO:HB3	1:L:405:LYS:HE3	1.35	1.07
1:C:60:ILE:HD13	1:C:60:ILE:H	1.08	1.07
1:C:400:PRO:HB3	1:C:405:LYS:HE3	1.35	1.07
1:D:4:HIS:HD2	2:P:178:ILE:HG13	1.00	1.07
1:A:400:PRO:HB3	1:A:405:LYS:HE3	1.35	1.07
1:H:60:ILE:HD13	1:H:60:ILE:H	1.08	1.07
1:I:4:HIS:HD2	2:U:178:ILE:HG13	1.00	1.07
1:G:60:ILE:H	1:G:60:ILE:HD13	1.08	1.07
1:E:399:LEU:H	1:E:401:PRO:HG2	0.95	1.07
1:H:399:LEU:H	1:H:401:PRO:HG2	0.95	1.07
1:D:60:ILE:H	1:D:60:ILE:HD13	1.08	1.06
1:D:400:PRO:HB3	1:D:405:LYS:HE3	1.35	1.06
1:I:400:PRO:HB3	1:I:405:LYS:HE3	1.35	1.06
1:I:60:ILE:HD13	1:I:60:ILE:H	1.08	1.06
1:F:4:HIS:HD2	2:R:178:ILE:HG13	1.00	1.06
1:A:61:ASN:O	1:F:337:ARG:HB2	1.54	1.05
1:B:399:LEU:H	1:B:401:PRO:HG2	0.95	1.05
1:G:4:HIS:HD2	2:S:178:ILE:HG13	1.00	1.05
1:K:399:LEU:H	1:K:401:PRO:HG2	0.95	1.05
1:H:4:HIS:HD2	2:T:178:ILE:HG13	1.00	1.04
1:C:4:HIS:HA	2:O:178:ILE:CD1	1.88	1.04
1:D:4:HIS:HA	2:P:178:ILE:CD1	1.88	1.04
1:D:399:LEU:H	1:D:401:PRO:HG2	0.95	1.04
1:I:4:HIS:HA	2:U:178:ILE:CD1	1.88	1.04
1:J:4:HIS:HA	2:V:178:ILE:CD1	1.88	1.04
1:B:4:HIS:HA	2:N:178:ILE:CD1	1.88	1.04
1:E:4:HIS:HD2	2:Q:178:ILE:HG13	1.00	1.04
1:E:4:HIS:HA	2:Q:178:ILE:CD1	1.88	1.04
1:H:4:HIS:HA	2:T:178:ILE:CD1	1.88	1.04
1:I:399:LEU:H	1:I:401:PRO:HG2	0.95	1.04
1:K:4:HIS:HA	2:W:178:ILE:CD1	1.88	1.04
1:C:399:LEU:H	1:C:401:PRO:HG2	0.95	1.03
1:E:400:PRO:HB3	1:E:405:LYS:HE3	1.35	1.03
1:H:400:PRO:HB3	1:H:405:LYS:HE3	1.34	1.03
1:J:399:LEU:H	1:J:401:PRO:HG2	0.95	1.03
1:F:400:PRO:HB3	1:F:405:LYS:HE3	1.35	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:400:PRO:HB3	1:G:405:LYS:HE3	1.34	1.03
1:I:4:HIS:CB	2:U:179:LYS:NZ	2.21	1.03
1:A:4:HIS:HA	2:M:178:ILE:CD1	1.88	1.03
1:D:4:HIS:CB	2:P:179:LYS:NZ	2.21	1.03
1:L:4:HIS:HA	2:X:178:ILE:CD1	1.88	1.03
2:P:239:LYS:O	2:P:239:LYS:CE	2.07	1.03
2:U:239:LYS:O	2:U:239:LYS:CE	2.07	1.03
1:F:4:HIS:HD2	2:R:178:ILE:CG1	1.72	1.03
2:U:311:LEU:O	2:U:312:ALA:CB	1.98	1.03
1:E:4:HIS:HD2	2:Q:178:ILE:CG1	1.72	1.02
1:G:4:HIS:HD2	2:S:178:ILE:CG1	1.72	1.02
1:G:4:HIS:HA	2:S:178:ILE:CD1	1.88	1.02
1:H:4:HIS:HD2	2:T:178:ILE:CG1	1.72	1.02
2:P:311:LEU:O	2:P:312:ALA:CB	1.98	1.02
2:S:239:LYS:O	2:S:239:LYS:CE	2.07	1.02
2:O:311:LEU:O	2:O:312:ALA:CB	1.98	1.02
2:R:239:LYS:O	2:R:239:LYS:CE	2.07	1.02
2:V:311:LEU:O	2:V:312:ALA:CB	1.98	1.02
1:F:4:HIS:HA	2:R:178:ILE:CD1	1.88	1.02
1:A:4:HIS:HD2	2:M:178:ILE:CG1	1.72	1.02
1:I:4:HIS:HB3	2:U:179:LYS:HZ2	1.25	1.02
1:K:4:HIS:HD2	2:W:178:ILE:CG1	1.72	1.02
2:O:239:LYS:O	2:O:239:LYS:CE	2.07	1.02
1:B:4:HIS:HD2	2:N:178:ILE:CG1	1.72	1.02
1:C:4:HIS:CB	2:O:179:LYS:NZ	2.21	1.02
1:J:4:HIS:HD2	2:V:178:ILE:CG1	1.72	1.02
1:L:4:HIS:HD2	2:X:178:ILE:CG1	1.72	1.02
2:T:239:LYS:O	2:T:239:LYS:CE	2.07	1.02
2:V:239:LYS:O	2:V:239:LYS:CE	2.07	1.02
1:C:4:HIS:HD2	2:O:178:ILE:CG1	1.72	1.01
1:E:4:HIS:HB3	2:Q:179:LYS:HZ2	1.24	1.01
1:G:4:HIS:CB	2:S:179:LYS:NZ	2.21	1.01
2:N:239:LYS:O	2:N:239:LYS:CE	2.07	1.01
2:Q:239:LYS:O	2:Q:239:LYS:CE	2.07	1.01
2:W:239:LYS:O	2:W:239:LYS:CE	2.07	1.01
1:D:4:HIS:HD2	2:P:178:ILE:CG1	1.72	1.01
1:J:4:HIS:CB	2:V:179:LYS:NZ	2.21	1.01
1:L:5:VAL:N	2:X:179:LYS:HZ1	1.56	1.01
1:F:4:HIS:CB	2:R:179:LYS:NZ	2.21	1.01
1:I:4:HIS:HD2	2:U:178:ILE:CG1	1.72	1.01
1:B:4:HIS:CB	2:N:179:LYS:NZ	2.21	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:4:HIS:CB	2:W:179:LYS:NZ	2.21	1.01
1:A:5:VAL:N	2:M:179:LYS:HZ1	1.56	1.01
1:E:4:HIS:CB	2:Q:179:LYS:NZ	2.21	1.01
2:X:239:LYS:O	2:X:239:LYS:CE	2.07	1.01
2:M:239:LYS:O	2:M:239:LYS:CE	2.07	1.00
1:D:4:HIS:HB3	2:P:179:LYS:HZ2	1.26	1.00
1:E:337:ARG:HB2	1:F:61:ASN:O	1.61	1.00
1:H:4:HIS:CB	2:T:179:LYS:NZ	2.21	1.00
1:H:61:ASN:O	1:I:337:ARG:HB2	1.61	1.00
1:H:4:HIS:HB3	2:T:179:LYS:HZ2	1.25	1.00
1:C:4:HIS:CA	2:O:178:ILE:HD12	1.91	1.00
1:D:4:HIS:CA	2:P:178:ILE:HD12	1.91	1.00
1:F:4:HIS:CA	2:R:178:ILE:HD12	1.91	1.00
1:K:61:ASN:O	1:L:337:ARG:HB2	1.61	1.00
1:H:4:HIS:CA	2:T:178:ILE:HD12	1.91	1.00
1:J:4:HIS:CA	2:V:178:ILE:HD12	1.91	1.00
2:Q:312:ALA:HB3	2:Q:317:ILE:CG2	1.92	1.00
2:T:312:ALA:HB3	2:T:317:ILE:CG2	1.92	1.00
2:W:31:THR:CG2	2:W:33:ILE:H	1.75	1.00
1:E:4:HIS:CA	2:Q:178:ILE:HD12	1.91	0.99
2:N:31:THR:CG2	2:N:33:ILE:H	1.75	0.99
2:O:312:ALA:HB3	2:O:317:ILE:CG2	1.92	0.99
2:V:312:ALA:HB3	2:V:317:ILE:CG2	1.92	0.99
1:B:4:HIS:CA	2:N:178:ILE:HD12	1.91	0.99
1:G:4:HIS:CA	2:S:178:ILE:HD12	1.91	0.99
1:I:4:HIS:CA	2:U:178:ILE:HD12	1.91	0.99
1:K:4:HIS:CA	2:W:178:ILE:HD12	1.91	0.99
2:M:31:THR:CG2	2:M:33:ILE:H	1.75	0.99
2:N:311:LEU:O	2:N:312:ALA:CB	1.98	0.99
2:V:31:THR:CG2	2:V:33:ILE:H	1.75	0.99
2:O:31:THR:CG2	2:O:33:ILE:H	1.75	0.99
2:W:311:LEU:O	2:W:312:ALA:CB	1.98	0.99
2:X:31:THR:CG2	2:X:33:ILE:H	1.75	0.99
1:A:4:HIS:CA	2:M:178:ILE:HD12	1.91	0.99
1:L:4:HIS:CA	2:X:178:ILE:HD12	1.91	0.99
2:Q:311:LEU:O	2:Q:312:ALA:CB	1.98	0.99
2:R:31:THR:CG2	2:R:33:ILE:H	1.75	0.99
2:S:31:THR:CG2	2:S:33:ILE:H	1.75	0.99
2:T:311:LEU:O	2:T:312:ALA:CB	1.98	0.99
1:A:4:HIS:CB	2:M:179:LYS:NZ	2.21	0.99
2:Q:31:THR:CG2	2:Q:33:ILE:H	1.75	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:31:THR:CG2	2:T:33:ILE:H	1.75	0.99
1:D:337:ARG:HB2	1:E:61:ASN:O	1.60	0.99
2:U:31:THR:CG2	2:U:33:ILE:H	1.75	0.99
2:R:312:ALA:HB3	2:R:317:ILE:CG2	1.92	0.98
1:B:337:ARG:HB2	1:C:61:ASN:O	1.60	0.98
1:L:4:HIS:CB	2:X:179:LYS:NZ	2.21	0.98
2:P:31:THR:CG2	2:P:33:ILE:H	1.75	0.98
2:M:312:ALA:HB3	2:M:317:ILE:CG2	1.92	0.98
2:S:312:ALA:HB3	2:S:317:ILE:CG2	1.92	0.98
2:X:312:ALA:HB3	2:X:317:ILE:CG2	1.92	0.98
1:K:4:HIS:HB3	2:W:179:LYS:HZ2	1.27	0.98
1:C:4:HIS:HB3	2:O:179:LYS:HZ2	1.26	0.98
1:K:5:VAL:N	2:W:179:LYS:HZ1	1.59	0.98
2:P:312:ALA:HB3	2:P:317:ILE:CG2	1.92	0.98
2:U:312:ALA:HB3	2:U:317:ILE:CG2	1.92	0.98
1:G:4:HIS:HB3	2:S:179:LYS:HZ2	1.29	0.98
2:N:312:ALA:HB3	2:N:317:ILE:CG2	1.92	0.98
2:W:312:ALA:HB3	2:W:317:ILE:CG2	1.92	0.98
1:F:4:HIS:HB3	2:R:179:LYS:HZ2	1.29	0.98
1:J:4:HIS:HB3	2:V:179:LYS:HZ2	1.26	0.98
1:L:4:HIS:HA	2:X:178:ILE:HD12	0.98	0.98
1:A:4:HIS:HA	2:M:178:ILE:HD12	0.98	0.97
1:B:4:HIS:HB3	2:N:179:LYS:HZ2	1.28	0.97
1:G:4:HIS:HA	2:S:178:ILE:HD12	0.98	0.97
1:J:4:HIS:HA	2:V:178:ILE:HD12	0.98	0.97
1:B:5:VAL:N	2:N:179:LYS:HZ1	1.58	0.97
1:C:4:HIS:HA	2:O:178:ILE:HD12	0.98	0.97
1:F:4:HIS:HA	2:R:178:ILE:HD12	0.98	0.97
1:D:4:HIS:HA	2:P:178:ILE:HD12	0.98	0.97
1:I:4:HIS:HA	2:U:178:ILE:HD12	0.98	0.97
1:H:5:VAL:N	2:T:179:LYS:HZ1	1.60	0.97
1:B:4:HIS:HA	2:N:178:ILE:HD12	0.98	0.96
1:E:4:HIS:HA	2:Q:178:ILE:HD12	0.98	0.96
1:K:4:HIS:HA	2:W:178:ILE:HD12	0.98	0.96
1:H:4:HIS:HA	2:T:178:ILE:HD12	0.98	0.96
2:P:239:LYS:O	2:P:239:LYS:CD	2.14	0.96
2:T:239:LYS:O	2:T:239:LYS:CD	2.14	0.96
2:U:239:LYS:O	2:U:239:LYS:CD	2.14	0.96
2:Q:239:LYS:O	2:Q:239:LYS:CD	2.14	0.96
1:F:5:VAL:N	2:R:179:LYS:HZ1	1.57	0.95
1:E:5:VAL:N	2:Q:179:LYS:HZ1	1.61	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:312:ALA:CB	2:T:317:ILE:CG2	2.45	0.95
2:Q:312:ALA:CB	2:Q:317:ILE:CG2	2.45	0.95
2:N:312:ALA:CB	2:N:317:ILE:CG2	2.45	0.95
2:O:239:LYS:O	2:O:239:LYS:CD	2.14	0.95
2:O:312:ALA:CB	2:O:317:ILE:CG2	2.45	0.95
2:V:312:ALA:CB	2:V:317:ILE:CG2	2.45	0.95
2:W:312:ALA:CB	2:W:317:ILE:CG2	2.45	0.95
2:R:312:ALA:CB	2:R:317:ILE:CG2	2.45	0.95
2:S:312:ALA:CB	2:S:317:ILE:CG2	2.45	0.95
2:V:239:LYS:O	2:V:239:LYS:CD	2.14	0.95
2:X:239:LYS:O	2:X:239:LYS:CD	2.14	0.95
2:M:312:ALA:CB	2:M:317:ILE:CG2	2.45	0.95
2:P:312:ALA:CB	2:P:317:ILE:CG2	2.45	0.95
2:M:239:LYS:O	2:M:239:LYS:CD	2.14	0.94
2:U:312:ALA:CB	2:U:317:ILE:CG2	2.45	0.94
2:X:312:ALA:CB	2:X:317:ILE:CG2	2.45	0.94
2:R:239:LYS:O	2:R:239:LYS:CD	2.14	0.94
2:N:239:LYS:O	2:N:239:LYS:CD	2.14	0.94
2:W:239:LYS:O	2:W:239:LYS:CD	2.14	0.94
2:S:239:LYS:O	2:S:239:LYS:CD	2.14	0.94
1:G:5:VAL:N	2:S:179:LYS:HZ1	1.58	0.94
1:C:235:ILE:HG21	1:C:367:PRO:HG3	1.49	0.94
1:J:235:ILE:HG21	1:J:367:PRO:HG3	1.49	0.94
1:L:4:HIS:HB3	2:X:179:LYS:HZ2	1.32	0.93
1:C:5:VAL:N	2:O:179:LYS:HZ1	1.60	0.93
1:K:235:ILE:HG21	1:K:367:PRO:HG3	1.49	0.93
1:B:235:ILE:HG21	1:B:367:PRO:HG3	1.49	0.93
1:K:60:ILE:H	1:K:60:ILE:CD1	1.82	0.93
1:B:60:ILE:H	1:B:60:ILE:CD1	1.82	0.92
1:J:5:VAL:N	2:V:179:LYS:HZ1	1.59	0.92
1:D:235:ILE:HG21	1:D:367:PRO:HG3	1.49	0.92
1:A:4:HIS:HB3	2:M:179:LYS:HZ2	1.33	0.92
1:I:235:ILE:HG21	1:I:367:PRO:HG3	1.49	0.92
1:G:235:ILE:HG21	1:G:367:PRO:HG3	1.49	0.92
1:A:235:ILE:HG21	1:A:367:PRO:HG3	1.49	0.92
1:L:235:ILE:HG21	1:L:367:PRO:HG3	1.49	0.92
1:F:235:ILE:HG21	1:F:367:PRO:HG3	1.49	0.91
1:D:60:ILE:H	1:D:60:ILE:CD1	1.82	0.91
1:I:5:VAL:N	2:U:179:LYS:HZ1	1.60	0.91
1:I:60:ILE:H	1:I:60:ILE:CD1	1.82	0.91
1:E:235:ILE:HG21	1:E:367:PRO:HG3	1.49	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:235:ILE:HG21	1:H:367:PRO:HG3	1.49	0.90
2:W:1:LYS:HA	2:W:54:GLY:O	1.72	0.90
1:J:395:ASN:HB3	1:J:400:PRO:HD2	1.54	0.90
2:N:1:LYS:HA	2:N:54:GLY:O	1.72	0.90
1:C:395:ASN:HB3	1:C:400:PRO:HD2	1.54	0.90
1:B:398:ASP:O	1:B:399:LEU:C	2.11	0.90
1:K:398:ASP:O	1:K:399:LEU:C	2.11	0.90
2:V:1:LYS:HA	2:V:54:GLY:O	1.72	0.90
2:X:1:LYS:HA	2:X:54:GLY:O	1.72	0.90
1:E:4:HIS:CB	2:Q:179:LYS:HZ2	1.82	0.90
2:M:1:LYS:HA	2:M:54:GLY:O	1.72	0.90
2:O:1:LYS:HA	2:O:54:GLY:O	1.72	0.90
1:D:5:VAL:N	2:P:179:LYS:HZ1	1.59	0.89
1:K:395:ASN:HB3	1:K:400:PRO:HD2	1.54	0.89
2:S:1:LYS:HA	2:S:54:GLY:O	1.72	0.89
1:E:60:ILE:H	1:E:60:ILE:CD1	1.82	0.89
1:G:60:ILE:HD13	1:G:60:ILE:N	1.87	0.89
1:C:60:ILE:H	1:C:60:ILE:CD1	1.82	0.89
2:R:1:LYS:HA	2:R:54:GLY:O	1.72	0.89
1:A:398:ASP:O	1:A:399:LEU:C	2.11	0.89
1:B:395:ASN:HB3	1:B:400:PRO:HD2	1.54	0.89
1:D:395:ASN:HB3	1:D:400:PRO:HD2	1.54	0.89
1:H:60:ILE:H	1:H:60:ILE:CD1	1.82	0.89
1:I:395:ASN:HB3	1:I:400:PRO:HD2	1.54	0.89
1:L:398:ASP:O	1:L:399:LEU:C	2.11	0.89
2:P:1:LYS:HA	2:P:54:GLY:O	1.72	0.89
1:A:4:HIS:CA	2:M:179:LYS:HZ3	1.84	0.89
1:F:60:ILE:HD13	1:F:60:ILE:N	1.87	0.89
2:U:1:LYS:HA	2:U:54:GLY:O	1.72	0.89
1:C:60:ILE:HD13	1:C:60:ILE:N	1.87	0.89
1:E:60:ILE:HD13	1:E:60:ILE:N	1.87	0.89
1:J:60:ILE:H	1:J:60:ILE:CD1	1.82	0.89
1:E:395:ASN:HB3	1:E:400:PRO:HD2	1.54	0.88
1:F:60:ILE:H	1:F:60:ILE:CD1	1.82	0.88
1:H:60:ILE:HD13	1:H:60:ILE:N	1.87	0.88
1:D:60:ILE:HD13	1:D:60:ILE:N	1.87	0.88
1:H:395:ASN:HB3	1:H:400:PRO:HD2	1.54	0.88
1:J:60:ILE:HD13	1:J:60:ILE:N	1.87	0.88
1:K:60:ILE:HD13	1:K:60:ILE:N	1.87	0.88
1:L:4:HIS:CA	2:X:179:LYS:HZ3	1.85	0.88
1:F:398:ASP:O	1:F:399:LEU:C	2.11	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:ILE:H	1:G:60:ILE:CD1	1.82	0.88
1:I:60:ILE:HD13	1:I:60:ILE:N	1.87	0.88
1:J:398:ASP:O	1:J:399:LEU:C	2.11	0.88
1:L:60:ILE:HD13	1:L:60:ILE:N	1.87	0.88
2:M:312:ALA:CB	2:M:317:ILE:HB	2.04	0.88
2:P:312:ALA:CB	2:P:317:ILE:HB	2.04	0.88
1:B:60:ILE:HD13	1:B:60:ILE:N	1.87	0.88
1:H:4:HIS:CB	2:T:179:LYS:HZ2	1.84	0.88
2:T:312:ALA:CB	2:T:317:ILE:HB	2.04	0.88
2:X:312:ALA:CB	2:X:317:ILE:HB	2.04	0.88
1:A:60:ILE:HD13	1:A:60:ILE:N	1.87	0.88
1:C:398:ASP:O	1:C:399:LEU:C	2.11	0.88
2:P:309:GLU:O	2:P:313:LYS:HE3	1.74	0.88
2:Q:309:GLU:O	2:Q:313:LYS:HE3	1.74	0.88
2:Q:312:ALA:CB	2:Q:317:ILE:HB	2.04	0.88
2:T:309:GLU:O	2:T:313:LYS:HE3	1.74	0.88
2:U:309:GLU:O	2:U:313:LYS:HE3	1.74	0.88
2:U:312:ALA:CB	2:U:317:ILE:HB	2.04	0.88
1:A:395:ASN:HB3	1:A:400:PRO:HD2	1.54	0.88
1:G:398:ASP:O	1:G:399:LEU:C	2.11	0.88
1:L:395:ASN:HB3	1:L:400:PRO:HD2	1.54	0.88
2:Q:1:LYS:HA	2:Q:54:GLY:O	1.72	0.87
2:N:312:ALA:CB	2:N:317:ILE:HB	2.04	0.87
2:O:312:ALA:CB	2:O:317:ILE:HB	2.04	0.87
2:V:312:ALA:CB	2:V:317:ILE:HB	2.04	0.87
2:W:312:ALA:CB	2:W:317:ILE:HB	2.04	0.87
1:I:4:HIS:CB	2:U:179:LYS:HZ2	1.83	0.87
2:R:312:ALA:CB	2:R:317:ILE:HB	2.04	0.87
2:T:1:LYS:HA	2:T:54:GLY:O	1.72	0.87
2:M:309:GLU:O	2:M:313:LYS:HE3	1.74	0.87
1:G:395:ASN:HB3	1:G:400:PRO:HD2	1.54	0.87
2:S:312:ALA:CB	2:S:317:ILE:HB	2.04	0.87
2:X:309:GLU:O	2:X:313:LYS:HE3	1.74	0.87
1:F:4:HIS:CA	2:R:179:LYS:HZ3	1.86	0.86
1:F:395:ASN:HB3	1:F:400:PRO:HD2	1.54	0.86
2:S:309:GLU:O	2:S:313:LYS:HE3	1.74	0.86
1:B:4:HIS:CA	2:N:179:LYS:HZ3	1.87	0.86
2:N:309:GLU:O	2:N:313:LYS:HE3	1.74	0.86
2:W:309:GLU:O	2:W:313:LYS:HE3	1.74	0.86
1:G:4:HIS:CA	2:S:179:LYS:HZ3	1.87	0.86
2:M:31:THR:HG23	2:M:33:ILE:N	1.91	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:31:THR:HG23	2:X:33:ILE:N	1.91	0.86
2:O:309:GLU:O	2:O:313:LYS:HE3	1.74	0.86
2:R:309:GLU:O	2:R:313:LYS:HE3	1.74	0.86
2:S:31:THR:HG23	2:S:33:ILE:N	1.91	0.86
2:V:309:GLU:O	2:V:313:LYS:HE3	1.74	0.85
2:R:31:THR:HG23	2:R:33:ILE:N	1.91	0.85
1:A:60:ILE:H	1:A:60:ILE:CD1	1.82	0.85
1:D:4:HIS:CB	2:P:179:LYS:HZ2	1.85	0.85
1:J:82:ASP:O	1:J:84:THR:HG22	1.76	0.85
1:K:4:HIS:CA	2:W:179:LYS:HZ3	1.89	0.85
2:V:31:THR:HG23	2:V:33:ILE:N	1.91	0.85
1:C:82:ASP:O	1:C:84:THR:HG22	1.76	0.85
1:E:458:HIS:HD2	1:E:460:VAL:H	1.25	0.85
2:O:31:THR:HG23	2:O:33:ILE:N	1.91	0.85
1:H:398:ASP:O	1:H:399:LEU:C	2.11	0.85
1:H:458:HIS:HD2	1:H:460:VAL:H	1.25	0.85
1:A:458:HIS:HD2	1:A:460:VAL:H	1.25	0.85
1:C:4:HIS:CA	2:O:179:LYS:HZ3	1.89	0.85
1:L:60:ILE:H	1:L:60:ILE:CD1	1.82	0.85
1:A:130:PRO:HB3	1:A:268:MET:HE3	1.59	0.85
1:D:458:HIS:HD2	1:D:460:VAL:H	1.25	0.85
1:E:82:ASP:O	1:E:84:THR:HG22	1.76	0.85
1:H:82:ASP:O	1:H:84:THR:HG22	1.76	0.85
1:I:61:ASN:O	1:J:337:ARG:CB	2.21	0.85
1:I:458:HIS:HD2	1:I:460:VAL:H	1.25	0.85
1:J:4:HIS:CA	2:V:179:LYS:HZ3	1.90	0.85
1:K:82:ASP:O	1:K:84:THR:HG22	1.76	0.85
1:L:130:PRO:HB3	1:L:268:MET:HE3	1.59	0.85
1:L:458:HIS:HD2	1:L:460:VAL:H	1.25	0.85
1:B:82:ASP:O	1:B:84:THR:HG22	1.76	0.85
1:I:130:PRO:HB3	1:I:268:MET:HE3	1.59	0.85
1:D:130:PRO:HB3	1:D:268:MET:HE3	1.59	0.84
1:E:398:ASP:O	1:E:399:LEU:C	2.11	0.84
2:P:31:THR:HG23	2:P:33:ILE:N	1.91	0.84
1:G:458:HIS:HD2	1:G:460:VAL:H	1.25	0.84
1:B:130:PRO:HB3	1:B:268:MET:HE3	1.59	0.84
1:D:4:HIS:CA	2:P:179:LYS:HZ3	1.89	0.84
1:I:82:ASP:O	1:I:84:THR:HG22	1.76	0.84
2:R:311:LEU:O	2:R:312:ALA:CB	1.98	0.84
2:X:311:LEU:O	2:X:312:ALA:CB	1.98	0.84
1:E:130:PRO:HB3	1:E:268:MET:HE3	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:130:PRO:HB3	1:H:268:MET:HE3	1.59	0.84
1:K:130:PRO:HB3	1:K:268:MET:HE3	1.59	0.84
2:N:31:THR:HG23	2:N:33:ILE:N	1.91	0.84
2:W:31:THR:HG23	2:W:33:ILE:N	1.91	0.84
1:D:82:ASP:O	1:D:84:THR:HG22	1.76	0.84
1:G:130:PRO:HB3	1:G:268:MET:HE3	1.59	0.84
1:J:130:PRO:HB3	1:J:268:MET:HE3	1.59	0.84
1:F:458:HIS:HD2	1:F:460:VAL:H	1.25	0.84
2:U:31:THR:HG23	2:U:33:ILE:N	1.91	0.84
1:C:130:PRO:HB3	1:C:268:MET:HE3	1.59	0.84
1:D:398:ASP:O	1:D:399:LEU:C	2.11	0.84
1:F:82:ASP:O	1:F:84:THR:HG22	1.76	0.84
1:F:130:PRO:HB3	1:F:268:MET:HE3	1.59	0.84
1:J:458:HIS:HD2	1:J:460:VAL:H	1.25	0.84
1:B:458:HIS:HD2	1:B:460:VAL:H	1.25	0.84
1:C:458:HIS:HD2	1:C:460:VAL:H	1.25	0.84
1:K:458:HIS:HD2	1:K:460:VAL:H	1.25	0.84
2:S:311:LEU:O	2:S:312:ALA:CB	1.98	0.84
1:I:398:ASP:O	1:I:399:LEU:C	2.11	0.83
1:H:4:HIS:CA	2:T:179:LYS:HZ3	1.90	0.83
2:M:311:LEU:O	2:M:312:ALA:CB	1.98	0.83
1:G:82:ASP:O	1:G:84:THR:HG22	1.76	0.83
1:I:4:HIS:CA	2:U:179:LYS:HZ3	1.90	0.83
2:P:312:ALA:HB3	2:P:317:ILE:HG21	1.61	0.83
2:T:31:THR:HG23	2:T:33:ILE:N	1.90	0.83
1:D:43:PHE:CB	2:P:370:LYS:CE	2.25	0.83
2:N:367:ARG:O	2:N:370:LYS:HB2	1.78	0.83
2:Q:31:THR:HG23	2:Q:33:ILE:N	1.91	0.83
2:U:312:ALA:HB3	2:U:317:ILE:HG21	1.61	0.83
2:V:367:ARG:O	2:V:370:LYS:HB2	1.78	0.83
2:W:367:ARG:O	2:W:370:LYS:HB2	1.78	0.83
1:A:43:PHE:CB	2:M:370:LYS:CE	2.25	0.83
2:O:367:ARG:O	2:O:370:LYS:HB2	1.78	0.83
1:L:82:ASP:O	1:L:84:THR:HG22	1.76	0.83
2:M:367:ARG:O	2:M:370:LYS:HB2	1.78	0.83
2:U:367:ARG:O	2:U:370:LYS:HB2	1.78	0.83
1:A:82:ASP:O	1:A:84:THR:HG22	1.76	0.83
1:I:43:PHE:CB	2:U:370:LYS:CE	2.25	0.83
2:W:239:LYS:O	2:W:239:LYS:CG	2.27	0.83
1:E:4:HIS:CA	2:Q:179:LYS:HZ3	1.92	0.82
2:N:239:LYS:O	2:N:239:LYS:CG	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:367:ARG:O	2:P:370:LYS:HB2	1.78	0.82
2:Q:367:ARG:O	2:Q:370:LYS:HB2	1.78	0.82
2:X:367:ARG:O	2:X:370:LYS:HB2	1.78	0.82
2:T:367:ARG:O	2:T:370:LYS:HB2	1.78	0.82
2:V:312:ALA:HB3	2:V:317:ILE:HG21	1.60	0.82
1:L:43:PHE:CB	2:X:370:LYS:CE	2.25	0.82
2:R:367:ARG:O	2:R:370:LYS:HB2	1.78	0.82
2:O:312:ALA:HB3	2:O:317:ILE:HG21	1.60	0.82
2:S:367:ARG:O	2:S:370:LYS:HB2	1.78	0.82
1:G:4:HIS:CB	2:S:179:LYS:HZ2	1.89	0.81
2:R:239:LYS:O	2:R:239:LYS:CG	2.27	0.81
2:X:312:ALA:HB3	2:X:317:ILE:HG21	1.60	0.81
1:C:399:LEU:HA	1:C:400:PRO:C	2.06	0.81
2:M:239:LYS:O	2:M:239:LYS:CG	2.27	0.81
2:M:312:ALA:HB3	2:M:317:ILE:HG21	1.60	0.81
2:S:239:LYS:O	2:S:239:LYS:CG	2.27	0.81
2:X:239:LYS:O	2:X:239:LYS:CG	2.27	0.81
1:D:399:LEU:HA	1:D:400:PRO:C	2.06	0.81
1:F:4:HIS:CB	2:R:179:LYS:HZ2	1.89	0.81
1:I:399:LEU:HA	1:I:400:PRO:C	2.06	0.81
1:J:399:LEU:HA	1:J:400:PRO:C	2.06	0.81
1:E:43:PHE:CB	2:Q:370:LYS:CE	2.25	0.81
1:G:43:PHE:CB	2:S:370:LYS:CE	2.25	0.81
2:P:33:ILE:HG12	2:P:275:LEU:HD13	1.63	0.81
2:S:312:ALA:HB3	2:S:317:ILE:HG21	1.60	0.81
2:U:33:ILE:HG12	2:U:275:LEU:HD13	1.63	0.81
1:C:398:ASP:O	1:C:399:LEU:O	1.99	0.81
1:J:398:ASP:O	1:J:399:LEU:O	1.99	0.81
1:L:399:LEU:HA	1:L:400:PRO:C	2.06	0.81
2:Q:33:ILE:HG12	2:Q:275:LEU:HD13	1.63	0.81
1:D:398:ASP:O	1:D:399:LEU:O	1.99	0.81
1:K:399:LEU:HA	1:K:400:PRO:C	2.06	0.81
1:A:337:ARG:CB	1:B:61:ASN:O	2.26	0.81
1:A:399:LEU:HA	1:A:400:PRO:C	2.06	0.81
1:I:398:ASP:O	1:I:399:LEU:O	1.99	0.81
2:P:239:LYS:O	2:P:239:LYS:CG	2.27	0.81
2:T:33:ILE:HG12	2:T:275:LEU:HD13	1.63	0.81
1:B:399:LEU:HA	1:B:400:PRO:C	2.06	0.81
2:M:295:LYS:C	2:M:295:LYS:HD3	2.06	0.81
2:R:312:ALA:HB3	2:R:317:ILE:HG21	1.60	0.81
1:E:399:LEU:HA	1:E:400:PRO:C	2.06	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:398:ASP:O	1:G:399:LEU:O	1.99	0.80
1:H:399:LEU:HA	1:H:400:PRO:C	2.06	0.80
2:O:33:ILE:HG12	2:O:275:LEU:HD13	1.63	0.80
2:X:295:LYS:C	2:X:295:LYS:HD3	2.06	0.80
1:B:398:ASP:O	1:B:399:LEU:O	1.99	0.80
1:F:43:PHE:CB	2:R:370:LYS:CE	2.25	0.80
1:F:398:ASP:O	1:F:399:LEU:O	1.99	0.80
2:N:312:ALA:HB3	2:N:317:ILE:HG21	1.60	0.80
2:R:295:LYS:HD3	2:R:295:LYS:C	2.06	0.80
2:W:312:ALA:HB3	2:W:317:ILE:HG21	1.61	0.80
1:H:43:PHE:CB	2:T:370:LYS:CE	2.24	0.80
1:K:398:ASP:O	1:K:399:LEU:O	1.99	0.80
2:N:295:LYS:C	2:N:295:LYS:HD3	2.06	0.80
2:Q:312:ALA:HB3	2:Q:317:ILE:HG21	1.60	0.80
2:U:239:LYS:O	2:U:239:LYS:CG	2.27	0.80
1:G:399:LEU:HA	1:G:400:PRO:C	2.06	0.80
2:S:295:LYS:C	2:S:295:LYS:HD3	2.06	0.80
2:V:33:ILE:HG12	2:V:275:LEU:HD13	1.63	0.80
2:W:295:LYS:HD3	2:W:295:LYS:C	2.07	0.80
1:A:398:ASP:O	1:A:399:LEU:O	1.99	0.80
2:T:312:ALA:HB3	2:T:317:ILE:HG21	1.60	0.80
1:C:43:PHE:CB	2:O:370:LYS:CE	2.25	0.80
1:L:398:ASP:O	1:L:399:LEU:O	1.99	0.80
2:R:33:ILE:HG12	2:R:275:LEU:HD13	1.63	0.80
2:V:295:LYS:C	2:V:295:LYS:HD3	2.06	0.80
1:E:398:ASP:O	1:E:399:LEU:O	1.99	0.80
2:S:33:ILE:HG12	2:S:275:LEU:HD13	1.63	0.80
1:F:399:LEU:HA	1:F:400:PRO:C	2.06	0.80
1:K:43:PHE:CB	2:W:370:LYS:CE	2.25	0.80
2:O:295:LYS:HD3	2:O:295:LYS:C	2.07	0.80
2:T:295:LYS:HD3	2:T:295:LYS:C	2.06	0.80
1:H:398:ASP:O	1:H:399:LEU:O	1.99	0.80
2:N:33:ILE:HG12	2:N:275:LEU:HD13	1.63	0.79
2:Q:239:LYS:O	2:Q:239:LYS:CG	2.27	0.79
1:J:43:PHE:CB	2:V:370:LYS:CE	2.25	0.79
2:M:33:ILE:HG12	2:M:275:LEU:HD13	1.63	0.79
2:O:239:LYS:O	2:O:239:LYS:CG	2.27	0.79
2:Q:295:LYS:C	2:Q:295:LYS:HD3	2.06	0.79
1:B:43:PHE:CB	2:N:370:LYS:CE	2.25	0.79
2:U:295:LYS:C	2:U:295:LYS:HD3	2.06	0.79
2:P:295:LYS:C	2:P:295:LYS:HD3	2.06	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:33:ILE:HG12	2:W:275:LEU:HD13	1.63	0.79
2:T:239:LYS:O	2:T:239:LYS:CG	2.27	0.79
2:X:33:ILE:HG12	2:X:275:LEU:HD13	1.63	0.79
2:V:239:LYS:O	2:V:239:LYS:CG	2.27	0.79
2:W:6:LYS:HA	2:W:33:ILE:HG23	1.65	0.79
2:N:6:LYS:HA	2:N:33:ILE:HG23	1.65	0.78
2:S:6:LYS:HA	2:S:33:ILE:HG23	1.65	0.78
2:T:6:LYS:HA	2:T:33:ILE:HG23	1.65	0.78
2:O:6:LYS:HA	2:O:33:ILE:HG23	1.65	0.78
2:U:6:LYS:HA	2:U:33:ILE:HG23	1.65	0.78
2:V:6:LYS:HA	2:V:33:ILE:HG23	1.65	0.78
2:P:6:LYS:HA	2:P:33:ILE:HG23	1.65	0.78
2:Q:6:LYS:HA	2:Q:33:ILE:HG23	1.65	0.78
2:M:6:LYS:HA	2:M:33:ILE:HG23	1.65	0.78
2:X:6:LYS:HA	2:X:33:ILE:HG23	1.65	0.78
2:R:6:LYS:HA	2:R:33:ILE:HG23	1.65	0.78
1:C:58:LYS:HD2	1:C:62:GLU:HB2	1.67	0.77
1:J:58:LYS:HD2	1:J:62:GLU:HB2	1.67	0.77
2:T:312:ALA:HB3	2:T:317:ILE:HG22	1.66	0.77
2:O:31:THR:HG23	2:O:33:ILE:HD12	1.67	0.77
2:Q:312:ALA:HB3	2:Q:317:ILE:HG22	1.67	0.77
2:V:31:THR:HG23	2:V:33:ILE:HD12	1.67	0.77
2:X:31:THR:HG23	2:X:33:ILE:HD12	1.67	0.77
1:A:5:VAL:CA	2:M:179:LYS:HZ1	1.97	0.76
1:D:58:LYS:HD2	1:D:62:GLU:HB2	1.67	0.76
1:I:58:LYS:HD2	1:I:62:GLU:HB2	1.67	0.76
2:M:31:THR:HG23	2:M:33:ILE:HD12	1.68	0.76
1:C:395:ASN:HB3	1:C:400:PRO:CD	2.16	0.76
1:J:395:ASN:HB3	1:J:400:PRO:CD	2.16	0.76
2:S:312:ALA:HB3	2:S:317:ILE:HG22	1.66	0.76
2:R:31:THR:HG23	2:R:33:ILE:HD12	1.67	0.76
1:D:3:GLU:CD	2:P:338:ALA:CB	2.59	0.76
2:M:312:ALA:CB	2:M:317:ILE:HG21	2.15	0.76
2:X:312:ALA:CB	2:X:317:ILE:HG21	2.15	0.76
1:A:3:GLU:CD	2:M:338:ALA:HB1	2.11	0.76
1:I:3:GLU:CD	2:U:338:ALA:CB	2.59	0.76
2:S:31:THR:HG23	2:S:33:ILE:HD12	1.67	0.76
2:U:31:THR:HG23	2:U:33:ILE:HD12	1.67	0.76
1:C:337:ARG:CB	1:D:61:ASN:O	2.27	0.76
1:D:44:GLU:HG3	2:P:370:LYS:NZ	2.01	0.76
1:D:395:ASN:HB3	1:D:400:PRO:CD	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:58:LYS:HD2	1:K:62:GLU:HB2	1.67	0.76
1:L:3:GLU:CD	2:X:338:ALA:HB1	2.11	0.76
2:N:31:THR:HG23	2:N:33:ILE:HD12	1.67	0.76
2:R:312:ALA:HB3	2:R:317:ILE:HG22	1.66	0.76
2:W:28:GLU:HA	2:W:31:THR:HG22	1.68	0.76
1:B:58:LYS:HD2	1:B:62:GLU:HB2	1.67	0.76
1:D:3:GLU:CD	2:P:338:ALA:HB1	2.11	0.76
1:H:3:GLU:CD	2:T:338:ALA:CB	2.59	0.76
1:I:3:GLU:CD	2:U:338:ALA:HB1	2.11	0.76
1:I:395:ASN:HB3	1:I:400:PRO:CD	2.16	0.76
1:J:3:GLU:CD	2:V:338:ALA:HB1	2.11	0.76
2:P:31:THR:HG23	2:P:33:ILE:HD12	1.67	0.76
2:P:136:ASP:OD2	2:P:203:HIS:HD2	1.69	0.76
2:W:31:THR:HG23	2:W:33:ILE:HD12	1.67	0.76
1:A:44:GLU:HG3	2:M:370:LYS:NZ	2.01	0.76
1:C:3:GLU:CD	2:O:338:ALA:HB1	2.11	0.76
1:E:3:GLU:CD	2:Q:338:ALA:CB	2.59	0.76
1:E:3:GLU:CD	2:Q:338:ALA:HB1	2.11	0.76
1:J:44:GLU:HG3	2:V:370:LYS:NZ	2.01	0.76
2:N:28:GLU:HA	2:N:31:THR:HG22	1.68	0.76
2:U:136:ASP:OD2	2:U:203:HIS:HD2	1.69	0.76
2:V:136:ASP:OD2	2:V:203:HIS:HD2	1.69	0.76
1:C:44:GLU:HG3	2:O:370:LYS:NZ	2.01	0.76
1:H:58:LYS:HD2	1:H:62:GLU:HB2	1.67	0.76
1:I:44:GLU:HG3	2:U:370:LYS:NZ	2.01	0.76
2:N:136:ASP:OD2	2:N:203:HIS:HD2	1.69	0.76
2:O:136:ASP:OD2	2:O:203:HIS:HD2	1.69	0.76
2:W:136:ASP:OD2	2:W:203:HIS:HD2	1.69	0.76
1:E:58:LYS:HD2	1:E:62:GLU:HB2	1.67	0.76
1:H:3:GLU:CD	2:T:338:ALA:HB1	2.11	0.76
2:O:28:GLU:HA	2:O:31:THR:HG22	1.68	0.76
2:R:312:ALA:HA	2:R:314:ASP:H	1.51	0.76
2:S:312:ALA:HA	2:S:314:ASP:H	1.51	0.76
2:T:31:THR:HG23	2:T:33:ILE:HD12	1.67	0.76
2:V:28:GLU:HA	2:V:31:THR:HG22	1.68	0.76
1:A:395:ASN:HB3	1:A:400:PRO:CD	2.16	0.75
1:B:44:GLU:HG3	2:N:370:LYS:NZ	2.01	0.75
1:C:3:GLU:CD	2:O:338:ALA:CB	2.59	0.75
1:K:3:GLU:CD	2:W:338:ALA:CB	2.59	0.75
1:K:3:GLU:CD	2:W:338:ALA:HB1	2.11	0.75
2:M:312:ALA:HB3	2:M:317:ILE:HG22	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:312:ALA:HA	2:M:314:ASP:H	1.51	0.75
2:P:312:ALA:HB3	2:P:317:ILE:HG22	1.66	0.75
1:B:3:GLU:CD	2:N:338:ALA:HB1	2.11	0.75
1:G:3:GLU:CD	2:S:338:ALA:HB1	2.11	0.75
1:K:395:ASN:HB3	1:K:400:PRO:CD	2.16	0.75
1:L:5:VAL:CA	2:X:179:LYS:HZ1	1.98	0.75
1:L:395:ASN:HB3	1:L:400:PRO:CD	2.16	0.75
2:Q:31:THR:HG23	2:Q:33:ILE:HD12	1.67	0.75
2:Q:312:ALA:HA	2:Q:314:ASP:H	1.51	0.75
2:T:312:ALA:HA	2:T:314:ASP:H	1.51	0.75
2:U:312:ALA:HB3	2:U:317:ILE:HG22	1.67	0.75
2:X:312:ALA:HA	2:X:314:ASP:H	1.51	0.75
1:B:395:ASN:HB3	1:B:400:PRO:CD	2.16	0.75
1:H:44:GLU:HG3	2:T:370:LYS:NZ	2.01	0.75
1:J:3:GLU:CD	2:V:338:ALA:CB	2.59	0.75
1:K:44:GLU:HG3	2:W:370:LYS:NZ	2.01	0.75
2:P:312:ALA:HA	2:P:314:ASP:H	1.51	0.75
2:Q:136:ASP:OD2	2:Q:203:HIS:HD2	1.69	0.75
2:X:312:ALA:HB3	2:X:317:ILE:HG22	1.66	0.75
1:B:3:GLU:CD	2:N:338:ALA:CB	2.59	0.75
1:E:44:GLU:HG3	2:Q:370:LYS:NZ	2.01	0.75
2:P:312:ALA:CB	2:P:317:ILE:HG21	2.15	0.75
2:Q:28:GLU:HA	2:Q:31:THR:HG22	1.68	0.75
2:T:136:ASP:OD2	2:T:203:HIS:HD2	1.69	0.75
2:U:312:ALA:HA	2:U:314:ASP:H	1.51	0.75
1:F:3:GLU:CD	2:R:338:ALA:HB1	2.11	0.75
1:F:395:ASN:HB3	1:F:400:PRO:CD	2.16	0.75
1:L:3:GLU:CD	2:X:338:ALA:CB	2.59	0.75
1:A:3:GLU:CD	2:M:338:ALA:CB	2.59	0.75
1:G:395:ASN:HB3	1:G:400:PRO:CD	2.16	0.75
1:H:395:ASN:HB3	1:H:400:PRO:CD	2.16	0.75
1:L:44:GLU:HG3	2:X:370:LYS:NZ	2.01	0.75
2:R:28:GLU:HA	2:R:31:THR:HG22	1.68	0.75
2:R:312:ALA:CB	2:R:317:ILE:HG21	2.15	0.75
2:T:28:GLU:HA	2:T:31:THR:HG22	1.68	0.75
2:U:312:ALA:CB	2:U:317:ILE:HG21	2.15	0.75
1:E:395:ASN:HB3	1:E:400:PRO:CD	2.16	0.75
1:B:7:THR:OG1	2:N:178:ILE:HD11	1.87	0.75
1:F:7:THR:OG1	2:R:178:ILE:HD11	1.87	0.75
1:G:3:GLU:CD	2:S:338:ALA:CB	2.59	0.75
2:S:312:ALA:CB	2:S:317:ILE:HG21	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:THR:OG1	2:M:178:ILE:HD11	1.87	0.75
1:F:58:LYS:HD2	1:F:62:GLU:HB2	1.67	0.75
1:G:7:THR:OG1	2:S:178:ILE:HD11	1.87	0.75
2:S:28:GLU:HA	2:S:31:THR:HG22	1.68	0.75
2:T:64:HIS:HD2	2:T:261:VAL:H	1.34	0.75
1:A:58:LYS:HD2	1:A:62:GLU:HB2	1.67	0.74
1:F:3:GLU:CD	2:R:338:ALA:CB	2.59	0.74
1:G:44:GLU:HG3	2:S:370:LYS:NZ	2.01	0.74
1:G:58:LYS:HD2	1:G:62:GLU:HB2	1.67	0.74
1:L:7:THR:OG1	2:X:178:ILE:HD11	1.88	0.74
2:M:136:ASP:OD2	2:M:203:HIS:HD2	1.69	0.74
2:Q:64:HIS:HD2	2:Q:261:VAL:H	1.34	0.74
2:X:28:GLU:HA	2:X:31:THR:HG22	1.68	0.74
2:X:136:ASP:OD2	2:X:203:HIS:HD2	1.69	0.74
1:A:248:ARG:HH21	1:A:248:ARG:CG	2.00	0.74
1:F:44:GLU:HG3	2:R:370:LYS:NZ	2.01	0.74
1:K:7:THR:OG1	2:W:178:ILE:HD11	1.87	0.74
2:O:312:ALA:CB	2:O:317:ILE:HG21	2.15	0.74
2:W:64:HIS:HD2	2:W:261:VAL:H	1.34	0.74
1:J:248:ARG:HH21	1:J:248:ARG:CG	2.00	0.74
1:L:58:LYS:HD2	1:L:62:GLU:HB2	1.67	0.74
1:C:248:ARG:HH21	1:C:248:ARG:CG	2.00	0.74
1:H:7:THR:OG1	2:T:178:ILE:HD11	1.87	0.74
1:L:248:ARG:CG	1:L:248:ARG:HH21	2.00	0.74
2:N:64:HIS:HD2	2:N:261:VAL:H	1.34	0.74
2:O:312:ALA:HA	2:O:314:ASP:H	1.51	0.74
1:C:7:THR:OG1	2:O:178:ILE:HD11	1.87	0.74
1:E:7:THR:OG1	2:Q:178:ILE:HD11	1.87	0.74
1:G:5:VAL:CA	2:S:179:LYS:HZ1	1.99	0.74
1:I:248:ARG:HH21	1:I:248:ARG:CG	2.00	0.74
1:J:7:THR:OG1	2:V:178:ILE:HD11	1.87	0.74
2:M:28:GLU:HA	2:M:31:THR:HG22	1.68	0.74
2:N:312:ALA:HB3	2:N:317:ILE:HG22	1.66	0.74
2:N:312:ALA:HA	2:N:314:ASP:H	1.51	0.74
2:O:312:ALA:HB3	2:O:317:ILE:HG22	1.66	0.74
2:U:28:GLU:HA	2:U:31:THR:HG22	1.68	0.74
2:V:312:ALA:CB	2:V:317:ILE:HG21	2.15	0.74
2:V:312:ALA:HB3	2:V:317:ILE:HG22	1.66	0.74
1:C:192:ARG:HH21	1:C:219:ASN:ND2	1.86	0.74
1:G:248:ARG:HH21	1:G:248:ARG:CG	2.00	0.74
1:J:192:ARG:HH21	1:J:219:ASN:ND2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:248:ARG:HH21	1:K:248:ARG:CG	2.00	0.74
2:S:64:HIS:HD2	2:S:261:VAL:H	1.34	0.74
1:B:248:ARG:HH21	1:B:248:ARG:CG	2.00	0.74
1:D:248:ARG:HH21	1:D:248:ARG:CG	2.00	0.74
2:P:64:HIS:HD2	2:P:261:VAL:H	1.34	0.74
2:V:312:ALA:HA	2:V:314:ASP:H	1.51	0.74
2:W:312:ALA:HA	2:W:314:ASP:H	1.51	0.74
2:R:64:HIS:HD2	2:R:261:VAL:H	1.34	0.74
1:F:5:VAL:CA	2:R:179:LYS:HZ1	1.99	0.74
2:P:28:GLU:HA	2:P:31:THR:HG22	1.68	0.74
2:Q:312:ALA:CB	2:Q:317:ILE:HG21	2.15	0.74
2:U:64:HIS:HD2	2:U:261:VAL:H	1.34	0.74
2:W:312:ALA:HB3	2:W:317:ILE:HG22	1.67	0.74
1:D:5:VAL:CA	2:P:179:LYS:HZ1	2.01	0.74
2:T:312:ALA:CB	2:T:317:ILE:HG21	2.15	0.74
1:F:248:ARG:HH21	1:F:248:ARG:CG	2.00	0.73
2:V:64:HIS:HD2	2:V:261:VAL:H	1.34	0.73
2:X:64:HIS:HD2	2:X:261:VAL:H	1.34	0.73
2:U:341:TYR:CD1	2:U:367:ARG:NH2	2.57	0.73
1:K:192:ARG:HH21	1:K:219:ASN:ND2	1.86	0.73
2:P:341:TYR:CD1	2:P:367:ARG:NH2	2.57	0.73
2:R:136:ASP:OD2	2:R:203:HIS:HD2	1.69	0.73
2:S:136:ASP:OD2	2:S:203:HIS:HD2	1.69	0.73
2:M:64:HIS:HD2	2:M:261:VAL:H	1.34	0.73
2:W:312:ALA:CB	2:W:317:ILE:CB	2.66	0.73
1:B:5:VAL:CA	2:N:179:LYS:HZ1	2.00	0.73
1:B:192:ARG:HH21	1:B:219:ASN:ND2	1.86	0.73
2:N:312:ALA:CB	2:N:317:ILE:CB	2.66	0.73
2:N:312:ALA:CB	2:N:317:ILE:HG21	2.15	0.73
2:O:64:HIS:HD2	2:O:261:VAL:H	1.34	0.73
2:Q:341:TYR:CD1	2:Q:367:ARG:NH2	2.57	0.73
2:T:341:TYR:CD1	2:T:367:ARG:NH2	2.57	0.73
2:W:312:ALA:CB	2:W:317:ILE:HG21	2.16	0.73
2:V:312:ALA:CB	2:V:317:ILE:CB	2.66	0.73
1:D:7:THR:OG1	2:P:178:ILE:HD11	1.87	0.73
1:D:192:ARG:HH21	1:D:219:ASN:ND2	1.86	0.73
1:I:7:THR:OG1	2:U:178:ILE:HD11	1.87	0.73
2:X:341:TYR:CD1	2:X:367:ARG:NH2	2.57	0.73
1:I:192:ARG:HH21	1:I:219:ASN:ND2	1.86	0.73
2:O:312:ALA:CB	2:O:317:ILE:CB	2.66	0.73
1:C:5:VAL:CA	2:O:179:LYS:HZ1	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:5:VAL:CA	2:V:179:LYS:HZ1	2.01	0.73
2:M:341:TYR:CD1	2:M:367:ARG:NH2	2.57	0.73
1:E:248:ARG:HH21	1:E:248:ARG:CG	2.00	0.73
2:N:341:TYR:CD1	2:N:367:ARG:NH2	2.57	0.73
2:O:341:TYR:CD1	2:O:367:ARG:NH2	2.57	0.73
2:S:312:ALA:CB	2:S:317:ILE:CB	2.66	0.73
2:U:27:PHE:O	2:U:31:THR:HB	1.89	0.73
2:W:341:TYR:CD1	2:W:367:ARG:NH2	2.57	0.73
2:X:312:ALA:CB	2:X:317:ILE:CB	2.66	0.73
1:G:192:ARG:HH21	1:G:219:ASN:ND2	1.86	0.72
1:H:248:ARG:HH21	1:H:248:ARG:CG	2.00	0.72
2:M:312:ALA:CB	2:M:317:ILE:CB	2.66	0.72
2:R:312:ALA:CB	2:R:317:ILE:CB	2.66	0.72
2:S:341:TYR:CD1	2:S:367:ARG:NH2	2.57	0.72
2:V:341:TYR:CD1	2:V:367:ARG:NH2	2.57	0.72
1:I:5:VAL:CA	2:U:179:LYS:HZ1	2.02	0.72
2:P:27:PHE:O	2:P:31:THR:HB	1.89	0.72
2:R:27:PHE:O	2:R:31:THR:HB	1.89	0.72
2:U:312:ALA:CB	2:U:317:ILE:CB	2.66	0.72
1:F:192:ARG:HH21	1:F:219:ASN:ND2	1.86	0.72
1:G:61:ASN:O	1:H:337:ARG:CB	2.28	0.72
1:H:5:VAL:CA	2:T:179:LYS:HZ1	2.02	0.72
2:O:27:PHE:O	2:O:31:THR:HB	1.89	0.72
2:T:27:PHE:O	2:T:31:THR:HB	1.89	0.72
1:E:192:ARG:HH21	1:E:219:ASN:ND2	1.86	0.72
2:P:312:ALA:CB	2:P:317:ILE:CB	2.66	0.72
2:Q:27:PHE:O	2:Q:31:THR:HB	1.89	0.72
2:T:312:ALA:CB	2:T:317:ILE:CB	2.66	0.72
2:Q:312:ALA:CB	2:Q:317:ILE:CB	2.66	0.72
2:R:341:TYR:CD1	2:R:367:ARG:NH2	2.57	0.72
1:H:192:ARG:HH21	1:H:219:ASN:ND2	1.86	0.72
1:K:5:VAL:CA	2:W:179:LYS:HZ1	2.01	0.72
2:P:312:ALA:HB1	2:P:317:ILE:HB	1.72	0.72
2:S:27:PHE:O	2:S:31:THR:HB	1.89	0.72
2:U:312:ALA:HB1	2:U:317:ILE:HB	1.72	0.72
2:V:27:PHE:O	2:V:31:THR:HB	1.89	0.72
1:J:4:HIS:CB	2:V:179:LYS:HZ2	1.85	0.72
2:N:27:PHE:O	2:N:31:THR:HB	1.89	0.72
1:F:96:THR:OG1	1:F:98:GLN:HB2	1.90	0.72
2:W:27:PHE:O	2:W:31:THR:HB	1.89	0.72
2:W:312:ALA:HB1	2:W:317:ILE:HB	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:64:HIS:HE1	2:X:330:MET:O	1.73	0.72
1:G:96:THR:OG1	1:G:98:GLN:HB2	1.90	0.72
1:L:192:ARG:HH21	1:L:219:ASN:ND2	1.86	0.72
2:M:64:HIS:HE1	2:M:330:MET:O	1.73	0.72
2:N:312:ALA:HB1	2:N:317:ILE:HB	1.72	0.72
1:A:192:ARG:HH21	1:A:219:ASN:ND2	1.86	0.71
1:E:5:VAL:CA	2:Q:179:LYS:HZ1	2.03	0.71
1:A:96:THR:OG1	1:A:98:GLN:HB2	1.90	0.71
1:L:96:THR:OG1	1:L:98:GLN:HB2	1.90	0.71
2:M:27:PHE:O	2:M:31:THR:HB	1.89	0.71
2:R:341:TYR:HD1	2:R:367:ARG:NH2	1.88	0.71
2:V:64:HIS:HE1	2:V:330:MET:O	1.73	0.71
2:M:312:ALA:HB1	2:M:317:ILE:HB	1.72	0.71
2:O:64:HIS:HE1	2:O:330:MET:O	1.73	0.71
2:X:27:PHE:O	2:X:31:THR:HB	1.89	0.71
2:S:341:TYR:HD1	2:S:367:ARG:NH2	1.88	0.71
2:U:64:HIS:HE1	2:U:330:MET:O	1.73	0.71
2:X:312:ALA:HB1	2:X:317:ILE:HB	1.72	0.71
1:H:96:THR:OG1	1:H:98:GLN:HB2	1.90	0.71
1:G:4:HIS:CD2	2:S:178:ILE:CG1	2.58	0.71
2:N:64:HIS:HE1	2:N:330:MET:O	1.73	0.71
2:P:64:HIS:HE1	2:P:330:MET:O	1.73	0.71
1:E:96:THR:OG1	1:E:98:GLN:HB2	1.90	0.71
2:T:312:ALA:HB1	2:T:317:ILE:HB	1.72	0.71
2:W:341:TYR:HD1	2:W:367:ARG:NH2	1.88	0.71
2:N:341:TYR:HD1	2:N:367:ARG:NH2	1.88	0.71
2:Q:312:ALA:HB1	2:Q:317:ILE:HB	1.72	0.71
2:S:64:HIS:HE1	2:S:330:MET:O	1.73	0.71
2:W:64:HIS:HE1	2:W:330:MET:O	1.73	0.71
2:Q:341:TYR:HD1	2:Q:367:ARG:NH2	1.88	0.71
2:R:64:HIS:HE1	2:R:330:MET:O	1.73	0.71
2:T:341:TYR:HD1	2:T:367:ARG:NH2	1.88	0.71
2:U:341:TYR:HD1	2:U:367:ARG:NH2	1.88	0.70
2:V:341:TYR:HD1	2:V:367:ARG:NH2	1.88	0.70
1:E:384:ASN:HD22	1:E:384:ASN:N	1.89	0.70
2:O:341:TYR:HD1	2:O:367:ARG:NH2	1.88	0.70
2:P:341:TYR:HD1	2:P:367:ARG:NH2	1.88	0.70
2:V:312:ALA:HB1	2:V:317:ILE:HB	1.72	0.70
1:B:7:THR:OG1	2:N:178:ILE:CD1	2.39	0.70
1:K:96:THR:OG1	1:K:98:GLN:HB2	1.90	0.70
1:B:96:THR:OG1	1:B:98:GLN:HB2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:THR:OG1	2:Q:178:ILE:CD1	2.39	0.70
1:G:384:ASN:HD22	1:G:384:ASN:N	1.89	0.70
1:H:384:ASN:HD22	1:H:384:ASN:N	1.89	0.70
1:K:7:THR:OG1	2:W:178:ILE:CD1	2.39	0.70
2:S:312:ALA:HB1	2:S:317:ILE:HB	1.72	0.70
2:T:64:HIS:HE1	2:T:330:MET:O	1.73	0.70
2:O:312:ALA:HB1	2:O:317:ILE:HB	1.72	0.70
2:Q:64:HIS:HE1	2:Q:330:MET:O	1.73	0.70
1:A:7:THR:OG1	2:M:178:ILE:CD1	2.39	0.70
1:A:320:LYS:NZ	1:G:461:GLU:OE1	2.24	0.70
1:H:7:THR:OG1	2:T:178:ILE:CD1	2.39	0.70
1:I:96:THR:OG1	1:I:98:GLN:HB2	1.90	0.70
1:D:7:THR:OG1	2:P:178:ILE:CD1	2.39	0.70
1:D:96:THR:OG1	1:D:98:GLN:HB2	1.90	0.70
1:F:399:LEU:H	1:F:401:PRO:CG	1.90	0.70
1:I:7:THR:OG1	2:U:178:ILE:CD1	2.39	0.70
1:L:7:THR:OG1	2:X:178:ILE:CD1	2.39	0.70
1:F:7:THR:OG1	2:R:178:ILE:CD1	2.39	0.70
1:F:384:ASN:N	1:F:384:ASN:HD22	1.89	0.70
1:J:7:THR:OG1	2:V:178:ILE:CD1	2.39	0.70
1:L:384:ASN:HD22	1:L:384:ASN:N	1.89	0.70
2:R:312:ALA:HB1	2:R:317:ILE:HB	1.72	0.70
2:Q:68:GLY:HA3	2:Q:332:ASN:O	1.92	0.69
2:T:68:GLY:HA3	2:T:332:ASN:O	1.92	0.69
1:A:384:ASN:HD22	1:A:384:ASN:N	1.89	0.69
1:C:7:THR:OG1	2:O:178:ILE:CD1	2.39	0.69
1:F:3:GLU:OE2	2:R:338:ALA:HB3	1.93	0.69
1:G:7:THR:OG1	2:S:178:ILE:CD1	2.39	0.69
1:B:384:ASN:HD22	1:B:384:ASN:N	1.89	0.69
1:G:3:GLU:OE2	2:S:338:ALA:HB3	1.93	0.69
2:U:68:GLY:HA3	2:U:332:ASN:O	1.92	0.69
1:A:399:LEU:N	1:A:401:PRO:CG	2.52	0.69
1:C:96:THR:OG1	1:C:98:GLN:HB2	1.90	0.69
1:D:384:ASN:HD22	1:D:384:ASN:N	1.89	0.69
1:H:4:HIS:CD2	2:T:178:ILE:CG1	2.58	0.69
1:K:384:ASN:HD22	1:K:384:ASN:N	1.89	0.69
2:P:68:GLY:HA3	2:P:332:ASN:O	1.92	0.69
2:X:341:TYR:HD1	2:X:367:ARG:NH2	1.88	0.69
1:H:3:GLU:OE2	2:T:338:ALA:HB3	1.93	0.69
1:I:384:ASN:N	1:I:384:ASN:HD22	1.89	0.69
1:J:96:THR:OG1	1:J:98:GLN:HB2	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:GLU:OE2	2:Q:338:ALA:HB3	1.93	0.69
1:L:399:LEU:N	1:L:401:PRO:CG	2.52	0.69
1:A:3:GLU:OE2	2:M:338:ALA:HB3	1.93	0.69
1:D:3:GLU:OE2	2:P:338:ALA:HB3	1.93	0.69
1:G:399:LEU:H	1:G:401:PRO:CG	1.90	0.69
1:I:3:GLU:OE2	2:U:338:ALA:HB3	1.93	0.69
1:J:30:HIS:H	1:K:180:PHE:HB3	1.58	0.69
2:M:341:TYR:HD1	2:M:367:ARG:NH2	1.88	0.69
1:D:4:HIS:CA	2:P:179:LYS:NZ	2.53	0.69
1:C:3:GLU:OE2	2:O:338:ALA:HB3	1.93	0.69
1:E:4:HIS:CA	2:Q:179:LYS:NZ	2.53	0.69
1:F:399:LEU:N	1:F:401:PRO:CG	2.52	0.69
1:G:399:LEU:N	1:G:401:PRO:CG	2.52	0.69
1:I:4:HIS:CA	2:U:179:LYS:NZ	2.53	0.68
1:J:384:ASN:HD22	1:J:384:ASN:N	1.89	0.68
1:L:3:GLU:OE2	2:X:338:ALA:HB3	1.93	0.68
2:W:59:ILE:HD12	2:W:280:LEU:HD11	1.75	0.68
2:N:59:ILE:HD12	2:N:280:LEU:HD11	1.75	0.68
2:O:68:GLY:HA3	2:O:332:ASN:O	1.92	0.68
2:X:68:GLY:HA3	2:X:332:ASN:O	1.92	0.68
1:G:337:ARG:CB	1:L:61:ASN:O	2.34	0.68
1:J:3:GLU:OE2	2:V:338:ALA:HB3	1.93	0.68
1:C:384:ASN:HD22	1:C:384:ASN:N	1.89	0.68
2:M:68:GLY:HA3	2:M:332:ASN:O	1.92	0.68
2:O:59:ILE:HD12	2:O:280:LEU:HD11	1.75	0.68
2:S:68:GLY:HA3	2:S:332:ASN:O	1.92	0.68
2:V:68:GLY:HA3	2:V:332:ASN:O	1.92	0.68
2:U:59:ILE:HD12	2:U:280:LEU:HD11	1.75	0.68
1:H:4:HIS:CA	2:T:179:LYS:NZ	2.53	0.68
1:K:4:HIS:CB	2:W:179:LYS:HZ2	1.86	0.68
2:V:59:ILE:HD12	2:V:280:LEU:HD11	1.75	0.68
2:P:59:ILE:HD12	2:P:280:LEU:HD11	1.75	0.68
1:A:4:HIS:CD2	2:M:178:ILE:CG1	2.58	0.68
1:E:399:LEU:HA	1:E:400:PRO:O	1.94	0.68
1:A:3:GLU:HG2	2:M:338:ALA:HB2	1.75	0.68
1:K:3:GLU:OE2	2:W:338:ALA:HB3	1.92	0.68
2:R:68:GLY:HA3	2:R:332:ASN:O	1.92	0.68
1:B:3:GLU:OE2	2:N:338:ALA:HB3	1.93	0.67
1:H:399:LEU:HA	1:H:400:PRO:O	1.94	0.67
1:I:3:GLU:HG2	2:U:338:ALA:HB2	1.75	0.67
1:I:399:LEU:HA	1:I:400:PRO:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:3:GLU:HG2	2:W:338:ALA:HB2	1.75	0.67
1:K:4:HIS:CA	2:W:179:LYS:NZ	2.53	0.67
1:L:3:GLU:HG2	2:X:338:ALA:HB2	1.75	0.67
2:S:43:LEU:CD1	2:S:60:ILE:HD11	2.24	0.67
1:F:4:HIS:CA	2:R:179:LYS:NZ	2.53	0.67
1:L:4:HIS:CD2	2:X:178:ILE:CG1	2.58	0.67
2:P:43:LEU:CD1	2:P:60:ILE:HD11	2.24	0.67
2:R:59:ILE:HD12	2:R:280:LEU:HD11	1.75	0.67
2:U:43:LEU:CD1	2:U:60:ILE:HD11	2.24	0.67
2:W:68:GLY:HA3	2:W:332:ASN:O	1.92	0.67
1:B:3:GLU:HG2	2:N:338:ALA:HB2	1.76	0.67
1:D:399:LEU:HA	1:D:400:PRO:O	1.94	0.67
1:L:295:LEU:O	1:L:388:PRO:CG	2.43	0.67
2:S:59:ILE:HD12	2:S:280:LEU:HD11	1.75	0.67
1:A:295:LEU:O	1:A:388:PRO:CG	2.43	0.67
1:D:3:GLU:HG2	2:P:338:ALA:HB2	1.75	0.67
2:N:68:GLY:HA3	2:N:332:ASN:O	1.92	0.67
2:R:43:LEU:CD1	2:R:60:ILE:HD11	2.24	0.67
2:M:59:ILE:HD12	2:M:280:LEU:HD11	1.75	0.67
2:V:43:LEU:CD1	2:V:60:ILE:HD11	2.24	0.67
2:X:59:ILE:HD12	2:X:280:LEU:HD11	1.75	0.67
1:G:4:HIS:CA	2:S:179:LYS:NZ	2.53	0.67
2:O:43:LEU:CD1	2:O:60:ILE:HD11	2.24	0.67
2:M:43:LEU:CD1	2:M:60:ILE:HD11	2.24	0.67
1:J:3:GLU:HG2	2:V:338:ALA:HB2	1.76	0.67
1:B:4:HIS:CB	2:N:179:LYS:HZ2	1.88	0.67
1:F:3:GLU:HG2	2:R:338:ALA:HB2	1.75	0.67
1:F:458:HIS:CD2	1:F:460:VAL:H	2.11	0.67
1:G:458:HIS:CD2	1:G:460:VAL:H	2.11	0.67
1:I:295:LEU:O	1:I:388:PRO:CG	2.43	0.67
1:K:399:LEU:HA	1:K:400:PRO:O	1.94	0.67
2:N:43:LEU:CD1	2:N:60:ILE:HD11	2.24	0.67
2:T:59:ILE:HD12	2:T:280:LEU:HD11	1.75	0.67
2:W:43:LEU:CD1	2:W:60:ILE:HD11	2.24	0.67
2:X:43:LEU:CD1	2:X:60:ILE:HD11	2.24	0.67
1:A:53:SER:HB2	1:F:179:TYR:CD2	2.30	0.67
1:B:295:LEU:O	1:B:388:PRO:CG	2.43	0.67
1:J:399:LEU:HA	1:J:400:PRO:O	1.94	0.67
2:W:312:ALA:HB2	2:W:317:ILE:HB	1.77	0.67
1:B:399:LEU:HA	1:B:400:PRO:O	1.94	0.66
1:C:3:GLU:HG2	2:O:338:ALA:HB2	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:HIS:CB	2:O:179:LYS:HZ2	1.85	0.66
1:D:295:LEU:O	1:D:388:PRO:CG	2.43	0.66
1:F:43:PHE:CD2	2:R:370:LYS:HG2	2.31	0.66
1:G:3:GLU:HG2	2:S:338:ALA:HB2	1.75	0.66
1:G:295:LEU:O	1:G:388:PRO:CG	2.43	0.66
1:H:43:PHE:CD2	2:T:370:LYS:HG2	2.31	0.66
1:K:295:LEU:O	1:K:388:PRO:CG	2.43	0.66
1:L:399:LEU:HA	1:L:400:PRO:O	1.94	0.66
2:N:312:ALA:HB2	2:N:317:ILE:HB	1.77	0.66
1:A:399:LEU:HA	1:A:400:PRO:O	1.94	0.66
1:E:3:GLU:HG2	2:Q:338:ALA:HB2	1.75	0.66
1:G:43:PHE:CD2	2:S:370:LYS:HG2	2.31	0.66
1:H:399:LEU:H	1:H:401:PRO:CG	1.90	0.66
2:O:83:LYS:O	2:O:87:ASP:HB2	1.96	0.66
2:Q:43:LEU:CD1	2:Q:60:ILE:HD11	2.24	0.66
2:Q:59:ILE:HD12	2:Q:280:LEU:HD11	1.75	0.66
2:V:83:LYS:O	2:V:87:ASP:HB2	1.96	0.66
1:C:4:HIS:CA	2:O:179:LYS:NZ	2.53	0.66
1:C:399:LEU:HA	1:C:400:PRO:O	1.94	0.66
1:D:3:GLU:OE1	2:P:368:ILE:HA	1.96	0.66
1:F:295:LEU:O	1:F:388:PRO:CG	2.43	0.66
1:H:3:GLU:HG2	2:T:338:ALA:HB2	1.75	0.66
2:N:83:LYS:O	2:N:87:ASP:HB2	1.96	0.66
2:T:43:LEU:CD1	2:T:60:ILE:HD11	2.24	0.66
1:E:43:PHE:CD2	2:Q:370:LYS:HG2	2.31	0.66
1:E:399:LEU:H	1:E:401:PRO:CG	1.90	0.66
1:L:43:PHE:CD2	2:X:370:LYS:HG2	2.31	0.66
1:A:3:GLU:OE2	2:M:338:ALA:CB	2.44	0.66
1:C:295:LEU:O	1:C:388:PRO:CG	2.43	0.66
1:F:3:GLU:OE2	2:R:338:ALA:CB	2.44	0.66
1:G:399:LEU:HA	1:G:400:PRO:O	1.94	0.66
1:I:3:GLU:OE1	2:U:368:ILE:HA	1.96	0.66
1:J:295:LEU:O	1:J:388:PRO:CG	2.43	0.66
2:W:83:LYS:O	2:W:87:ASP:HB2	1.96	0.66
1:A:43:PHE:CD2	2:M:370:LYS:HG2	2.31	0.66
1:E:3:GLU:OE1	2:Q:368:ILE:HA	1.96	0.66
1:G:3:GLU:OE2	2:S:338:ALA:CB	2.44	0.66
1:H:3:GLU:OE1	2:T:368:ILE:HA	1.96	0.66
1:K:3:GLU:OE2	2:W:338:ALA:CB	2.44	0.66
1:K:43:PHE:CD2	2:W:370:LYS:HG2	2.30	0.66
1:L:3:GLU:OE2	2:X:338:ALA:CB	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:PHE:CD2	2:P:370:LYS:HG2	2.31	0.66
1:F:399:LEU:HA	1:F:400:PRO:O	1.94	0.66
1:B:43:PHE:CD2	2:N:370:LYS:HG2	2.31	0.66
1:E:295:LEU:O	1:E:388:PRO:CG	2.43	0.66
1:H:295:LEU:O	1:H:388:PRO:CG	2.43	0.66
2:P:237:THR:O	2:P:237:THR:HG22	1.96	0.66
2:U:237:THR:O	2:U:237:THR:HG22	1.96	0.66
1:B:3:GLU:OE2	2:N:338:ALA:CB	2.44	0.66
1:C:43:PHE:CD2	2:O:370:LYS:HG2	2.31	0.66
1:I:43:PHE:CD2	2:U:370:LYS:HG2	2.31	0.66
1:J:4:HIS:CA	2:V:179:LYS:NZ	2.53	0.66
1:J:43:PHE:CD2	2:V:370:LYS:HG2	2.31	0.66
1:C:3:GLU:OE1	2:O:368:ILE:HA	1.96	0.66
1:G:3:GLU:OE1	2:S:368:ILE:HA	1.96	0.66
1:J:3:GLU:OE1	2:V:368:ILE:HA	1.96	0.66
2:V:312:ALA:HB2	2:V:317:ILE:HB	1.77	0.66
2:O:312:ALA:HB2	2:O:317:ILE:HB	1.77	0.65
1:A:365:ALA:O	1:A:367:PRO:HD3	1.96	0.65
1:A:458:HIS:CD2	1:A:460:VAL:H	2.11	0.65
1:F:3:GLU:OE1	2:R:368:ILE:HA	1.96	0.65
1:L:365:ALA:O	1:L:367:PRO:HD3	1.96	0.65
2:U:83:LYS:O	2:U:87:ASP:HB2	1.96	0.65
1:G:30:HIS:H	1:H:180:PHE:HB3	1.62	0.65
1:I:3:GLU:OE2	2:U:338:ALA:CB	2.44	0.65
2:P:83:LYS:O	2:P:87:ASP:HB2	1.96	0.65
1:D:3:GLU:OE2	2:P:338:ALA:CB	2.44	0.65
2:M:83:LYS:O	2:M:87:ASP:HB2	1.96	0.65
2:Q:312:ALA:HB2	2:Q:317:ILE:HB	1.77	0.65
2:T:312:ALA:HB2	2:T:317:ILE:HB	1.77	0.65
2:R:312:ALA:HB2	2:R:317:ILE:HB	1.77	0.65
1:A:43:PHE:CG	2:M:370:LYS:HG2	2.32	0.65
1:E:3:GLU:OE2	2:Q:338:ALA:CB	2.44	0.65
1:L:458:HIS:CD2	1:L:460:VAL:H	2.11	0.65
1:D:461:GLU:OE1	1:J:320:LYS:NZ	2.26	0.65
1:J:3:GLU:OE2	2:V:338:ALA:CB	2.44	0.65
1:K:43:PHE:CG	2:W:370:LYS:HG2	2.32	0.65
2:S:83:LYS:O	2:S:87:ASP:HB2	1.96	0.65
1:A:29:GLN:OE1	1:F:181:PRO:HD3	1.96	0.65
1:B:43:PHE:CG	2:N:370:LYS:HG2	2.32	0.65
1:H:399:LEU:N	1:H:401:PRO:CG	2.52	0.65
1:I:30:HIS:H	1:J:180:PHE:HB3	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:83:LYS:O	2:R:87:ASP:HB2	1.96	0.65
1:C:3:GLU:OE2	2:O:338:ALA:CB	2.44	0.65
1:D:43:PHE:CG	2:P:370:LYS:HG2	2.32	0.65
1:H:3:GLU:OE2	2:T:338:ALA:CB	2.44	0.65
1:J:61:ASN:O	1:K:337:ARG:CB	2.34	0.65
2:P:312:ALA:HB2	2:P:317:ILE:HB	1.77	0.65
2:R:43:LEU:HD13	2:R:60:ILE:HD11	1.79	0.65
2:X:83:LYS:O	2:X:87:ASP:HB2	1.96	0.65
1:F:43:PHE:CG	2:R:370:LYS:HG2	2.32	0.65
1:L:3:GLU:OE1	2:X:368:ILE:HA	1.96	0.65
1:L:43:PHE:CG	2:X:370:LYS:HG2	2.32	0.65
2:S:43:LEU:HD13	2:S:60:ILE:HD11	1.79	0.65
2:X:237:THR:O	2:X:237:THR:HG22	1.96	0.65
2:X:369:THR:CA	2:X:370:LYS:N	2.59	0.65
1:A:3:GLU:OE1	2:M:368:ILE:HA	1.96	0.64
1:B:365:ALA:O	1:B:367:PRO:HD3	1.96	0.64
1:F:365:ALA:O	1:F:367:PRO:HD3	1.96	0.64
1:I:43:PHE:CG	2:U:370:LYS:HG2	2.32	0.64
2:M:237:THR:O	2:M:237:THR:HG22	1.96	0.64
2:Q:237:THR:HG22	2:Q:237:THR:O	1.96	0.64
2:S:312:ALA:HB2	2:S:317:ILE:HB	1.77	0.64
2:T:43:LEU:HD13	2:T:60:ILE:HD11	1.79	0.64
2:T:83:LYS:O	2:T:87:ASP:HB2	1.96	0.64
1:A:4:HIS:CA	2:M:179:LYS:NZ	2.53	0.64
1:C:43:PHE:CG	2:O:370:LYS:HG2	2.32	0.64
1:C:179:TYR:CD2	1:D:53:SER:HB2	2.32	0.64
1:J:43:PHE:CG	2:V:370:LYS:HG2	2.32	0.64
1:K:365:ALA:O	1:K:367:PRO:HD3	1.96	0.64
2:Q:43:LEU:HD13	2:Q:60:ILE:HD11	1.79	0.64
1:B:458:HIS:CD2	1:B:460:VAL:H	2.11	0.64
1:E:365:ALA:O	1:E:367:PRO:HD3	1.96	0.64
1:E:399:LEU:N	1:E:401:PRO:CG	2.52	0.64
1:G:43:PHE:CG	2:S:370:LYS:HG2	2.32	0.64
1:G:365:ALA:O	1:G:367:PRO:HD3	1.97	0.64
2:M:312:ALA:HB2	2:M:317:ILE:HB	1.77	0.64
2:N:237:THR:HG22	2:N:237:THR:O	1.96	0.64
2:Q:83:LYS:O	2:Q:87:ASP:HB2	1.96	0.64
2:W:237:THR:O	2:W:237:THR:HG22	1.96	0.64
2:X:312:ALA:HB2	2:X:317:ILE:HB	1.77	0.64
1:B:3:GLU:OE1	2:N:368:ILE:HA	1.96	0.64
1:B:170:GLY:HA2	1:B:172:ARG:NH2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:LEU:N	1:C:401:PRO:CG	2.52	0.64
1:H:53:SER:HB2	1:I:179:TYR:CD2	2.32	0.64
1:K:170:GLY:HA2	1:K:172:ARG:NH2	2.13	0.64
2:T:237:THR:O	2:T:237:THR:HG22	1.96	0.64
2:U:43:LEU:HD13	2:U:60:ILE:HD11	1.79	0.64
2:U:312:ALA:HB2	2:U:317:ILE:HB	1.77	0.64
1:A:170:GLY:HA2	1:A:172:ARG:NH2	2.13	0.64
1:C:458:HIS:CD2	1:C:460:VAL:H	2.11	0.64
1:D:170:GLY:HA2	1:D:172:ARG:NH2	2.13	0.64
1:E:43:PHE:CG	2:Q:370:LYS:HG2	2.32	0.64
1:E:461:GLU:OE1	1:K:320:LYS:NZ	2.27	0.64
1:I:170:GLY:HA2	1:I:172:ARG:NH2	2.13	0.64
1:J:365:ALA:O	1:J:367:PRO:HD3	1.96	0.64
1:K:3:GLU:OE1	2:W:368:ILE:HA	1.96	0.64
2:N:369:THR:CA	2:N:370:LYS:N	2.59	0.64
2:P:43:LEU:HD13	2:P:60:ILE:HD11	1.80	0.64
1:B:211:HIS:HD2	1:B:212:GLU:O	1.81	0.64
1:H:43:PHE:CG	2:T:370:LYS:HG2	2.32	0.64
1:J:399:LEU:N	1:J:401:PRO:CG	2.52	0.64
1:K:211:HIS:HD2	1:K:212:GLU:O	1.81	0.64
1:K:458:HIS:CD2	1:K:460:VAL:H	2.12	0.64
1:L:170:GLY:HA2	1:L:172:ARG:NH2	2.13	0.64
2:V:237:THR:HG22	2:V:237:THR:O	1.96	0.64
2:W:369:THR:CA	2:W:370:LYS:N	2.59	0.64
1:C:365:ALA:O	1:C:367:PRO:HD3	1.96	0.64
1:D:399:LEU:H	1:D:401:PRO:CG	1.90	0.64
1:J:170:GLY:HA2	1:J:172:ARG:NH2	2.13	0.64
1:L:3:GLU:HG2	2:X:338:ALA:CB	2.28	0.64
1:L:4:HIS:CA	2:X:179:LYS:NZ	2.53	0.64
2:M:43:LEU:HD13	2:M:60:ILE:HD11	1.79	0.64
2:O:237:THR:O	2:O:237:THR:HG22	1.96	0.64
2:Q:59:ILE:CD1	2:Q:280:LEU:HD21	2.28	0.64
2:R:59:ILE:CD1	2:R:280:LEU:HD21	2.28	0.64
2:S:59:ILE:CD1	2:S:280:LEU:HD21	2.28	0.64
2:S:237:THR:HG22	2:S:237:THR:O	1.96	0.64
1:D:4:HIS:CD2	2:P:178:ILE:CG1	2.58	0.64
1:I:365:ALA:O	1:I:367:PRO:HD3	1.96	0.64
2:M:59:ILE:CD1	2:M:280:LEU:HD21	2.28	0.64
2:T:59:ILE:CD1	2:T:280:LEU:HD21	2.28	0.64
2:X:59:ILE:CD1	2:X:280:LEU:HD21	2.28	0.64
1:A:3:GLU:HG2	2:M:338:ALA:CB	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:GLY:HA2	1:C:172:ARG:NH2	2.13	0.64
1:H:365:ALA:O	1:H:367:PRO:HD3	1.96	0.64
1:I:211:HIS:HD2	1:I:212:GLU:O	1.81	0.64
1:J:458:HIS:CD2	1:J:460:VAL:H	2.11	0.64
2:M:369:THR:CA	2:M:370:LYS:N	2.59	0.64
2:R:237:THR:O	2:R:237:THR:HG22	1.96	0.64
1:C:3:GLU:HG2	2:O:338:ALA:CB	2.28	0.64
1:D:211:HIS:HD2	1:D:212:GLU:O	1.81	0.64
1:D:320:LYS:NZ	1:J:461:GLU:OE1	2.28	0.64
1:D:458:HIS:CD2	1:D:460:VAL:H	2.11	0.64
1:E:320:LYS:NZ	1:K:461:GLU:OE1	2.27	0.64
2:P:59:ILE:CD1	2:P:280:LEU:HD21	2.28	0.64
2:X:43:LEU:HD13	2:X:60:ILE:HD11	1.79	0.64
1:D:3:GLU:HG2	2:P:338:ALA:CB	2.28	0.63
1:D:365:ALA:O	1:D:367:PRO:HD3	1.96	0.63
1:E:458:HIS:CD2	1:E:460:VAL:H	2.11	0.63
1:F:3:GLU:HG2	2:R:338:ALA:CB	2.28	0.63
1:F:386:ILE:O	1:F:388:PRO:HD3	1.99	0.63
1:G:3:GLU:HG2	2:S:338:ALA:CB	2.28	0.63
1:G:386:ILE:O	1:G:388:PRO:HD3	1.99	0.63
1:I:3:GLU:HG2	2:U:338:ALA:CB	2.28	0.63
1:J:3:GLU:HG2	2:V:338:ALA:CB	2.28	0.63
1:J:211:HIS:HD2	1:J:212:GLU:O	1.81	0.63
2:O:43:LEU:HD13	2:O:60:ILE:HD11	1.79	0.63
2:T:369:THR:CA	2:T:370:LYS:N	2.59	0.63
2:U:59:ILE:CD1	2:U:280:LEU:HD21	2.28	0.63
2:V:43:LEU:HD13	2:V:60:ILE:HD11	1.79	0.63
1:C:211:HIS:HD2	1:C:212:GLU:O	1.81	0.63
1:E:170:GLY:HA2	1:E:172:ARG:NH2	2.13	0.63
1:E:211:HIS:HD2	1:E:212:GLU:O	1.81	0.63
1:G:211:HIS:HD2	1:G:212:GLU:O	1.81	0.63
1:H:211:HIS:HD2	1:H:212:GLU:O	1.81	0.63
1:I:458:HIS:CD2	1:I:460:VAL:H	2.11	0.63
1:E:386:ILE:O	1:E:388:PRO:HD3	1.99	0.63
1:I:4:HIS:CD2	2:U:178:ILE:CG1	2.59	0.63
1:I:399:LEU:H	1:I:401:PRO:CG	1.90	0.63
2:O:59:ILE:CD1	2:O:280:LEU:HD21	2.28	0.63
2:Q:369:THR:CA	2:Q:370:LYS:N	2.59	0.63
1:H:386:ILE:O	1:H:388:PRO:HD3	1.99	0.63
1:J:399:LEU:H	1:J:401:PRO:CG	1.90	0.63
2:V:59:ILE:CD1	2:V:280:LEU:HD21	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ILE:O	1:A:388:PRO:HD3	1.99	0.63
1:E:235:ILE:CG2	1:E:367:PRO:HG3	2.28	0.63
1:H:3:GLU:HG2	2:T:338:ALA:CB	2.28	0.63
1:H:170:GLY:HA2	1:H:172:ARG:NH2	2.13	0.63
1:H:458:HIS:CD2	1:H:460:VAL:H	2.11	0.63
2:N:43:LEU:HD13	2:N:60:ILE:HD11	1.79	0.63
1:E:3:GLU:HG2	2:Q:338:ALA:CB	2.28	0.63
1:F:211:HIS:HD2	1:F:212:GLU:O	1.81	0.63
1:F:320:LYS:NZ	1:L:461:GLU:OE1	2.27	0.63
1:H:235:ILE:CG2	1:H:367:PRO:HG3	2.28	0.63
1:K:3:GLU:HG2	2:W:338:ALA:CB	2.28	0.63
1:L:386:ILE:O	1:L:388:PRO:HD3	1.99	0.63
2:N:59:ILE:CD1	2:N:280:LEU:HD21	2.28	0.63
2:W:59:ILE:CD1	2:W:280:LEU:HD21	2.28	0.63
1:F:170:GLY:HA2	1:F:172:ARG:NH2	2.13	0.63
1:K:396:LEU:HD12	1:K:398:ASP:H	1.64	0.63
2:S:369:THR:CA	2:S:370:LYS:N	2.59	0.63
2:W:43:LEU:HD13	2:W:60:ILE:HD11	1.79	0.63
1:B:3:GLU:HG2	2:N:338:ALA:CB	2.28	0.63
1:B:396:LEU:HD12	1:B:398:ASP:H	1.64	0.63
1:G:170:GLY:HA2	1:G:172:ARG:NH2	2.13	0.63
2:O:48:PRO:O	2:O:52:ALA:HB2	1.99	0.63
2:V:48:PRO:O	2:V:52:ALA:HB2	1.99	0.63
1:A:211:HIS:HD2	1:A:212:GLU:O	1.81	0.63
1:E:396:LEU:HD12	1:E:398:ASP:H	1.64	0.63
1:H:396:LEU:HD12	1:H:398:ASP:H	1.64	0.63
1:L:211:HIS:HD2	1:L:212:GLU:O	1.81	0.63
2:R:369:THR:CA	2:R:370:LYS:N	2.59	0.63
1:G:396:LEU:HD12	1:G:398:ASP:H	1.64	0.62
2:S:48:PRO:O	2:S:52:ALA:HB2	1.99	0.62
2:W:309:GLU:O	2:W:313:LYS:CE	2.47	0.62
1:D:396:LEU:HD12	1:D:398:ASP:H	1.64	0.62
2:N:309:GLU:O	2:N:313:LYS:CE	2.47	0.62
2:Q:48:PRO:O	2:Q:52:ALA:HB2	1.99	0.62
2:R:48:PRO:O	2:R:52:ALA:HB2	1.99	0.62
2:T:48:PRO:O	2:T:52:ALA:HB2	1.99	0.62
1:B:4:HIS:CD2	2:N:178:ILE:CG1	2.58	0.62
1:F:396:LEU:HD12	1:F:398:ASP:H	1.64	0.62
1:I:396:LEU:HD12	1:I:398:ASP:H	1.64	0.62
2:M:48:PRO:O	2:M:52:ALA:HB2	1.99	0.62
2:P:48:PRO:O	2:P:52:ALA:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:48:PRO:O	2:X:52:ALA:HB2	1.99	0.62
1:I:386:ILE:O	1:I:388:PRO:HD3	1.99	0.62
1:K:383:LYS:C	1:K:384:ASN:HD22	2.08	0.62
2:U:369:THR:CA	2:U:370:LYS:N	2.59	0.62
1:A:396:LEU:HD12	1:A:398:ASP:H	1.64	0.62
1:C:396:LEU:HD12	1:C:398:ASP:H	1.64	0.62
1:D:386:ILE:O	1:D:388:PRO:HD3	1.99	0.62
1:L:396:LEU:HD12	1:L:398:ASP:H	1.64	0.62
2:U:48:PRO:O	2:U:52:ALA:HB2	1.99	0.62
1:B:383:LYS:C	1:B:384:ASN:HD22	2.08	0.62
1:C:399:LEU:H	1:C:401:PRO:CG	1.90	0.62
1:I:399:LEU:N	1:I:401:PRO:CG	2.52	0.62
1:K:4:HIS:CD2	2:W:178:ILE:CG1	2.58	0.62
2:O:369:THR:CA	2:O:370:LYS:N	2.59	0.62
2:N:48:PRO:O	2:N:52:ALA:HB2	1.99	0.62
2:P:369:THR:CA	2:P:370:LYS:N	2.59	0.62
2:V:369:THR:CA	2:V:370:LYS:N	2.59	0.62
1:B:4:HIS:CA	2:N:179:LYS:NZ	2.53	0.62
1:E:383:LYS:C	1:E:384:ASN:HD22	2.08	0.62
1:J:396:LEU:HD12	1:J:398:ASP:H	1.64	0.62
2:W:48:PRO:O	2:W:52:ALA:HB2	1.99	0.62
1:C:235:ILE:CG2	1:C:367:PRO:HG3	2.27	0.62
1:D:399:LEU:N	1:D:401:PRO:CG	2.52	0.62
1:G:383:LYS:C	1:G:384:ASN:HD22	2.08	0.62
1:H:383:LYS:C	1:H:384:ASN:HD22	2.08	0.62
1:J:386:ILE:O	1:J:388:PRO:HD3	1.99	0.62
2:M:309:GLU:O	2:M:313:LYS:CE	2.47	0.62
2:Q:309:GLU:O	2:Q:313:LYS:CE	2.47	0.62
1:A:383:LYS:C	1:A:384:ASN:HD22	2.08	0.61
1:B:386:ILE:O	1:B:388:PRO:HD3	1.99	0.61
1:C:386:ILE:O	1:C:388:PRO:HD3	1.99	0.61
1:F:383:LYS:C	1:F:384:ASN:HD22	2.08	0.61
1:J:383:LYS:C	1:J:384:ASN:HD22	2.08	0.61
1:K:399:LEU:N	1:K:401:PRO:CG	2.52	0.61
2:R:1:LYS:CA	2:R:54:GLY:O	2.48	0.61
2:T:309:GLU:O	2:T:313:LYS:CE	2.47	0.61
1:B:427:PHE:CE1	1:B:428:LEU:HD13	2.35	0.61
1:C:383:LYS:C	1:C:384:ASN:HD22	2.08	0.61
1:K:386:ILE:O	1:K:388:PRO:HD3	1.99	0.61
1:L:383:LYS:C	1:L:384:ASN:HD22	2.08	0.61
2:X:309:GLU:O	2:X:313:LYS:CE	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:LEU:N	1:B:401:PRO:CG	2.52	0.61
1:C:427:PHE:CE1	1:C:428:LEU:HD13	2.35	0.61
1:D:383:LYS:C	1:D:384:ASN:HD22	2.08	0.61
1:I:383:LYS:C	1:I:384:ASN:HD22	2.08	0.61
1:K:427:PHE:CE1	1:K:428:LEU:HD13	2.36	0.61
1:B:155:GLU:OE1	1:B:211:HIS:HE1	1.83	0.61
1:J:235:ILE:CG2	1:J:367:PRO:HG3	2.28	0.61
1:J:427:PHE:CE1	1:J:428:LEU:HD13	2.35	0.61
1:K:7:THR:HG21	2:W:335:GLN:OE1	2.01	0.61
1:K:155:GLU:OE1	1:K:211:HIS:HE1	1.83	0.61
2:S:1:LYS:CA	2:S:54:GLY:O	2.48	0.61
1:L:155:GLU:OE1	1:L:211:HIS:HE1	1.83	0.61
1:A:7:THR:HG21	2:M:335:GLN:OE1	2.01	0.61
1:A:155:GLU:OE1	1:A:211:HIS:HE1	1.83	0.61
1:C:4:HIS:CD2	2:O:178:ILE:CG1	2.58	0.61
1:D:7:THR:HG21	2:P:335:GLN:OE1	2.01	0.61
1:D:235:ILE:CG2	1:D:367:PRO:HG3	2.28	0.61
1:F:7:THR:HG21	2:R:335:GLN:OE1	2.01	0.61
1:G:7:THR:HG21	2:S:335:GLN:OE1	2.01	0.61
1:I:7:THR:HG21	2:U:335:GLN:OE1	2.01	0.61
1:K:53:SER:HB2	1:L:179:TYR:CD2	2.35	0.61
1:L:7:THR:HG21	2:X:335:GLN:OE1	2.01	0.61
1:A:180:PHE:HB3	1:B:30:HIS:H	1.65	0.61
1:B:7:THR:HG21	2:N:335:GLN:OE1	2.01	0.61
1:C:7:THR:HG21	2:O:335:GLN:OE1	2.01	0.61
1:J:7:THR:HG21	2:V:335:GLN:OE1	2.01	0.61
1:L:334:TYR:CE2	1:L:391:PRO:HG3	2.36	0.61
2:U:149:PHE:CE1	2:U:204:MET:HE1	2.36	0.61
2:X:149:PHE:CE1	2:X:204:MET:HE1	2.36	0.61
1:A:334:TYR:CE2	1:A:391:PRO:HG3	2.36	0.61
1:A:461:GLU:OE1	1:G:320:LYS:NZ	2.25	0.61
1:B:360:PHE:CG	1:B:361:PRO:HD3	2.35	0.61
1:D:427:PHE:CE1	1:D:428:LEU:HD13	2.35	0.61
1:E:155:GLU:OE1	1:E:211:HIS:HE1	1.83	0.61
1:K:360:PHE:CG	1:K:361:PRO:HD3	2.35	0.61
2:M:149:PHE:CE1	2:M:204:MET:HE1	2.36	0.61
2:P:149:PHE:CE1	2:P:204:MET:HE1	2.36	0.61
1:C:180:PHE:HB3	1:D:30:HIS:H	1.66	0.61
1:D:155:GLU:OE1	1:D:211:HIS:HE1	1.83	0.61
1:F:360:PHE:CG	1:F:361:PRO:HD3	2.35	0.61
1:H:155:GLU:OE1	1:H:211:HIS:HE1	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:155:GLU:OE1	1:I:211:HIS:HE1	1.83	0.61
1:I:235:ILE:CG2	1:I:367:PRO:HG3	2.28	0.61
2:Q:45:GLU:O	2:Q:48:PRO:HD2	2.01	0.61
2:T:45:GLU:O	2:T:48:PRO:HD2	2.01	0.61
1:C:334:TYR:CE2	1:C:391:PRO:HG3	2.36	0.60
1:E:427:PHE:CE1	1:E:428:LEU:HD13	2.35	0.60
1:H:360:PHE:CG	1:H:361:PRO:HD3	2.35	0.60
1:I:427:PHE:CE1	1:I:428:LEU:HD13	2.36	0.60
1:J:155:GLU:OE1	1:J:211:HIS:HE1	1.83	0.60
1:K:29:GLN:OE1	1:L:181:PRO:HD3	2.01	0.60
2:O:45:GLU:O	2:O:48:PRO:HD2	2.01	0.60
2:O:149:PHE:CE1	2:O:204:MET:HE1	2.36	0.60
2:S:45:GLU:O	2:S:48:PRO:HD2	2.01	0.60
2:S:149:PHE:CE1	2:S:204:MET:HE1	2.36	0.60
2:U:45:GLU:O	2:U:48:PRO:HD2	2.01	0.60
1:A:427:PHE:CE1	1:A:428:LEU:HD13	2.36	0.60
1:E:360:PHE:CG	1:E:361:PRO:HD3	2.35	0.60
1:H:427:PHE:CE1	1:H:428:LEU:HD13	2.36	0.60
1:L:427:PHE:CE1	1:L:428:LEU:HD13	2.36	0.60
2:P:45:GLU:O	2:P:48:PRO:HD2	2.01	0.60
2:Q:149:PHE:CE1	2:Q:204:MET:HE1	2.36	0.60
2:R:45:GLU:O	2:R:48:PRO:HD2	2.01	0.60
2:T:149:PHE:CE1	2:T:204:MET:HE1	2.36	0.60
2:V:45:GLU:O	2:V:48:PRO:HD2	2.01	0.60
2:W:149:PHE:CE1	2:W:204:MET:HE1	2.36	0.60
1:C:155:GLU:OE1	1:C:211:HIS:HE1	1.83	0.60
1:C:248:ARG:HH21	1:C:248:ARG:HG2	1.65	0.60
1:H:334:TYR:CE2	1:H:391:PRO:HG3	2.36	0.60
1:J:4:HIS:CD2	2:V:178:ILE:CG1	2.58	0.60
1:J:248:ARG:HH21	1:J:248:ARG:HG2	1.66	0.60
2:N:149:PHE:CE1	2:N:204:MET:HE1	2.36	0.60
2:P:309:GLU:O	2:P:313:LYS:CE	2.47	0.60
2:V:149:PHE:CE1	2:V:204:MET:HE1	2.36	0.60
1:E:7:THR:HG21	2:Q:335:GLN:OE1	2.01	0.60
1:E:334:TYR:CE2	1:E:391:PRO:HG3	2.36	0.60
1:J:323:VAL:O	1:J:325:GLY:N	2.35	0.60
1:J:334:TYR:CE2	1:J:391:PRO:HG3	2.36	0.60
1:L:3:GLU:OE1	2:X:367:ARG:O	2.20	0.60
2:N:45:GLU:O	2:N:48:PRO:HD2	2.01	0.60
2:R:149:PHE:CE1	2:R:204:MET:HE1	2.36	0.60
2:W:45:GLU:O	2:W:48:PRO:HD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:OE1	2:M:367:ARG:O	2.20	0.60
1:C:320:LYS:NZ	1:I:461:GLU:OE1	2.30	0.60
1:C:323:VAL:O	1:C:325:GLY:N	2.35	0.60
1:D:334:TYR:CE2	1:D:391:PRO:HG3	2.36	0.60
1:D:360:PHE:CG	1:D:361:PRO:HD3	2.35	0.60
1:E:180:PHE:HB3	1:F:30:HIS:H	1.66	0.60
1:G:360:PHE:CG	1:G:361:PRO:HD3	2.35	0.60
1:H:7:THR:HG21	2:T:335:GLN:OE1	2.01	0.60
1:I:360:PHE:CG	1:I:361:PRO:HD3	2.35	0.60
2:P:1:LYS:CA	2:P:54:GLY:O	2.48	0.60
1:F:461:GLU:OE1	1:L:320:LYS:NZ	2.30	0.60
1:I:334:TYR:CE2	1:I:391:PRO:HG3	2.36	0.60
2:N:1:LYS:CA	2:N:54:GLY:O	2.48	0.60
2:U:309:GLU:O	2:U:313:LYS:CE	2.47	0.60
2:W:1:LYS:CA	2:W:54:GLY:O	2.48	0.60
1:B:334:TYR:CE2	1:B:391:PRO:HG3	2.36	0.60
1:E:248:ARG:HH21	1:E:248:ARG:HG2	1.66	0.60
1:E:323:VAL:O	1:E:325:GLY:N	2.35	0.60
1:F:155:GLU:OE1	1:F:211:HIS:HE1	1.83	0.60
1:G:334:TYR:CE2	1:G:391:PRO:HG3	2.36	0.60
1:G:427:PHE:CE1	1:G:428:LEU:HD13	2.36	0.60
1:K:334:TYR:CE2	1:K:391:PRO:HG3	2.36	0.60
2:R:309:GLU:O	2:R:313:LYS:CE	2.47	0.60
2:U:1:LYS:CA	2:U:54:GLY:O	2.48	0.60
1:C:181:PRO:HD3	1:D:29:GLN:OE1	2.01	0.60
1:F:427:PHE:CE1	1:F:428:LEU:HD13	2.36	0.60
1:H:248:ARG:HH21	1:H:248:ARG:HG2	1.66	0.60
1:B:3:GLU:OE1	2:N:367:ARG:O	2.20	0.60
1:F:3:GLU:OE1	2:R:367:ARG:O	2.20	0.60
1:H:323:VAL:O	1:H:325:GLY:N	2.35	0.60
2:T:64:HIS:CD2	2:T:261:VAL:H	2.19	0.60
1:B:248:ARG:HH21	1:B:248:ARG:HG2	1.66	0.60
1:F:334:TYR:CE2	1:F:391:PRO:HG3	2.36	0.60
1:G:155:GLU:OE1	1:G:211:HIS:HE1	1.83	0.60
1:I:3:GLU:OE1	2:U:367:ARG:O	2.19	0.60
1:K:248:ARG:HH21	1:K:248:ARG:HG2	1.66	0.60
2:X:45:GLU:O	2:X:48:PRO:HD2	2.01	0.60
1:I:248:ARG:HH21	1:I:248:ARG:HG2	1.66	0.59
2:S:309:GLU:O	2:S:313:LYS:CE	2.47	0.59
1:D:3:GLU:OE1	2:P:367:ARG:O	2.20	0.59
1:G:3:GLU:OE1	2:S:367:ARG:O	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:3:GLU:OE1	2:W:367:ARG:O	2.20	0.59
2:M:45:GLU:O	2:M:48:PRO:HD2	2.01	0.59
2:Q:64:HIS:CD2	2:Q:261:VAL:H	2.19	0.59
1:D:248:ARG:HH21	1:D:248:ARG:HG2	1.65	0.59
1:J:43:PHE:CG	2:V:370:LYS:HE2	2.32	0.59
1:A:235:ILE:CG2	1:A:367:PRO:HG3	2.27	0.59
1:A:323:VAL:O	1:A:325:GLY:N	2.35	0.59
1:B:323:VAL:O	1:B:325:GLY:N	2.35	0.59
1:K:323:VAL:O	1:K:325:GLY:N	2.35	0.59
1:D:181:PRO:HD3	1:E:29:GLN:OE1	2.02	0.59
1:I:323:VAL:O	1:I:325:GLY:N	2.35	0.59
1:A:248:ARG:HH21	1:A:248:ARG:HG2	1.66	0.59
1:J:3:GLU:OE1	2:V:367:ARG:O	2.20	0.59
1:K:360:PHE:CE2	1:K:361:PRO:HD3	2.37	0.59
2:O:136:ASP:O	2:O:140:LYS:HB2	2.02	0.59
2:V:136:ASP:O	2:V:140:LYS:HB2	2.03	0.59
1:B:360:PHE:CE2	1:B:361:PRO:HD3	2.37	0.59
1:C:3:GLU:OE1	2:O:367:ARG:O	2.20	0.59
1:C:43:PHE:CG	2:O:370:LYS:HE2	2.32	0.59
1:D:44:GLU:HG3	2:P:370:LYS:HZ3	1.67	0.59
1:L:323:VAL:O	1:L:325:GLY:N	2.35	0.59
2:W:136:ASP:O	2:W:140:LYS:HB2	2.03	0.59
1:D:323:VAL:O	1:D:325:GLY:N	2.35	0.59
1:G:180:PHE:HB3	1:L:30:HIS:H	1.68	0.59
1:I:332:LEU:HB2	1:I:408:PRO:HB2	1.85	0.59
1:L:235:ILE:CG2	1:L:367:PRO:HG3	2.28	0.59
2:N:136:ASP:O	2:N:140:LYS:HB2	2.03	0.59
1:C:18:ASP:OD2	1:C:30:HIS:HD2	1.86	0.59
1:D:332:LEU:HB2	1:D:408:PRO:HB2	1.85	0.59
1:F:44:GLU:HG3	2:R:370:LYS:HZ3	1.68	0.59
1:I:44:GLU:HG3	2:U:370:LYS:HZ3	1.67	0.59
1:J:360:PHE:CE2	1:J:361:PRO:HD3	2.36	0.59
1:L:248:ARG:HH21	1:L:248:ARG:HG2	1.66	0.59
1:C:360:PHE:CE2	1:C:361:PRO:HD3	2.37	0.58
1:D:18:ASP:OD2	1:D:30:HIS:HD2	1.86	0.58
1:E:118:THR:OG1	1:E:120:ILE:HG13	2.03	0.58
1:F:248:ARG:HH21	1:F:248:ARG:HG2	1.66	0.58
1:H:3:GLU:OE1	2:T:367:ARG:O	2.20	0.58
1:J:118:THR:OG1	1:J:120:ILE:HG13	2.03	0.58
2:U:64:HIS:CD2	2:U:261:VAL:H	2.19	0.58
1:B:399:LEU:H	1:B:401:PRO:CG	1.90	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:THR:OG1	1:C:120:ILE:HG13	2.04	0.58
1:G:323:VAL:O	1:G:325:GLY:N	2.35	0.58
1:G:332:LEU:HB2	1:G:408:PRO:HB2	1.85	0.58
1:H:44:GLU:HG3	2:T:370:LYS:HZ3	1.67	0.58
1:H:118:THR:OG1	1:H:120:ILE:HG13	2.04	0.58
1:I:18:ASP:OD2	1:I:30:HIS:HD2	1.86	0.58
1:J:18:ASP:OD2	1:J:30:HIS:HD2	1.86	0.58
1:K:399:LEU:H	1:K:401:PRO:CG	1.90	0.58
2:U:3:GLU:O	2:U:4:GLU:CB	2.51	0.58
1:B:18:ASP:OD2	1:B:30:HIS:HD2	1.86	0.58
1:E:3:GLU:OE1	2:Q:367:ARG:O	2.20	0.58
2:P:64:HIS:CD2	2:P:261:VAL:H	2.19	0.58
2:Q:136:ASP:O	2:Q:140:LYS:HB2	2.03	0.58
2:T:136:ASP:O	2:T:140:LYS:HB2	2.02	0.58
2:U:136:ASP:O	2:U:140:LYS:HB2	2.02	0.58
1:C:360:PHE:CG	1:C:361:PRO:HD3	2.35	0.58
1:I:53:SER:HB2	1:J:179:TYR:CD2	2.38	0.58
1:K:18:ASP:OD2	1:K:30:HIS:HD2	1.86	0.58
2:M:136:ASP:O	2:M:140:LYS:HB2	2.02	0.58
2:P:3:GLU:O	2:P:4:GLU:CB	2.51	0.58
2:X:136:ASP:O	2:X:140:LYS:HB2	2.02	0.58
1:E:44:GLU:HG3	2:Q:370:LYS:HZ3	1.66	0.58
1:F:323:VAL:O	1:F:325:GLY:N	2.35	0.58
1:I:118:THR:OG1	1:I:120:ILE:HG13	2.04	0.58
2:O:136:ASP:OD2	2:O:140:LYS:NZ	2.35	0.58
2:P:136:ASP:O	2:P:140:LYS:HB2	2.02	0.58
1:D:118:THR:OG1	1:D:120:ILE:HG13	2.04	0.58
1:F:332:LEU:HB2	1:F:408:PRO:HB2	1.85	0.58
1:H:18:ASP:OD2	1:H:30:HIS:HD2	1.86	0.58
2:M:1:LYS:CA	2:M:54:GLY:O	2.48	0.58
2:R:136:ASP:O	2:R:140:LYS:HB2	2.02	0.58
2:X:1:LYS:CA	2:X:54:GLY:O	2.48	0.58
1:A:18:ASP:OD2	1:A:30:HIS:HD2	1.86	0.58
1:C:332:LEU:HB2	1:C:408:PRO:HB2	1.85	0.58
1:E:18:ASP:OD2	1:E:30:HIS:HD2	1.86	0.58
1:E:82:ASP:O	1:E:84:THR:CG2	2.51	0.58
1:H:82:ASP:O	1:H:84:THR:CG2	2.51	0.58
1:J:332:LEU:HB2	1:J:408:PRO:HB2	1.85	0.58
2:S:136:ASP:O	2:S:140:LYS:HB2	2.02	0.58
1:B:235:ILE:CG2	1:B:367:PRO:HG3	2.28	0.58
1:D:192:ARG:HH21	1:D:219:ASN:HD22	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:GLU:HG3	2:S:370:LYS:HZ3	1.66	0.58
1:I:192:ARG:HH21	1:I:219:ASN:HD22	1.52	0.58
2:V:1:LYS:CA	2:V:54:GLY:O	2.48	0.58
1:C:308:ILE:HG21	1:C:374:LEU:HD13	1.86	0.58
1:F:443:ILE:O	1:F:447:ARG:HG3	2.04	0.58
1:G:248:ARG:HH21	1:G:248:ARG:HG2	1.66	0.58
1:J:44:GLU:HG3	2:V:370:LYS:HZ3	1.68	0.58
1:J:360:PHE:CG	1:J:361:PRO:HD3	2.35	0.58
1:K:235:ILE:CG2	1:K:367:PRO:HG3	2.27	0.58
2:O:1:LYS:CA	2:O:54:GLY:O	2.48	0.58
1:A:43:PHE:CB	2:M:370:LYS:CD	2.82	0.58
1:C:180:PHE:O	1:D:29:GLN:HA	2.04	0.58
1:D:308:ILE:HG21	1:D:374:LEU:HD13	1.86	0.58
1:F:18:ASP:OD2	1:F:30:HIS:HD2	1.86	0.58
1:G:443:ILE:O	1:G:447:ARG:HG3	2.04	0.58
1:I:43:PHE:CG	2:U:370:LYS:HE2	2.32	0.58
2:M:128:THR:HG22	2:M:131:GLU:H	1.69	0.58
2:N:128:THR:HG22	2:N:131:GLU:H	1.69	0.58
2:V:3:GLU:O	2:V:4:GLU:CB	2.51	0.58
2:V:64:HIS:CD2	2:V:261:VAL:H	2.19	0.58
1:B:43:PHE:CG	2:N:370:LYS:HE2	2.32	0.57
1:B:308:ILE:HG21	1:B:374:LEU:HD13	1.86	0.57
1:E:43:PHE:CB	2:Q:370:LYS:CD	2.82	0.57
1:G:53:SER:HB2	1:H:179:TYR:CD2	2.40	0.57
1:H:332:LEU:HB2	1:H:408:PRO:HB2	1.85	0.57
1:J:308:ILE:HG21	1:J:374:LEU:HD13	1.86	0.57
1:K:43:PHE:CB	2:W:370:LYS:CD	2.82	0.57
1:K:308:ILE:HG21	1:K:374:LEU:HD13	1.86	0.57
1:L:18:ASP:OD2	1:L:30:HIS:HD2	1.86	0.57
2:M:136:ASP:OD2	2:M:203:HIS:CD2	2.56	0.57
2:Q:128:THR:HG22	2:Q:131:GLU:H	1.69	0.57
2:R:3:GLU:O	2:R:4:GLU:CB	2.51	0.57
2:T:128:THR:HG22	2:T:131:GLU:H	1.69	0.57
2:W:128:THR:HG22	2:W:131:GLU:H	1.69	0.57
2:X:128:THR:HG22	2:X:131:GLU:H	1.69	0.57
1:A:44:GLU:HG3	2:M:370:LYS:HZ3	1.67	0.57
1:B:179:TYR:CD2	1:C:53:SER:HB2	2.38	0.57
1:E:443:ILE:O	1:E:447:ARG:HG3	2.04	0.57
1:G:18:ASP:OD2	1:G:30:HIS:HD2	1.87	0.57
1:G:192:ARG:HH21	1:G:219:ASN:HD22	1.52	0.57
1:H:43:PHE:CB	2:T:370:LYS:CD	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:308:ILE:HG21	1:H:374:LEU:HD13	1.86	0.57
1:H:443:ILE:O	1:H:447:ARG:HG3	2.04	0.57
1:K:43:PHE:CG	2:W:370:LYS:HE2	2.32	0.57
1:K:332:LEU:HB2	1:K:408:PRO:HB2	1.85	0.57
1:L:43:PHE:CB	2:X:370:LYS:CD	2.82	0.57
1:L:332:LEU:HB2	1:L:408:PRO:HB2	1.85	0.57
2:O:3:GLU:O	2:O:4:GLU:CB	2.51	0.57
2:S:128:THR:HG22	2:S:131:GLU:H	1.69	0.57
1:A:118:THR:OG1	1:A:120:ILE:HG13	2.03	0.57
1:A:192:ARG:HH21	1:A:219:ASN:HD22	1.52	0.57
1:A:308:ILE:HG21	1:A:374:LEU:HD13	1.86	0.57
1:A:332:LEU:HB2	1:A:408:PRO:HB2	1.85	0.57
1:A:360:PHE:CG	1:A:361:PRO:HD3	2.35	0.57
1:B:43:PHE:CB	2:N:370:LYS:CD	2.82	0.57
1:B:332:LEU:HB2	1:B:408:PRO:HB2	1.85	0.57
1:C:44:GLU:HG3	2:O:370:LYS:HZ3	1.67	0.57
1:D:43:PHE:CG	2:P:370:LYS:HE2	2.32	0.57
1:E:332:LEU:HB2	1:E:408:PRO:HB2	1.85	0.57
1:I:308:ILE:HG21	1:I:374:LEU:HD13	1.86	0.57
1:L:308:ILE:HG21	1:L:374:LEU:HD13	1.86	0.57
2:O:64:HIS:CD2	2:O:261:VAL:H	2.19	0.57
2:R:128:THR:HG22	2:R:131:GLU:H	1.69	0.57
2:S:3:GLU:O	2:S:4:GLU:CB	2.51	0.57
2:V:295:LYS:HD3	2:V:296:ASP:N	2.19	0.57
2:W:295:LYS:HD3	2:W:296:ASP:N	2.19	0.57
2:X:136:ASP:OD2	2:X:203:HIS:CD2	2.56	0.57
1:E:308:ILE:HG21	1:E:374:LEU:HD13	1.86	0.57
1:F:43:PHE:CB	2:R:370:LYS:CD	2.82	0.57
1:F:120:ILE:HD13	1:F:382:ILE:HG21	1.87	0.57
1:G:120:ILE:HD13	1:G:382:ILE:HG21	1.87	0.57
1:H:332:LEU:CB	1:H:408:PRO:HB2	2.35	0.57
1:I:360:PHE:CE2	1:I:361:PRO:HD3	2.36	0.57
1:K:192:ARG:HH21	1:K:219:ASN:HD22	1.52	0.57
2:N:295:LYS:HD3	2:N:296:ASP:N	2.19	0.57
2:O:309:GLU:O	2:O:313:LYS:CE	2.47	0.57
2:P:128:THR:HG22	2:P:131:GLU:H	1.69	0.57
2:T:1:LYS:CA	2:T:54:GLY:O	2.48	0.57
1:A:443:ILE:O	1:A:447:ARG:HG3	2.04	0.57
1:B:118:THR:OG1	1:B:120:ILE:HG13	2.03	0.57
1:B:192:ARG:HH21	1:B:219:ASN:HD22	1.52	0.57
1:E:332:LEU:CB	1:E:408:PRO:HB2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:PHE:CB	2:S:370:LYS:CD	2.82	0.57
1:G:308:ILE:HG21	1:G:374:LEU:HD13	1.86	0.57
1:K:118:THR:OG1	1:K:120:ILE:HG13	2.03	0.57
1:L:118:THR:OG1	1:L:120:ILE:HG13	2.04	0.57
1:L:192:ARG:HH21	1:L:219:ASN:HD22	1.52	0.57
2:O:295:LYS:HD3	2:O:296:ASP:N	2.19	0.57
2:Q:1:LYS:CA	2:Q:54:GLY:O	2.48	0.57
2:U:128:THR:HG22	2:U:131:GLU:H	1.69	0.57
1:D:360:PHE:CE2	1:D:361:PRO:HD3	2.36	0.57
1:F:235:ILE:CG2	1:F:367:PRO:HG3	2.28	0.57
1:F:308:ILE:HG21	1:F:374:LEU:HD13	1.86	0.57
1:L:443:ILE:O	1:L:447:ARG:HG3	2.04	0.57
2:N:64:HIS:CD2	2:N:261:VAL:H	2.19	0.57
2:S:136:ASP:OD2	2:S:203:HIS:CD2	2.56	0.57
2:V:309:GLU:O	2:V:313:LYS:CE	2.47	0.57
2:W:64:HIS:CD2	2:W:261:VAL:H	2.19	0.57
1:A:360:PHE:CE2	1:A:361:PRO:HD3	2.36	0.57
1:F:192:ARG:HH21	1:F:219:ASN:HD22	1.52	0.57
1:G:399:LEU:CA	1:G:400:PRO:C	2.78	0.57
1:L:360:PHE:CG	1:L:361:PRO:HD3	2.35	0.57
1:I:332:LEU:CB	1:I:408:PRO:HB2	2.35	0.57
1:L:360:PHE:CE2	1:L:361:PRO:HD3	2.37	0.57
2:O:128:THR:HG22	2:O:131:GLU:H	1.69	0.57
2:R:136:ASP:OD2	2:R:203:HIS:CD2	2.56	0.57
2:V:128:THR:HG22	2:V:131:GLU:H	1.69	0.57
1:A:120:ILE:HD13	1:A:382:ILE:HG21	1.87	0.57
1:D:332:LEU:CB	1:D:408:PRO:HB2	2.35	0.57
1:F:399:LEU:CA	1:F:400:PRO:C	2.78	0.57
1:J:443:ILE:O	1:J:447:ARG:HG3	2.04	0.57
2:Q:3:GLU:O	2:Q:4:GLU:CB	2.51	0.57
1:B:326:TYR:HA	1:B:396:LEU:HD13	1.87	0.57
1:D:82:ASP:O	1:D:84:THR:CG2	2.51	0.57
1:K:443:ILE:O	1:K:447:ARG:HG3	2.04	0.57
1:L:120:ILE:HD13	1:L:382:ILE:HG21	1.87	0.57
2:Q:136:ASP:OD2	2:Q:140:LYS:NZ	2.35	0.57
1:J:332:LEU:CB	1:J:408:PRO:HB2	2.35	0.56
1:L:44:GLU:HG3	2:X:370:LYS:HZ3	1.68	0.56
2:T:3:GLU:O	2:T:4:GLU:CB	2.51	0.56
2:X:64:HIS:CD2	2:X:261:VAL:H	2.19	0.56
2:X:295:LYS:HD3	2:X:296:ASP:N	2.19	0.56
1:C:332:LEU:CB	1:C:408:PRO:HB2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:PHE:CB	2:P:370:LYS:CD	2.82	0.56
1:I:82:ASP:O	1:I:84:THR:CG2	2.51	0.56
1:K:326:TYR:HA	1:K:396:LEU:HD13	1.88	0.56
2:M:295:LYS:HD3	2:M:296:ASP:N	2.19	0.56
1:A:326:TYR:HA	1:A:396:LEU:HD13	1.88	0.56
1:B:443:ILE:O	1:B:447:ARG:HG3	2.04	0.56
1:C:192:ARG:HH21	1:C:219:ASN:HD22	1.52	0.56
1:C:340:SER:HB3	1:C:396:LEU:HA	1.88	0.56
1:C:443:ILE:O	1:C:447:ARG:HG3	2.04	0.56
1:D:443:ILE:O	1:D:447:ARG:HG3	2.04	0.56
1:D:460:VAL:HG12	1:D:464:LEU:HD22	1.88	0.56
1:E:192:ARG:HH21	1:E:219:ASN:HD22	1.52	0.56
1:E:460:VAL:HG12	1:E:464:LEU:HD22	1.88	0.56
1:F:118:THR:OG1	1:F:120:ILE:HG13	2.04	0.56
1:F:326:TYR:HA	1:F:396:LEU:HD13	1.87	0.56
1:F:360:PHE:CE2	1:F:361:PRO:HD3	2.36	0.56
1:F:460:VAL:HG12	1:F:464:LEU:HD22	1.88	0.56
1:G:460:VAL:HG12	1:G:464:LEU:HD22	1.88	0.56
1:H:192:ARG:HH21	1:H:219:ASN:HD22	1.52	0.56
1:H:360:PHE:CE2	1:H:361:PRO:HD3	2.36	0.56
1:H:460:VAL:HG12	1:H:464:LEU:HD22	1.88	0.56
1:I:340:SER:HB3	1:I:396:LEU:HA	1.87	0.56
1:I:460:VAL:HG12	1:I:464:LEU:HD22	1.88	0.56
1:J:326:TYR:HA	1:J:396:LEU:HD13	1.87	0.56
1:L:326:TYR:HA	1:L:396:LEU:HD13	1.87	0.56
2:M:3:GLU:O	2:M:4:GLU:CB	2.51	0.56
2:N:3:GLU:O	2:N:4:GLU:CB	2.51	0.56
2:U:295:LYS:HD3	2:U:296:ASP:N	2.19	0.56
2:W:3:GLU:O	2:W:4:GLU:CB	2.51	0.56
2:X:3:GLU:O	2:X:4:GLU:CB	2.51	0.56
1:B:120:ILE:HD13	1:B:382:ILE:HG21	1.87	0.56
1:D:340:SER:HB3	1:D:396:LEU:HA	1.87	0.56
1:D:399:LEU:CA	1:D:400:PRO:C	2.78	0.56
1:E:340:SER:HB3	1:E:396:LEU:HA	1.87	0.56
1:F:340:SER:HB3	1:F:396:LEU:HA	1.87	0.56
1:G:326:TYR:HA	1:G:396:LEU:HD13	1.87	0.56
1:G:340:SER:HB3	1:G:396:LEU:HA	1.88	0.56
1:I:43:PHE:CB	2:U:370:LYS:CD	2.82	0.56
1:J:340:SER:HB3	1:J:396:LEU:HA	1.88	0.56
1:K:332:LEU:CB	1:K:408:PRO:HB2	2.35	0.56
2:M:30:ASP:OD1	2:M:283:TYR:OH	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:295:LYS:HD3	2:P:296:ASP:N	2.19	0.56
2:X:30:ASP:OD1	2:X:283:TYR:OH	2.24	0.56
1:B:332:LEU:CB	1:B:408:PRO:HB2	2.35	0.56
1:C:326:TYR:HA	1:C:396:LEU:HD13	1.88	0.56
1:E:360:PHE:CE2	1:E:361:PRO:HD3	2.36	0.56
1:G:118:THR:OG1	1:G:120:ILE:HG13	2.04	0.56
1:I:443:ILE:O	1:I:447:ARG:HG3	2.04	0.56
1:J:360:PHE:CD2	1:J:361:PRO:CD	2.74	0.56
1:J:460:VAL:HG12	1:J:464:LEU:HD22	1.88	0.56
1:A:399:LEU:CA	1:A:400:PRO:C	2.78	0.56
1:B:44:GLU:HG3	2:N:370:LYS:HZ3	1.67	0.56
1:B:460:VAL:HG12	1:B:464:LEU:HD22	1.88	0.56
1:G:179:TYR:CD2	1:L:53:SER:HB2	2.40	0.56
1:G:360:PHE:CE2	1:G:361:PRO:HD3	2.37	0.56
1:H:340:SER:HB3	1:H:396:LEU:HA	1.88	0.56
1:I:399:LEU:CA	1:I:400:PRO:C	2.78	0.56
1:K:120:ILE:HD13	1:K:382:ILE:HG21	1.87	0.56
1:K:460:VAL:HG12	1:K:464:LEU:HD22	1.88	0.56
2:M:64:HIS:CD2	2:M:261:VAL:H	2.19	0.56
1:A:332:LEU:CB	1:A:408:PRO:HB2	2.35	0.56
1:C:120:ILE:HD13	1:C:382:ILE:HG21	1.87	0.56
1:G:235:ILE:CG2	1:G:367:PRO:HG3	2.28	0.56
1:J:43:PHE:CB	2:V:370:LYS:CD	2.82	0.56
1:J:192:ARG:HH21	1:J:219:ASN:HD22	1.52	0.56
1:K:398:ASP:O	1:K:399:LEU:HG	2.06	0.56
1:L:43:PHE:CG	2:X:370:LYS:HE2	2.32	0.56
1:L:399:LEU:CA	1:L:400:PRO:C	2.78	0.56
2:S:30:ASP:OD1	2:S:283:TYR:OH	2.24	0.56
2:S:64:HIS:CD2	2:S:261:VAL:H	2.19	0.56
1:B:340:SER:HB3	1:B:396:LEU:HA	1.88	0.56
1:B:398:ASP:O	1:B:399:LEU:HG	2.06	0.56
1:C:460:VAL:HG12	1:C:464:LEU:HD22	1.88	0.56
1:H:326:TYR:HA	1:H:396:LEU:HD13	1.87	0.56
1:J:120:ILE:HD13	1:J:382:ILE:HG21	1.87	0.56
1:K:340:SER:HB3	1:K:396:LEU:HA	1.88	0.56
1:L:332:LEU:CB	1:L:408:PRO:HB2	2.35	0.56
2:S:295:LYS:HD3	2:S:296:ASP:N	2.19	0.56
1:A:43:PHE:CG	2:M:370:LYS:HE2	2.32	0.56
1:A:82:ASP:O	1:A:84:THR:CG2	2.51	0.56
1:A:398:ASP:O	1:A:399:LEU:HG	2.06	0.56
1:A:460:VAL:HG12	1:A:464:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:PHE:CB	2:O:370:LYS:CD	2.82	0.56
1:E:326:TYR:HA	1:E:396:LEU:HD13	1.87	0.56
1:H:399:LEU:CA	1:H:400:PRO:C	2.78	0.56
1:L:398:ASP:O	1:L:399:LEU:HG	2.06	0.56
2:R:30:ASP:OD1	2:R:283:TYR:OH	2.24	0.56
2:R:295:LYS:HD3	2:R:296:ASP:N	2.19	0.56
1:A:179:TYR:CD2	1:B:53:SER:HB2	2.40	0.56
1:A:340:SER:HB3	1:A:396:LEU:HA	1.88	0.56
1:C:360:PHE:CD2	1:C:361:PRO:CD	2.74	0.56
1:D:403:GLU:C	1:D:405:LYS:H	2.14	0.56
1:G:332:LEU:CB	1:G:408:PRO:HB2	2.35	0.56
1:I:29:GLN:HA	1:J:180:PHE:O	2.06	0.56
1:I:326:TYR:HA	1:I:396:LEU:HD13	1.87	0.56
1:I:403:GLU:C	1:I:405:LYS:H	2.14	0.56
1:K:3:GLU:CG	2:W:338:ALA:CB	2.84	0.56
1:K:44:GLU:HG3	2:W:370:LYS:HZ3	1.67	0.56
2:R:64:HIS:CD2	2:R:261:VAL:H	2.19	0.56
2:T:295:LYS:HD3	2:T:296:ASP:N	2.19	0.56
1:D:326:TYR:HA	1:D:396:LEU:HD13	1.87	0.55
1:F:332:LEU:CB	1:F:408:PRO:HB2	2.35	0.55
1:L:82:ASP:O	1:L:84:THR:CG2	2.51	0.55
1:L:114:TYR:CD2	1:L:431:GLY:HA3	2.41	0.55
1:L:460:VAL:HG12	1:L:464:LEU:HD22	1.88	0.55
1:E:399:LEU:CA	1:E:400:PRO:C	2.78	0.55
1:F:398:ASP:O	1:F:399:LEU:HG	2.06	0.55
1:G:398:ASP:O	1:G:399:LEU:HG	2.06	0.55
1:H:403:GLU:C	1:H:405:LYS:H	2.14	0.55
1:L:340:SER:HB3	1:L:396:LEU:HA	1.88	0.55
1:B:3:GLU:CG	2:N:338:ALA:CB	2.85	0.55
1:D:120:ILE:HD13	1:D:382:ILE:HG21	1.87	0.55
1:E:398:ASP:O	1:E:399:LEU:HG	2.06	0.55
1:I:120:ILE:HD13	1:I:382:ILE:HG21	1.87	0.55
2:N:30:ASP:OD1	2:N:283:TYR:OH	2.24	0.55
2:Q:295:LYS:HD3	2:Q:296:ASP:N	2.19	0.55
1:A:114:TYR:CD2	1:A:431:GLY:HA3	2.41	0.55
1:E:403:GLU:C	1:E:405:LYS:H	2.14	0.55
1:H:398:ASP:O	1:H:399:LEU:HG	2.06	0.55
1:J:398:ASP:O	1:J:399:LEU:HG	2.06	0.55
1:J:399:LEU:CA	1:J:400:PRO:C	2.78	0.55
2:W:30:ASP:OD1	2:W:283:TYR:OH	2.24	0.55
1:C:399:LEU:CA	1:C:400:PRO:C	2.78	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:TYR:CD2	1:E:53:SER:HB2	2.41	0.55
1:E:3:GLU:CG	2:Q:338:ALA:CB	2.85	0.55
1:H:3:GLU:CG	2:T:338:ALA:CB	2.85	0.55
1:H:120:ILE:HD13	1:H:382:ILE:HG21	1.87	0.55
1:J:3:GLU:CG	2:V:338:ALA:CB	2.85	0.55
1:C:3:GLU:CG	2:O:338:ALA:CB	2.85	0.55
1:C:82:ASP:O	1:C:84:THR:CG2	2.51	0.55
1:C:398:ASP:O	1:C:399:LEU:HG	2.06	0.55
1:E:120:ILE:HD13	1:E:382:ILE:HG21	1.87	0.55
1:E:360:PHE:CD2	1:E:361:PRO:CD	2.74	0.55
2:P:136:ASP:OD2	2:P:203:HIS:CD2	2.56	0.55
1:A:3:GLU:CG	2:M:338:ALA:CB	2.84	0.55
1:F:3:GLU:CG	2:R:338:ALA:CB	2.85	0.55
1:G:3:GLU:CG	2:S:338:ALA:CB	2.85	0.55
1:L:3:GLU:CG	2:X:338:ALA:CB	2.85	0.55
2:N:329:ILE:HG23	2:N:329:ILE:O	2.06	0.55
2:U:140:LYS:HD2	2:U:144:LYS:O	2.07	0.55
2:W:329:ILE:HG23	2:W:329:ILE:O	2.06	0.55
1:A:399:LEU:H	1:A:401:PRO:CG	1.90	0.55
2:P:140:LYS:HD2	2:P:144:LYS:O	2.07	0.55
1:D:180:PHE:HB3	1:E:30:HIS:H	1.70	0.55
1:G:360:PHE:CD2	1:G:361:PRO:CD	2.74	0.55
1:J:82:ASP:O	1:J:84:THR:CG2	2.51	0.55
2:Q:140:LYS:HD2	2:Q:144:LYS:O	2.07	0.55
2:R:312:ALA:CB	2:R:317:ILE:HG22	2.32	0.55
2:T:140:LYS:HD2	2:T:144:LYS:O	2.07	0.55
2:V:329:ILE:HG23	2:V:329:ILE:O	2.06	0.55
1:C:114:TYR:CD2	1:C:431:GLY:HA3	2.41	0.55
1:D:398:ASP:O	1:D:399:LEU:HG	2.06	0.55
1:F:4:HIS:CD2	2:R:178:ILE:CG1	2.58	0.55
1:H:114:TYR:CD2	1:H:431:GLY:HA3	2.41	0.55
1:H:360:PHE:CD2	1:H:361:PRO:CD	2.74	0.55
2:O:140:LYS:HD2	2:O:144:LYS:O	2.07	0.55
2:O:329:ILE:HG23	2:O:329:ILE:O	2.06	0.55
2:T:30:ASP:OD1	2:T:283:TYR:OH	2.24	0.55
2:U:136:ASP:OD2	2:U:203:HIS:CD2	2.56	0.55
2:X:329:ILE:O	2:X:329:ILE:HG23	2.06	0.55
1:D:114:TYR:CD2	1:D:431:GLY:HA3	2.41	0.54
1:E:114:TYR:CD2	1:E:431:GLY:HA3	2.41	0.54
1:I:114:TYR:CD2	1:I:431:GLY:HA3	2.41	0.54
1:I:398:ASP:O	1:I:399:LEU:HG	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:114:TYR:CD2	1:K:431:GLY:HA3	2.41	0.54
1:L:128:PRO:HD2	1:L:231:LYS:HE2	1.89	0.54
2:V:140:LYS:HD2	2:V:144:LYS:O	2.07	0.54
1:B:114:TYR:CD2	1:B:431:GLY:HA3	2.41	0.54
1:B:128:PRO:HD2	1:B:231:LYS:HE2	1.89	0.54
1:F:114:TYR:CD2	1:F:431:GLY:HA3	2.41	0.54
1:G:114:TYR:CD2	1:G:431:GLY:HA3	2.41	0.54
1:J:114:TYR:CD2	1:J:431:GLY:HA3	2.41	0.54
1:K:128:PRO:HD2	1:K:231:LYS:HE2	1.89	0.54
2:M:329:ILE:O	2:M:329:ILE:HG23	2.06	0.54
2:Q:30:ASP:OD1	2:Q:283:TYR:OH	2.24	0.54
2:V:30:ASP:OD1	2:V:283:TYR:OH	2.24	0.54
1:A:128:PRO:HD2	1:A:231:LYS:HE2	1.89	0.54
2:M:136:ASP:OD2	2:M:140:LYS:NZ	2.35	0.54
2:R:329:ILE:HG23	2:R:329:ILE:O	2.06	0.54
2:S:140:LYS:HD2	2:S:144:LYS:O	2.07	0.54
2:U:30:ASP:OD1	2:U:283:TYR:OH	2.24	0.54
1:B:180:PHE:HB3	1:C:30:HIS:H	1.73	0.54
1:D:3:GLU:CG	2:P:338:ALA:CB	2.85	0.54
1:E:248:ARG:HG2	1:E:248:ARG:NH2	2.23	0.54
1:F:248:ARG:HG2	1:F:248:ARG:NH2	2.23	0.54
1:H:248:ARG:HG2	1:H:248:ARG:NH2	2.23	0.54
2:O:30:ASP:OD1	2:O:283:TYR:OH	2.24	0.54
2:P:30:ASP:OD1	2:P:283:TYR:OH	2.24	0.54
2:Q:136:ASP:OD2	2:Q:203:HIS:CD2	2.56	0.54
2:R:140:LYS:HD2	2:R:144:LYS:O	2.07	0.54
2:S:312:ALA:CB	2:S:317:ILE:HG22	2.32	0.54
1:C:403:GLU:C	1:C:405:LYS:H	2.14	0.54
1:F:403:GLU:C	1:F:405:LYS:H	2.14	0.54
1:L:399:LEU:H	1:L:401:PRO:CG	1.90	0.54
2:M:140:LYS:HD2	2:M:144:LYS:O	2.07	0.54
2:N:140:LYS:HD2	2:N:144:LYS:O	2.07	0.54
1:A:29:GLN:HA	1:F:180:PHE:O	2.08	0.54
1:A:403:GLU:C	1:A:405:LYS:H	2.14	0.54
1:G:248:ARG:HG2	1:G:248:ARG:NH2	2.23	0.54
1:I:3:GLU:CG	2:U:338:ALA:CB	2.85	0.54
1:I:128:PRO:HD2	1:I:231:LYS:HE2	1.89	0.54
1:J:403:GLU:C	1:J:405:LYS:H	2.14	0.54
1:K:360:PHE:CD2	1:K:361:PRO:CD	2.74	0.54
2:Q:329:ILE:HG23	2:Q:329:ILE:O	2.06	0.54
2:U:329:ILE:O	2:U:329:ILE:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:369:THR:C	2:U:370:LYS:CA	2.75	0.54
1:D:128:PRO:HD2	1:D:231:LYS:HE2	1.89	0.54
1:G:29:GLN:OE1	1:H:181:PRO:HD3	2.07	0.54
1:H:248:ARG:CG	1:H:248:ARG:NH2	2.67	0.54
1:J:128:PRO:HD2	1:J:231:LYS:HE2	1.89	0.54
2:P:369:THR:C	2:P:370:LYS:CA	2.75	0.54
1:B:360:PHE:CD2	1:B:361:PRO:CD	2.74	0.54
1:B:399:LEU:CA	1:B:400:PRO:C	2.78	0.54
1:G:403:GLU:C	1:G:405:LYS:H	2.14	0.54
1:H:128:PRO:HD2	1:H:231:LYS:HE2	1.89	0.54
1:K:403:GLU:C	1:K:405:LYS:H	2.14	0.54
1:L:403:GLU:C	1:L:405:LYS:H	2.14	0.54
2:S:132:ILE:N	2:S:133:PRO:CD	2.71	0.54
2:S:329:ILE:HG23	2:S:329:ILE:O	2.06	0.54
2:T:132:ILE:N	2:T:133:PRO:CD	2.71	0.54
2:T:136:ASP:OD2	2:T:203:HIS:CD2	2.56	0.54
2:T:329:ILE:HG23	2:T:329:ILE:O	2.06	0.54
2:W:140:LYS:HD2	2:W:144:LYS:O	2.07	0.54
1:B:403:GLU:C	1:B:405:LYS:H	2.14	0.54
1:E:248:ARG:CG	1:E:248:ARG:NH2	2.67	0.54
1:F:82:ASP:O	1:F:84:THR:CG2	2.51	0.54
1:F:128:PRO:HD2	1:F:231:LYS:HE2	1.89	0.54
2:M:132:ILE:N	2:M:133:PRO:CD	2.71	0.54
2:O:136:ASP:OD2	2:O:203:HIS:CD2	2.56	0.54
2:P:329:ILE:HG23	2:P:329:ILE:O	2.06	0.54
2:Q:19:GLY:O	2:Q:23:VAL:HG23	2.08	0.54
2:Q:132:ILE:N	2:Q:133:PRO:CD	2.71	0.54
2:R:132:ILE:N	2:R:133:PRO:CD	2.71	0.54
2:X:132:ILE:N	2:X:133:PRO:CD	2.71	0.54
2:X:140:LYS:HD2	2:X:144:LYS:O	2.07	0.54
1:C:128:PRO:HD2	1:C:231:LYS:HE2	1.89	0.54
1:K:29:GLN:HA	1:L:180:PHE:O	2.08	0.54
2:O:19:GLY:O	2:O:23:VAL:HG23	2.08	0.54
2:V:19:GLY:O	2:V:23:VAL:HG23	2.08	0.54
1:D:248:ARG:HG2	1:D:248:ARG:NH2	2.23	0.53
1:E:128:PRO:HD2	1:E:231:LYS:HE2	1.89	0.53
1:J:29:GLN:HA	1:K:180:PHE:O	2.07	0.53
1:K:399:LEU:CA	1:K:400:PRO:C	2.78	0.53
2:T:19:GLY:O	2:T:23:VAL:HG23	2.08	0.53
1:F:360:PHE:CD2	1:F:361:PRO:CD	2.74	0.53
1:I:29:GLN:HB3	1:J:180:PHE:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:248:ARG:HG2	1:I:248:ARG:NH2	2.23	0.53
1:J:29:GLN:OE1	1:K:181:PRO:HD3	2.08	0.53
2:N:132:ILE:N	2:N:133:PRO:CD	2.71	0.53
2:O:132:ILE:N	2:O:133:PRO:CD	2.71	0.53
2:P:132:ILE:N	2:P:133:PRO:CD	2.71	0.53
2:U:132:ILE:N	2:U:133:PRO:CD	2.71	0.53
2:W:132:ILE:N	2:W:133:PRO:CD	2.71	0.53
1:A:248:ARG:HG2	1:A:248:ARG:NH2	2.23	0.53
1:B:82:ASP:O	1:B:84:THR:CG2	2.51	0.53
1:G:43:PHE:CG	2:S:370:LYS:HE2	2.32	0.53
1:G:128:PRO:HD2	1:G:231:LYS:HE2	1.89	0.53
1:K:82:ASP:O	1:K:84:THR:CG2	2.51	0.53
2:U:136:ASP:OD2	2:U:140:LYS:NZ	2.35	0.53
2:V:132:ILE:N	2:V:133:PRO:CD	2.71	0.53
2:V:136:ASP:OD2	2:V:203:HIS:CD2	2.56	0.53
1:B:456:THR:O	1:H:458:HIS:HE1	1.91	0.53
1:G:82:ASP:O	1:G:84:THR:CG2	2.51	0.53
1:H:7:THR:HG1	2:T:178:ILE:HD11	1.73	0.53
1:K:30:HIS:H	1:L:180:PHE:HB3	1.73	0.53
2:W:19:GLY:O	2:W:23:VAL:HG23	2.08	0.53
1:L:248:ARG:HG2	1:L:248:ARG:NH2	2.23	0.53
2:N:19:GLY:O	2:N:23:VAL:HG23	2.08	0.53
2:P:136:ASP:OD2	2:P:140:LYS:NZ	2.35	0.53
2:P:202:LYS:HA	2:P:202:LYS:HE2	1.91	0.53
2:R:34:LYS:HG2	2:R:34:LYS:O	2.09	0.53
2:S:19:GLY:O	2:S:23:VAL:HG23	2.08	0.53
2:S:202:LYS:HE2	2:S:202:LYS:HA	1.91	0.53
2:T:202:LYS:HE2	2:T:202:LYS:HA	1.91	0.53
1:C:248:ARG:HG2	1:C:248:ARG:NH2	2.23	0.53
1:J:248:ARG:HG2	1:J:248:ARG:NH2	2.23	0.53
2:N:202:LYS:HE2	2:N:202:LYS:HA	1.91	0.53
2:O:202:LYS:HE2	2:O:202:LYS:HA	1.91	0.53
2:Q:202:LYS:HE2	2:Q:202:LYS:HA	1.91	0.53
2:R:19:GLY:O	2:R:23:VAL:HG23	2.08	0.53
2:S:34:LYS:O	2:S:34:LYS:HG2	2.09	0.53
2:V:202:LYS:HE2	2:V:202:LYS:HA	1.91	0.53
1:B:248:ARG:HG2	1:B:248:ARG:NH2	2.23	0.53
1:H:29:GLN:HA	1:I:180:PHE:O	2.09	0.53
1:K:248:ARG:HG2	1:K:248:ARG:NH2	2.23	0.53
2:M:202:LYS:HA	2:M:202:LYS:HE2	1.91	0.53
2:O:335:GLN:NE2	2:O:335:GLN:H	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:19:GLY:O	2:P:23:VAL:HG23	2.08	0.53
2:X:202:LYS:HA	2:X:202:LYS:HE2	1.91	0.53
1:B:7:THR:HG1	2:N:178:ILE:HD11	1.74	0.53
1:F:43:PHE:CG	2:R:370:LYS:HE2	2.32	0.53
1:L:360:PHE:CD2	1:L:361:PRO:CD	2.74	0.53
2:R:202:LYS:HE2	2:R:202:LYS:HA	1.91	0.53
2:T:312:ALA:CB	2:T:317:ILE:HG22	2.32	0.53
2:U:19:GLY:O	2:U:23:VAL:HG23	2.08	0.53
2:U:202:LYS:HA	2:U:202:LYS:HE2	1.91	0.53
2:V:335:GLN:NE2	2:V:335:GLN:H	2.07	0.53
2:W:202:LYS:HE2	2:W:202:LYS:HA	1.91	0.53
1:B:320:LYS:NZ	1:H:461:GLU:OE1	2.35	0.52
2:N:335:GLN:NE2	2:N:335:GLN:H	2.07	0.52
1:K:7:THR:HG1	2:W:178:ILE:HD11	1.74	0.52
1:A:360:PHE:CD2	1:A:361:PRO:CD	2.74	0.52
1:J:7:THR:HG1	2:V:178:ILE:HD11	1.75	0.52
2:M:19:GLY:O	2:M:23:VAL:HG23	2.08	0.52
2:M:335:GLN:NE2	2:M:335:GLN:H	2.07	0.52
2:W:335:GLN:NE2	2:W:335:GLN:H	2.08	0.52
1:A:30:HIS:H	1:F:180:PHE:HB3	1.73	0.52
1:C:7:THR:HG1	2:O:178:ILE:HD11	1.75	0.52
1:C:16:PHE:HB2	1:C:84:THR:HB	1.92	0.52
1:D:295:LEU:O	1:D:388:PRO:HG3	2.09	0.52
1:J:16:PHE:HB2	1:J:84:THR:HB	1.92	0.52
2:Q:335:GLN:NE2	2:Q:335:GLN:H	2.07	0.52
2:X:335:GLN:NE2	2:X:335:GLN:H	2.07	0.52
1:K:295:LEU:O	1:K:388:PRO:HG3	2.09	0.52
2:T:335:GLN:NE2	2:T:335:GLN:H	2.08	0.52
2:X:19:GLY:O	2:X:23:VAL:HG23	2.08	0.52
1:B:248:ARG:HH21	1:B:248:ARG:HG3	1.75	0.52
1:B:295:LEU:O	1:B:388:PRO:HG3	2.09	0.52
1:D:7:THR:HG1	2:P:178:ILE:HD11	1.75	0.52
1:E:16:PHE:HB2	1:E:84:THR:HB	1.92	0.52
1:H:16:PHE:HB2	1:H:84:THR:HB	1.92	0.52
1:I:16:PHE:HB2	1:I:84:THR:HB	1.92	0.52
1:I:295:LEU:O	1:I:388:PRO:HG3	2.09	0.52
1:K:248:ARG:HH21	1:K:248:ARG:HG3	1.75	0.52
2:P:322:GLU:O	2:P:326:LYS:HG3	2.10	0.52
2:T:322:GLU:O	2:T:326:LYS:HG3	2.10	0.52
2:X:34:LYS:HG2	2:X:34:LYS:O	2.09	0.52
2:X:369:THR:C	2:X:370:LYS:CA	2.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:PHE:HB2	1:D:84:THR:HB	1.92	0.52
1:D:456:THR:O	1:J:458:HIS:HE1	1.93	0.52
2:Q:312:ALA:CB	2:Q:317:ILE:HG22	2.32	0.52
2:Q:322:GLU:O	2:Q:326:LYS:HG3	2.10	0.52
2:U:322:GLU:O	2:U:326:LYS:HG3	2.10	0.52
1:E:295:LEU:O	1:E:388:PRO:HG3	2.09	0.52
2:O:9:ILE:HG21	2:O:20:LEU:HD21	1.92	0.52
2:U:9:ILE:HG21	2:U:20:LEU:HD21	1.92	0.52
2:V:369:THR:C	2:V:370:LYS:CA	2.75	0.52
1:B:16:PHE:HB2	1:B:84:THR:HB	1.92	0.52
1:K:16:PHE:HB2	1:K:84:THR:HB	1.92	0.52
2:N:34:LYS:O	2:N:34:LYS:HG2	2.09	0.52
2:O:322:GLU:O	2:O:326:LYS:HG3	2.10	0.52
2:T:9:ILE:HG21	2:T:20:LEU:HD21	1.92	0.52
2:V:9:ILE:HG21	2:V:20:LEU:HD21	1.92	0.52
2:V:34:LYS:O	2:V:34:LYS:HG2	2.09	0.52
2:W:34:LYS:HG2	2:W:34:LYS:O	2.09	0.52
1:A:295:LEU:O	1:A:388:PRO:HG3	2.09	0.52
1:B:461:GLU:OE1	1:H:320:LYS:NZ	2.33	0.52
1:H:295:LEU:O	1:H:388:PRO:HG3	2.09	0.52
1:I:7:THR:HG1	2:U:178:ILE:HD11	1.75	0.52
2:M:34:LYS:HG2	2:M:34:LYS:O	2.09	0.52
2:O:34:LYS:HG2	2:O:34:LYS:O	2.09	0.52
2:P:9:ILE:HG21	2:P:20:LEU:HD21	1.92	0.52
2:Q:9:ILE:HG21	2:Q:20:LEU:HD21	1.92	0.52
2:R:322:GLU:O	2:R:326:LYS:HG3	2.10	0.52
2:S:322:GLU:O	2:S:326:LYS:HG3	2.10	0.52
2:W:312:ALA:HB2	2:W:317:ILE:CB	2.39	0.52
2:W:369:THR:C	2:W:370:LYS:CA	2.75	0.52
1:G:29:GLN:HA	1:H:180:PHE:O	2.11	0.51
1:J:29:GLN:HB3	1:K:180:PHE:HB2	1.92	0.51
2:N:136:ASP:OD2	2:N:203:HIS:CD2	2.56	0.51
2:O:82:ASP:O	2:O:85:PHE:N	2.43	0.51
2:R:9:ILE:HG21	2:R:20:LEU:HD21	1.92	0.51
2:R:82:ASP:O	2:R:85:PHE:N	2.43	0.51
2:S:82:ASP:O	2:S:85:PHE:N	2.43	0.51
2:U:82:ASP:O	2:U:85:PHE:N	2.43	0.51
2:V:322:GLU:O	2:V:326:LYS:HG3	2.10	0.51
2:M:82:ASP:O	2:M:85:PHE:N	2.43	0.51
2:N:312:ALA:HB2	2:N:317:ILE:CB	2.39	0.51
2:N:367:ARG:HA	2:N:370:LYS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:369:THR:C	2:N:370:LYS:CA	2.75	0.51
2:P:82:ASP:O	2:P:85:PHE:N	2.44	0.51
2:S:9:ILE:HG21	2:S:20:LEU:HD21	1.92	0.51
2:V:82:ASP:O	2:V:85:PHE:N	2.43	0.51
1:I:29:GLN:HB3	1:J:180:PHE:CB	2.40	0.51
2:M:322:GLU:O	2:M:326:LYS:HG3	2.10	0.51
2:N:322:GLU:O	2:N:326:LYS:HG3	2.10	0.51
2:Q:82:ASP:O	2:Q:85:PHE:N	2.43	0.51
2:U:34:LYS:O	2:U:34:LYS:HG2	2.09	0.51
2:W:136:ASP:OD2	2:W:203:HIS:CD2	2.56	0.51
2:W:322:GLU:O	2:W:326:LYS:HG3	2.10	0.51
2:X:82:ASP:O	2:X:85:PHE:N	2.43	0.51
2:X:367:ARG:HA	2:X:370:LYS:HD2	1.93	0.51
1:C:180:PHE:HB2	1:D:29:GLN:HB3	1.92	0.51
1:G:180:PHE:O	1:L:29:GLN:HA	2.10	0.51
1:J:295:LEU:O	1:J:388:PRO:HG3	2.09	0.51
2:M:9:ILE:HG21	2:M:20:LEU:HD21	1.92	0.51
2:M:369:THR:C	2:M:370:LYS:CA	2.76	0.51
2:P:34:LYS:O	2:P:34:LYS:HG2	2.09	0.51
2:P:363:ASP:O	2:P:367:ARG:HG3	2.11	0.51
2:S:335:GLN:NE2	2:S:335:GLN:H	2.07	0.51
2:T:82:ASP:O	2:T:85:PHE:N	2.43	0.51
2:U:363:ASP:O	2:U:367:ARG:HG3	2.10	0.51
2:V:363:ASP:O	2:V:367:ARG:HG3	2.10	0.51
2:W:367:ARG:HA	2:W:370:LYS:HD2	1.93	0.51
2:X:322:GLU:O	2:X:326:LYS:HG3	2.10	0.51
1:B:458:HIS:HE1	1:H:456:THR:O	1.93	0.51
1:C:295:LEU:O	1:C:388:PRO:HG3	2.09	0.51
1:D:248:ARG:CG	1:D:248:ARG:NH2	2.67	0.51
1:G:16:PHE:HB2	1:G:84:THR:HB	1.92	0.51
1:I:29:GLN:OE1	1:J:181:PRO:HD3	2.10	0.51
1:J:248:ARG:HH21	1:J:248:ARG:HG3	1.75	0.51
2:O:363:ASP:O	2:O:367:ARG:HG3	2.11	0.51
2:Q:363:ASP:O	2:Q:367:ARG:HG3	2.11	0.51
2:U:335:GLN:NE2	2:U:335:GLN:H	2.08	0.51
2:X:9:ILE:HG21	2:X:20:LEU:HD21	1.92	0.51
1:E:7:THR:HG1	2:Q:178:ILE:HD11	1.75	0.51
1:H:29:GLN:OE1	1:I:181:PRO:HD3	2.10	0.51
2:O:369:THR:C	2:O:370:LYS:CA	2.75	0.51
2:P:335:GLN:NE2	2:P:335:GLN:H	2.07	0.51
2:T:363:ASP:O	2:T:367:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:PHE:CB	1:D:29:GLN:HB3	2.41	0.51
1:C:248:ARG:HH21	1:C:248:ARG:HG3	1.75	0.51
1:F:16:PHE:HB2	1:F:84:THR:HB	1.92	0.51
1:F:256:MET:HG3	1:L:466:TYR:HA	1.91	0.51
2:N:82:ASP:O	2:N:85:PHE:N	2.44	0.51
2:R:335:GLN:NE2	2:R:335:GLN:H	2.07	0.51
2:W:82:ASP:O	2:W:85:PHE:N	2.43	0.51
1:A:16:PHE:HB2	1:A:84:THR:HB	1.92	0.51
1:A:256:MET:HG3	1:G:466:TYR:HA	1.91	0.51
1:D:458:HIS:HE1	1:J:456:THR:O	1.94	0.51
1:G:396:LEU:O	1:G:400:PRO:HG2	2.11	0.51
2:M:367:ARG:HA	2:M:370:LYS:HD2	1.93	0.51
2:N:9:ILE:HG21	2:N:20:LEU:HD21	1.92	0.51
2:W:9:ILE:HG21	2:W:20:LEU:HD21	1.92	0.51
1:F:318:SER:OG	1:F:362:ASP:OD2	2.27	0.51
1:H:396:LEU:O	1:H:400:PRO:HG2	2.11	0.51
1:I:248:ARG:CG	1:I:248:ARG:NH2	2.66	0.51
1:I:360:PHE:CD2	1:I:361:PRO:CD	2.74	0.51
1:J:396:LEU:O	1:J:400:PRO:HG2	2.11	0.51
1:L:16:PHE:HB2	1:L:84:THR:HB	1.92	0.51
1:L:311:LEU:HD22	1:L:369:LEU:HB3	1.93	0.51
1:D:360:PHE:CD2	1:D:361:PRO:CD	2.74	0.51
1:G:7:THR:HG1	2:S:178:ILE:HD11	1.75	0.51
1:J:53:SER:HB2	1:K:179:TYR:CD2	2.46	0.51
1:A:311:LEU:HD22	1:A:369:LEU:HB3	1.93	0.50
1:B:181:PRO:HD3	1:C:29:GLN:OE1	2.10	0.50
1:C:396:LEU:O	1:C:400:PRO:HG2	2.11	0.50
1:F:396:LEU:O	1:F:400:PRO:HG2	2.12	0.50
1:G:295:LEU:O	1:G:388:PRO:HG3	2.09	0.50
1:L:295:LEU:O	1:L:388:PRO:HG3	2.09	0.50
2:T:34:LYS:O	2:T:34:LYS:HG2	2.09	0.50
1:B:311:LEU:HD22	1:B:369:LEU:HB3	1.93	0.50
1:E:396:LEU:O	1:E:400:PRO:HG2	2.12	0.50
1:F:295:LEU:O	1:F:388:PRO:HG3	2.09	0.50
1:G:318:SER:OG	1:G:362:ASP:OD2	2.27	0.50
1:I:396:LEU:O	1:I:400:PRO:HG2	2.11	0.50
2:Q:34:LYS:O	2:Q:34:LYS:HG2	2.09	0.50
2:S:136:ASP:OD2	2:S:140:LYS:NZ	2.35	0.50
1:D:396:LEU:O	1:D:400:PRO:HG2	2.12	0.50
1:I:248:ARG:HH21	1:I:248:ARG:HG3	1.75	0.50
1:I:311:LEU:HD22	1:I:369:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:311:LEU:HD22	1:K:369:LEU:HB3	1.93	0.50
1:C:461:GLU:OE1	1:I:320:LYS:NZ	2.33	0.50
2:N:85:PHE:CD1	2:N:85:PHE:C	2.90	0.50
2:N:239:LYS:NZ	2:N:241:ASN:HB2	2.27	0.50
2:R:363:ASP:O	2:R:367:ARG:HG3	2.11	0.50
2:T:367:ARG:HA	2:T:370:LYS:HD2	1.93	0.50
2:W:85:PHE:C	2:W:85:PHE:CD1	2.89	0.50
1:C:454:ARG:O	1:I:320:LYS:HG3	2.11	0.50
2:O:239:LYS:NZ	2:O:241:ASN:HB2	2.27	0.50
2:S:363:ASP:O	2:S:367:ARG:HG3	2.10	0.50
2:U:239:LYS:NZ	2:U:241:ASN:HB2	2.27	0.50
2:V:239:LYS:NZ	2:V:241:ASN:HB2	2.27	0.50
1:A:396:LEU:O	1:A:400:PRO:HG2	2.11	0.50
1:C:458:HIS:HE1	1:I:456:THR:O	1.95	0.50
1:D:248:ARG:HH21	1:D:248:ARG:HG3	1.75	0.50
1:F:7:THR:HG1	2:R:178:ILE:HD11	1.75	0.50
1:J:335:SER:HB2	1:J:392:MET:O	2.12	0.50
2:M:363:ASP:O	2:M:367:ARG:HG3	2.11	0.50
2:P:239:LYS:NZ	2:P:241:ASN:HB2	2.27	0.50
2:Q:239:LYS:NZ	2:Q:241:ASN:HB2	2.27	0.50
2:T:239:LYS:NZ	2:T:241:ASN:HB2	2.27	0.50
2:W:239:LYS:NZ	2:W:241:ASN:HB2	2.27	0.50
1:D:311:LEU:HD22	1:D:369:LEU:HB3	1.93	0.50
1:L:255:PHE:HB3	1:L:363:PRO:HB2	1.94	0.50
1:L:396:LEU:O	1:L:400:PRO:HG2	2.11	0.50
2:O:85:PHE:C	2:O:85:PHE:CD1	2.90	0.50
2:T:85:PHE:CD1	2:T:85:PHE:C	2.90	0.50
2:V:85:PHE:CD1	2:V:85:PHE:C	2.90	0.50
2:X:85:PHE:CD1	2:X:85:PHE:C	2.89	0.50
2:X:363:ASP:O	2:X:367:ARG:HG3	2.11	0.50
1:B:192:ARG:HD3	1:B:219:ASN:HD22	1.77	0.50
1:B:335:SER:HB2	1:B:392:MET:O	2.12	0.50
1:C:192:ARG:HD3	1:C:219:ASN:HD22	1.77	0.50
1:E:43:PHE:CG	2:Q:370:LYS:HE2	2.32	0.50
1:E:192:ARG:HD3	1:E:219:ASN:HD22	1.77	0.50
1:F:311:LEU:HD22	1:F:369:LEU:HB3	1.93	0.50
1:F:335:SER:HB2	1:F:392:MET:O	2.12	0.50
1:H:43:PHE:CG	2:T:370:LYS:HE2	2.32	0.50
1:H:248:ARG:HH21	1:H:248:ARG:HG3	1.75	0.50
1:J:192:ARG:HD3	1:J:219:ASN:HD22	1.77	0.50
1:K:192:ARG:HD3	1:K:219:ASN:HD22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:335:SER:HB2	1:K:392:MET:O	2.12	0.50
2:M:85:PHE:CD1	2:M:85:PHE:C	2.89	0.50
2:P:85:PHE:CD1	2:P:85:PHE:C	2.90	0.50
2:Q:237:THR:O	2:Q:237:THR:CG2	2.60	0.50
2:Q:367:ARG:HA	2:Q:370:LYS:HD2	1.93	0.50
2:U:367:ARG:HA	2:U:370:LYS:HD2	1.93	0.50
2:X:212:ILE:HD13	2:X:212:ILE:N	2.27	0.50
1:B:396:LEU:O	1:B:400:PRO:HG2	2.11	0.50
1:C:28:GLU:OE1	1:C:88:ARG:NH1	2.45	0.50
1:C:335:SER:HB2	1:C:392:MET:O	2.12	0.50
1:E:43:PHE:HB3	2:Q:370:LYS:CD	2.28	0.50
1:G:335:SER:HB2	1:G:392:MET:O	2.12	0.50
1:J:28:GLU:OE1	1:J:88:ARG:NH1	2.45	0.50
1:J:311:LEU:HD22	1:J:369:LEU:HB3	1.93	0.50
1:K:255:PHE:HB3	1:K:363:PRO:HB2	1.94	0.50
1:K:396:LEU:O	1:K:400:PRO:HG2	2.11	0.50
2:M:212:ILE:HD13	2:M:212:ILE:N	2.27	0.50
2:O:367:ARG:HA	2:O:370:LYS:HD2	1.93	0.50
2:P:367:ARG:HA	2:P:370:LYS:HD2	1.93	0.50
2:Q:85:PHE:CD1	2:Q:85:PHE:C	2.90	0.50
2:U:85:PHE:CD1	2:U:85:PHE:C	2.89	0.50
2:V:136:ASP:OD2	2:V:140:LYS:NZ	2.35	0.50
1:A:454:ARG:O	1:G:320:LYS:HG3	2.12	0.49
1:B:255:PHE:HB3	1:B:363:PRO:HB2	1.94	0.49
1:C:248:ARG:CG	1:C:248:ARG:NH2	2.67	0.49
1:E:248:ARG:HH21	1:E:248:ARG:HG3	1.75	0.49
1:G:192:ARG:HD3	1:G:219:ASN:HD22	1.77	0.49
1:H:192:ARG:HD3	1:H:219:ASN:HD22	1.77	0.49
2:S:85:PHE:CD1	2:S:85:PHE:C	2.89	0.49
2:S:367:ARG:HA	2:S:370:LYS:HD2	1.93	0.49
2:T:237:THR:O	2:T:237:THR:CG2	2.60	0.49
1:A:255:PHE:HB3	1:A:363:PRO:HB2	1.94	0.49
1:B:124:VAL:HG13	1:B:274:LEU:HD21	1.94	0.49
1:C:311:LEU:HD22	1:C:369:LEU:HB3	1.93	0.49
1:F:192:ARG:HD3	1:F:219:ASN:HD22	1.77	0.49
1:G:29:GLN:HB3	1:H:180:PHE:HB2	1.94	0.49
2:N:237:THR:O	2:N:237:THR:CG2	2.60	0.49
2:R:136:ASP:OD2	2:R:140:LYS:NZ	2.35	0.49
2:R:367:ARG:HA	2:R:370:LYS:HD2	1.93	0.49
2:T:212:ILE:HD13	2:T:212:ILE:N	2.27	0.49
2:U:312:ALA:HB2	2:U:317:ILE:CB	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:367:ARG:HA	2:V:370:LYS:HD2	1.93	0.49
2:W:237:THR:O	2:W:237:THR:CG2	2.60	0.49
1:A:124:VAL:HG13	1:A:274:LEU:HD21	1.94	0.49
1:G:311:LEU:HD22	1:G:369:LEU:HB3	1.93	0.49
1:K:124:VAL:HG13	1:K:274:LEU:HD21	1.94	0.49
1:L:124:VAL:HG13	1:L:274:LEU:HD21	1.94	0.49
2:Q:212:ILE:HD13	2:Q:212:ILE:N	2.27	0.49
2:W:363:ASP:O	2:W:367:ARG:HG3	2.10	0.49
2:X:312:ALA:HB2	2:X:317:ILE:CB	2.39	0.49
1:B:180:PHE:O	1:C:29:GLN:HA	2.13	0.49
1:E:124:VAL:HG13	1:E:274:LEU:HD21	1.94	0.49
1:E:256:MET:HG3	1:K:466:TYR:HA	1.94	0.49
1:K:43:PHE:HB3	2:W:370:LYS:CD	2.28	0.49
2:M:312:ALA:HB2	2:M:317:ILE:CB	2.39	0.49
2:P:312:ALA:HB2	2:P:317:ILE:CB	2.39	0.49
1:D:335:SER:HB2	1:D:392:MET:O	2.12	0.49
1:H:124:VAL:HG13	1:H:274:LEU:HD21	1.94	0.49
1:I:192:ARG:HD3	1:I:219:ASN:HD22	1.77	0.49
2:M:239:LYS:NZ	2:M:241:ASN:HB2	2.27	0.49
2:N:212:ILE:HD13	2:N:212:ILE:N	2.27	0.49
2:N:363:ASP:O	2:N:367:ARG:HG3	2.11	0.49
2:Q:312:ALA:HB2	2:Q:317:ILE:CB	2.39	0.49
2:R:85:PHE:C	2:R:85:PHE:CD1	2.90	0.49
2:W:212:ILE:HD13	2:W:212:ILE:N	2.27	0.49
1:A:335:SER:HB2	1:A:392:MET:O	2.12	0.49
1:D:124:VAL:HG13	1:D:274:LEU:HD21	1.94	0.49
1:D:192:ARG:HD3	1:D:219:ASN:HD22	1.77	0.49
1:F:364:ALA:HA	1:L:468:VAL:HG13	1.95	0.49
1:G:181:PRO:HD3	1:L:29:GLN:OE1	2.13	0.49
1:G:248:ARG:HH21	1:G:248:ARG:HG3	1.75	0.49
1:I:124:VAL:HG13	1:I:274:LEU:HD21	1.94	0.49
1:I:335:SER:HB2	1:I:392:MET:O	2.12	0.49
2:O:312:ALA:HB2	2:O:317:ILE:CB	2.39	0.49
2:S:239:LYS:NZ	2:S:241:ASN:HB2	2.27	0.49
2:V:312:ALA:HB2	2:V:317:ILE:CB	2.39	0.49
1:B:43:PHE:HB3	2:N:370:LYS:CD	2.28	0.49
1:C:180:PHE:O	1:C:181:PRO:C	2.54	0.49
1:E:311:LEU:HD22	1:E:369:LEU:HB3	1.93	0.49
1:J:248:ARG:CG	1:J:248:ARG:NH2	2.67	0.49
1:L:335:SER:HB2	1:L:392:MET:O	2.12	0.49
2:M:136:ASP:HB3	2:M:203:HIS:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:239:LYS:NZ	2:R:241:ASN:HB2	2.27	0.49
2:T:312:ALA:HB2	2:T:317:ILE:CB	2.39	0.49
2:U:6:LYS:HA	2:U:33:ILE:CG2	2.41	0.49
2:X:239:LYS:NZ	2:X:241:ASN:HB2	2.27	0.49
1:A:192:ARG:HD3	1:A:219:ASN:HD22	1.77	0.49
1:E:255:PHE:HB3	1:E:363:PRO:HB2	1.94	0.49
1:E:335:SER:HB2	1:E:392:MET:O	2.12	0.49
1:H:335:SER:HB2	1:H:392:MET:O	2.12	0.49
2:N:136:ASP:OD2	2:N:140:LYS:NZ	2.35	0.49
2:N:147:LEU:O	2:N:148:MET:HG2	2.13	0.49
2:O:237:THR:O	2:O:237:THR:CG2	2.60	0.49
2:R:237:THR:O	2:R:237:THR:CG2	2.60	0.49
2:S:237:THR:O	2:S:237:THR:CG2	2.60	0.49
2:U:237:THR:O	2:U:237:THR:CG2	2.60	0.49
2:W:136:ASP:OD2	2:W:140:LYS:NZ	2.35	0.49
2:X:136:ASP:HB3	2:X:203:HIS:CD2	2.48	0.49
1:D:255:PHE:HB3	1:D:363:PRO:HB2	1.94	0.49
1:F:255:PHE:HB3	1:F:363:PRO:HB2	1.94	0.49
2:P:6:LYS:HA	2:P:33:ILE:CG2	2.41	0.49
2:P:212:ILE:HD13	2:P:212:ILE:N	2.27	0.49
2:R:136:ASP:HB3	2:R:203:HIS:CD2	2.48	0.49
2:S:212:ILE:HD13	2:S:212:ILE:N	2.27	0.49
2:U:212:ILE:HD13	2:U:212:ILE:N	2.27	0.49
2:V:212:ILE:HD13	2:V:212:ILE:N	2.27	0.49
2:W:147:LEU:O	2:W:148:MET:HG2	2.13	0.49
2:X:147:LEU:O	2:X:148:MET:HG2	2.13	0.49
1:E:4:HIS:CD2	2:Q:178:ILE:CG1	2.58	0.49
1:E:181:PRO:HD3	1:F:29:GLN:OE1	2.12	0.49
1:G:28:GLU:OE1	1:G:88:ARG:NH1	2.45	0.49
1:H:311:LEU:HD22	1:H:369:LEU:HB3	1.93	0.49
1:I:255:PHE:HB3	1:I:363:PRO:HB2	1.94	0.49
1:J:124:VAL:HG13	1:J:274:LEU:HD21	1.94	0.49
1:J:180:PHE:O	1:J:181:PRO:C	2.54	0.49
1:L:192:ARG:HD3	1:L:219:ASN:HD22	1.77	0.49
2:M:147:LEU:O	2:M:148:MET:HG2	2.13	0.49
2:N:136:ASP:HB3	2:N:203:HIS:CD2	2.48	0.49
2:O:212:ILE:HD13	2:O:212:ILE:N	2.27	0.49
2:P:237:THR:O	2:P:237:THR:CG2	2.60	0.49
2:R:212:ILE:HD13	2:R:212:ILE:N	2.27	0.49
2:S:136:ASP:HB3	2:S:203:HIS:CD2	2.48	0.49
1:C:255:PHE:HB3	1:C:363:PRO:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:124:VAL:HG13	1:G:274:LEU:HD21	1.94	0.48
1:H:255:PHE:HB3	1:H:363:PRO:HB2	1.94	0.48
2:M:61:PHE:HA	2:M:263:SER:O	2.13	0.48
2:O:6:LYS:HA	2:O:33:ILE:CG2	2.41	0.48
2:Q:61:PHE:HA	2:Q:263:SER:O	2.13	0.48
2:S:61:PHE:HA	2:S:263:SER:O	2.13	0.48
2:S:312:ALA:HB2	2:S:317:ILE:CB	2.39	0.48
2:T:61:PHE:HA	2:T:263:SER:O	2.13	0.48
2:V:6:LYS:HA	2:V:33:ILE:CG2	2.41	0.48
2:V:237:THR:O	2:V:237:THR:CG2	2.60	0.48
2:W:136:ASP:HB3	2:W:203:HIS:CD2	2.48	0.48
2:X:136:ASP:OD2	2:X:140:LYS:NZ	2.35	0.48
1:C:124:VAL:HG13	1:C:274:LEU:HD21	1.94	0.48
1:F:456:THR:O	1:L:458:HIS:HE1	1.96	0.48
1:G:255:PHE:HB3	1:G:363:PRO:HB2	1.94	0.48
2:R:61:PHE:HA	2:R:263:SER:O	2.13	0.48
2:R:147:LEU:O	2:R:148:MET:HG2	2.13	0.48
2:T:147:LEU:O	2:T:148:MET:HG2	2.13	0.48
2:X:61:PHE:HA	2:X:263:SER:O	2.13	0.48
1:C:22:THR:HG22	1:C:23:ASP:O	2.14	0.48
1:E:466:TYR:HA	1:K:256:MET:HG3	1.94	0.48
1:F:124:VAL:HG13	1:F:274:LEU:HD21	1.94	0.48
1:F:248:ARG:HH21	1:F:248:ARG:HG3	1.75	0.48
1:K:22:THR:HG22	1:K:23:ASP:O	2.14	0.48
2:N:277:LYS:O	2:N:281:GLU:HG3	2.13	0.48
2:Q:147:LEU:O	2:Q:148:MET:HG2	2.13	0.48
2:S:147:LEU:O	2:S:148:MET:HG2	2.13	0.48
2:V:277:LYS:O	2:V:281:GLU:HG3	2.13	0.48
2:W:277:LYS:O	2:W:281:GLU:HG3	2.13	0.48
1:A:180:PHE:O	1:B:29:GLN:HA	2.14	0.48
1:B:22:THR:HG22	1:B:23:ASP:O	2.14	0.48
1:B:180:PHE:O	1:B:181:PRO:C	2.54	0.48
1:J:22:THR:HG22	1:J:23:ASP:O	2.14	0.48
1:J:255:PHE:HB3	1:J:363:PRO:HB2	1.94	0.48
2:O:147:LEU:O	2:O:148:MET:HG2	2.13	0.48
2:R:277:LYS:O	2:R:281:GLU:HG3	2.13	0.48
2:S:369:THR:C	2:S:370:LYS:CA	2.75	0.48
2:T:136:ASP:OD2	2:T:140:LYS:NZ	2.35	0.48
1:D:396:LEU:H	1:D:396:LEU:HG	1.46	0.48
1:F:28:GLU:OE1	1:F:88:ARG:NH1	2.45	0.48
1:K:180:PHE:O	1:K:181:PRO:C	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:277:LYS:O	2:O:281:GLU:HG3	2.13	0.48
2:T:136:ASP:HB3	2:T:203:HIS:CD2	2.48	0.48
2:U:277:LYS:O	2:U:281:GLU:HG3	2.13	0.48
1:E:398:ASP:OD1	1:E:399:LEU:HD23	2.14	0.48
1:F:364:ALA:HA	1:L:468:VAL:CG1	2.44	0.48
1:H:30:HIS:H	1:I:180:PHE:HB3	1.78	0.48
1:H:398:ASP:OD1	1:H:399:LEU:HD23	2.14	0.48
1:K:248:ARG:CG	1:K:248:ARG:NH2	2.67	0.48
2:P:61:PHE:HA	2:P:263:SER:O	2.13	0.48
2:P:277:LYS:O	2:P:281:GLU:HG3	2.13	0.48
2:R:312:ALA:HB2	2:R:317:ILE:CB	2.39	0.48
2:U:61:PHE:HA	2:U:263:SER:O	2.13	0.48
2:V:64:HIS:CE1	2:V:330:MET:O	2.62	0.48
2:V:147:LEU:O	2:V:148:MET:HG2	2.13	0.48
1:B:248:ARG:CG	1:B:248:ARG:NH2	2.67	0.48
1:J:329:PRO:O	1:J:342:SER:HB3	2.14	0.48
2:S:277:LYS:O	2:S:281:GLU:HG3	2.13	0.48
1:A:180:PHE:O	1:A:181:PRO:C	2.54	0.48
1:B:329:PRO:O	1:B:342:SER:HB3	2.14	0.48
1:C:329:PRO:O	1:C:342:SER:HB3	2.14	0.48
1:E:43:PHE:HB3	2:Q:370:LYS:NZ	2.22	0.48
1:F:458:HIS:HE1	1:L:456:THR:O	1.96	0.48
1:G:398:ASP:OD1	1:G:399:LEU:HD23	2.14	0.48
1:H:43:PHE:HB3	2:T:370:LYS:NZ	2.22	0.48
1:I:28:GLU:OE1	1:I:88:ARG:NH1	2.45	0.48
1:I:398:ASP:OD1	1:I:399:LEU:HD23	2.14	0.48
1:K:398:ASP:OD1	1:K:399:LEU:HD23	2.14	0.48
2:P:136:ASP:HB3	2:P:203:HIS:CD2	2.48	0.48
2:Q:136:ASP:HB3	2:Q:203:HIS:CD2	2.48	0.48
2:Q:277:LYS:O	2:Q:281:GLU:HG3	2.13	0.48
1:A:7:THR:HG1	2:M:178:ILE:HD11	1.75	0.48
1:A:22:THR:HG22	1:A:23:ASP:O	2.13	0.48
1:A:61:ASN:O	1:F:337:ARG:CB	2.44	0.48
1:B:398:ASP:OD1	1:B:399:LEU:HD23	2.14	0.48
1:C:398:ASP:OD1	1:C:399:LEU:HD23	2.14	0.48
1:D:22:THR:HG22	1:D:23:ASP:O	2.14	0.48
1:D:398:ASP:OD1	1:D:399:LEU:HD23	2.14	0.48
1:G:329:PRO:O	1:G:342:SER:HB3	2.14	0.48
1:J:29:GLN:HB3	1:K:180:PHE:CB	2.44	0.48
1:K:329:PRO:O	1:K:342:SER:HB3	2.14	0.48
2:O:136:ASP:HB3	2:O:203:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:147:LEU:O	2:P:148:MET:HG2	2.13	0.48
2:Q:6:LYS:HA	2:Q:33:ILE:CG2	2.41	0.48
2:T:277:LYS:O	2:T:281:GLU:HG3	2.13	0.48
2:U:136:ASP:HB3	2:U:203:HIS:CD2	2.48	0.48
2:V:136:ASP:HB3	2:V:203:HIS:CD2	2.48	0.48
1:E:22:THR:HG22	1:E:23:ASP:O	2.14	0.48
1:E:179:TYR:CD2	1:F:53:SER:HB2	2.49	0.48
1:E:320:LYS:HG3	1:K:454:ARG:O	2.13	0.48
1:F:329:PRO:O	1:F:342:SER:HB3	2.14	0.48
1:F:398:ASP:OD1	1:F:399:LEU:HD23	2.14	0.48
1:H:22:THR:HG22	1:H:23:ASP:O	2.14	0.48
1:I:22:THR:HG22	1:I:23:ASP:O	2.14	0.48
1:J:398:ASP:OD1	1:J:399:LEU:HD23	2.14	0.48
1:L:7:THR:HG1	2:X:178:ILE:HD11	1.75	0.48
2:N:61:PHE:HA	2:N:263:SER:O	2.13	0.48
2:V:61:PHE:HA	2:V:263:SER:O	2.13	0.48
1:A:398:ASP:OD1	1:A:399:LEU:HD23	2.14	0.47
1:D:28:GLU:OE1	1:D:88:ARG:NH1	2.45	0.47
1:E:454:ARG:O	1:K:320:LYS:HG3	2.13	0.47
1:G:22:THR:HG22	1:G:23:ASP:O	2.14	0.47
1:L:22:THR:HG22	1:L:23:ASP:O	2.14	0.47
1:L:180:PHE:O	1:L:181:PRO:C	2.54	0.47
2:T:6:LYS:HA	2:T:33:ILE:CG2	2.41	0.47
2:X:277:LYS:O	2:X:281:GLU:HG3	2.13	0.47
1:L:43:PHE:HB3	2:X:370:LYS:CD	2.28	0.47
1:L:398:ASP:OD1	1:L:399:LEU:HD23	2.14	0.47
2:N:6:LYS:HA	2:N:33:ILE:CG2	2.41	0.47
2:O:61:PHE:HA	2:O:263:SER:O	2.13	0.47
2:O:64:HIS:CE1	2:O:330:MET:O	2.62	0.47
2:R:369:THR:C	2:R:370:LYS:CA	2.75	0.47
2:U:147:LEU:O	2:U:148:MET:HG2	2.13	0.47
2:W:6:LYS:HA	2:W:33:ILE:CG2	2.41	0.47
2:W:61:PHE:HA	2:W:263:SER:O	2.13	0.47
1:D:124:VAL:HG13	1:D:274:LEU:CD2	2.45	0.47
1:F:22:THR:HG22	1:F:23:ASP:O	2.13	0.47
1:I:124:VAL:HG13	1:I:274:LEU:CD2	2.45	0.47
2:M:277:LYS:O	2:M:281:GLU:HG3	2.13	0.47
2:Q:62:TRP:CD1	2:Q:66:ARG:HG3	2.50	0.47
2:S:62:TRP:CD1	2:S:66:ARG:HG3	2.50	0.47
1:F:180:PHE:O	1:F:181:PRO:C	2.54	0.47
1:G:124:VAL:HG13	1:G:274:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:100:TYR:CE2	1:J:102:ARG:HB2	2.50	0.47
1:J:124:VAL:HG13	1:J:274:LEU:CD2	2.45	0.47
2:T:62:TRP:CD1	2:T:66:ARG:HG3	2.50	0.47
2:U:62:TRP:CD1	2:U:66:ARG:HG3	2.50	0.47
1:A:124:VAL:HG13	1:A:274:LEU:CD2	2.45	0.47
1:A:329:PRO:O	1:A:342:SER:HB3	2.14	0.47
1:B:28:GLU:OE1	1:B:88:ARG:NH1	2.45	0.47
1:C:100:TYR:CE2	1:C:102:ARG:HB2	2.50	0.47
1:C:124:VAL:HG13	1:C:274:LEU:CD2	2.45	0.47
1:C:465:TYR:O	1:C:468:VAL:HB	2.15	0.47
1:I:100:TYR:CE2	1:I:102:ARG:HB2	2.50	0.47
1:L:248:ARG:HH21	1:L:248:ARG:HG3	1.75	0.47
2:P:62:TRP:CD1	2:P:66:ARG:HG3	2.50	0.47
2:R:62:TRP:CD1	2:R:66:ARG:HG3	2.50	0.47
1:A:181:PRO:HD3	1:B:29:GLN:OE1	2.14	0.47
1:F:124:VAL:HG13	1:F:274:LEU:CD2	2.45	0.47
1:J:465:TYR:O	1:J:468:VAL:HB	2.15	0.47
1:K:28:GLU:OE1	1:K:88:ARG:NH1	2.45	0.47
1:B:100:TYR:CE2	1:B:102:ARG:HB2	2.50	0.47
1:D:100:TYR:CE2	1:D:102:ARG:HB2	2.50	0.47
1:D:180:PHE:O	1:D:181:PRO:C	2.54	0.47
1:E:271:HIS:CD2	1:E:357:GLU:HG3	2.50	0.47
1:F:100:TYR:CE2	1:F:102:ARG:HB2	2.50	0.47
1:F:465:TYR:O	1:F:468:VAL:HB	2.15	0.47
1:G:43:PHE:HB3	2:S:370:LYS:CD	2.28	0.47
1:G:180:PHE:O	1:G:181:PRO:C	2.54	0.47
1:I:271:HIS:CD2	1:I:357:GLU:HG3	2.50	0.47
1:I:329:PRO:O	1:I:342:SER:HB3	2.14	0.47
1:K:100:TYR:CE2	1:K:102:ARG:HB2	2.50	0.47
1:K:295:LEU:O	1:K:388:PRO:HG2	2.15	0.47
1:L:4:HIS:HD2	2:X:178:ILE:CD1	2.27	0.47
1:L:124:VAL:HG13	1:L:274:LEU:CD2	2.45	0.47
1:L:329:PRO:O	1:L:342:SER:HB3	2.14	0.47
1:A:4:HIS:HD2	2:M:178:ILE:CD1	2.27	0.47
1:A:248:ARG:CG	1:A:248:ARG:NH2	2.67	0.47
1:B:295:LEU:O	1:B:388:PRO:HG2	2.15	0.47
1:C:396:LEU:HB2	1:C:397:TYR:H	1.36	0.47
1:D:271:HIS:CD2	1:D:357:GLU:HG3	2.50	0.47
1:D:329:PRO:O	1:D:342:SER:HB3	2.14	0.47
1:E:329:PRO:O	1:E:342:SER:HB3	2.14	0.47
1:H:271:HIS:CD2	1:H:357:GLU:HG3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:237:THR:O	2:M:237:THR:CG2	2.60	0.47
2:O:62:TRP:CD1	2:O:66:ARG:HG3	2.49	0.47
2:X:237:THR:O	2:X:237:THR:CG2	2.60	0.47
1:A:100:TYR:CE2	1:A:102:ARG:HB2	2.50	0.47
1:A:248:ARG:HH21	1:A:248:ARG:HG3	1.75	0.47
1:A:320:LYS:HG3	1:G:454:ARG:O	2.15	0.47
1:B:124:VAL:HG13	1:B:274:LEU:CD2	2.45	0.47
1:B:465:TYR:O	1:B:468:VAL:HB	2.15	0.47
1:D:465:TYR:O	1:D:468:VAL:HB	2.15	0.47
1:E:5:VAL:HG23	2:Q:179:LYS:HZ1	1.80	0.47
1:F:271:HIS:CD2	1:F:357:GLU:HG3	2.50	0.47
1:G:100:TYR:CE2	1:G:102:ARG:HB2	2.50	0.47
1:G:271:HIS:CD2	1:G:357:GLU:HG3	2.50	0.47
1:G:465:TYR:O	1:G:468:VAL:HB	2.15	0.47
1:H:100:TYR:CE2	1:H:102:ARG:HB2	2.50	0.47
1:H:465:TYR:O	1:H:468:VAL:HB	2.15	0.47
1:I:180:PHE:O	1:I:181:PRO:C	2.54	0.47
1:K:465:TYR:O	1:K:468:VAL:HB	2.15	0.47
2:T:31:THR:HG23	2:T:33:ILE:CD1	2.42	0.47
2:V:62:TRP:CD1	2:V:66:ARG:HG3	2.50	0.47
2:X:62:TRP:CD1	2:X:66:ARG:HG3	2.50	0.47
1:C:271:HIS:CD2	1:C:357:GLU:HG3	2.50	0.47
1:C:295:LEU:O	1:C:388:PRO:HG2	2.15	0.47
1:E:100:TYR:CE2	1:E:102:ARG:HB2	2.50	0.47
1:E:180:PHE:O	1:F:29:GLN:HA	2.15	0.47
1:E:465:TYR:O	1:E:468:VAL:HB	2.15	0.47
1:F:4:HIS:HD2	2:R:178:ILE:CD1	2.27	0.47
1:H:329:PRO:O	1:H:342:SER:HB3	2.14	0.47
1:I:465:TYR:O	1:I:468:VAL:HB	2.15	0.47
1:J:295:LEU:O	1:J:388:PRO:HG2	2.15	0.47
1:K:124:VAL:HG13	1:K:274:LEU:CD2	2.45	0.47
1:L:465:TYR:O	1:L:468:VAL:HB	2.15	0.47
2:M:62:TRP:CD1	2:M:66:ARG:HG3	2.50	0.47
2:N:82:ASP:C	2:N:84:ALA:N	2.73	0.47
1:F:295:LEU:O	1:F:388:PRO:HG2	2.15	0.46
1:J:232:ALA:HB1	1:J:367:PRO:HB2	1.97	0.46
1:J:271:HIS:CD2	1:J:357:GLU:HG3	2.50	0.46
1:L:100:TYR:CE2	1:L:102:ARG:HB2	2.50	0.46
2:M:82:ASP:C	2:M:84:ALA:N	2.73	0.46
2:Q:31:THR:HG23	2:Q:33:ILE:CD1	2.42	0.46
2:W:82:ASP:C	2:W:84:ALA:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:82:ASP:C	2:X:84:ALA:N	2.73	0.46
1:A:295:LEU:O	1:A:388:PRO:HG2	2.15	0.46
1:A:465:TYR:O	1:A:468:VAL:HB	2.15	0.46
1:C:232:ALA:HB1	1:C:367:PRO:HB2	1.97	0.46
1:C:320:LYS:HG3	1:I:454:ARG:O	2.15	0.46
1:C:455:MET:HG2	1:I:323:VAL:HG11	1.97	0.46
1:D:235:ILE:HD13	1:D:235:ILE:HA	1.82	0.46
1:E:232:ALA:HB1	1:E:367:PRO:HB2	1.97	0.46
2:N:290:LEU:HD23	2:N:290:LEU:HA	1.73	0.46
2:R:136:ASP:CG	2:R:203:HIS:HD2	2.24	0.46
2:S:136:ASP:CG	2:S:203:HIS:HD2	2.24	0.46
2:T:31:THR:CG2	2:T:33:ILE:HD12	2.43	0.46
2:W:62:TRP:CD1	2:W:66:ARG:HG3	2.49	0.46
1:E:124:VAL:HG13	1:E:274:LEU:CD2	2.45	0.46
1:G:4:HIS:HD2	2:S:178:ILE:CD1	2.27	0.46
1:H:124:VAL:HG13	1:H:274:LEU:CD2	2.44	0.46
1:K:4:HIS:CD2	2:W:178:ILE:CD1	2.98	0.46
1:L:248:ARG:CG	1:L:248:ARG:NH2	2.67	0.46
2:N:62:TRP:CD1	2:N:66:ARG:HG3	2.50	0.46
2:Q:31:THR:CG2	2:Q:33:ILE:HD12	2.43	0.46
1:C:4:HIS:CD2	2:O:178:ILE:CD1	2.99	0.46
1:C:456:THR:O	1:I:458:HIS:HE1	1.98	0.46
1:E:41:GLU:OE2	1:E:45:GLU:OE2	2.34	0.46
1:F:4:HIS:CD2	2:R:178:ILE:CD1	2.99	0.46
1:G:295:LEU:O	1:G:388:PRO:HG2	2.15	0.46
1:J:4:HIS:CD2	2:V:178:ILE:CD1	2.99	0.46
1:J:396:LEU:HB2	1:J:397:TYR:H	1.36	0.46
1:K:43:PHE:HB3	2:W:370:LYS:NZ	2.22	0.46
1:L:295:LEU:O	1:L:388:PRO:HG2	2.15	0.46
2:M:136:ASP:CG	2:M:203:HIS:HD2	2.24	0.46
2:Q:136:ASP:CG	2:Q:203:HIS:HD2	2.24	0.46
2:T:136:ASP:CG	2:T:203:HIS:HD2	2.24	0.46
1:B:43:PHE:HB3	2:N:370:LYS:NZ	2.22	0.46
1:D:41:GLU:OE2	1:D:45:GLU:OE2	2.34	0.46
1:E:4:HIS:CD2	2:Q:178:ILE:CD1	2.99	0.46
1:G:3:GLU:O	1:G:7:THR:HG23	2.16	0.46
1:H:41:GLU:OE2	1:H:45:GLU:OE2	2.34	0.46
1:H:128:PRO:HA	1:H:269:HIS:O	2.16	0.46
1:H:232:ALA:HB1	1:H:367:PRO:HB2	1.97	0.46
1:I:41:GLU:OE2	1:I:45:GLU:OE2	2.34	0.46
1:K:387:HIS:HA	1:K:388:PRO:HD2	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:6:LYS:HA	2:M:33:ILE:CG2	2.41	0.46
2:T:290:LEU:HD23	2:T:290:LEU:HA	1.73	0.46
2:W:290:LEU:HD23	2:W:290:LEU:HA	1.73	0.46
1:A:3:GLU:O	1:A:7:THR:HG23	2.16	0.46
1:B:4:HIS:CD2	2:N:178:ILE:CD1	2.99	0.46
1:B:232:ALA:HB1	1:B:367:PRO:HB2	1.97	0.46
1:F:232:ALA:HB1	1:F:367:PRO:HB2	1.97	0.46
1:G:232:ALA:HB1	1:G:367:PRO:HB2	1.97	0.46
1:H:403:GLU:C	1:H:405:LYS:N	2.74	0.46
1:K:232:ALA:HB1	1:K:367:PRO:HB2	1.97	0.46
1:L:3:GLU:O	1:L:7:THR:HG23	2.16	0.46
2:M:41:ASP:O	2:M:42:LYS:HB2	2.16	0.46
2:Q:290:LEU:HD23	2:Q:290:LEU:HA	1.73	0.46
2:X:136:ASP:CG	2:X:203:HIS:HD2	2.24	0.46
1:A:271:HIS:CD2	1:A:357:GLU:HG3	2.50	0.46
1:B:271:HIS:CD2	1:B:357:GLU:HG3	2.50	0.46
1:C:3:GLU:O	1:C:7:THR:HG23	2.16	0.46
1:D:466:TYR:HA	1:J:256:MET:HG3	1.97	0.46
1:E:128:PRO:HA	1:E:269:HIS:O	2.16	0.46
1:E:403:GLU:C	1:E:405:LYS:N	2.74	0.46
1:H:4:HIS:CD2	2:T:178:ILE:CD1	2.99	0.46
1:H:180:PHE:O	1:H:181:PRO:C	2.54	0.46
1:K:271:HIS:CD2	1:K:357:GLU:HG3	2.50	0.46
2:U:64:HIS:CE1	2:U:330:MET:O	2.62	0.46
2:X:41:ASP:O	2:X:42:LYS:HB2	2.16	0.46
1:A:4:HIS:CD2	2:M:178:ILE:CD1	2.98	0.46
1:A:170:GLY:HA2	1:A:172:ARG:HH22	1.81	0.46
1:B:320:LYS:HG3	1:H:454:ARG:O	2.16	0.46
1:B:323:VAL:HG11	1:H:455:MET:HG2	1.98	0.46
1:C:128:PRO:HA	1:C:269:HIS:O	2.16	0.46
1:C:256:MET:HG3	1:I:466:TYR:HA	1.98	0.46
1:C:403:GLU:C	1:C:405:LYS:N	2.74	0.46
1:F:3:GLU:O	1:F:7:THR:HG23	2.16	0.46
1:F:254:THR:HB	1:L:466:TYR:CE1	2.51	0.46
1:H:5:VAL:HG23	2:T:179:LYS:HZ1	1.81	0.46
1:I:295:LEU:O	1:I:388:PRO:HG2	2.15	0.46
1:J:128:PRO:HA	1:J:269:HIS:O	2.16	0.46
1:J:403:GLU:C	1:J:405:LYS:N	2.74	0.46
1:K:128:PRO:HA	1:K:269:HIS:O	2.16	0.46
1:L:170:GLY:HA2	1:L:172:ARG:HH22	1.81	0.46
2:X:6:LYS:HA	2:X:33:ILE:CG2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:PRO:HA	1:B:269:HIS:O	2.16	0.46
1:B:387:HIS:HA	1:B:388:PRO:HD2	1.73	0.46
1:D:128:PRO:HA	1:D:269:HIS:O	2.16	0.46
1:F:128:PRO:HA	1:F:269:HIS:O	2.16	0.46
1:I:5:VAL:HG23	2:U:179:LYS:HZ1	1.81	0.46
1:I:232:ALA:HB1	1:I:367:PRO:HB2	1.97	0.46
1:J:3:GLU:O	1:J:7:THR:HG23	2.16	0.46
1:L:41:GLU:OE2	1:L:45:GLU:OE2	2.34	0.46
2:P:144:LYS:HE2	2:P:221:GLU:HA	1.98	0.46
2:Q:144:LYS:HE2	2:Q:221:GLU:HA	1.98	0.46
2:R:82:ASP:C	2:R:84:ALA:N	2.73	0.46
2:S:144:LYS:HE2	2:S:221:GLU:HA	1.98	0.46
2:S:290:LEU:HD23	2:S:290:LEU:HA	1.73	0.46
1:E:295:LEU:O	1:E:388:PRO:HG2	2.15	0.46
1:F:403:GLU:C	1:F:405:LYS:N	2.74	0.46
1:G:4:HIS:CD2	2:S:178:ILE:CD1	2.99	0.46
1:G:41:GLU:OE2	1:G:45:GLU:OE2	2.34	0.46
1:G:128:PRO:HA	1:G:269:HIS:O	2.16	0.46
1:K:41:GLU:OE2	1:K:45:GLU:OE2	2.34	0.46
1:L:271:HIS:CD2	1:L:357:GLU:HG3	2.50	0.46
2:R:6:LYS:HA	2:R:33:ILE:CG2	2.41	0.46
2:S:6:LYS:HA	2:S:33:ILE:CG2	2.41	0.46
2:S:82:ASP:C	2:S:84:ALA:N	2.73	0.46
2:T:64:HIS:CE1	2:T:330:MET:O	2.62	0.46
2:T:82:ASP:C	2:T:84:ALA:N	2.73	0.46
2:U:144:LYS:HE2	2:U:221:GLU:HA	1.98	0.46
1:A:41:GLU:OE2	1:A:45:GLU:OE2	2.34	0.45
1:B:41:GLU:OE2	1:B:45:GLU:OE2	2.34	0.45
1:D:295:LEU:O	1:D:388:PRO:HG2	2.15	0.45
1:G:313:ASN:HD21	1:G:360:PHE:HD2	1.64	0.45
1:H:295:LEU:O	1:H:388:PRO:HG2	2.15	0.45
1:I:128:PRO:HA	1:I:269:HIS:O	2.16	0.45
1:J:387:HIS:HA	1:J:388:PRO:HD2	1.73	0.45
1:K:235:ILE:HD13	1:K:235:ILE:HA	1.82	0.45
2:P:64:HIS:CE1	2:P:330:MET:O	2.62	0.45
2:R:41:ASP:O	2:R:42:LYS:HB2	2.16	0.45
2:R:144:LYS:HE2	2:R:221:GLU:HA	1.98	0.45
2:T:144:LYS:HE2	2:T:221:GLU:HA	1.98	0.45
2:W:312:ALA:CB	2:W:317:ILE:HG22	2.32	0.45
2:X:31:THR:HG23	2:X:33:ILE:CD1	2.42	0.45
1:D:180:PHE:O	1:E:29:GLN:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:ALA:HB1	1:D:367:PRO:HB2	1.97	0.45
1:E:180:PHE:O	1:E:181:PRO:C	2.54	0.45
1:G:29:GLN:HB3	1:H:180:PHE:CB	2.46	0.45
1:G:170:GLY:HA2	1:G:172:ARG:HH22	1.81	0.45
1:G:403:GLU:C	1:G:405:LYS:N	2.74	0.45
1:L:4:HIS:CD2	2:X:178:ILE:CD1	2.99	0.45
2:N:31:THR:CG2	2:N:33:ILE:HD12	2.43	0.45
2:S:41:ASP:O	2:S:42:LYS:HB2	2.16	0.45
2:W:59:ILE:HG21	2:W:59:ILE:HD13	1.70	0.45
1:A:403:GLU:C	1:A:405:LYS:N	2.74	0.45
1:A:466:TYR:HA	1:G:256:MET:HG3	1.97	0.45
1:B:235:ILE:HD13	1:B:235:ILE:HA	1.82	0.45
1:C:41:GLU:OE2	1:C:45:GLU:OE2	2.34	0.45
1:D:3:GLU:O	1:D:7:THR:HG23	2.16	0.45
1:F:41:GLU:OE2	1:F:45:GLU:OE2	2.34	0.45
1:I:4:HIS:CD2	2:U:178:ILE:CD1	2.99	0.45
1:I:403:GLU:C	1:I:405:LYS:N	2.74	0.45
2:N:312:ALA:CB	2:N:317:ILE:HG22	2.32	0.45
2:O:144:LYS:HE2	2:O:221:GLU:HA	1.98	0.45
2:U:59:ILE:HG21	2:U:59:ILE:HD13	1.70	0.45
2:V:41:ASP:O	2:V:42:LYS:HB2	2.16	0.45
2:V:82:ASP:C	2:V:84:ALA:N	2.73	0.45
2:W:31:THR:CG2	2:W:33:ILE:HD12	2.43	0.45
2:X:312:ALA:CB	2:X:317:ILE:HG22	2.32	0.45
1:B:313:ASN:HD21	1:B:360:PHE:HD2	1.65	0.45
1:E:3:GLU:O	1:E:7:THR:HG23	2.16	0.45
1:E:28:GLU:OE1	1:E:88:ARG:NH1	2.45	0.45
1:K:313:ASN:HD21	1:K:360:PHE:HD2	1.65	0.45
2:O:41:ASP:O	2:O:42:LYS:HB2	2.16	0.45
2:O:82:ASP:C	2:O:84:ALA:N	2.73	0.45
2:Q:82:ASP:C	2:Q:84:ALA:N	2.73	0.45
2:R:64:HIS:CE1	2:R:330:MET:O	2.62	0.45
2:R:290:LEU:HD23	2:R:290:LEU:HA	1.73	0.45
2:V:31:THR:HG23	2:V:33:ILE:CD1	2.42	0.45
2:V:144:LYS:HE2	2:V:221:GLU:HA	1.98	0.45
2:W:31:THR:HG23	2:W:33:ILE:CD1	2.42	0.45
1:A:31:VAL:HG23	1:F:210:HIS:HB3	1.97	0.45
1:D:4:HIS:CD2	2:P:178:ILE:CD1	2.99	0.45
1:D:170:GLY:HA2	1:D:172:ARG:HH22	1.81	0.45
1:F:313:ASN:HD21	1:F:360:PHE:HD2	1.65	0.45
1:H:3:GLU:O	1:H:7:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:170:GLY:HA2	1:I:172:ARG:HH22	1.81	0.45
1:J:41:GLU:OE2	1:J:45:GLU:OE2	2.34	0.45
1:J:313:ASN:HD21	1:J:360:PHE:HD2	1.64	0.45
1:L:313:ASN:HD21	1:L:360:PHE:HD2	1.65	0.45
1:L:403:GLU:C	1:L:405:LYS:N	2.74	0.45
2:Q:64:HIS:CE1	2:Q:330:MET:O	2.62	0.45
1:A:139:ARG:HD3	1:F:163:LYS:HG2	1.99	0.45
1:A:313:ASN:HD21	1:A:360:PHE:HD2	1.65	0.45
1:B:320:LYS:HG2	1:H:455:MET:C	2.42	0.45
1:C:313:ASN:HD21	1:C:360:PHE:HD2	1.65	0.45
1:C:328:ALA:HA	1:C:329:PRO:HD3	1.73	0.45
1:F:170:GLY:HA2	1:F:172:ARG:HH22	1.81	0.45
1:F:454:ARG:O	1:L:320:LYS:HG3	2.16	0.45
1:I:3:GLU:O	1:I:7:THR:HG23	2.16	0.45
2:N:31:THR:HG23	2:N:33:ILE:CD1	2.42	0.45
2:N:41:ASP:O	2:N:42:LYS:HB2	2.16	0.45
1:A:232:ALA:HB1	1:A:367:PRO:HB2	1.97	0.45
1:A:396:LEU:HB2	1:A:397:TYR:H	1.36	0.45
1:C:387:HIS:HA	1:C:388:PRO:HD2	1.73	0.45
1:D:5:VAL:HG23	2:P:179:LYS:HZ1	1.82	0.45
1:D:403:GLU:C	1:D:405:LYS:N	2.74	0.45
1:H:4:HIS:HD2	2:T:178:ILE:CD1	2.27	0.45
1:H:313:ASN:HD21	1:H:360:PHE:HD2	1.64	0.45
2:M:31:THR:HG23	2:M:33:ILE:CD1	2.42	0.45
2:U:41:ASP:O	2:U:42:LYS:HB2	2.16	0.45
2:W:41:ASP:O	2:W:42:LYS:HB2	2.16	0.45
1:D:396:LEU:HB2	1:D:397:TYR:H	1.36	0.45
1:H:28:GLU:OE1	1:H:88:ARG:NH1	2.45	0.45
2:O:31:THR:HG23	2:O:33:ILE:CD1	2.42	0.45
2:P:41:ASP:O	2:P:42:LYS:HB2	2.16	0.45
2:U:290:LEU:HD23	2:U:290:LEU:HA	1.73	0.45
1:A:180:PHE:HB2	1:B:29:GLN:HB3	1.99	0.45
1:B:3:GLU:O	1:B:7:THR:HG23	2.16	0.45
1:C:4:HIS:HD2	2:O:178:ILE:CD1	2.27	0.45
1:D:324:PRO:HB3	1:D:397:TYR:CD2	2.52	0.45
1:E:4:HIS:HD2	2:Q:178:ILE:CD1	2.27	0.45
1:J:4:HIS:HD2	2:V:178:ILE:CD1	2.27	0.45
1:J:31:VAL:HG23	1:K:210:HIS:HB3	1.98	0.45
1:L:396:LEU:HB2	1:L:397:TYR:H	1.36	0.45
2:M:312:ALA:CB	2:M:317:ILE:HG22	2.32	0.45
2:P:290:LEU:HD23	2:P:290:LEU:HA	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:270:SER:HA	2:R:271:PRO:HD3	1.74	0.45
2:S:64:HIS:CE1	2:S:330:MET:O	2.62	0.45
1:D:468:VAL:HG13	1:J:364:ALA:HA	1.99	0.45
1:E:313:ASN:HD21	1:E:360:PHE:HD2	1.65	0.45
1:I:324:PRO:HB3	1:I:397:TYR:CD2	2.52	0.45
1:J:34:PRO:HG2	1:K:206:VAL:O	2.17	0.45
1:L:128:PRO:HA	1:L:269:HIS:O	2.16	0.45
1:L:232:ALA:HB1	1:L:367:PRO:HB2	1.97	0.45
2:M:144:LYS:HE2	2:M:221:GLU:HA	1.98	0.45
2:N:239:LYS:HZ3	2:N:241:ASN:HB2	1.82	0.45
2:P:82:ASP:C	2:P:84:ALA:N	2.73	0.45
2:Q:41:ASP:O	2:Q:42:LYS:HB2	2.16	0.45
2:U:97:VAL:O	2:U:104:ILE:HG12	2.17	0.45
2:X:6:LYS:HD2	2:X:8:VAL:HG23	1.99	0.45
1:A:128:PRO:HA	1:A:269:HIS:O	2.16	0.44
1:A:324:PRO:HB3	1:A:397:TYR:CE2	2.52	0.44
1:C:65:MET:HA	1:C:94:PRO:HG3	2.00	0.44
1:G:458:HIS:CD2	1:G:459:PRO:HD2	2.52	0.44
1:I:396:LEU:HB2	1:I:397:TYR:H	1.36	0.44
1:K:3:GLU:O	1:K:7:THR:HG23	2.16	0.44
1:K:4:HIS:HD2	2:W:178:ILE:CD1	2.27	0.44
1:L:43:PHE:HB3	2:X:370:LYS:NZ	2.22	0.44
2:M:6:LYS:HD2	2:M:8:VAL:HG23	1.99	0.44
2:P:59:ILE:HG21	2:P:59:ILE:HD13	1.70	0.44
2:P:97:VAL:O	2:P:104:ILE:HG12	2.17	0.44
2:U:82:ASP:C	2:U:84:ALA:N	2.73	0.44
2:W:136:ASP:CG	2:W:203:HIS:HD2	2.24	0.44
2:X:144:LYS:HE2	2:X:221:GLU:HA	1.98	0.44
1:C:324:PRO:HB3	1:C:397:TYR:CD2	2.52	0.44
1:E:324:PRO:HB3	1:E:397:TYR:CD2	2.52	0.44
1:H:324:PRO:HB3	1:H:397:TYR:CD2	2.52	0.44
1:J:65:MET:HA	1:J:94:PRO:HG3	2.00	0.44
2:Q:369:THR:C	2:Q:370:LYS:CA	2.75	0.44
2:T:41:ASP:O	2:T:42:LYS:HB2	2.16	0.44
2:W:239:LYS:HZ3	2:W:241:ASN:HB2	1.82	0.44
1:A:340:SER:HB3	1:A:396:LEU:HB3	1.99	0.44
1:A:458:HIS:CD2	1:A:459:PRO:HD2	2.52	0.44
1:E:276:LYS:HG2	1:E:277:ASN:ND2	2.32	0.44
1:F:7:THR:OG1	2:R:178:ILE:HD13	2.18	0.44
1:J:324:PRO:HB3	1:J:397:TYR:CD2	2.52	0.44
1:K:458:HIS:CD2	1:K:459:PRO:HD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:324:PRO:HB3	1:L:397:TYR:CD2	2.52	0.44
1:L:324:PRO:HB3	1:L:397:TYR:CE2	2.53	0.44
2:P:128:THR:CG2	2:P:131:GLU:H	2.31	0.44
2:U:128:THR:CG2	2:U:131:GLU:H	2.31	0.44
2:V:136:ASP:CG	2:V:203:HIS:HD2	2.24	0.44
2:W:270:SER:HA	2:W:271:PRO:HD3	1.74	0.44
2:X:64:HIS:CE1	2:X:330:MET:O	2.62	0.44
2:X:97:VAL:O	2:X:104:ILE:HG12	2.17	0.44
2:X:270:SER:HA	2:X:271:PRO:HD3	1.74	0.44
1:A:65:MET:HA	1:A:94:PRO:HG3	2.00	0.44
1:A:324:PRO:HB3	1:A:397:TYR:CD2	2.52	0.44
1:B:65:MET:HA	1:B:94:PRO:HG3	1.99	0.44
1:B:458:HIS:CD2	1:B:459:PRO:HD2	2.52	0.44
1:C:458:HIS:CD2	1:C:459:PRO:HD2	2.52	0.44
1:D:65:MET:HA	1:D:94:PRO:HG3	2.00	0.44
1:E:458:HIS:CD2	1:E:459:PRO:HD2	2.52	0.44
1:F:73:THR:HG21	1:F:88:ARG:HB3	2.00	0.44
1:F:275:ALA:HA	1:F:281:LEU:HD13	2.00	0.44
1:H:276:LYS:HG2	1:H:277:ASN:ND2	2.33	0.44
1:L:65:MET:HA	1:L:94:PRO:HG3	2.00	0.44
1:L:458:HIS:CD2	1:L:459:PRO:HD2	2.52	0.44
2:M:97:VAL:O	2:M:104:ILE:HG12	2.17	0.44
2:M:270:SER:HA	2:M:271:PRO:HD3	1.74	0.44
2:N:97:VAL:O	2:N:104:ILE:HG12	2.17	0.44
2:N:128:THR:CG2	2:N:131:GLU:H	2.31	0.44
2:N:136:ASP:CG	2:N:203:HIS:HD2	2.24	0.44
2:N:144:LYS:HE2	2:N:221:GLU:HA	1.98	0.44
2:N:270:SER:HA	2:N:271:PRO:HD3	1.74	0.44
2:O:31:THR:CG2	2:O:33:ILE:HD12	2.43	0.44
2:O:128:THR:CG2	2:O:131:GLU:H	2.31	0.44
2:Q:97:VAL:O	2:Q:104:ILE:HG12	2.17	0.44
2:R:31:THR:HG23	2:R:33:ILE:CD1	2.42	0.44
2:R:97:VAL:O	2:R:104:ILE:HG12	2.17	0.44
2:T:97:VAL:O	2:T:104:ILE:HG12	2.17	0.44
2:T:312:ALA:HB2	2:T:317:ILE:CG2	2.45	0.44
2:U:31:THR:HG23	2:U:33:ILE:CD1	2.42	0.44
2:V:128:THR:CG2	2:V:131:GLU:H	2.31	0.44
2:W:128:THR:CG2	2:W:131:GLU:H	2.31	0.44
1:A:7:THR:OG1	2:M:178:ILE:HD13	2.18	0.44
1:A:276:LYS:HG2	1:A:277:ASN:ND2	2.33	0.44
1:B:4:HIS:HD2	2:N:178:ILE:CD1	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:ASN:HD21	1:D:360:PHE:HD2	1.65	0.44
1:E:5:VAL:CG2	2:Q:179:LYS:HZ1	2.30	0.44
1:E:65:MET:HA	1:E:94:PRO:HG3	2.00	0.44
1:F:458:HIS:CD2	1:F:459:PRO:HD2	2.52	0.44
1:G:7:THR:OG1	2:S:178:ILE:HD13	2.18	0.44
1:G:324:PRO:HB3	1:G:397:TYR:CE2	2.53	0.44
1:H:65:MET:HA	1:H:94:PRO:HG3	2.00	0.44
1:H:275:ALA:HA	1:H:281:LEU:HD13	2.00	0.44
1:I:65:MET:HA	1:I:94:PRO:HG3	2.00	0.44
1:I:313:ASN:HD21	1:I:360:PHE:HD2	1.65	0.44
1:J:328:ALA:HA	1:J:329:PRO:HD3	1.73	0.44
1:L:276:LYS:HG2	1:L:277:ASN:ND2	2.33	0.44
2:M:64:HIS:CE1	2:M:330:MET:O	2.62	0.44
2:S:31:THR:HG23	2:S:33:ILE:CD1	2.42	0.44
2:W:97:VAL:O	2:W:104:ILE:HG12	2.17	0.44
2:W:144:LYS:HE2	2:W:221:GLU:HA	1.98	0.44
1:A:29:GLN:HB3	1:F:180:PHE:HB2	2.00	0.44
1:A:73:THR:HG21	1:A:88:ARG:HB3	2.00	0.44
1:B:17:VAL:HG12	1:B:19:LEU:HD13	2.00	0.44
1:B:403:GLU:C	1:B:405:LYS:N	2.74	0.44
1:D:340:SER:HB3	1:D:396:LEU:HB3	1.99	0.44
1:E:275:ALA:HA	1:E:281:LEU:HD13	2.00	0.44
1:G:73:THR:HG21	1:G:88:ARG:HB3	2.00	0.44
1:I:340:SER:HB3	1:I:396:LEU:HB3	1.99	0.44
1:J:5:VAL:CG2	2:V:179:LYS:HZ1	2.31	0.44
1:K:17:VAL:HG12	1:K:19:LEU:HD13	2.00	0.44
1:K:65:MET:HA	1:K:94:PRO:HG3	2.00	0.44
2:O:290:LEU:HD23	2:O:290:LEU:HA	1.73	0.44
2:P:31:THR:HG23	2:P:33:ILE:CD1	2.42	0.44
2:P:136:ASP:CG	2:P:203:HIS:HD2	2.24	0.44
2:T:270:SER:HA	2:T:271:PRO:HD3	1.74	0.44
2:U:136:ASP:CG	2:U:203:HIS:HD2	2.24	0.44
1:C:5:VAL:CG2	2:O:179:LYS:HZ1	2.31	0.44
1:E:309:ASN:HD22	1:E:313:ASN:HD22	1.66	0.44
1:F:65:MET:HA	1:F:94:PRO:HG3	2.00	0.44
1:G:65:MET:HA	1:G:94:PRO:HG3	2.00	0.44
1:G:275:ALA:HA	1:G:281:LEU:HD13	2.00	0.44
1:H:5:VAL:CG2	2:T:179:LYS:HZ1	2.30	0.44
1:H:324:PRO:HB3	1:H:397:TYR:CE2	2.52	0.44
1:H:458:HIS:CD2	1:H:459:PRO:HD2	2.53	0.44
1:I:324:PRO:HB3	1:I:397:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:398:ASP:C	1:I:399:LEU:HG	2.43	0.44
1:L:28:GLU:OE1	1:L:88:ARG:NH1	2.45	0.44
1:L:340:SER:HB3	1:L:396:LEU:HB3	2.00	0.44
2:M:128:THR:CG2	2:M:131:GLU:H	2.31	0.44
2:O:136:ASP:CG	2:O:203:HIS:HD2	2.24	0.44
2:Q:128:THR:CG2	2:Q:131:GLU:H	2.31	0.44
2:S:97:VAL:O	2:S:104:ILE:HG12	2.17	0.44
2:V:290:LEU:HD23	2:V:290:LEU:HA	1.73	0.44
1:A:215:THR:O	1:A:216:ALA:HB3	2.18	0.44
1:B:340:SER:HB3	1:B:396:LEU:HB3	1.99	0.44
1:C:275:ALA:HA	1:C:281:LEU:HD13	2.00	0.44
1:D:324:PRO:HB3	1:D:397:TYR:CE2	2.52	0.44
1:E:324:PRO:HB3	1:E:397:TYR:CE2	2.52	0.44
1:F:324:PRO:HB3	1:F:397:TYR:CD2	2.52	0.44
1:F:324:PRO:HB3	1:F:397:TYR:CE2	2.52	0.44
1:G:324:PRO:HB3	1:G:397:TYR:CD2	2.52	0.44
1:H:309:ASN:HD22	1:H:313:ASN:HD22	1.66	0.44
1:J:5:VAL:HG23	2:V:179:LYS:HZ1	1.82	0.44
1:J:458:HIS:CD2	1:J:459:PRO:HD2	2.52	0.44
1:K:340:SER:HB3	1:K:396:LEU:HB3	1.99	0.44
2:O:132:ILE:N	2:O:133:PRO:HD3	2.33	0.44
2:P:312:ALA:CB	2:P:317:ILE:HG22	2.32	0.44
2:T:128:THR:CG2	2:T:131:GLU:H	2.31	0.44
2:T:369:THR:C	2:T:370:LYS:CA	2.75	0.44
2:V:132:ILE:N	2:V:133:PRO:HD3	2.33	0.44
1:A:43:PHE:HB3	2:M:370:LYS:NZ	2.22	0.44
1:B:276:LYS:HG2	1:B:277:ASN:ND2	2.33	0.44
1:C:5:VAL:HG23	2:O:179:LYS:HZ1	1.82	0.44
1:D:275:ALA:HA	1:D:281:LEU:HD13	2.00	0.44
1:D:398:ASP:C	1:D:399:LEU:HG	2.43	0.44
1:G:180:PHE:HB2	1:L:29:GLN:HB3	2.00	0.44
1:I:275:ALA:HA	1:I:281:LEU:HD13	2.00	0.44
1:J:170:GLY:HA2	1:J:172:ARG:HH22	1.81	0.44
1:J:275:ALA:HA	1:J:281:LEU:HD13	2.00	0.44
1:J:324:PRO:HB3	1:J:397:TYR:CE2	2.52	0.44
1:J:340:SER:HB3	1:J:396:LEU:HB3	1.99	0.44
1:K:276:LYS:HG2	1:K:277:ASN:ND2	2.32	0.44
1:L:73:THR:HG21	1:L:88:ARG:HB3	2.00	0.44
1:L:215:THR:O	1:L:216:ALA:HB3	2.18	0.44
2:N:132:ILE:N	2:N:133:PRO:HD3	2.33	0.44
2:O:97:VAL:O	2:O:104:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:139:LEU:HA	2:P:142:LYS:HE3	2.00	0.44
2:U:6:LYS:HD2	2:U:8:VAL:HG23	1.99	0.44
2:U:139:LEU:HA	2:U:142:LYS:HE3	2.00	0.44
2:V:31:THR:CG2	2:V:33:ILE:HD12	2.43	0.44
2:W:132:ILE:N	2:W:133:PRO:HD3	2.33	0.44
2:X:128:THR:CG2	2:X:131:GLU:H	2.31	0.44
1:B:324:PRO:HB3	1:B:397:TYR:CD2	2.52	0.43
1:C:324:PRO:HB3	1:C:397:TYR:CE2	2.52	0.43
1:J:7:THR:OG1	2:V:178:ILE:HD13	2.18	0.43
1:J:276:LYS:HG2	1:J:277:ASN:ND2	2.33	0.43
1:K:5:VAL:HG23	2:W:179:LYS:HZ1	1.83	0.43
1:K:324:PRO:HB3	1:K:397:TYR:CD2	2.52	0.43
2:P:6:LYS:HD2	2:P:8:VAL:HG23	1.99	0.43
2:Q:312:ALA:HB2	2:Q:317:ILE:CG2	2.45	0.43
2:S:132:ILE:N	2:S:133:PRO:HD3	2.33	0.43
2:S:311:LEU:HD12	2:S:311:LEU:HA	1.89	0.43
2:V:59:ILE:HG21	2:V:59:ILE:HD13	1.70	0.43
2:V:97:VAL:O	2:V:104:ILE:HG12	2.17	0.43
2:X:148:MET:HE3	2:X:216:ALA:CB	2.48	0.43
1:A:29:GLN:HB3	1:F:180:PHE:CB	2.49	0.43
1:C:7:THR:OG1	2:O:178:ILE:HD13	2.18	0.43
1:C:276:LYS:HG2	1:C:277:ASN:ND2	2.33	0.43
1:D:137:ASP:HB3	1:D:152:ASP:HB3	2.01	0.43
1:D:328:ALA:HA	1:D:329:PRO:HD3	1.73	0.43
1:E:398:ASP:C	1:E:399:LEU:HG	2.43	0.43
1:F:276:LYS:HG2	1:F:277:ASN:ND2	2.33	0.43
1:G:309:ASN:HD22	1:G:313:ASN:HD22	1.66	0.43
1:H:398:ASP:C	1:H:399:LEU:HG	2.43	0.43
1:I:5:VAL:CG2	2:U:179:LYS:HZ1	2.31	0.43
1:I:137:ASP:HB3	1:I:152:ASP:HB3	2.01	0.43
1:I:276:LYS:HG2	1:I:277:ASN:ND2	2.33	0.43
1:J:73:THR:HG21	1:J:88:ARG:HB3	2.00	0.43
1:K:275:ALA:HA	1:K:281:LEU:HD13	2.00	0.43
1:K:403:GLU:C	1:K:405:LYS:N	2.74	0.43
2:M:139:LEU:HA	2:M:142:LYS:HE3	2.00	0.43
2:Q:270:SER:HA	2:Q:271:PRO:HD3	1.74	0.43
2:R:132:ILE:N	2:R:133:PRO:HD3	2.33	0.43
2:S:6:LYS:HD2	2:S:8:VAL:HG23	1.99	0.43
1:A:28:GLU:OE1	1:A:88:ARG:NH1	2.45	0.43
1:A:328:ALA:HA	1:A:329:PRO:HD3	1.73	0.43
1:B:125:LEU:O	1:B:272:MET:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ALA:HA	1:B:281:LEU:HD13	2.00	0.43
1:C:17:VAL:HG12	1:C:19:LEU:HD13	2.00	0.43
1:C:170:GLY:HA2	1:C:172:ARG:HH22	1.81	0.43
1:C:455:MET:C	1:I:320:LYS:HG2	2.43	0.43
1:D:276:LYS:HG2	1:D:277:ASN:ND2	2.33	0.43
1:E:328:ALA:HA	1:E:329:PRO:HD3	1.73	0.43
1:F:309:ASN:HD22	1:F:313:ASN:HD22	1.66	0.43
1:F:398:ASP:C	1:F:399:LEU:HG	2.43	0.43
1:G:180:PHE:CB	1:L:29:GLN:HB3	2.48	0.43
1:G:276:LYS:HG2	1:G:277:ASN:ND2	2.33	0.43
1:H:7:THR:OG1	2:T:178:ILE:HD13	2.18	0.43
1:I:309:ASN:HD22	1:I:313:ASN:HD22	1.66	0.43
1:I:458:HIS:CD2	1:I:459:PRO:HD2	2.52	0.43
1:L:235:ILE:HD13	1:L:235:ILE:HA	1.82	0.43
1:L:275:ALA:HA	1:L:281:LEU:HD13	2.00	0.43
2:M:148:MET:HE3	2:M:216:ALA:CB	2.48	0.43
2:N:148:MET:HE3	2:N:216:ALA:CB	2.48	0.43
2:P:59:ILE:HD11	2:P:280:LEU:HD21	2.00	0.43
2:P:132:ILE:N	2:P:133:PRO:HD3	2.33	0.43
2:U:312:ALA:CB	2:U:317:ILE:HG22	2.32	0.43
2:W:148:MET:HE3	2:W:216:ALA:CB	2.48	0.43
2:X:139:LEU:HA	2:X:142:LYS:HE3	2.00	0.43
1:A:275:ALA:HA	1:A:281:LEU:HD13	2.00	0.43
1:C:73:THR:HG21	1:C:88:ARG:HB3	2.00	0.43
1:C:210:HIS:HB3	1:D:31:VAL:HG23	1.99	0.43
1:C:340:SER:HB3	1:C:396:LEU:HB3	1.99	0.43
1:D:5:VAL:CG2	2:P:179:LYS:HZ1	2.31	0.43
1:D:468:VAL:CG1	1:J:364:ALA:HA	2.49	0.43
1:F:125:LEU:O	1:F:272:MET:HA	2.19	0.43
1:J:17:VAL:HG12	1:J:19:LEU:HD13	2.00	0.43
1:J:398:ASP:C	1:J:399:LEU:HG	2.43	0.43
2:M:132:ILE:N	2:M:133:PRO:HD3	2.33	0.43
2:N:139:LEU:HA	2:N:142:LYS:HE3	2.00	0.43
2:R:6:LYS:HD2	2:R:8:VAL:HG23	1.99	0.43
2:R:59:ILE:HD11	2:R:280:LEU:HD21	2.00	0.43
2:S:59:ILE:HD11	2:S:280:LEU:HD21	2.00	0.43
2:S:270:SER:HA	2:S:271:PRO:HD3	1.74	0.43
2:U:132:ILE:N	2:U:133:PRO:HD3	2.33	0.43
2:V:148:MET:HE3	2:V:216:ALA:CB	2.48	0.43
2:W:139:LEU:HA	2:W:142:LYS:HE3	2.00	0.43
2:W:362:LYS:C	2:W:362:LYS:HE2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:246:VAL:H	2:X:246:VAL:HG23	1.58	0.43
1:D:73:THR:HG21	1:D:88:ARG:HB3	2.00	0.43
1:E:137:ASP:HB3	1:E:152:ASP:HB3	2.01	0.43
1:H:125:LEU:O	1:H:272:MET:HA	2.19	0.43
1:I:17:VAL:HG12	1:I:19:LEU:HD13	2.00	0.43
1:I:73:THR:HG21	1:I:88:ARG:HB3	2.00	0.43
1:K:125:LEU:O	1:K:272:MET:HA	2.19	0.43
2:N:362:LYS:HE2	2:N:362:LYS:C	2.44	0.43
2:P:239:LYS:HZ3	2:P:241:ASN:HB2	1.82	0.43
2:Q:321:MET:HB3	2:Q:321:MET:HE2	1.71	0.43
2:R:311:LEU:HD12	2:R:311:LEU:HA	1.88	0.43
2:U:59:ILE:HD11	2:U:280:LEU:HD21	2.00	0.43
2:W:312:ALA:HB2	2:W:317:ILE:CG2	2.45	0.43
2:X:132:ILE:N	2:X:133:PRO:HD3	2.33	0.43
1:A:180:PHE:CB	1:B:29:GLN:HB3	2.49	0.43
1:B:73:THR:HG21	1:B:88:ARG:HB3	2.00	0.43
1:B:324:PRO:HB3	1:B:397:TYR:CE2	2.53	0.43
1:B:344:ARG:NH1	1:B:346:PRO:HA	2.34	0.43
1:C:309:ASN:HD22	1:C:313:ASN:HD22	1.66	0.43
1:D:7:THR:OG1	2:P:178:ILE:HD13	2.18	0.43
1:D:309:ASN:HD22	1:D:313:ASN:HD22	1.66	0.43
1:D:458:HIS:CD2	1:D:459:PRO:HD2	2.53	0.43
1:E:7:THR:OG1	2:Q:178:ILE:HD13	2.18	0.43
1:E:125:LEU:O	1:E:272:MET:HA	2.19	0.43
1:J:236:GLN:OE1	1:J:236:GLN:HA	2.19	0.43
1:J:309:ASN:HD22	1:J:313:ASN:HD22	1.66	0.43
1:K:73:THR:HG21	1:K:88:ARG:HB3	2.00	0.43
1:K:215:THR:O	1:K:216:ALA:HB3	2.18	0.43
1:K:324:PRO:HB3	1:K:397:TYR:CE2	2.52	0.43
2:M:290:LEU:HA	2:M:290:LEU:HD23	1.73	0.43
2:M:362:LYS:C	2:M:362:LYS:HE2	2.44	0.43
2:N:312:ALA:HB2	2:N:317:ILE:CG2	2.45	0.43
2:O:148:MET:HE3	2:O:216:ALA:CB	2.48	0.43
2:P:148:MET:HE3	2:P:216:ALA:CB	2.48	0.43
2:Q:6:LYS:HD2	2:Q:8:VAL:HG23	1.99	0.43
2:T:132:ILE:N	2:T:133:PRO:HD3	2.33	0.43
2:V:6:LYS:HD2	2:V:8:VAL:HG23	1.99	0.43
2:V:362:LYS:HE2	2:V:362:LYS:C	2.44	0.43
2:X:362:LYS:C	2:X:362:LYS:HE2	2.44	0.43
1:A:235:ILE:HD13	1:A:235:ILE:HA	1.82	0.43
1:B:236:GLN:OE1	1:B:236:GLN:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:ARG:O	1:H:320:LYS:HG3	2.17	0.43
1:C:236:GLN:HA	1:C:236:GLN:OE1	2.19	0.43
1:C:398:ASP:C	1:C:399:LEU:HG	2.43	0.43
1:D:17:VAL:HG12	1:D:19:LEU:HD13	2.00	0.43
1:E:170:GLY:HA2	1:E:172:ARG:HH22	1.81	0.43
1:E:231:LYS:HD2	1:E:231:LYS:HA	1.74	0.43
1:F:256:MET:CG	1:L:466:TYR:HA	2.49	0.43
1:G:125:LEU:O	1:G:272:MET:HA	2.19	0.43
1:G:398:ASP:C	1:G:399:LEU:HG	2.43	0.43
1:H:334:TYR:HA	1:H:343:ILE:O	2.19	0.43
1:I:7:THR:OG1	2:U:178:ILE:HD13	2.18	0.43
1:K:236:GLN:HA	1:K:236:GLN:OE1	2.19	0.43
1:K:344:ARG:NH1	1:K:346:PRO:HA	2.34	0.43
1:L:125:LEU:O	1:L:272:MET:HA	2.19	0.43
2:N:6:LYS:HD2	2:N:8:VAL:HG23	1.99	0.43
2:O:6:LYS:HD2	2:O:8:VAL:HG23	1.99	0.43
2:O:312:ALA:CB	2:O:317:ILE:HG22	2.32	0.43
2:O:362:LYS:C	2:O:362:LYS:HE2	2.44	0.43
2:Q:148:MET:HE3	2:Q:216:ALA:CB	2.48	0.43
2:S:128:THR:CG2	2:S:131:GLU:H	2.31	0.43
2:U:148:MET:HE3	2:U:216:ALA:CB	2.48	0.43
2:U:311:LEU:HD12	2:U:311:LEU:HA	1.89	0.43
2:W:59:ILE:HD11	2:W:280:LEU:HD21	2.00	0.43
1:A:125:LEU:O	1:A:272:MET:HA	2.19	0.43
1:B:215:THR:O	1:B:216:ALA:HB3	2.18	0.43
1:D:320:LYS:HG3	1:J:454:ARG:O	2.18	0.43
1:D:332:LEU:HD22	1:D:409:GLN:C	2.44	0.43
1:F:340:SER:HB3	1:F:396:LEU:HB3	1.99	0.43
1:H:137:ASP:HB3	1:H:152:ASP:HB3	2.01	0.43
1:H:170:GLY:HA2	1:H:172:ARG:HH22	1.81	0.43
1:H:231:LYS:HA	1:H:231:LYS:HD2	1.74	0.43
1:I:328:ALA:HA	1:I:329:PRO:HD3	1.73	0.43
1:K:5:VAL:CG2	2:W:179:LYS:HZ1	2.32	0.43
1:L:344:ARG:NH1	1:L:346:PRO:HA	2.34	0.43
2:N:59:ILE:HD11	2:N:280:LEU:HD21	2.00	0.43
2:Q:132:ILE:N	2:Q:133:PRO:HD3	2.33	0.43
2:S:59:ILE:HG21	2:S:59:ILE:HD13	1.70	0.43
2:S:139:LEU:HA	2:S:142:LYS:HE3	2.00	0.43
2:S:148:MET:HE3	2:S:216:ALA:CB	2.48	0.43
2:T:6:LYS:HD2	2:T:8:VAL:HG23	1.99	0.43
2:W:6:LYS:HD2	2:W:8:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:MET:CG	1:G:466:TYR:HA	2.49	0.43
1:B:398:ASP:C	1:B:399:LEU:HG	2.43	0.43
1:D:318:SER:OG	1:D:362:ASP:OD2	2.27	0.43
1:D:334:TYR:HA	1:D:343:ILE:O	2.19	0.43
1:E:332:LEU:HD22	1:E:409:GLN:C	2.44	0.43
1:E:334:TYR:HA	1:E:343:ILE:O	2.19	0.43
1:H:328:ALA:HA	1:H:329:PRO:HD3	1.73	0.43
1:H:340:SER:HB3	1:H:396:LEU:HB3	1.99	0.43
1:I:332:LEU:HD22	1:I:409:GLN:C	2.44	0.43
1:I:344:ARG:NH1	1:I:346:PRO:HA	2.33	0.43
1:K:29:GLN:HB3	1:L:180:PHE:HB2	2.01	0.43
1:K:398:ASP:C	1:K:399:LEU:HG	2.43	0.43
1:L:398:ASP:C	1:L:399:LEU:HG	2.43	0.43
2:R:31:THR:CG2	2:R:33:ILE:HD12	2.43	0.43
2:R:128:THR:CG2	2:R:131:GLU:H	2.31	0.43
2:R:139:LEU:HA	2:R:142:LYS:HE3	2.00	0.43
2:R:148:MET:HE3	2:R:216:ALA:CB	2.48	0.43
2:T:148:MET:HE3	2:T:216:ALA:CB	2.48	0.43
1:A:344:ARG:NH1	1:A:346:PRO:HA	2.34	0.43
1:B:137:ASP:HB3	1:B:152:ASP:HB3	2.01	0.43
1:C:125:LEU:O	1:C:272:MET:HA	2.19	0.43
1:C:231:LYS:HA	1:C:231:LYS:HD2	1.74	0.43
1:D:125:LEU:O	1:D:272:MET:HA	2.19	0.43
1:D:344:ARG:NH1	1:D:346:PRO:HA	2.34	0.43
1:E:73:THR:HG21	1:E:88:ARG:HB3	2.00	0.43
1:E:340:SER:HB3	1:E:396:LEU:HB3	1.99	0.43
1:E:344:ARG:NH1	1:E:346:PRO:HA	2.34	0.43
1:F:332:LEU:HD22	1:F:409:GLN:C	2.44	0.43
1:J:344:ARG:NH1	1:J:346:PRO:HA	2.33	0.43
2:O:59:ILE:HG21	2:O:59:ILE:HD13	1.70	0.43
2:R:362:LYS:C	2:R:362:LYS:HE2	2.44	0.43
1:A:17:VAL:HG12	1:A:19:LEU:HD13	2.00	0.42
1:A:137:ASP:HB3	1:A:152:ASP:HB3	2.01	0.42
1:E:215:THR:O	1:E:216:ALA:HB3	2.18	0.42
1:E:272:MET:HE3	1:E:272:MET:HB2	1.97	0.42
1:F:231:LYS:HA	1:F:231:LYS:HD2	1.74	0.42
1:G:332:LEU:HD22	1:G:409:GLN:C	2.44	0.42
1:G:340:SER:HB3	1:G:396:LEU:HB3	1.99	0.42
1:H:73:THR:HG21	1:H:88:ARG:HB3	2.00	0.42
1:H:215:THR:O	1:H:216:ALA:HB3	2.18	0.42
1:H:332:LEU:HD22	1:H:409:GLN:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:125:LEU:O	1:I:272:MET:HA	2.19	0.42
1:I:215:THR:O	1:I:216:ALA:HB3	2.18	0.42
1:I:334:TYR:HA	1:I:343:ILE:O	2.19	0.42
1:K:137:ASP:HB3	1:K:152:ASP:HB3	2.01	0.42
2:P:270:SER:HA	2:P:271:PRO:HD3	1.74	0.42
2:R:59:ILE:HG21	2:R:59:ILE:HD13	1.70	0.42
2:V:312:ALA:CB	2:V:317:ILE:HG22	2.32	0.42
2:X:59:ILE:HD11	2:X:280:LEU:HD21	2.00	0.42
1:A:30:HIS:HB3	1:F:182:VAL:HG12	2.01	0.42
1:A:398:ASP:C	1:A:399:LEU:HG	2.43	0.42
1:B:5:VAL:HG23	2:N:179:LYS:HZ1	1.84	0.42
1:C:334:TYR:HA	1:C:343:ILE:O	2.19	0.42
1:C:344:ARG:NH1	1:C:346:PRO:HA	2.34	0.42
1:D:130:PRO:HB3	1:D:268:MET:CE	2.42	0.42
1:D:215:THR:O	1:D:216:ALA:HB3	2.18	0.42
1:F:17:VAL:HG12	1:F:19:LEU:HD13	2.00	0.42
1:G:334:TYR:HA	1:G:343:ILE:O	2.19	0.42
1:H:17:VAL:HG12	1:H:19:LEU:HD13	2.00	0.42
1:H:344:ARG:NH1	1:H:346:PRO:HA	2.34	0.42
1:I:130:PRO:HB3	1:I:268:MET:CE	2.41	0.42
1:J:334:TYR:HA	1:J:343:ILE:O	2.19	0.42
1:K:29:GLN:HB3	1:L:180:PHE:CB	2.49	0.42
1:L:137:ASP:HB3	1:L:152:ASP:HB3	2.01	0.42
2:P:311:LEU:HD12	2:P:311:LEU:HA	1.88	0.42
2:Q:139:LEU:HA	2:Q:142:LYS:HE3	2.00	0.42
2:S:362:LYS:HE2	2:S:362:LYS:C	2.44	0.42
2:X:77:ALA:HB2	2:X:273:LYS:HE2	2.01	0.42
1:B:309:ASN:HD22	1:B:313:ASN:HD22	1.66	0.42
1:B:332:LEU:HD22	1:B:409:GLN:C	2.44	0.42
1:E:17:VAL:HG12	1:E:19:LEU:HD13	2.00	0.42
1:E:456:THR:O	1:K:458:HIS:HE1	2.02	0.42
1:H:68:MET:HA	1:H:69:PRO:HD2	1.94	0.42
1:I:43:PHE:HB3	2:U:370:LYS:NZ	2.22	0.42
1:J:125:LEU:O	1:J:272:MET:HA	2.19	0.42
1:J:137:ASP:HB3	1:J:152:ASP:HB3	2.01	0.42
1:K:332:LEU:HD22	1:K:409:GLN:C	2.44	0.42
1:L:17:VAL:HG12	1:L:19:LEU:HD13	2.00	0.42
1:L:332:LEU:HD22	1:L:409:GLN:C	2.44	0.42
2:M:59:ILE:HD11	2:M:280:LEU:HD21	2.00	0.42
2:Q:362:LYS:C	2:Q:362:LYS:HE2	2.44	0.42
2:T:59:ILE:HD11	2:T:280:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:139:LEU:HA	2:T:142:LYS:HE3	2.00	0.42
1:A:309:ASN:HD22	1:A:313:ASN:HD22	1.66	0.42
1:A:332:LEU:HD22	1:A:409:GLN:C	2.44	0.42
1:E:68:MET:HA	1:E:69:PRO:HD2	1.94	0.42
1:G:17:VAL:HG12	1:G:19:LEU:HD13	2.00	0.42
1:G:215:THR:O	1:G:216:ALA:HB3	2.18	0.42
1:G:236:GLN:OE1	1:G:236:GLN:HA	2.19	0.42
1:H:272:MET:HE3	1:H:272:MET:HB2	1.97	0.42
1:J:215:THR:O	1:J:216:ALA:HB3	2.18	0.42
1:K:309:ASN:HD22	1:K:313:ASN:HD22	1.66	0.42
1:L:328:ALA:HA	1:L:329:PRO:HD3	1.73	0.42
2:M:77:ALA:HB2	2:M:273:LYS:HE2	2.01	0.42
2:M:246:VAL:H	2:M:246:VAL:HG23	1.58	0.42
2:Q:59:ILE:HD11	2:Q:280:LEU:HD21	2.00	0.42
2:R:42:LYS:HD2	2:R:42:LYS:N	2.35	0.42
2:S:31:THR:CG2	2:S:33:ILE:HD12	2.43	0.42
2:T:321:MET:HB3	2:T:321:MET:HE2	1.71	0.42
2:U:77:ALA:HB2	2:U:273:LYS:HE2	2.01	0.42
1:B:5:VAL:CG2	2:N:179:LYS:HZ1	2.32	0.42
1:B:334:TYR:HA	1:B:343:ILE:O	2.19	0.42
1:C:137:ASP:HB3	1:C:152:ASP:HB3	2.01	0.42
1:C:215:THR:O	1:C:216:ALA:HB3	2.18	0.42
1:D:6:LEU:HD12	2:P:370:LYS:O	2.20	0.42
1:F:130:PRO:HB3	1:F:268:MET:CE	2.41	0.42
1:G:344:ARG:NH1	1:G:346:PRO:HA	2.34	0.42
1:L:309:ASN:HD22	1:L:313:ASN:HD22	1.66	0.42
2:N:64:HIS:CE1	2:N:330:MET:O	2.62	0.42
2:O:139:LEU:HA	2:O:142:LYS:HE3	2.00	0.42
2:P:362:LYS:C	2:P:362:LYS:HE2	2.44	0.42
2:R:163:ALA:HA	2:R:256:LYS:HD3	2.02	0.42
2:S:42:LYS:N	2:S:42:LYS:HD2	2.35	0.42
2:S:163:ALA:HA	2:S:256:LYS:HD3	2.02	0.42
2:T:163:ALA:HA	2:T:256:LYS:HD3	2.02	0.42
2:T:362:LYS:C	2:T:362:LYS:HE2	2.44	0.42
2:U:270:SER:HA	2:U:271:PRO:HD3	1.74	0.42
1:A:364:ALA:HA	1:G:468:VAL:HG13	2.01	0.42
1:B:466:TYR:HA	1:H:256:MET:HG3	2.01	0.42
1:C:332:LEU:HD12	1:C:332:LEU:HA	1.90	0.42
1:E:138:ILE:O	1:E:138:ILE:HG23	2.20	0.42
1:F:215:THR:O	1:F:216:ALA:HB3	2.18	0.42
1:F:236:GLN:OE1	1:F:236:GLN:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:334:TYR:HA	1:F:343:ILE:O	2.19	0.42
1:I:6:LEU:HD12	2:U:370:LYS:O	2.20	0.42
1:I:332:LEU:HB2	1:I:408:PRO:CB	2.50	0.42
2:M:42:LYS:N	2:M:42:LYS:HD2	2.35	0.42
2:N:77:ALA:HB2	2:N:273:LYS:HE2	2.01	0.42
2:P:77:ALA:HB2	2:P:273:LYS:HE2	2.01	0.42
2:Q:163:ALA:HA	2:Q:256:LYS:HD3	2.02	0.42
2:V:139:LEU:HA	2:V:142:LYS:HE3	2.00	0.42
2:W:64:HIS:CE1	2:W:330:MET:O	2.62	0.42
1:E:236:GLN:OE1	1:E:236:GLN:HA	2.19	0.42
1:F:332:LEU:HB2	1:F:408:PRO:CB	2.50	0.42
1:F:396:LEU:HB2	1:F:397:TYR:H	1.36	0.42
1:G:130:PRO:HB3	1:G:268:MET:CE	2.41	0.42
1:H:138:ILE:O	1:H:138:ILE:HG23	2.20	0.42
1:I:138:ILE:O	1:I:138:ILE:HG23	2.20	0.42
1:K:334:TYR:HA	1:K:343:ILE:O	2.19	0.42
1:L:236:GLN:OE1	1:L:236:GLN:HA	2.18	0.42
1:L:396:LEU:H	1:L:396:LEU:HG	1.46	0.42
2:M:31:THR:CG2	2:M:33:ILE:N	2.60	0.42
2:U:362:LYS:C	2:U:362:LYS:HE2	2.44	0.42
2:W:77:ALA:HB2	2:W:273:LYS:HE2	2.01	0.42
2:X:31:THR:CG2	2:X:33:ILE:N	2.60	0.42
2:X:42:LYS:N	2:X:42:LYS:HD2	2.35	0.42
2:X:290:LEU:HA	2:X:290:LEU:HD23	1.73	0.42
1:A:6:LEU:HD12	2:M:370:LYS:O	2.19	0.42
1:A:130:PRO:HB3	1:A:268:MET:CE	2.41	0.42
1:A:334:TYR:HA	1:A:343:ILE:O	2.19	0.42
1:D:43:PHE:HB3	2:P:370:LYS:NZ	2.22	0.42
1:D:332:LEU:HB2	1:D:408:PRO:CB	2.50	0.42
1:F:344:ARG:NH1	1:F:346:PRO:HA	2.34	0.42
1:H:29:GLN:HB3	1:I:180:PHE:CB	2.49	0.42
1:H:236:GLN:OE1	1:H:236:GLN:HA	2.19	0.42
1:K:328:ALA:HA	1:K:329:PRO:HD3	1.73	0.42
2:O:125:PRO:HA	2:O:126:PRO:HD3	1.82	0.42
1:A:387:HIS:HA	1:A:388:PRO:HD2	1.73	0.42
1:B:320:LYS:HG2	1:H:455:MET:O	2.19	0.42
1:C:332:LEU:HD22	1:C:409:GLN:C	2.44	0.42
1:D:138:ILE:O	1:D:138:ILE:HG23	2.20	0.42
1:G:5:VAL:CG2	2:S:179:LYS:HZ1	2.33	0.42
1:J:231:LYS:HA	1:J:231:LYS:HD2	1.74	0.42
1:L:334:TYR:HA	1:L:343:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:31:THR:CG2	2:P:33:ILE:HD12	2.43	0.42
2:U:312:ALA:HB2	2:U:317:ILE:CG2	2.45	0.42
2:U:312:ALA:HB2	2:U:317:ILE:HG21	2.00	0.42
2:V:125:PRO:HA	2:V:126:PRO:HD3	1.82	0.42
1:A:236:GLN:OE1	1:A:236:GLN:HA	2.19	0.42
1:A:332:LEU:HB2	1:A:408:PRO:CB	2.50	0.42
1:A:456:THR:O	1:G:458:HIS:HE1	2.02	0.42
1:C:281:LEU:HB3	1:C:293:GLN:OE1	2.20	0.42
1:D:281:LEU:HB3	1:D:293:GLN:OE1	2.20	0.42
1:F:5:VAL:CG2	2:R:179:LYS:HZ1	2.33	0.42
1:F:433:VAL:HG12	1:F:434:PHE:CD2	2.55	0.42
1:G:384:ASN:N	1:G:384:ASN:ND2	2.60	0.42
1:J:281:LEU:HB3	1:J:293:GLN:OE1	2.20	0.42
1:J:332:LEU:HB2	1:J:408:PRO:CB	2.50	0.42
1:J:332:LEU:HD22	1:J:409:GLN:C	2.44	0.42
1:K:31:VAL:HG23	1:L:210:HIS:HB3	2.01	0.42
1:L:130:PRO:HB3	1:L:268:MET:CE	2.41	0.42
1:L:387:HIS:HA	1:L:388:PRO:HD2	1.73	0.42
2:M:330:MET:HA	2:M:331:PRO:HD3	1.79	0.42
2:P:312:ALA:HB2	2:P:317:ILE:CG2	2.44	0.42
2:P:312:ALA:HB2	2:P:317:ILE:HG21	2.00	0.42
2:Q:77:ALA:HB2	2:Q:273:LYS:HE2	2.01	0.42
2:U:31:THR:CG2	2:U:33:ILE:HD12	2.43	0.42
2:V:312:ALA:HB2	2:V:317:ILE:CG2	2.45	0.42
1:A:91:ILE:HB	1:A:103:ASP:HB2	2.02	0.41
1:C:332:LEU:HB2	1:C:408:PRO:CB	2.50	0.41
1:D:230:LYS:O	1:D:234:GLU:HG3	2.20	0.41
1:E:6:LEU:HD12	2:Q:370:LYS:O	2.20	0.41
1:G:230:LYS:O	1:G:234:GLU:HG3	2.20	0.41
1:I:230:LYS:O	1:I:234:GLU:HG3	2.20	0.41
1:I:281:LEU:HB3	1:I:293:GLN:OE1	2.20	0.41
1:J:332:LEU:HD12	1:J:332:LEU:HA	1.90	0.41
1:L:91:ILE:HB	1:L:103:ASP:HB2	2.02	0.41
2:N:59:ILE:HG21	2:N:59:ILE:HD13	1.70	0.41
2:O:27:PHE:O	2:O:31:THR:CB	2.66	0.41
2:P:31:THR:CG2	2:P:33:ILE:N	2.60	0.41
2:T:42:LYS:N	2:T:42:LYS:HD2	2.35	0.41
2:V:246:VAL:H	2:V:246:VAL:HG23	1.58	0.41
2:V:312:ALA:HB2	2:V:317:ILE:HG21	2.00	0.41
1:C:433:VAL:HG12	1:C:434:PHE:CD2	2.55	0.41
1:F:91:ILE:HB	1:F:103:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:LYS:O	1:F:234:GLU:HG3	2.21	0.41
1:F:296:TYR:HB3	1:F:382:ILE:HA	2.03	0.41
1:G:137:ASP:HB3	1:G:152:ASP:HB3	2.01	0.41
1:G:433:VAL:HG12	1:G:434:PHE:CD2	2.56	0.41
1:H:6:LEU:HD12	2:T:370:LYS:O	2.20	0.41
1:H:433:VAL:HG12	1:H:434:PHE:CD2	2.55	0.41
1:I:4:HIS:HD2	2:U:178:ILE:CD1	2.27	0.41
1:K:91:ILE:HB	1:K:103:ASP:HB2	2.02	0.41
1:L:296:TYR:HB3	1:L:382:ILE:HA	2.02	0.41
1:L:332:LEU:HB2	1:L:408:PRO:CB	2.50	0.41
2:N:121:LEU:HD23	2:N:121:LEU:HA	1.86	0.41
2:O:312:ALA:HB2	2:O:317:ILE:CG2	2.45	0.41
2:Q:42:LYS:N	2:Q:42:LYS:HD2	2.35	0.41
2:S:10:TRP:CD1	2:S:57:PRO:HB3	2.55	0.41
2:T:77:ALA:HB2	2:T:273:LYS:HE2	2.01	0.41
2:U:163:ALA:HA	2:U:256:LYS:HD3	2.02	0.41
1:B:91:ILE:HB	1:B:103:ASP:HB2	2.03	0.41
1:D:364:ALA:HA	1:J:468:VAL:HG13	2.03	0.41
1:D:454:ARG:O	1:J:320:LYS:HG3	2.20	0.41
1:F:466:TYR:HA	1:L:256:MET:HG3	2.01	0.41
1:G:91:ILE:HB	1:G:103:ASP:HB2	2.02	0.41
1:G:396:LEU:H	1:G:396:LEU:HG	1.46	0.41
1:I:34:PRO:HG2	1:J:206:VAL:O	2.20	0.41
1:J:272:MET:HE3	1:J:272:MET:HB2	1.97	0.41
1:J:433:VAL:HG12	1:J:434:PHE:CD2	2.56	0.41
2:P:72:GLN:O	2:P:72:GLN:HG2	2.20	0.41
2:Q:72:GLN:O	2:Q:72:GLN:HG2	2.20	0.41
2:R:10:TRP:CD1	2:R:57:PRO:HB3	2.56	0.41
2:R:31:THR:CG2	2:R:33:ILE:N	2.60	0.41
2:T:72:GLN:O	2:T:72:GLN:HG2	2.20	0.41
2:W:121:LEU:HD23	2:W:121:LEU:HA	1.86	0.41
1:A:296:TYR:HB3	1:A:382:ILE:HA	2.03	0.41
1:B:206:VAL:O	1:C:34:PRO:HG2	2.20	0.41
1:B:230:LYS:O	1:B:234:GLU:HG3	2.20	0.41
1:B:328:ALA:HA	1:B:329:PRO:HD3	1.73	0.41
1:B:332:LEU:HB2	1:B:408:PRO:CB	2.50	0.41
1:D:4:HIS:HD2	2:P:178:ILE:CD1	2.27	0.41
1:D:256:MET:HG3	1:J:466:TYR:HA	2.02	0.41
1:E:433:VAL:HG12	1:E:434:PHE:CD2	2.55	0.41
2:O:163:ALA:HA	2:O:256:LYS:HD3	2.02	0.41
2:O:312:ALA:HB2	2:O:317:ILE:HG21	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:125:PRO:HA	2:P:126:PRO:HD3	1.82	0.41
2:Q:10:TRP:CD1	2:Q:57:PRO:HB3	2.56	0.41
2:R:27:PHE:O	2:R:31:THR:CB	2.66	0.41
2:T:10:TRP:CD1	2:T:57:PRO:HB3	2.56	0.41
2:U:72:GLN:O	2:U:72:GLN:HG2	2.20	0.41
2:V:27:PHE:O	2:V:31:THR:CB	2.66	0.41
1:A:281:LEU:HB3	1:A:293:GLN:OE1	2.20	0.41
1:A:433:VAL:HG12	1:A:434:PHE:CD2	2.55	0.41
1:B:6:LEU:HD12	2:N:370:LYS:O	2.20	0.41
1:C:272:MET:HE3	1:C:272:MET:HB2	1.97	0.41
1:E:458:HIS:HE1	1:K:456:THR:O	2.03	0.41
1:F:5:VAL:HG23	2:R:179:LYS:HZ1	1.86	0.41
1:G:6:LEU:HD12	2:S:370:LYS:O	2.20	0.41
1:G:296:TYR:HB3	1:G:382:ILE:HA	2.03	0.41
1:I:384:ASN:N	1:I:384:ASN:ND2	2.60	0.41
1:I:433:VAL:HG12	1:I:434:PHE:CD2	2.56	0.41
1:K:230:LYS:O	1:K:234:GLU:HG3	2.20	0.41
1:K:332:LEU:HB2	1:K:408:PRO:CB	2.50	0.41
1:L:6:LEU:HD12	2:X:370:LYS:O	2.20	0.41
2:N:42:LYS:N	2:N:42:LYS:HD2	2.35	0.41
2:N:163:ALA:HA	2:N:256:LYS:HD3	2.02	0.41
2:P:163:ALA:HA	2:P:256:LYS:HD3	2.02	0.41
2:W:163:ALA:HA	2:W:256:LYS:HD3	2.02	0.41
2:W:312:ALA:HB2	2:W:317:ILE:HG21	2.00	0.41
2:X:31:THR:CG2	2:X:33:ILE:CD1	2.99	0.41
2:X:312:ALA:HB2	2:X:317:ILE:HG21	2.00	0.41
1:A:105:ARG:HH21	1:A:105:ARG:HD3	1.76	0.41
1:B:281:LEU:HB3	1:B:293:GLN:OE1	2.20	0.41
1:C:91:ILE:HB	1:C:103:ASP:HB2	2.02	0.41
1:D:433:VAL:HG12	1:D:434:PHE:CD2	2.56	0.41
1:E:230:LYS:O	1:E:234:GLU:HG3	2.21	0.41
1:F:6:LEU:HD12	2:R:370:LYS:O	2.20	0.41
1:F:384:ASN:N	1:F:384:ASN:ND2	2.60	0.41
1:G:5:VAL:HG23	2:S:179:LYS:HZ1	1.86	0.41
1:H:332:LEU:HB2	1:H:408:PRO:CB	2.49	0.41
1:H:396:LEU:H	1:H:396:LEU:HG	1.46	0.41
1:I:236:GLN:OE1	1:I:236:GLN:HA	2.19	0.41
1:K:6:LEU:HD12	2:W:370:LYS:O	2.20	0.41
1:L:433:VAL:HG12	1:L:434:PHE:CD2	2.55	0.41
2:M:163:ALA:HA	2:M:256:LYS:HD3	2.02	0.41
2:N:312:ALA:HB2	2:N:317:ILE:HG21	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:31:THR:CG2	2:O:33:ILE:CD1	2.99	0.41
2:O:77:ALA:HB2	2:O:273:LYS:HE2	2.01	0.41
2:U:42:LYS:HD2	2:U:42:LYS:N	2.35	0.41
2:U:125:PRO:HA	2:U:126:PRO:HD3	1.82	0.41
2:V:31:THR:CG2	2:V:33:ILE:CD1	2.99	0.41
2:V:163:ALA:HA	2:V:256:LYS:HD3	2.02	0.41
1:A:364:ALA:HA	1:G:468:VAL:CG1	2.50	0.41
1:E:206:VAL:O	1:F:34:PRO:HG2	2.20	0.41
1:E:281:LEU:HB3	1:E:293:GLN:OE1	2.20	0.41
1:F:281:LEU:HB3	1:F:293:GLN:OE1	2.20	0.41
1:G:231:LYS:HA	1:G:231:LYS:HD2	1.74	0.41
1:H:281:LEU:HB3	1:H:293:GLN:OE1	2.20	0.41
1:I:387:HIS:HA	1:I:388:PRO:HD2	1.73	0.41
1:J:6:LEU:HD12	2:V:370:LYS:O	2.20	0.41
1:L:281:LEU:HB3	1:L:293:GLN:OE1	2.20	0.41
2:M:31:THR:CG2	2:M:33:ILE:CD1	2.99	0.41
2:O:72:GLN:O	2:O:72:GLN:HG2	2.20	0.41
2:U:31:THR:CG2	2:U:33:ILE:N	2.60	0.41
2:U:106:TYR:HA	2:U:107:PRO:HD3	1.86	0.41
2:W:42:LYS:N	2:W:42:LYS:HD2	2.35	0.41
2:X:163:ALA:HA	2:X:256:LYS:HD3	2.02	0.41
1:A:230:LYS:O	1:A:234:GLU:HG3	2.20	0.41
1:A:458:HIS:HE1	1:G:456:THR:O	2.03	0.41
1:D:384:ASN:N	1:D:384:ASN:ND2	2.60	0.41
1:E:296:TYR:HB3	1:E:382:ILE:HA	2.03	0.41
1:E:332:LEU:HB2	1:E:408:PRO:CB	2.50	0.41
1:F:387:HIS:HA	1:F:388:PRO:HD2	1.73	0.41
1:H:230:LYS:O	1:H:234:GLU:HG3	2.21	0.41
1:I:68:MET:HA	1:I:69:PRO:HD2	1.94	0.41
1:I:114:TYR:O	1:I:118:THR:HG23	2.21	0.41
1:K:139:ARG:HD3	1:L:163:LYS:HG2	2.01	0.41
1:K:281:LEU:HB3	1:K:293:GLN:OE1	2.20	0.41
2:M:10:TRP:CD1	2:M:57:PRO:HB3	2.55	0.41
2:N:330:MET:HA	2:N:331:PRO:HD3	1.79	0.41
2:P:121:LEU:HA	2:P:121:LEU:HD23	1.86	0.41
2:R:77:ALA:HB2	2:R:273:LYS:HE2	2.01	0.41
1:C:6:LEU:HD12	2:O:370:LYS:O	2.20	0.41
1:C:230:LYS:O	1:C:234:GLU:HG3	2.20	0.41
1:D:114:TYR:O	1:D:118:THR:HG23	2.21	0.41
1:D:192:ARG:NH2	1:D:219:ASN:ND2	2.63	0.41
1:D:231:LYS:HA	1:D:231:LYS:HD2	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:GLN:OE1	1:D:236:GLN:HA	2.19	0.41
1:D:387:HIS:HA	1:D:388:PRO:HD2	1.73	0.41
1:E:364:ALA:HA	1:K:468:VAL:HG13	2.03	0.41
1:F:137:ASP:HB3	1:F:152:ASP:HB3	2.01	0.41
1:G:105:ARG:HH21	1:G:105:ARG:HD3	1.76	0.41
1:G:138:ILE:O	1:G:138:ILE:HG23	2.20	0.41
1:H:296:TYR:HB3	1:H:382:ILE:HA	2.03	0.41
1:I:192:ARG:NH2	1:I:219:ASN:ND2	2.63	0.41
1:J:91:ILE:HB	1:J:103:ASP:HB2	2.03	0.41
1:J:230:LYS:O	1:J:234:GLU:HG3	2.21	0.41
1:K:231:LYS:HD2	1:K:231:LYS:HA	1.74	0.41
1:L:105:ARG:HH21	1:L:105:ARG:HD3	1.76	0.41
1:L:230:LYS:O	1:L:234:GLU:HG3	2.21	0.41
2:M:312:ALA:HB2	2:M:317:ILE:HG21	2.00	0.41
2:O:42:LYS:N	2:O:42:LYS:HD2	2.35	0.41
2:O:246:VAL:H	2:O:246:VAL:HG23	1.58	0.41
2:P:42:LYS:N	2:P:42:LYS:HD2	2.35	0.41
2:P:366:THR:O	2:P:370:LYS:HG3	2.21	0.41
2:S:27:PHE:O	2:S:31:THR:CB	2.66	0.41
2:S:77:ALA:HB2	2:S:273:LYS:HE2	2.01	0.41
2:T:31:THR:CG2	2:T:33:ILE:N	2.60	0.41
2:U:366:THR:O	2:U:370:LYS:HG3	2.21	0.41
2:V:72:GLN:O	2:V:72:GLN:HG2	2.20	0.41
2:V:77:ALA:HB2	2:V:273:LYS:HE2	2.01	0.41
2:V:366:THR:O	2:V:370:LYS:HG3	2.21	0.41
2:X:72:GLN:O	2:X:72:GLN:HG2	2.20	0.41
2:X:149:PHE:CD1	2:X:204:MET:HE1	2.56	0.41
2:X:330:MET:HA	2:X:331:PRO:HD3	1.79	0.41
1:A:396:LEU:H	1:A:396:LEU:HG	1.46	0.41
1:B:231:LYS:HD2	1:B:231:LYS:HA	1.74	0.41
1:B:296:TYR:HB3	1:B:382:ILE:HA	2.03	0.41
1:B:433:VAL:HG12	1:B:434:PHE:CD2	2.55	0.41
1:D:182:VAL:HG12	1:E:30:HIS:HB3	2.03	0.41
1:E:125:LEU:HD12	1:E:125:LEU:HA	1.91	0.41
1:G:281:LEU:HB3	1:G:293:GLN:OE1	2.20	0.41
1:H:91:ILE:HB	1:H:103:ASP:HB2	2.02	0.41
1:I:294:ALA:O	1:I:298:ILE:HG13	2.21	0.41
2:M:149:PHE:CD1	2:M:204:MET:HE1	2.56	0.41
2:O:366:THR:O	2:O:370:LYS:HG3	2.21	0.41
2:V:270:SER:HA	2:V:271:PRO:HD3	1.74	0.41
2:W:31:THR:CG2	2:W:33:ILE:CD1	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:330:MET:HA	2:W:331:PRO:HD3	1.79	0.41
2:X:10:TRP:CD1	2:X:57:PRO:HB3	2.56	0.41
1:D:294:ALA:O	1:D:298:ILE:HG13	2.22	0.40
1:F:138:ILE:HG23	1:F:138:ILE:O	2.20	0.40
1:F:294:ALA:O	1:F:298:ILE:HG13	2.21	0.40
1:F:320:LYS:HG3	1:L:454:ARG:O	2.21	0.40
1:F:466:TYR:CE1	1:L:254:THR:HB	2.56	0.40
1:H:34:PRO:HG2	1:I:206:VAL:O	2.22	0.40
1:H:61:ASN:O	1:I:337:ARG:CB	2.50	0.40
1:I:3:GLU:CD	2:U:368:ILE:HA	2.46	0.40
1:K:296:TYR:HB3	1:K:382:ILE:HA	2.03	0.40
1:K:433:VAL:HG12	1:K:434:PHE:CD2	2.55	0.40
2:N:31:THR:CG2	2:N:33:ILE:CD1	2.99	0.40
2:N:149:PHE:CD1	2:N:204:MET:HE1	2.56	0.40
2:O:330:MET:HA	2:O:331:PRO:HD3	1.79	0.40
2:O:361:LEU:HD23	2:O:361:LEU:HA	1.96	0.40
2:P:10:TRP:CD1	2:P:57:PRO:HB3	2.55	0.40
2:U:10:TRP:CD1	2:U:57:PRO:HB3	2.56	0.40
2:U:121:LEU:HA	2:U:121:LEU:HD23	1.86	0.40
2:V:42:LYS:N	2:V:42:LYS:HD2	2.35	0.40
2:W:149:PHE:CD1	2:W:204:MET:HE1	2.56	0.40
2:X:106:TYR:HA	2:X:107:PRO:HD3	1.87	0.40
2:X:268:ALA:O	2:X:273:LYS:NZ	2.48	0.40
1:C:138:ILE:O	1:C:138:ILE:HG23	2.20	0.40
1:D:91:ILE:HB	1:D:103:ASP:HB2	2.02	0.40
1:E:114:TYR:O	1:E:118:THR:HG23	2.21	0.40
1:E:313:ASN:HB3	1:E:318:SER:HB3	2.03	0.40
1:F:105:ARG:HH21	1:F:105:ARG:HD3	1.76	0.40
1:G:294:ALA:O	1:G:298:ILE:HG13	2.22	0.40
1:H:313:ASN:HB3	1:H:318:SER:HB3	2.03	0.40
1:H:396:LEU:HB2	1:H:397:TYR:H	1.36	0.40
1:I:91:ILE:HB	1:I:103:ASP:HB2	2.02	0.40
2:R:72:GLN:O	2:R:72:GLN:HG2	2.20	0.40
2:T:366:THR:O	2:T:370:LYS:HG3	2.21	0.40
2:W:47:PHE:HB3	2:W:48:PRO:HD3	2.03	0.40
1:A:5:VAL:H	2:M:179:LYS:NZ	2.04	0.40
1:B:254:THR:HB	1:H:466:TYR:CE1	2.56	0.40
1:C:114:TYR:O	1:C:118:THR:HG23	2.21	0.40
1:D:3:GLU:CD	2:P:368:ILE:HA	2.46	0.40
1:D:68:MET:HA	1:D:69:PRO:HD2	1.94	0.40
1:D:364:ALA:HA	1:J:468:VAL:CG1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:ILE:HB	1:E:103:ASP:HB2	2.03	0.40
1:G:272:MET:HE3	1:G:272:MET:HB2	1.97	0.40
1:G:396:LEU:HB2	1:G:397:TYR:H	1.36	0.40
1:J:294:ALA:O	1:J:298:ILE:HG13	2.21	0.40
1:K:130:PRO:HB3	1:K:268:MET:CE	2.41	0.40
1:L:138:ILE:O	1:L:138:ILE:HG23	2.20	0.40
2:M:72:GLN:O	2:M:72:GLN:HG2	2.20	0.40
2:N:47:PHE:HB3	2:N:48:PRO:HD3	2.03	0.40
2:N:258:PHE:CG	2:N:330:MET:HG2	2.57	0.40
2:O:59:ILE:HD11	2:O:280:LEU:HD21	2.00	0.40
2:O:218:ASN:HD21	2:O:235:ILE:HG12	1.87	0.40
2:P:47:PHE:HB3	2:P:48:PRO:HD3	2.03	0.40
2:P:106:TYR:HA	2:P:107:PRO:HD3	1.87	0.40
2:P:348:ILE:HD13	2:P:348:ILE:HG21	1.93	0.40
2:Q:366:THR:O	2:Q:370:LYS:HG3	2.21	0.40
2:R:149:PHE:CD1	2:R:204:MET:HE1	2.56	0.40
2:S:72:GLN:O	2:S:72:GLN:HG2	2.20	0.40
2:S:149:PHE:CD1	2:S:204:MET:HE1	2.56	0.40
2:U:47:PHE:HB3	2:U:48:PRO:HD3	2.03	0.40
2:W:218:ASN:HD21	2:W:235:ILE:HG12	1.87	0.40
1:A:138:ILE:O	1:A:138:ILE:HG23	2.20	0.40
1:B:130:PRO:HB3	1:B:268:MET:CE	2.41	0.40
1:B:138:ILE:O	1:B:138:ILE:HG23	2.20	0.40
1:D:296:TYR:HB3	1:D:382:ILE:HA	2.03	0.40
1:F:313:ASN:HB3	1:F:318:SER:HB3	2.03	0.40
1:F:455:MET:HG2	1:L:323:VAL:HG11	2.03	0.40
1:G:43:PHE:HB3	2:S:370:LYS:NZ	2.22	0.40
1:H:114:TYR:O	1:H:118:THR:HG23	2.21	0.40
1:J:138:ILE:O	1:J:138:ILE:HG23	2.20	0.40
1:J:235:ILE:HD13	1:J:235:ILE:HA	1.82	0.40
2:N:218:ASN:HD21	2:N:235:ILE:HG12	1.87	0.40
2:Q:31:THR:CG2	2:Q:33:ILE:N	2.60	0.40
2:Q:31:THR:CG2	2:Q:33:ILE:CD1	2.99	0.40
2:R:31:THR:CG2	2:R:33:ILE:CD1	2.99	0.40
2:S:330:MET:HA	2:S:331:PRO:HD3	1.79	0.40
2:V:149:PHE:CD1	2:V:204:MET:HE1	2.56	0.40
2:V:311:LEU:HD12	2:V:311:LEU:HA	1.88	0.40
1:A:294:ALA:O	1:A:298:ILE:HG13	2.21	0.40
1:B:180:PHE:CB	1:C:29:GLN:HB3	2.52	0.40
1:B:364:ALA:HA	1:H:468:VAL:CG1	2.51	0.40
1:C:125:LEU:HD12	1:C:125:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:ALA:O	1:C:298:ILE:HG13	2.21	0.40
1:E:396:LEU:H	1:E:396:LEU:HG	1.46	0.40
1:F:396:LEU:H	1:F:396:LEU:HG	1.46	0.40
1:I:296:TYR:HB3	1:I:382:ILE:HA	2.03	0.40
1:J:114:TYR:O	1:J:118:THR:HG23	2.21	0.40
1:K:138:ILE:O	1:K:138:ILE:HG23	2.20	0.40
1:L:303:LYS:HD2	1:L:386:ILE:HD13	2.04	0.40
2:N:10:TRP:CD1	2:N:57:PRO:HB3	2.55	0.40
2:P:31:THR:CG2	2:P:33:ILE:CD1	2.99	0.40
2:Q:361:LEU:HD23	2:Q:361:LEU:HA	1.96	0.40
2:S:31:THR:CG2	2:S:33:ILE:CD1	2.99	0.40
2:S:366:THR:O	2:S:370:LYS:HG3	2.21	0.40
2:T:31:THR:CG2	2:T:33:ILE:CD1	2.99	0.40
2:T:149:PHE:CD1	2:T:204:MET:HE1	2.56	0.40
2:U:31:THR:CG2	2:U:33:ILE:CD1	2.99	0.40
2:V:59:ILE:HD11	2:V:280:LEU:HD21	2.00	0.40
2:V:218:ASN:HD21	2:V:235:ILE:HG12	1.87	0.40
2:W:10:TRP:CD1	2:W:57:PRO:HB3	2.55	0.40
2:W:258:PHE:CG	2:W:330:MET:HG2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	7	36
1	B	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	7	36
1	C	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	7	36
1	D	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	7	36
1	E	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	7	36
1	G	464/466 (100%)	425 (92%)	31 (7%)	8 (2%)	7	36
1	H	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	7	36
1	I	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	7	36
1	J	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	7	36
1	K	464/466 (100%)	424 (91%)	32 (7%)	8 (2%)	7	36
1	L	464/466 (100%)	425 (92%)	31 (7%)	8 (2%)	7	36
2	M	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	16	54
2	N	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	16	54
2	O	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	16	54
2	P	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	16	54
2	Q	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	16	54
2	R	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	16	54
2	S	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	16	54
2	T	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	16	54
2	U	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	16	54
2	V	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	16	54
2	W	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	16	54
2	X	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	16	54
All	All	9984/10032 (100%)	9278 (93%)	574 (6%)	132 (1%)	12	42

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	PHE
1	A	400	PRO
1	A	401	PRO
1	B	180	PHE
1	B	400	PRO
1	B	401	PRO
1	C	180	PHE
1	C	400	PRO
1	C	401	PRO
1	D	180	PHE
1	D	400	PRO

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Mol	Chain	Res	Type
1	D	401	PRO
1	E	180	PHE
1	E	400	PRO
1	E	401	PRO
1	F	180	PHE
1	F	400	PRO
1	F	401	PRO
1	G	180	PHE
1	G	400	PRO
1	G	401	PRO
1	H	180	PHE
1	H	400	PRO
1	H	401	PRO
1	I	180	PHE
1	I	400	PRO
1	I	401	PRO
1	J	180	PHE
1	J	400	PRO
1	J	401	PRO
1	K	180	PHE
1	K	400	PRO
1	K	401	PRO
1	L	180	PHE
1	L	400	PRO
1	L	401	PRO
2	M	4	GLU
2	N	4	GLU
2	O	4	GLU
2	P	4	GLU
2	Q	4	GLU
2	R	4	GLU
2	S	4	GLU
2	T	4	GLU
2	U	4	GLU
2	V	4	GLU
2	W	4	GLU
2	X	4	GLU
1	A	170	GLY
1	B	170	GLY
1	C	170	GLY
1	D	170	GLY
1	E	170	GLY

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Mol	Chain	Res	Type
1	F	170	GLY
1	G	170	GLY
1	H	170	GLY
1	I	170	GLY
1	J	170	GLY
1	K	170	GLY
1	L	170	GLY
2	M	83	LYS
2	N	83	LYS
2	O	83	LYS
2	P	83	LYS
2	Q	83	LYS
2	R	83	LYS
2	S	83	LYS
2	T	83	LYS
2	U	83	LYS
2	V	83	LYS
2	W	83	LYS
2	X	83	LYS
1	A	324	PRO
1	A	338	ASN
1	A	394	LYS
1	B	324	PRO
1	B	338	ASN
1	B	394	LYS
1	C	324	PRO
1	C	338	ASN
1	C	394	LYS
1	D	324	PRO
1	D	338	ASN
1	D	394	LYS
1	E	324	PRO
1	E	338	ASN
1	E	394	LYS
1	F	324	PRO
1	F	338	ASN
1	F	394	LYS
1	G	324	PRO
1	G	338	ASN
1	G	394	LYS
1	H	324	PRO
1	H	338	ASN

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Mol	Chain	Res	Type
1	H	394	LYS
1	I	324	PRO
1	I	338	ASN
1	I	394	LYS
1	J	324	PRO
1	J	338	ASN
1	J	394	LYS
1	K	324	PRO
1	K	338	ASN
1	K	394	LYS
1	L	324	PRO
1	L	338	ASN
1	L	394	LYS
1	A	396	LEU
1	B	396	LEU
1	C	396	LEU
1	D	396	LEU
1	E	396	LEU
1	F	396	LEU
1	G	396	LEU
1	H	396	LEU
1	I	396	LEU
1	J	396	LEU
1	K	396	LEU
1	L	396	LEU
2	M	2	ILE
2	N	2	ILE
2	O	2	ILE
2	P	2	ILE
2	Q	2	ILE
2	R	2	ILE
2	S	2	ILE
2	T	2	ILE
2	U	2	ILE
2	V	2	ILE
2	W	2	ILE
2	X	2	ILE

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 PDB entries followed by that with respect to all EM

entries.

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	383/383 (100%)	344 (90%)	39 (10%)	7	23
1	B	383/383 (100%)	344 (90%)	39 (10%)	7	23
1	C	383/383 (100%)	344 (90%)	39 (10%)	7	23
1	D	383/383 (100%)	344 (90%)	39 (10%)	7	23
1	E	383/383 (100%)	344 (90%)	39 (10%)	7	23
1	F	383/383 (100%)	344 (90%)	39 (10%)	7	23
1	G	383/383 (100%)	344 (90%)	39 (10%)	7	23
1	H	383/383 (100%)	344 (90%)	39 (10%)	7	23
1	I	383/383 (100%)	344 (90%)	39 (10%)	7	23
1	J	383/383 (100%)	344 (90%)	39 (10%)	7	23
1	K	383/383 (100%)	344 (90%)	39 (10%)	7	23
1	L	383/383 (100%)	344 (90%)	39 (10%)	7	23
2	M	292/297 (98%)	246 (84%)	46 (16%)	2	11
2	N	292/297 (98%)	246 (84%)	46 (16%)	2	11
2	O	292/297 (98%)	246 (84%)	46 (16%)	2	11
2	P	292/297 (98%)	246 (84%)	46 (16%)	2	11
2	Q	292/297 (98%)	246 (84%)	46 (16%)	2	11
2	R	292/297 (98%)	246 (84%)	46 (16%)	2	11
2	S	292/297 (98%)	246 (84%)	46 (16%)	2	11
2	T	292/297 (98%)	246 (84%)	46 (16%)	2	11
2	U	292/297 (98%)	246 (84%)	46 (16%)	2	11
2	V	292/297 (98%)	246 (84%)	46 (16%)	2	11
2	W	292/297 (98%)	246 (84%)	46 (16%)	2	11
2	X	292/297 (98%)	246 (84%)	46 (16%)	2	11
All	All	8100/8160 (99%)	7080 (87%)	1020 (13%)	6	16

All (1020) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU

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Mol	Chain	Res	Type
1	A	19	LEU
1	A	60	ILE
1	A	62	GLU
1	A	63	SER
1	A	64	ASP
1	A	65	MET
1	A	84	THR
1	A	88	ARG
1	A	96	THR
1	A	98	GLN
1	A	102	ARG
1	A	115	LEU
1	A	124	VAL
1	A	125	LEU
1	A	165	GLU
1	A	179	TYR
1	A	183	PRO
1	A	209	HIS
1	A	235	ILE
1	A	248	ARG
1	A	264	ASN
1	A	320	LYS
1	A	324	PRO
1	A	326	TYR
1	A	332	LEU
1	A	337	ARG
1	A	343	ILE
1	A	374	LEU
1	A	375	LEU
1	A	384	ASN
1	A	394	LYS
1	A	396	LEU
1	A	397	TYR
1	A	399	LEU
1	A	428	LEU
1	A	447	ARG
1	A	464	LEU
1	A	468	VAL
1	B	6	LEU
1	B	19	LEU
1	B	60	ILE
1	B	62	GLU

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Mol	Chain	Res	Type
1	B	63	SER
1	B	64	ASP
1	B	65	MET
1	B	84	THR
1	B	88	ARG
1	B	96	THR
1	B	98	GLN
1	B	102	ARG
1	B	115	LEU
1	B	124	VAL
1	B	125	LEU
1	B	165	GLU
1	B	179	TYR
1	B	183	PRO
1	B	209	HIS
1	B	235	ILE
1	B	248	ARG
1	B	264	ASN
1	B	320	LYS
1	B	324	PRO
1	B	326	TYR
1	B	332	LEU
1	B	337	ARG
1	B	343	ILE
1	B	374	LEU
1	B	375	LEU
1	B	384	ASN
1	B	394	LYS
1	B	396	LEU
1	B	397	TYR
1	B	399	LEU
1	B	428	LEU
1	B	447	ARG
1	B	464	LEU
1	B	468	VAL
1	C	6	LEU
1	C	19	LEU
1	C	60	ILE
1	C	62	GLU
1	C	63	SER
1	C	64	ASP
1	C	65	MET

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Mol	Chain	Res	Type
1	C	84	THR
1	C	88	ARG
1	C	96	THR
1	C	98	GLN
1	C	102	ARG
1	C	115	LEU
1	C	124	VAL
1	C	125	LEU
1	C	165	GLU
1	C	179	TYR
1	C	183	PRO
1	C	209	HIS
1	C	235	ILE
1	C	248	ARG
1	C	264	ASN
1	C	320	LYS
1	C	324	PRO
1	C	326	TYR
1	C	332	LEU
1	C	337	ARG
1	C	343	ILE
1	C	374	LEU
1	C	375	LEU
1	C	384	ASN
1	C	394	LYS
1	C	396	LEU
1	C	397	TYR
1	C	399	LEU
1	C	428	LEU
1	C	447	ARG
1	C	464	LEU
1	C	468	VAL
1	D	6	LEU
1	D	19	LEU
1	D	60	ILE
1	D	62	GLU
1	D	63	SER
1	D	64	ASP
1	D	65	MET
1	D	84	THR
1	D	88	ARG
1	D	96	THR

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Mol	Chain	Res	Type
1	D	98	GLN
1	D	102	ARG
1	D	115	LEU
1	D	124	VAL
1	D	125	LEU
1	D	165	GLU
1	D	179	TYR
1	D	183	PRO
1	D	209	HIS
1	D	235	ILE
1	D	248	ARG
1	D	264	ASN
1	D	320	LYS
1	D	324	PRO
1	D	326	TYR
1	D	332	LEU
1	D	337	ARG
1	D	343	ILE
1	D	374	LEU
1	D	375	LEU
1	D	384	ASN
1	D	394	LYS
1	D	396	LEU
1	D	397	TYR
1	D	399	LEU
1	D	428	LEU
1	D	447	ARG
1	D	464	LEU
1	D	468	VAL
1	E	6	LEU
1	E	19	LEU
1	E	60	ILE
1	E	62	GLU
1	E	63	SER
1	E	64	ASP
1	E	65	MET
1	E	84	THR
1	E	88	ARG
1	E	96	THR
1	E	98	GLN
1	E	102	ARG
1	E	115	LEU

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Mol	Chain	Res	Type
1	E	124	VAL
1	E	125	LEU
1	E	165	GLU
1	E	179	TYR
1	E	183	PRO
1	E	209	HIS
1	E	235	ILE
1	E	248	ARG
1	E	264	ASN
1	E	320	LYS
1	E	324	PRO
1	E	326	TYR
1	E	332	LEU
1	E	337	ARG
1	E	343	ILE
1	E	374	LEU
1	E	375	LEU
1	E	384	ASN
1	E	394	LYS
1	E	396	LEU
1	E	397	TYR
1	E	399	LEU
1	E	428	LEU
1	E	447	ARG
1	E	464	LEU
1	E	468	VAL
1	F	6	LEU
1	F	19	LEU
1	F	60	ILE
1	F	62	GLU
1	F	63	SER
1	F	64	ASP
1	F	65	MET
1	F	84	THR
1	F	88	ARG
1	F	96	THR
1	F	98	GLN
1	F	102	ARG
1	F	115	LEU
1	F	124	VAL
1	F	125	LEU
1	F	165	GLU

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Mol	Chain	Res	Type
1	F	179	TYR
1	F	183	PRO
1	F	209	HIS
1	F	235	ILE
1	F	248	ARG
1	F	264	ASN
1	F	320	LYS
1	F	324	PRO
1	F	326	TYR
1	F	332	LEU
1	F	337	ARG
1	F	343	ILE
1	F	374	LEU
1	F	375	LEU
1	F	384	ASN
1	F	394	LYS
1	F	396	LEU
1	F	397	TYR
1	F	399	LEU
1	F	428	LEU
1	F	447	ARG
1	F	464	LEU
1	F	468	VAL
1	G	6	LEU
1	G	19	LEU
1	G	60	ILE
1	G	62	GLU
1	G	63	SER
1	G	64	ASP
1	G	65	MET
1	G	84	THR
1	G	88	ARG
1	G	96	THR
1	G	98	GLN
1	G	102	ARG
1	G	115	LEU
1	G	124	VAL
1	G	125	LEU
1	G	165	GLU
1	G	179	TYR
1	G	183	PRO
1	G	209	HIS

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Mol	Chain	Res	Type
1	G	235	ILE
1	G	248	ARG
1	G	264	ASN
1	G	320	LYS
1	G	324	PRO
1	G	326	TYR
1	G	332	LEU
1	G	337	ARG
1	G	343	ILE
1	G	374	LEU
1	G	375	LEU
1	G	384	ASN
1	G	394	LYS
1	G	396	LEU
1	G	397	TYR
1	G	399	LEU
1	G	428	LEU
1	G	447	ARG
1	G	464	LEU
1	G	468	VAL
1	H	6	LEU
1	H	19	LEU
1	H	60	ILE
1	H	62	GLU
1	H	63	SER
1	H	64	ASP
1	H	65	MET
1	H	84	THR
1	H	88	ARG
1	H	96	THR
1	H	98	GLN
1	H	102	ARG
1	H	115	LEU
1	H	124	VAL
1	H	125	LEU
1	H	165	GLU
1	H	179	TYR
1	H	183	PRO
1	H	209	HIS
1	H	235	ILE
1	H	248	ARG
1	H	264	ASN

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Mol	Chain	Res	Type
1	H	320	LYS
1	H	324	PRO
1	H	326	TYR
1	H	332	LEU
1	H	337	ARG
1	H	343	ILE
1	H	374	LEU
1	H	375	LEU
1	H	384	ASN
1	H	394	LYS
1	H	396	LEU
1	H	397	TYR
1	H	399	LEU
1	H	428	LEU
1	H	447	ARG
1	H	464	LEU
1	H	468	VAL
1	I	6	LEU
1	I	19	LEU
1	I	60	ILE
1	I	62	GLU
1	I	63	SER
1	I	64	ASP
1	I	65	MET
1	I	84	THR
1	I	88	ARG
1	I	96	THR
1	I	98	GLN
1	I	102	ARG
1	I	115	LEU
1	I	124	VAL
1	I	125	LEU
1	I	165	GLU
1	I	179	TYR
1	I	183	PRO
1	I	209	HIS
1	I	235	ILE
1	I	248	ARG
1	I	264	ASN
1	I	320	LYS
1	I	324	PRO
1	I	326	TYR

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Mol	Chain	Res	Type
1	I	332	LEU
1	I	337	ARG
1	I	343	ILE
1	I	374	LEU
1	I	375	LEU
1	I	384	ASN
1	I	394	LYS
1	I	396	LEU
1	I	397	TYR
1	I	399	LEU
1	I	428	LEU
1	I	447	ARG
1	I	464	LEU
1	I	468	VAL
1	J	6	LEU
1	J	19	LEU
1	J	60	ILE
1	J	62	GLU
1	J	63	SER
1	J	64	ASP
1	J	65	MET
1	J	84	THR
1	J	88	ARG
1	J	96	THR
1	J	98	GLN
1	J	102	ARG
1	J	115	LEU
1	J	124	VAL
1	J	125	LEU
1	J	165	GLU
1	J	179	TYR
1	J	183	PRO
1	J	209	HIS
1	J	235	ILE
1	J	248	ARG
1	J	264	ASN
1	J	320	LYS
1	J	324	PRO
1	J	326	TYR
1	J	332	LEU
1	J	337	ARG
1	J	343	ILE

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Mol	Chain	Res	Type
1	J	374	LEU
1	J	375	LEU
1	J	384	ASN
1	J	394	LYS
1	J	396	LEU
1	J	397	TYR
1	J	399	LEU
1	J	428	LEU
1	J	447	ARG
1	J	464	LEU
1	J	468	VAL
1	K	6	LEU
1	K	19	LEU
1	K	60	ILE
1	K	62	GLU
1	K	63	SER
1	K	64	ASP
1	K	65	MET
1	K	84	THR
1	K	88	ARG
1	K	96	THR
1	K	98	GLN
1	K	102	ARG
1	K	115	LEU
1	K	124	VAL
1	K	125	LEU
1	K	165	GLU
1	K	179	TYR
1	K	183	PRO
1	K	209	HIS
1	K	235	ILE
1	K	248	ARG
1	K	264	ASN
1	K	320	LYS
1	K	324	PRO
1	K	326	TYR
1	K	332	LEU
1	K	337	ARG
1	K	343	ILE
1	K	374	LEU
1	K	375	LEU
1	K	384	ASN

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Mol	Chain	Res	Type
1	K	394	LYS
1	K	396	LEU
1	K	397	TYR
1	K	399	LEU
1	K	428	LEU
1	K	447	ARG
1	K	464	LEU
1	K	468	VAL
1	L	6	LEU
1	L	19	LEU
1	L	60	ILE
1	L	62	GLU
1	L	63	SER
1	L	64	ASP
1	L	65	MET
1	L	84	THR
1	L	88	ARG
1	L	96	THR
1	L	98	GLN
1	L	102	ARG
1	L	115	LEU
1	L	124	VAL
1	L	125	LEU
1	L	165	GLU
1	L	179	TYR
1	L	183	PRO
1	L	209	HIS
1	L	235	ILE
1	L	248	ARG
1	L	264	ASN
1	L	320	LYS
1	L	324	PRO
1	L	326	TYR
1	L	332	LEU
1	L	337	ARG
1	L	343	ILE
1	L	374	LEU
1	L	375	LEU
1	L	384	ASN
1	L	394	LYS
1	L	396	LEU
1	L	397	TYR

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Mol	Chain	Res	Type
1	L	399	LEU
1	L	428	LEU
1	L	447	ARG
1	L	464	LEU
1	L	468	VAL
2	M	6	LYS
2	M	26	LYS
2	M	30	ASP
2	M	31	THR
2	M	34	LYS
2	M	42	LYS
2	M	45	GLU
2	M	46	LYS
2	M	50	VAL
2	M	53	THR
2	M	59	ILE
2	M	83	LYS
2	M	87	ASP
2	M	89	LEU
2	M	98	ARG
2	M	115	LEU
2	M	127	LYS
2	M	128	THR
2	M	135	LEU
2	M	138	GLU
2	M	140	LYS
2	M	142	LYS
2	M	148	MET
2	M	160	LEU
2	M	173	ASN
2	M	175	LYS
2	M	202	LYS
2	M	204	MET
2	M	212	ILE
2	M	239	LYS
2	M	240	VAL
2	M	246	VAL
2	M	253	GLN
2	M	258	PHE
2	M	274	GLU
2	M	291	GLU
2	M	295	LYS

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Mol	Chain	Res	Type
2	M	309	GLU
2	M	311	LEU
2	M	313	LYS
2	M	317	ILE
2	M	328	GLU
2	M	329	ILE
2	M	337	SER
2	M	341	TYR
2	M	354	ARG
2	N	6	LYS
2	N	26	LYS
2	N	30	ASP
2	N	31	THR
2	N	34	LYS
2	N	42	LYS
2	N	45	GLU
2	N	46	LYS
2	N	50	VAL
2	N	53	THR
2	N	59	ILE
2	N	83	LYS
2	N	87	ASP
2	N	89	LEU
2	N	98	ARG
2	N	115	LEU
2	N	127	LYS
2	N	128	THR
2	N	135	LEU
2	N	138	GLU
2	N	140	LYS
2	N	142	LYS
2	N	148	MET
2	N	160	LEU
2	N	173	ASN
2	N	175	LYS
2	N	202	LYS
2	N	204	MET
2	N	212	ILE
2	N	239	LYS
2	N	240	VAL
2	N	246	VAL
2	N	253	GLN

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Mol	Chain	Res	Type
2	N	258	PHE
2	N	274	GLU
2	N	291	GLU
2	N	295	LYS
2	N	309	GLU
2	N	311	LEU
2	N	313	LYS
2	N	317	ILE
2	N	328	GLU
2	N	329	ILE
2	N	337	SER
2	N	341	TYR
2	N	354	ARG
2	O	6	LYS
2	O	26	LYS
2	O	30	ASP
2	O	31	THR
2	O	34	LYS
2	O	42	LYS
2	O	45	GLU
2	O	46	LYS
2	O	50	VAL
2	O	53	THR
2	O	59	ILE
2	O	83	LYS
2	O	87	ASP
2	O	89	LEU
2	O	98	ARG
2	O	115	LEU
2	O	127	LYS
2	O	128	THR
2	O	135	LEU
2	O	138	GLU
2	O	140	LYS
2	O	142	LYS
2	O	148	MET
2	O	160	LEU
2	O	173	ASN
2	O	175	LYS
2	O	202	LYS
2	O	204	MET
2	O	212	ILE

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Mol	Chain	Res	Type
2	O	239	LYS
2	O	240	VAL
2	O	246	VAL
2	O	253	GLN
2	O	258	PHE
2	O	274	GLU
2	O	291	GLU
2	O	295	LYS
2	O	309	GLU
2	O	311	LEU
2	O	313	LYS
2	O	317	ILE
2	O	328	GLU
2	O	329	ILE
2	O	337	SER
2	O	341	TYR
2	O	354	ARG
2	P	6	LYS
2	P	26	LYS
2	P	30	ASP
2	P	31	THR
2	P	34	LYS
2	P	42	LYS
2	P	45	GLU
2	P	46	LYS
2	P	50	VAL
2	P	53	THR
2	P	59	ILE
2	P	83	LYS
2	P	87	ASP
2	P	89	LEU
2	P	98	ARG
2	P	115	LEU
2	P	127	LYS
2	P	128	THR
2	P	135	LEU
2	P	138	GLU
2	P	140	LYS
2	P	142	LYS
2	P	148	MET
2	P	160	LEU
2	P	173	ASN

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Mol	Chain	Res	Type
2	P	175	LYS
2	P	202	LYS
2	P	204	MET
2	P	212	ILE
2	P	239	LYS
2	P	240	VAL
2	P	246	VAL
2	P	253	GLN
2	P	258	PHE
2	P	274	GLU
2	P	291	GLU
2	P	295	LYS
2	P	309	GLU
2	P	311	LEU
2	P	313	LYS
2	P	317	ILE
2	P	328	GLU
2	P	329	ILE
2	P	337	SER
2	P	341	TYR
2	P	354	ARG
2	Q	6	LYS
2	Q	26	LYS
2	Q	30	ASP
2	Q	31	THR
2	Q	34	LYS
2	Q	42	LYS
2	Q	45	GLU
2	Q	46	LYS
2	Q	50	VAL
2	Q	53	THR
2	Q	59	ILE
2	Q	83	LYS
2	Q	87	ASP
2	Q	89	LEU
2	Q	98	ARG
2	Q	115	LEU
2	Q	127	LYS
2	Q	128	THR
2	Q	135	LEU
2	Q	138	GLU
2	Q	140	LYS

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Mol	Chain	Res	Type
2	Q	142	LYS
2	Q	148	MET
2	Q	160	LEU
2	Q	173	ASN
2	Q	175	LYS
2	Q	202	LYS
2	Q	204	MET
2	Q	212	ILE
2	Q	239	LYS
2	Q	240	VAL
2	Q	246	VAL
2	Q	253	GLN
2	Q	258	PHE
2	Q	274	GLU
2	Q	291	GLU
2	Q	295	LYS
2	Q	309	GLU
2	Q	311	LEU
2	Q	313	LYS
2	Q	317	ILE
2	Q	328	GLU
2	Q	329	ILE
2	Q	337	SER
2	Q	341	TYR
2	Q	354	ARG
2	R	6	LYS
2	R	26	LYS
2	R	30	ASP
2	R	31	THR
2	R	34	LYS
2	R	42	LYS
2	R	45	GLU
2	R	46	LYS
2	R	50	VAL
2	R	53	THR
2	R	59	ILE
2	R	83	LYS
2	R	87	ASP
2	R	89	LEU
2	R	98	ARG
2	R	115	LEU
2	R	127	LYS

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Mol	Chain	Res	Type
2	R	128	THR
2	R	135	LEU
2	R	138	GLU
2	R	140	LYS
2	R	142	LYS
2	R	148	MET
2	R	160	LEU
2	R	173	ASN
2	R	175	LYS
2	R	202	LYS
2	R	204	MET
2	R	212	ILE
2	R	239	LYS
2	R	240	VAL
2	R	246	VAL
2	R	253	GLN
2	R	258	PHE
2	R	274	GLU
2	R	291	GLU
2	R	295	LYS
2	R	309	GLU
2	R	311	LEU
2	R	313	LYS
2	R	317	ILE
2	R	328	GLU
2	R	329	ILE
2	R	337	SER
2	R	341	TYR
2	R	354	ARG
2	S	6	LYS
2	S	26	LYS
2	S	30	ASP
2	S	31	THR
2	S	34	LYS
2	S	42	LYS
2	S	45	GLU
2	S	46	LYS
2	S	50	VAL
2	S	53	THR
2	S	59	ILE
2	S	83	LYS
2	S	87	ASP

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Mol	Chain	Res	Type
2	S	89	LEU
2	S	98	ARG
2	S	115	LEU
2	S	127	LYS
2	S	128	THR
2	S	135	LEU
2	S	138	GLU
2	S	140	LYS
2	S	142	LYS
2	S	148	MET
2	S	160	LEU
2	S	173	ASN
2	S	175	LYS
2	S	202	LYS
2	S	204	MET
2	S	212	ILE
2	S	239	LYS
2	S	240	VAL
2	S	246	VAL
2	S	253	GLN
2	S	258	PHE
2	S	274	GLU
2	S	291	GLU
2	S	295	LYS
2	S	309	GLU
2	S	311	LEU
2	S	313	LYS
2	S	317	ILE
2	S	328	GLU
2	S	329	ILE
2	S	337	SER
2	S	341	TYR
2	S	354	ARG
2	T	6	LYS
2	T	26	LYS
2	T	30	ASP
2	T	31	THR
2	T	34	LYS
2	T	42	LYS
2	T	45	GLU
2	T	46	LYS
2	T	50	VAL

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Mol	Chain	Res	Type
2	T	53	THR
2	T	59	ILE
2	T	83	LYS
2	T	87	ASP
2	T	89	LEU
2	T	98	ARG
2	T	115	LEU
2	T	127	LYS
2	T	128	THR
2	T	135	LEU
2	T	138	GLU
2	T	140	LYS
2	T	142	LYS
2	T	148	MET
2	T	160	LEU
2	T	173	ASN
2	T	175	LYS
2	T	202	LYS
2	T	204	MET
2	T	212	ILE
2	T	239	LYS
2	T	240	VAL
2	T	246	VAL
2	T	253	GLN
2	T	258	PHE
2	T	274	GLU
2	T	291	GLU
2	T	295	LYS
2	T	309	GLU
2	T	311	LEU
2	T	313	LYS
2	T	317	ILE
2	T	328	GLU
2	T	329	ILE
2	T	337	SER
2	T	341	TYR
2	T	354	ARG
2	U	6	LYS
2	U	26	LYS
2	U	30	ASP
2	U	31	THR
2	U	34	LYS

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Mol	Chain	Res	Type
2	U	42	LYS
2	U	45	GLU
2	U	46	LYS
2	U	50	VAL
2	U	53	THR
2	U	59	ILE
2	U	83	LYS
2	U	87	ASP
2	U	89	LEU
2	U	98	ARG
2	U	115	LEU
2	U	127	LYS
2	U	128	THR
2	U	135	LEU
2	U	138	GLU
2	U	140	LYS
2	U	142	LYS
2	U	148	MET
2	U	160	LEU
2	U	173	ASN
2	U	175	LYS
2	U	202	LYS
2	U	204	MET
2	U	212	ILE
2	U	239	LYS
2	U	240	VAL
2	U	246	VAL
2	U	253	GLN
2	U	258	PHE
2	U	274	GLU
2	U	291	GLU
2	U	295	LYS
2	U	309	GLU
2	U	311	LEU
2	U	313	LYS
2	U	317	ILE
2	U	328	GLU
2	U	329	ILE
2	U	337	SER
2	U	341	TYR
2	U	354	ARG
2	V	6	LYS

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Mol	Chain	Res	Type
2	V	26	LYS
2	V	30	ASP
2	V	31	THR
2	V	34	LYS
2	V	42	LYS
2	V	45	GLU
2	V	46	LYS
2	V	50	VAL
2	V	53	THR
2	V	59	ILE
2	V	83	LYS
2	V	87	ASP
2	V	89	LEU
2	V	98	ARG
2	V	115	LEU
2	V	127	LYS
2	V	128	THR
2	V	135	LEU
2	V	138	GLU
2	V	140	LYS
2	V	142	LYS
2	V	148	MET
2	V	160	LEU
2	V	173	ASN
2	V	175	LYS
2	V	202	LYS
2	V	204	MET
2	V	212	ILE
2	V	239	LYS
2	V	240	VAL
2	V	246	VAL
2	V	253	GLN
2	V	258	PHE
2	V	274	GLU
2	V	291	GLU
2	V	295	LYS
2	V	309	GLU
2	V	311	LEU
2	V	313	LYS
2	V	317	ILE
2	V	328	GLU
2	V	329	ILE

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Mol	Chain	Res	Type
2	V	337	SER
2	V	341	TYR
2	V	354	ARG
2	W	6	LYS
2	W	26	LYS
2	W	30	ASP
2	W	31	THR
2	W	34	LYS
2	W	42	LYS
2	W	45	GLU
2	W	46	LYS
2	W	50	VAL
2	W	53	THR
2	W	59	ILE
2	W	83	LYS
2	W	87	ASP
2	W	89	LEU
2	W	98	ARG
2	W	115	LEU
2	W	127	LYS
2	W	128	THR
2	W	135	LEU
2	W	138	GLU
2	W	140	LYS
2	W	142	LYS
2	W	148	MET
2	W	160	LEU
2	W	173	ASN
2	W	175	LYS
2	W	202	LYS
2	W	204	MET
2	W	212	ILE
2	W	239	LYS
2	W	240	VAL
2	W	246	VAL
2	W	253	GLN
2	W	258	PHE
2	W	274	GLU
2	W	291	GLU
2	W	295	LYS
2	W	309	GLU
2	W	311	LEU

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Mol	Chain	Res	Type
2	W	313	LYS
2	W	317	ILE
2	W	328	GLU
2	W	329	ILE
2	W	337	SER
2	W	341	TYR
2	W	354	ARG
2	X	6	LYS
2	X	26	LYS
2	X	30	ASP
2	X	31	THR
2	X	34	LYS
2	X	42	LYS
2	X	45	GLU
2	X	46	LYS
2	X	50	VAL
2	X	53	THR
2	X	59	ILE
2	X	83	LYS
2	X	87	ASP
2	X	89	LEU
2	X	98	ARG
2	X	115	LEU
2	X	127	LYS
2	X	128	THR
2	X	135	LEU
2	X	138	GLU
2	X	140	LYS
2	X	142	LYS
2	X	148	MET
2	X	160	LEU
2	X	173	ASN
2	X	175	LYS
2	X	202	LYS
2	X	204	MET
2	X	212	ILE
2	X	239	LYS
2	X	240	VAL
2	X	246	VAL
2	X	253	GLN
2	X	258	PHE
2	X	274	GLU

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Mol	Chain	Res	Type
2	X	291	GLU
2	X	295	LYS
2	X	309	GLU
2	X	311	LEU
2	X	313	LYS
2	X	317	ILE
2	X	328	GLU
2	X	329	ILE
2	X	337	SER
2	X	341	TYR
2	X	354	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (258) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	30	HIS
1	A	61	ASN
1	A	189	GLN
1	A	211	HIS
1	A	218	GLN
1	A	219	ASN
1	A	244	ASN
1	A	264	ASN
1	A	277	ASN
1	A	313	ASN
1	A	384	ASN
1	A	409	GLN
1	A	458	HIS
1	B	10	ASN
1	B	30	HIS
1	B	61	ASN
1	B	189	GLN
1	B	211	HIS
1	B	218	GLN
1	B	219	ASN
1	B	244	ASN
1	B	264	ASN
1	B	277	ASN
1	B	313	ASN
1	B	384	ASN
1	B	409	GLN

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Mol	Chain	Res	Type
1	B	458	HIS
1	C	10	ASN
1	C	30	HIS
1	C	189	GLN
1	C	211	HIS
1	C	218	GLN
1	C	219	ASN
1	C	244	ASN
1	C	264	ASN
1	C	277	ASN
1	C	313	ASN
1	C	384	ASN
1	C	409	GLN
1	C	458	HIS
1	D	10	ASN
1	D	30	HIS
1	D	61	ASN
1	D	189	GLN
1	D	211	HIS
1	D	218	GLN
1	D	219	ASN
1	D	244	ASN
1	D	264	ASN
1	D	277	ASN
1	D	313	ASN
1	D	384	ASN
1	D	409	GLN
1	D	458	HIS
1	E	10	ASN
1	E	30	HIS
1	E	61	ASN
1	E	189	GLN
1	E	211	HIS
1	E	218	GLN
1	E	219	ASN
1	E	244	ASN
1	E	264	ASN
1	E	277	ASN
1	E	313	ASN
1	E	384	ASN
1	E	409	GLN
1	E	458	HIS

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Mol	Chain	Res	Type
1	F	10	ASN
1	F	30	HIS
1	F	189	GLN
1	F	211	HIS
1	F	218	GLN
1	F	219	ASN
1	F	244	ASN
1	F	264	ASN
1	F	277	ASN
1	F	313	ASN
1	F	384	ASN
1	F	409	GLN
1	F	458	HIS
1	G	10	ASN
1	G	30	HIS
1	G	61	ASN
1	G	189	GLN
1	G	211	HIS
1	G	218	GLN
1	G	219	ASN
1	G	244	ASN
1	G	264	ASN
1	G	277	ASN
1	G	313	ASN
1	G	384	ASN
1	G	409	GLN
1	G	458	HIS
1	H	10	ASN
1	H	30	HIS
1	H	189	GLN
1	H	211	HIS
1	H	218	GLN
1	H	219	ASN
1	H	244	ASN
1	H	264	ASN
1	H	277	ASN
1	H	313	ASN
1	H	384	ASN
1	H	409	GLN
1	H	458	HIS
1	I	10	ASN
1	I	30	HIS

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Mol	Chain	Res	Type
1	I	61	ASN
1	I	189	GLN
1	I	211	HIS
1	I	218	GLN
1	I	219	ASN
1	I	244	ASN
1	I	264	ASN
1	I	277	ASN
1	I	313	ASN
1	I	384	ASN
1	I	409	GLN
1	I	458	HIS
1	J	10	ASN
1	J	30	HIS
1	J	61	ASN
1	J	189	GLN
1	J	211	HIS
1	J	218	GLN
1	J	219	ASN
1	J	244	ASN
1	J	264	ASN
1	J	277	ASN
1	J	313	ASN
1	J	384	ASN
1	J	409	GLN
1	J	458	HIS
1	K	10	ASN
1	K	30	HIS
1	K	189	GLN
1	K	211	HIS
1	K	218	GLN
1	K	219	ASN
1	K	244	ASN
1	K	264	ASN
1	K	277	ASN
1	K	313	ASN
1	K	384	ASN
1	K	409	GLN
1	K	458	HIS
1	L	10	ASN
1	L	30	HIS
1	L	61	ASN

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Mol	Chain	Res	Type
1	L	189	GLN
1	L	211	HIS
1	L	218	GLN
1	L	219	ASN
1	L	244	ASN
1	L	264	ASN
1	L	277	ASN
1	L	313	ASN
1	L	384	ASN
1	L	409	GLN
1	L	458	HIS
2	M	18	ASN
2	M	49	GLN
2	M	64	HIS
2	M	201	ASN
2	M	203	HIS
2	M	205	ASN
2	M	218	ASN
2	M	272	ASN
2	N	18	ASN
2	N	49	GLN
2	N	64	HIS
2	N	203	HIS
2	N	205	ASN
2	N	218	ASN
2	N	272	ASN
2	O	18	ASN
2	O	49	GLN
2	O	64	HIS
2	O	203	HIS
2	O	205	ASN
2	O	218	ASN
2	O	272	ASN
2	O	325	GLN
2	P	18	ASN
2	P	49	GLN
2	P	64	HIS
2	P	201	ASN
2	P	203	HIS
2	P	205	ASN
2	P	218	ASN
2	P	272	ASN

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Mol	Chain	Res	Type
2	P	325	GLN
2	Q	18	ASN
2	Q	49	GLN
2	Q	64	HIS
2	Q	203	HIS
2	Q	205	ASN
2	Q	218	ASN
2	Q	272	ASN
2	R	18	ASN
2	R	49	GLN
2	R	64	HIS
2	R	173	ASN
2	R	203	HIS
2	R	205	ASN
2	R	218	ASN
2	R	272	ASN
2	S	18	ASN
2	S	49	GLN
2	S	64	HIS
2	S	173	ASN
2	S	203	HIS
2	S	205	ASN
2	S	218	ASN
2	S	272	ASN
2	T	18	ASN
2	T	49	GLN
2	T	64	HIS
2	T	203	HIS
2	T	205	ASN
2	T	218	ASN
2	T	272	ASN
2	U	18	ASN
2	U	49	GLN
2	U	64	HIS
2	U	201	ASN
2	U	203	HIS
2	U	205	ASN
2	U	218	ASN
2	U	272	ASN
2	U	325	GLN
2	V	18	ASN
2	V	49	GLN

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Mol	Chain	Res	Type
2	V	64	HIS
2	V	203	HIS
2	V	205	ASN
2	V	218	ASN
2	V	272	ASN
2	V	325	GLN
2	W	18	ASN
2	W	49	GLN
2	W	64	HIS
2	W	203	HIS
2	W	205	ASN
2	W	218	ASN
2	W	272	ASN
2	X	18	ASN
2	X	49	GLN
2	X	64	HIS
2	X	173	ASN
2	X	203	HIS
2	X	205	ASN
2	X	218	ASN
2	X	272	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	Y	1	3	12,12,12	1.19	1 (8%)	17,17,17	2.24	5 (29%)
3	GLC	Y	2	3	11,11,12	1.52	1 (9%)	15,15,17	1.45	1 (6%)
3	GLC	Z	1	3	12,12,12	1.20	1 (8%)	17,17,17	2.25	5 (29%)
3	GLC	Z	2	3	11,11,12	1.51	1 (9%)	15,15,17	1.44	1 (6%)
3	GLC	a	1	3	12,12,12	1.20	1 (8%)	17,17,17	2.25	5 (29%)
3	GLC	a	2	3	11,11,12	1.52	1 (9%)	15,15,17	1.45	1 (6%)
3	GLC	b	1	3	12,12,12	1.19	1 (8%)	17,17,17	2.24	5 (29%)
3	GLC	b	2	3	11,11,12	1.52	1 (9%)	15,15,17	1.45	1 (6%)
3	GLC	c	1	3	12,12,12	1.19	1 (8%)	17,17,17	2.24	5 (29%)
3	GLC	c	2	3	11,11,12	1.52	1 (9%)	15,15,17	1.45	1 (6%)
3	GLC	d	1	3	12,12,12	1.20	1 (8%)	17,17,17	2.24	5 (29%)
3	GLC	d	2	3	11,11,12	1.52	1 (9%)	15,15,17	1.45	1 (6%)
3	GLC	e	1	3	12,12,12	1.19	1 (8%)	17,17,17	2.24	5 (29%)
3	GLC	e	2	3	11,11,12	1.51	1 (9%)	15,15,17	1.45	1 (6%)
3	GLC	f	1	3	12,12,12	1.19	1 (8%)	17,17,17	2.25	5 (29%)
3	GLC	f	2	3	11,11,12	1.52	1 (9%)	15,15,17	1.44	1 (6%)
3	GLC	g	1	3	12,12,12	1.18	1 (8%)	17,17,17	2.24	5 (29%)
3	GLC	g	2	3	11,11,12	1.53	1 (9%)	15,15,17	1.45	1 (6%)
3	GLC	h	1	3	12,12,12	1.19	1 (8%)	17,17,17	2.24	5 (29%)
3	GLC	h	2	3	11,11,12	1.52	1 (9%)	15,15,17	1.45	1 (6%)
3	GLC	i	1	3	12,12,12	1.18	1 (8%)	17,17,17	2.24	5 (29%)
3	GLC	i	2	3	11,11,12	1.52	1 (9%)	15,15,17	1.44	1 (6%)
3	GLC	j	1	3	12,12,12	1.19	1 (8%)	17,17,17	2.24	5 (29%)
3	GLC	j	2	3	11,11,12	1.53	1 (9%)	15,15,17	1.45	1 (6%)

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
3	GLC	Y	1	3	-	0/2/22/22	0/1/1/1
3	GLC	Y	2	3	-	0/2/19/22	0/1/1/1
3	GLC	Z	1	3	-	0/2/22/22	0/1/1/1
3	GLC	Z	2	3	-	0/2/19/22	0/1/1/1
3	GLC	a	1	3	-	0/2/22/22	0/1/1/1
3	GLC	a	2	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	b	1	3	-	0/2/22/22	0/1/1/1
3	GLC	b	2	3	-	0/2/19/22	0/1/1/1
3	GLC	c	1	3	-	0/2/22/22	0/1/1/1
3	GLC	c	2	3	-	0/2/19/22	0/1/1/1
3	GLC	d	1	3	-	0/2/22/22	0/1/1/1
3	GLC	d	2	3	-	0/2/19/22	0/1/1/1
3	GLC	e	1	3	-	0/2/22/22	0/1/1/1
3	GLC	e	2	3	-	0/2/19/22	0/1/1/1
3	GLC	f	1	3	-	0/2/22/22	0/1/1/1
3	GLC	f	2	3	-	0/2/19/22	0/1/1/1
3	GLC	g	1	3	-	0/2/22/22	0/1/1/1
3	GLC	g	2	3	-	0/2/19/22	0/1/1/1
3	GLC	h	1	3	-	0/2/22/22	0/1/1/1
3	GLC	h	2	3	-	0/2/19/22	0/1/1/1
3	GLC	i	1	3	-	0/2/22/22	0/1/1/1
3	GLC	i	2	3	-	0/2/19/22	0/1/1/1
3	GLC	j	1	3	-	0/2/22/22	0/1/1/1
3	GLC	j	2	3	-	0/2/19/22	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	g	2	GLC	O5-C1	-3.97	1.37	1.43
3	j	2	GLC	O5-C1	-3.97	1.37	1.43
3	c	2	GLC	O5-C1	-3.95	1.37	1.43
3	f	2	GLC	O5-C1	-3.95	1.37	1.43
3	h	2	GLC	O5-C1	-3.95	1.37	1.43
3	i	2	GLC	O5-C1	-3.95	1.37	1.43
3	Y	2	GLC	O5-C1	-3.94	1.37	1.43
3	b	2	GLC	O5-C1	-3.93	1.37	1.43
3	a	2	GLC	O5-C1	-3.92	1.37	1.43
3	Z	2	GLC	O5-C1	-3.92	1.37	1.43
3	d	2	GLC	O5-C1	-3.91	1.37	1.43
3	e	2	GLC	O5-C1	-3.90	1.37	1.43
3	d	1	GLC	O5-C1	-2.29	1.37	1.42
3	a	1	GLC	O5-C1	-2.27	1.37	1.42
3	Z	1	GLC	O5-C1	-2.27	1.37	1.42
3	j	1	GLC	O5-C1	-2.26	1.37	1.42
3	c	1	GLC	O5-C1	-2.26	1.37	1.42
3	Y	1	GLC	O5-C1	-2.25	1.37	1.42
3	g	1	GLC	O5-C1	-2.25	1.37	1.42
3	h	1	GLC	O5-C1	-2.25	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	f	1	GLC	O5-C1	-2.25	1.37	1.42
3	e	1	GLC	O5-C1	-2.24	1.37	1.42
3	b	1	GLC	O5-C1	-2.23	1.37	1.42
3	i	1	GLC	O5-C1	-2.20	1.37	1.42

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	1	GLC	C1-O5-C5	6.08	125.41	113.65
3	Z	1	GLC	C1-O5-C5	6.06	125.38	113.65
3	d	1	GLC	C1-O5-C5	6.06	125.38	113.65
3	j	1	GLC	C1-O5-C5	6.06	125.37	113.65
3	c	1	GLC	C1-O5-C5	6.05	125.36	113.65
3	h	1	GLC	C1-O5-C5	6.05	125.36	113.65
3	f	1	GLC	C1-O5-C5	6.05	125.35	113.65
3	g	1	GLC	C1-O5-C5	6.05	125.35	113.65
3	Y	1	GLC	C1-O5-C5	6.04	125.34	113.65
3	e	1	GLC	C1-O5-C5	6.04	125.33	113.65
3	b	1	GLC	C1-O5-C5	6.03	125.32	113.65
3	i	1	GLC	C1-O5-C5	6.02	125.29	113.65
3	j	2	GLC	C1-O5-C5	4.23	117.85	112.19
3	b	2	GLC	C1-O5-C5	4.22	117.84	112.19
3	d	2	GLC	C1-O5-C5	4.21	117.83	112.19
3	c	2	GLC	C1-O5-C5	4.21	117.83	112.19
3	g	2	GLC	C1-O5-C5	4.21	117.83	112.19
3	h	2	GLC	C1-O5-C5	4.21	117.83	112.19
3	e	2	GLC	C1-O5-C5	4.21	117.82	112.19
3	f	2	GLC	C1-O5-C5	4.21	117.82	112.19
3	a	2	GLC	C1-O5-C5	4.20	117.82	112.19
3	Y	2	GLC	C1-O5-C5	4.20	117.81	112.19
3	i	2	GLC	C1-O5-C5	4.20	117.81	112.19
3	Z	2	GLC	C1-O5-C5	4.18	117.79	112.19
3	b	1	GLC	O1-C1-O5	-3.96	98.64	110.41
3	e	1	GLC	O1-C1-O5	-3.95	98.67	110.41
3	i	1	GLC	O1-C1-O5	-3.95	98.68	110.41
3	g	1	GLC	O1-C1-O5	-3.94	98.70	110.41
3	f	1	GLC	O1-C1-O5	-3.94	98.70	110.41
3	h	1	GLC	O1-C1-O5	-3.94	98.70	110.41
3	c	1	GLC	O1-C1-O5	-3.94	98.70	110.41
3	j	1	GLC	O1-C1-O5	-3.94	98.71	110.41
3	a	1	GLC	O1-C1-O5	-3.94	98.72	110.41
3	Z	1	GLC	O1-C1-O5	-3.94	98.72	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	1	GLC	O1-C1-O5	-3.93	98.73	110.41
3	d	1	GLC	O1-C1-O5	-3.93	98.74	110.41
3	e	1	GLC	O5-C1-C2	3.73	116.85	110.30
3	f	1	GLC	O5-C1-C2	3.72	116.84	110.30
3	Y	1	GLC	O5-C1-C2	3.72	116.83	110.30
3	b	1	GLC	O5-C1-C2	3.71	116.83	110.30
3	c	1	GLC	O5-C1-C2	3.71	116.82	110.30
3	Z	1	GLC	O5-C1-C2	3.70	116.81	110.30
3	d	1	GLC	O5-C1-C2	3.70	116.81	110.30
3	h	1	GLC	O5-C1-C2	3.70	116.81	110.30
3	i	1	GLC	O5-C1-C2	3.70	116.81	110.30
3	g	1	GLC	O5-C1-C2	3.69	116.80	110.30
3	j	1	GLC	O5-C1-C2	3.69	116.79	110.30
3	a	1	GLC	O5-C1-C2	3.68	116.76	110.30
3	a	1	GLC	O6-C6-C5	-2.58	102.56	111.33
3	f	1	GLC	O6-C6-C5	-2.57	102.58	111.33
3	e	1	GLC	O6-C6-C5	-2.57	102.59	111.33
3	b	1	GLC	O6-C6-C5	-2.57	102.60	111.33
3	h	1	GLC	O6-C6-C5	-2.56	102.61	111.33
3	Z	1	GLC	O6-C6-C5	-2.56	102.61	111.33
3	i	1	GLC	O6-C6-C5	-2.56	102.61	111.33
3	j	1	GLC	O6-C6-C5	-2.56	102.62	111.33
3	d	1	GLC	O6-C6-C5	-2.56	102.62	111.33
3	Y	1	GLC	O6-C6-C5	-2.56	102.62	111.33
3	g	1	GLC	O6-C6-C5	-2.56	102.63	111.33
3	c	1	GLC	O6-C6-C5	-2.55	102.64	111.33
3	f	1	GLC	O4-C4-C5	-2.20	103.90	109.32
3	Z	1	GLC	O4-C4-C5	-2.19	103.92	109.32
3	b	1	GLC	O4-C4-C5	-2.19	103.92	109.32
3	c	1	GLC	O4-C4-C5	-2.18	103.95	109.32
3	d	1	GLC	O4-C4-C5	-2.18	103.96	109.32
3	h	1	GLC	O4-C4-C5	-2.18	103.97	109.32
3	Y	1	GLC	O4-C4-C5	-2.17	103.97	109.32
3	j	1	GLC	O4-C4-C5	-2.17	103.97	109.32
3	a	1	GLC	O4-C4-C5	-2.17	103.97	109.32
3	g	1	GLC	O4-C4-C5	-2.17	103.98	109.32
3	i	1	GLC	O4-C4-C5	-2.17	103.99	109.32
3	e	1	GLC	O4-C4-C5	-2.16	104.01	109.32

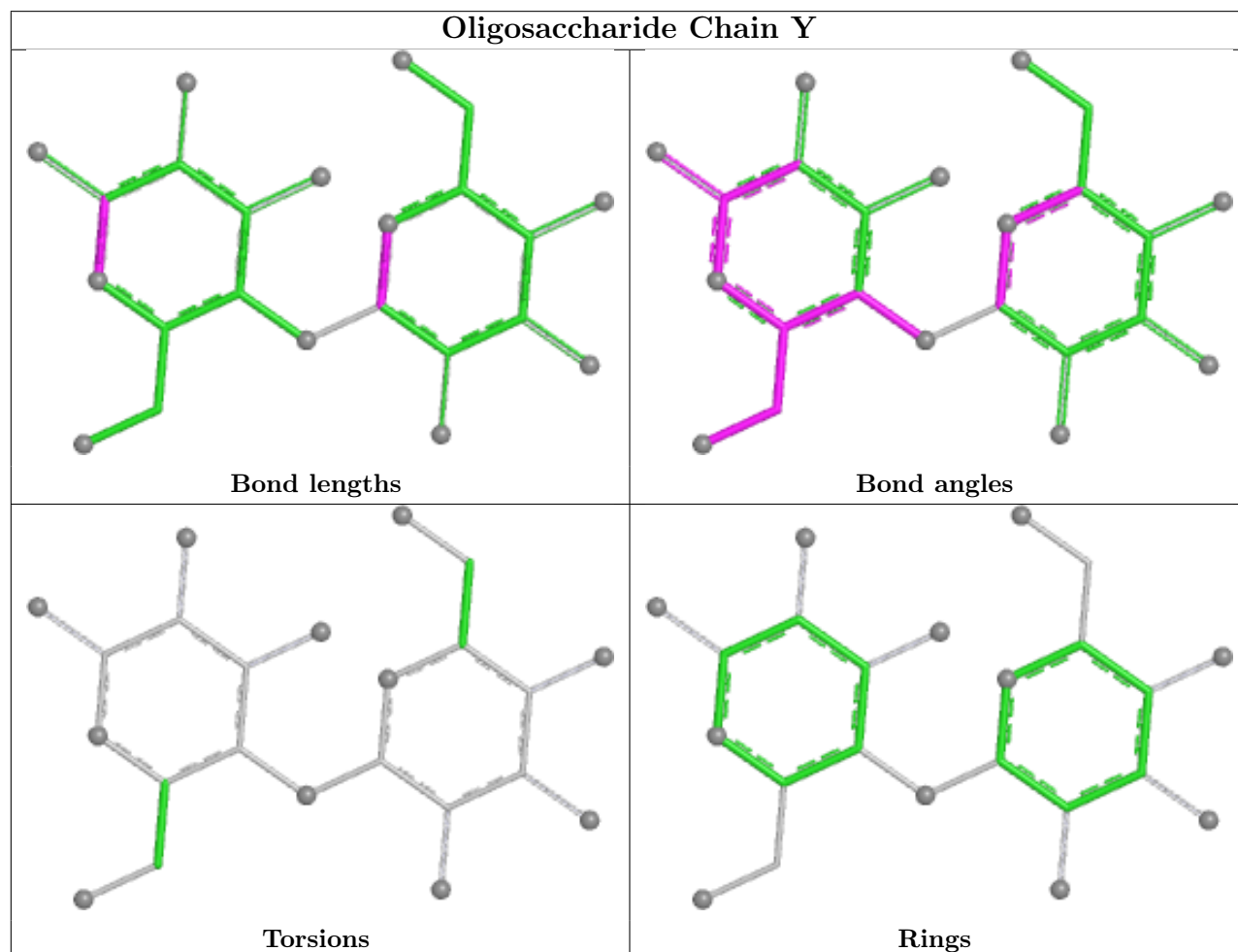
There are no chirality outliers.

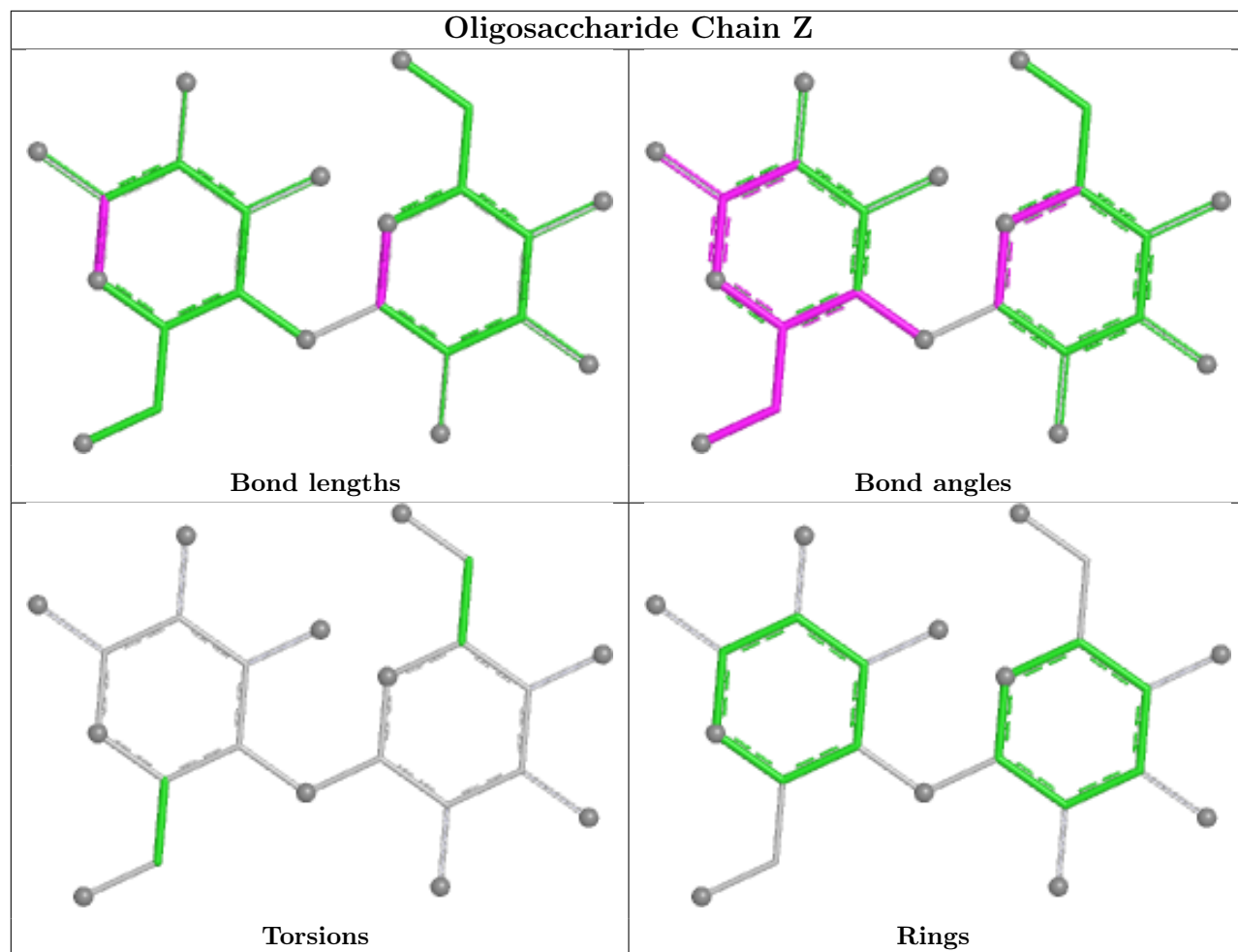
There are no torsion outliers.

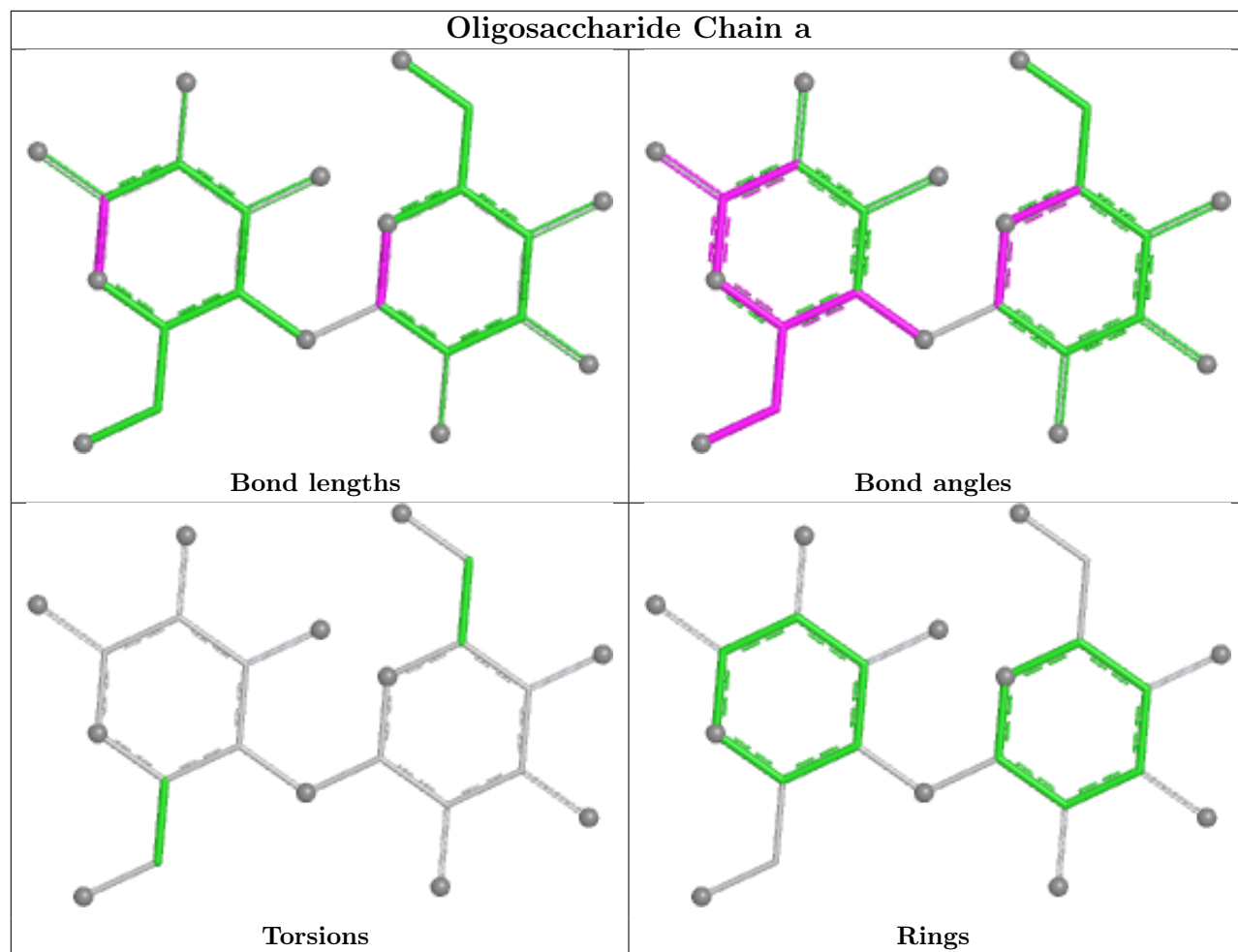
There are no ring outliers.

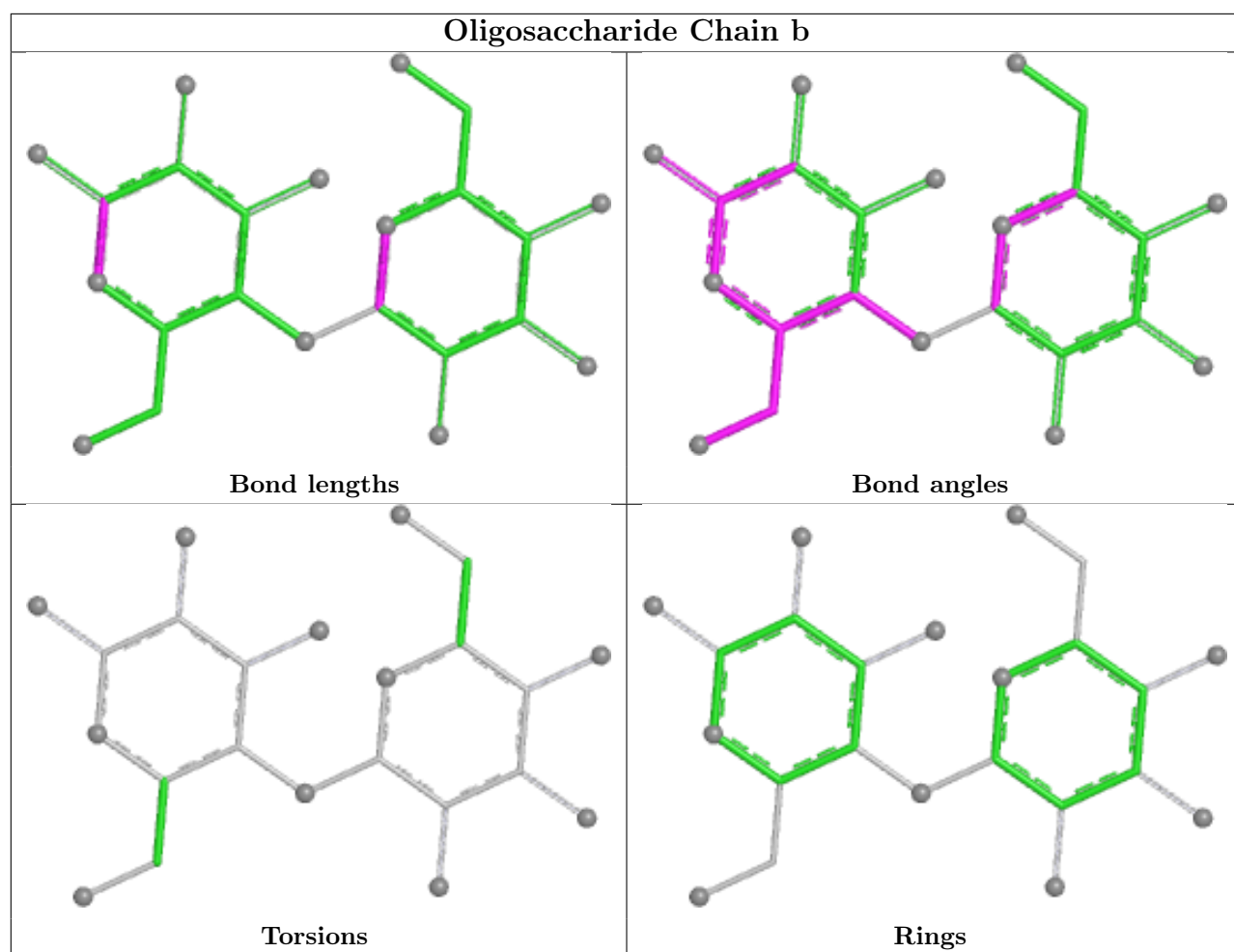
No monomer is involved in short contacts.

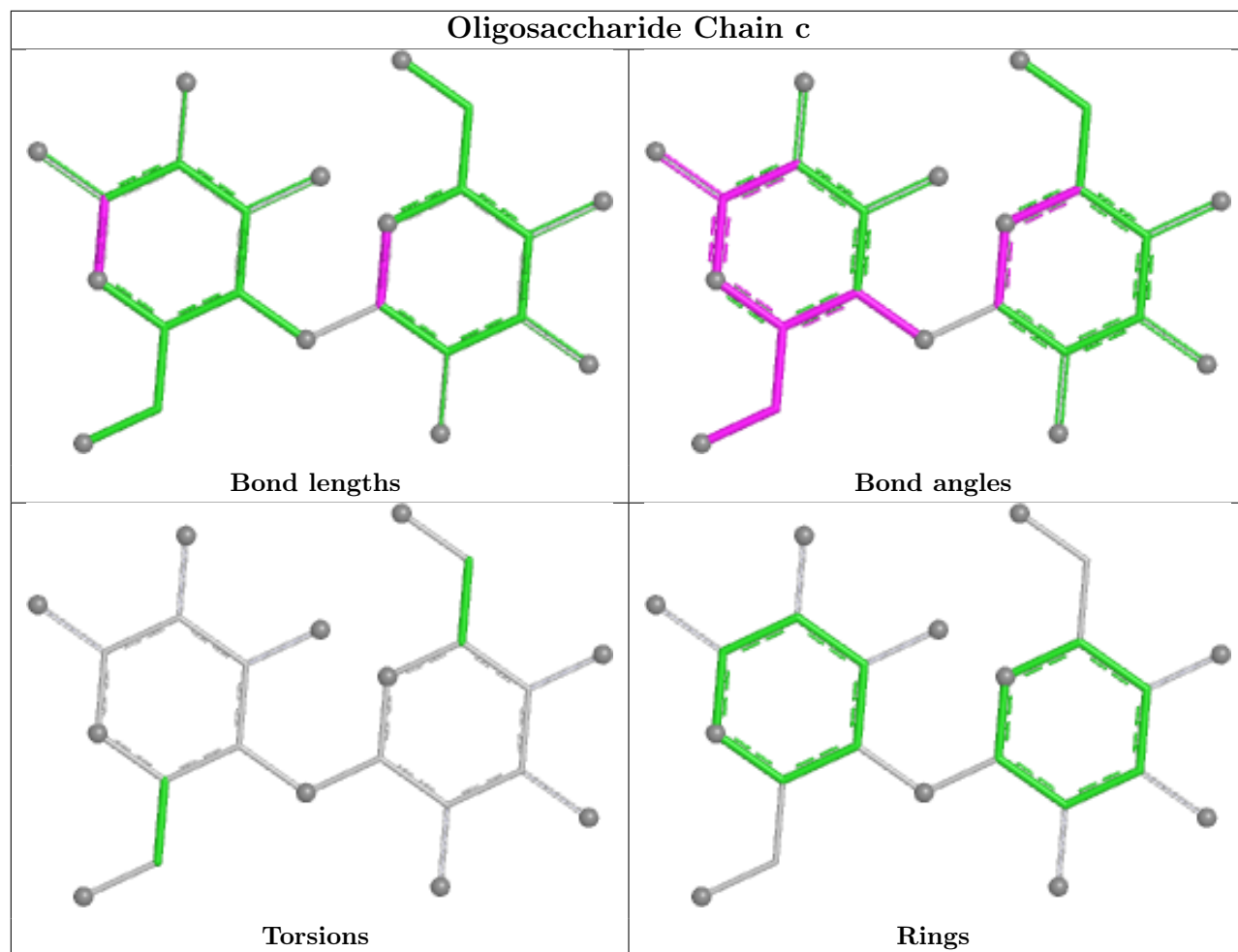
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

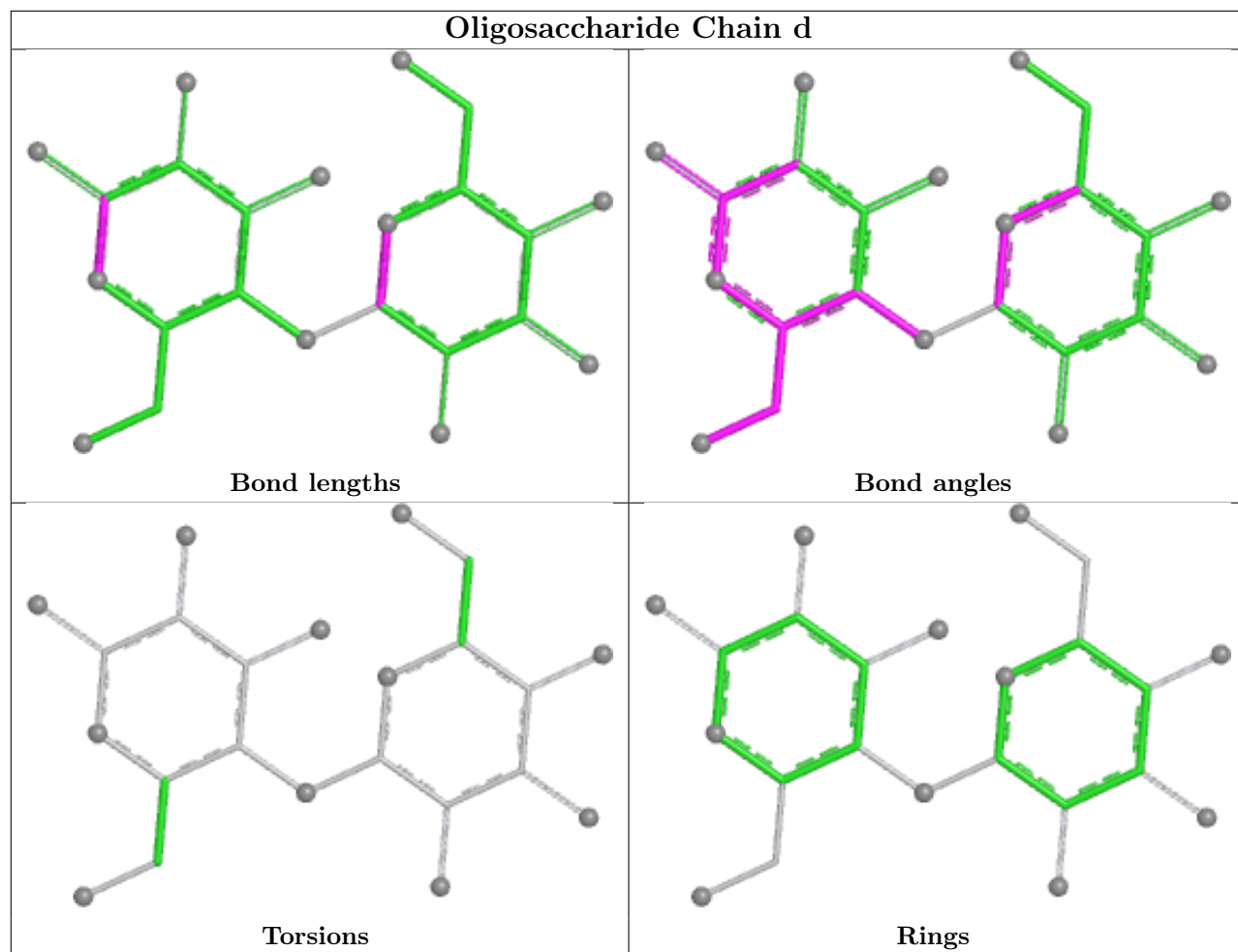


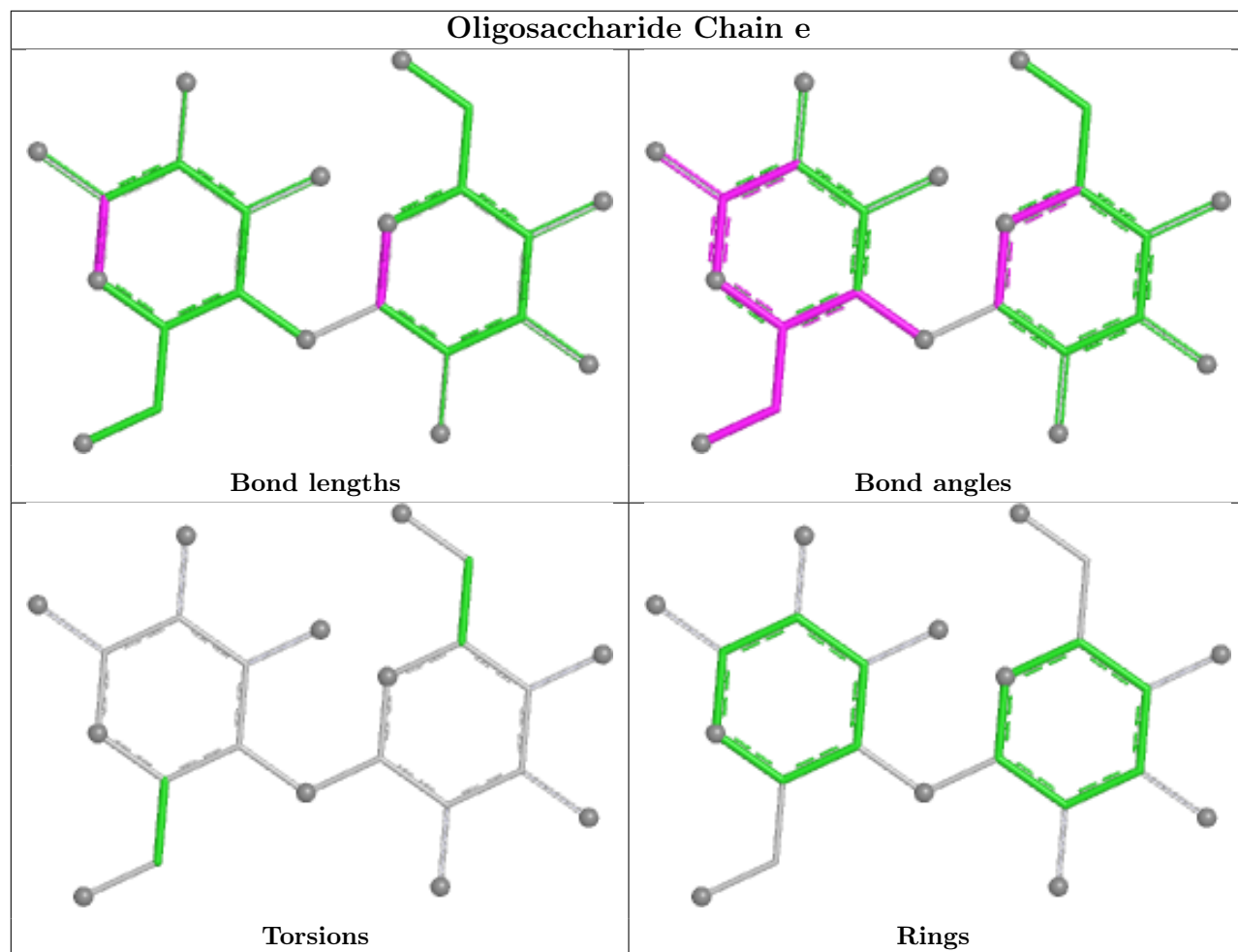


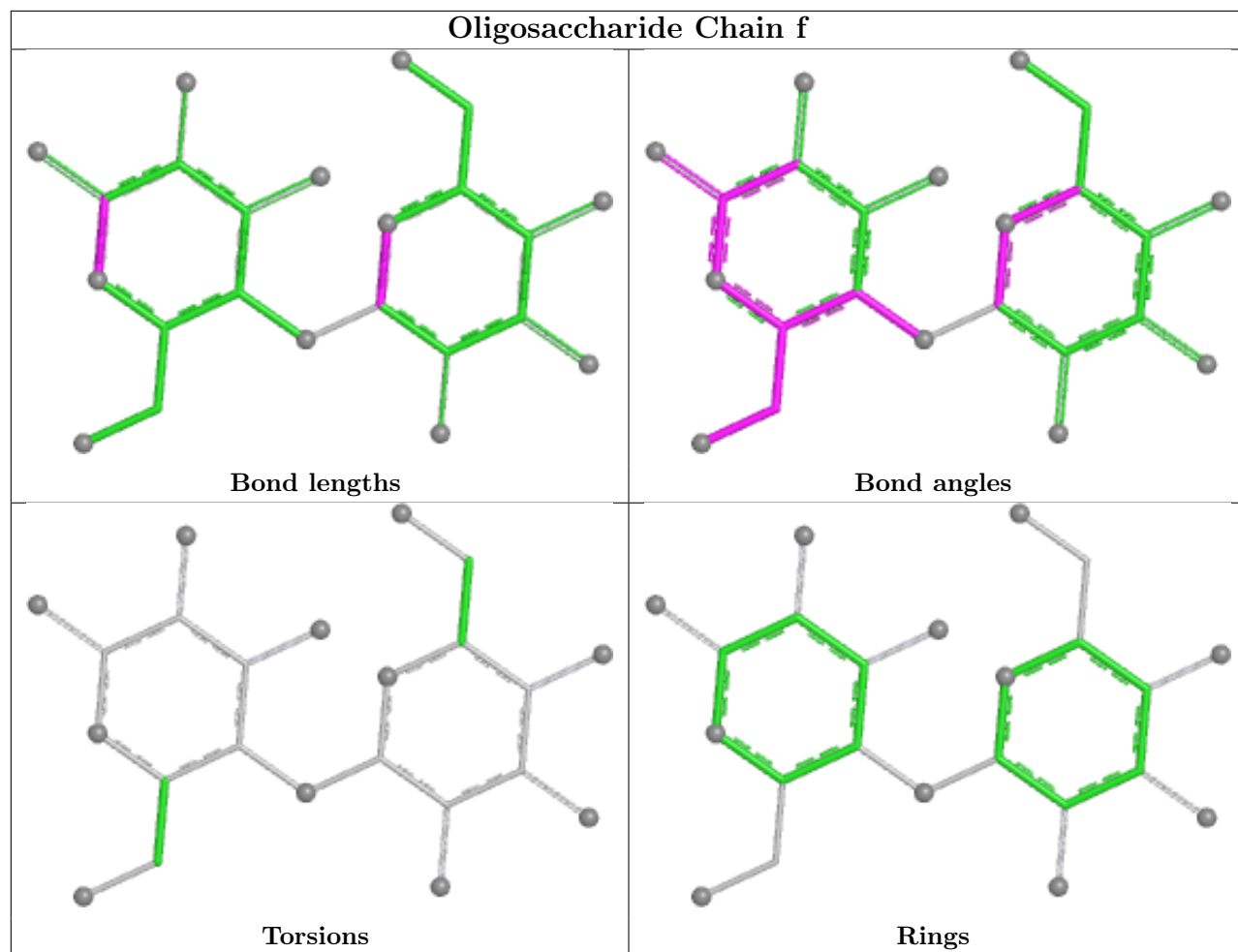


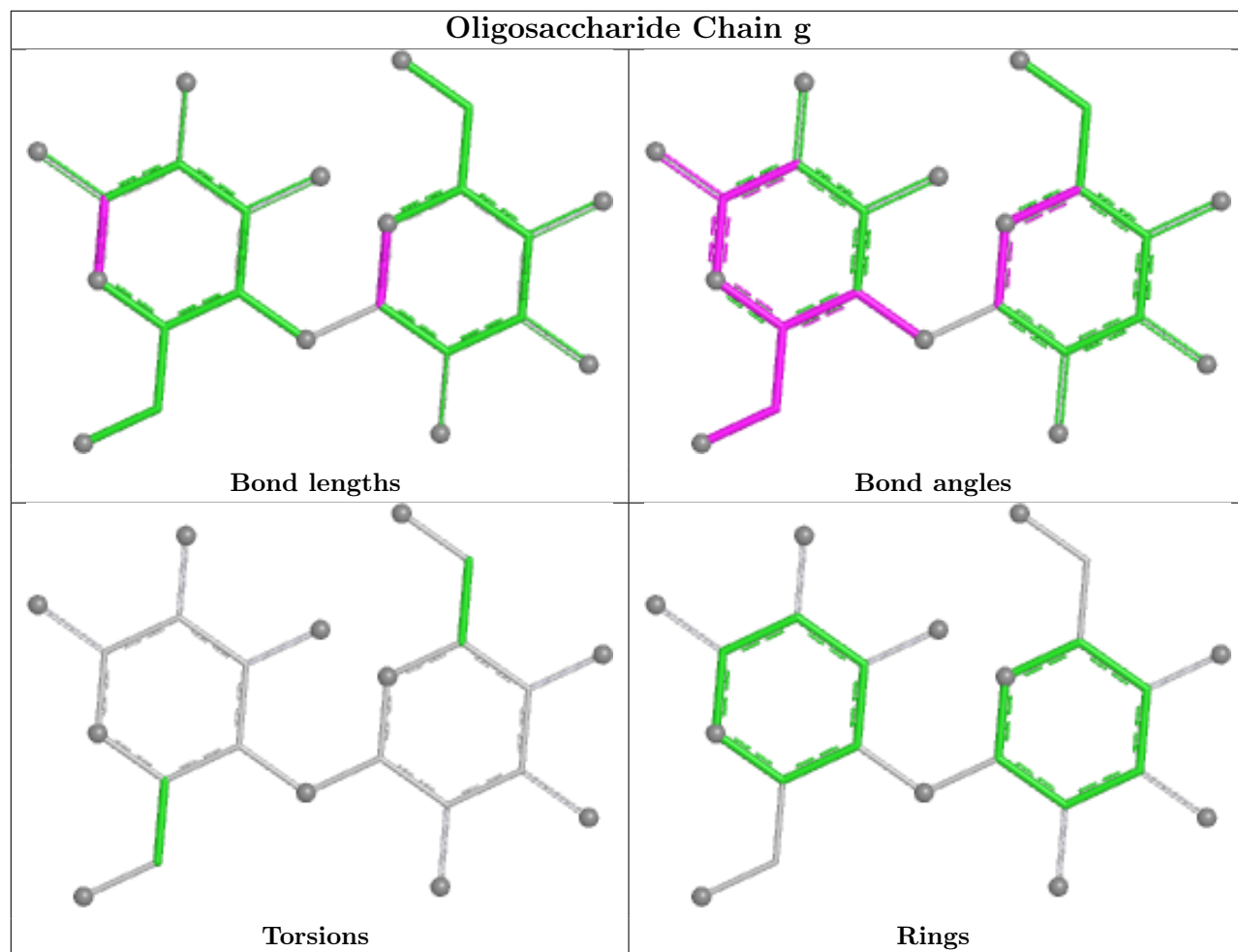


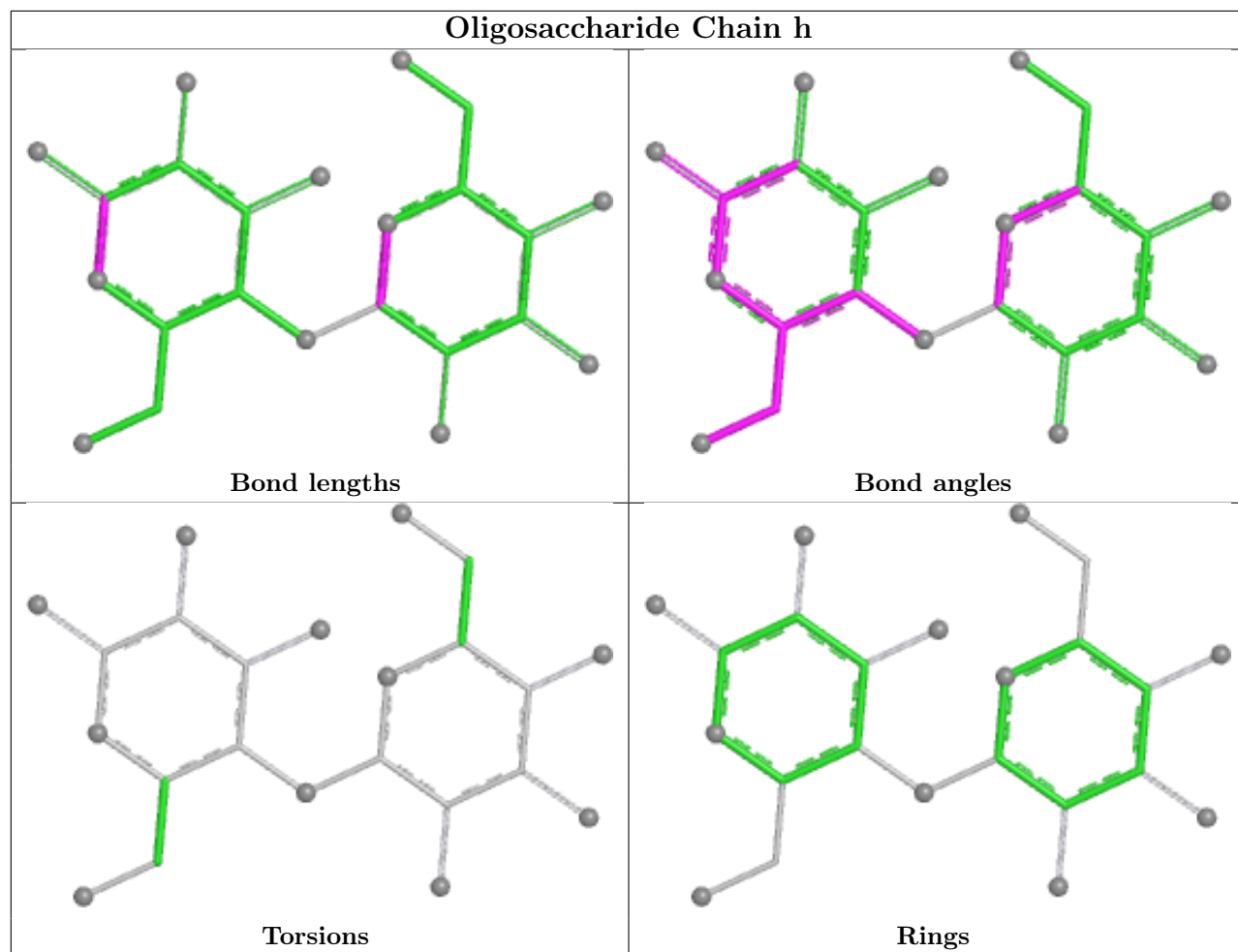


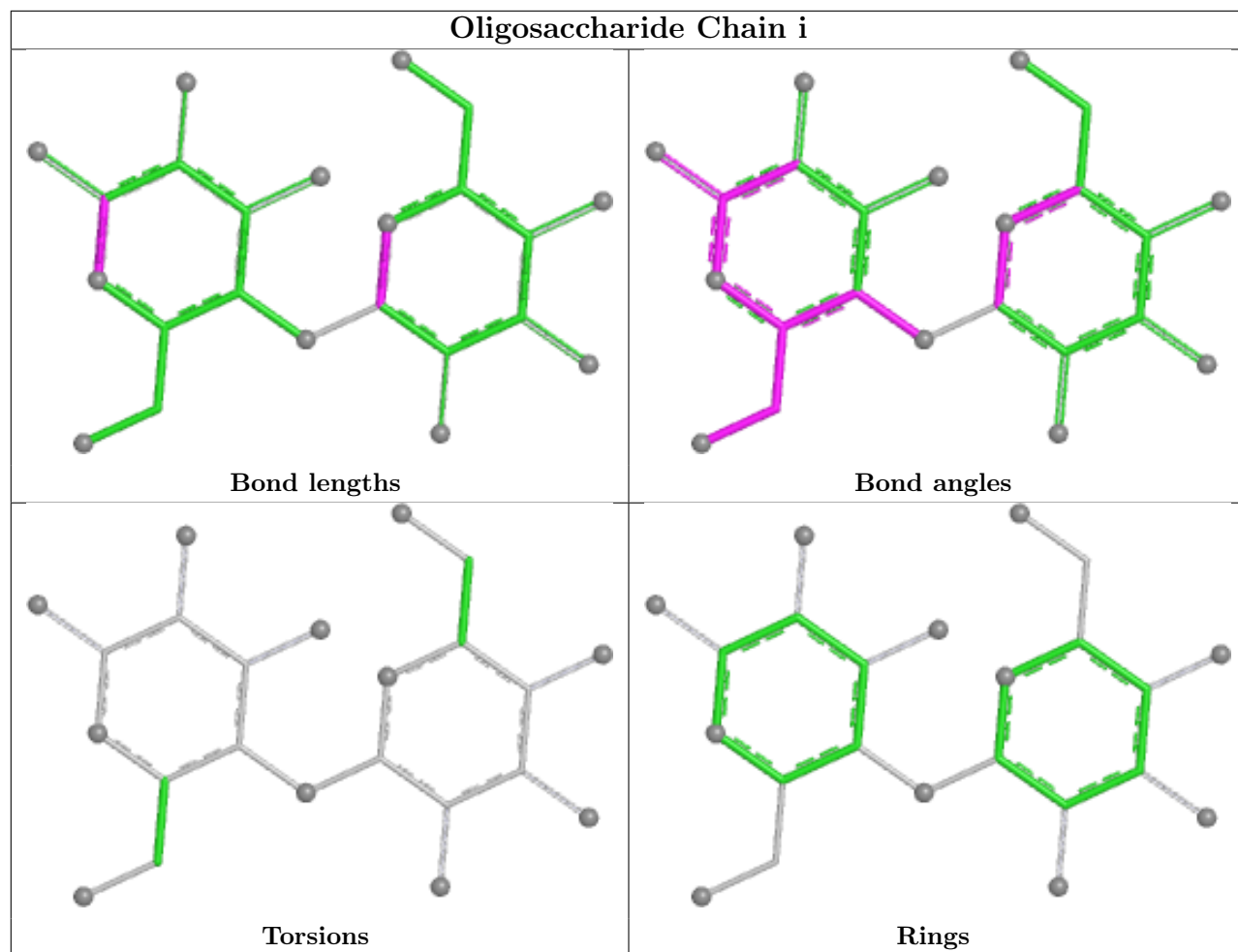


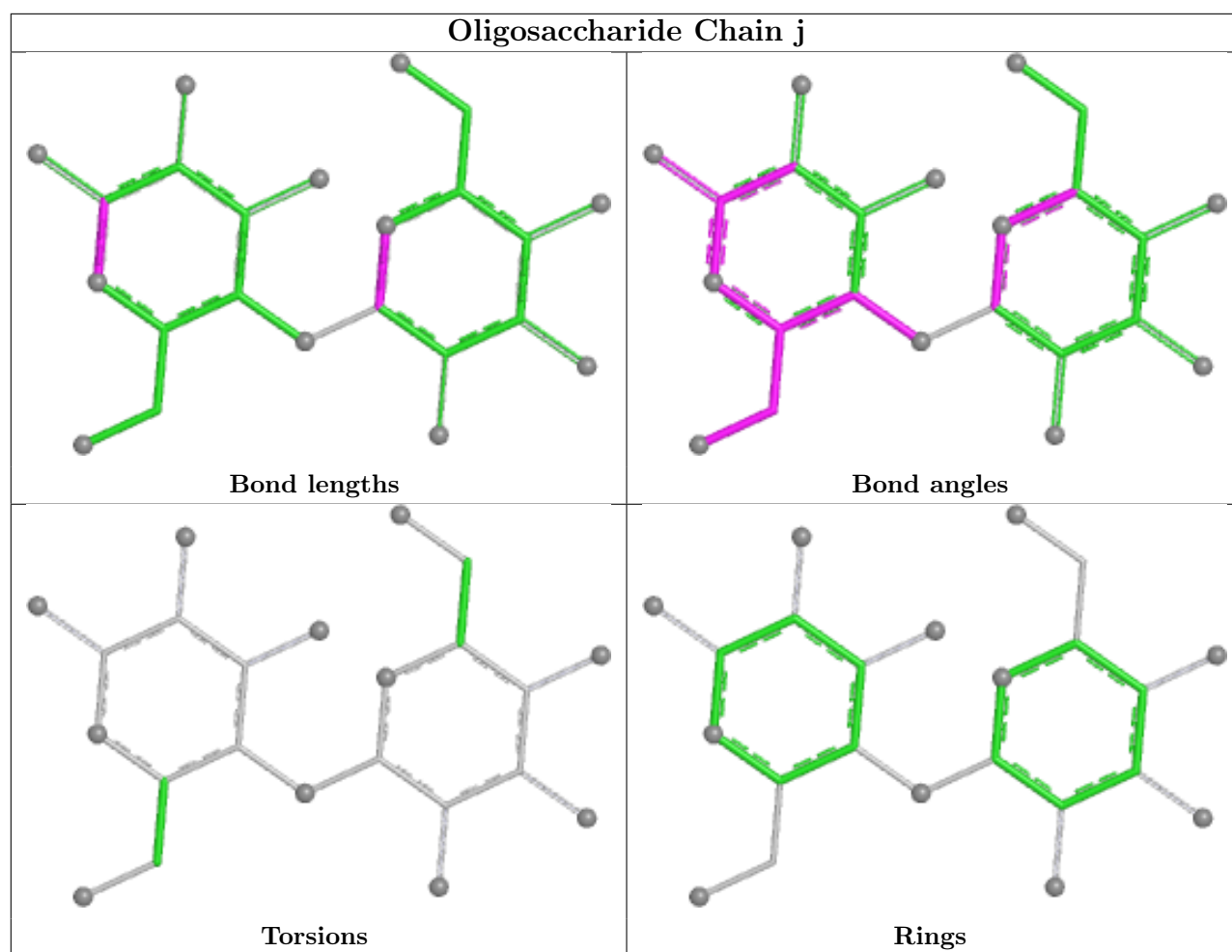












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	M	1
2	O	1
2	P	1
2	Q	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
2	T	1
2	N	1
2	R	1
2	S	1
2	U	1
2	V	1
2	W	1
2	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	369:THR	C	370:LYS	N	1.68
1	O	369:THR	C	370:LYS	N	1.68
1	P	369:THR	C	370:LYS	N	1.68
1	Q	369:THR	C	370:LYS	N	1.68
1	T	369:THR	C	370:LYS	N	1.68
1	N	369:THR	C	370:LYS	N	1.67
1	R	369:THR	C	370:LYS	N	1.67
1	S	369:THR	C	370:LYS	N	1.67
1	U	369:THR	C	370:LYS	N	1.67
1	V	369:THR	C	370:LYS	N	1.67
1	W	369:THR	C	370:LYS	N	1.67
1	X	369:THR	C	370:LYS	N	1.67

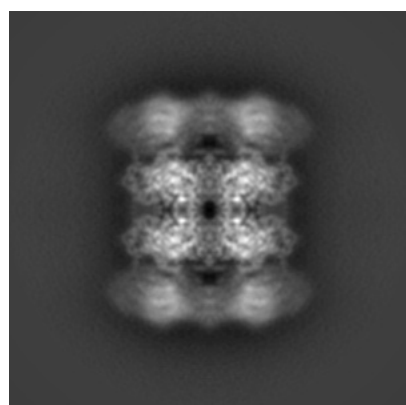
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4039. These allow visual inspection of the internal detail of the map and identification of artifacts.

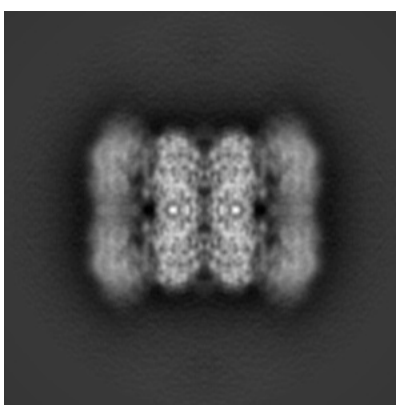
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

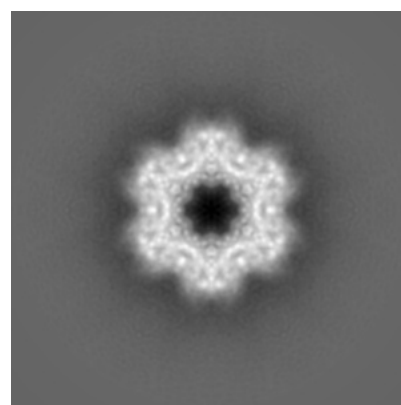
6.1.1 Primary map



X



Y

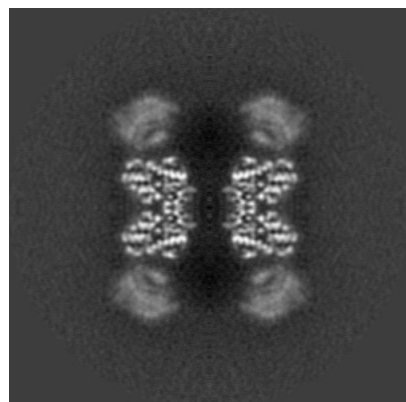


Z

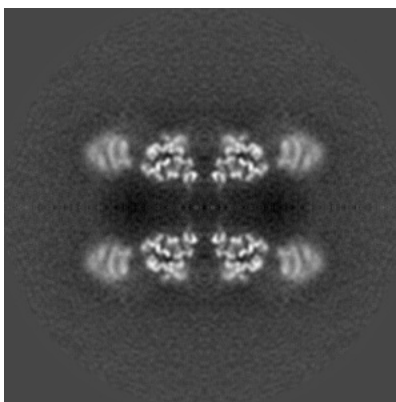
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

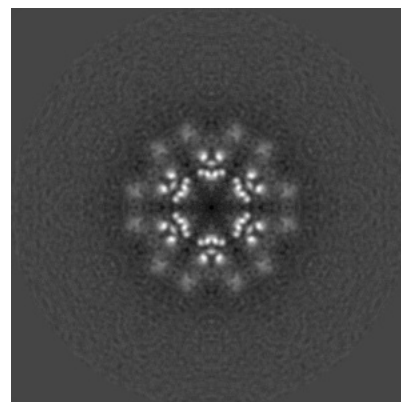
6.2.1 Primary map



X Index: 200



Y Index: 200

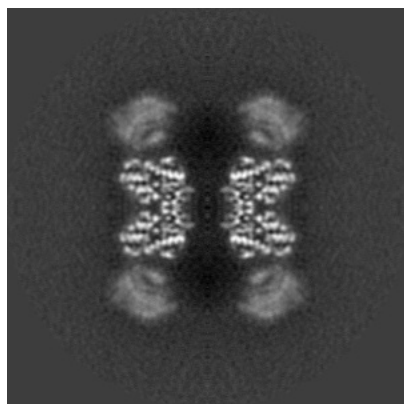


Z Index: 200

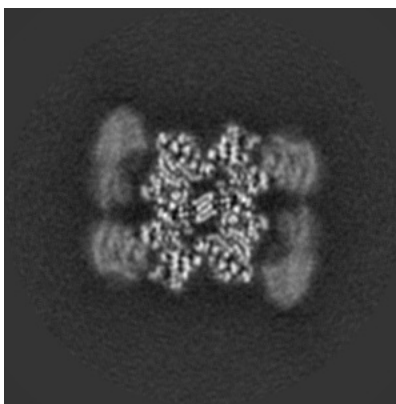
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

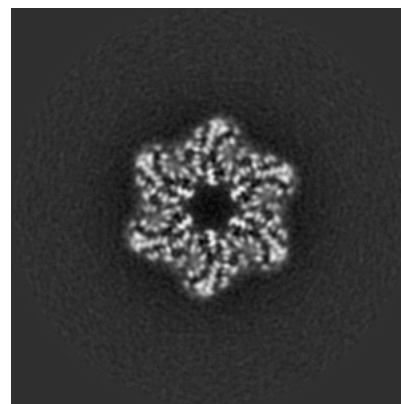
6.3.1 Primary map



X Index: 200



Y Index: 166

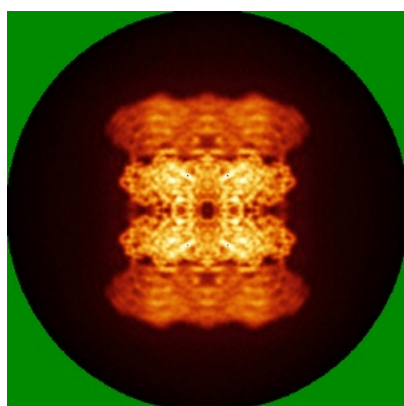


Z Index: 169

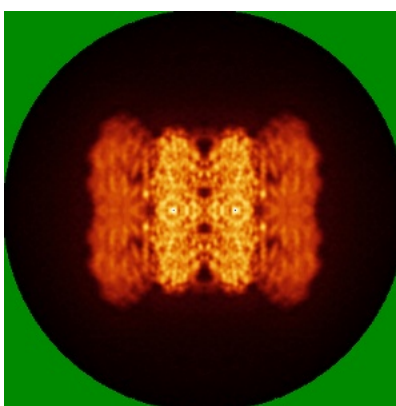
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

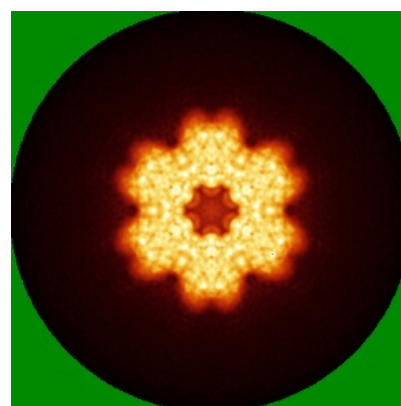
6.4.1 Primary map



X



Y

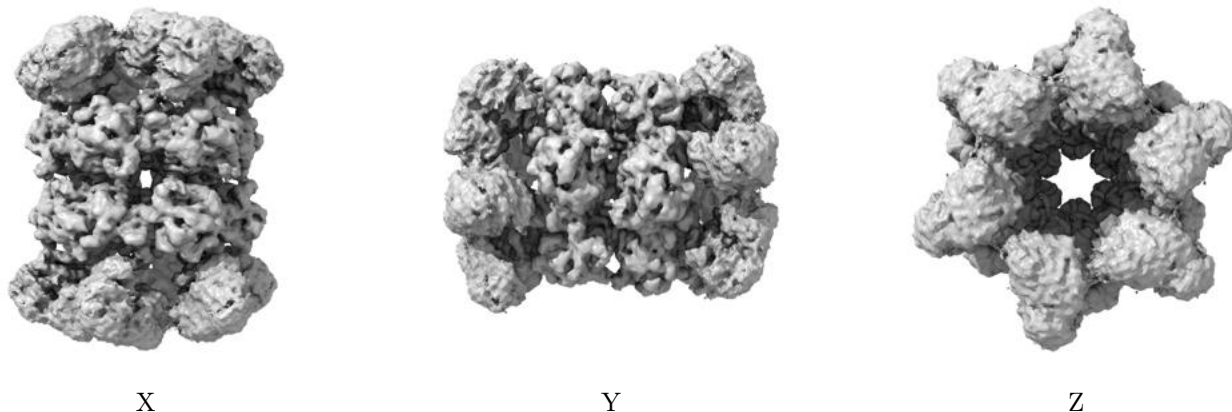


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

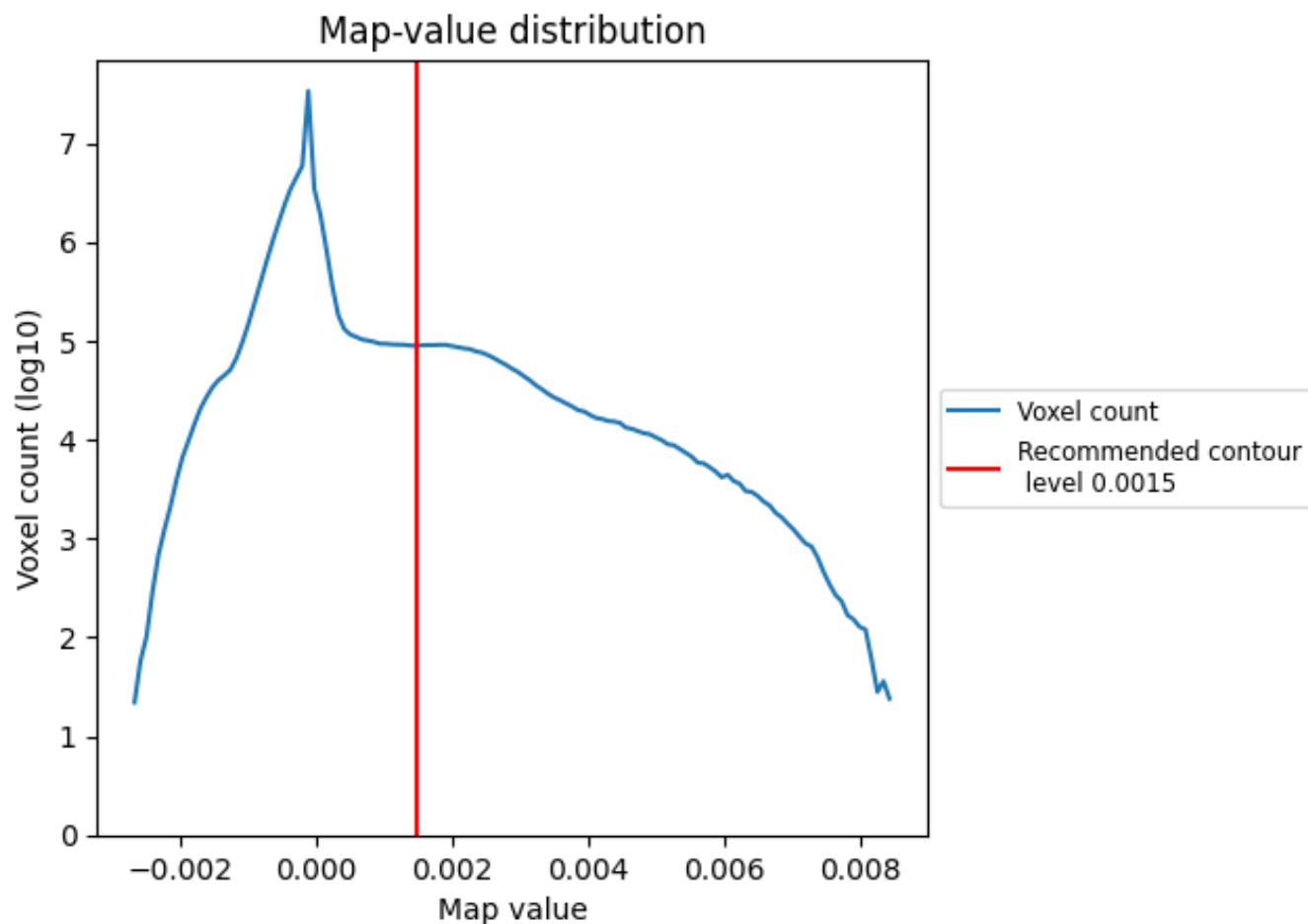
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

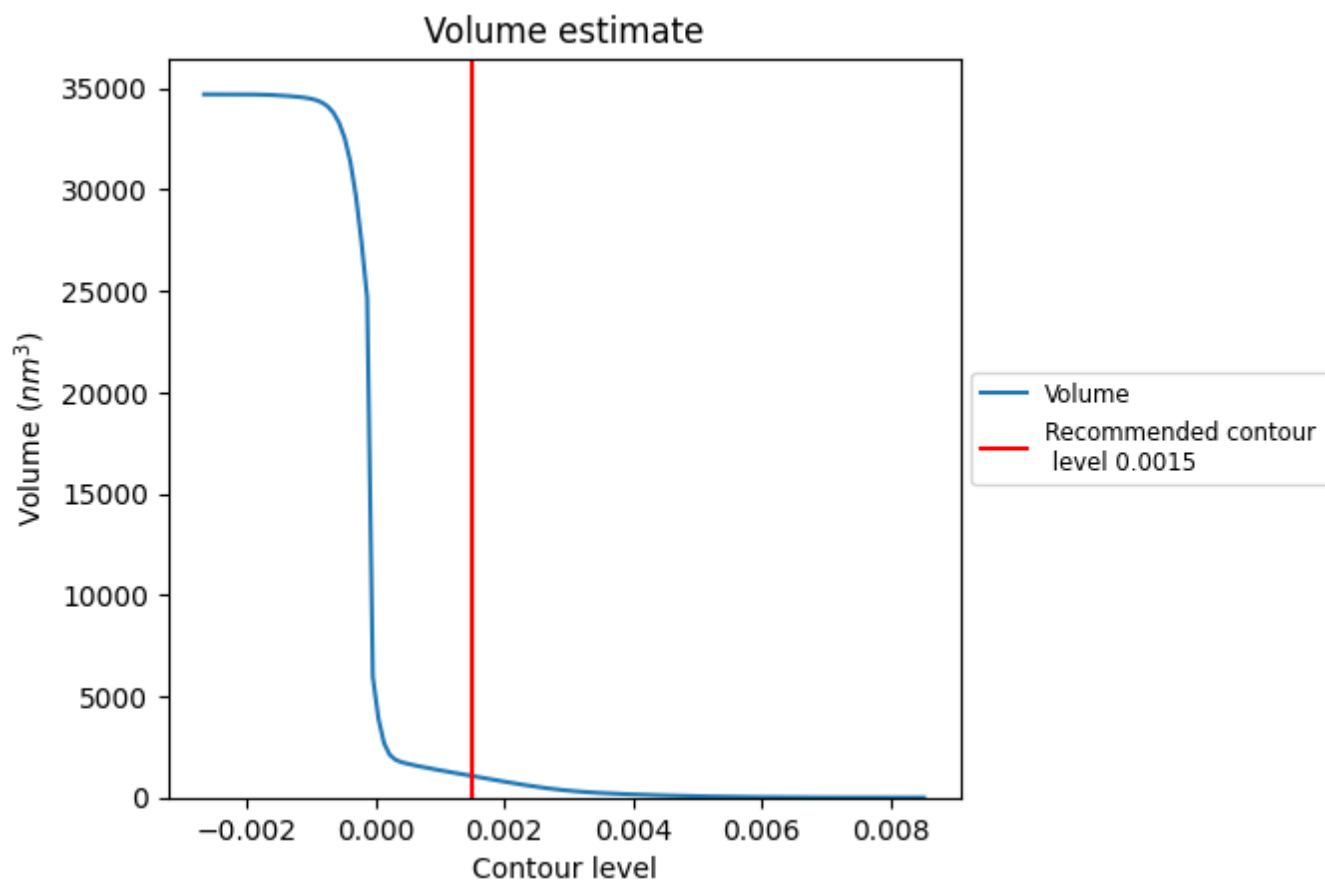
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

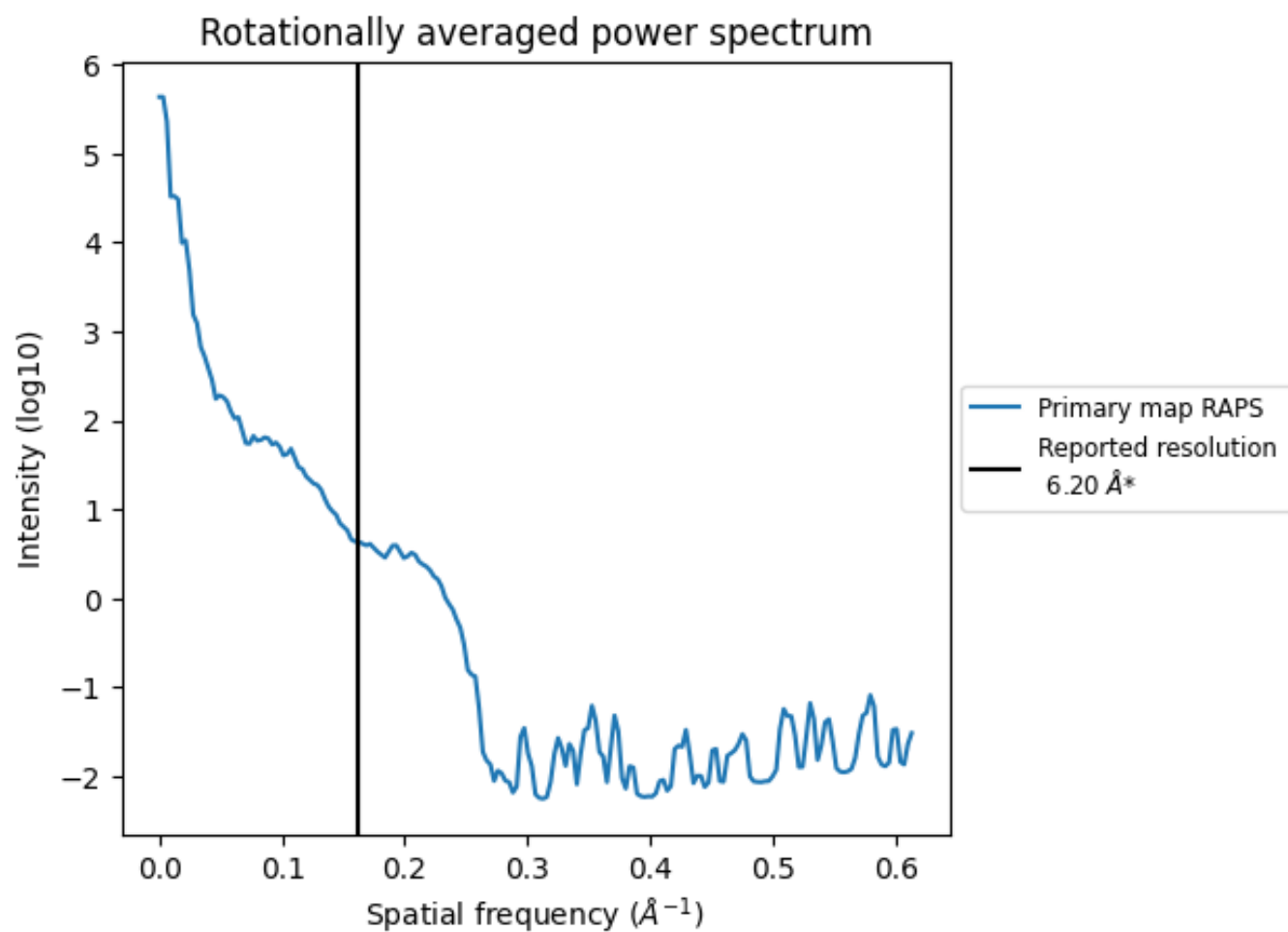
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1067 nm^3 ; this corresponds to an approximate mass of 964 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.161 Å⁻¹

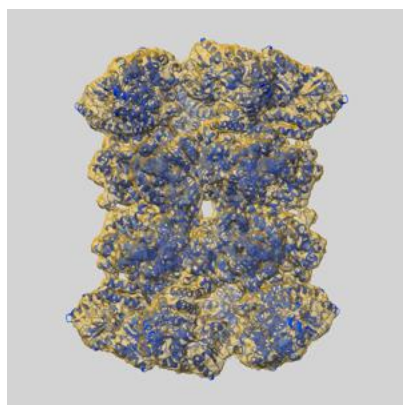
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

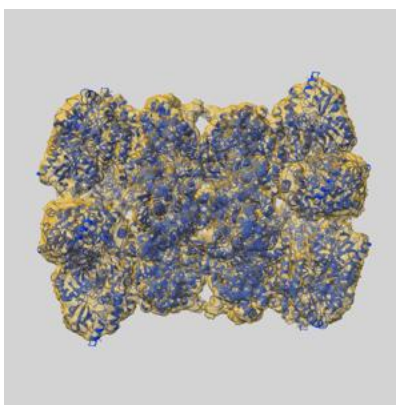
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4039 and PDB model 5LDF. Per-residue inclusion information can be found in section 3 on page 8.

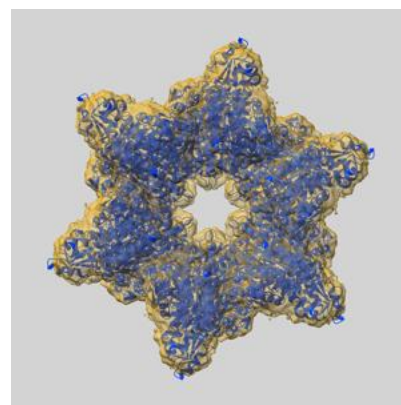
9.1 Map-model overlay [i](#)



X



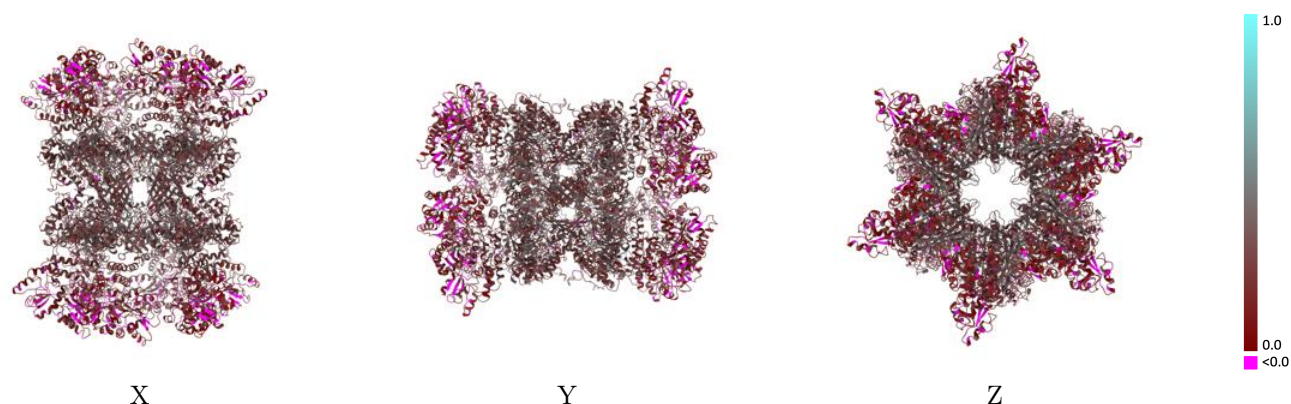
Y



Z

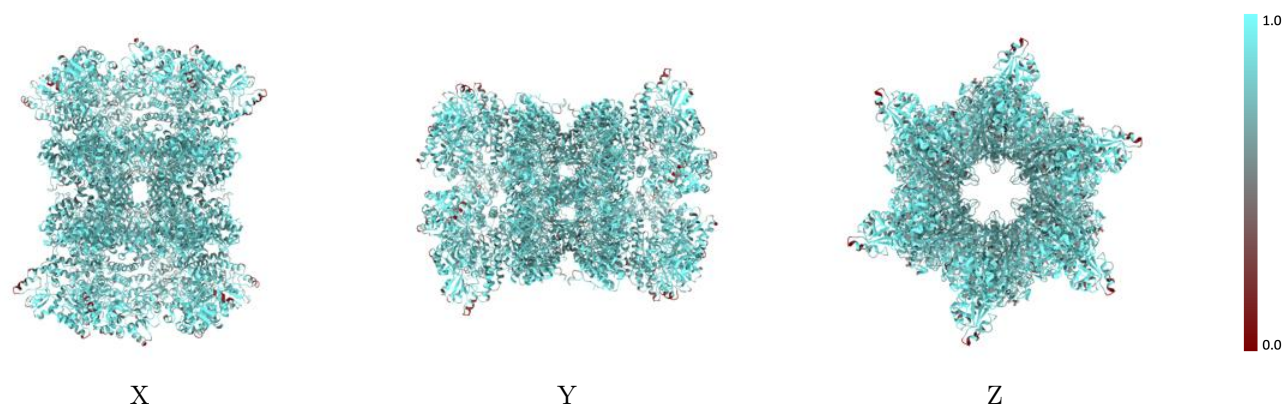
The images above show the 3D surface view of the map at the recommended contour level 0.0015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



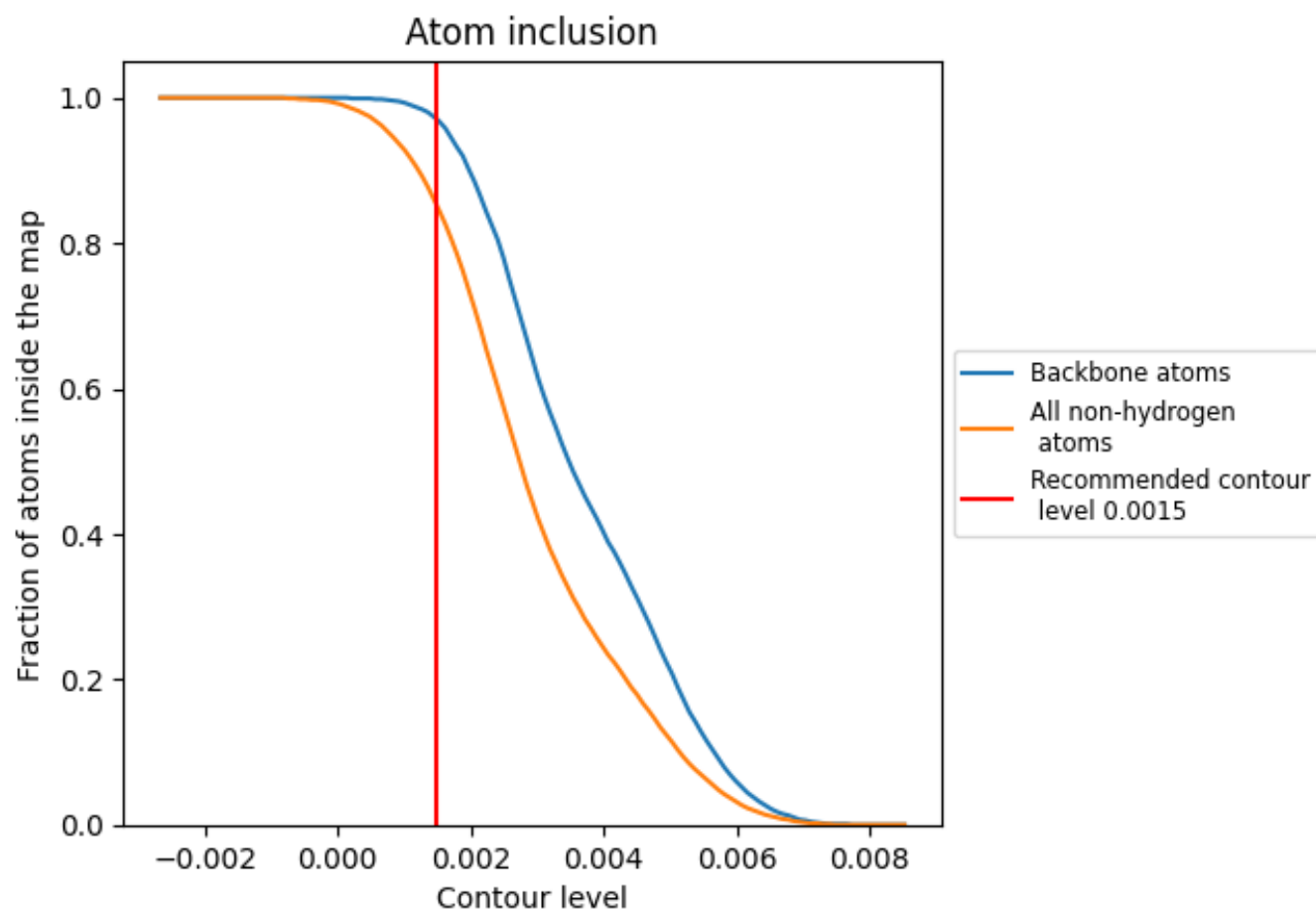
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8510	 0.2390
A	 0.8570	 0.3150
B	 0.8560	 0.3110
C	 0.8530	 0.3040
D	 0.8560	 0.3080
E	 0.8550	 0.3110
F	 0.8540	 0.3050
G	 0.8580	 0.3150
H	 0.8530	 0.3080
I	 0.8570	 0.3140
J	 0.8560	 0.3150
K	 0.8560	 0.3130
L	 0.8530	 0.3070
M	 0.8440	 0.1500
N	 0.8440	 0.1500
O	 0.8460	 0.1440
P	 0.8440	 0.1430
Q	 0.8450	 0.1450
R	 0.8460	 0.1460
S	 0.8450	 0.1480
T	 0.8450	 0.1470
U	 0.8440	 0.1490
V	 0.8460	 0.1510
W	 0.8460	 0.1500
X	 0.8440	 0.1500
Y	 0.8700	 0.2270
Z	 0.8700	 0.2200
a	 0.8260	 0.1720
b	 0.8260	 0.1850
c	 0.8700	 0.2020
d	 0.8260	 0.1720
e	 0.8700	 0.2320
f	 0.8700	 0.2180
g	 0.8700	 0.2260
h	 0.9130	 0.2260



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Chain	Atom inclusion	Q-score
i	 0.8700	 0.2350
j	 0.8700	 0.2230