



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:00 PM BST

PDB ID : 3J9I
EMDB ID: : EMD-5623
Title : Thermoplasma acidophilum 20S proteasome
Authors : Li, X.; Mooney, P.; Zheng, S.; Booth, C.; Braunfeld, M.B.; Gubbens, S.;
Agard, D.A.; Cheng, Y.
Deposited on : 2015-02-02
Resolution : 3.30 Å(reported)
Based on PDB ID : 1PMA

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

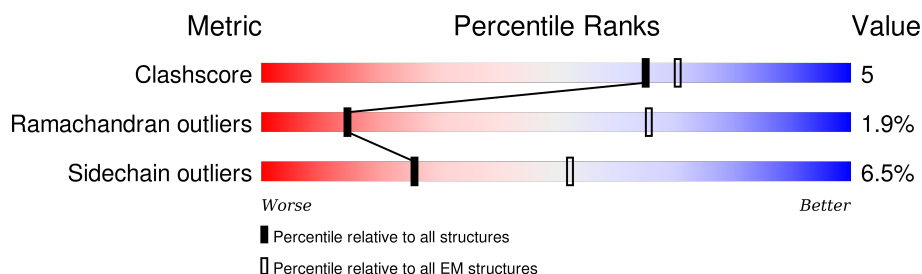
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.













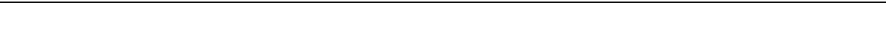

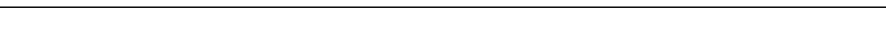
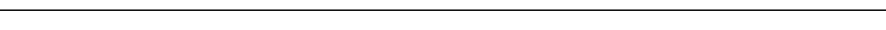





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	224	74% 21% .
1	B	224	74% 21% .
1	C	224	74% 21% .
1	D	224	74% 21% .
1	E	224	74% 21% .
1	F	224	74% 21% .
1	G	224	74% 21% .
1	O	224	74% 21% .
1	P	224	74% 21% .

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Mol	Chain	Length	Quality of chain
1	Q	224	
1	R	224	
1	S	224	
1	T	224	
1	U	224	
2	1	203	
2	2	203	
2	H	203	
2	I	203	
2	J	203	
2	K	203	
2	L	203	
2	M	203	
2	N	203	
2	V	203	
2	W	203	
2	X	203	
2	Y	203	
2	Z	203	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 46228 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 Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	F	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	T	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	G	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	U	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	A	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	O	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	B	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	P	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	C	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	Q	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	D	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	R	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		
1	E	224	Total	C	N	O	S	0	0
			1744	1107	296	338	3		

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		

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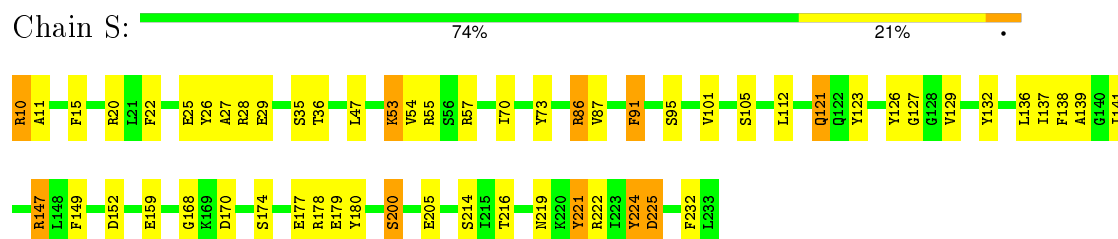
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	1	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	N	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	2	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	H	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	V	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	I	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	W	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	J	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	X	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	K	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	Y	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	L	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		

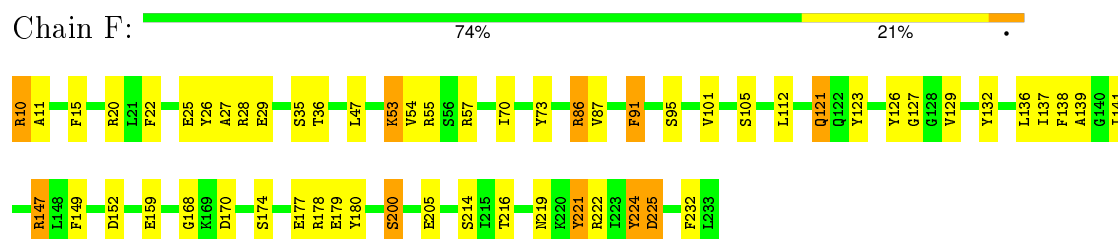
3 Residue-property plots

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

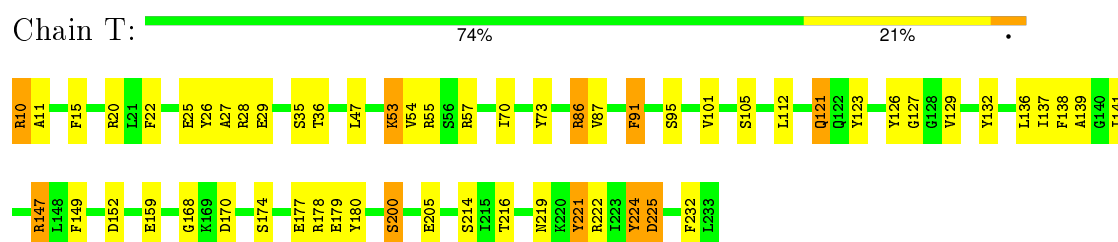
- Molecule 1: Proteasome subunit alpha



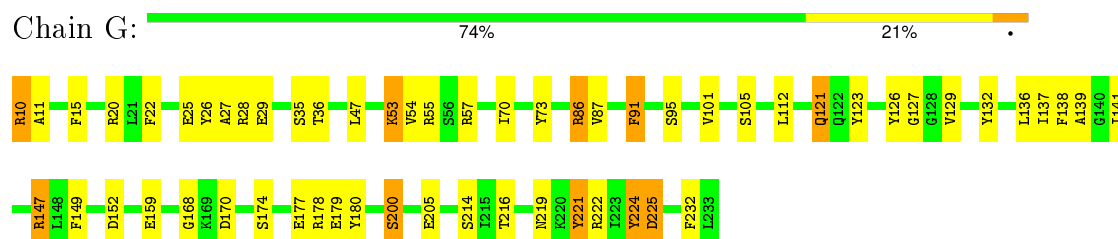
- Molecule 1: Proteasome subunit alpha



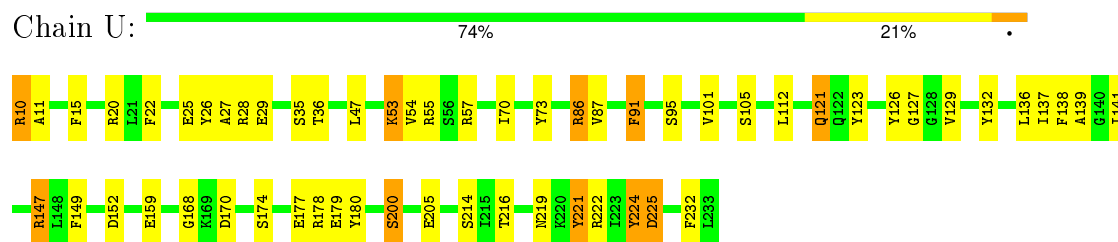
- Molecule 1: Proteasome subunit alpha



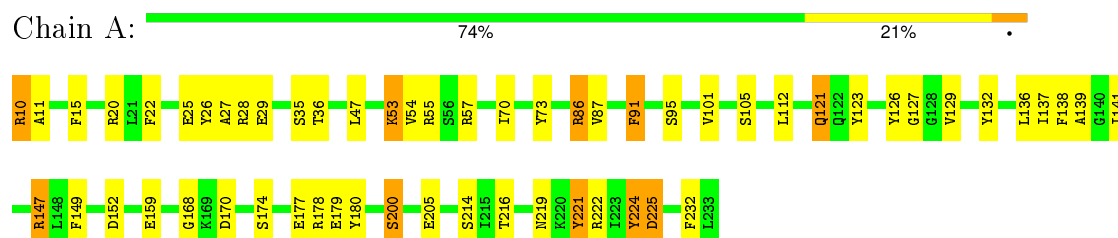
- Molecule 1: Proteasome subunit alpha



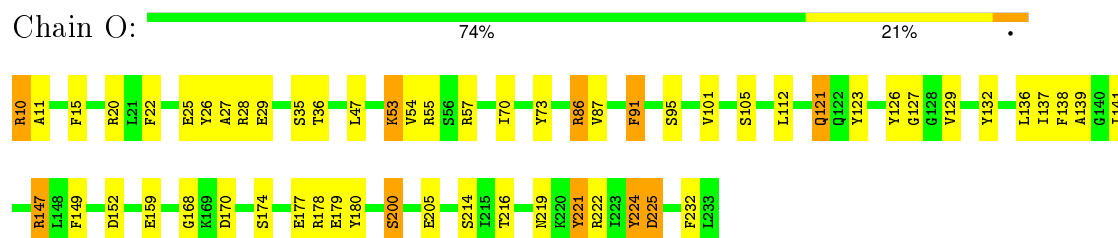
- Molecule 1: Proteasome subunit alpha



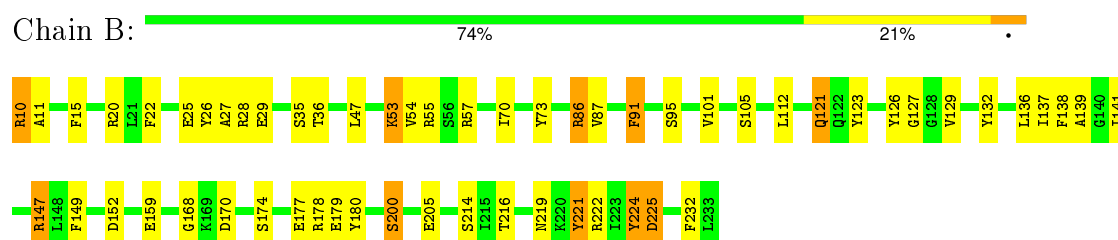
- Molecule 1: Proteasome subunit alpha



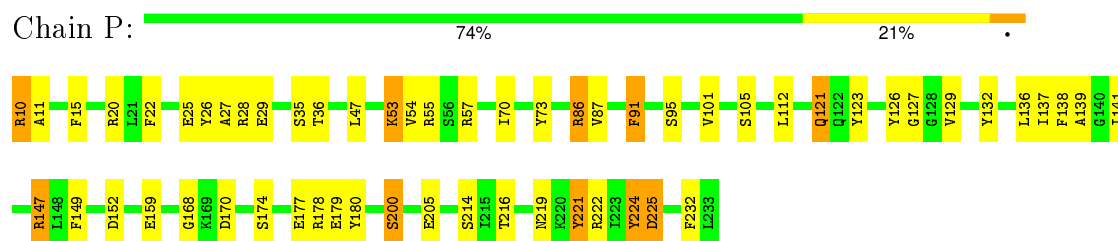
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

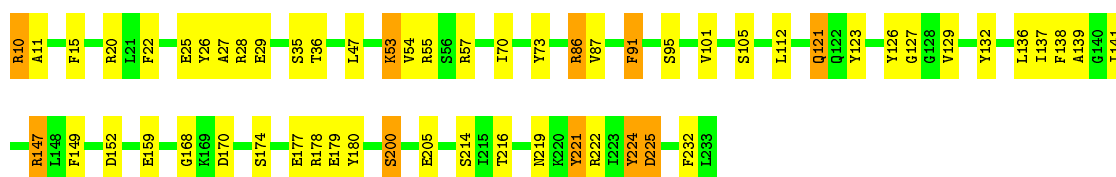


- Molecule 1: Proteasome subunit alpha

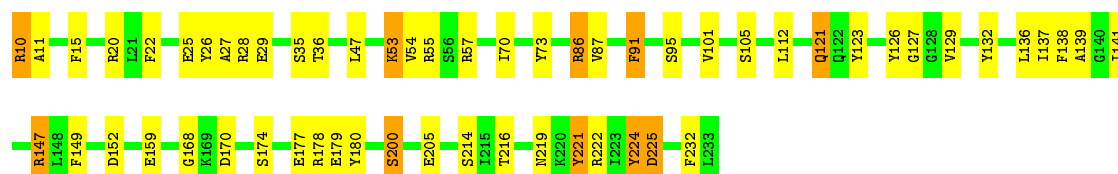


- Molecule 1: Proteasome subunit alpha

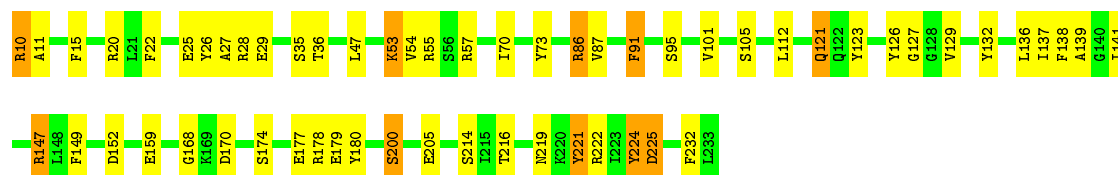




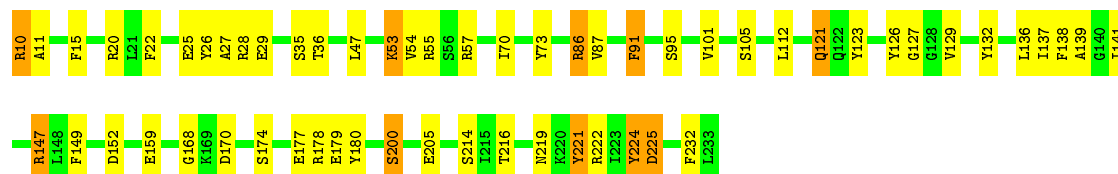
- Molecule 1: Proteasome subunit alpha



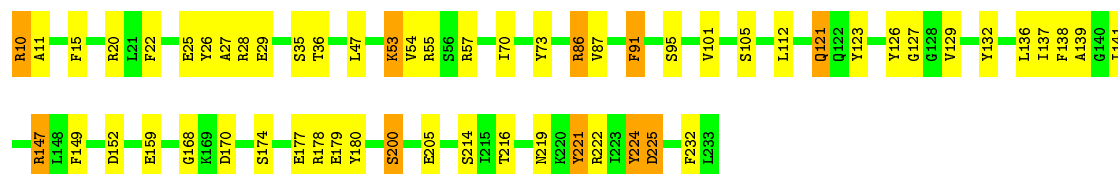
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

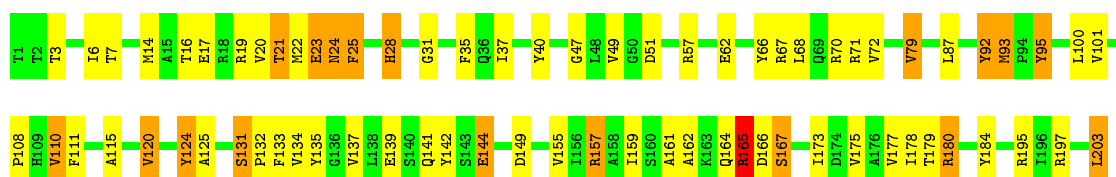


- Molecule 1: Proteasome subunit alpha



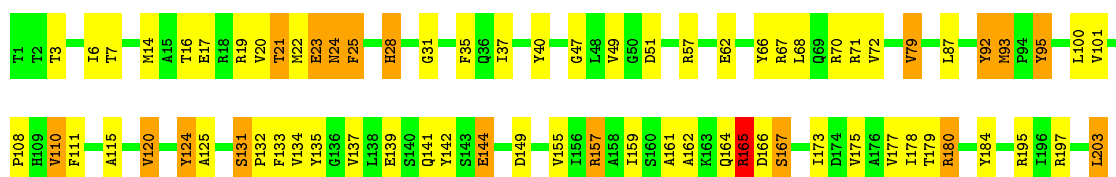
- Molecule 2: Proteasome subunit beta





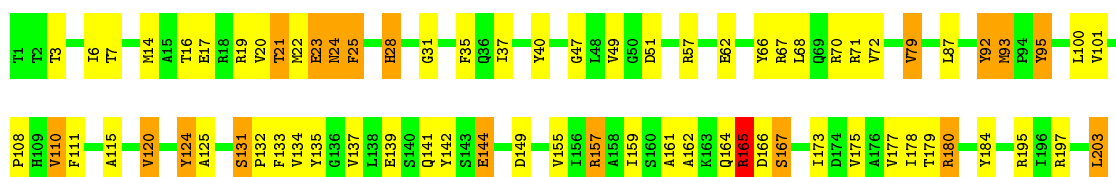
• Molecule 2: Proteasome subunit beta

Chain M:



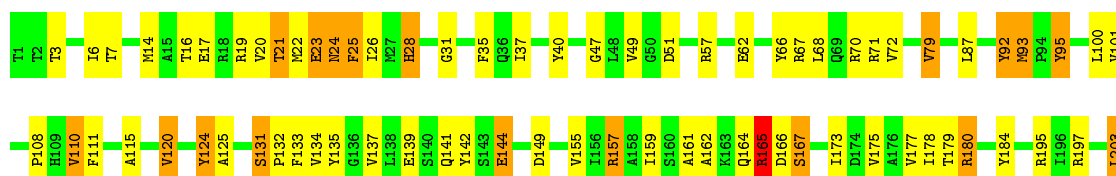
• Molecule 2: Proteasome subunit beta

Chain 1:



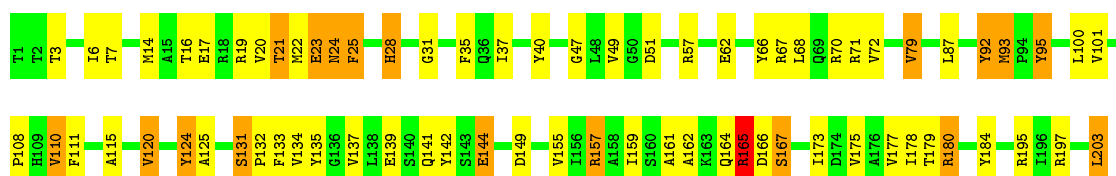
• Molecule 2: Proteasome subunit beta

Chain N:



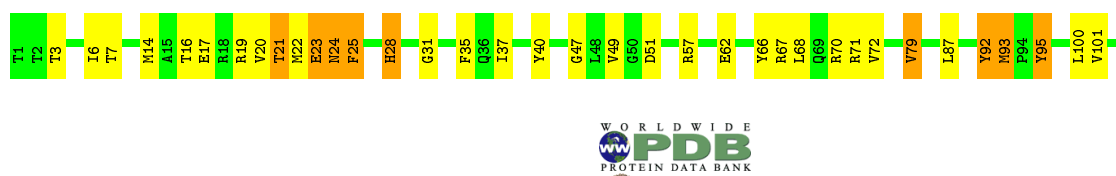
• Molecule 2: Proteasome subunit beta

Chain 2:



• Molecule 2: Proteasome subunit beta

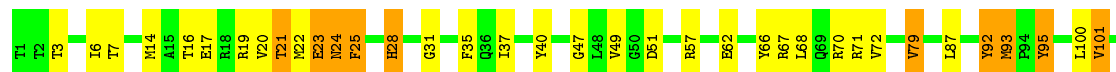
Chain H:





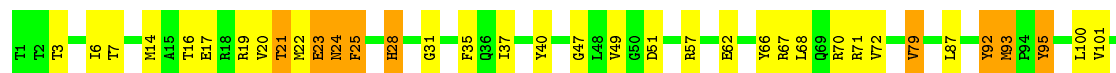
• Molecule 2: Proteasome subunit beta

Chain V: 64% 27% 9%



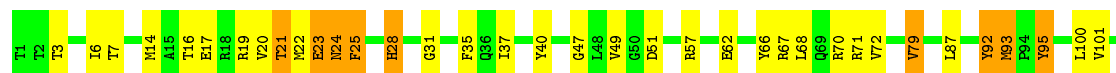
• Molecule 2: Proteasome subunit beta

Chain I: 64% 27% 9%



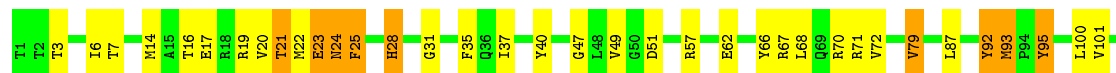
• Molecule 2: Proteasome subunit beta

Chain W: 64% 27% 9%



• Molecule 2: Proteasome subunit beta

Chain J: 64% 27% 9%



• Molecule 2: Proteasome subunit beta

Chain X: 64% 27% 9%





• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	126729	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each Particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 >2	RMSZ	# Z >2
1	A	1.73	19/1767 (1.1%)	2.01	45/2380 (1.9%)
1	B	1.73	19/1767 (1.1%)	2.01	44/2380 (1.8%)
1	C	1.73	17/1767 (1.0%)	2.01	45/2380 (1.9%)
1	D	1.73	19/1767 (1.1%)	2.01	45/2380 (1.9%)
1	E	1.73	19/1767 (1.1%)	2.01	44/2380 (1.8%)
1	F	1.73	18/1767 (1.0%)	2.01	45/2380 (1.9%)
1	G	1.73	19/1767 (1.1%)	2.01	44/2380 (1.8%)
1	O	1.73	17/1767 (1.0%)	2.01	44/2380 (1.8%)
1	P	1.73	19/1767 (1.1%)	2.01	45/2380 (1.9%)
1	Q	1.73	19/1767 (1.1%)	2.01	44/2380 (1.8%)
1	R	1.73	19/1767 (1.1%)	2.01	45/2380 (1.9%)
1	S	1.73	19/1767 (1.1%)	2.01	44/2380 (1.8%)
1	T	1.73	18/1767 (1.0%)	2.01	45/2380 (1.9%)
1	U	1.73	17/1767 (1.0%)	2.01	45/2380 (1.9%)
2	1	1.66	12/1577 (0.8%)	2.08	53/2129 (2.5%)
2	2	1.66	12/1577 (0.8%)	2.08	53/2129 (2.5%)
2	H	1.66	12/1577 (0.8%)	2.08	53/2129 (2.5%)
2	I	1.66	12/1577 (0.8%)	2.08	53/2129 (2.5%)
2	J	1.66	12/1577 (0.8%)	2.08	53/2129 (2.5%)
2	K	1.66	12/1577 (0.8%)	2.08	53/2129 (2.5%)
2	L	1.66	12/1577 (0.8%)	2.08	53/2129 (2.5%)
2	M	1.66	12/1577 (0.8%)	2.08	53/2129 (2.5%)
2	N	1.66	12/1577 (0.8%)	2.08	53/2129 (2.5%)
2	V	1.66	12/1577 (0.8%)	2.08	53/2129 (2.5%)
2	W	1.66	12/1577 (0.8%)	2.08	53/2129 (2.5%)
2	X	1.66	12/1577 (0.8%)	2.08	53/2129 (2.5%)
2	Y	1.66	12/1577 (0.8%)	2.08	53/2129 (2.5%)
2	Z	1.66	12/1577 (0.8%)	2.08	53/2129 (2.5%)
All	All	1.70	426/46816 (0.9%)	2.04	1366/63126 (2.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	4
1	G	0	4
1	O	0	4
1	P	0	4
1	Q	0	4
1	R	0	4
1	S	0	4
1	T	0	4
1	U	0	4
2	1	0	8
2	2	0	8
2	H	0	8
2	I	0	8
2	J	0	8
2	K	0	8
2	L	0	8
2	M	0	8
2	N	0	8
2	V	0	8
2	W	0	8
2	X	0	8
2	Y	0	8
2	Z	0	8
All	All	0	168

All (426) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	92	TYR	CG-CD1	8.79	1.50	1.39
2	Z	92	TYR	CG-CD1	8.78	1.50	1.39
2	M	92	TYR	CG-CD1	8.78	1.50	1.39
2	1	92	TYR	CG-CD1	8.78	1.50	1.39
2	I	92	TYR	CG-CD1	8.78	1.50	1.39
2	N	92	TYR	CG-CD1	8.78	1.50	1.39
2	H	92	TYR	CG-CD1	8.78	1.50	1.39
2	X	92	TYR	CG-CD1	8.78	1.50	1.39
2	Y	92	TYR	CG-CD1	8.78	1.50	1.39
2	W	92	TYR	CG-CD1	8.78	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	92	TYR	CG-CD1	8.78	1.50	1.39
2	J	92	TYR	CG-CD1	8.78	1.50	1.39
2	L	92	TYR	CG-CD1	8.78	1.50	1.39
2	K	92	TYR	CG-CD1	8.78	1.50	1.39
1	F	28	ARG	CD-NE	7.89	1.59	1.46
1	P	28	ARG	CD-NE	7.89	1.59	1.46
1	Q	28	ARG	CD-NE	7.89	1.59	1.46
1	U	28	ARG	CD-NE	7.88	1.59	1.46
1	D	28	ARG	CD-NE	7.88	1.59	1.46
1	A	28	ARG	CD-NE	7.88	1.59	1.46
1	R	28	ARG	CD-NE	7.88	1.59	1.46
1	S	28	ARG	CD-NE	7.88	1.59	1.46
1	B	28	ARG	CD-NE	7.88	1.59	1.46
1	T	28	ARG	CD-NE	7.87	1.59	1.46
1	C	28	ARG	CD-NE	7.87	1.59	1.46
1	G	28	ARG	CD-NE	7.86	1.59	1.46
1	O	28	ARG	CD-NE	7.86	1.59	1.46
1	E	28	ARG	CD-NE	7.86	1.59	1.46
1	F	10	ARG	NE-CZ	7.16	1.42	1.33
1	P	10	ARG	NE-CZ	7.16	1.42	1.33
1	O	10	ARG	NE-CZ	7.12	1.42	1.33
1	E	10	ARG	NE-CZ	7.12	1.42	1.33
1	U	10	ARG	NE-CZ	7.12	1.42	1.33
1	Q	10	ARG	NE-CZ	7.12	1.42	1.33
1	D	10	ARG	NE-CZ	7.12	1.42	1.33
1	T	10	ARG	NE-CZ	7.11	1.42	1.33
1	C	10	ARG	NE-CZ	7.11	1.42	1.33
1	A	10	ARG	NE-CZ	7.11	1.42	1.33
1	R	10	ARG	NE-CZ	7.11	1.42	1.33
1	S	10	ARG	NE-CZ	7.09	1.42	1.33
1	B	10	ARG	NE-CZ	7.09	1.42	1.33
1	G	10	ARG	NE-CZ	7.05	1.42	1.33
2	H	47	GLY	CA-C	-6.93	1.40	1.51
2	L	47	GLY	CA-C	-6.92	1.40	1.51
2	K	47	GLY	CA-C	-6.92	1.40	1.51
2	N	47	GLY	CA-C	-6.90	1.40	1.51
2	Z	47	GLY	CA-C	-6.89	1.40	1.51
2	I	47	GLY	CA-C	-6.89	1.40	1.51
2	V	47	GLY	CA-C	-6.89	1.40	1.51
2	Y	47	GLY	CA-C	-6.88	1.40	1.51
2	2	47	GLY	CA-C	-6.85	1.40	1.51
2	M	47	GLY	CA-C	-6.85	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	47	GLY	CA-C	-6.85	1.40	1.51
2	1	47	GLY	CA-C	-6.84	1.41	1.51
2	J	47	GLY	CA-C	-6.84	1.41	1.51
2	X	47	GLY	CA-C	-6.84	1.41	1.51
2	Y	180	ARG	CD-NE	6.83	1.58	1.46
2	L	180	ARG	CD-NE	6.82	1.58	1.46
2	2	180	ARG	CD-NE	6.81	1.58	1.46
2	K	180	ARG	CD-NE	6.81	1.58	1.46
2	Z	180	ARG	CD-NE	6.81	1.58	1.46
2	H	180	ARG	CD-NE	6.81	1.58	1.46
2	I	180	ARG	CD-NE	6.81	1.58	1.46
2	M	180	ARG	CD-NE	6.81	1.58	1.46
2	W	180	ARG	CD-NE	6.81	1.58	1.46
2	1	180	ARG	CD-NE	6.80	1.58	1.46
2	N	180	ARG	CD-NE	6.80	1.58	1.46
2	X	180	ARG	CD-NE	6.80	1.58	1.46
2	V	180	ARG	CD-NE	6.79	1.57	1.46
2	J	180	ARG	CD-NE	6.79	1.57	1.46
2	2	144	GLU	CG-CD	6.78	1.62	1.51
2	X	144	GLU	CG-CD	6.78	1.62	1.51
2	M	144	GLU	CG-CD	6.78	1.62	1.51
2	H	144	GLU	CG-CD	6.78	1.62	1.51
2	Y	144	GLU	CG-CD	6.78	1.62	1.51
2	J	144	GLU	CG-CD	6.77	1.62	1.51
2	Z	144	GLU	CG-CD	6.77	1.62	1.51
2	I	144	GLU	CG-CD	6.77	1.62	1.51
2	W	144	GLU	CG-CD	6.77	1.62	1.51
2	V	144	GLU	CG-CD	6.77	1.62	1.51
2	L	144	GLU	CG-CD	6.77	1.62	1.51
2	K	144	GLU	CG-CD	6.76	1.62	1.51
2	N	144	GLU	CG-CD	6.76	1.62	1.51
2	1	144	GLU	CG-CD	6.75	1.62	1.51
2	J	167	SER	CA-CB	6.55	1.62	1.52
2	M	167	SER	CA-CB	6.55	1.62	1.52
2	N	167	SER	CA-CB	6.55	1.62	1.52
2	H	167	SER	CA-CB	6.55	1.62	1.52
2	Z	167	SER	CA-CB	6.53	1.62	1.52
2	2	167	SER	CA-CB	6.53	1.62	1.52
2	I	167	SER	CA-CB	6.53	1.62	1.52
2	K	167	SER	CA-CB	6.53	1.62	1.52
2	Y	167	SER	CA-CB	6.53	1.62	1.52
2	W	167	SER	CA-CB	6.51	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	167	SER	CA-CB	6.50	1.62	1.52
2	X	167	SER	CA-CB	6.50	1.62	1.52
2	V	167	SER	CA-CB	6.50	1.62	1.52
2	L	167	SER	CA-CB	6.50	1.62	1.52
1	P	25	GLU	CD-OE2	6.26	1.32	1.25
1	D	179	GLU	CD-OE2	6.25	1.32	1.25
1	C	179	GLU	CD-OE2	6.25	1.32	1.25
1	O	25	GLU	CD-OE2	6.24	1.32	1.25
1	G	179	GLU	CD-OE2	6.24	1.32	1.25
1	R	25	GLU	CD-OE2	6.22	1.32	1.25
1	S	25	GLU	CD-OE2	6.22	1.32	1.25
1	B	25	GLU	CD-OE2	6.22	1.32	1.25
1	T	179	GLU	CD-OE2	6.22	1.32	1.25
1	U	25	GLU	CD-OE2	6.22	1.32	1.25
1	D	25	GLU	CD-OE2	6.22	1.32	1.25
1	T	25	GLU	CD-OE2	6.22	1.32	1.25
1	C	25	GLU	CD-OE2	6.22	1.32	1.25
1	A	25	GLU	CD-OE2	6.20	1.32	1.25
1	G	25	GLU	CD-OE2	6.20	1.32	1.25
1	Q	25	GLU	CD-OE2	6.20	1.32	1.25
1	F	25	GLU	CD-OE2	6.19	1.32	1.25
1	E	25	GLU	CD-OE2	6.19	1.32	1.25
1	O	179	GLU	CD-OE2	6.17	1.32	1.25
1	E	179	GLU	CD-OE2	6.17	1.32	1.25
1	S	179	GLU	CD-OE2	6.17	1.32	1.25
1	B	179	GLU	CD-OE2	6.17	1.32	1.25
1	Q	179	GLU	CD-OE2	6.17	1.32	1.25
1	U	179	GLU	CD-OE2	6.17	1.32	1.25
1	A	179	GLU	CD-OE2	6.17	1.32	1.25
1	R	179	GLU	CD-OE2	6.17	1.32	1.25
1	F	179	GLU	CD-OE2	6.16	1.32	1.25
1	P	179	GLU	CD-OE2	6.16	1.32	1.25
1	T	232	PHE	CG-CD1	6.08	1.47	1.38
1	U	232	PHE	CG-CD1	6.07	1.47	1.38
1	C	232	PHE	CG-CD1	6.07	1.47	1.38
1	S	232	PHE	CG-CD1	6.04	1.47	1.38
1	A	232	PHE	CG-CD1	6.04	1.47	1.38
1	B	232	PHE	CG-CD1	6.04	1.47	1.38
1	R	232	PHE	CG-CD1	6.04	1.47	1.38
1	O	232	PHE	CG-CD1	6.03	1.47	1.38
1	P	232	PHE	CG-CD1	6.03	1.47	1.38
1	D	232	PHE	CG-CD1	6.03	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	232	PHE	CG-CD1	6.03	1.47	1.38
1	C	127	GLY	CA-C	-6.02	1.42	1.51
1	T	127	GLY	CA-C	-6.01	1.42	1.51
1	Q	232	PHE	CG-CD1	6.01	1.47	1.38
1	D	127	GLY	CA-C	-6.00	1.42	1.51
1	R	73	TYR	CE2-CZ	-6.00	1.30	1.38
1	A	127	GLY	CA-C	-6.00	1.42	1.51
1	O	127	GLY	CA-C	-6.00	1.42	1.51
1	R	127	GLY	CA-C	-6.00	1.42	1.51
1	E	127	GLY	CA-C	-6.00	1.42	1.51
1	F	232	PHE	CG-CD1	5.99	1.47	1.38
1	G	232	PHE	CG-CD1	5.99	1.47	1.38
1	A	73	TYR	CE2-CZ	-5.99	1.30	1.38
1	S	127	GLY	CA-C	-5.99	1.42	1.51
1	F	127	GLY	CA-C	-5.99	1.42	1.51
1	B	127	GLY	CA-C	-5.99	1.42	1.51
1	P	127	GLY	CA-C	-5.99	1.42	1.51
1	G	127	GLY	CA-C	-5.98	1.42	1.51
1	Q	127	GLY	CA-C	-5.98	1.42	1.51
1	Q	73	TYR	CE2-CZ	-5.97	1.30	1.38
1	T	73	TYR	CE2-CZ	-5.96	1.30	1.38
1	C	73	TYR	CE2-CZ	-5.96	1.30	1.38
1	U	127	GLY	CA-C	-5.96	1.42	1.51
1	S	73	TYR	CE2-CZ	-5.95	1.30	1.38
1	B	73	TYR	CE2-CZ	-5.95	1.30	1.38
1	F	73	TYR	CE2-CZ	-5.93	1.30	1.38
1	O	73	TYR	CE2-CZ	-5.93	1.30	1.38
1	P	73	TYR	CE2-CZ	-5.93	1.30	1.38
1	E	73	TYR	CE2-CZ	-5.93	1.30	1.38
1	G	73	TYR	CE2-CZ	-5.92	1.30	1.38
1	U	73	TYR	CE2-CZ	-5.91	1.30	1.38
1	D	73	TYR	CE2-CZ	-5.91	1.30	1.38
2	2	111	PHE	CA-C	-5.77	1.38	1.52
2	M	111	PHE	CA-C	-5.76	1.38	1.52
2	L	111	PHE	CA-C	-5.75	1.38	1.52
2	N	111	PHE	CA-C	-5.75	1.38	1.52
2	W	111	PHE	CA-C	-5.75	1.38	1.52
2	X	111	PHE	CA-C	-5.75	1.38	1.52
2	Z	111	PHE	CA-C	-5.75	1.38	1.52
2	I	111	PHE	CA-C	-5.75	1.38	1.52
1	C	28	ARG	NE-CZ	5.75	1.40	1.33
2	H	111	PHE	CA-C	-5.74	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	111	PHE	CA-C	-5.74	1.38	1.52
2	V	111	PHE	CA-C	-5.74	1.38	1.52
2	1	111	PHE	CA-C	-5.74	1.38	1.52
2	J	111	PHE	CA-C	-5.74	1.38	1.52
2	K	111	PHE	CA-C	-5.74	1.38	1.52
1	O	26	TYR	CG-CD2	5.73	1.46	1.39
1	E	26	TYR	CG-CD2	5.73	1.46	1.39
1	F	26	TYR	CG-CD2	5.72	1.46	1.39
1	P	26	TYR	CG-CD2	5.72	1.46	1.39
1	Q	26	TYR	CG-CD2	5.72	1.46	1.39
1	S	26	TYR	CG-CD2	5.71	1.46	1.39
1	B	26	TYR	CG-CD2	5.71	1.46	1.39
1	O	28	ARG	NE-CZ	5.71	1.40	1.33
1	E	28	ARG	NE-CZ	5.71	1.40	1.33
1	T	26	TYR	CG-CD2	5.71	1.46	1.39
1	C	26	TYR	CG-CD2	5.71	1.46	1.39
1	U	28	ARG	NE-CZ	5.70	1.40	1.33
1	G	26	TYR	CG-CD2	5.69	1.46	1.39
1	R	26	TYR	CG-CD2	5.69	1.46	1.39
1	D	26	TYR	CG-CD2	5.69	1.46	1.39
1	G	28	ARG	NE-CZ	5.68	1.40	1.33
1	Q	28	ARG	NE-CZ	5.68	1.40	1.33
1	U	26	TYR	CG-CD2	5.68	1.46	1.39
1	S	28	ARG	NE-CZ	5.67	1.40	1.33
1	B	28	ARG	NE-CZ	5.67	1.40	1.33
1	T	28	ARG	NE-CZ	5.67	1.40	1.33
1	Q	159	GLU	CG-CD	5.67	1.60	1.51
1	F	159	GLU	CG-CD	5.67	1.60	1.51
1	P	159	GLU	CG-CD	5.67	1.60	1.51
1	F	28	ARG	NE-CZ	5.65	1.40	1.33
1	F	95	SER	CB-OG	-5.65	1.34	1.42
1	P	28	ARG	NE-CZ	5.65	1.40	1.33
1	T	159	GLU	CG-CD	5.65	1.60	1.51
1	A	26	TYR	CG-CD2	5.65	1.46	1.39
1	C	159	GLU	CG-CD	5.65	1.60	1.51
1	U	159	GLU	CG-CD	5.65	1.60	1.51
1	A	159	GLU	CG-CD	5.65	1.60	1.51
1	D	28	ARG	NE-CZ	5.65	1.40	1.33
1	R	159	GLU	CG-CD	5.65	1.60	1.51
1	R	28	ARG	NE-CZ	5.64	1.40	1.33
1	S	159	GLU	CG-CD	5.64	1.60	1.51
1	B	159	GLU	CG-CD	5.64	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	159	GLU	CG-CD	5.64	1.60	1.51
1	G	159	GLU	CG-CD	5.63	1.60	1.51
2	V	165	ARG	CZ-NH1	5.63	1.40	1.33
2	J	165	ARG	CZ-NH1	5.63	1.40	1.33
1	Q	95	SER	CB-OG	-5.63	1.34	1.42
2	L	165	ARG	CZ-NH1	5.63	1.40	1.33
1	U	95	SER	CB-OG	-5.63	1.34	1.42
1	D	95	SER	CB-OG	-5.63	1.34	1.42
1	R	95	SER	CB-OG	-5.62	1.34	1.42
1	T	95	SER	CB-OG	-5.61	1.34	1.42
1	A	28	ARG	NE-CZ	5.61	1.40	1.33
2	H	165	ARG	CZ-NH1	5.61	1.40	1.33
1	C	95	SER	CB-OG	-5.61	1.34	1.42
1	S	95	SER	CB-OG	-5.61	1.34	1.42
1	O	159	GLU	CG-CD	5.61	1.60	1.51
1	B	95	SER	CB-OG	-5.61	1.34	1.42
1	D	159	GLU	CG-CD	5.61	1.60	1.51
2	Y	165	ARG	CZ-NH1	5.60	1.40	1.33
2	N	165	ARG	CZ-NH1	5.60	1.40	1.33
2	X	165	ARG	CZ-NH1	5.60	1.40	1.33
1	E	95	SER	CB-OG	-5.60	1.34	1.42
1	G	95	SER	CB-OG	-5.59	1.34	1.42
1	A	95	SER	CB-OG	-5.59	1.34	1.42
2	Z	165	ARG	CZ-NH1	5.58	1.40	1.33
2	I	165	ARG	CZ-NH1	5.58	1.40	1.33
2	M	165	ARG	CZ-NH1	5.58	1.40	1.33
1	P	95	SER	CB-OG	-5.58	1.34	1.42
2	W	165	ARG	CZ-NH1	5.58	1.40	1.33
2	2	165	ARG	CZ-NH1	5.58	1.40	1.33
2	K	165	ARG	CZ-NH1	5.58	1.40	1.33
2	1	165	ARG	CZ-NH1	5.56	1.40	1.33
1	O	95	SER	CB-OG	-5.55	1.35	1.42
1	F	180	TYR	CZ-OH	5.55	1.47	1.37
1	G	180	TYR	CZ-OH	5.55	1.47	1.37
1	R	180	TYR	CZ-OH	5.54	1.47	1.37
1	T	180	TYR	CZ-OH	5.54	1.47	1.37
1	A	180	TYR	CZ-OH	5.54	1.47	1.37
1	C	180	TYR	CZ-OH	5.54	1.47	1.37
1	S	180	TYR	CZ-OH	5.54	1.47	1.37
1	B	180	TYR	CZ-OH	5.54	1.47	1.37
1	U	180	TYR	CZ-OH	5.54	1.47	1.37
1	O	180	TYR	CZ-OH	5.54	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	180	TYR	CZ-OH	5.54	1.47	1.37
1	Q	180	TYR	CZ-OH	5.54	1.47	1.37
1	E	180	TYR	CZ-OH	5.54	1.47	1.37
1	D	180	TYR	CZ-OH	5.53	1.47	1.37
2	J	67	ARG	CZ-NH1	5.52	1.40	1.33
2	1	67	ARG	CZ-NH1	5.51	1.40	1.33
2	V	165	ARG	CZ-NH2	5.50	1.40	1.33
1	T	174	SER	CA-CB	5.50	1.61	1.52
2	2	67	ARG	CZ-NH1	5.50	1.40	1.33
2	2	165	ARG	CZ-NH2	5.50	1.40	1.33
2	K	165	ARG	CZ-NH2	5.50	1.40	1.33
1	A	174	SER	CA-CB	5.50	1.61	1.52
1	C	174	SER	CA-CB	5.50	1.61	1.52
1	R	174	SER	CA-CB	5.50	1.61	1.52
2	1	165	ARG	CZ-NH2	5.50	1.40	1.33
2	J	165	ARG	CZ-NH2	5.50	1.40	1.33
1	S	174	SER	CA-CB	5.49	1.61	1.52
2	Z	165	ARG	CZ-NH2	5.49	1.40	1.33
1	G	174	SER	CA-CB	5.49	1.61	1.52
1	B	174	SER	CA-CB	5.49	1.61	1.52
2	I	165	ARG	CZ-NH2	5.49	1.40	1.33
1	Q	174	SER	CA-CB	5.49	1.61	1.52
2	H	165	ARG	CZ-NH2	5.49	1.40	1.33
1	O	174	SER	CA-CB	5.49	1.61	1.52
1	E	174	SER	CA-CB	5.49	1.61	1.52
2	L	165	ARG	CZ-NH2	5.49	1.40	1.33
1	F	174	SER	CA-CB	5.49	1.61	1.52
1	U	174	SER	CA-CB	5.49	1.61	1.52
1	P	174	SER	CA-CB	5.49	1.61	1.52
1	D	174	SER	CA-CB	5.49	1.61	1.52
2	N	165	ARG	CZ-NH2	5.48	1.40	1.33
2	X	165	ARG	CZ-NH2	5.48	1.40	1.33
2	X	67	ARG	CZ-NH1	5.48	1.40	1.33
2	Y	165	ARG	CZ-NH2	5.48	1.40	1.33
2	M	165	ARG	CZ-NH2	5.47	1.40	1.33
2	W	165	ARG	CZ-NH2	5.47	1.40	1.33
2	Z	67	ARG	CZ-NH1	5.47	1.40	1.33
2	I	67	ARG	CZ-NH1	5.47	1.40	1.33
2	H	67	ARG	CZ-NH1	5.46	1.40	1.33
2	Y	67	ARG	CZ-NH1	5.46	1.40	1.33
2	M	133	PHE	CG-CD1	5.46	1.47	1.38
2	V	133	PHE	CG-CD1	5.46	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	133	PHE	CG-CD1	5.46	1.47	1.38
2	L	133	PHE	CG-CD1	5.46	1.47	1.38
2	2	133	PHE	CG-CD1	5.45	1.47	1.38
2	K	133	PHE	CG-CD1	5.45	1.47	1.38
2	N	133	PHE	CG-CD1	5.45	1.47	1.38
2	V	67	ARG	CZ-NH1	5.45	1.40	1.33
2	X	133	PHE	CG-CD1	5.45	1.47	1.38
2	L	67	ARG	CZ-NH1	5.45	1.40	1.33
2	1	133	PHE	CG-CD1	5.45	1.47	1.38
2	J	133	PHE	CG-CD1	5.45	1.47	1.38
2	K	67	ARG	CZ-NH1	5.45	1.40	1.33
2	Z	133	PHE	CG-CD1	5.45	1.47	1.38
2	M	67	ARG	CZ-NH1	5.45	1.40	1.33
2	I	133	PHE	CG-CD1	5.45	1.47	1.38
2	W	67	ARG	CZ-NH1	5.45	1.40	1.33
2	N	67	ARG	CZ-NH1	5.44	1.40	1.33
2	H	133	PHE	CG-CD1	5.44	1.47	1.38
2	Y	133	PHE	CG-CD1	5.44	1.47	1.38
2	L	67	ARG	NE-CZ	5.35	1.40	1.33
2	M	67	ARG	NE-CZ	5.33	1.40	1.33
2	Y	164	GLN	CA-C	-5.32	1.39	1.52
2	W	67	ARG	NE-CZ	5.31	1.40	1.33
2	1	67	ARG	NE-CZ	5.31	1.40	1.33
2	V	67	ARG	NE-CZ	5.30	1.40	1.33
2	N	164	GLN	CA-C	-5.30	1.39	1.52
2	X	164	GLN	CA-C	-5.30	1.39	1.52
2	H	164	GLN	CA-C	-5.30	1.39	1.52
2	J	164	GLN	CA-C	-5.30	1.39	1.52
2	2	67	ARG	NE-CZ	5.30	1.40	1.33
2	K	67	ARG	NE-CZ	5.30	1.40	1.33
2	V	164	GLN	CA-C	-5.29	1.39	1.52
2	K	164	GLN	CA-C	-5.29	1.39	1.52
2	L	164	GLN	CA-C	-5.29	1.39	1.52
2	Z	164	GLN	CA-C	-5.29	1.39	1.52
2	I	164	GLN	CA-C	-5.29	1.39	1.52
2	M	164	GLN	CA-C	-5.29	1.39	1.52
2	2	164	GLN	CA-C	-5.29	1.39	1.52
2	W	164	GLN	CA-C	-5.29	1.39	1.52
2	Z	67	ARG	NE-CZ	5.28	1.40	1.33
2	I	67	ARG	NE-CZ	5.28	1.40	1.33
2	1	164	GLN	CA-C	-5.28	1.39	1.52
2	H	67	ARG	NE-CZ	5.27	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	67	ARG	NE-CZ	5.27	1.40	1.33
2	J	67	ARG	NE-CZ	5.26	1.39	1.33
2	N	67	ARG	NE-CZ	5.25	1.39	1.33
2	X	67	ARG	NE-CZ	5.25	1.39	1.33
1	P	105	SER	CA-CB	5.24	1.60	1.52
1	O	105	SER	CA-CB	5.24	1.60	1.52
1	R	105	SER	CA-CB	5.24	1.60	1.52
1	U	105	SER	CA-CB	5.23	1.60	1.52
1	D	105	SER	CA-CB	5.23	1.60	1.52
1	T	105	SER	CA-CB	5.22	1.60	1.52
1	G	105	SER	CA-CB	5.20	1.60	1.52
1	Q	105	SER	CA-CB	5.20	1.60	1.52
1	S	105	SER	CA-CB	5.19	1.60	1.52
1	B	105	SER	CA-CB	5.19	1.60	1.52
1	F	105	SER	CA-CB	5.19	1.60	1.52
1	A	105	SER	CA-CB	5.19	1.60	1.52
1	C	105	SER	CA-CB	5.19	1.60	1.52
1	R	29	GLU	CG-CD	-5.18	1.44	1.51
1	E	105	SER	CA-CB	5.18	1.60	1.52
1	C	29	GLU	CG-CD	-5.17	1.44	1.51
1	T	29	GLU	CG-CD	-5.16	1.44	1.51
1	U	29	GLU	CG-CD	-5.16	1.44	1.51
1	D	29	GLU	CG-CD	-5.16	1.44	1.51
1	E	29	GLU	CG-CD	-5.16	1.44	1.51
1	G	29	GLU	CG-CD	-5.16	1.44	1.51
1	Q	29	GLU	CG-CD	-5.16	1.44	1.51
1	S	29	GLU	CG-CD	-5.14	1.44	1.51
1	B	29	GLU	CG-CD	-5.14	1.44	1.51
1	P	29	GLU	CG-CD	-5.12	1.44	1.51
1	A	29	GLU	CG-CD	-5.12	1.44	1.51
1	Q	224	TYR	CE2-CZ	5.11	1.45	1.38
1	O	29	GLU	CG-CD	-5.10	1.44	1.51
1	R	180	TYR	CE2-CZ	5.10	1.45	1.38
1	F	29	GLU	CG-CD	-5.09	1.44	1.51
1	F	224	TYR	CE2-CZ	5.09	1.45	1.38
1	U	224	TYR	CE2-CZ	5.09	1.45	1.38
1	P	224	TYR	CE2-CZ	5.09	1.45	1.38
1	D	224	TYR	CE2-CZ	5.09	1.45	1.38
1	S	224	TYR	CE2-CZ	5.08	1.45	1.38
1	B	224	TYR	CE2-CZ	5.08	1.45	1.38
1	A	224	TYR	CE2-CZ	5.07	1.45	1.38
1	R	224	TYR	CE2-CZ	5.07	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	224	TYR	CE2-CZ	5.06	1.45	1.38
1	C	224	TYR	CE2-CZ	5.06	1.45	1.38
1	E	57	ARG	NE-CZ	5.06	1.39	1.33
1	E	224	TYR	CE2-CZ	5.06	1.45	1.38
1	D	57	ARG	NE-CZ	5.06	1.39	1.33
1	A	28	ARG	CZ-NH1	5.05	1.39	1.33
1	R	28	ARG	CZ-NH1	5.05	1.39	1.33
1	G	28	ARG	CZ-NH1	5.04	1.39	1.33
1	A	180	TYR	CE2-CZ	5.04	1.45	1.38
1	T	57	ARG	NE-CZ	5.04	1.39	1.33
1	O	224	TYR	CE2-CZ	5.04	1.45	1.38
1	C	57	ARG	NE-CZ	5.04	1.39	1.33
1	F	180	TYR	CE2-CZ	5.04	1.45	1.38
1	G	224	TYR	CE2-CZ	5.04	1.45	1.38
1	P	28	ARG	CZ-NH1	5.04	1.39	1.33
1	S	180	TYR	CE2-CZ	5.02	1.45	1.38
1	B	180	TYR	CE2-CZ	5.02	1.45	1.38
1	S	57	ARG	NE-CZ	5.02	1.39	1.33
1	G	180	TYR	CE2-CZ	5.02	1.45	1.38
1	B	57	ARG	NE-CZ	5.02	1.39	1.33
1	Q	180	TYR	CE2-CZ	5.02	1.45	1.38
1	O	28	ARG	CZ-NH1	5.02	1.39	1.33
1	P	180	TYR	CE2-CZ	5.02	1.45	1.38
1	E	28	ARG	CZ-NH1	5.02	1.39	1.33
1	A	57	ARG	NE-CZ	5.01	1.39	1.33
1	R	57	ARG	NE-CZ	5.01	1.39	1.33
1	U	180	TYR	CE2-CZ	5.01	1.45	1.38
1	D	28	ARG	CZ-NH1	5.01	1.39	1.33
1	D	180	TYR	CE2-CZ	5.01	1.45	1.38
1	E	180	TYR	CE2-CZ	5.01	1.45	1.38
1	T	180	TYR	CE2-CZ	5.01	1.45	1.38
1	F	57	ARG	NE-CZ	5.01	1.39	1.33
1	P	57	ARG	NE-CZ	5.01	1.39	1.33
1	G	57	ARG	NE-CZ	5.00	1.39	1.33
1	Q	28	ARG	CZ-NH1	5.00	1.39	1.33
1	Q	57	ARG	NE-CZ	5.00	1.39	1.33
1	S	28	ARG	CZ-NH1	5.00	1.39	1.33
1	B	28	ARG	CZ-NH1	5.00	1.39	1.33

All (1366) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	135	TYR	CB-CG-CD1	-14.47	112.32	121.00
2	X	135	TYR	CB-CG-CD1	-14.46	112.33	121.00
2	W	135	TYR	CB-CG-CD1	-14.44	112.33	121.00
2	2	135	TYR	CB-CG-CD1	-14.42	112.35	121.00
2	K	135	TYR	CB-CG-CD1	-14.42	112.35	121.00
2	Z	135	TYR	CB-CG-CD1	-14.39	112.37	121.00
2	I	135	TYR	CB-CG-CD1	-14.39	112.37	121.00
2	J	135	TYR	CB-CG-CD1	-14.37	112.38	121.00
2	M	135	TYR	CB-CG-CD1	-14.37	112.38	121.00
2	N	135	TYR	CB-CG-CD1	-14.37	112.38	121.00
2	H	135	TYR	CB-CG-CD1	-14.36	112.39	121.00
2	Y	135	TYR	CB-CG-CD1	-14.36	112.39	121.00
2	V	135	TYR	CB-CG-CD1	-14.35	112.39	121.00
2	L	135	TYR	CB-CG-CD1	-14.34	112.39	121.00
2	N	180	ARG	NE-CZ-NH1	14.16	127.38	120.30
2	X	180	ARG	NE-CZ-NH1	14.15	127.37	120.30
2	Y	180	ARG	NE-CZ-NH1	14.14	127.37	120.30
2	V	180	ARG	NE-CZ-NH1	14.14	127.37	120.30
2	W	180	ARG	NE-CZ-NH1	14.12	127.36	120.30
2	1	180	ARG	NE-CZ-NH1	14.11	127.36	120.30
2	Z	180	ARG	NE-CZ-NH1	14.11	127.35	120.30
2	I	180	ARG	NE-CZ-NH1	14.11	127.35	120.30
2	J	180	ARG	NE-CZ-NH1	14.11	127.36	120.30
2	M	180	ARG	NE-CZ-NH1	14.10	127.35	120.30
2	2	180	ARG	NE-CZ-NH1	14.10	127.35	120.30
2	K	180	ARG	NE-CZ-NH1	14.10	127.35	120.30
2	L	180	ARG	NE-CZ-NH1	14.08	127.34	120.30
2	H	180	ARG	NE-CZ-NH1	14.06	127.33	120.30
1	E	73	TYR	CB-CG-CD1	-14.03	112.58	121.00
1	G	73	TYR	CB-CG-CD1	-14.02	112.59	121.00
1	P	73	TYR	CB-CG-CD1	-14.02	112.59	121.00
1	Q	73	TYR	CB-CG-CD1	-14.02	112.59	121.00
1	F	73	TYR	CB-CG-CD1	-14.01	112.59	121.00
1	C	73	TYR	CB-CG-CD1	-14.01	112.59	121.00
1	U	73	TYR	CB-CG-CD1	-14.01	112.60	121.00
1	O	73	TYR	CB-CG-CD1	-14.00	112.60	121.00
1	D	73	TYR	CB-CG-CD1	-14.00	112.60	121.00
1	S	73	TYR	CB-CG-CD1	-14.00	112.60	121.00
1	B	73	TYR	CB-CG-CD1	-14.00	112.60	121.00
1	R	73	TYR	CB-CG-CD1	-13.97	112.62	121.00
1	T	73	TYR	CB-CG-CD1	-13.96	112.62	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	TYR	CB-CG-CD1	-13.95	112.63	121.00
1	A	132	TYR	CB-CG-CD1	-13.48	112.91	121.00
1	R	132	TYR	CB-CG-CD1	-13.48	112.91	121.00
1	G	132	TYR	CB-CG-CD1	-13.46	112.92	121.00
2	J	25	PHE	CB-CG-CD1	13.45	130.22	120.80
1	O	132	TYR	CB-CG-CD1	-13.44	112.93	121.00
1	C	132	TYR	CB-CG-CD1	-13.43	112.94	121.00
1	F	132	TYR	CB-CG-CD1	-13.43	112.94	121.00
1	P	132	TYR	CB-CG-CD1	-13.43	112.94	121.00
1	E	132	TYR	CB-CG-CD1	-13.43	112.94	121.00
2	N	25	PHE	CB-CG-CD1	13.41	130.19	120.80
1	S	132	TYR	CB-CG-CD1	-13.41	112.95	121.00
1	B	132	TYR	CB-CG-CD1	-13.41	112.95	121.00
2	1	25	PHE	CB-CG-CD1	13.40	130.18	120.80
2	V	25	PHE	CB-CG-CD1	13.40	130.18	120.80
1	Q	132	TYR	CB-CG-CD1	-13.40	112.96	121.00
2	Y	25	PHE	CB-CG-CD1	13.40	130.18	120.80
2	Z	25	PHE	CB-CG-CD1	13.39	130.18	120.80
2	M	25	PHE	CB-CG-CD1	13.39	130.18	120.80
2	I	25	PHE	CB-CG-CD1	13.39	130.18	120.80
2	W	25	PHE	CB-CG-CD1	13.39	130.18	120.80
1	U	132	TYR	CB-CG-CD1	-13.38	112.97	121.00
1	T	132	TYR	CB-CG-CD1	-13.38	112.97	121.00
2	L	25	PHE	CB-CG-CD1	13.37	130.16	120.80
2	2	25	PHE	CB-CG-CD1	13.37	130.16	120.80
2	H	25	PHE	CB-CG-CD1	13.37	130.16	120.80
2	K	25	PHE	CB-CG-CD1	13.37	130.16	120.80
2	X	25	PHE	CB-CG-CD1	13.33	130.13	120.80
1	D	132	TYR	CB-CG-CD1	-13.33	113.00	121.00
1	G	22	PHE	CB-CG-CD2	-12.78	111.85	120.80
1	C	22	PHE	CB-CG-CD2	-12.76	111.87	120.80
1	O	22	PHE	CB-CG-CD2	-12.75	111.88	120.80
1	Q	22	PHE	CB-CG-CD2	-12.75	111.88	120.80
1	E	22	PHE	CB-CG-CD2	-12.75	111.88	120.80
1	T	22	PHE	CB-CG-CD2	-12.75	111.88	120.80
1	S	22	PHE	CB-CG-CD2	-12.74	111.88	120.80
1	B	22	PHE	CB-CG-CD2	-12.74	111.88	120.80
1	U	22	PHE	CB-CG-CD2	-12.72	111.89	120.80
1	D	22	PHE	CB-CG-CD2	-12.72	111.89	120.80
1	A	22	PHE	CB-CG-CD2	-12.72	111.89	120.80
1	R	22	PHE	CB-CG-CD2	-12.72	111.89	120.80
1	P	22	PHE	CB-CG-CD2	-12.70	111.91	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	22	PHE	CB-CG-CD2	-12.68	111.92	120.80
2	N	165	ARG	NE-CZ-NH2	11.38	125.99	120.30
2	H	165	ARG	NE-CZ-NH2	11.35	125.97	120.30
2	W	165	ARG	NE-CZ-NH2	11.34	125.97	120.30
2	Y	165	ARG	NE-CZ-NH2	11.34	125.97	120.30
2	L	165	ARG	NE-CZ-NH2	11.32	125.96	120.30
2	1	165	ARG	NE-CZ-NH2	11.31	125.96	120.30
2	J	165	ARG	NE-CZ-NH2	11.31	125.96	120.30
2	X	165	ARG	NE-CZ-NH2	11.30	125.95	120.30
2	Z	165	ARG	NE-CZ-NH2	11.29	125.95	120.30
2	I	165	ARG	NE-CZ-NH2	11.29	125.95	120.30
2	V	165	ARG	NE-CZ-NH2	11.28	125.94	120.30
2	M	165	ARG	NE-CZ-NH2	11.26	125.93	120.30
2	2	165	ARG	NE-CZ-NH2	11.26	125.93	120.30
2	K	165	ARG	NE-CZ-NH2	11.26	125.93	120.30
2	J	25	PHE	CB-CG-CD2	-11.21	112.95	120.80
2	N	25	PHE	CB-CG-CD2	-11.20	112.96	120.80
2	V	25	PHE	CB-CG-CD2	-11.18	112.97	120.80
2	Z	25	PHE	CB-CG-CD2	-11.17	112.98	120.80
2	I	25	PHE	CB-CG-CD2	-11.17	112.98	120.80
2	M	25	PHE	CB-CG-CD2	-11.17	112.98	120.80
2	W	25	PHE	CB-CG-CD2	-11.17	112.98	120.80
2	X	25	PHE	CB-CG-CD2	-11.17	112.98	120.80
2	2	25	PHE	CB-CG-CD2	-11.16	112.99	120.80
2	K	25	PHE	CB-CG-CD2	-11.16	112.99	120.80
2	L	25	PHE	CB-CG-CD2	-11.15	112.99	120.80
2	H	25	PHE	CB-CG-CD2	-11.15	113.00	120.80
2	Y	25	PHE	CB-CG-CD2	-11.15	113.00	120.80
2	1	25	PHE	CB-CG-CD2	-11.14	113.00	120.80
1	Q	222	ARG	NE-CZ-NH2	10.43	125.52	120.30
1	P	222	ARG	NE-CZ-NH2	10.41	125.50	120.30
1	T	222	ARG	NE-CZ-NH2	10.40	125.50	120.30
1	C	222	ARG	NE-CZ-NH2	10.40	125.50	120.30
1	U	222	ARG	NE-CZ-NH2	10.39	125.50	120.30
1	D	222	ARG	NE-CZ-NH2	10.39	125.50	120.30
1	G	222	ARG	NE-CZ-NH2	10.39	125.49	120.30
1	F	222	ARG	NE-CZ-NH2	10.38	125.49	120.30
1	S	222	ARG	NE-CZ-NH2	10.38	125.49	120.30
1	B	222	ARG	NE-CZ-NH2	10.38	125.49	120.30
1	O	222	ARG	NE-CZ-NH2	10.35	125.48	120.30
1	E	222	ARG	NE-CZ-NH2	10.35	125.48	120.30
1	A	222	ARG	NE-CZ-NH2	10.32	125.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	222	ARG	NE-CZ-NH2	10.32	125.46	120.30
1	Q	22	PHE	CB-CG-CD1	10.07	127.85	120.80
1	G	22	PHE	CB-CG-CD1	10.06	127.84	120.80
1	E	22	PHE	CB-CG-CD1	10.04	127.83	120.80
1	D	22	PHE	CB-CG-CD1	10.04	127.83	120.80
1	S	22	PHE	CB-CG-CD1	10.04	127.83	120.80
1	O	22	PHE	CB-CG-CD1	10.04	127.83	120.80
1	B	22	PHE	CB-CG-CD1	10.04	127.83	120.80
1	U	22	PHE	CB-CG-CD1	10.04	127.83	120.80
1	T	22	PHE	CB-CG-CD1	10.03	127.82	120.80
1	A	22	PHE	CB-CG-CD1	10.03	127.82	120.80
1	R	22	PHE	CB-CG-CD1	10.03	127.82	120.80
1	P	22	PHE	CB-CG-CD1	10.03	127.82	120.80
1	C	22	PHE	CB-CG-CD1	10.02	127.81	120.80
1	F	22	PHE	CB-CG-CD1	10.01	127.80	120.80
1	P	86	ARG	NE-CZ-NH2	-9.97	115.32	120.30
1	Q	86	ARG	NE-CZ-NH2	-9.97	115.32	120.30
1	A	86	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	R	86	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	E	86	ARG	NE-CZ-NH2	-9.94	115.33	120.30
1	T	86	ARG	NE-CZ-NH2	-9.93	115.34	120.30
1	C	86	ARG	NE-CZ-NH2	-9.93	115.34	120.30
1	S	86	ARG	NE-CZ-NH2	-9.93	115.34	120.30
1	B	86	ARG	NE-CZ-NH2	-9.93	115.34	120.30
1	G	86	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	O	86	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	D	86	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	F	86	ARG	NE-CZ-NH2	-9.89	115.36	120.30
1	U	86	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	Q	147	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	P	147	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	R	147	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	E	147	ARG	NE-CZ-NH1	9.83	125.21	120.30
1	O	147	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	U	147	ARG	NE-CZ-NH1	9.81	125.20	120.30
1	F	147	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	T	147	ARG	NE-CZ-NH1	9.79	125.20	120.30
1	C	147	ARG	NE-CZ-NH1	9.79	125.20	120.30
1	A	147	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	S	147	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	B	147	ARG	NE-CZ-NH1	9.78	125.19	120.30
2	Y	157	ARG	NE-CZ-NH1	9.76	125.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	157	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	G	147	ARG	NE-CZ-NH1	9.72	125.16	120.30
2	1	157	ARG	NE-CZ-NH1	9.71	125.15	120.30
2	Z	157	ARG	NE-CZ-NH1	9.70	125.15	120.30
2	I	157	ARG	NE-CZ-NH1	9.70	125.15	120.30
2	J	157	ARG	NE-CZ-NH1	9.69	125.15	120.30
1	D	147	ARG	NE-CZ-NH1	9.69	125.15	120.30
2	N	157	ARG	NE-CZ-NH1	9.68	125.14	120.30
2	M	157	ARG	NE-CZ-NH1	9.68	125.14	120.30
2	W	157	ARG	NE-CZ-NH1	9.68	125.14	120.30
2	H	157	ARG	NE-CZ-NH1	9.68	125.14	120.30
2	2	157	ARG	NE-CZ-NH1	9.67	125.14	120.30
2	V	157	ARG	NE-CZ-NH1	9.67	125.14	120.30
2	X	157	ARG	NE-CZ-NH1	9.66	125.13	120.30
2	K	157	ARG	NE-CZ-NH1	9.66	125.13	120.30
2	M	40	TYR	CB-CG-CD2	9.52	126.71	121.00
2	W	40	TYR	CB-CG-CD2	9.52	126.71	121.00
2	K	40	TYR	CB-CG-CD2	9.52	126.71	121.00
2	V	40	TYR	CB-CG-CD2	9.51	126.70	121.00
2	2	40	TYR	CB-CG-CD2	9.50	126.70	121.00
2	X	40	TYR	CB-CG-CD2	9.49	126.69	121.00
2	Z	40	TYR	CB-CG-CD2	9.49	126.69	121.00
2	1	40	TYR	CB-CG-CD2	9.49	126.69	121.00
2	I	40	TYR	CB-CG-CD2	9.49	126.69	121.00
2	J	40	TYR	CB-CG-CD2	9.49	126.69	121.00
1	A	180	TYR	CB-CG-CD2	-9.46	115.32	121.00
2	H	40	TYR	CB-CG-CD2	9.46	126.68	121.00
2	Y	40	TYR	CB-CG-CD2	9.46	126.68	121.00
2	L	40	TYR	CB-CG-CD2	9.46	126.67	121.00
2	N	40	TYR	CB-CG-CD2	9.46	126.67	121.00
1	E	180	TYR	CB-CG-CD2	-9.45	115.33	121.00
1	F	180	TYR	CB-CG-CD2	-9.45	115.33	121.00
1	P	180	TYR	CB-CG-CD2	-9.42	115.35	121.00
1	S	180	TYR	CB-CG-CD2	-9.41	115.35	121.00
1	O	180	TYR	CB-CG-CD2	-9.41	115.36	121.00
1	B	180	TYR	CB-CG-CD2	-9.41	115.35	121.00
1	G	180	TYR	CB-CG-CD2	-9.40	115.36	121.00
1	Q	180	TYR	CB-CG-CD2	-9.40	115.36	121.00
1	R	180	TYR	CB-CG-CD2	-9.39	115.37	121.00
1	U	180	TYR	CB-CG-CD2	-9.38	115.37	121.00
1	D	180	TYR	CB-CG-CD2	-9.38	115.37	121.00
1	T	180	TYR	CB-CG-CD2	-9.38	115.37	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	TYR	CB-CG-CD2	-9.38	115.37	121.00
2	2	184	TYR	CB-CG-CD2	-8.89	115.67	121.00
2	V	184	TYR	CB-CG-CD2	-8.89	115.67	121.00
2	W	184	TYR	CB-CG-CD2	-8.87	115.68	121.00
2	1	184	TYR	CB-CG-CD2	-8.86	115.68	121.00
2	J	184	TYR	CB-CG-CD2	-8.86	115.68	121.00
2	M	184	TYR	CB-CG-CD2	-8.86	115.69	121.00
2	L	184	TYR	CB-CG-CD2	-8.85	115.69	121.00
2	Z	184	TYR	CB-CG-CD2	-8.84	115.70	121.00
2	I	184	TYR	CB-CG-CD2	-8.84	115.70	121.00
1	A	10	ARG	NE-CZ-NH2	-8.83	115.89	120.30
2	H	184	TYR	CB-CG-CD2	-8.83	115.70	121.00
1	R	10	ARG	NE-CZ-NH2	-8.83	115.89	120.30
2	N	184	TYR	CB-CG-CD2	-8.82	115.71	121.00
2	X	184	TYR	CB-CG-CD2	-8.82	115.71	121.00
1	D	10	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	Q	10	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	T	10	ARG	NE-CZ-NH2	-8.79	115.90	120.30
1	C	10	ARG	NE-CZ-NH2	-8.79	115.90	120.30
2	K	184	TYR	CB-CG-CD2	-8.79	115.72	121.00
1	S	10	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	B	10	ARG	NE-CZ-NH2	-8.78	115.91	120.30
2	Y	184	TYR	CB-CG-CD2	-8.78	115.73	121.00
1	O	10	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	F	10	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	P	10	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	U	10	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	G	10	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	E	10	ARG	NE-CZ-NH2	-8.76	115.92	120.30
2	1	135	TYR	CB-CG-CD2	8.45	126.07	121.00
2	X	135	TYR	CB-CG-CD2	8.41	126.05	121.00
2	J	135	TYR	CB-CG-CD2	8.39	126.04	121.00
2	L	135	TYR	CB-CG-CD2	8.36	126.02	121.00
2	H	135	TYR	CB-CG-CD2	8.36	126.02	121.00
2	Y	135	TYR	CB-CG-CD2	8.36	126.02	121.00
2	2	135	TYR	CB-CG-CD2	8.36	126.02	121.00
2	W	135	TYR	CB-CG-CD2	8.36	126.02	121.00
2	K	135	TYR	CB-CG-CD2	8.36	126.02	121.00
2	Z	135	TYR	CB-CG-CD2	8.36	126.01	121.00
2	I	135	TYR	CB-CG-CD2	8.36	126.01	121.00
2	M	135	TYR	CB-CG-CD2	8.32	125.99	121.00
2	Y	157	ARG	NE-CZ-NH2	-8.32	116.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	135	TYR	CB-CG-CD2	8.31	125.99	121.00
2	V	135	TYR	CB-CG-CD2	8.31	125.98	121.00
2	2	142	TYR	CD1-CE1-CZ	-8.29	112.34	119.80
2	1	142	TYR	CD1-CE1-CZ	-8.29	112.34	119.80
2	J	142	TYR	CD1-CE1-CZ	-8.29	112.34	119.80
2	K	142	TYR	CD1-CE1-CZ	-8.29	112.34	119.80
2	L	157	ARG	NE-CZ-NH2	-8.28	116.16	120.30
2	M	142	TYR	CD1-CE1-CZ	-8.28	112.35	119.80
2	W	142	TYR	CD1-CE1-CZ	-8.28	112.35	119.80
2	L	142	TYR	CD1-CE1-CZ	-8.28	112.35	119.80
2	V	142	TYR	CD1-CE1-CZ	-8.27	112.36	119.80
2	N	142	TYR	CD1-CE1-CZ	-8.26	112.37	119.80
2	H	142	TYR	CD1-CE1-CZ	-8.26	112.37	119.80
2	X	142	TYR	CD1-CE1-CZ	-8.26	112.37	119.80
2	Z	142	TYR	CD1-CE1-CZ	-8.26	112.37	119.80
2	I	142	TYR	CD1-CE1-CZ	-8.26	112.37	119.80
2	Y	142	TYR	CD1-CE1-CZ	-8.25	112.37	119.80
2	N	157	ARG	NE-CZ-NH2	-8.22	116.19	120.30
2	Z	157	ARG	NE-CZ-NH2	-8.22	116.19	120.30
2	I	157	ARG	NE-CZ-NH2	-8.22	116.19	120.30
2	2	157	ARG	NE-CZ-NH2	-8.21	116.19	120.30
2	M	157	ARG	NE-CZ-NH2	-8.21	116.19	120.30
2	V	157	ARG	NE-CZ-NH2	-8.21	116.19	120.30
2	W	157	ARG	NE-CZ-NH2	-8.21	116.19	120.30
2	X	157	ARG	NE-CZ-NH2	-8.19	116.20	120.30
2	H	157	ARG	NE-CZ-NH2	-8.19	116.21	120.30
2	1	157	ARG	NE-CZ-NH2	-8.18	116.21	120.30
2	J	157	ARG	NE-CZ-NH2	-8.17	116.21	120.30
2	K	157	ARG	NE-CZ-NH2	-8.17	116.21	120.30
2	V	166	ASP	CB-CG-OD1	7.89	125.40	118.30
2	L	166	ASP	CB-CG-OD1	7.89	125.40	118.30
2	J	166	ASP	CB-CG-OD1	7.88	125.39	118.30
2	2	166	ASP	CB-CG-OD1	7.87	125.38	118.30
2	K	166	ASP	CB-CG-OD1	7.87	125.38	118.30
2	Y	166	ASP	CB-CG-OD1	7.87	125.38	118.30
2	Z	166	ASP	CB-CG-OD1	7.86	125.38	118.30
2	M	166	ASP	CB-CG-OD1	7.86	125.38	118.30
2	I	166	ASP	CB-CG-OD1	7.86	125.38	118.30
2	W	166	ASP	CB-CG-OD1	7.86	125.38	118.30
2	1	166	ASP	CB-CG-OD1	7.86	125.37	118.30
2	N	166	ASP	CB-CG-OD1	7.85	125.37	118.30
2	X	166	ASP	CB-CG-OD1	7.85	125.37	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	166	ASP	CB-CG-OD1	7.85	125.37	118.30
1	Q	91	PHE	CB-CG-CD1	-7.73	115.39	120.80
2	2	166	ASP	CB-CG-OD2	-7.72	111.35	118.30
2	K	166	ASP	CB-CG-OD2	-7.72	111.35	118.30
2	M	166	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	O	91	PHE	CB-CG-CD1	-7.72	115.39	120.80
1	E	91	PHE	CB-CG-CD1	-7.72	115.39	120.80
1	G	91	PHE	CB-CG-CD1	-7.72	115.40	120.80
2	1	166	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	C	91	PHE	CB-CG-CD1	-7.71	115.41	120.80
2	X	166	ASP	CB-CG-OD2	-7.71	111.36	118.30
2	J	166	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	U	91	PHE	CB-CG-CD1	-7.70	115.41	120.80
1	S	91	PHE	CB-CG-CD1	-7.69	115.41	120.80
1	B	91	PHE	CB-CG-CD1	-7.69	115.41	120.80
1	A	91	PHE	CB-CG-CD1	-7.69	115.42	120.80
1	R	91	PHE	CB-CG-CD1	-7.69	115.42	120.80
2	Z	166	ASP	CB-CG-OD2	-7.68	111.38	118.30
2	I	166	ASP	CB-CG-OD2	-7.68	111.38	118.30
2	N	166	ASP	CB-CG-OD2	-7.67	111.39	118.30
1	D	91	PHE	CB-CG-CD1	-7.67	115.43	120.80
2	W	166	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	T	91	PHE	CB-CG-CD1	-7.67	115.43	120.80
2	V	166	ASP	CB-CG-OD2	-7.66	111.41	118.30
2	L	166	ASP	CB-CG-OD2	-7.66	111.41	118.30
2	Y	166	ASP	CB-CG-OD2	-7.65	111.41	118.30
1	F	91	PHE	CB-CG-CD1	-7.65	115.45	120.80
1	P	91	PHE	CB-CG-CD1	-7.65	115.45	120.80
2	H	166	ASP	CB-CG-OD2	-7.64	111.42	118.30
2	1	203	LEU	CB-CG-CD1	7.56	123.85	111.00
2	2	203	LEU	CB-CG-CD1	7.56	123.85	111.00
2	K	203	LEU	CB-CG-CD1	7.56	123.85	111.00
2	Y	203	LEU	CB-CG-CD1	7.56	123.85	111.00
2	Z	203	LEU	CB-CG-CD1	7.56	123.84	111.00
2	I	203	LEU	CB-CG-CD1	7.56	123.84	111.00
2	M	203	LEU	CB-CG-CD1	7.55	123.84	111.00
2	X	203	LEU	CB-CG-CD1	7.55	123.84	111.00
2	N	203	LEU	CB-CG-CD1	7.55	123.84	111.00
2	V	203	LEU	CB-CG-CD1	7.55	123.84	111.00
2	H	203	LEU	CB-CG-CD1	7.55	123.83	111.00
2	L	203	LEU	CB-CG-CD1	7.55	123.83	111.00
2	J	203	LEU	CB-CG-CD1	7.54	123.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	203	LEU	CB-CG-CD1	7.54	123.82	111.00
2	W	177	VAL	CA-CB-CG1	7.48	122.12	110.90
2	M	177	VAL	CA-CB-CG1	7.48	122.11	110.90
2	X	177	VAL	CA-CB-CG1	7.47	122.11	110.90
2	V	177	VAL	CA-CB-CG1	7.47	122.11	110.90
2	L	177	VAL	CA-CB-CG1	7.47	122.11	110.90
2	2	177	VAL	CA-CB-CG1	7.47	122.11	110.90
2	K	177	VAL	CA-CB-CG1	7.47	122.11	110.90
2	N	177	VAL	CA-CB-CG1	7.46	122.10	110.90
2	J	177	VAL	CA-CB-CG1	7.46	122.09	110.90
2	Z	177	VAL	CA-CB-CG1	7.46	122.09	110.90
2	I	177	VAL	CA-CB-CG1	7.46	122.09	110.90
2	H	177	VAL	CA-CB-CG1	7.44	122.06	110.90
2	Y	177	VAL	CA-CB-CG1	7.44	122.06	110.90
2	1	177	VAL	CA-CB-CG1	7.44	122.06	110.90
2	2	51	ASP	CB-CG-OD2	-7.37	111.66	118.30
2	J	51	ASP	CB-CG-OD2	-7.37	111.67	118.30
2	W	51	ASP	CB-CG-OD2	-7.35	111.68	118.30
2	K	51	ASP	CB-CG-OD2	-7.34	111.70	118.30
2	H	51	ASP	CB-CG-OD2	-7.34	111.70	118.30
2	V	51	ASP	CB-CG-OD2	-7.32	111.71	118.30
2	L	51	ASP	CB-CG-OD2	-7.32	111.71	118.30
2	1	51	ASP	CB-CG-OD2	-7.32	111.71	118.30
2	Z	51	ASP	CB-CG-OD2	-7.32	111.71	118.30
2	I	51	ASP	CB-CG-OD2	-7.32	111.71	118.30
2	N	51	ASP	CB-CG-OD2	-7.32	111.72	118.30
2	X	51	ASP	CB-CG-OD2	-7.32	111.72	118.30
2	M	51	ASP	CB-CG-OD2	-7.31	111.72	118.30
2	Y	51	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	T	15	PHE	CB-CG-CD2	7.29	125.90	120.80
1	C	15	PHE	CB-CG-CD2	7.29	125.90	120.80
1	U	15	PHE	CB-CG-CD2	7.27	125.89	120.80
1	D	15	PHE	CB-CG-CD2	7.27	125.89	120.80
1	S	15	PHE	CB-CG-CD2	7.27	125.89	120.80
1	B	15	PHE	CB-CG-CD2	7.27	125.89	120.80
1	U	221	TYR	CG-CD1-CE1	-7.26	115.49	121.30
1	F	15	PHE	CB-CG-CD2	7.26	125.88	120.80
1	A	221	TYR	CG-CD1-CE1	-7.26	115.50	121.30
1	P	15	PHE	CB-CG-CD2	7.26	125.88	120.80
1	R	221	TYR	CG-CD1-CE1	-7.26	115.50	121.30
1	O	15	PHE	CB-CG-CD2	7.25	125.88	120.80
1	E	15	PHE	CB-CG-CD2	7.25	125.88	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	15	PHE	CB-CG-CD2	7.25	125.88	120.80
1	Q	15	PHE	CB-CG-CD2	7.25	125.88	120.80
1	A	15	PHE	CB-CG-CD2	7.24	125.87	120.80
1	R	15	PHE	CB-CG-CD2	7.24	125.87	120.80
1	T	221	TYR	CG-CD1-CE1	-7.24	115.51	121.30
1	C	221	TYR	CG-CD1-CE1	-7.24	115.51	121.30
1	S	221	TYR	CG-CD1-CE1	-7.24	115.51	121.30
1	B	221	TYR	CG-CD1-CE1	-7.24	115.51	121.30
1	Q	221	TYR	CG-CD1-CE1	-7.23	115.52	121.30
1	F	221	TYR	CG-CD1-CE1	-7.21	115.53	121.30
1	O	221	TYR	CG-CD1-CE1	-7.21	115.53	121.30
1	E	221	TYR	CG-CD1-CE1	-7.21	115.53	121.30
1	G	221	TYR	CG-CD1-CE1	-7.19	115.55	121.30
1	T	132	TYR	CG-CD2-CE2	-7.18	115.55	121.30
1	D	221	TYR	CG-CD1-CE1	-7.18	115.55	121.30
1	P	221	TYR	CG-CD1-CE1	-7.18	115.56	121.30
1	G	132	TYR	CG-CD2-CE2	-7.17	115.56	121.30
1	D	132	TYR	CG-CD2-CE2	-7.16	115.57	121.30
1	Q	132	TYR	CG-CD2-CE2	-7.13	115.60	121.30
1	A	132	TYR	CG-CD2-CE2	-7.12	115.60	121.30
1	R	132	TYR	CG-CD2-CE2	-7.12	115.60	121.30
1	S	132	TYR	CG-CD2-CE2	-7.12	115.60	121.30
1	U	132	TYR	CG-CD2-CE2	-7.12	115.60	121.30
1	B	132	TYR	CG-CD2-CE2	-7.12	115.60	121.30
1	C	132	TYR	CG-CD2-CE2	-7.12	115.60	121.30
1	O	132	TYR	CG-CD2-CE2	-7.12	115.61	121.30
1	E	132	TYR	CG-CD2-CE2	-7.12	115.61	121.30
1	U	57	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	D	57	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	F	132	TYR	CG-CD2-CE2	-7.08	115.63	121.30
1	P	132	TYR	CG-CD2-CE2	-7.08	115.64	121.30
1	E	57	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	57	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	R	57	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	O	57	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	S	57	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	B	57	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	Q	57	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	T	152	ASP	CB-CG-OD1	-7.00	112.00	118.30
1	C	152	ASP	CB-CG-OD1	-7.00	112.00	118.30
1	E	152	ASP	CB-CG-OD1	-7.00	112.00	118.30
1	G	57	ARG	NE-CZ-NH2	-7.00	116.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	152	ASP	CB-CG-OD1	-7.00	112.00	118.30
1	T	57	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	57	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	F	152	ASP	CB-CG-OD1	-6.99	112.01	118.30
1	S	152	ASP	CB-CG-OD1	-6.99	112.01	118.30
1	B	152	ASP	CB-CG-OD1	-6.99	112.01	118.30
1	F	57	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	P	57	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	O	152	ASP	CB-CG-OD1	-6.98	112.02	118.30
1	R	152	ASP	CB-CG-OD1	-6.98	112.02	118.30
1	G	152	ASP	CB-CG-OD1	-6.97	112.02	118.30
1	Q	152	ASP	CB-CG-OD1	-6.97	112.02	118.30
1	A	152	ASP	CB-CG-OD1	-6.97	112.03	118.30
1	D	152	ASP	CB-CG-OD1	-6.95	112.05	118.30
1	U	152	ASP	CB-CG-OD1	-6.95	112.05	118.30
2	Y	71	ARG	NE-CZ-NH2	6.91	123.75	120.30
2	J	71	ARG	NE-CZ-NH2	6.89	123.75	120.30
2	M	71	ARG	NE-CZ-NH2	6.88	123.74	120.30
2	W	71	ARG	NE-CZ-NH2	6.88	123.74	120.30
2	K	71	ARG	NE-CZ-NH2	6.87	123.73	120.30
2	1	71	ARG	NE-CZ-NH2	6.86	123.73	120.30
2	Z	71	ARG	NE-CZ-NH2	6.84	123.72	120.30
2	N	71	ARG	NE-CZ-NH2	6.84	123.72	120.30
2	I	71	ARG	NE-CZ-NH2	6.84	123.72	120.30
2	X	71	ARG	NE-CZ-NH2	6.84	123.72	120.30
2	N	24	ASN	O-C-N	-6.83	111.78	122.70
2	H	71	ARG	NE-CZ-NH2	6.83	123.71	120.30
2	X	24	ASN	O-C-N	-6.81	111.80	122.70
2	V	24	ASN	O-C-N	-6.81	111.81	122.70
2	H	24	ASN	O-C-N	-6.80	111.81	122.70
2	W	24	ASN	O-C-N	-6.80	111.81	122.70
2	Y	24	ASN	O-C-N	-6.80	111.81	122.70
2	Z	24	ASN	O-C-N	-6.80	111.82	122.70
2	I	24	ASN	O-C-N	-6.80	111.82	122.70
2	L	24	ASN	O-C-N	-6.80	111.82	122.70
2	V	71	ARG	NE-CZ-NH2	6.80	123.70	120.30
2	L	71	ARG	NE-CZ-NH2	6.80	123.70	120.30
2	2	71	ARG	NE-CZ-NH2	6.79	123.70	120.30
2	M	24	ASN	O-C-N	-6.79	111.84	122.70
2	2	24	ASN	O-C-N	-6.79	111.84	122.70
2	K	24	ASN	O-C-N	-6.79	111.84	122.70
2	1	24	ASN	O-C-N	-6.78	111.85	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	24	ASN	O-C-N	-6.78	111.85	122.70
2	1	184	TYR	CG-CD2-CE2	-6.77	115.88	121.30
2	J	184	TYR	CG-CD2-CE2	-6.77	115.88	121.30
2	W	57	ARG	NE-CZ-NH1	6.76	123.68	120.30
2	2	184	TYR	CG-CD2-CE2	-6.76	115.90	121.30
2	V	184	TYR	CG-CD2-CE2	-6.75	115.90	121.30
2	M	57	ARG	NE-CZ-NH1	6.75	123.67	120.30
2	H	184	TYR	CG-CD2-CE2	-6.75	115.90	121.30
2	2	57	ARG	NE-CZ-NH1	6.73	123.66	120.30
2	L	184	TYR	CG-CD2-CE2	-6.72	115.92	121.30
2	H	57	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	Y	57	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	L	57	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	X	57	ARG	NE-CZ-NH1	6.71	123.66	120.30
2	Z	184	TYR	CG-CD2-CE2	-6.71	115.93	121.30
2	M	184	TYR	CG-CD2-CE2	-6.71	115.93	121.30
2	I	184	TYR	CG-CD2-CE2	-6.71	115.93	121.30
2	N	57	ARG	NE-CZ-NH1	6.71	123.65	120.30
2	J	57	ARG	NE-CZ-NH1	6.70	123.65	120.30
2	1	57	ARG	NE-CZ-NH1	6.70	123.65	120.30
2	W	184	TYR	CG-CD2-CE2	-6.69	115.95	121.30
2	L	110	VAL	CA-CB-CG1	6.69	120.94	110.90
2	N	184	TYR	CG-CD2-CE2	-6.69	115.95	121.30
2	V	57	ARG	NE-CZ-NH1	6.69	123.64	120.30
2	X	184	TYR	CG-CD2-CE2	-6.69	115.95	121.30
2	Y	110	VAL	CA-CB-CG1	6.69	120.93	110.90
2	Z	57	ARG	NE-CZ-NH1	6.69	123.64	120.30
2	I	57	ARG	NE-CZ-NH1	6.69	123.64	120.30
2	2	110	VAL	CA-CB-CG1	6.68	120.92	110.90
2	K	184	TYR	CG-CD2-CE2	-6.68	115.95	121.30
2	W	110	VAL	CA-CB-CG1	6.68	120.92	110.90
2	Z	110	VAL	CA-CB-CG1	6.68	120.92	110.90
2	I	110	VAL	CA-CB-CG1	6.68	120.92	110.90
2	K	57	ARG	NE-CZ-NH1	6.67	123.64	120.30
2	Y	124	TYR	N-CA-CB	6.67	122.61	110.60
2	1	110	VAL	CA-CB-CG1	6.67	120.91	110.90
2	V	110	VAL	CA-CB-CG1	6.67	120.91	110.90
2	J	110	VAL	CA-CB-CG1	6.67	120.91	110.90
2	X	110	VAL	CA-CB-CG1	6.67	120.91	110.90
2	H	110	VAL	CA-CB-CG1	6.67	120.90	110.90
2	M	110	VAL	CA-CB-CG1	6.67	120.90	110.90
2	K	110	VAL	CA-CB-CG1	6.67	120.90	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	124	TYR	N-CA-CB	6.67	122.60	110.60
2	J	124	TYR	N-CA-CB	6.66	122.59	110.60
2	Y	184	TYR	CG-CD2-CE2	-6.66	115.97	121.30
2	V	124	TYR	N-CA-CB	6.66	122.59	110.60
2	2	124	TYR	N-CA-CB	6.66	122.59	110.60
2	L	124	TYR	N-CA-CB	6.66	122.58	110.60
2	N	110	VAL	CA-CB-CG1	6.65	120.88	110.90
2	H	124	TYR	N-CA-CB	6.65	122.57	110.60
2	Z	124	TYR	N-CA-CB	6.65	122.57	110.60
2	1	124	TYR	N-CA-CB	6.65	122.57	110.60
2	I	124	TYR	N-CA-CB	6.65	122.57	110.60
2	K	124	TYR	N-CA-CB	6.65	122.57	110.60
2	M	124	TYR	N-CA-CB	6.65	122.56	110.60
2	W	124	TYR	N-CA-CB	6.65	122.56	110.60
2	N	124	TYR	N-CA-CB	6.63	122.54	110.60
1	U	73	TYR	CB-CG-CD2	6.62	124.97	121.00
1	C	73	TYR	CB-CG-CD2	6.62	124.97	121.00
1	E	73	TYR	CB-CG-CD2	6.61	124.96	121.00
1	G	73	TYR	CB-CG-CD2	6.60	124.96	121.00
1	P	73	TYR	CB-CG-CD2	6.60	124.96	121.00
1	D	73	TYR	CB-CG-CD2	6.59	124.95	121.00
1	O	73	TYR	CB-CG-CD2	6.58	124.95	121.00
1	F	232	PHE	CB-CG-CD2	-6.57	116.20	120.80
1	G	126	TYR	CG-CD2-CE2	-6.57	116.05	121.30
1	S	73	TYR	CB-CG-CD2	6.56	124.94	121.00
1	B	73	TYR	CB-CG-CD2	6.56	124.94	121.00
1	Q	73	TYR	CB-CG-CD2	6.56	124.94	121.00
1	R	232	PHE	CB-CG-CD2	-6.56	116.21	120.80
1	F	73	TYR	CB-CG-CD2	6.55	124.93	121.00
1	E	232	PHE	CB-CG-CD2	-6.55	116.22	120.80
1	G	232	PHE	CB-CG-CD2	-6.55	116.22	120.80
1	P	232	PHE	CB-CG-CD2	-6.55	116.22	120.80
1	Q	232	PHE	CB-CG-CD2	-6.55	116.22	120.80
1	T	126	TYR	CG-CD2-CE2	-6.53	116.07	121.30
1	A	73	TYR	CB-CG-CD2	6.53	124.92	121.00
1	C	126	TYR	CG-CD2-CE2	-6.53	116.07	121.30
1	R	73	TYR	CB-CG-CD2	6.53	124.92	121.00
1	D	126	TYR	CG-CD2-CE2	-6.53	116.08	121.30
1	S	232	PHE	CB-CG-CD2	-6.53	116.23	120.80
1	B	232	PHE	CB-CG-CD2	-6.53	116.23	120.80
1	U	126	TYR	CG-CD2-CE2	-6.53	116.08	121.30
1	O	126	TYR	CG-CD2-CE2	-6.53	116.08	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	126	TYR	CG-CD2-CE2	-6.53	116.08	121.30
1	E	126	TYR	CG-CD2-CE2	-6.52	116.08	121.30
1	C	232	PHE	CB-CG-CD2	-6.52	116.24	120.80
1	Q	73	TYR	CG-CD2-CE2	-6.51	116.09	121.30
1	D	232	PHE	CB-CG-CD2	-6.51	116.24	120.80
1	S	126	TYR	CG-CD2-CE2	-6.51	116.09	121.30
1	T	73	TYR	CB-CG-CD2	6.51	124.91	121.00
1	B	126	TYR	CG-CD2-CE2	-6.51	116.09	121.30
1	Q	126	TYR	CG-CD2-CE2	-6.51	116.09	121.30
1	R	126	TYR	CG-CD2-CE2	-6.50	116.10	121.30
1	T	232	PHE	CB-CG-CD2	-6.50	116.25	120.80
1	O	232	PHE	CB-CG-CD2	-6.50	116.25	120.80
1	A	126	TYR	CG-CD2-CE2	-6.50	116.10	121.30
1	F	126	TYR	CG-CD2-CE2	-6.49	116.11	121.30
1	U	232	PHE	CB-CG-CD2	-6.48	116.26	120.80
1	F	73	TYR	CG-CD2-CE2	-6.48	116.12	121.30
1	A	232	PHE	CB-CG-CD2	-6.47	116.27	120.80
1	T	73	TYR	CG-CD2-CE2	-6.47	116.12	121.30
1	R	73	TYR	CG-CD2-CE2	-6.46	116.13	121.30
1	G	73	TYR	CG-CD2-CE2	-6.46	116.13	121.30
1	S	73	TYR	CG-CD2-CE2	-6.46	116.14	121.30
1	B	73	TYR	CG-CD2-CE2	-6.46	116.14	121.30
1	A	73	TYR	CG-CD2-CE2	-6.45	116.14	121.30
1	O	73	TYR	CG-CD2-CE2	-6.45	116.14	121.30
1	P	73	TYR	CG-CD2-CE2	-6.44	116.15	121.30
1	C	73	TYR	CG-CD2-CE2	-6.43	116.15	121.30
2	W	131	SER	N-CA-CB	6.43	120.15	110.50
1	E	73	TYR	CG-CD2-CE2	-6.43	116.16	121.30
2	2	131	SER	N-CA-CB	6.43	120.14	110.50
2	K	131	SER	N-CA-CB	6.43	120.14	110.50
2	N	131	SER	N-CA-CB	6.43	120.14	110.50
2	X	131	SER	N-CA-CB	6.43	120.14	110.50
1	D	73	TYR	CG-CD2-CE2	-6.42	116.17	121.30
2	Y	131	SER	N-CA-CB	6.42	120.12	110.50
2	Z	131	SER	N-CA-CB	6.40	120.11	110.50
2	I	131	SER	N-CA-CB	6.40	120.11	110.50
2	H	131	SER	N-CA-CB	6.40	120.10	110.50
2	L	131	SER	N-CA-CB	6.40	120.10	110.50
2	J	131	SER	N-CA-CB	6.40	120.10	110.50
1	U	73	TYR	CG-CD2-CE2	-6.40	116.18	121.30
2	V	131	SER	N-CA-CB	6.40	120.09	110.50
2	M	131	SER	N-CA-CB	6.39	120.09	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	131	SER	N-CA-CB	6.38	120.07	110.50
2	K	135	TYR	CG-CD1-CE1	-6.38	116.20	121.30
1	G	200	SER	N-CA-CB	-6.36	100.95	110.50
2	N	24	ASN	CA-C-N	6.36	131.20	117.20
1	C	200	SER	N-CA-CB	-6.36	100.95	110.50
2	W	135	TYR	CG-CD1-CE1	-6.36	116.21	121.30
1	Q	200	SER	N-CA-CB	-6.36	100.96	110.50
1	T	200	SER	N-CA-CB	-6.36	100.97	110.50
2	1	24	ASN	CA-C-N	6.36	131.18	117.20
2	J	24	ASN	CA-C-N	6.36	131.18	117.20
1	D	200	SER	N-CA-CB	-6.36	100.97	110.50
2	K	92	TYR	CG-CD1-CE1	-6.36	116.22	121.30
1	F	200	SER	N-CA-CB	-6.35	100.97	110.50
2	W	24	ASN	CA-C-N	6.35	131.18	117.20
2	H	24	ASN	CA-C-N	6.35	131.17	117.20
2	Y	24	ASN	CA-C-N	6.35	131.17	117.20
2	M	24	ASN	CA-C-N	6.35	131.17	117.20
2	Z	24	ASN	CA-C-N	6.35	131.16	117.20
2	2	24	ASN	CA-C-N	6.35	131.16	117.20
2	I	24	ASN	CA-C-N	6.35	131.16	117.20
1	S	200	SER	N-CA-CB	-6.34	100.98	110.50
2	1	135	TYR	CG-CD1-CE1	-6.34	116.22	121.30
2	V	24	ASN	CA-C-N	6.34	131.16	117.20
1	B	200	SER	N-CA-CB	-6.34	100.98	110.50
1	U	200	SER	N-CA-CB	-6.34	100.99	110.50
1	A	200	SER	N-CA-CB	-6.34	100.99	110.50
2	V	92	TYR	CG-CD1-CE1	-6.34	116.23	121.30
2	J	92	TYR	CG-CD1-CE1	-6.34	116.23	121.30
2	X	24	ASN	CA-C-N	6.34	131.15	117.20
1	R	200	SER	N-CA-CB	-6.34	100.99	110.50
2	L	92	TYR	CG-CD1-CE1	-6.34	116.23	121.30
1	O	200	SER	N-CA-CB	-6.34	100.99	110.50
2	L	24	ASN	CA-C-N	6.34	131.14	117.20
2	M	92	TYR	CG-CD1-CE1	-6.34	116.23	121.30
2	N	92	TYR	CG-CD1-CE1	-6.34	116.23	121.30
1	P	200	SER	N-CA-CB	-6.34	101.00	110.50
2	X	92	TYR	CG-CD1-CE1	-6.34	116.23	121.30
2	2	135	TYR	CG-CD1-CE1	-6.33	116.23	121.30
2	H	92	TYR	CG-CD1-CE1	-6.33	116.23	121.30
2	W	92	TYR	CG-CD1-CE1	-6.33	116.23	121.30
2	X	135	TYR	CG-CD1-CE1	-6.33	116.23	121.30
1	E	200	SER	N-CA-CB	-6.33	101.00	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	24	ASN	CA-C-N	6.33	131.13	117.20
2	M	135	TYR	CG-CD1-CE1	-6.32	116.24	121.30
2	Z	92	TYR	CG-CD1-CE1	-6.32	116.24	121.30
2	1	92	TYR	CG-CD1-CE1	-6.32	116.24	121.30
2	I	92	TYR	CG-CD1-CE1	-6.32	116.24	121.30
2	Y	92	TYR	CG-CD1-CE1	-6.32	116.25	121.30
2	Z	135	TYR	CG-CD1-CE1	-6.31	116.25	121.30
2	N	135	TYR	CG-CD1-CE1	-6.31	116.25	121.30
2	I	135	TYR	CG-CD1-CE1	-6.31	116.25	121.30
2	2	92	TYR	CG-CD1-CE1	-6.29	116.27	121.30
2	H	135	TYR	CG-CD1-CE1	-6.29	116.27	121.30
2	Y	135	TYR	CG-CD1-CE1	-6.29	116.27	121.30
1	T	225	ASP	CB-CG-OD1	6.29	123.96	118.30
2	V	135	TYR	CG-CD1-CE1	-6.28	116.27	121.30
2	L	135	TYR	CG-CD1-CE1	-6.27	116.28	121.30
1	C	225	ASP	CB-CG-OD1	6.27	123.94	118.30
2	J	135	TYR	CG-CD1-CE1	-6.27	116.29	121.30
1	A	225	ASP	CB-CG-OD1	6.26	123.94	118.30
1	R	225	ASP	CB-CG-OD1	6.26	123.94	118.30
1	P	225	ASP	CB-CG-OD1	6.26	123.94	118.30
1	S	225	ASP	CB-CG-OD1	6.26	123.94	118.30
1	B	225	ASP	CB-CG-OD1	6.26	123.94	118.30
1	D	225	ASP	CB-CG-OD1	6.26	123.93	118.30
1	F	225	ASP	CB-CG-OD1	6.25	123.92	118.30
1	O	225	ASP	CB-CG-OD1	6.25	123.92	118.30
1	E	225	ASP	CB-CG-OD1	6.25	123.92	118.30
1	U	225	ASP	CB-CG-OD1	6.24	123.91	118.30
1	Q	225	ASP	CB-CG-OD1	6.24	123.92	118.30
2	K	21	THR	C-N-CA	6.24	137.29	121.70
1	G	225	ASP	CB-CG-OD1	6.23	123.91	118.30
2	H	21	THR	C-N-CA	6.23	137.28	121.70
2	1	79	VAL	CA-CB-CG1	6.23	120.25	110.90
2	N	21	THR	C-N-CA	6.23	137.28	121.70
2	X	21	THR	C-N-CA	6.23	137.28	121.70
2	M	79	VAL	CA-CB-CG1	6.23	120.24	110.90
2	M	21	THR	C-N-CA	6.22	137.26	121.70
1	O	138	PHE	CB-CG-CD1	6.22	125.16	120.80
2	2	21	THR	C-N-CA	6.22	137.26	121.70
2	L	21	THR	C-N-CA	6.22	137.25	121.70
2	Z	21	THR	C-N-CA	6.22	137.25	121.70
2	I	21	THR	C-N-CA	6.22	137.25	121.70
2	Y	21	THR	C-N-CA	6.22	137.24	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	79	VAL	CA-CB-CG1	6.21	120.22	110.90
2	V	79	VAL	CA-CB-CG1	6.21	120.22	110.90
2	V	21	THR	C-N-CA	6.21	137.22	121.70
2	W	21	THR	C-N-CA	6.21	137.22	121.70
2	J	79	VAL	CA-CB-CG1	6.21	120.21	110.90
2	2	79	VAL	CA-CB-CG1	6.21	120.21	110.90
1	C	138	PHE	CB-CG-CD1	6.21	125.14	120.80
2	X	79	VAL	CA-CB-CG1	6.21	120.21	110.90
2	K	79	VAL	CA-CB-CG1	6.21	120.21	110.90
2	L	79	VAL	CA-CB-CG1	6.21	120.21	110.90
2	Z	79	VAL	CA-CB-CG1	6.20	120.20	110.90
1	U	138	PHE	CB-CG-CD1	6.20	125.14	120.80
2	I	79	VAL	CA-CB-CG1	6.20	120.20	110.90
1	D	138	PHE	CB-CG-CD1	6.20	125.14	120.80
2	H	79	VAL	CA-CB-CG1	6.20	120.20	110.90
2	Y	79	VAL	CA-CB-CG1	6.20	120.20	110.90
1	T	138	PHE	CB-CG-CD1	6.20	125.14	120.80
2	J	203	LEU	N-CA-CB	6.20	122.79	110.40
2	J	21	THR	C-N-CA	6.20	137.19	121.70
2	1	21	THR	C-N-CA	6.19	137.19	121.70
2	1	203	LEU	N-CA-CB	6.19	122.79	110.40
2	N	79	VAL	CA-CB-CG1	6.19	120.19	110.90
2	2	203	LEU	N-CA-CB	6.19	122.77	110.40
2	L	203	LEU	N-CA-CB	6.18	122.76	110.40
1	G	27	ALA	N-CA-CB	6.18	118.75	110.10
1	C	27	ALA	N-CA-CB	6.18	118.75	110.10
1	F	27	ALA	N-CA-CB	6.17	118.75	110.10
1	D	27	ALA	N-CA-CB	6.17	118.74	110.10
2	Z	203	LEU	N-CA-CB	6.17	122.74	110.40
2	H	203	LEU	N-CA-CB	6.17	122.74	110.40
2	I	203	LEU	N-CA-CB	6.17	122.74	110.40
2	W	203	LEU	N-CA-CB	6.17	122.73	110.40
1	S	138	PHE	CB-CG-CD1	6.16	125.11	120.80
2	V	203	LEU	N-CA-CB	6.16	122.72	110.40
1	B	138	PHE	CB-CG-CD1	6.16	125.11	120.80
2	X	203	LEU	N-CA-CB	6.16	122.72	110.40
1	E	138	PHE	CB-CG-CD1	6.16	125.11	120.80
1	S	27	ALA	N-CA-CB	6.16	118.72	110.10
1	B	27	ALA	N-CA-CB	6.16	118.72	110.10
1	P	27	ALA	N-CA-CB	6.16	118.72	110.10
2	K	203	LEU	N-CA-CB	6.16	122.72	110.40
2	M	203	LEU	N-CA-CB	6.16	122.71	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	203	LEU	N-CA-CB	6.16	122.71	110.40
1	A	138	PHE	CB-CG-CD1	6.16	125.11	120.80
2	Y	203	LEU	N-CA-CB	6.16	122.71	110.40
1	A	27	ALA	N-CA-CB	6.15	118.71	110.10
1	O	27	ALA	N-CA-CB	6.14	118.70	110.10
1	E	27	ALA	N-CA-CB	6.14	118.70	110.10
1	G	138	PHE	CB-CG-CD1	6.14	125.10	120.80
1	U	27	ALA	N-CA-CB	6.14	118.69	110.10
1	R	138	PHE	CB-CG-CD1	6.14	125.09	120.80
1	R	27	ALA	N-CA-CB	6.13	118.69	110.10
1	Q	27	ALA	N-CA-CB	6.13	118.69	110.10
1	T	27	ALA	N-CA-CB	6.13	118.68	110.10
1	F	138	PHE	CB-CG-CD1	6.12	125.08	120.80
1	Q	138	PHE	CB-CG-CD1	6.12	125.08	120.80
1	A	10	ARG	NH1-CZ-NH2	6.11	126.12	119.40
1	P	138	PHE	CB-CG-CD1	6.11	125.08	120.80
1	R	10	ARG	NH1-CZ-NH2	6.11	126.12	119.40
1	D	10	ARG	NH1-CZ-NH2	6.11	126.12	119.40
1	T	10	ARG	NH1-CZ-NH2	6.09	126.10	119.40
1	C	10	ARG	NH1-CZ-NH2	6.09	126.10	119.40
1	U	10	ARG	NH1-CZ-NH2	6.08	126.09	119.40
1	F	10	ARG	NH1-CZ-NH2	6.08	126.08	119.40
1	U	224	TYR	CA-CB-CG	6.08	124.95	113.40
1	P	10	ARG	NH1-CZ-NH2	6.08	126.08	119.40
1	C	224	TYR	CA-CB-CG	6.07	124.94	113.40
1	Q	10	ARG	NH1-CZ-NH2	6.07	126.08	119.40
1	O	224	TYR	CA-CB-CG	6.07	124.93	113.40
1	D	224	TYR	CA-CB-CG	6.07	124.94	113.40
1	S	224	TYR	CA-CB-CG	6.07	124.93	113.40
1	B	224	TYR	CA-CB-CG	6.07	124.93	113.40
1	S	10	ARG	NH1-CZ-NH2	6.07	126.07	119.40
1	F	224	TYR	CA-CB-CG	6.07	124.92	113.40
1	G	224	TYR	CA-CB-CG	6.07	124.92	113.40
1	B	10	ARG	NH1-CZ-NH2	6.07	126.07	119.40
1	P	224	TYR	CA-CB-CG	6.07	124.92	113.40
1	Q	224	TYR	CA-CB-CG	6.07	124.92	113.40
1	T	224	TYR	CA-CB-CG	6.06	124.92	113.40
1	A	224	TYR	CA-CB-CG	6.06	124.92	113.40
1	R	224	TYR	CA-CB-CG	6.06	124.92	113.40
1	O	10	ARG	NH1-CZ-NH2	6.06	126.06	119.40
1	E	224	TYR	CA-CB-CG	6.06	124.91	113.40
1	E	10	ARG	NH1-CZ-NH2	6.05	126.06	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	10	ARG	NH1-CZ-NH2	6.05	126.05	119.40
1	G	147	ARG	CD-NE-CZ	-5.99	115.21	123.60
1	Q	147	ARG	CD-NE-CZ	-5.99	115.21	123.60
1	P	147	ARG	CD-NE-CZ	-5.99	115.22	123.60
1	R	147	ARG	CD-NE-CZ	-5.98	115.22	123.60
1	E	147	ARG	CD-NE-CZ	-5.98	115.22	123.60
1	D	147	ARG	CD-NE-CZ	-5.98	115.23	123.60
1	S	147	ARG	CD-NE-CZ	-5.98	115.23	123.60
1	U	15	PHE	CD1-CE1-CZ	-5.98	112.93	120.10
1	B	147	ARG	CD-NE-CZ	-5.98	115.23	123.60
1	T	147	ARG	CD-NE-CZ	-5.98	115.23	123.60
1	O	147	ARG	CD-NE-CZ	-5.98	115.23	123.60
1	A	147	ARG	CD-NE-CZ	-5.97	115.24	123.60
2	W	133	PHE	CB-CG-CD1	-5.97	116.62	120.80
1	U	147	ARG	CD-NE-CZ	-5.97	115.24	123.60
1	D	15	PHE	CD1-CE1-CZ	-5.97	112.94	120.10
1	C	147	ARG	CD-NE-CZ	-5.97	115.24	123.60
1	F	147	ARG	CD-NE-CZ	-5.96	115.25	123.60
1	F	15	PHE	CD1-CE1-CZ	-5.96	112.94	120.10
1	T	15	PHE	CD1-CE1-CZ	-5.96	112.95	120.10
2	V	133	PHE	CB-CG-CD1	-5.95	116.63	120.80
2	L	133	PHE	CB-CG-CD1	-5.95	116.63	120.80
2	M	133	PHE	CB-CG-CD1	-5.95	116.64	120.80
1	S	15	PHE	CD1-CE1-CZ	-5.94	112.97	120.10
1	B	15	PHE	CD1-CE1-CZ	-5.94	112.97	120.10
1	G	15	PHE	CD1-CE1-CZ	-5.94	112.97	120.10
1	A	15	PHE	CD1-CE1-CZ	-5.94	112.97	120.10
1	O	15	PHE	CD1-CE1-CZ	-5.93	112.98	120.10
1	E	15	PHE	CD1-CE1-CZ	-5.93	112.98	120.10
2	2	133	PHE	CB-CG-CD1	-5.93	116.65	120.80
1	Q	15	PHE	CD1-CE1-CZ	-5.93	112.98	120.10
2	K	133	PHE	CB-CG-CD1	-5.93	116.65	120.80
1	C	15	PHE	CD1-CE1-CZ	-5.92	112.99	120.10
2	N	133	PHE	CB-CG-CD1	-5.92	116.65	120.80
2	1	133	PHE	CB-CG-CD1	-5.92	116.66	120.80
2	J	133	PHE	CB-CG-CD1	-5.92	116.66	120.80
2	Z	133	PHE	CB-CG-CD1	-5.91	116.66	120.80
2	I	133	PHE	CB-CG-CD1	-5.91	116.66	120.80
1	P	15	PHE	CD1-CE1-CZ	-5.91	113.01	120.10
1	R	15	PHE	CD1-CE1-CZ	-5.90	113.02	120.10
2	X	133	PHE	CB-CG-CD1	-5.89	116.68	120.80
2	Y	133	PHE	CB-CG-CD1	-5.88	116.68	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	51	ASP	CB-CG-OD1	5.88	123.59	118.30
2	W	51	ASP	CB-CG-OD1	5.88	123.59	118.30
2	J	135	TYR	N-CA-CB	5.87	121.16	110.60
2	2	51	ASP	CB-CG-OD1	5.86	123.58	118.30
2	K	51	ASP	CB-CG-OD1	5.86	123.58	118.30
2	L	135	TYR	N-CA-CB	5.86	121.15	110.60
2	H	133	PHE	CB-CG-CD1	-5.86	116.70	120.80
2	V	51	ASP	CB-CG-OD1	5.86	123.57	118.30
2	L	51	ASP	CB-CG-OD1	5.86	123.57	118.30
2	X	135	TYR	N-CA-CB	5.86	121.14	110.60
2	Z	51	ASP	CB-CG-OD1	5.85	123.57	118.30
2	1	51	ASP	CB-CG-OD1	5.85	123.57	118.30
2	H	51	ASP	CB-CG-OD1	5.85	123.57	118.30
2	V	135	TYR	N-CA-CB	5.85	121.13	110.60
2	I	51	ASP	CB-CG-OD1	5.85	123.57	118.30
2	J	51	ASP	CB-CG-OD1	5.85	123.57	118.30
2	M	135	TYR	N-CA-CB	5.85	121.13	110.60
2	W	135	TYR	N-CA-CB	5.85	121.13	110.60
2	K	197	ARG	NE-CZ-NH2	-5.85	117.38	120.30
2	H	135	TYR	N-CA-CB	5.85	121.12	110.60
2	Y	135	TYR	N-CA-CB	5.85	121.12	110.60
2	1	135	TYR	N-CA-CB	5.84	121.12	110.60
2	Z	135	TYR	N-CA-CB	5.84	121.12	110.60
2	I	135	TYR	N-CA-CB	5.84	121.12	110.60
1	P	214	SER	N-CA-CB	5.83	119.24	110.50
2	2	135	TYR	N-CA-CB	5.83	121.08	110.60
1	O	214	SER	N-CA-CB	5.83	119.24	110.50
2	K	135	TYR	N-CA-CB	5.83	121.08	110.60
1	F	138	PHE	CB-CG-CD2	-5.82	116.72	120.80
1	T	214	SER	N-CA-CB	5.82	119.23	110.50
1	A	214	SER	N-CA-CB	5.82	119.23	110.50
1	T	138	PHE	CB-CG-CD2	-5.82	116.72	120.80
2	N	51	ASP	CB-CG-OD1	5.82	123.54	118.30
1	C	138	PHE	CB-CG-CD2	-5.82	116.72	120.80
2	Y	51	ASP	CB-CG-OD1	5.82	123.54	118.30
2	N	135	TYR	N-CA-CB	5.82	121.07	110.60
1	E	214	SER	N-CA-CB	5.81	119.22	110.50
1	O	149	PHE	N-CA-CB	5.81	121.06	110.60
1	E	149	PHE	N-CA-CB	5.81	121.06	110.60
1	U	214	SER	N-CA-CB	5.81	119.22	110.50
1	F	149	PHE	N-CA-CB	5.81	121.06	110.60
1	G	149	PHE	N-CA-CB	5.81	121.06	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	197	ARG	NE-CZ-NH2	-5.81	117.39	120.30
2	X	197	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	U	149	PHE	N-CA-CB	5.81	121.05	110.60
2	X	51	ASP	CB-CG-OD1	5.81	123.53	118.30
1	D	149	PHE	N-CA-CB	5.81	121.06	110.60
1	S	149	PHE	N-CA-CB	5.81	121.05	110.60
1	B	149	PHE	N-CA-CB	5.81	121.05	110.60
1	R	149	PHE	N-CA-CB	5.81	121.05	110.60
1	T	149	PHE	N-CA-CB	5.80	121.05	110.60
1	P	149	PHE	N-CA-CB	5.80	121.05	110.60
1	A	149	PHE	N-CA-CB	5.80	121.04	110.60
1	O	138	PHE	CB-CG-CD2	-5.80	116.74	120.80
1	D	214	SER	N-CA-CB	5.80	119.20	110.50
1	R	214	SER	N-CA-CB	5.80	119.20	110.50
1	F	214	SER	N-CA-CB	5.80	119.20	110.50
2	Y	23	GLU	N-CA-CB	5.80	121.04	110.60
2	1	23	GLU	N-CA-CB	5.80	121.04	110.60
2	V	23	GLU	N-CA-CB	5.80	121.04	110.60
1	Q	149	PHE	N-CA-CB	5.80	121.04	110.60
1	C	149	PHE	N-CA-CB	5.80	121.03	110.60
1	S	214	SER	N-CA-CB	5.79	119.19	110.50
2	2	23	GLU	N-CA-CB	5.79	121.03	110.60
1	B	214	SER	N-CA-CB	5.79	119.19	110.50
2	J	23	GLU	N-CA-CB	5.79	121.03	110.60
2	L	23	GLU	N-CA-CB	5.79	121.03	110.60
1	E	138	PHE	CB-CG-CD2	-5.79	116.75	120.80
2	J	197	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	Z	197	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	G	138	PHE	CB-CG-CD2	-5.79	116.75	120.80
2	2	197	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	I	197	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	M	197	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	W	197	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	Z	23	GLU	N-CA-CB	5.78	121.01	110.60
2	M	162	ALA	CB-CA-C	-5.78	101.42	110.10
2	I	23	GLU	N-CA-CB	5.78	121.01	110.60
2	W	162	ALA	CB-CA-C	-5.78	101.42	110.10
1	S	138	PHE	CB-CG-CD2	-5.78	116.75	120.80
1	B	138	PHE	CB-CG-CD2	-5.78	116.75	120.80
1	C	214	SER	N-CA-CB	5.78	119.17	110.50
2	K	162	ALA	CB-CA-C	-5.78	101.43	110.10
1	G	214	SER	N-CA-CB	5.78	119.17	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	214	SER	N-CA-CB	5.78	119.17	110.50
2	Z	162	ALA	CB-CA-C	-5.78	101.44	110.10
2	M	23	GLU	N-CA-CB	5.78	121.00	110.60
2	H	23	GLU	N-CA-CB	5.78	121.00	110.60
2	I	162	ALA	CB-CA-C	-5.78	101.44	110.10
2	1	162	ALA	CB-CA-C	-5.77	101.44	110.10
2	N	23	GLU	N-CA-CB	5.77	120.99	110.60
2	J	162	ALA	CB-CA-C	-5.77	101.44	110.10
2	X	162	ALA	CB-CA-C	-5.77	101.44	110.10
2	K	23	GLU	N-CA-CB	5.77	120.99	110.60
2	W	23	GLU	N-CA-CB	5.77	120.99	110.60
2	X	23	GLU	N-CA-CB	5.77	120.99	110.60
2	V	197	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	P	138	PHE	CB-CG-CD2	-5.77	116.76	120.80
2	L	197	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	Q	138	PHE	CB-CG-CD2	-5.77	116.76	120.80
2	N	162	ALA	CB-CA-C	-5.76	101.45	110.10
2	H	162	ALA	CB-CA-C	-5.76	101.45	110.10
2	V	162	ALA	CB-CA-C	-5.76	101.45	110.10
1	R	138	PHE	CB-CG-CD2	-5.76	116.77	120.80
2	Y	162	ALA	CB-CA-C	-5.76	101.45	110.10
2	L	162	ALA	CB-CA-C	-5.76	101.45	110.10
2	1	197	ARG	NE-CZ-NH2	-5.76	117.42	120.30
2	2	162	ALA	CB-CA-C	-5.76	101.46	110.10
1	U	138	PHE	CB-CG-CD2	-5.75	116.77	120.80
1	A	138	PHE	CB-CG-CD2	-5.75	116.77	120.80
1	D	138	PHE	CB-CG-CD2	-5.75	116.78	120.80
2	Y	197	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	G	200	SER	C-N-CA	5.74	136.05	121.70
1	U	200	SER	C-N-CA	5.74	136.05	121.70
2	H	197	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	Q	200	SER	C-N-CA	5.74	136.05	121.70
1	F	200	SER	C-N-CA	5.74	136.04	121.70
1	S	200	SER	C-N-CA	5.73	136.03	121.70
1	O	200	SER	C-N-CA	5.73	136.03	121.70
1	B	200	SER	C-N-CA	5.73	136.03	121.70
1	R	200	SER	C-N-CA	5.73	136.03	121.70
1	A	200	SER	C-N-CA	5.73	136.03	121.70
1	E	200	SER	C-N-CA	5.73	136.03	121.70
1	P	200	SER	C-N-CA	5.73	136.02	121.70
1	D	200	SER	C-N-CA	5.73	136.02	121.70
1	T	200	SER	C-N-CA	5.72	136.01	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	SER	C-N-CA	5.72	136.01	121.70
1	Q	170	ASP	O-C-N	5.72	131.86	122.70
2	X	72	VAL	CG1-CB-CG2	5.72	120.06	110.90
1	R	170	ASP	O-C-N	5.72	131.85	122.70
1	E	170	ASP	O-C-N	5.72	131.85	122.70
1	P	170	ASP	O-C-N	5.72	131.84	122.70
2	M	72	VAL	CG1-CB-CG2	5.71	120.04	110.90
1	D	170	ASP	O-C-N	5.71	131.84	122.70
1	T	170	ASP	O-C-N	5.71	131.83	122.70
2	2	72	VAL	CG1-CB-CG2	5.71	120.03	110.90
1	A	170	ASP	O-C-N	5.71	131.83	122.70
2	K	72	VAL	CG1-CB-CG2	5.71	120.03	110.90
2	N	72	VAL	CG1-CB-CG2	5.71	120.03	110.90
2	Z	72	VAL	CG1-CB-CG2	5.71	120.03	110.90
2	I	72	VAL	CG1-CB-CG2	5.71	120.03	110.90
2	H	40	TYR	CB-CG-CD1	-5.70	117.58	121.00
2	Y	72	VAL	CG1-CB-CG2	5.70	120.03	110.90
2	L	72	VAL	CG1-CB-CG2	5.70	120.02	110.90
1	G	170	ASP	O-C-N	5.70	131.82	122.70
2	1	72	VAL	CG1-CB-CG2	5.70	120.02	110.90
2	W	72	VAL	CG1-CB-CG2	5.70	120.02	110.90
2	X	40	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	S	170	ASP	O-C-N	5.70	131.81	122.70
1	B	170	ASP	O-C-N	5.70	131.81	122.70
2	M	40	TYR	CB-CG-CD1	-5.69	117.58	121.00
1	U	170	ASP	O-C-N	5.69	131.81	122.70
1	O	170	ASP	O-C-N	5.69	131.81	122.70
2	W	40	TYR	CB-CG-CD1	-5.69	117.58	121.00
2	V	72	VAL	CG1-CB-CG2	5.69	120.01	110.90
2	J	72	VAL	CG1-CB-CG2	5.69	120.01	110.90
2	H	72	VAL	CG1-CB-CG2	5.69	120.00	110.90
1	F	170	ASP	O-C-N	5.69	131.80	122.70
2	Y	40	TYR	CB-CG-CD1	-5.68	117.59	121.00
2	1	40	TYR	CB-CG-CD1	-5.68	117.59	121.00
2	J	40	TYR	CB-CG-CD1	-5.68	117.59	121.00
2	K	40	TYR	CB-CG-CD1	-5.68	117.59	121.00
2	Z	40	TYR	CB-CG-CD1	-5.67	117.60	121.00
2	I	40	TYR	CB-CG-CD1	-5.67	117.60	121.00
2	N	40	TYR	CB-CG-CD1	-5.67	117.60	121.00
2	2	40	TYR	CB-CG-CD1	-5.67	117.60	121.00
1	P	73	TYR	CG-CD1-CE1	-5.67	116.77	121.30
2	V	40	TYR	CB-CG-CD1	-5.66	117.60	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	ASP	O-C-N	5.66	131.76	122.70
1	F	73	TYR	CG-CD1-CE1	-5.66	116.77	121.30
2	J	111	PHE	CB-CG-CD1	-5.66	116.84	120.80
1	E	73	TYR	CG-CD1-CE1	-5.66	116.78	121.30
2	L	40	TYR	CB-CG-CD1	-5.66	117.61	121.00
2	1	111	PHE	CB-CG-CD1	-5.65	116.85	120.80
2	N	195	ARG	NE-CZ-NH1	5.65	123.12	120.30
2	Y	111	PHE	CB-CG-CD1	-5.65	116.85	120.80
1	R	73	TYR	CG-CD1-CE1	-5.64	116.78	121.30
2	W	195	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	1	195	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	H	195	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	C	73	TYR	CG-CD1-CE1	-5.64	116.79	121.30
1	T	73	TYR	CG-CD1-CE1	-5.64	116.79	121.30
1	S	73	TYR	CG-CD1-CE1	-5.63	116.79	121.30
1	B	73	TYR	CG-CD1-CE1	-5.63	116.79	121.30
2	2	195	ARG	NE-CZ-NH1	5.63	123.12	120.30
2	K	195	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	D	73	TYR	CG-CD1-CE1	-5.63	116.80	121.30
2	M	195	ARG	NE-CZ-NH1	5.63	123.11	120.30
2	Y	125	ALA	N-CA-CB	5.63	117.98	110.10
1	U	73	TYR	CG-CD1-CE1	-5.62	116.80	121.30
2	M	62	GLU	O-C-N	-5.62	113.71	122.70
1	G	73	TYR	CG-CD1-CE1	-5.62	116.80	121.30
1	Q	73	TYR	CG-CD1-CE1	-5.62	116.80	121.30
2	Z	111	PHE	CB-CG-CD1	-5.62	116.87	120.80
2	1	125	ALA	N-CA-CB	5.62	117.97	110.10
1	U	101	VAL	CA-CB-CG1	5.62	119.33	110.90
1	A	73	TYR	CG-CD1-CE1	-5.62	116.80	121.30
2	I	111	PHE	CB-CG-CD1	-5.62	116.87	120.80
2	Z	195	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	N	115	ALA	CB-CA-C	-5.62	101.68	110.10
2	I	195	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	L	125	ALA	N-CA-CB	5.62	117.96	110.10
1	P	101	VAL	CA-CB-CG1	5.61	119.32	110.90
2	L	115	ALA	CB-CA-C	-5.61	101.68	110.10
1	O	73	TYR	CG-CD1-CE1	-5.61	116.81	121.30
2	W	62	GLU	O-C-N	-5.61	113.72	122.70
1	A	101	VAL	CA-CB-CG1	5.61	119.31	110.90
2	V	62	GLU	O-C-N	-5.61	113.72	122.70
2	Y	115	ALA	CB-CA-C	-5.61	101.69	110.10
2	L	62	GLU	O-C-N	-5.61	113.72	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	123	TYR	CB-CG-CD2	-5.61	117.64	121.00
2	H	125	ALA	N-CA-CB	5.61	117.95	110.10
1	Q	123	TYR	CB-CG-CD2	-5.61	117.64	121.00
1	T	101	VAL	CA-CB-CG1	5.61	119.31	110.90
1	O	101	VAL	CA-CB-CG1	5.61	119.31	110.90
1	C	101	VAL	CA-CB-CG1	5.61	119.31	110.90
2	J	125	ALA	N-CA-CB	5.61	117.95	110.10
1	E	101	VAL	CA-CB-CG1	5.61	119.31	110.90
1	F	101	VAL	CA-CB-CG1	5.60	119.31	110.90
1	S	101	VAL	CA-CB-CG1	5.60	119.30	110.90
1	B	101	VAL	CA-CB-CG1	5.60	119.30	110.90
1	Q	101	VAL	CA-CB-CG1	5.60	119.31	110.90
1	D	101	VAL	CA-CB-CG1	5.60	119.31	110.90
2	Z	125	ALA	N-CA-CB	5.60	117.94	110.10
2	H	115	ALA	CB-CA-C	-5.60	101.70	110.10
2	I	125	ALA	N-CA-CB	5.60	117.94	110.10
2	L	195	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	2	125	ALA	N-CA-CB	5.60	117.94	110.10
2	V	125	ALA	N-CA-CB	5.60	117.94	110.10
2	X	125	ALA	N-CA-CB	5.60	117.94	110.10
2	K	125	ALA	N-CA-CB	5.60	117.94	110.10
2	N	125	ALA	N-CA-CB	5.60	117.94	110.10
2	X	62	GLU	O-C-N	-5.60	113.74	122.70
2	1	115	ALA	CB-CA-C	-5.60	101.71	110.10
2	V	111	PHE	CB-CG-CD1	-5.60	116.88	120.80
2	L	111	PHE	CB-CG-CD1	-5.60	116.88	120.80
2	X	111	PHE	CB-CG-CD1	-5.59	116.88	120.80
1	G	101	VAL	CA-CB-CG1	5.59	119.29	110.90
2	Z	62	GLU	O-C-N	-5.59	113.76	122.70
2	Z	115	ALA	CB-CA-C	-5.59	101.72	110.10
2	1	62	GLU	O-C-N	-5.59	113.76	122.70
2	V	115	ALA	CB-CA-C	-5.59	101.72	110.10
2	I	62	GLU	O-C-N	-5.59	113.76	122.70
2	I	115	ALA	CB-CA-C	-5.59	101.72	110.10
2	J	62	GLU	O-C-N	-5.59	113.76	122.70
2	X	115	ALA	CB-CA-C	-5.59	101.72	110.10
2	X	195	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	R	101	VAL	CA-CB-CG1	5.59	119.28	110.90
1	P	123	TYR	CB-CG-CD2	-5.59	117.65	121.00
2	W	125	ALA	N-CA-CB	5.59	117.92	110.10
2	M	115	ALA	CB-CA-C	-5.58	101.72	110.10
2	W	115	ALA	CB-CA-C	-5.58	101.72	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	195	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	2	111	PHE	CB-CG-CD1	-5.58	116.89	120.80
2	K	111	PHE	CB-CG-CD1	-5.58	116.89	120.80
2	L	124	TYR	CB-CG-CD1	-5.58	117.65	121.00
2	J	115	ALA	CB-CA-C	-5.58	101.73	110.10
2	K	115	ALA	CB-CA-C	-5.58	101.73	110.10
2	N	62	GLU	O-C-N	-5.58	113.78	122.70
2	2	115	ALA	CB-CA-C	-5.58	101.74	110.10
2	M	125	ALA	N-CA-CB	5.57	117.90	110.10
2	H	62	GLU	O-C-N	-5.57	113.79	122.70
1	O	123	TYR	CB-CG-CD2	-5.57	117.66	121.00
2	Y	62	GLU	O-C-N	-5.57	113.79	122.70
1	U	123	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	S	123	TYR	CB-CG-CD2	-5.57	117.66	121.00
2	2	62	GLU	O-C-N	-5.57	113.79	122.70
1	B	123	TYR	CB-CG-CD2	-5.57	117.66	121.00
2	1	124	TYR	CB-CG-CD1	-5.57	117.66	121.00
2	Y	195	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	E	123	TYR	CB-CG-CD2	-5.56	117.66	121.00
1	T	123	TYR	CB-CG-CD2	-5.56	117.67	121.00
2	N	111	PHE	CB-CG-CD1	-5.56	116.91	120.80
1	C	123	TYR	CB-CG-CD2	-5.56	117.67	121.00
2	H	111	PHE	CB-CG-CD1	-5.56	116.91	120.80
2	V	124	TYR	CB-CG-CD1	-5.55	117.67	121.00
2	K	62	GLU	O-C-N	-5.55	113.81	122.70
1	Q	222	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	F	222	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	O	205	GLU	N-CA-CB	5.54	120.57	110.60
2	V	195	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	T	205	GLU	N-CA-CB	5.54	120.57	110.60
1	D	205	GLU	N-CA-CB	5.54	120.56	110.60
1	G	205	GLU	N-CA-CB	5.53	120.56	110.60
1	A	123	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	Q	205	GLU	N-CA-CB	5.53	120.56	110.60
1	R	123	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	R	205	GLU	N-CA-CB	5.53	120.56	110.60
1	U	205	GLU	N-CA-CB	5.53	120.56	110.60
1	A	205	GLU	N-CA-CB	5.53	120.55	110.60
1	P	205	GLU	N-CA-CB	5.53	120.55	110.60
2	M	111	PHE	CB-CG-CD1	-5.53	116.93	120.80
2	W	111	PHE	CB-CG-CD1	-5.53	116.93	120.80
1	S	205	GLU	N-CA-CB	5.53	120.55	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	222	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	B	205	GLU	N-CA-CB	5.53	120.55	110.60
1	E	205	GLU	N-CA-CB	5.53	120.55	110.60
2	Z	124	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	U	222	ARG	NE-CZ-NH1	-5.52	117.54	120.30
2	I	124	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	C	205	GLU	N-CA-CB	5.52	120.54	110.60
1	F	123	TYR	CB-CG-CD2	-5.52	117.69	121.00
2	N	124	TYR	CB-CG-CD1	-5.52	117.69	121.00
2	X	124	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	D	123	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	P	222	ARG	NE-CZ-NH1	-5.52	117.54	120.30
2	W	124	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	F	205	GLU	N-CA-CB	5.51	120.52	110.60
2	H	124	TYR	CB-CG-CD1	-5.51	117.69	121.00
2	Y	124	TYR	CB-CG-CD1	-5.51	117.69	121.00
1	T	222	ARG	NE-CZ-NH1	-5.50	117.55	120.30
2	2	124	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	C	222	ARG	NE-CZ-NH1	-5.50	117.55	120.30
2	K	124	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	O	222	ARG	NE-CZ-NH1	-5.50	117.55	120.30
2	J	124	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	S	222	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	B	222	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	D	222	ARG	NE-CZ-NH1	-5.48	117.56	120.30
2	M	124	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	T	139	ALA	N-CA-CB	-5.47	102.45	110.10
2	N	134	VAL	CA-CB-CG2	5.46	119.09	110.90
1	O	139	ALA	N-CA-CB	-5.46	102.46	110.10
2	V	134	VAL	CA-CB-CG2	5.46	119.08	110.90
1	A	222	ARG	NE-CZ-NH1	-5.45	117.57	120.30
2	X	134	VAL	CA-CB-CG2	5.45	119.08	110.90
1	R	222	ARG	NE-CZ-NH1	-5.45	117.57	120.30
1	F	139	ALA	N-CA-CB	-5.45	102.47	110.10
2	J	134	VAL	CA-CB-CG2	5.45	119.08	110.90
1	P	139	ALA	N-CA-CB	-5.45	102.47	110.10
1	C	139	ALA	N-CA-CB	-5.45	102.48	110.10
1	E	222	ARG	NE-CZ-NH1	-5.44	117.58	120.30
2	1	134	VAL	CA-CB-CG2	5.44	119.06	110.90
1	U	139	ALA	N-CA-CB	-5.44	102.48	110.10
1	D	139	ALA	N-CA-CB	-5.44	102.48	110.10
2	2	134	VAL	CA-CB-CG2	5.44	119.06	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	134	VAL	CA-CB-CG2	5.44	119.06	110.90
1	S	139	ALA	N-CA-CB	-5.43	102.49	110.10
1	G	152	ASP	N-CA-CB	-5.43	100.82	110.60
1	A	139	ALA	N-CA-CB	-5.43	102.49	110.10
1	B	139	ALA	N-CA-CB	-5.43	102.49	110.10
2	Z	134	VAL	CA-CB-CG2	5.43	119.05	110.90
2	I	134	VAL	CA-CB-CG2	5.43	119.05	110.90
1	E	139	ALA	N-CA-CB	-5.43	102.50	110.10
1	A	152	ASP	N-CA-CB	-5.43	100.83	110.60
1	Q	139	ALA	N-CA-CB	-5.43	102.50	110.10
2	M	134	VAL	CA-CB-CG2	5.42	119.04	110.90
1	O	152	ASP	N-CA-CB	-5.42	100.84	110.60
2	W	134	VAL	CA-CB-CG2	5.42	119.04	110.90
2	Y	134	VAL	CA-CB-CG2	5.42	119.04	110.90
1	G	139	ALA	N-CA-CB	-5.42	102.51	110.10
1	R	139	ALA	N-CA-CB	-5.42	102.51	110.10
1	S	152	ASP	N-CA-CB	-5.42	100.85	110.60
1	B	152	ASP	N-CA-CB	-5.42	100.85	110.60
1	F	152	ASP	N-CA-CB	-5.42	100.85	110.60
1	Q	152	ASP	N-CA-CB	-5.42	100.85	110.60
1	P	152	ASP	N-CA-CB	-5.42	100.85	110.60
1	D	152	ASP	N-CA-CB	-5.42	100.85	110.60
2	K	134	VAL	CA-CB-CG2	5.41	119.02	110.90
1	G	91	PHE	CB-CG-CD2	5.41	124.59	120.80
1	T	152	ASP	N-CA-CB	-5.41	100.86	110.60
1	U	152	ASP	N-CA-CB	-5.41	100.86	110.60
1	R	152	ASP	N-CA-CB	-5.41	100.87	110.60
1	U	105	SER	N-CA-CB	5.41	118.61	110.50
2	H	134	VAL	CA-CB-CG2	5.41	119.01	110.90
1	D	105	SER	N-CA-CB	5.41	118.61	110.50
1	A	105	SER	N-CA-CB	5.40	118.61	110.50
1	T	105	SER	N-CA-CB	5.40	118.60	110.50
1	G	105	SER	N-CA-CB	5.40	118.60	110.50
1	C	152	ASP	N-CA-CB	-5.40	100.88	110.60
1	O	105	SER	N-CA-CB	5.40	118.60	110.50
1	R	105	SER	N-CA-CB	5.40	118.60	110.50
1	E	105	SER	N-CA-CB	5.40	118.60	110.50
1	U	91	PHE	CB-CG-CD2	5.40	124.58	120.80
1	E	152	ASP	N-CA-CB	-5.40	100.89	110.60
2	X	93	MET	N-CA-C	-5.39	96.44	111.00
1	S	105	SER	N-CA-CB	5.39	118.59	110.50
1	B	105	SER	N-CA-CB	5.39	118.59	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	93	MET	N-CA-C	-5.39	96.44	111.00
1	C	105	SER	N-CA-CB	5.39	118.59	110.50
1	Q	105	SER	N-CA-CB	5.39	118.58	110.50
2	Z	93	MET	N-CA-C	-5.38	96.46	111.00
2	2	149	ASP	CB-CG-OD2	5.38	123.15	118.30
2	V	93	MET	N-CA-C	-5.38	96.46	111.00
2	I	93	MET	N-CA-C	-5.38	96.46	111.00
2	W	93	MET	N-CA-C	-5.38	96.46	111.00
2	N	93	MET	N-CA-C	-5.38	96.47	111.00
2	H	93	MET	N-CA-C	-5.38	96.47	111.00
2	H	149	ASP	CB-CG-OD2	5.38	123.14	118.30
1	F	105	SER	N-CA-CB	5.38	118.57	110.50
2	J	149	ASP	CB-CG-OD2	5.38	123.14	118.30
1	P	105	SER	N-CA-CB	5.38	118.57	110.50
1	D	91	PHE	CB-CG-CD2	5.37	124.56	120.80
2	L	93	MET	N-CA-C	-5.37	96.49	111.00
2	K	93	MET	N-CA-C	-5.37	96.50	111.00
2	M	93	MET	N-CA-C	-5.37	96.50	111.00
2	Y	93	MET	N-CA-C	-5.37	96.50	111.00
2	1	93	MET	N-CA-C	-5.37	96.50	111.00
2	N	149	ASP	CB-CG-OD2	5.37	123.13	118.30
2	J	93	MET	N-CA-C	-5.37	96.50	111.00
1	Q	91	PHE	CB-CG-CD2	5.37	124.56	120.80
2	X	149	ASP	CB-CG-OD2	5.37	123.13	118.30
1	E	91	PHE	CB-CG-CD2	5.36	124.55	120.80
2	Z	149	ASP	CB-CG-OD2	5.36	123.12	118.30
2	I	149	ASP	CB-CG-OD2	5.36	123.12	118.30
2	1	149	ASP	CB-CG-OD2	5.35	123.12	118.30
1	O	91	PHE	CB-CG-CD2	5.34	124.54	120.80
2	V	149	ASP	CB-CG-OD2	5.34	123.11	118.30
2	Y	149	ASP	CB-CG-OD2	5.34	123.11	118.30
2	L	149	ASP	CB-CG-OD2	5.34	123.11	118.30
1	T	91	PHE	CB-CG-CD2	5.34	124.54	120.80
1	C	91	PHE	CB-CG-CD2	5.34	124.54	120.80
1	S	91	PHE	CB-CG-CD2	5.34	124.54	120.80
1	B	91	PHE	CB-CG-CD2	5.34	124.54	120.80
2	M	149	ASP	CB-CG-OD2	5.33	123.09	118.30
2	W	149	ASP	CB-CG-OD2	5.32	123.09	118.30
2	K	180	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	F	91	PHE	CB-CG-CD2	5.32	124.52	120.80
1	P	91	PHE	CB-CG-CD2	5.32	124.52	120.80
2	K	149	ASP	CB-CG-OD2	5.31	123.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	180	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	W	180	ARG	NE-CZ-NH2	-5.29	117.65	120.30
2	1	110	VAL	N-CA-CB	5.29	123.13	111.50
2	J	110	VAL	N-CA-CB	5.29	123.13	111.50
2	J	180	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	J	14	MET	CG-SD-CE	-5.28	91.75	100.20
2	H	110	VAL	N-CA-CB	5.28	123.11	111.50
2	W	14	MET	CG-SD-CE	-5.28	91.76	100.20
2	Y	110	VAL	N-CA-CB	5.28	123.11	111.50
2	Z	110	VAL	N-CA-CB	5.28	123.11	111.50
2	I	110	VAL	N-CA-CB	5.28	123.11	111.50
2	W	110	VAL	N-CA-CB	5.28	123.11	111.50
2	2	14	MET	CG-SD-CE	-5.27	91.76	100.20
2	N	110	VAL	N-CA-CB	5.27	123.10	111.50
2	2	110	VAL	N-CA-CB	5.27	123.10	111.50
2	H	14	MET	CG-SD-CE	-5.27	91.76	100.20
2	K	14	MET	CG-SD-CE	-5.27	91.76	100.20
2	Y	14	MET	CG-SD-CE	-5.27	91.76	100.20
2	L	110	VAL	N-CA-CB	5.27	123.10	111.50
2	2	101	VAL	CA-CB-CG1	5.27	118.81	110.90
2	2	180	ARG	NE-CZ-NH2	-5.27	117.67	120.30
2	N	14	MET	CG-SD-CE	-5.27	91.77	100.20
1	A	91	PHE	CB-CG-CD2	5.27	124.49	120.80
2	X	14	MET	CG-SD-CE	-5.27	91.77	100.20
2	K	110	VAL	N-CA-CB	5.27	123.09	111.50
1	R	91	PHE	CB-CG-CD2	5.27	124.49	120.80
2	V	14	MET	CG-SD-CE	-5.27	91.78	100.20
2	Y	101	VAL	CA-CB-CG1	5.27	118.80	110.90
2	V	110	VAL	N-CA-CB	5.26	123.08	111.50
2	M	110	VAL	N-CA-CB	5.26	123.08	111.50
2	L	180	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	Z	14	MET	CG-SD-CE	-5.26	91.78	100.20
2	I	14	MET	CG-SD-CE	-5.26	91.78	100.20
2	Y	180	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	1	14	MET	CG-SD-CE	-5.26	91.78	100.20
2	W	101	VAL	CA-CB-CG1	5.26	118.79	110.90
2	J	101	VAL	CA-CB-CG1	5.25	118.78	110.90
2	M	14	MET	CG-SD-CE	-5.25	91.80	100.20
2	1	101	VAL	CA-CB-CG1	5.25	118.77	110.90
2	V	101	VAL	CA-CB-CG1	5.25	118.77	110.90
2	V	142	TYR	CG-CD1-CE1	5.25	125.50	121.30
2	M	101	VAL	CA-CB-CG1	5.25	118.77	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	101	VAL	CA-CB-CG1	5.25	118.77	110.90
2	X	110	VAL	N-CA-CB	5.25	123.04	111.50
2	Z	101	VAL	CA-CB-CG1	5.24	118.77	110.90
2	2	142	TYR	CG-CD1-CE1	5.24	125.50	121.30
2	I	101	VAL	CA-CB-CG1	5.24	118.77	110.90
2	K	142	TYR	CG-CD1-CE1	5.24	125.50	121.30
2	L	14	MET	CG-SD-CE	-5.24	91.81	100.20
2	H	101	VAL	CA-CB-CG1	5.24	118.76	110.90
2	V	180	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	M	142	TYR	CG-CD1-CE1	5.24	125.49	121.30
2	1	142	TYR	CG-CD1-CE1	5.24	125.49	121.30
2	W	142	TYR	CG-CD1-CE1	5.24	125.49	121.30
2	J	142	TYR	CG-CD1-CE1	5.24	125.49	121.30
2	K	101	VAL	CA-CB-CG1	5.24	118.75	110.90
1	T	15	PHE	CB-CG-CD1	-5.23	117.14	120.80
1	C	15	PHE	CB-CG-CD1	-5.23	117.14	120.80
2	X	101	VAL	CA-CB-CG1	5.23	118.75	110.90
2	Z	180	ARG	NE-CZ-NH2	-5.23	117.69	120.30
2	I	180	ARG	NE-CZ-NH2	-5.23	117.69	120.30
2	L	101	VAL	CA-CB-CG1	5.23	118.74	110.90
2	N	180	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	Q	15	PHE	CB-CG-CD1	-5.22	117.14	120.80
1	O	15	PHE	CB-CG-CD1	-5.22	117.14	120.80
1	E	15	PHE	CB-CG-CD1	-5.22	117.14	120.80
1	P	15	PHE	CB-CG-CD1	-5.22	117.15	120.80
1	D	15	PHE	CB-CG-CD1	-5.22	117.15	120.80
1	S	15	PHE	CB-CG-CD1	-5.22	117.15	120.80
1	B	15	PHE	CB-CG-CD1	-5.22	117.15	120.80
2	L	142	TYR	CG-CD1-CE1	5.22	125.47	121.30
1	G	15	PHE	CB-CG-CD1	-5.21	117.15	120.80
1	U	15	PHE	CB-CG-CD1	-5.21	117.15	120.80
1	F	15	PHE	CB-CG-CD1	-5.21	117.15	120.80
2	N	142	TYR	CG-CD1-CE1	5.21	125.47	121.30
1	A	15	PHE	CB-CG-CD1	-5.21	117.15	120.80
2	H	142	TYR	CG-CD1-CE1	5.21	125.47	121.30
1	R	15	PHE	CB-CG-CD1	-5.21	117.15	120.80
2	Y	142	TYR	CG-CD1-CE1	5.21	125.47	121.30
2	Z	142	TYR	CG-CD1-CE1	5.20	125.46	121.30
2	I	142	TYR	CG-CD1-CE1	5.20	125.46	121.30
2	M	180	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	P	178	ARG	NE-CZ-NH2	5.20	122.90	120.30
2	H	180	ARG	NE-CZ-NH2	-5.19	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	178	ARG	NE-CZ-NH2	5.19	122.89	120.30
2	X	142	TYR	CG-CD1-CE1	5.18	125.44	121.30
2	1	180	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	E	178	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	T	132	TYR	CD1-CG-CD2	5.15	123.57	117.90
1	S	178	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	B	178	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	G	132	TYR	CD1-CG-CD2	5.14	123.56	117.90
1	Q	132	TYR	CD1-CG-CD2	5.14	123.56	117.90
1	G	178	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	A	178	ARG	NE-CZ-NH2	5.14	122.87	120.30
2	H	161	ALA	N-CA-CB	5.14	117.29	110.10
1	C	132	TYR	CD1-CG-CD2	5.14	123.55	117.90
1	D	132	TYR	CD1-CG-CD2	5.14	123.55	117.90
2	X	161	ALA	N-CA-CB	5.13	117.29	110.10
2	Y	161	ALA	N-CA-CB	5.13	117.29	110.10
1	A	132	TYR	CD1-CG-CD2	5.13	123.54	117.90
2	V	161	ALA	N-CA-CB	5.13	117.28	110.10
1	R	132	TYR	CD1-CG-CD2	5.13	123.54	117.90
2	L	161	ALA	N-CA-CB	5.13	117.28	110.10
1	F	178	ARG	NE-CZ-NH2	5.12	122.86	120.30
2	K	161	ALA	N-CA-CB	5.12	117.27	110.10
1	S	132	TYR	CD1-CG-CD2	5.12	123.53	117.90
2	Z	161	ALA	N-CA-CB	5.12	117.27	110.10
1	B	132	TYR	CD1-CG-CD2	5.12	123.53	117.90
2	I	161	ALA	N-CA-CB	5.12	117.27	110.10
2	1	161	ALA	N-CA-CB	5.12	117.27	110.10
1	O	132	TYR	CD1-CG-CD2	5.12	123.53	117.90
2	J	161	ALA	N-CA-CB	5.12	117.27	110.10
1	E	132	TYR	CD1-CG-CD2	5.12	123.53	117.90
2	M	35	PHE	N-CA-CB	5.11	119.80	110.60
2	M	161	ALA	N-CA-CB	5.11	117.26	110.10
2	W	161	ALA	N-CA-CB	5.11	117.26	110.10
2	L	35	PHE	N-CA-CB	5.11	119.81	110.60
2	J	35	PHE	N-CA-CB	5.11	119.80	110.60
2	N	161	ALA	N-CA-CB	5.11	117.25	110.10
1	C	178	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	U	132	TYR	CD1-CG-CD2	5.11	123.52	117.90
1	R	178	ARG	NE-CZ-NH2	5.11	122.85	120.30
2	Z	35	PHE	N-CA-CB	5.11	119.79	110.60
1	F	132	TYR	CD1-CG-CD2	5.11	123.52	117.90
2	I	35	PHE	N-CA-CB	5.11	119.79	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	35	PHE	N-CA-CB	5.11	119.79	110.60
1	P	132	TYR	CD1-CG-CD2	5.10	123.51	117.90
2	X	35	PHE	N-CA-CB	5.10	119.78	110.60
2	V	35	PHE	N-CA-CB	5.10	119.78	110.60
2	2	161	ALA	N-CA-CB	5.10	117.23	110.10
2	2	35	PHE	N-CA-CB	5.09	119.77	110.60
1	D	178	ARG	NE-CZ-NH2	5.09	122.85	120.30
2	Y	35	PHE	N-CA-CB	5.09	119.76	110.60
2	N	35	PHE	N-CA-CB	5.09	119.76	110.60
2	K	35	PHE	N-CA-CB	5.09	119.76	110.60
2	1	35	PHE	N-CA-CB	5.09	119.76	110.60
2	H	35	PHE	N-CA-CB	5.08	119.75	110.60
1	O	178	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	Q	178	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	U	178	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	A	10	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	R	10	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	T	10	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	U	10	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	C	10	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	D	10	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	F	10	ARG	NE-CZ-NH1	-5.01	117.80	120.30
1	P	10	ARG	NE-CZ-NH1	-5.01	117.80	120.30

There are no chirality outliers.

All (168) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	124	TYR	Sidechain
2	1	165	ARG	Sidechain
2	1	180	ARG	Sidechain
2	1	24	ASN	Peptide
2	1	28	HIS	Sidechain
2	1	66	TYR	Sidechain
2	1	70	ARG	Sidechain
2	1	95	TYR	Sidechain
2	2	124	TYR	Sidechain
2	2	165	ARG	Sidechain
2	2	180	ARG	Sidechain
2	2	24	ASN	Peptide
2	2	28	HIS	Sidechain
2	2	66	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	2	70	ARG	Sidechain
2	2	95	TYR	Sidechain
1	A	147	ARG	Sidechain
1	A	20	ARG	Sidechain
1	A	86	ARG	Sidechain
1	A	91	PHE	Sidechain
1	B	147	ARG	Sidechain
1	B	20	ARG	Sidechain
1	B	86	ARG	Sidechain
1	B	91	PHE	Sidechain
1	C	147	ARG	Sidechain
1	C	20	ARG	Sidechain
1	C	86	ARG	Sidechain
1	C	91	PHE	Sidechain
1	D	147	ARG	Sidechain
1	D	20	ARG	Sidechain
1	D	86	ARG	Sidechain
1	D	91	PHE	Sidechain
1	E	147	ARG	Sidechain
1	E	20	ARG	Sidechain
1	E	86	ARG	Sidechain
1	E	91	PHE	Sidechain
1	F	147	ARG	Sidechain
1	F	20	ARG	Sidechain
1	F	86	ARG	Sidechain
1	F	91	PHE	Sidechain
1	G	147	ARG	Sidechain
1	G	20	ARG	Sidechain
1	G	86	ARG	Sidechain
1	G	91	PHE	Sidechain
2	H	124	TYR	Sidechain
2	H	165	ARG	Sidechain
2	H	180	ARG	Sidechain
2	H	24	ASN	Peptide
2	H	28	HIS	Sidechain
2	H	66	TYR	Sidechain
2	H	70	ARG	Sidechain
2	H	95	TYR	Sidechain
2	I	124	TYR	Sidechain
2	I	165	ARG	Sidechain
2	I	180	ARG	Sidechain
2	I	24	ASN	Peptide

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Mol	Chain	Res	Type	Group
2	I	28	HIS	Sidechain
2	I	66	TYR	Sidechain
2	I	70	ARG	Sidechain
2	I	95	TYR	Sidechain
2	J	124	TYR	Sidechain
2	J	165	ARG	Sidechain
2	J	180	ARG	Sidechain
2	J	24	ASN	Peptide
2	J	28	HIS	Sidechain
2	J	66	TYR	Sidechain
2	J	70	ARG	Sidechain
2	J	95	TYR	Sidechain
2	K	124	TYR	Sidechain
2	K	165	ARG	Sidechain
2	K	180	ARG	Sidechain
2	K	24	ASN	Peptide
2	K	28	HIS	Sidechain
2	K	66	TYR	Sidechain
2	K	70	ARG	Sidechain
2	K	95	TYR	Sidechain
2	L	124	TYR	Sidechain
2	L	165	ARG	Sidechain
2	L	180	ARG	Sidechain
2	L	24	ASN	Peptide
2	L	28	HIS	Sidechain
2	L	66	TYR	Sidechain
2	L	70	ARG	Sidechain
2	L	95	TYR	Sidechain
2	M	124	TYR	Sidechain
2	M	165	ARG	Sidechain
2	M	180	ARG	Sidechain
2	M	24	ASN	Peptide
2	M	28	HIS	Sidechain
2	M	66	TYR	Sidechain
2	M	70	ARG	Sidechain
2	M	95	TYR	Sidechain
2	N	124	TYR	Sidechain
2	N	165	ARG	Sidechain
2	N	180	ARG	Sidechain
2	N	24	ASN	Peptide
2	N	28	HIS	Sidechain
2	N	66	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	N	70	ARG	Sidechain
2	N	95	TYR	Sidechain
1	O	147	ARG	Sidechain
1	O	20	ARG	Sidechain
1	O	86	ARG	Sidechain
1	O	91	PHE	Sidechain
1	P	147	ARG	Sidechain
1	P	20	ARG	Sidechain
1	P	86	ARG	Sidechain
1	P	91	PHE	Sidechain
1	Q	147	ARG	Sidechain
1	Q	20	ARG	Sidechain
1	Q	86	ARG	Sidechain
1	Q	91	PHE	Sidechain
1	R	147	ARG	Sidechain
1	R	20	ARG	Sidechain
1	R	86	ARG	Sidechain
1	R	91	PHE	Sidechain
1	S	147	ARG	Sidechain
1	S	20	ARG	Sidechain
1	S	86	ARG	Sidechain
1	S	91	PHE	Sidechain
1	T	147	ARG	Sidechain
1	T	20	ARG	Sidechain
1	T	86	ARG	Sidechain
1	T	91	PHE	Sidechain
1	U	147	ARG	Sidechain
1	U	20	ARG	Sidechain
1	U	86	ARG	Sidechain
1	U	91	PHE	Sidechain
2	V	124	TYR	Sidechain
2	V	165	ARG	Sidechain
2	V	180	ARG	Sidechain
2	V	24	ASN	Peptide
2	V	28	HIS	Sidechain
2	V	66	TYR	Sidechain
2	V	70	ARG	Sidechain
2	V	95	TYR	Sidechain
2	W	124	TYR	Sidechain
2	W	165	ARG	Sidechain
2	W	180	ARG	Sidechain
2	W	24	ASN	Peptide

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Mol	Chain	Res	Type	Group
2	W	28	HIS	Sidechain
2	W	66	TYR	Sidechain
2	W	70	ARG	Sidechain
2	W	95	TYR	Sidechain
2	X	124	TYR	Sidechain
2	X	165	ARG	Sidechain
2	X	180	ARG	Sidechain
2	X	24	ASN	Peptide
2	X	28	HIS	Sidechain
2	X	66	TYR	Sidechain
2	X	70	ARG	Sidechain
2	X	95	TYR	Sidechain
2	Y	124	TYR	Sidechain
2	Y	165	ARG	Sidechain
2	Y	180	ARG	Sidechain
2	Y	24	ASN	Peptide
2	Y	28	HIS	Sidechain
2	Y	66	TYR	Sidechain
2	Y	70	ARG	Sidechain
2	Y	95	TYR	Sidechain
2	Z	124	TYR	Sidechain
2	Z	165	ARG	Sidechain
2	Z	180	ARG	Sidechain
2	Z	24	ASN	Peptide
2	Z	28	HIS	Sidechain
2	Z	66	TYR	Sidechain
2	Z	70	ARG	Sidechain
2	Z	95	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1744	0	1782	23	0
1	B	1744	0	1782	23	0
1	C	1744	0	1782	23	0
1	D	1744	0	1782	23	0
1	E	1744	0	1782	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1744	0	1782	24	0
1	G	1744	0	1782	23	0
1	O	1744	0	1782	23	0
1	P	1744	0	1782	24	0
1	Q	1744	0	1782	23	0
1	R	1744	0	1782	23	0
1	S	1744	0	1782	23	0
1	T	1744	0	1782	23	0
1	U	1744	0	1782	23	0
2	1	1558	0	1609	31	0
2	2	1558	0	1609	31	0
2	H	1558	0	1609	32	0
2	I	1558	0	1609	31	0
2	J	1558	0	1609	31	0
2	K	1558	0	1609	31	0
2	L	1558	0	1609	31	0
2	M	1558	0	1609	30	0
2	N	1558	0	1609	31	0
2	V	1558	0	1609	32	0
2	W	1558	0	1609	30	0
2	X	1558	0	1609	31	0
2	Y	1558	0	1609	32	0
2	Z	1558	0	1609	31	0
All	All	46228	0	47474	479	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 5.

All (479) 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:S:11:ALA:CB	1:T:10:ARG:CZ	1.95	1.44
1:B:11:ALA:CB	1:C:10:ARG:CZ	1.95	1.43
1:T:11:ALA:CB	1:U:10:ARG:CZ	1.95	1.43
1:A:11:ALA:CB	1:B:10:ARG:CZ	1.95	1.43
1:S:10:ARG:CZ	1:R:11:ALA:CB	1.95	1.43
1:C:11:ALA:CB	1:D:10:ARG:CZ	1.95	1.43
1:G:11:ALA:CB	1:A:10:ARG:CZ	1.95	1.42
1:Q:11:ALA:CB	1:R:10:ARG:CZ	1.95	1.42
1:U:11:ALA:CB	1:O:10:ARG:CZ	1.95	1.42
1:O:11:ALA:CB	1:P:10:ARG:CZ	1.95	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:ARG:CZ	1:E:11:ALA:CB	1.95	1.42
1:F:11:ALA:CB	1:G:10:ARG:CZ	1.95	1.42
1:D:11:ALA:CB	1:E:10:ARG:CZ	1.95	1.42
1:P:11:ALA:CB	1:Q:10:ARG:CZ	1.95	1.41
1:A:11:ALA:HB1	1:B:10:ARG:NH1	1.03	1.36
1:S:10:ARG:NH1	1:R:11:ALA:HB1	1.03	1.36
1:G:11:ALA:HB1	1:A:10:ARG:NH1	1.03	1.35
1:Q:11:ALA:HB1	1:R:10:ARG:NH1	1.03	1.35
1:S:11:ALA:HB1	1:T:10:ARG:NH1	1.03	1.35
1:B:11:ALA:HB1	1:C:10:ARG:NH1	1.03	1.34
1:F:11:ALA:HB1	1:G:10:ARG:NH1	1.03	1.34
1:P:11:ALA:HB1	1:Q:10:ARG:NH1	1.03	1.34
1:S:11:ALA:HB1	1:T:10:ARG:CZ	1.58	1.33
1:B:11:ALA:HB1	1:C:10:ARG:CZ	1.58	1.33
1:T:11:ALA:HB1	1:U:10:ARG:CZ	1.58	1.32
1:T:11:ALA:HB1	1:U:10:ARG:NH1	1.03	1.32
1:C:11:ALA:HB1	1:D:10:ARG:CZ	1.58	1.32
1:C:11:ALA:HB1	1:D:10:ARG:NH1	1.03	1.32
1:F:10:ARG:NH1	1:E:11:ALA:HB1	1.03	1.31
1:G:11:ALA:HB1	1:A:10:ARG:CZ	1.58	1.31
1:Q:11:ALA:HB1	1:R:10:ARG:CZ	1.58	1.31
1:U:11:ALA:HB1	1:O:10:ARG:NH1	1.03	1.31
1:O:11:ALA:HB1	1:P:10:ARG:NH1	1.03	1.31
1:P:11:ALA:HB1	1:Q:10:ARG:CZ	1.58	1.31
1:F:11:ALA:HB1	1:G:10:ARG:CZ	1.58	1.31
1:D:11:ALA:HB1	1:E:10:ARG:NH1	1.03	1.31
1:U:11:ALA:HB1	1:O:10:ARG:CZ	1.58	1.29
1:Q:11:ALA:CB	1:R:10:ARG:NH1	1.95	1.29
1:D:11:ALA:HB1	1:E:10:ARG:CZ	1.58	1.29
1:S:10:ARG:CZ	1:R:11:ALA:HB1	1.58	1.29
1:G:11:ALA:CB	1:A:10:ARG:NH1	1.95	1.29
1:A:11:ALA:HB1	1:B:10:ARG:CZ	1.58	1.28
1:B:11:ALA:CB	1:C:10:ARG:NH1	1.95	1.27
1:S:11:ALA:CB	1:T:10:ARG:NH1	1.95	1.27
1:F:11:ALA:CB	1:G:10:ARG:NH1	1.95	1.27
1:P:11:ALA:CB	1:Q:10:ARG:NH1	1.95	1.27
1:T:11:ALA:CB	1:U:10:ARG:NH1	1.96	1.26
1:C:11:ALA:CB	1:D:10:ARG:NH1	1.96	1.26
1:A:11:ALA:CB	1:B:10:ARG:NH1	1.95	1.26
1:S:10:ARG:NH1	1:R:11:ALA:CB	1.95	1.25
1:O:11:ALA:HB1	1:P:10:ARG:CZ	1.58	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:11:ALA:CB	1:O:10:ARG:NH1	1.95	1.24
1:F:10:ARG:CZ	1:E:11:ALA:HB1	1.58	1.24
1:D:11:ALA:CB	1:E:10:ARG:NH1	1.95	1.24
1:F:10:ARG:NH1	1:E:11:ALA:CB	1.95	1.24
1:O:11:ALA:CB	1:P:10:ARG:NH1	1.95	1.24
1:D:11:ALA:HB2	1:E:10:ARG:CZ	1.64	1.22
1:U:11:ALA:HB2	1:O:10:ARG:CZ	1.64	1.22
1:S:10:ARG:CZ	1:R:11:ALA:HB2	1.64	1.15
1:A:11:ALA:HB2	1:B:10:ARG:CZ	1.64	1.15
1:G:11:ALA:HB2	1:A:10:ARG:CZ	1.64	1.14
1:Q:11:ALA:HB2	1:R:10:ARG:CZ	1.64	1.14
1:S:11:ALA:HB2	1:T:10:ARG:CZ	1.64	1.13
1:B:11:ALA:HB2	1:C:10:ARG:CZ	1.64	1.13
1:U:11:ALA:HB2	1:O:10:ARG:NH2	1.65	1.12
1:F:11:ALA:HB2	1:G:10:ARG:NH2	1.65	1.12
1:D:11:ALA:HB2	1:E:10:ARG:NH2	1.65	1.12
1:P:11:ALA:HB2	1:Q:10:ARG:NH2	1.65	1.12
1:P:11:ALA:HB2	1:Q:10:ARG:CZ	1.64	1.11
1:F:11:ALA:HB2	1:G:10:ARG:CZ	1.64	1.11
1:S:10:ARG:NH2	1:R:11:ALA:HB2	1.65	1.10
1:A:11:ALA:HB2	1:B:10:ARG:NH2	1.65	1.10
1:F:10:ARG:NH2	1:E:11:ALA:HB2	1.65	1.10
1:O:11:ALA:HB2	1:P:10:ARG:NH2	1.65	1.09
1:S:11:ALA:HB2	1:T:10:ARG:NH2	1.65	1.09
1:B:11:ALA:HB2	1:C:10:ARG:NH2	1.65	1.09
1:G:11:ALA:HB2	1:A:10:ARG:NH2	1.65	1.09
1:Q:11:ALA:HB2	1:R:10:ARG:NH2	1.65	1.09
1:T:11:ALA:HB2	1:U:10:ARG:CZ	1.64	1.09
1:T:11:ALA:HB2	1:U:10:ARG:NH2	1.65	1.08
1:C:11:ALA:HB2	1:D:10:ARG:CZ	1.64	1.08
1:C:11:ALA:HB2	1:D:10:ARG:NH2	1.65	1.08
1:O:11:ALA:HB2	1:P:10:ARG:CZ	1.64	1.08
1:F:10:ARG:CZ	1:E:11:ALA:HB2	1.64	1.07
1:O:11:ALA:HB1	1:P:10:ARG:HH12	1.22	1.00
1:F:10:ARG:HH12	1:E:11:ALA:HB1	1.22	1.00
1:U:11:ALA:HB1	1:O:10:ARG:HH12	1.22	0.98
1:D:11:ALA:HB1	1:E:10:ARG:HH12	1.22	0.98
1:F:11:ALA:HB1	1:G:10:ARG:HH12	1.22	0.98
1:P:11:ALA:HB1	1:Q:10:ARG:HH12	1.22	0.98
2:V:167:SER:O	2:J:167:SER:HB2	1.64	0.97
2:N:167:SER:O	2:Y:167:SER:HB2	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:167:SER:HB2	2:L:167:SER:O	1.64	0.97
2:Z:167:SER:HB2	2:M:167:SER:O	1.64	0.97
2:Z:167:SER:O	2:M:167:SER:HB2	1.64	0.97
2:H:167:SER:HB2	2:X:167:SER:O	1.64	0.97
2:V:167:SER:HB2	2:J:167:SER:O	1.64	0.97
2:H:167:SER:O	2:X:167:SER:HB2	1.64	0.97
2:I:167:SER:O	2:W:167:SER:HB2	1.64	0.97
2:1:167:SER:O	2:L:167:SER:HB2	1.64	0.97
2:I:167:SER:HB2	2:W:167:SER:O	1.64	0.97
2:N:167:SER:HB2	2:Y:167:SER:O	1.64	0.97
2:1:28:HIS:CD2	2:2:120:VAL:HG11	2.02	0.95
2:N:28:HIS:CD2	2:H:120:VAL:HG11	2.02	0.95
2:J:28:HIS:CD2	2:K:120:VAL:HG11	2.02	0.95
2:X:28:HIS:CD2	2:Y:120:VAL:HG11	2.02	0.95
2:2:167:SER:HB2	2:K:167:SER:O	1.64	0.95
2:V:28:HIS:CD2	2:W:120:VAL:HG11	2.02	0.95
2:M:28:HIS:CD2	2:N:120:VAL:HG11	2.02	0.95
2:M:120:VAL:HG11	2:L:28:HIS:CD2	2.02	0.95
2:W:28:HIS:CD2	2:X:120:VAL:HG11	2.02	0.95
2:2:167:SER:O	2:K:167:SER:HB2	1.64	0.94
2:I:28:HIS:CD2	2:J:120:VAL:HG11	2.02	0.94
2:Z:28:HIS:CD2	2:1:120:VAL:HG11	2.02	0.94
2:K:28:HIS:CD2	2:L:120:VAL:HG11	2.02	0.94
2:2:28:HIS:CD2	2:V:120:VAL:HG11	2.02	0.94
1:B:11:ALA:HB1	1:C:10:ARG:HH12	1.22	0.94
2:Z:120:VAL:HG11	2:Y:28:HIS:CD2	2.02	0.94
2:H:28:HIS:CD2	2:I:120:VAL:HG11	2.02	0.93
1:S:11:ALA:HB1	1:T:10:ARG:HH12	1.22	0.93
1:T:11:ALA:HB1	1:U:10:ARG:HH12	1.22	0.93
1:C:11:ALA:HB1	1:D:10:ARG:HH12	1.22	0.93
1:Q:11:ALA:HB1	1:R:10:ARG:HH12	1.22	0.93
1:G:11:ALA:HB1	1:A:10:ARG:HH12	1.22	0.93
1:A:11:ALA:HB1	1:B:10:ARG:HH12	1.22	0.92
1:S:10:ARG:HH12	1:R:11:ALA:HB1	1.22	0.92
2:1:203:LEU:OXT	2:L:203:LEU:OXT	1.92	0.88
2:V:203:LEU:OXT	2:J:203:LEU:OXT	1.92	0.88
2:H:203:LEU:OXT	2:X:203:LEU:OXT	1.92	0.87
2:N:203:LEU:OXT	2:Y:203:LEU:OXT	1.92	0.87
2:I:203:LEU:OXT	2:W:203:LEU:OXT	1.92	0.86
2:Z:203:LEU:OXT	2:M:203:LEU:OXT	1.92	0.86
1:Q:11:ALA:CB	1:R:10:ARG:NH2	2.31	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:ALA:CB	1:A:10:ARG:NH2	2.31	0.86
2:2:203:LEU:OXT	2:K:203:LEU:OXT	1.92	0.86
1:S:11:ALA:CB	1:T:10:ARG:NH2	2.31	0.84
1:B:11:ALA:CB	1:C:10:ARG:NH2	2.31	0.84
1:T:11:ALA:CB	1:U:10:ARG:NH2	2.32	0.83
2:M:28:HIS:CD2	2:N:120:VAL:CG1	2.62	0.83
2:W:28:HIS:CD2	2:X:120:VAL:CG1	2.62	0.83
1:A:11:ALA:CB	1:B:10:ARG:NH2	2.31	0.83
2:V:28:HIS:CD2	2:W:120:VAL:CG1	2.62	0.83
2:M:120:VAL:CG1	2:L:28:HIS:CD2	2.62	0.83
2:K:28:HIS:CD2	2:L:120:VAL:CG1	2.62	0.83
2:2:28:HIS:CD2	2:V:120:VAL:CG1	2.62	0.83
1:S:10:ARG:NH2	1:R:11:ALA:CB	2.31	0.83
1:C:11:ALA:CB	1:D:10:ARG:NH2	2.32	0.83
2:N:28:HIS:CD2	2:H:120:VAL:CG1	2.62	0.82
2:X:28:HIS:CD2	2:Y:120:VAL:CG1	2.62	0.82
2:I:28:HIS:CD2	2:J:120:VAL:CG1	2.62	0.82
2:Z:28:HIS:CD2	2:1:120:VAL:CG1	2.62	0.82
2:1:28:HIS:CD2	2:2:120:VAL:CG1	2.62	0.82
2:J:28:HIS:CD2	2:K:120:VAL:CG1	2.62	0.82
2:Z:120:VAL:CG1	2:Y:28:HIS:CD2	2.62	0.81
2:H:28:HIS:CD2	2:I:120:VAL:CG1	2.62	0.81
1:F:10:ARG:NH2	1:E:11:ALA:CB	2.31	0.80
1:O:11:ALA:CB	1:P:10:ARG:NH2	2.32	0.79
1:U:11:ALA:CB	1:O:10:ARG:NH2	2.32	0.75
1:D:11:ALA:CB	1:E:10:ARG:NH2	2.32	0.75
1:F:11:ALA:CB	1:G:10:ARG:NH2	2.32	0.74
1:P:11:ALA:CB	1:Q:10:ARG:NH2	2.31	0.74
1:D:54:VAL:O	1:D:55:ARG:NH1	2.29	0.66
1:U:54:VAL:O	1:U:55:ARG:NH1	2.29	0.65
1:O:54:VAL:O	1:O:55:ARG:NH1	2.29	0.65
1:P:54:VAL:O	1:P:55:ARG:NH1	2.29	0.65
1:E:54:VAL:O	1:E:55:ARG:NH1	2.29	0.65
1:F:54:VAL:O	1:F:55:ARG:NH1	2.29	0.65
1:S:54:VAL:O	1:S:55:ARG:NH1	2.29	0.65
1:B:54:VAL:O	1:B:55:ARG:NH1	2.29	0.65
1:R:54:VAL:O	1:R:55:ARG:NH1	2.29	0.65
1:A:54:VAL:O	1:A:55:ARG:NH1	2.29	0.65
1:C:54:VAL:O	1:C:55:ARG:NH1	2.29	0.65
1:T:54:VAL:O	1:T:55:ARG:NH1	2.29	0.65
1:Q:54:VAL:O	1:Q:55:ARG:NH1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:VAL:O	1:G:55:ARG:NH1	2.29	0.65
2:N:167:SER:O	2:Y:167:SER:CB	2.45	0.61
2:H:167:SER:CB	2:X:167:SER:O	2.45	0.61
2:N:167:SER:CB	2:Y:167:SER:O	2.45	0.61
2:H:167:SER:O	2:X:167:SER:CB	2.45	0.61
2:I:167:SER:CB	2:W:167:SER:O	2.45	0.60
2:Z:167:SER:CB	2:M:167:SER:O	2.45	0.59
2:Z:167:SER:O	2:M:167:SER:CB	2.45	0.59
2:I:167:SER:O	2:W:167:SER:CB	2.45	0.59
2:V:167:SER:O	2:J:167:SER:CB	2.45	0.57
2:I:167:SER:CB	2:L:167:SER:O	2.45	0.57
2:V:167:SER:CB	2:J:167:SER:O	2.45	0.57
2:I:167:SER:O	2:L:167:SER:CB	2.45	0.56
2:2:167:SER:CB	2:K:167:SER:O	2.45	0.56
2:2:167:SER:O	2:K:167:SER:CB	2.45	0.56
2:J:28:HIS:CD2	2:K:120:VAL:HG13	2.41	0.56
2:I:28:HIS:CD2	2:2:120:VAL:HG13	2.41	0.55
2:X:6:ILE:HD12	2:X:155:VAL:HG23	1.89	0.55
2:N:6:ILE:HD12	2:N:155:VAL:HG23	1.89	0.55
2:H:6:ILE:HD12	2:H:155:VAL:HG23	1.89	0.55
2:Y:6:ILE:HD12	2:Y:155:VAL:HG23	1.89	0.55
2:W:6:ILE:HD12	2:W:155:VAL:HG23	1.89	0.55
2:I:6:ILE:HD12	2:I:155:VAL:HG23	1.89	0.55
2:M:6:ILE:HD12	2:M:155:VAL:HG23	1.89	0.55
2:Z:6:ILE:HD12	2:Z:155:VAL:HG23	1.89	0.55
2:I:6:ILE:HD12	2:I:155:VAL:HG23	1.89	0.55
2:2:28:HIS:CD2	2:V:120:VAL:HG13	2.41	0.55
2:K:28:HIS:CD2	2:L:120:VAL:HG13	2.41	0.55
2:J:6:ILE:HD12	2:J:155:VAL:HG23	1.89	0.55
2:V:28:HIS:CD2	2:W:120:VAL:HG13	2.41	0.54
2:M:120:VAL:HG13	2:L:28:HIS:CD2	2.41	0.54
2:Z:28:HIS:CD2	2:I:120:VAL:HG13	2.41	0.54
2:V:6:ILE:HD12	2:V:155:VAL:HG23	1.89	0.54
2:2:6:ILE:HD12	2:2:155:VAL:HG23	1.89	0.54
2:I:28:HIS:CD2	2:J:120:VAL:HG13	2.41	0.54
2:K:6:ILE:HD12	2:K:155:VAL:HG23	1.89	0.54
2:L:6:ILE:HD12	2:L:155:VAL:HG23	1.89	0.54
2:H:28:HIS:CD2	2:I:120:VAL:HG13	2.41	0.54
2:Z:93:MET:HB3	2:I:92:TYR:CE2	2.43	0.54
2:Z:120:VAL:HG13	2:Y:28:HIS:CD2	2.41	0.54
2:I:93:MET:HB3	2:J:92:TYR:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:92:TYR:CE2	2:Y:93:MET:HB3	2.43	0.54
2:H:93:MET:HB3	2:I:92:TYR:CE2	2.43	0.54
1:T:36:THR:HB	1:T:168:GLY:H	1.73	0.53
2:1:93:MET:HB3	2:2:92:TYR:CE2	2.43	0.53
1:C:36:THR:HB	1:C:168:GLY:H	1.73	0.53
2:J:93:MET:HB3	2:K:92:TYR:CE2	2.43	0.53
1:U:36:THR:HB	1:U:168:GLY:H	1.73	0.53
2:X:93:MET:HB3	2:Y:92:TYR:CE2	2.43	0.53
1:D:36:THR:HB	1:D:168:GLY:H	1.73	0.53
2:N:93:MET:HB3	2:H:92:TYR:CE2	2.43	0.53
1:G:36:THR:HB	1:G:168:GLY:H	1.73	0.53
2:M:92:TYR:CE2	2:L:93:MET:HB3	2.43	0.53
1:P:36:THR:HB	1:P:168:GLY:H	1.73	0.53
2:V:93:MET:HB3	2:W:92:TYR:CE2	2.43	0.53
2:W:93:MET:HB3	2:X:92:TYR:CE2	2.43	0.53
2:M:93:MET:HB3	2:N:92:TYR:CE2	2.43	0.53
1:Q:36:THR:HB	1:Q:168:GLY:H	1.73	0.53
1:F:36:THR:HB	1:F:168:GLY:H	1.74	0.53
2:2:93:MET:HB3	2:V:92:TYR:CE2	2.43	0.53
2:N:28:HIS:CD2	2:H:120:VAL:HG13	2.41	0.53
2:M:28:HIS:CD2	2:N:120:VAL:HG13	2.41	0.53
2:W:28:HIS:CD2	2:X:120:VAL:HG13	2.41	0.53
2:K:93:MET:HB3	2:L:92:TYR:CE2	2.43	0.53
2:X:28:HIS:CD2	2:Y:120:VAL:HG13	2.41	0.53
1:T:35:SER:HB2	1:T:53:LYS:HG2	1.91	0.52
1:C:35:SER:HB2	1:C:53:LYS:HG2	1.91	0.52
1:D:35:SER:HB2	1:D:53:LYS:HG2	1.91	0.52
1:A:36:THR:HB	1:A:168:GLY:H	1.73	0.52
1:R:36:THR:HB	1:R:168:GLY:H	1.73	0.52
1:Q:35:SER:HB2	1:Q:53:LYS:HG2	1.91	0.52
1:E:35:SER:HB2	1:E:53:LYS:HG2	1.91	0.52
1:G:35:SER:HB2	1:G:53:LYS:HG2	1.91	0.52
1:O:35:SER:HB2	1:O:53:LYS:HG2	1.91	0.52
2:V:141:GLN:HE22	2:V:157:ARG:HE	1.58	0.52
1:R:35:SER:HB2	1:R:53:LYS:HG2	1.91	0.52
1:B:36:THR:HB	1:B:168:GLY:H	1.73	0.52
2:L:141:GLN:HE22	2:L:157:ARG:HE	1.58	0.52
1:B:35:SER:HB2	1:B:53:LYS:HG2	1.91	0.51
2:2:141:GLN:HE22	2:2:157:ARG:HE	1.58	0.51
1:S:36:THR:HB	1:S:168:GLY:H	1.73	0.51
1:O:36:THR:HB	1:O:168:GLY:H	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:35:SER:HB2	1:S:53:LYS:HG2	1.91	0.51
1:A:35:SER:HB2	1:A:53:LYS:HG2	1.91	0.51
2:K:141:GLN:HE22	2:K:157:ARG:HE	1.58	0.51
1:P:35:SER:HB2	1:P:53:LYS:HG2	1.91	0.51
2:M:141:GLN:HE22	2:M:157:ARG:HE	1.58	0.51
2:W:141:GLN:HE22	2:W:157:ARG:HE	1.58	0.51
1:F:35:SER:HB2	1:F:53:LYS:HG2	1.91	0.51
1:E:36:THR:HB	1:E:168:GLY:H	1.74	0.51
2:1:141:GLN:HE22	2:1:157:ARG:HE	1.58	0.51
2:N:141:GLN:HE22	2:N:157:ARG:HE	1.58	0.51
2:J:141:GLN:HE22	2:J:157:ARG:HE	1.58	0.51
2:X:141:GLN:HE22	2:X:157:ARG:HE	1.58	0.51
1:U:35:SER:HB2	1:U:53:LYS:HG2	1.92	0.51
2:1:28:HIS:HD2	2:2:120:VAL:HG11	1.72	0.50
2:J:28:HIS:HD2	2:K:120:VAL:HG11	1.72	0.50
2:Z:141:GLN:HE22	2:Z:157:ARG:HE	1.58	0.50
2:H:141:GLN:HE22	2:H:157:ARG:HE	1.58	0.50
2:I:141:GLN:HE22	2:I:157:ARG:HE	1.58	0.50
2:Y:141:GLN:HE22	2:Y:157:ARG:HE	1.58	0.50
2:M:165:ARG:HD3	2:1:139:GLU:OE1	2.14	0.48
2:W:165:ARG:HD3	2:J:139:GLU:OE1	2.14	0.48
2:2:139:GLU:OE1	2:L:165:ARG:HD3	2.14	0.48
2:V:165:ARG:HD3	2:K:139:GLU:OE1	2.14	0.48
2:Z:28:HIS:HD2	2:1:120:VAL:HG11	1.72	0.48
2:I:28:HIS:HD2	2:J:120:VAL:HG11	1.72	0.48
2:Z:139:GLU:OE1	2:N:165:ARG:HD3	2.14	0.48
2:I:139:GLU:OE1	2:X:165:ARG:HD3	2.14	0.48
2:V:139:GLU:OE1	2:K:165:ARG:HD3	2.14	0.48
2:2:165:ARG:HD3	2:L:139:GLU:OE1	2.14	0.48
1:T:121:GLN:HE21	1:U:87:VAL:HG21	1.79	0.48
1:C:121:GLN:HE21	1:D:87:VAL:HG21	1.79	0.48
2:N:28:HIS:HD2	2:H:120:VAL:HG11	1.72	0.47
2:X:28:HIS:HD2	2:Y:120:VAL:HG11	1.72	0.47
2:W:139:GLU:OE1	2:J:165:ARG:HD3	2.14	0.47
1:S:121:GLN:HE21	1:T:87:VAL:HG21	1.79	0.47
2:M:139:GLU:OE1	2:1:165:ARG:HD3	2.14	0.47
2:M:120:VAL:HG13	2:L:28:HIS:NE2	2.30	0.47
1:D:121:GLN:HE21	1:E:87:VAL:HG21	1.79	0.47
1:B:121:GLN:HE21	1:C:87:VAL:HG21	1.79	0.47
2:H:139:GLU:OE1	2:Y:165:ARG:HD3	2.14	0.47
1:U:121:GLN:HE21	1:O:87:VAL:HG21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:28:HIS:NE2	2:2:120:VAL:HG13	2.30	0.47
2:J:28:HIS:NE2	2:K:120:VAL:HG13	2.30	0.47
2:V:28:HIS:NE2	2:W:120:VAL:HG13	2.30	0.47
2:2:28:HIS:NE2	2:V:120:VAL:HG13	2.30	0.47
2:W:7:THR:HG23	2:W:108:PRO:HB2	1.97	0.47
2:Z:165:ARG:HD3	2:N:139:GLU:OE1	2.14	0.47
2:H:165:ARG:HD3	2:Y:139:GLU:OE1	2.14	0.47
1:S:87:VAL:HG21	1:R:121:GLN:HE21	1.79	0.47
2:K:28:HIS:NE2	2:L:120:VAL:HG13	2.30	0.47
1:A:121:GLN:HE21	1:B:87:VAL:HG21	1.79	0.47
2:X:159:ILE:HB	2:X:173:ILE:HD12	1.97	0.47
2:M:7:THR:HG23	2:M:108:PRO:HB2	1.97	0.47
2:I:165:ARG:HD3	2:X:139:GLU:OE1	2.14	0.47
2:H:28:HIS:NE2	2:I:120:VAL:HG13	2.30	0.47
2:Y:159:ILE:HB	2:Y:173:ILE:HD12	1.97	0.47
2:N:28:HIS:NE2	2:H:120:VAL:HG13	2.30	0.47
2:X:28:HIS:NE2	2:Y:120:VAL:HG13	2.30	0.47
2:Z:120:VAL:HG13	2:Y:28:HIS:NE2	2.30	0.47
2:Z:120:VAL:HG11	2:Y:28:HIS:HD2	1.72	0.47
2:H:28:HIS:HD2	2:I:120:VAL:HG11	1.72	0.47
2:H:159:ILE:HB	2:H:173:ILE:HD12	1.97	0.47
2:K:7:THR:HG23	2:K:108:PRO:HB2	1.97	0.47
1:O:121:GLN:HE21	1:P:87:VAL:HG21	1.79	0.47
2:N:159:ILE:HB	2:N:173:ILE:HD12	1.97	0.47
1:Q:121:GLN:HE21	1:R:87:VAL:HG21	1.79	0.47
2:J:159:ILE:HB	2:J:173:ILE:HD12	1.97	0.47
1:G:121:GLN:HE21	1:A:87:VAL:HG21	1.79	0.47
1:P:121:GLN:HE21	1:Q:87:VAL:HG21	1.79	0.47
2:X:7:THR:HG23	2:X:108:PRO:HB2	1.97	0.47
2:I:159:ILE:HB	2:I:173:ILE:HD12	1.97	0.47
1:F:87:VAL:HG21	1:E:121:GLN:HE21	1.79	0.47
2:1:159:ILE:HB	2:1:173:ILE:HD12	1.97	0.47
2:N:7:THR:HG23	2:N:108:PRO:HB2	1.97	0.47
2:1:7:THR:HG23	2:1:108:PRO:HB2	1.97	0.47
2:2:7:THR:HG23	2:2:108:PRO:HB2	1.97	0.47
2:Z:159:ILE:HB	2:Z:173:ILE:HD12	1.97	0.47
1:F:121:GLN:HE21	1:G:87:VAL:HG21	1.79	0.47
2:J:7:THR:HG23	2:J:108:PRO:HB2	1.97	0.47
2:M:28:HIS:NE2	2:N:120:VAL:HG13	2.30	0.47
2:Z:28:HIS:NE2	2:1:120:VAL:HG13	2.30	0.47
2:M:159:ILE:HB	2:M:173:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:7:THR:HG23	2:H:108:PRO:HB2	1.97	0.47
2:K:159:ILE:HB	2:K:173:ILE:HD12	1.97	0.47
2:W:28:HIS:NE2	2:X:120:VAL:HG13	2.30	0.46
2:I:28:HIS:NE2	2:J:120:VAL:HG13	2.30	0.46
2:Y:7:THR:HG23	2:Y:108:PRO:HB2	1.97	0.46
2:2:159:ILE:HB	2:2:173:ILE:HD12	1.97	0.46
2:L:159:ILE:HB	2:L:173:ILE:HD12	1.97	0.46
2:V:159:ILE:HB	2:V:173:ILE:HD12	1.97	0.46
2:W:159:ILE:HB	2:W:173:ILE:HD12	1.97	0.46
2:I:7:THR:HG23	2:I:108:PRO:HB2	1.97	0.46
2:V:7:THR:HG23	2:V:108:PRO:HB2	1.97	0.46
2:L:7:THR:HG23	2:L:108:PRO:HB2	1.97	0.46
2:Z:7:THR:HG23	2:Z:108:PRO:HB2	1.97	0.46
2:V:87:LEU:HD23	2:V:95:TYR:CD2	2.52	0.45
2:K:87:LEU:HD23	2:K:95:TYR:CD2	2.52	0.45
2:L:87:LEU:HD23	2:L:95:TYR:CD2	2.52	0.45
1:U:70:ILE:HG21	1:U:112:LEU:HD21	1.98	0.45
2:2:87:LEU:HD23	2:2:95:TYR:CD2	2.52	0.45
1:D:70:ILE:HG21	1:D:112:LEU:HD21	1.98	0.45
1:T:70:ILE:HG21	1:T:112:LEU:HD21	1.98	0.45
2:I:87:LEU:HD23	2:I:95:TYR:CD2	2.52	0.45
2:J:87:LEU:HD23	2:J:95:TYR:CD2	2.52	0.45
2:Z:87:LEU:HD23	2:Z:95:TYR:CD2	2.52	0.45
1:O:70:ILE:HG21	1:O:112:LEU:HD21	1.98	0.45
1:C:70:ILE:HG21	1:C:112:LEU:HD21	1.98	0.45
1:E:70:ILE:HG21	1:E:112:LEU:HD21	1.98	0.45
2:1:87:LEU:HD23	2:1:95:TYR:CD2	2.52	0.45
1:R:70:ILE:HG21	1:R:112:LEU:HD21	1.98	0.44
2:W:87:LEU:HD23	2:W:95:TYR:CD2	2.52	0.44
1:A:70:ILE:HG21	1:A:112:LEU:HD21	1.98	0.44
2:M:87:LEU:HD23	2:M:95:TYR:CD2	2.52	0.44
1:G:70:ILE:HG21	1:G:112:LEU:HD21	1.98	0.44
2:H:87:LEU:HD23	2:H:95:TYR:CD2	2.52	0.44
1:Q:70:ILE:HG21	1:Q:112:LEU:HD21	1.99	0.44
2:Y:87:LEU:HD23	2:Y:95:TYR:CD2	2.52	0.44
2:N:87:LEU:HD23	2:N:95:TYR:CD2	2.52	0.44
1:P:70:ILE:HG21	1:P:112:LEU:HD21	1.98	0.44
1:S:70:ILE:HG21	1:S:112:LEU:HD21	1.98	0.44
1:F:70:ILE:HG21	1:F:112:LEU:HD21	1.98	0.44
2:X:87:LEU:HD23	2:X:95:TYR:CD2	2.52	0.44
1:B:70:ILE:HG21	1:B:112:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:131:SER:HB3	2:X:132:PRO:HD3	2.00	0.43
2:W:131:SER:HB3	2:W:132:PRO:HD3	2.00	0.43
2:N:131:SER:HB3	2:N:132:PRO:HD3	2.00	0.43
2:1:131:SER:HB3	2:1:132:PRO:HD3	2.00	0.43
2:M:131:SER:HB3	2:M:132:PRO:HD3	2.00	0.43
2:2:131:SER:HB3	2:2:132:PRO:HD3	2.00	0.43
2:1:3:THR:HG22	2:1:16:THR:HG22	1.99	0.43
2:H:132:PRO:HB2	2:Y:132:PRO:HB2	2.01	0.43
1:P:54:VAL:HG13	1:P:54:VAL:O	2.19	0.43
2:J:131:SER:HB3	2:J:132:PRO:HD3	2.00	0.43
2:I:3:THR:HG22	2:I:16:THR:HG22	1.99	0.43
2:K:131:SER:HB3	2:K:132:PRO:HD3	2.00	0.43
2:V:131:SER:HB3	2:V:132:PRO:HD3	2.00	0.43
2:Z:3:THR:HG22	2:Z:16:THR:HG22	1.99	0.43
2:X:3:THR:HG22	2:X:16:THR:HG22	1.99	0.43
1:F:54:VAL:O	1:F:54:VAL:HG13	2.19	0.43
1:S:54:VAL:O	1:S:54:VAL:HG13	2.19	0.43
1:B:54:VAL:O	1:B:54:VAL:HG13	2.19	0.43
1:R:54:VAL:HG13	1:R:54:VAL:O	2.19	0.43
2:Z:132:PRO:HB2	2:N:132:PRO:HB2	2.01	0.43
2:L:131:SER:HB3	2:L:132:PRO:HD3	2.00	0.43
2:N:3:THR:HG22	2:N:16:THR:HG22	1.99	0.43
2:J:3:THR:HG22	2:J:16:THR:HG22	1.99	0.43
1:A:54:VAL:HG13	1:A:54:VAL:O	2.19	0.43
2:I:132:PRO:HB2	2:X:132:PRO:HB2	2.01	0.43
2:H:131:SER:HB3	2:H:132:PRO:HD3	2.00	0.43
2:L:3:THR:HG22	2:L:16:THR:HG22	1.99	0.43
2:W:3:THR:HG22	2:W:16:THR:HG22	1.99	0.43
1:T:54:VAL:HG13	1:T:54:VAL:O	2.19	0.43
2:Y:131:SER:HB3	2:Y:132:PRO:HD3	2.00	0.43
2:M:3:THR:HG22	2:M:16:THR:HG22	1.99	0.43
1:U:54:VAL:O	1:U:54:VAL:HG13	2.19	0.43
2:V:3:THR:HG22	2:V:16:THR:HG22	1.99	0.43
2:Y:3:THR:HG22	2:Y:16:THR:HG22	1.99	0.43
1:C:54:VAL:O	1:C:54:VAL:HG13	2.19	0.43
2:W:132:PRO:CB	2:J:132:PRO:HB2	2.49	0.43
2:W:132:PRO:HB2	2:J:132:PRO:CB	2.49	0.43
2:M:132:PRO:HB2	2:1:132:PRO:CB	2.49	0.43
1:D:54:VAL:HG13	1:D:54:VAL:O	2.19	0.42
2:Z:132:PRO:CB	2:N:132:PRO:HB2	2.49	0.42
2:M:132:PRO:CB	2:1:132:PRO:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:VAL:O	1:G:54:VAL:HG13	2.19	0.42
1:F:53:LYS:HA	1:F:53:LYS:HD3	1.78	0.42
2:H:3:THR:HG22	2:H:16:THR:HG22	1.99	0.42
1:Q:54:VAL:HG13	1:Q:54:VAL:O	2.19	0.42
1:P:53:LYS:HA	1:P:53:LYS:HD3	1.78	0.42
2:I:132:PRO:CB	2:X:132:PRO:HB2	2.49	0.42
2:K:3:THR:HG22	2:K:16:THR:HG22	1.99	0.42
2:2:3:THR:HG22	2:2:16:THR:HG22	1.99	0.42
2:2:132:PRO:CB	2:L:132:PRO:HB2	2.49	0.42
2:V:132:PRO:HB2	2:K:132:PRO:CB	2.49	0.42
2:I:132:PRO:HB2	2:X:132:PRO:CB	2.49	0.42
2:Z:131:SER:HB3	2:Z:132:PRO:HD3	2.00	0.42
2:V:132:PRO:CB	2:K:132:PRO:HB2	2.49	0.42
2:Z:132:PRO:HB2	2:N:132:PRO:CB	2.49	0.42
2:2:132:PRO:HB2	2:L:132:PRO:CB	2.49	0.42
1:E:54:VAL:O	1:E:54:VAL:HG13	2.19	0.42
2:I:131:SER:HB3	2:I:132:PRO:HD3	2.00	0.42
2:H:132:PRO:HB2	2:Y:132:PRO:CB	2.49	0.42
1:O:54:VAL:HG13	1:O:54:VAL:O	2.19	0.42
2:H:132:PRO:CB	2:Y:132:PRO:HB2	2.49	0.42
2:W:21:THR:O	2:W:21:THR:HG23	2.20	0.42
2:M:21:THR:O	2:M:21:THR:HG23	2.20	0.42
2:2:132:PRO:HB2	2:L:132:PRO:HB2	2.00	0.42
2:M:120:VAL:HG11	2:L:28:HIS:HD2	1.72	0.41
2:V:132:PRO:HB2	2:K:132:PRO:HB2	2.01	0.41
2:W:132:PRO:HB2	2:J:132:PRO:HB2	2.01	0.41
2:L:21:THR:HG23	2:L:21:THR:O	2.20	0.41
2:Y:21:THR:HG23	2:Y:21:THR:O	2.20	0.41
2:H:21:THR:O	2:H:21:THR:HG23	2.20	0.41
2:V:28:HIS:HD2	2:W:120:VAL:HG11	1.72	0.41
2:M:132:PRO:HB2	2:1:132:PRO:HB2	2.01	0.41
2:Y:20:VAL:HG23	2:Y:31:GLY:HA3	2.03	0.41
2:X:21:THR:HG23	2:X:21:THR:O	2.20	0.41
2:N:21:THR:O	2:N:21:THR:HG23	2.20	0.41
2:V:21:THR:O	2:V:21:THR:HG23	2.20	0.41
2:K:20:VAL:HG23	2:K:31:GLY:HA3	2.03	0.41
2:L:20:VAL:HG23	2:L:31:GLY:HA3	2.03	0.41
2:H:20:VAL:HG23	2:H:31:GLY:HA3	2.03	0.41
2:V:20:VAL:HG23	2:V:31:GLY:HA3	2.03	0.41
2:2:20:VAL:HG23	2:2:31:GLY:HA3	2.03	0.41
2:K:21:THR:HG23	2:K:21:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:28:HIS:HD2	2:L:120:VAL:HG11	1.72	0.41
2:N:20:VAL:HG23	2:N:31:GLY:HA3	2.03	0.41
2:J:21:THR:O	2:J:21:THR:HG23	2.20	0.41
2:2:21:THR:HG23	2:2:21:THR:O	2.20	0.41
2:X:20:VAL:HG23	2:X:31:GLY:HA3	2.03	0.41
2:2:28:HIS:HD2	2:V:120:VAL:HG11	1.72	0.41
2:M:20:VAL:HG23	2:M:31:GLY:HA3	2.03	0.41
2:Z:20:VAL:HG23	2:Z:31:GLY:HA3	2.03	0.41
2:Z:21:THR:HG23	2:Z:21:THR:O	2.20	0.41
2:I:21:THR:O	2:I:21:THR:HG23	2.20	0.41
2:1:21:THR:HG23	2:1:21:THR:O	2.20	0.41
2:W:20:VAL:HG23	2:W:31:GLY:HA3	2.03	0.41
2:I:20:VAL:HG23	2:I:31:GLY:HA3	2.03	0.40
2:J:20:VAL:HG23	2:J:31:GLY:HA3	2.03	0.40
2:H:167:SER:HB3	2:X:26:ILE:HG21	2.04	0.40
2:N:26:ILE:HG21	2:Y:167:SER:HB3	2.04	0.40
2:1:20:VAL:HG23	2:1:31:GLY:HA3	2.03	0.40
2:V:101:VAL:HG12	2:V:113:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	21	60
1	B	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	21	60
1	C	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	21	60
1	D	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	21	60
1	E	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	21	60
1	F	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	21	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	21	60
1	O	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	21	60
1	P	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	21	60
1	Q	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	21	60
1	R	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	21	60
1	S	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	21	60
1	T	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	21	60
1	U	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	21	60
2	1	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	5	33
2	2	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	5	33
2	H	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	5	33
2	I	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	5	33
2	J	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	5	33
2	K	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	5	33
2	L	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	5	33
2	M	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	5	33
2	N	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	5	33
2	V	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	5	33
2	W	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	5	33
2	X	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	5	33
2	Y	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	5	33
2	Z	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	5	33
All	All	5922/5978 (99%)	5334 (90%)	476 (8%)	112 (2%)	14	45

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Z	25	PHE
2	M	25	PHE
2	1	25	PHE
2	N	25	PHE
2	2	25	PHE
2	H	25	PHE
2	V	25	PHE

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Mol	Chain	Res	Type
2	I	25	PHE
2	W	25	PHE
2	J	25	PHE
2	X	25	PHE
2	K	25	PHE
2	Y	25	PHE
2	L	25	PHE
1	S	200	SER
2	Z	22	MET
2	Z	23	GLU
1	F	200	SER
2	M	22	MET
2	M	23	GLU
1	T	200	SER
2	1	22	MET
2	1	23	GLU
1	G	200	SER
2	N	22	MET
2	N	23	GLU
1	U	200	SER
2	2	22	MET
2	2	23	GLU
1	A	200	SER
2	H	22	MET
2	H	23	GLU
1	O	200	SER
2	V	22	MET
2	V	23	GLU
1	B	200	SER
2	I	22	MET
2	I	23	GLU
1	P	200	SER
2	W	22	MET
2	W	23	GLU
1	C	200	SER
2	J	22	MET
2	J	23	GLU
1	Q	200	SER
2	X	22	MET
2	X	23	GLU
1	D	200	SER
2	K	22	MET

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Mol	Chain	Res	Type
2	K	23	GLU
1	R	200	SER
2	Y	22	MET
2	Y	23	GLU
1	E	200	SER
2	L	22	MET
2	L	23	GLU
2	Z	49	VAL
2	M	49	VAL
2	1	49	VAL
2	N	49	VAL
2	2	49	VAL
2	H	49	VAL
2	V	49	VAL
2	I	49	VAL
2	W	49	VAL
2	J	49	VAL
2	X	49	VAL
2	K	49	VAL
2	Y	49	VAL
2	L	49	VAL
2	Z	19	ARG
2	M	19	ARG
2	1	19	ARG
2	N	19	ARG
2	2	19	ARG
2	H	19	ARG
2	V	19	ARG
2	I	19	ARG
2	W	19	ARG
2	J	19	ARG
2	X	19	ARG
2	K	19	ARG
2	Y	19	ARG
2	L	19	ARG
1	S	129	VAL
1	F	129	VAL
1	T	129	VAL
1	G	129	VAL
1	U	129	VAL
1	A	129	VAL
1	O	129	VAL

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Mol	Chain	Res	Type
1	B	129	VAL
1	P	129	VAL
1	C	129	VAL
1	Q	129	VAL
1	D	129	VAL
1	R	129	VAL
1	E	129	VAL
2	Z	110	VAL
2	M	110	VAL
2	1	110	VAL
2	N	110	VAL
2	2	110	VAL
2	H	110	VAL
2	V	110	VAL
2	I	110	VAL
2	W	110	VAL
2	J	110	VAL
2	X	110	VAL
2	K	110	VAL
2	Y	110	VAL
2	L	110	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	186/186 (100%)	174 (94%)	12 (6%)	21	59
1	B	186/186 (100%)	174 (94%)	12 (6%)	21	59
1	C	186/186 (100%)	174 (94%)	12 (6%)	21	59
1	D	186/186 (100%)	174 (94%)	12 (6%)	21	59
1	E	186/186 (100%)	174 (94%)	12 (6%)	21	59
1	F	186/186 (100%)	174 (94%)	12 (6%)	21	59
1	G	186/186 (100%)	174 (94%)	12 (6%)	21	59
1	O	186/186 (100%)	174 (94%)	12 (6%)	21	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	186/186 (100%)	174 (94%)	12 (6%)	21	59
1	Q	186/186 (100%)	174 (94%)	12 (6%)	21	59
1	R	186/186 (100%)	174 (94%)	12 (6%)	21	59
1	S	186/186 (100%)	174 (94%)	12 (6%)	21	59
1	T	186/186 (100%)	174 (94%)	12 (6%)	21	59
1	U	186/186 (100%)	174 (94%)	12 (6%)	21	59
2	1	170/170 (100%)	159 (94%)	11 (6%)	21	59
2	2	170/170 (100%)	159 (94%)	11 (6%)	21	59
2	H	170/170 (100%)	159 (94%)	11 (6%)	21	59
2	I	170/170 (100%)	159 (94%)	11 (6%)	21	59
2	J	170/170 (100%)	159 (94%)	11 (6%)	21	59
2	K	170/170 (100%)	159 (94%)	11 (6%)	21	59
2	L	170/170 (100%)	159 (94%)	11 (6%)	21	59
2	M	170/170 (100%)	159 (94%)	11 (6%)	21	59
2	N	170/170 (100%)	159 (94%)	11 (6%)	21	59
2	V	170/170 (100%)	159 (94%)	11 (6%)	21	59
2	W	170/170 (100%)	159 (94%)	11 (6%)	21	59
2	X	170/170 (100%)	159 (94%)	11 (6%)	21	59
2	Y	170/170 (100%)	159 (94%)	11 (6%)	21	59
2	Z	170/170 (100%)	159 (94%)	11 (6%)	21	59
All	All	4984/4984 (100%)	4662 (94%)	322 (6%)	26	59

All (322) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	47	LEU
1	S	53	LYS
1	S	121	GLN
1	S	136	LEU
1	S	137	ILE
1	S	141	ILE
1	S	177	GLU
1	S	216	THR
1	S	219	ASN
1	S	221	TYR

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Mol	Chain	Res	Type
1	S	224	TYR
1	S	225	ASP
2	Z	17	GLU
2	Z	37	ILE
2	Z	68	LEU
2	Z	79	VAL
2	Z	100	LEU
2	Z	120	VAL
2	Z	137	VAL
2	Z	144	GLU
2	Z	175	VAL
2	Z	178	ILE
2	Z	179	THR
1	F	47	LEU
1	F	53	LYS
1	F	121	GLN
1	F	136	LEU
1	F	137	ILE
1	F	141	ILE
1	F	177	GLU
1	F	216	THR
1	F	219	ASN
1	F	221	TYR
1	F	224	TYR
1	F	225	ASP
2	M	17	GLU
2	M	37	ILE
2	M	68	LEU
2	M	79	VAL
2	M	100	LEU
2	M	120	VAL
2	M	137	VAL
2	M	144	GLU
2	M	175	VAL
2	M	178	ILE
2	M	179	THR
1	T	47	LEU
1	T	53	LYS
1	T	121	GLN
1	T	136	LEU
1	T	137	ILE
1	T	141	ILE

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Mol	Chain	Res	Type
1	T	177	GLU
1	T	216	THR
1	T	219	ASN
1	T	221	TYR
1	T	224	TYR
1	T	225	ASP
2	1	17	GLU
2	1	37	ILE
2	1	68	LEU
2	1	79	VAL
2	1	100	LEU
2	1	120	VAL
2	1	137	VAL
2	1	144	GLU
2	1	175	VAL
2	1	178	ILE
2	1	179	THR
1	G	47	LEU
1	G	53	LYS
1	G	121	GLN
1	G	136	LEU
1	G	137	ILE
1	G	141	ILE
1	G	177	GLU
1	G	216	THR
1	G	219	ASN
1	G	221	TYR
1	G	224	TYR
1	G	225	ASP
2	N	17	GLU
2	N	37	ILE
2	N	68	LEU
2	N	79	VAL
2	N	100	LEU
2	N	120	VAL
2	N	137	VAL
2	N	144	GLU
2	N	175	VAL
2	N	178	ILE
2	N	179	THR
1	U	47	LEU
1	U	53	LYS

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Mol	Chain	Res	Type
1	U	121	GLN
1	U	136	LEU
1	U	137	ILE
1	U	141	ILE
1	U	177	GLU
1	U	216	THR
1	U	219	ASN
1	U	221	TYR
1	U	224	TYR
1	U	225	ASP
2	2	17	GLU
2	2	37	ILE
2	2	68	LEU
2	2	79	VAL
2	2	100	LEU
2	2	120	VAL
2	2	137	VAL
2	2	144	GLU
2	2	175	VAL
2	2	178	ILE
2	2	179	THR
1	A	47	LEU
1	A	53	LYS
1	A	121	GLN
1	A	136	LEU
1	A	137	ILE
1	A	141	ILE
1	A	177	GLU
1	A	216	THR
1	A	219	ASN
1	A	221	TYR
1	A	224	TYR
1	A	225	ASP
2	H	17	GLU
2	H	37	ILE
2	H	68	LEU
2	H	79	VAL
2	H	100	LEU
2	H	120	VAL
2	H	137	VAL
2	H	144	GLU
2	H	175	VAL

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Mol	Chain	Res	Type
2	H	178	ILE
2	H	179	THR
1	O	47	LEU
1	O	53	LYS
1	O	121	GLN
1	O	136	LEU
1	O	137	ILE
1	O	141	ILE
1	O	177	GLU
1	O	216	THR
1	O	219	ASN
1	O	221	TYR
1	O	224	TYR
1	O	225	ASP
2	V	17	GLU
2	V	37	ILE
2	V	68	LEU
2	V	79	VAL
2	V	100	LEU
2	V	120	VAL
2	V	137	VAL
2	V	144	GLU
2	V	175	VAL
2	V	178	ILE
2	V	179	THR
1	B	47	LEU
1	B	53	LYS
1	B	121	GLN
1	B	136	LEU
1	B	137	ILE
1	B	141	ILE
1	B	177	GLU
1	B	216	THR
1	B	219	ASN
1	B	221	TYR
1	B	224	TYR
1	B	225	ASP
2	I	17	GLU
2	I	37	ILE
2	I	68	LEU
2	I	79	VAL
2	I	100	LEU

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Mol	Chain	Res	Type
2	I	120	VAL
2	I	137	VAL
2	I	144	GLU
2	I	175	VAL
2	I	178	ILE
2	I	179	THR
1	P	47	LEU
1	P	53	LYS
1	P	121	GLN
1	P	136	LEU
1	P	137	ILE
1	P	141	ILE
1	P	177	GLU
1	P	216	THR
1	P	219	ASN
1	P	221	TYR
1	P	224	TYR
1	P	225	ASP
2	W	17	GLU
2	W	37	ILE
2	W	68	LEU
2	W	79	VAL
2	W	100	LEU
2	W	120	VAL
2	W	137	VAL
2	W	144	GLU
2	W	175	VAL
2	W	178	ILE
2	W	179	THR
1	C	47	LEU
1	C	53	LYS
1	C	121	GLN
1	C	136	LEU
1	C	137	ILE
1	C	141	ILE
1	C	177	GLU
1	C	216	THR
1	C	219	ASN
1	C	221	TYR
1	C	224	TYR
1	C	225	ASP
2	J	17	GLU

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Mol	Chain	Res	Type
2	J	37	ILE
2	J	68	LEU
2	J	79	VAL
2	J	100	LEU
2	J	120	VAL
2	J	137	VAL
2	J	144	GLU
2	J	175	VAL
2	J	178	ILE
2	J	179	THR
1	Q	47	LEU
1	Q	53	LYS
1	Q	121	GLN
1	Q	136	LEU
1	Q	137	ILE
1	Q	141	ILE
1	Q	177	GLU
1	Q	216	THR
1	Q	219	ASN
1	Q	221	TYR
1	Q	224	TYR
1	Q	225	ASP
2	X	17	GLU
2	X	37	ILE
2	X	68	LEU
2	X	79	VAL
2	X	100	LEU
2	X	120	VAL
2	X	137	VAL
2	X	144	GLU
2	X	175	VAL
2	X	178	ILE
2	X	179	THR
1	D	47	LEU
1	D	53	LYS
1	D	121	GLN
1	D	136	LEU
1	D	137	ILE
1	D	141	ILE
1	D	177	GLU
1	D	216	THR
1	D	219	ASN

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Mol	Chain	Res	Type
1	D	221	TYR
1	D	224	TYR
1	D	225	ASP
2	K	17	GLU
2	K	37	ILE
2	K	68	LEU
2	K	79	VAL
2	K	100	LEU
2	K	120	VAL
2	K	137	VAL
2	K	144	GLU
2	K	175	VAL
2	K	178	ILE
2	K	179	THR
1	R	47	LEU
1	R	53	LYS
1	R	121	GLN
1	R	136	LEU
1	R	137	ILE
1	R	141	ILE
1	R	177	GLU
1	R	216	THR
1	R	219	ASN
1	R	221	TYR
1	R	224	TYR
1	R	225	ASP
2	Y	17	GLU
2	Y	37	ILE
2	Y	68	LEU
2	Y	79	VAL
2	Y	100	LEU
2	Y	120	VAL
2	Y	137	VAL
2	Y	144	GLU
2	Y	175	VAL
2	Y	178	ILE
2	Y	179	THR
1	E	47	LEU
1	E	53	LYS
1	E	121	GLN
1	E	136	LEU
1	E	137	ILE

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Mol	Chain	Res	Type
1	E	141	ILE
1	E	177	GLU
1	E	216	THR
1	E	219	ASN
1	E	221	TYR
1	E	224	TYR
1	E	225	ASP
2	L	17	GLU
2	L	37	ILE
2	L	68	LEU
2	L	79	VAL
2	L	100	LEU
2	L	120	VAL
2	L	137	VAL
2	L	144	GLU
2	L	175	VAL
2	L	178	ILE
2	L	179	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	121	GLN
2	Z	141	GLN
2	Z	191	GLN
1	F	121	GLN
2	M	141	GLN
2	M	191	GLN
1	T	121	GLN
2	1	191	GLN
1	G	121	GLN
2	N	191	GLN
1	U	121	GLN
2	2	191	GLN
1	A	121	GLN
2	H	141	GLN
2	H	191	GLN
1	O	121	GLN
2	V	141	GLN
2	V	191	GLN
1	B	121	GLN
2	I	141	GLN

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Mol	Chain	Res	Type
2	I	191	GLN
1	P	121	GLN
2	W	141	GLN
2	W	191	GLN
1	C	121	GLN
2	J	191	GLN
1	Q	121	GLN
2	X	191	GLN
1	D	121	GLN
2	K	191	GLN
1	R	121	GLN
2	Y	191	GLN
1	E	121	GLN
2	L	141	GLN
2	L	191	GLN

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](#)

There are no carbohydrates in this entry.

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](#)

There are no chain breaks in this entry.