



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 11:25 PM UTC

PDB ID : 3J9I / pdb_00003j9i
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 initial model : 1PMA

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

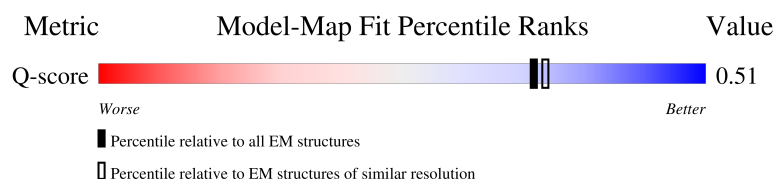
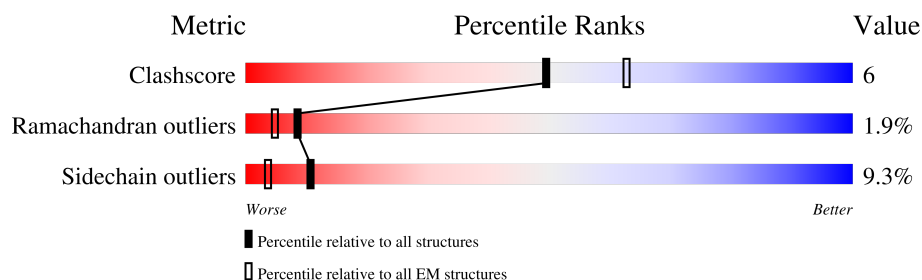
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	224	15% 41% 50% 9%
1	B	224	14% 41% 50% 9%
1	C	224	14% 40% 51% 9%
1	D	224	15% 40% 51% 9%

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Mol	Chain	Length	Quality of chain
1	E	224	
1	F	224	
1	G	224	
1	O	224	
1	P	224	
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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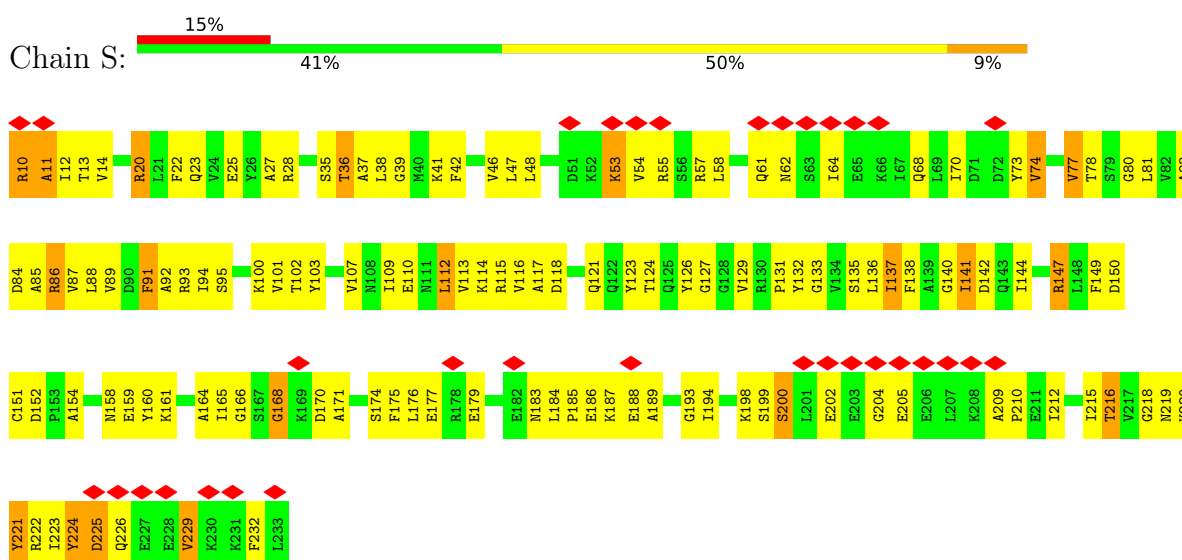
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	1	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	N	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	2	203	Total	C	N	O	S	0	0
			1558	985	264	298	11		
2	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		

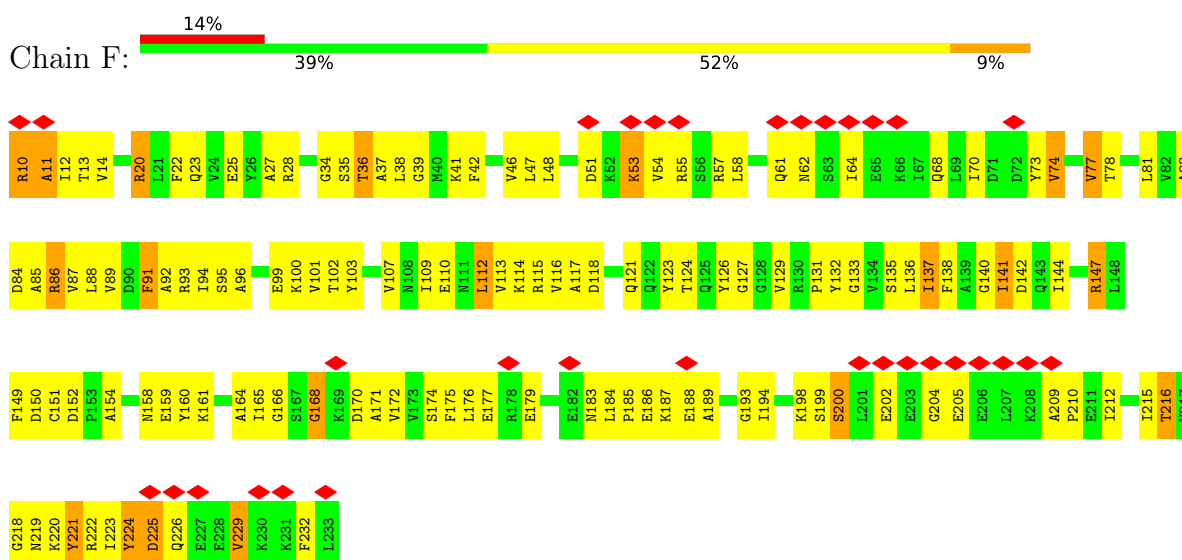
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

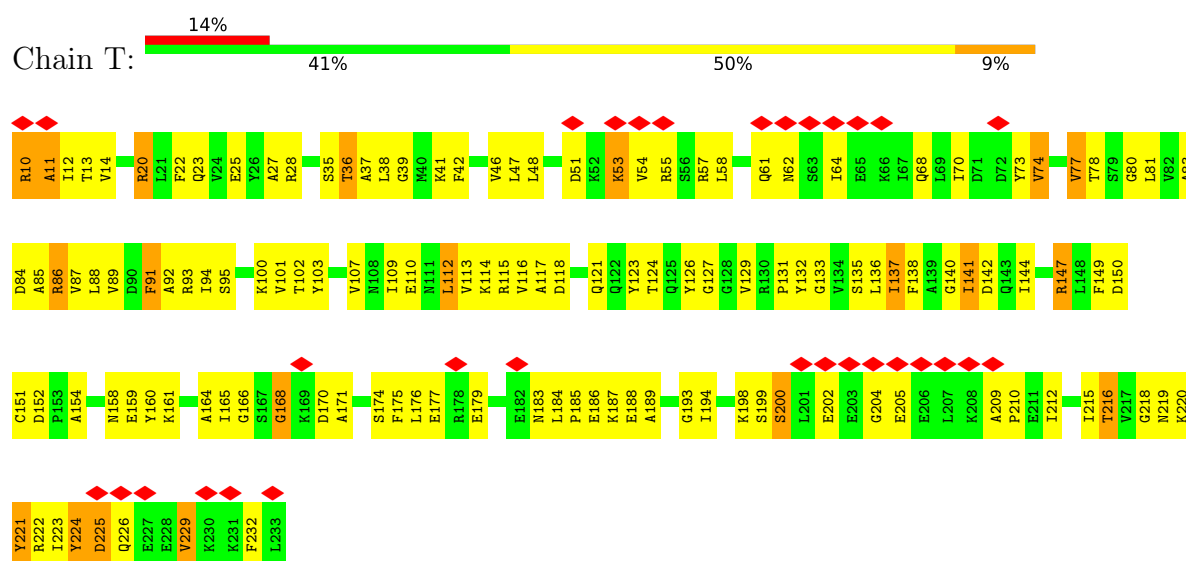
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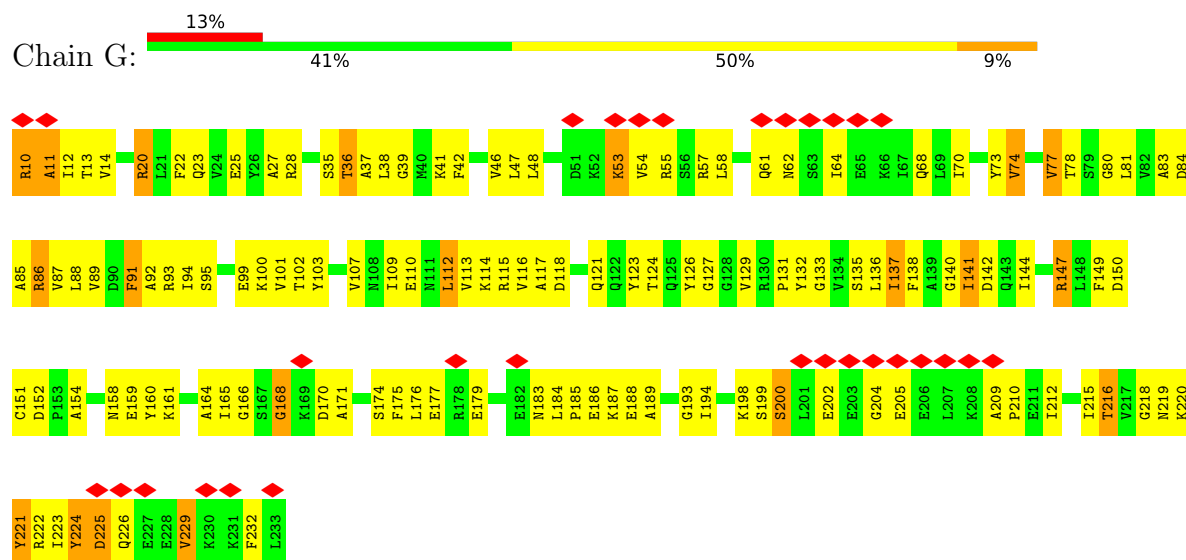
• Molecule 1: Proteasome subunit alpha



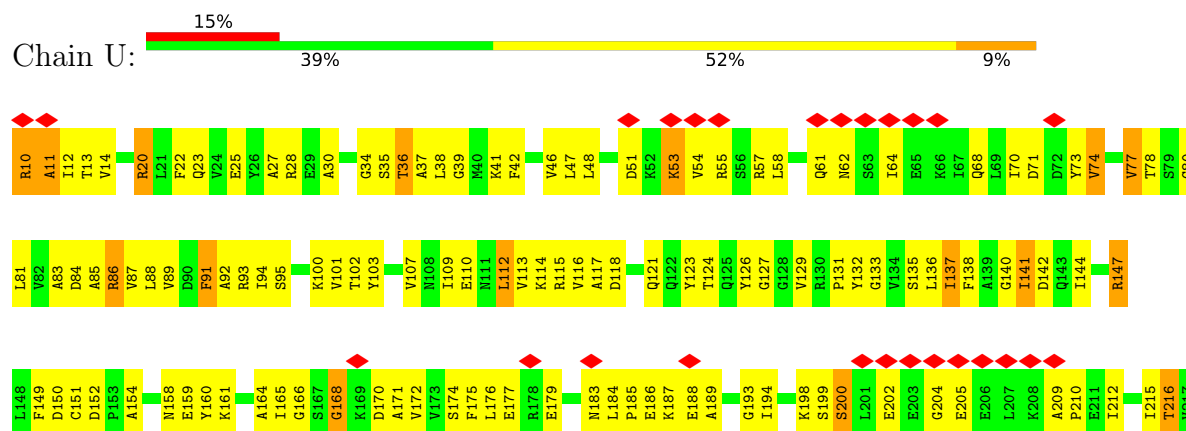
• Molecule 1: Proteasome subunit alpha

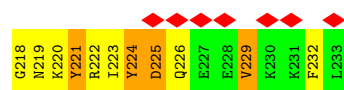


• Molecule 1: Proteasome subunit alpha

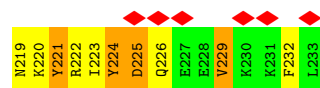
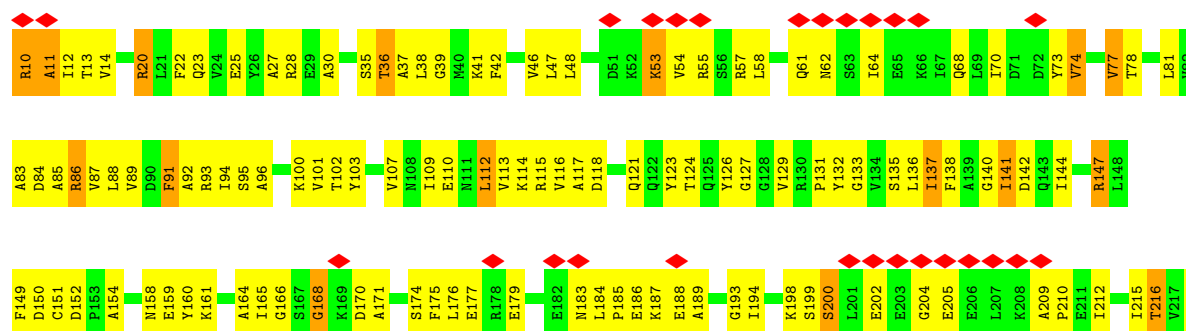
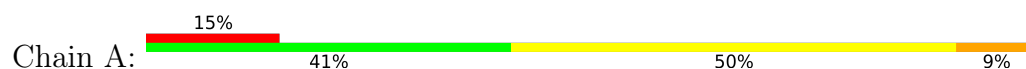


• Molecule 1: Proteasome subunit alpha

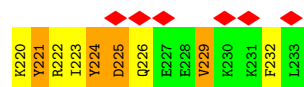
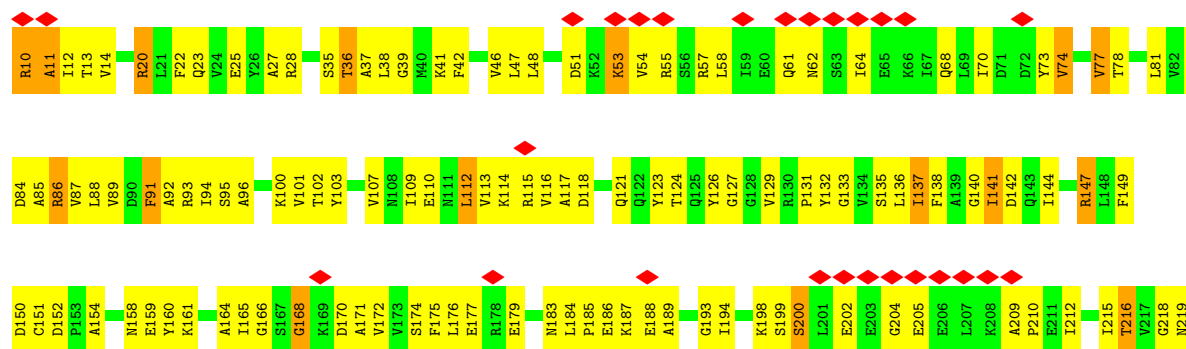




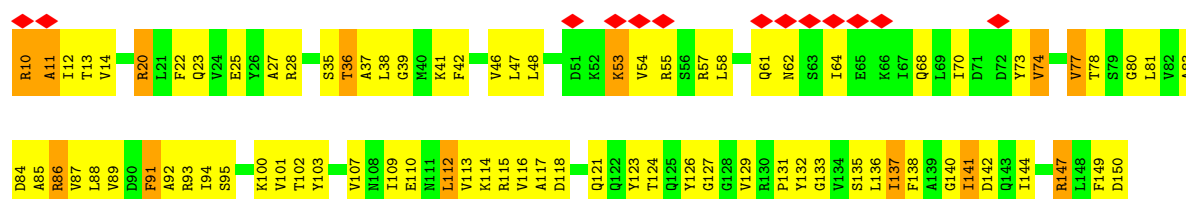
• Molecule 1: Proteasome subunit alpha

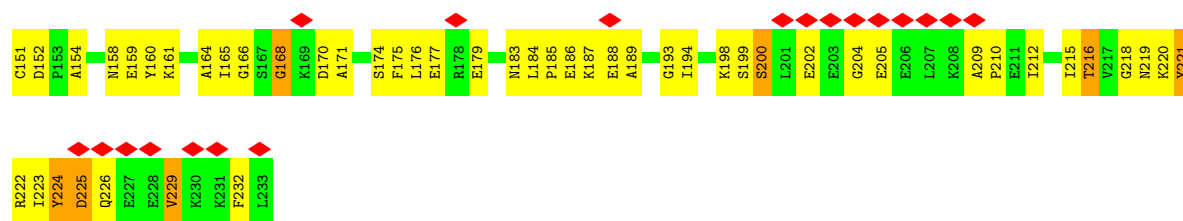


• Molecule 1: Proteasome subunit alpha

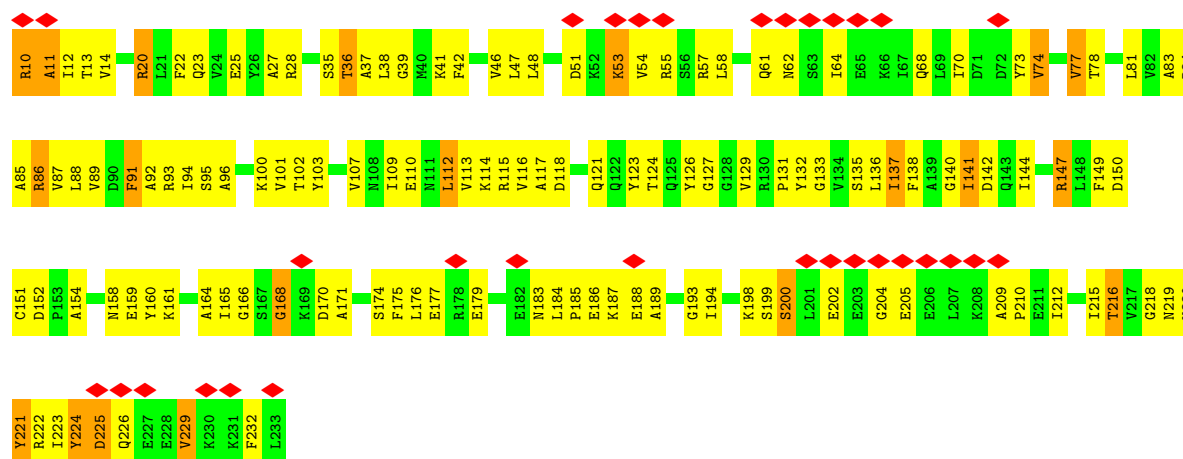


• Molecule 1: Proteasome subunit alpha

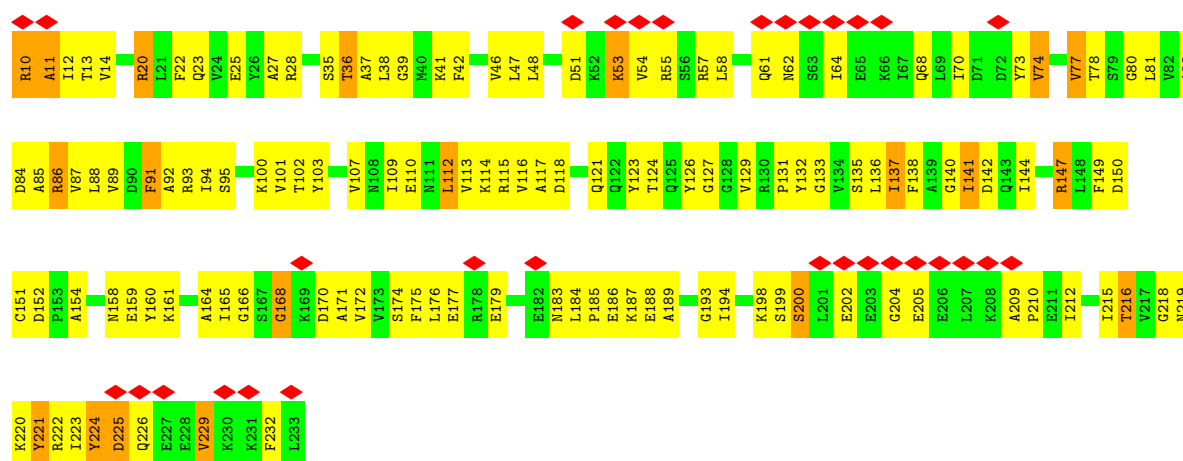




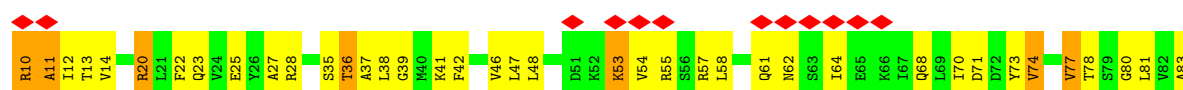
• Molecule 1: Proteasome subunit alpha

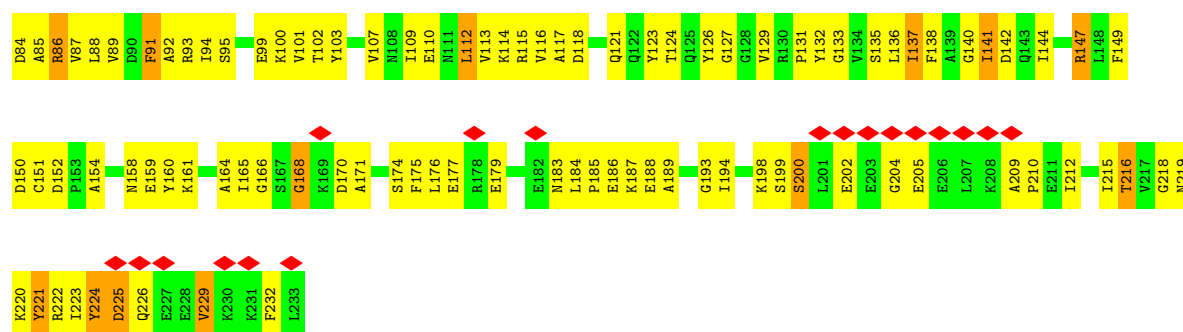


• Molecule 1: Proteasome subunit alpha

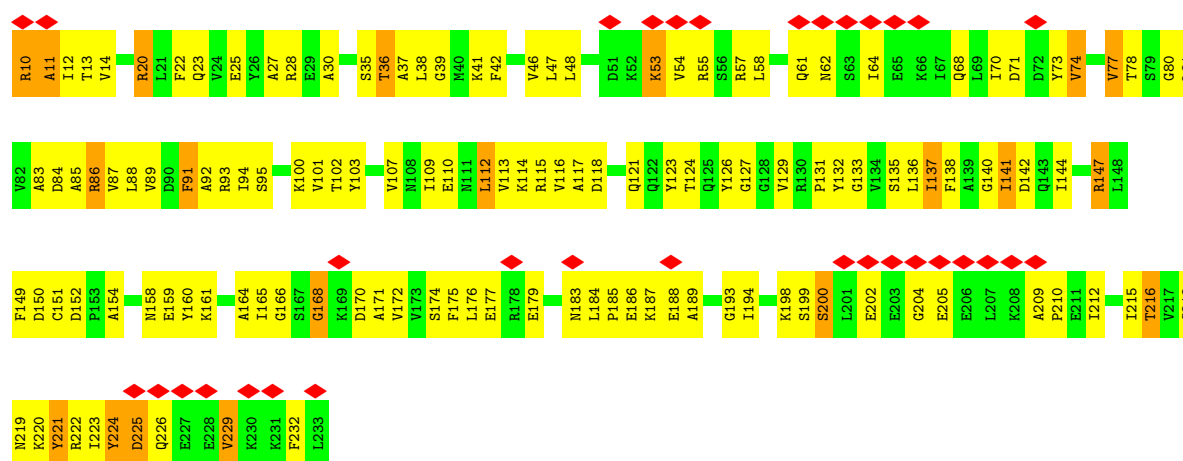


• Molecule 1: Proteasome subunit alpha

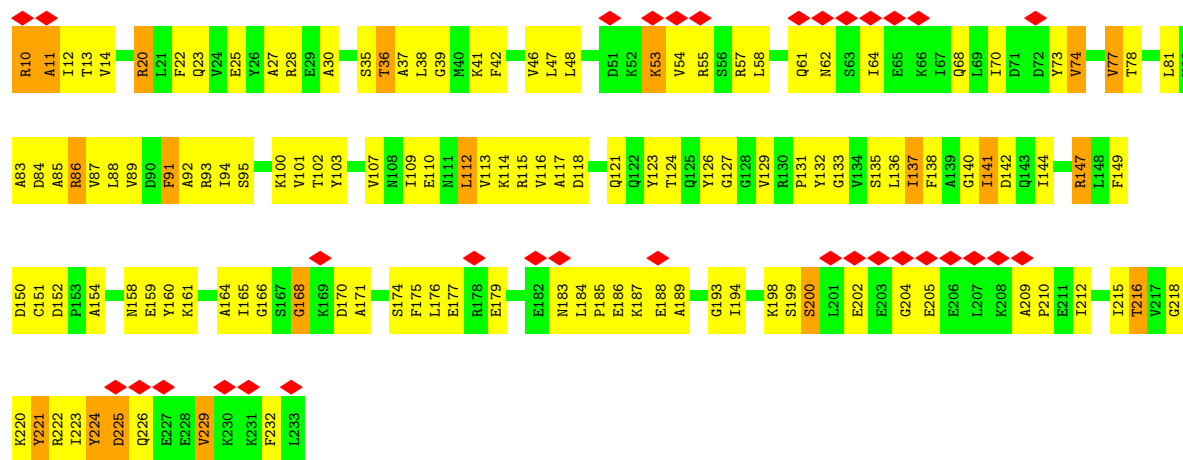




• Molecule 1: Proteasome subunit alpha

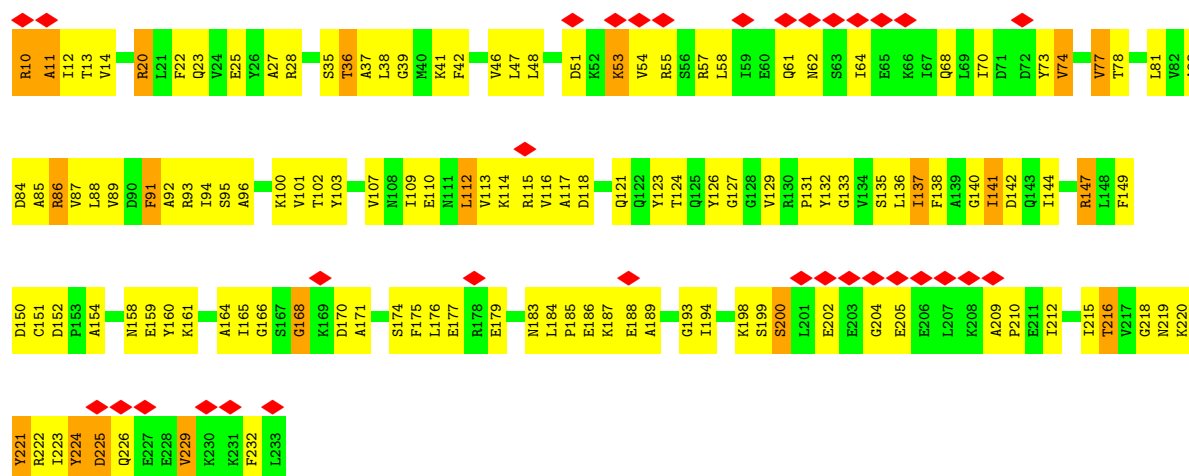


• Molecule 1: Proteasome subunit alpha

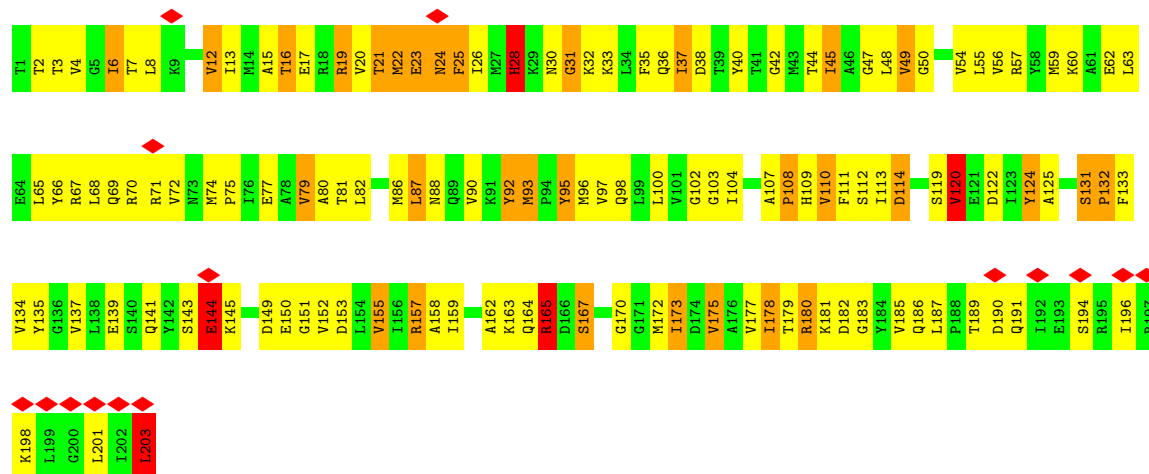


• Molecule 1: Proteasome subunit alpha

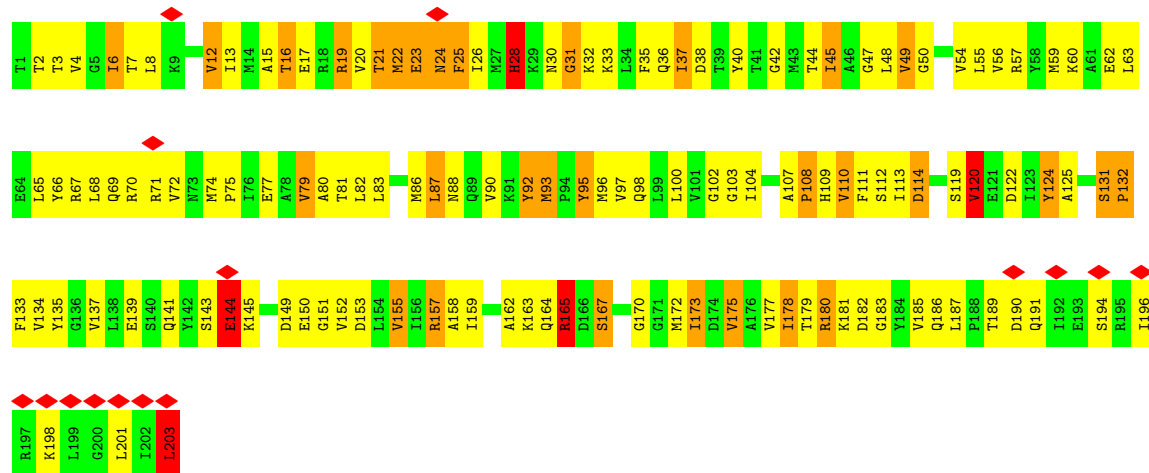




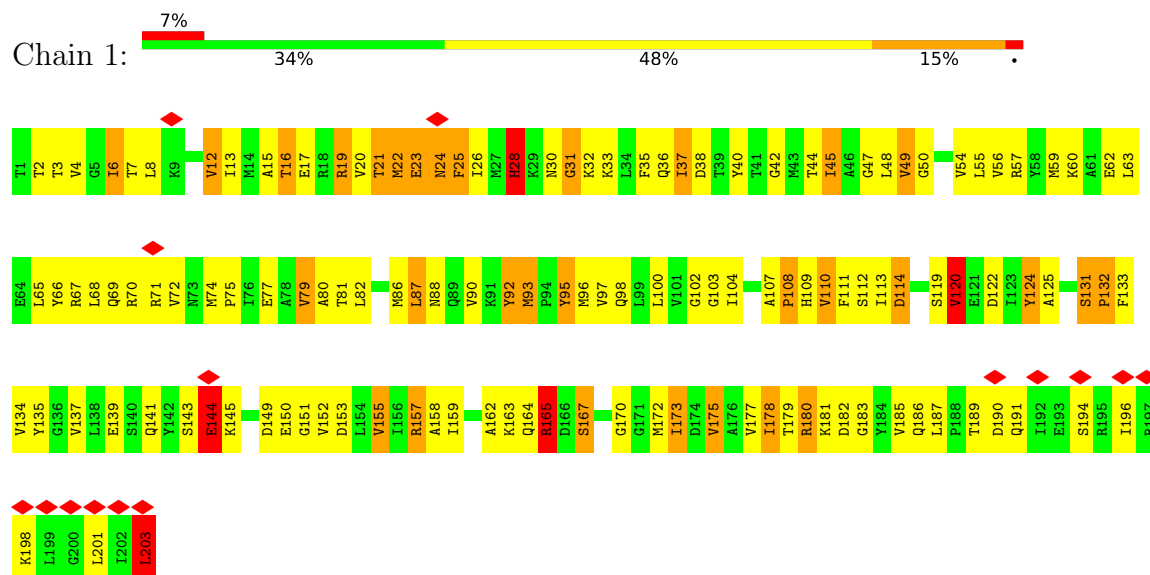
• Molecule 2: Proteasome subunit beta



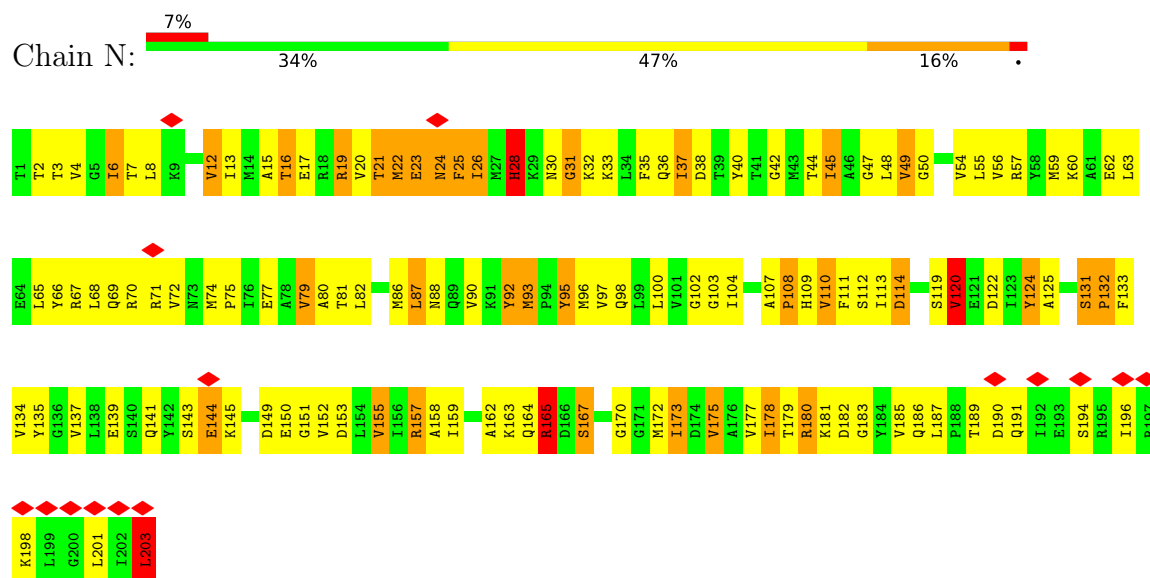
• Molecule 2: Proteasome subunit beta



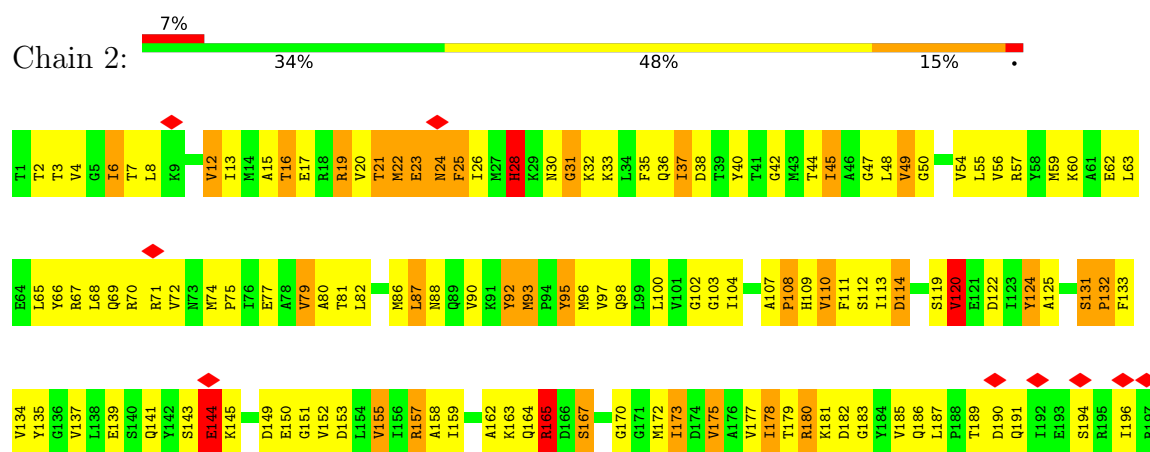
- Molecule 2: Proteasome subunit beta

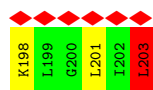


- Molecule 2: Proteasome subunit beta

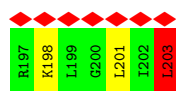
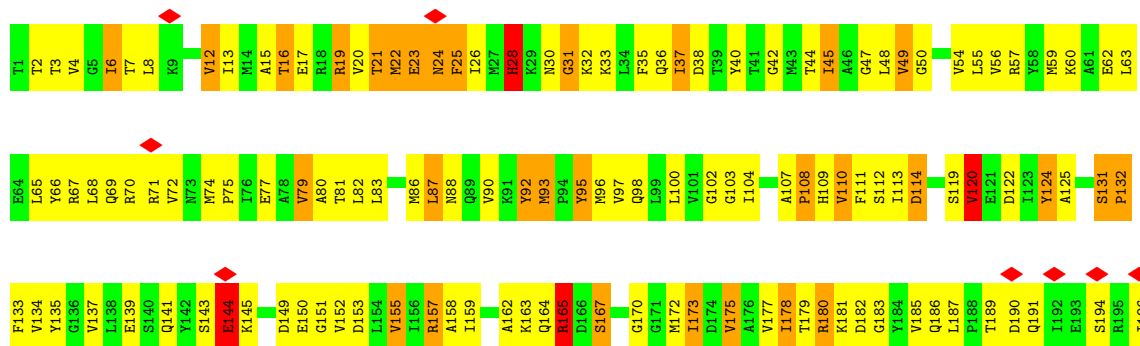


- Molecule 2: Proteasome subunit beta

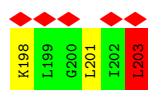
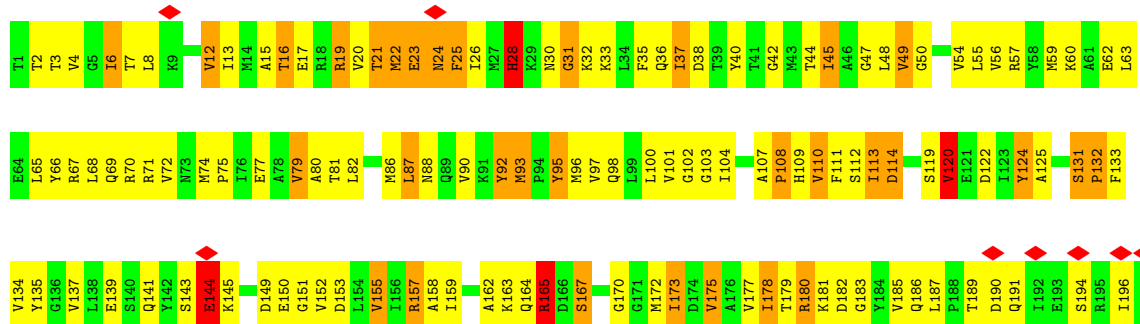




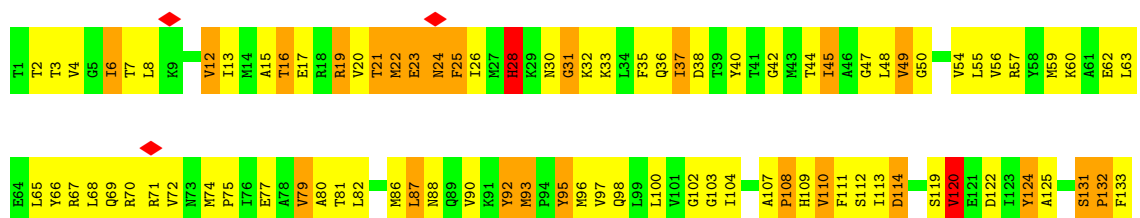
• Molecule 2: Proteasome subunit beta

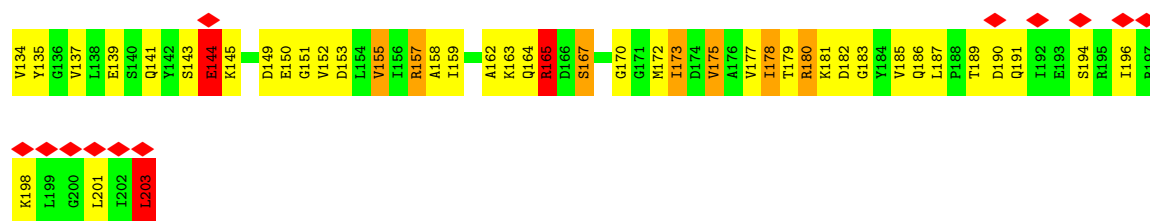


• Molecule 2: Proteasome subunit beta

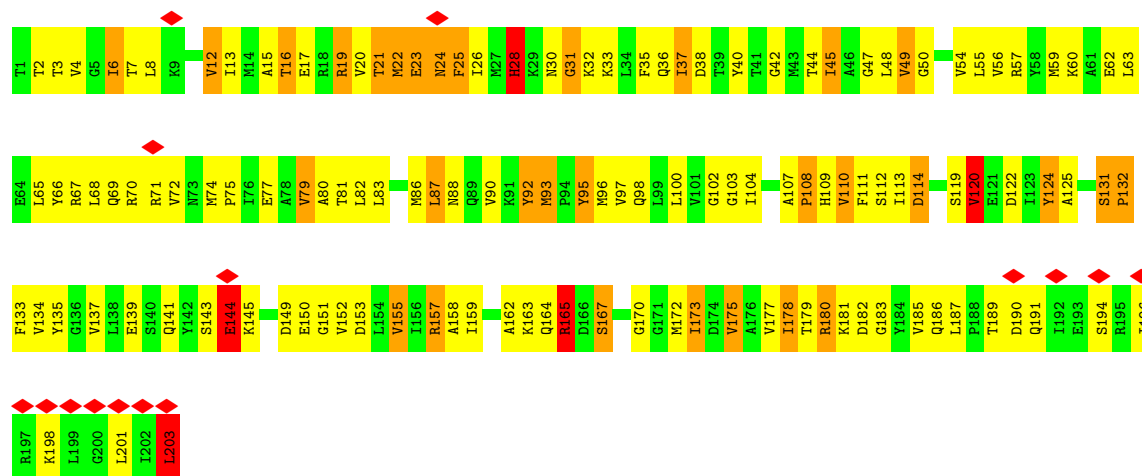


• Molecule 2: Proteasome subunit beta

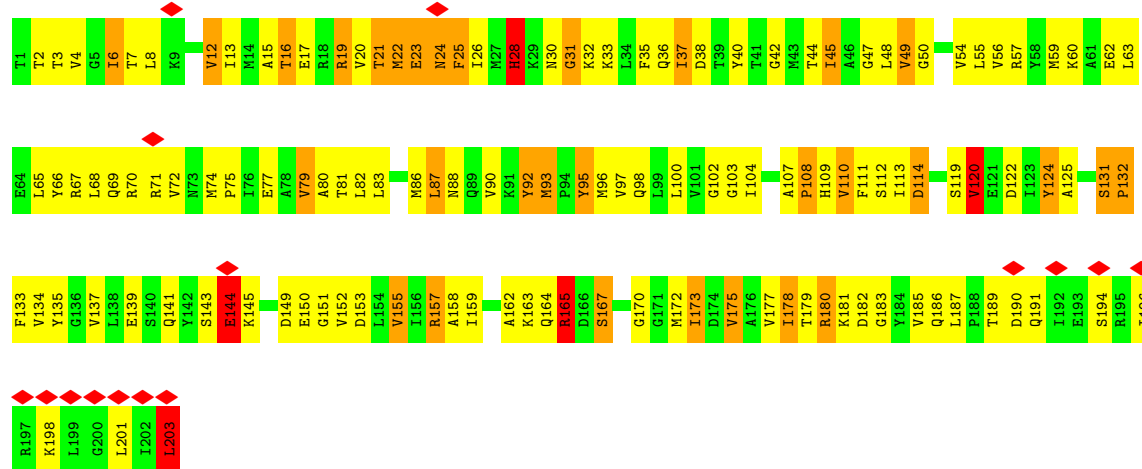




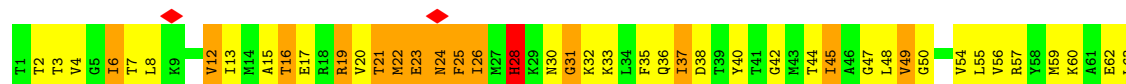
• Molecule 2: Proteasome subunit beta

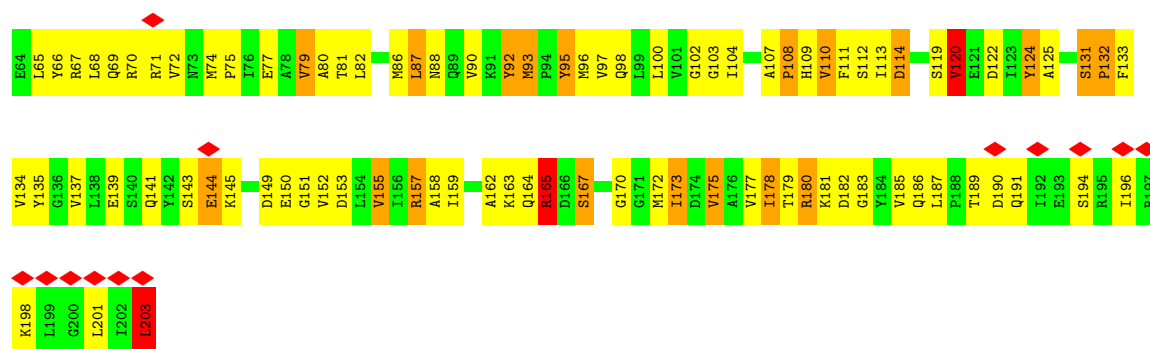


• Molecule 2: Proteasome subunit beta

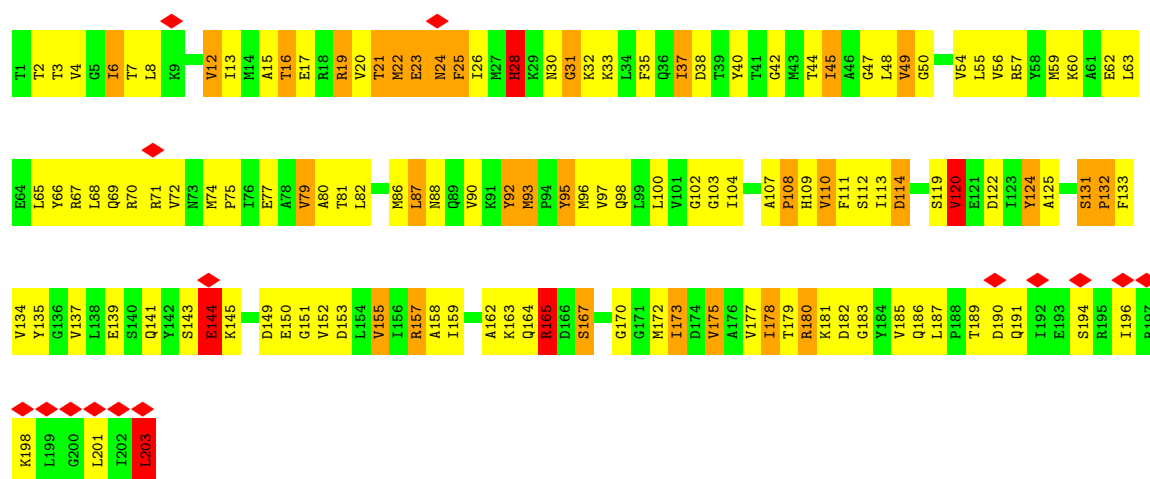


• Molecule 2: Proteasome subunit beta

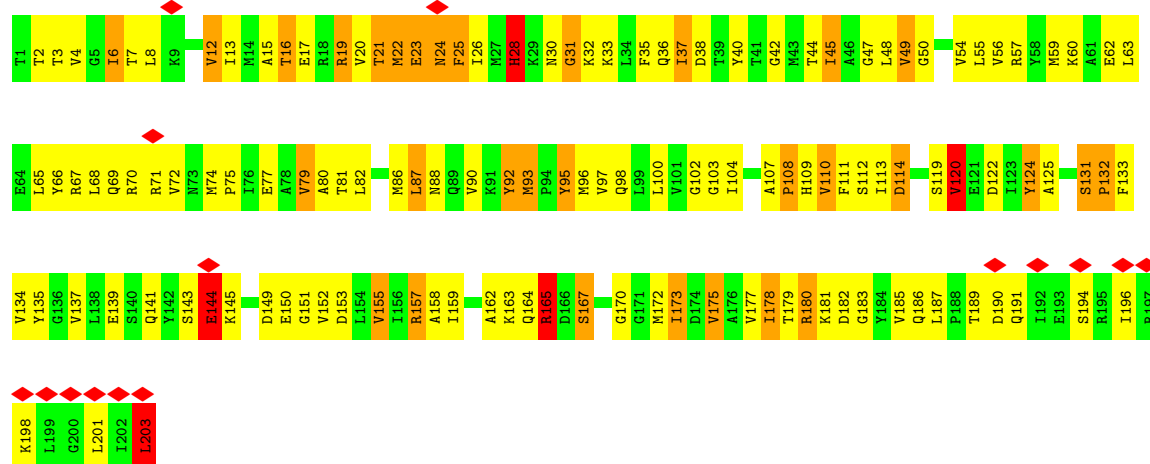




• Molecule 2: Proteasome subunit beta

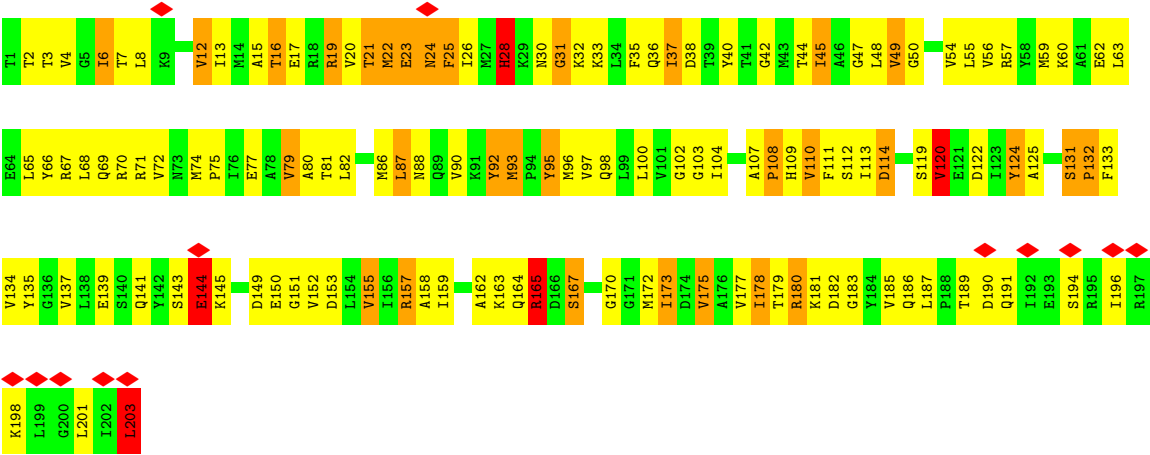


• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D7	Depositor
Number of particles used	126729	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	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
Maximum map value	1.200	Depositor
Minimum map value	-0.555	Depositor
Average map value	-0.008	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.25	Depositor
Map size ($\text{\AA}$)	311.1936, 311.1936, 311.1936	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2156, 1.2156, 1.2156	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 > 5$	RMSZ	# $ Z > 5$
1	A	2.27	63/1767 (3.6%)	2.48	119/2380 (5.0%)
1	B	2.27	62/1767 (3.5%)	2.48	119/2380 (5.0%)
1	C	2.27	64/1767 (3.6%)	2.48	119/2380 (5.0%)
1	D	2.27	66/1767 (3.7%)	2.48	119/2380 (5.0%)
1	E	2.27	63/1767 (3.6%)	2.48	119/2380 (5.0%)
1	F	2.27	66/1767 (3.7%)	2.48	120/2380 (5.0%)
1	G	2.27	64/1767 (3.6%)	2.48	119/2380 (5.0%)
1	O	2.27	64/1767 (3.6%)	2.48	119/2380 (5.0%)
1	P	2.27	64/1767 (3.6%)	2.48	119/2380 (5.0%)
1	Q	2.27	65/1767 (3.7%)	2.48	119/2380 (5.0%)
1	R	2.27	62/1767 (3.5%)	2.48	119/2380 (5.0%)
1	S	2.27	62/1767 (3.5%)	2.48	119/2380 (5.0%)
1	T	2.27	63/1767 (3.6%)	2.48	119/2380 (5.0%)
1	U	2.27	66/1767 (3.7%)	2.48	120/2380 (5.0%)
2	1	2.28	66/1577 (4.2%)	2.53	114/2129 (5.4%)
2	2	2.28	67/1577 (4.2%)	2.53	113/2129 (5.3%)
2	H	2.28	67/1577 (4.2%)	2.53	113/2129 (5.3%)
2	I	2.28	66/1577 (4.2%)	2.53	113/2129 (5.3%)
2	J	2.28	67/1577 (4.2%)	2.53	113/2129 (5.3%)
2	K	2.28	66/1577 (4.2%)	2.53	113/2129 (5.3%)
2	L	2.28	66/1577 (4.2%)	2.53	114/2129 (5.4%)
2	M	2.28	67/1577 (4.2%)	2.53	112/2129 (5.3%)
2	N	2.28	66/1577 (4.2%)	2.53	114/2129 (5.4%)
2	V	2.28	65/1577 (4.1%)	2.53	113/2129 (5.3%)
2	W	2.28	67/1577 (4.2%)	2.53	113/2129 (5.3%)
2	X	2.28	65/1577 (4.1%)	2.53	113/2129 (5.3%)
2	Y	2.28	65/1577 (4.1%)	2.53	114/2129 (5.4%)
2	Z	2.28	66/1577 (4.2%)	2.53	113/2129 (5.3%)
All	All	2.27	1820/46816 (3.9%)	2.50	3253/63126 (5.2%)

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 (1820) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	111	PHE	CA-C	-12.29	1.38	1.52
2	M	111	PHE	CA-C	-12.28	1.38	1.52
2	L	111	PHE	CA-C	-12.25	1.38	1.52
2	N	111	PHE	CA-C	-12.25	1.38	1.52
2	X	111	PHE	CA-C	-12.25	1.38	1.52
2	Z	111	PHE	CA-C	-12.24	1.38	1.52
2	I	111	PHE	CA-C	-12.24	1.38	1.52
2	W	111	PHE	CA-C	-12.24	1.38	1.52
2	H	111	PHE	CA-C	-12.24	1.38	1.52
2	Y	111	PHE	CA-C	-12.24	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	111	PHE	CA-C	-12.23	1.38	1.52
2	1	111	PHE	CA-C	-12.23	1.38	1.52
2	J	111	PHE	CA-C	-12.23	1.38	1.52
2	K	111	PHE	CA-C	-12.22	1.38	1.52
2	Y	164	GLN	CA-C	-10.60	1.39	1.52
2	N	164	GLN	CA-C	-10.57	1.39	1.52
2	H	164	GLN	CA-C	-10.57	1.39	1.52
2	J	164	GLN	CA-C	-10.57	1.39	1.52
2	X	164	GLN	CA-C	-10.57	1.39	1.52
2	K	164	GLN	CA-C	-10.55	1.39	1.52
2	V	164	GLN	CA-C	-10.55	1.39	1.52
2	L	164	GLN	CA-C	-10.55	1.39	1.52
2	Z	164	GLN	CA-C	-10.54	1.39	1.52
2	M	164	GLN	CA-C	-10.54	1.39	1.52
2	2	164	GLN	CA-C	-10.54	1.39	1.52
2	I	164	GLN	CA-C	-10.54	1.39	1.52
2	W	164	GLN	CA-C	-10.54	1.39	1.52
2	1	164	GLN	CA-C	-10.52	1.39	1.52
1	F	28	ARG	CD-NE	9.72	1.59	1.46
1	P	28	ARG	CD-NE	9.72	1.59	1.46
1	Q	28	ARG	CD-NE	9.72	1.59	1.46
1	U	28	ARG	CD-NE	9.71	1.59	1.46
1	A	28	ARG	CD-NE	9.71	1.59	1.46
1	D	28	ARG	CD-NE	9.71	1.59	1.46
1	R	28	ARG	CD-NE	9.71	1.59	1.46
1	S	28	ARG	CD-NE	9.71	1.59	1.46
1	B	28	ARG	CD-NE	9.71	1.59	1.46
1	T	28	ARG	CD-NE	9.70	1.59	1.46
1	C	28	ARG	CD-NE	9.70	1.59	1.46
1	G	28	ARG	CD-NE	9.68	1.59	1.46
1	O	28	ARG	CD-NE	9.68	1.59	1.46
1	E	28	ARG	CD-NE	9.68	1.59	1.46
1	P	39	GLY	C-N	9.33	1.45	1.33
1	U	39	GLY	C-N	9.29	1.44	1.33
1	O	39	GLY	C-N	9.29	1.44	1.33
1	E	39	GLY	C-N	9.29	1.44	1.33
1	S	39	GLY	C-N	9.28	1.44	1.33
1	T	39	GLY	C-N	9.29	1.44	1.33
1	B	39	GLY	C-N	9.28	1.44	1.33
1	C	39	GLY	C-N	9.29	1.44	1.33
1	F	39	GLY	C-N	9.28	1.44	1.33
1	D	39	GLY	C-N	9.28	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	GLY	C-N	9.27	1.44	1.33
1	R	39	GLY	C-N	9.27	1.44	1.33
1	G	39	GLY	C-N	9.26	1.44	1.33
1	Q	39	GLY	C-N	9.26	1.44	1.33
1	F	10	ARG	NE-CZ	8.47	1.42	1.33
1	P	10	ARG	NE-CZ	8.47	1.42	1.33
2	Y	180	ARG	CD-NE	8.44	1.58	1.46
1	O	10	ARG	NE-CZ	8.42	1.42	1.33
1	E	10	ARG	NE-CZ	8.42	1.42	1.33
2	L	180	ARG	CD-NE	8.42	1.58	1.46
1	U	10	ARG	NE-CZ	8.42	1.42	1.33
2	2	180	ARG	CD-NE	8.42	1.58	1.46
1	Q	10	ARG	NE-CZ	8.42	1.42	1.33
1	D	10	ARG	NE-CZ	8.42	1.42	1.33
2	K	180	ARG	CD-NE	8.42	1.58	1.46
2	Z	180	ARG	CD-NE	8.41	1.58	1.46
2	H	180	ARG	CD-NE	8.41	1.58	1.46
2	M	180	ARG	CD-NE	8.41	1.58	1.46
2	I	180	ARG	CD-NE	8.41	1.58	1.46
2	W	180	ARG	CD-NE	8.41	1.58	1.46
1	T	10	ARG	NE-CZ	8.41	1.42	1.33
1	C	10	ARG	NE-CZ	8.41	1.42	1.33
1	A	10	ARG	NE-CZ	8.40	1.42	1.33
1	R	10	ARG	NE-CZ	8.40	1.42	1.33
2	1	180	ARG	CD-NE	8.40	1.58	1.46
2	N	180	ARG	CD-NE	8.40	1.58	1.46
2	X	180	ARG	CD-NE	8.39	1.58	1.46
2	V	180	ARG	CD-NE	8.39	1.57	1.46
2	J	180	ARG	CD-NE	8.39	1.57	1.46
1	S	10	ARG	NE-CZ	8.38	1.42	1.33
1	B	10	ARG	NE-CZ	8.38	1.42	1.33
1	G	10	ARG	NE-CZ	8.33	1.42	1.33
1	P	116	VAL	CA-C	-8.06	1.42	1.52
1	O	116	VAL	CA-C	-8.05	1.42	1.52
1	E	116	VAL	CA-C	-8.04	1.42	1.52
1	T	116	VAL	CA-C	-8.04	1.42	1.52
1	U	116	VAL	CA-C	-8.04	1.42	1.52
1	G	116	VAL	CA-C	-8.04	1.42	1.52
1	Q	116	VAL	CA-C	-8.04	1.42	1.52
1	F	116	VAL	CA-C	-8.04	1.42	1.52
1	R	116	VAL	CA-C	-8.03	1.42	1.52
1	S	116	VAL	CA-C	-8.03	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	VAL	CA-C	-8.03	1.42	1.52
1	A	116	VAL	CA-C	-8.01	1.42	1.52
1	D	116	VAL	CA-C	-8.01	1.42	1.52
1	C	116	VAL	CA-C	-8.01	1.42	1.52
2	H	47	GLY	CA-C	-7.89	1.40	1.51
2	L	47	GLY	CA-C	-7.88	1.40	1.51
2	K	47	GLY	CA-C	-7.87	1.40	1.51
2	N	47	GLY	CA-C	-7.85	1.40	1.51
2	Z	47	GLY	CA-C	-7.84	1.40	1.51
2	I	47	GLY	CA-C	-7.84	1.40	1.51
2	V	47	GLY	CA-C	-7.84	1.40	1.51
2	Y	47	GLY	CA-C	-7.82	1.40	1.51
2	2	47	GLY	CA-C	-7.80	1.40	1.51
2	M	47	GLY	CA-C	-7.80	1.40	1.51
2	W	47	GLY	CA-C	-7.80	1.40	1.51
2	1	47	GLY	CA-C	-7.79	1.41	1.51
2	J	47	GLY	CA-C	-7.79	1.41	1.51
2	X	47	GLY	CA-C	-7.78	1.41	1.51
1	O	160	TYR	CA-C	-7.68	1.42	1.53
1	C	160	TYR	CA-C	-7.68	1.42	1.53
1	A	160	TYR	CA-C	-7.67	1.42	1.53
1	S	160	TYR	CA-C	-7.66	1.42	1.53
1	B	160	TYR	CA-C	-7.66	1.42	1.53
1	F	160	TYR	CA-C	-7.65	1.42	1.53
1	P	160	TYR	CA-C	-7.65	1.42	1.53
1	R	160	TYR	CA-C	-7.64	1.42	1.53
1	D	160	TYR	CA-C	-7.64	1.42	1.53
1	U	160	TYR	CA-C	-7.64	1.42	1.53
1	E	160	TYR	CA-C	-7.64	1.42	1.53
1	G	160	TYR	CA-C	-7.63	1.42	1.53
1	Q	160	TYR	CA-C	-7.63	1.42	1.53
1	T	160	TYR	CA-C	-7.63	1.42	1.53
1	G	22	PHE	CA-C	-7.58	1.42	1.52
1	D	22	PHE	CA-C	-7.58	1.42	1.52
1	R	22	PHE	CA-C	-7.58	1.42	1.52
1	E	22	PHE	CA-C	-7.58	1.42	1.52
1	S	22	PHE	CA-C	-7.55	1.42	1.52
1	B	22	PHE	CA-C	-7.55	1.42	1.52
1	O	22	PHE	CA-C	-7.54	1.42	1.52
1	T	22	PHE	CA-C	-7.54	1.42	1.52
1	C	22	PHE	CA-C	-7.54	1.42	1.52
1	A	22	PHE	CA-C	-7.53	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	22	PHE	CA-C	-7.53	1.42	1.52
1	U	84	ASP	N-CA	7.52	1.55	1.46
1	F	22	PHE	CA-C	-7.52	1.42	1.52
1	U	22	PHE	CA-C	-7.52	1.42	1.52
1	P	22	PHE	CA-C	-7.52	1.42	1.52
1	E	84	ASP	N-CA	7.52	1.55	1.46
1	T	84	ASP	N-CA	7.50	1.55	1.46
1	A	84	ASP	N-CA	7.50	1.55	1.46
1	C	84	ASP	N-CA	7.50	1.55	1.46
2	1	190	ASP	N-CA	-7.48	1.37	1.46
1	O	84	ASP	N-CA	7.47	1.55	1.46
1	G	84	ASP	N-CA	7.46	1.55	1.46
1	Q	84	ASP	N-CA	7.46	1.55	1.46
1	S	84	ASP	N-CA	7.46	1.55	1.46
1	B	84	ASP	N-CA	7.46	1.55	1.46
2	V	190	ASP	N-CA	-7.45	1.37	1.46
2	L	190	ASP	N-CA	-7.45	1.37	1.46
2	H	190	ASP	N-CA	-7.44	1.37	1.46
1	D	84	ASP	N-CA	7.44	1.55	1.46
2	Y	190	ASP	N-CA	-7.44	1.37	1.46
1	R	84	ASP	N-CA	7.44	1.55	1.46
1	F	84	ASP	N-CA	7.42	1.55	1.46
1	P	84	ASP	N-CA	7.42	1.55	1.46
2	Z	190	ASP	N-CA	-7.42	1.37	1.46
2	I	190	ASP	N-CA	-7.42	1.37	1.46
2	2	190	ASP	N-CA	-7.41	1.37	1.46
2	K	190	ASP	N-CA	-7.41	1.37	1.46
2	J	190	ASP	N-CA	-7.41	1.37	1.46
2	N	190	ASP	N-CA	-7.40	1.37	1.46
2	X	190	ASP	N-CA	-7.40	1.37	1.46
2	M	190	ASP	N-CA	-7.39	1.37	1.46
2	W	190	ASP	N-CA	-7.39	1.37	1.46
1	P	184	LEU	CA-C	-7.36	1.44	1.52
1	F	184	LEU	CA-C	-7.34	1.45	1.52
1	G	184	LEU	CA-C	-7.34	1.45	1.52
1	T	184	LEU	CA-C	-7.33	1.45	1.52
1	O	184	LEU	CA-C	-7.33	1.45	1.52
1	U	184	LEU	CA-C	-7.31	1.45	1.52
1	D	184	LEU	CA-C	-7.31	1.45	1.52
2	1	74	MET	CA-C	-7.31	1.44	1.52
1	S	184	LEU	CA-C	-7.30	1.45	1.52
1	B	184	LEU	CA-C	-7.30	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	145	LYS	N-CA	-7.30	1.37	1.46
2	N	145	LYS	N-CA	-7.30	1.37	1.46
1	E	184	LEU	CA-C	-7.30	1.45	1.52
1	A	184	LEU	CA-C	-7.29	1.45	1.52
1	R	184	LEU	CA-C	-7.29	1.45	1.52
1	C	184	LEU	CA-C	-7.29	1.45	1.52
2	N	74	MET	CA-C	-7.28	1.44	1.52
2	2	74	MET	CA-C	-7.28	1.44	1.52
1	Q	184	LEU	CA-C	-7.28	1.45	1.52
2	H	74	MET	CA-C	-7.27	1.44	1.52
1	A	220	LYS	CA-C	-7.27	1.43	1.53
2	W	145	LYS	N-CA	-7.27	1.37	1.46
1	F	220	LYS	CA-C	-7.27	1.43	1.53
2	M	74	MET	CA-C	-7.27	1.44	1.52
2	W	74	MET	CA-C	-7.27	1.44	1.52
1	D	220	LYS	CA-C	-7.26	1.43	1.53
2	Z	74	MET	CA-C	-7.26	1.44	1.52
2	I	74	MET	CA-C	-7.26	1.44	1.52
2	J	74	MET	CA-C	-7.26	1.44	1.52
1	G	220	LYS	CA-C	-7.25	1.43	1.53
1	Q	220	LYS	CA-C	-7.25	1.43	1.53
2	Y	145	LYS	N-CA	-7.25	1.37	1.46
2	L	74	MET	CA-C	-7.25	1.44	1.52
1	S	220	LYS	CA-C	-7.25	1.43	1.53
1	B	220	LYS	CA-C	-7.25	1.43	1.53
1	R	220	LYS	CA-C	-7.25	1.43	1.53
2	H	145	LYS	N-CA	-7.25	1.37	1.46
1	T	220	LYS	CA-C	-7.24	1.43	1.53
1	O	220	LYS	CA-C	-7.24	1.43	1.53
1	P	220	LYS	CA-C	-7.24	1.43	1.53
1	C	220	LYS	CA-C	-7.24	1.43	1.53
1	E	220	LYS	CA-C	-7.24	1.43	1.53
1	U	220	LYS	CA-C	-7.24	1.43	1.53
2	V	74	MET	CA-C	-7.24	1.44	1.52
2	X	145	LYS	N-CA	-7.24	1.37	1.46
2	Z	145	LYS	N-CA	-7.24	1.37	1.46
2	I	145	LYS	N-CA	-7.24	1.37	1.46
2	Y	74	MET	CA-C	-7.24	1.44	1.52
1	A	174	SER	CA-C	-7.24	1.43	1.52
2	K	74	MET	CA-C	-7.23	1.44	1.52
2	X	74	MET	CA-C	-7.22	1.44	1.52
1	T	174	SER	CA-C	-7.22	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	145	LYS	N-CA	-7.22	1.37	1.46
2	2	145	LYS	N-CA	-7.22	1.37	1.46
2	K	145	LYS	N-CA	-7.22	1.37	1.46
1	R	174	SER	CA-C	-7.22	1.43	1.52
2	L	145	LYS	N-CA	-7.21	1.37	1.46
1	G	174	SER	CA-C	-7.21	1.43	1.52
1	Q	174	SER	CA-C	-7.21	1.43	1.52
1	U	109	ILE	CA-CB	-7.20	1.44	1.54
1	D	109	ILE	CA-CB	-7.20	1.44	1.54
1	S	174	SER	CA-C	-7.19	1.43	1.52
1	B	174	SER	CA-C	-7.19	1.43	1.52
2	M	145	LYS	N-CA	-7.19	1.37	1.46
1	U	174	SER	CA-C	-7.19	1.43	1.52
1	D	174	SER	CA-C	-7.19	1.43	1.52
2	X	97	VAL	N-CA	-7.18	1.37	1.46
1	F	174	SER	CA-C	-7.17	1.43	1.52
1	P	174	SER	CA-C	-7.17	1.43	1.52
1	T	221	TYR	N-CA	-7.17	1.37	1.46
1	C	221	TYR	N-CA	-7.17	1.37	1.46
2	V	145	LYS	N-CA	-7.17	1.37	1.46
1	O	174	SER	CA-C	-7.17	1.43	1.52
1	R	221	TYR	N-CA	-7.16	1.37	1.46
2	V	97	VAL	N-CA	-7.16	1.37	1.46
1	T	109	ILE	CA-CB	-7.16	1.44	1.54
1	C	109	ILE	CA-CB	-7.16	1.44	1.54
1	S	109	ILE	CA-CB	-7.16	1.44	1.54
1	F	221	TYR	N-CA	-7.16	1.37	1.46
1	B	109	ILE	CA-CB	-7.16	1.44	1.54
1	P	221	TYR	N-CA	-7.16	1.37	1.46
1	G	221	TYR	N-CA	-7.16	1.37	1.46
1	Q	221	TYR	N-CA	-7.16	1.37	1.46
1	U	221	TYR	N-CA	-7.16	1.37	1.46
1	C	174	SER	CA-C	-7.16	1.43	1.52
1	D	221	TYR	N-CA	-7.16	1.37	1.46
1	S	221	TYR	N-CA	-7.15	1.37	1.46
1	B	221	TYR	N-CA	-7.15	1.37	1.46
1	A	109	ILE	CA-CB	-7.15	1.44	1.54
1	O	221	TYR	N-CA	-7.15	1.37	1.46
1	R	109	ILE	CA-CB	-7.15	1.44	1.54
2	H	97	VAL	N-CA	-7.15	1.37	1.46
2	Y	97	VAL	N-CA	-7.15	1.37	1.46
2	M	97	VAL	N-CA	-7.14	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	109	ILE	CA-CB	-7.14	1.44	1.54
1	E	109	ILE	CA-CB	-7.14	1.44	1.54
1	A	221	TYR	N-CA	-7.14	1.37	1.46
1	F	109	ILE	CA-CB	-7.13	1.44	1.54
1	G	109	ILE	CA-CB	-7.13	1.44	1.54
1	P	109	ILE	CA-CB	-7.13	1.44	1.54
1	Q	109	ILE	CA-CB	-7.13	1.44	1.54
2	N	97	VAL	N-CA	-7.13	1.37	1.46
1	E	221	TYR	N-CA	-7.13	1.37	1.46
1	E	174	SER	CA-C	-7.12	1.43	1.52
2	L	63	LEU	CA-C	-7.12	1.43	1.52
2	Z	97	VAL	N-CA	-7.12	1.37	1.46
2	1	97	VAL	N-CA	-7.12	1.37	1.46
2	I	97	VAL	N-CA	-7.12	1.37	1.46
2	J	97	VAL	N-CA	-7.12	1.37	1.46
2	L	97	VAL	N-CA	-7.11	1.37	1.46
2	1	63	LEU	CA-C	-7.10	1.43	1.52
2	J	63	LEU	CA-C	-7.10	1.43	1.52
2	2	63	LEU	CA-C	-7.10	1.43	1.52
2	K	63	LEU	CA-C	-7.10	1.43	1.52
2	2	97	VAL	N-CA	-7.09	1.37	1.46
2	K	97	VAL	N-CA	-7.09	1.37	1.46
2	M	63	LEU	CA-C	-7.09	1.43	1.52
2	Z	63	LEU	CA-C	-7.08	1.43	1.52
2	I	63	LEU	CA-C	-7.08	1.43	1.52
2	V	63	LEU	CA-C	-7.08	1.43	1.52
1	R	140	GLY	CA-C	-7.08	1.43	1.51
2	N	63	LEU	CA-C	-7.07	1.43	1.52
2	X	63	LEU	CA-C	-7.07	1.43	1.52
2	H	63	LEU	CA-C	-7.06	1.43	1.52
2	Y	63	LEU	CA-C	-7.06	1.43	1.52
2	W	97	VAL	N-CA	-7.06	1.38	1.46
1	D	140	GLY	CA-C	-7.06	1.44	1.51
2	H	40	TYR	CA-C	-7.05	1.44	1.53
2	Y	40	TYR	CA-C	-7.05	1.44	1.53
2	W	63	LEU	CA-C	-7.05	1.43	1.52
2	N	40	TYR	CA-C	-7.04	1.44	1.53
2	J	40	TYR	CA-C	-7.04	1.44	1.53
1	T	140	GLY	CA-C	-7.03	1.44	1.51
1	C	140	GLY	CA-C	-7.03	1.44	1.51
2	K	40	TYR	CA-C	-7.03	1.44	1.53
2	2	40	TYR	CA-C	-7.03	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	40	TYR	CA-C	-7.02	1.44	1.53
2	I	40	TYR	CA-C	-7.02	1.44	1.53
1	S	140	GLY	CA-C	-7.01	1.44	1.51
1	O	140	GLY	CA-C	-7.01	1.44	1.51
1	B	140	GLY	CA-C	-7.01	1.44	1.51
2	X	40	TYR	CA-C	-7.01	1.44	1.53
1	E	140	GLY	CA-C	-7.01	1.44	1.51
2	M	40	TYR	CA-C	-7.01	1.44	1.53
2	W	40	TYR	CA-C	-7.01	1.44	1.53
1	A	102	THR	CA-C	-7.01	1.44	1.53
1	O	102	THR	CA-C	-7.00	1.44	1.53
1	Q	102	THR	CA-C	-7.00	1.44	1.53
1	F	110	GLU	CA-C	-6.99	1.43	1.52
2	1	40	TYR	CA-C	-6.99	1.44	1.53
1	G	140	GLY	CA-C	-6.99	1.44	1.51
1	A	140	GLY	CA-C	-6.99	1.44	1.51
1	Q	140	GLY	CA-C	-6.99	1.44	1.51
2	V	40	TYR	CA-C	-6.99	1.44	1.53
2	L	40	TYR	CA-C	-6.99	1.44	1.53
1	U	140	GLY	CA-C	-6.98	1.44	1.51
1	G	102	THR	CA-C	-6.98	1.44	1.53
1	F	140	GLY	CA-C	-6.98	1.44	1.51
1	P	140	GLY	CA-C	-6.98	1.44	1.51
1	E	27	ALA	CA-C	-6.97	1.44	1.52
1	S	102	THR	CA-C	-6.95	1.44	1.53
1	B	102	THR	CA-C	-6.95	1.44	1.53
1	O	110	GLU	CA-C	-6.94	1.43	1.52
1	E	110	GLU	CA-C	-6.94	1.43	1.52
1	S	110	GLU	CA-C	-6.94	1.43	1.52
1	B	110	GLU	CA-C	-6.94	1.43	1.52
1	R	102	THR	CA-C	-6.94	1.44	1.53
1	T	102	THR	CA-C	-6.94	1.44	1.53
1	C	102	THR	CA-C	-6.94	1.44	1.53
2	N	65	LEU	CA-C	-6.93	1.44	1.52
1	U	102	THR	CA-C	-6.93	1.44	1.53
1	D	102	THR	CA-C	-6.93	1.44	1.53
1	A	110	GLU	CA-C	-6.93	1.43	1.52
1	R	110	GLU	CA-C	-6.93	1.43	1.52
1	E	102	THR	CA-C	-6.93	1.44	1.53
1	F	102	THR	CA-C	-6.93	1.44	1.53
1	P	102	THR	CA-C	-6.93	1.44	1.53
2	1	65	LEU	CA-C	-6.92	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	110	GLU	CA-C	-6.92	1.43	1.52
2	J	65	LEU	CA-C	-6.92	1.44	1.52
1	A	27	ALA	CA-C	-6.92	1.44	1.52
1	G	110	GLU	CA-C	-6.92	1.43	1.52
2	M	65	LEU	CA-C	-6.92	1.44	1.52
2	H	65	LEU	CA-C	-6.92	1.44	1.52
2	W	65	LEU	CA-C	-6.92	1.44	1.52
2	Y	65	LEU	CA-C	-6.92	1.44	1.52
1	F	27	ALA	CA-C	-6.91	1.44	1.52
1	P	27	ALA	CA-C	-6.91	1.44	1.52
2	2	65	LEU	CA-C	-6.91	1.44	1.52
1	O	27	ALA	CA-C	-6.91	1.44	1.52
2	K	65	LEU	CA-C	-6.91	1.44	1.52
1	U	110	GLU	CA-C	-6.91	1.43	1.52
1	D	110	GLU	CA-C	-6.91	1.43	1.52
1	S	27	ALA	CA-C	-6.90	1.44	1.52
1	T	110	GLU	CA-C	-6.90	1.43	1.52
1	B	27	ALA	CA-C	-6.90	1.44	1.52
1	C	110	GLU	CA-C	-6.90	1.43	1.52
1	Q	110	GLU	CA-C	-6.89	1.43	1.52
2	Z	65	LEU	CA-C	-6.89	1.44	1.52
2	I	65	LEU	CA-C	-6.89	1.44	1.52
1	U	27	ALA	CA-C	-6.89	1.44	1.52
1	D	27	ALA	CA-C	-6.89	1.44	1.52
1	R	27	ALA	CA-C	-6.89	1.44	1.52
2	V	65	LEU	CA-C	-6.88	1.44	1.52
2	L	65	LEU	CA-C	-6.88	1.44	1.52
1	T	27	ALA	CA-C	-6.88	1.44	1.52
1	G	27	ALA	CA-C	-6.88	1.44	1.52
1	C	27	ALA	CA-C	-6.88	1.44	1.52
1	Q	27	ALA	CA-C	-6.88	1.44	1.52
2	X	65	LEU	CA-C	-6.87	1.44	1.52
2	J	163	LYS	C-N	6.80	1.43	1.33
1	C	28	ARG	NE-CZ	6.79	1.40	1.33
2	H	163	LYS	C-N	6.78	1.43	1.33
2	V	163	LYS	C-N	6.78	1.43	1.33
2	L	163	LYS	C-N	6.78	1.43	1.33
2	K	163	LYS	C-N	6.77	1.43	1.33
2	Y	163	LYS	C-N	6.75	1.43	1.33
2	Z	163	LYS	C-N	6.75	1.43	1.33
1	O	28	ARG	NE-CZ	6.75	1.40	1.33
2	I	163	LYS	C-N	6.75	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	163	LYS	C-N	6.75	1.43	1.33
2	X	163	LYS	C-N	6.75	1.43	1.33
1	E	28	ARG	NE-CZ	6.75	1.40	1.33
2	1	163	LYS	C-N	6.74	1.43	1.33
1	U	28	ARG	NE-CZ	6.74	1.40	1.33
2	M	163	LYS	C-N	6.74	1.43	1.33
2	W	163	LYS	C-N	6.74	1.43	1.33
1	O	144	ILE	CA-CB	-6.73	1.45	1.54
1	P	144	ILE	CA-CB	-6.72	1.45	1.54
1	U	144	ILE	CA-CB	-6.72	1.45	1.54
2	2	163	LYS	C-N	6.72	1.43	1.33
1	G	28	ARG	NE-CZ	6.72	1.40	1.33
1	Q	28	ARG	NE-CZ	6.72	1.40	1.33
1	F	93	ARG	CA-C	-6.71	1.44	1.52
1	S	144	ILE	CA-CB	-6.71	1.45	1.54
1	B	144	ILE	CA-CB	-6.71	1.45	1.54
1	S	28	ARG	NE-CZ	6.71	1.40	1.33
1	T	144	ILE	CA-CB	-6.71	1.45	1.54
1	B	28	ARG	NE-CZ	6.71	1.40	1.33
1	C	144	ILE	CA-CB	-6.71	1.45	1.54
1	G	144	ILE	CA-CB	-6.71	1.45	1.54
1	Q	144	ILE	CA-CB	-6.71	1.45	1.54
1	T	28	ARG	NE-CZ	6.70	1.40	1.33
1	E	144	ILE	CA-CB	-6.70	1.45	1.54
1	D	144	ILE	CA-CB	-6.70	1.45	1.54
1	S	93	ARG	CA-C	-6.69	1.44	1.52
1	B	93	ARG	CA-C	-6.69	1.44	1.52
1	F	28	ARG	NE-CZ	6.68	1.40	1.33
1	G	93	ARG	CA-C	-6.68	1.44	1.52
1	P	28	ARG	NE-CZ	6.68	1.40	1.33
1	Q	93	ARG	CA-C	-6.68	1.44	1.52
1	T	93	ARG	CA-C	-6.68	1.44	1.52
1	C	93	ARG	CA-C	-6.68	1.44	1.52
1	O	93	ARG	CA-C	-6.68	1.44	1.52
1	E	93	ARG	CA-C	-6.68	1.44	1.52
1	D	28	ARG	NE-CZ	6.67	1.40	1.33
1	U	93	ARG	CA-C	-6.67	1.44	1.52
1	D	93	ARG	CA-C	-6.67	1.44	1.52
1	R	28	ARG	NE-CZ	6.67	1.40	1.33
1	A	93	ARG	CA-C	-6.67	1.44	1.52
1	F	144	ILE	CA-CB	-6.67	1.45	1.54
1	A	144	ILE	CA-CB	-6.67	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	144	ILE	CA-CB	-6.67	1.45	1.54
1	P	93	ARG	CA-C	-6.66	1.44	1.52
1	R	93	ARG	CA-C	-6.66	1.44	1.52
1	A	28	ARG	NE-CZ	6.63	1.40	1.33
2	Y	149	ASP	CA-C	-6.63	1.44	1.52
2	V	42	GLY	N-CA	6.63	1.51	1.44
2	V	149	ASP	CA-C	-6.62	1.44	1.52
2	L	149	ASP	CA-C	-6.62	1.44	1.52
2	N	149	ASP	CA-C	-6.62	1.44	1.52
2	H	149	ASP	CA-C	-6.62	1.44	1.52
2	Z	149	ASP	CA-C	-6.61	1.44	1.52
2	I	149	ASP	CA-C	-6.61	1.44	1.52
2	K	149	ASP	CA-C	-6.61	1.44	1.52
2	1	149	ASP	CA-C	-6.61	1.44	1.52
2	2	149	ASP	CA-C	-6.61	1.44	1.52
2	J	149	ASP	CA-C	-6.61	1.44	1.52
2	X	149	ASP	CA-C	-6.61	1.44	1.52
2	M	149	ASP	CA-C	-6.60	1.44	1.52
2	W	149	ASP	CA-C	-6.60	1.44	1.52
2	M	42	GLY	N-CA	6.58	1.51	1.44
2	W	42	GLY	N-CA	6.58	1.51	1.44
2	2	42	GLY	N-CA	6.58	1.51	1.44
2	L	42	GLY	N-CA	6.58	1.51	1.44
2	H	42	GLY	N-CA	6.56	1.51	1.44
2	Z	42	GLY	N-CA	6.54	1.51	1.44
2	I	42	GLY	N-CA	6.54	1.51	1.44
2	J	42	GLY	N-CA	6.54	1.51	1.44
1	R	141	ILE	CA-C	-6.53	1.44	1.52
1	A	141	ILE	CA-C	-6.53	1.44	1.52
1	P	141	ILE	CA-C	-6.53	1.44	1.52
1	T	141	ILE	CA-C	-6.53	1.44	1.52
1	U	141	ILE	CA-C	-6.50	1.44	1.52
1	D	141	ILE	CA-C	-6.50	1.44	1.52
1	S	141	ILE	CA-C	-6.50	1.44	1.52
2	N	42	GLY	N-CA	6.50	1.51	1.44
1	B	141	ILE	CA-C	-6.50	1.44	1.52
2	X	42	GLY	N-CA	6.50	1.51	1.44
2	K	42	GLY	N-CA	6.50	1.51	1.44
1	G	222	ARG	CA-C	6.49	1.60	1.52
1	Q	222	ARG	CA-C	6.49	1.60	1.52
1	D	222	ARG	CA-C	6.49	1.60	1.52
2	Y	42	GLY	N-CA	6.49	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	141	ILE	CA-C	-6.48	1.44	1.52
1	O	222	ARG	CA-C	6.48	1.60	1.52
1	E	141	ILE	CA-C	-6.48	1.44	1.52
1	E	222	ARG	CA-C	6.48	1.60	1.52
1	F	141	ILE	CA-C	-6.48	1.44	1.52
2	1	42	GLY	N-CA	6.48	1.51	1.44
1	F	222	ARG	CA-C	6.48	1.60	1.52
1	P	222	ARG	CA-C	6.48	1.60	1.52
1	C	141	ILE	CA-C	-6.48	1.44	1.52
1	S	222	ARG	CA-C	6.48	1.60	1.52
1	A	222	ARG	CA-C	6.48	1.60	1.52
1	B	222	ARG	CA-C	6.48	1.60	1.52
1	R	222	ARG	CA-C	6.48	1.60	1.52
1	G	141	ILE	CA-C	-6.47	1.44	1.52
1	C	222	ARG	CA-C	6.47	1.60	1.52
1	Q	141	ILE	CA-C	-6.47	1.44	1.52
1	U	222	ARG	CA-C	6.46	1.60	1.52
1	T	222	ARG	CA-C	6.46	1.60	1.52
2	M	13	ILE	CA-C	-6.46	1.45	1.52
2	1	13	ILE	CA-C	-6.45	1.45	1.52
2	J	13	ILE	CA-C	-6.45	1.45	1.52
2	Z	13	ILE	CA-C	-6.43	1.45	1.52
2	I	13	ILE	CA-C	-6.43	1.45	1.52
2	H	13	ILE	CA-C	-6.43	1.45	1.52
2	Y	13	ILE	CA-C	-6.43	1.45	1.52
2	2	13	ILE	CA-C	-6.42	1.45	1.52
2	K	13	ILE	CA-C	-6.42	1.45	1.52
2	N	13	ILE	CA-C	-6.41	1.45	1.52
2	X	13	ILE	CA-C	-6.41	1.45	1.52
1	C	127	GLY	CA-C	-6.41	1.42	1.52
1	A	151	CYS	C-N	6.41	1.40	1.32
1	R	151	CYS	C-N	6.41	1.40	1.32
1	T	127	GLY	CA-C	-6.40	1.42	1.52
1	D	127	GLY	CA-C	-6.40	1.42	1.52
1	A	127	GLY	CA-C	-6.39	1.42	1.52
1	O	127	GLY	CA-C	-6.39	1.42	1.52
1	R	127	GLY	CA-C	-6.39	1.42	1.52
1	E	127	GLY	CA-C	-6.39	1.42	1.52
2	V	13	ILE	CA-C	-6.38	1.45	1.52
2	L	13	ILE	CA-C	-6.38	1.45	1.52
2	W	13	ILE	CA-C	-6.38	1.45	1.52
1	S	127	GLY	CA-C	-6.38	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	127	GLY	CA-C	-6.38	1.42	1.52
1	B	127	GLY	CA-C	-6.38	1.42	1.52
1	P	127	GLY	CA-C	-6.38	1.42	1.52
1	T	20	ARG	CA-C	-6.38	1.44	1.52
1	C	20	ARG	CA-C	-6.38	1.44	1.52
1	G	127	GLY	CA-C	-6.37	1.42	1.52
1	Q	127	GLY	CA-C	-6.37	1.42	1.52
1	P	151	CYS	C-N	6.37	1.40	1.32
1	G	151	CYS	C-N	6.36	1.40	1.32
1	T	151	CYS	C-N	6.35	1.40	1.32
1	C	151	CYS	C-N	6.35	1.40	1.32
1	U	127	GLY	CA-C	-6.35	1.42	1.52
1	Q	92	ALA	CA-C	-6.35	1.44	1.52
1	S	151	CYS	C-N	6.35	1.40	1.32
1	B	151	CYS	C-N	6.35	1.40	1.32
1	T	92	ALA	CA-C	-6.34	1.44	1.52
1	P	92	ALA	CA-C	-6.34	1.44	1.52
1	U	92	ALA	CA-C	-6.34	1.44	1.52
1	U	151	CYS	C-N	6.34	1.40	1.32
1	D	151	CYS	C-N	6.34	1.40	1.32
1	A	20	ARG	CA-C	-6.33	1.45	1.52
1	R	20	ARG	CA-C	-6.33	1.45	1.52
1	U	20	ARG	CA-C	-6.33	1.45	1.52
1	D	20	ARG	CA-C	-6.33	1.45	1.52
2	L	67	ARG	NE-CZ	6.32	1.40	1.33
1	G	20	ARG	CA-C	-6.32	1.45	1.52
1	O	151	CYS	C-N	6.31	1.40	1.32
1	E	151	CYS	C-N	6.31	1.40	1.32
1	F	20	ARG	CA-C	-6.31	1.45	1.52
1	A	64	ILE	CA-C	-6.31	1.45	1.52
1	O	20	ARG	CA-C	-6.31	1.45	1.52
1	P	20	ARG	CA-C	-6.31	1.45	1.52
1	E	20	ARG	CA-C	-6.31	1.45	1.52
1	G	92	ALA	CA-C	-6.31	1.44	1.52
1	D	92	ALA	CA-C	-6.31	1.44	1.52
1	S	92	ALA	CA-C	-6.31	1.44	1.52
1	B	92	ALA	CA-C	-6.31	1.44	1.52
1	S	20	ARG	CA-C	-6.31	1.45	1.52
1	A	92	ALA	CA-C	-6.31	1.44	1.52
1	B	20	ARG	CA-C	-6.31	1.45	1.52
1	R	92	ALA	CA-C	-6.31	1.44	1.52
1	C	92	ALA	CA-C	-6.30	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	92	ALA	CA-C	-6.30	1.44	1.52
1	O	92	ALA	CA-C	-6.30	1.44	1.52
1	Q	151	CYS	C-N	6.30	1.40	1.32
1	F	151	CYS	C-N	6.30	1.40	1.32
2	M	67	ARG	NE-CZ	6.30	1.40	1.33
1	E	92	ALA	CA-C	-6.29	1.44	1.52
1	F	64	ILE	CA-C	-6.29	1.45	1.52
1	P	64	ILE	CA-C	-6.29	1.45	1.52
1	Q	20	ARG	CA-C	-6.29	1.45	1.52
1	U	64	ILE	CA-C	-6.28	1.45	1.52
2	W	67	ARG	NE-CZ	6.27	1.40	1.33
2	1	67	ARG	NE-CZ	6.27	1.40	1.33
2	V	67	ARG	NE-CZ	6.27	1.40	1.33
2	2	67	ARG	NE-CZ	6.26	1.40	1.33
2	K	67	ARG	NE-CZ	6.26	1.40	1.33
1	O	64	ILE	CA-C	-6.25	1.45	1.52
1	E	64	ILE	CA-C	-6.25	1.45	1.52
1	S	64	ILE	CA-C	-6.24	1.45	1.52
1	B	64	ILE	CA-C	-6.24	1.45	1.52
2	Z	67	ARG	NE-CZ	6.24	1.40	1.33
2	I	67	ARG	NE-CZ	6.24	1.40	1.33
2	H	67	ARG	NE-CZ	6.23	1.40	1.33
1	R	64	ILE	CA-C	-6.23	1.45	1.52
2	Y	67	ARG	NE-CZ	6.23	1.40	1.33
1	D	64	ILE	CA-C	-6.22	1.45	1.52
2	K	189	THR	C-N	6.22	1.42	1.33
2	J	67	ARG	NE-CZ	6.21	1.39	1.33
2	N	67	ARG	NE-CZ	6.21	1.39	1.33
2	X	67	ARG	NE-CZ	6.21	1.39	1.33
2	2	189	THR	C-N	6.20	1.42	1.33
2	1	189	THR	C-N	6.20	1.42	1.33
1	G	64	ILE	CA-C	-6.20	1.45	1.52
2	V	189	THR	C-N	6.19	1.42	1.33
2	L	189	THR	C-N	6.19	1.42	1.33
2	N	189	THR	C-N	6.19	1.42	1.33
2	H	189	THR	C-N	6.19	1.42	1.33
2	Y	189	THR	C-N	6.19	1.42	1.33
2	Z	189	THR	C-N	6.17	1.42	1.33
2	I	189	THR	C-N	6.17	1.42	1.33
2	X	189	THR	C-N	6.17	1.42	1.33
1	T	64	ILE	CA-C	-6.17	1.45	1.52
1	C	64	ILE	CA-C	-6.17	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	189	THR	C-N	6.16	1.42	1.33
2	W	189	THR	C-N	6.16	1.42	1.33
1	Q	64	ILE	CA-C	-6.16	1.45	1.52
2	J	189	THR	C-N	6.16	1.42	1.33
1	T	88	LEU	C-N	6.13	1.41	1.33
2	N	24	ASN	CA-C	-6.13	1.45	1.52
1	C	88	LEU	C-N	6.13	1.41	1.33
2	X	24	ASN	CA-C	-6.13	1.45	1.52
2	W	24	ASN	CA-C	-6.12	1.45	1.52
1	Q	88	LEU	C-N	6.12	1.41	1.33
1	F	88	LEU	C-N	6.12	1.41	1.33
1	U	88	LEU	C-N	6.10	1.41	1.33
1	O	88	LEU	C-N	6.10	1.41	1.33
1	D	88	LEU	C-N	6.10	1.41	1.33
1	S	88	LEU	C-N	6.10	1.41	1.33
1	B	88	LEU	C-N	6.10	1.41	1.33
1	E	88	LEU	C-N	6.10	1.41	1.33
2	K	24	ASN	CA-C	-6.10	1.45	1.52
2	V	24	ASN	CA-C	-6.09	1.45	1.52
2	L	24	ASN	CA-C	-6.09	1.45	1.52
2	Z	24	ASN	CA-C	-6.09	1.45	1.52
2	H	24	ASN	CA-C	-6.09	1.45	1.52
2	I	24	ASN	CA-C	-6.09	1.45	1.52
2	Y	24	ASN	CA-C	-6.09	1.45	1.52
1	A	83	ALA	N-CA	-6.08	1.39	1.46
1	C	109	ILE	C-N	6.08	1.42	1.33
1	R	83	ALA	N-CA	-6.08	1.39	1.46
2	1	24	ASN	CA-C	-6.08	1.45	1.52
1	G	109	ILE	C-N	6.08	1.42	1.33
2	J	24	ASN	CA-C	-6.08	1.45	1.52
1	U	83	ALA	N-CA	-6.07	1.39	1.46
2	2	24	ASN	CA-C	-6.07	1.45	1.52
1	D	83	ALA	N-CA	-6.07	1.39	1.46
2	M	24	ASN	CA-C	-6.07	1.45	1.52
1	F	109	ILE	C-N	6.06	1.41	1.33
1	A	88	LEU	C-N	6.06	1.41	1.33
1	P	109	ILE	C-N	6.06	1.41	1.33
1	R	88	LEU	C-N	6.06	1.41	1.33
1	P	88	LEU	C-N	6.06	1.41	1.33
1	U	109	ILE	C-N	6.05	1.41	1.33
1	D	109	ILE	C-N	6.05	1.41	1.33
1	G	83	ALA	N-CA	-6.05	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	83	ALA	N-CA	-6.05	1.39	1.46
1	S	83	ALA	N-CA	-6.04	1.39	1.46
1	O	83	ALA	N-CA	-6.04	1.39	1.46
1	B	83	ALA	N-CA	-6.04	1.39	1.46
1	E	83	ALA	N-CA	-6.04	1.39	1.46
2	L	33	LYS	N-CA	-6.04	1.38	1.46
1	T	109	ILE	C-N	6.04	1.41	1.33
1	G	88	LEU	C-N	6.04	1.41	1.33
1	A	41	LYS	CA-C	-6.04	1.45	1.52
1	R	41	LYS	CA-C	-6.04	1.45	1.52
2	K	109	HIS	CB-CG	6.04	1.58	1.50
2	X	109	HIS	CB-CG	6.04	1.58	1.50
1	S	109	ILE	C-N	6.04	1.41	1.33
1	F	83	ALA	N-CA	-6.04	1.39	1.46
2	V	109	HIS	CB-CG	6.04	1.58	1.50
1	B	109	ILE	C-N	6.04	1.41	1.33
1	P	83	ALA	N-CA	-6.04	1.39	1.46
2	L	109	HIS	CB-CG	6.04	1.58	1.50
1	A	109	ILE	C-N	6.03	1.41	1.33
1	R	109	ILE	C-N	6.03	1.41	1.33
2	M	33	LYS	N-CA	-6.03	1.38	1.46
2	W	33	LYS	N-CA	-6.03	1.38	1.46
1	E	109	ILE	C-N	6.03	1.41	1.33
2	J	33	LYS	N-CA	-6.02	1.38	1.46
1	U	41	LYS	CA-C	-6.02	1.45	1.52
2	I	109	HIS	CB-CG	6.02	1.58	1.50
1	O	41	LYS	CA-C	-6.02	1.45	1.52
1	E	41	LYS	CA-C	-6.02	1.45	1.52
2	Z	109	HIS	CB-CG	6.02	1.58	1.50
2	I	109	HIS	CB-CG	6.02	1.58	1.50
1	F	41	LYS	CA-C	-6.01	1.45	1.52
2	I	178	ILE	C-N	6.01	1.41	1.33
1	G	41	LYS	CA-C	-6.01	1.45	1.52
1	P	41	LYS	CA-C	-6.01	1.45	1.52
2	W	109	HIS	CB-CG	6.01	1.58	1.50
1	Q	41	LYS	CA-C	-6.01	1.45	1.52
1	Q	109	ILE	C-N	6.01	1.41	1.33
1	D	41	LYS	CA-C	-6.01	1.45	1.52
2	I	33	LYS	N-CA	-6.01	1.38	1.46
2	H	109	HIS	CB-CG	6.01	1.58	1.50
2	Y	109	HIS	CB-CG	6.01	1.58	1.50
2	M	109	HIS	CB-CG	6.00	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	41	LYS	CA-C	-6.00	1.45	1.52
1	C	41	LYS	CA-C	-6.00	1.45	1.52
1	S	41	LYS	CA-C	-6.00	1.45	1.52
1	G	135	SER	CA-C	-6.00	1.45	1.52
1	B	41	LYS	CA-C	-6.00	1.45	1.52
1	Q	135	SER	CA-C	-6.00	1.45	1.52
1	U	135	SER	CA-C	-6.00	1.45	1.52
2	H	33	LYS	N-CA	-6.00	1.38	1.46
2	H	178	ILE	C-N	6.00	1.41	1.33
2	V	178	ILE	C-N	6.00	1.41	1.33
2	Y	33	LYS	N-CA	-6.00	1.38	1.46
2	Y	178	ILE	C-N	6.00	1.41	1.33
2	L	178	ILE	C-N	6.00	1.41	1.33
1	T	83	ALA	N-CA	-6.00	1.39	1.46
1	C	83	ALA	N-CA	-6.00	1.39	1.46
1	F	135	SER	CA-C	-6.00	1.45	1.52
1	P	135	SER	CA-C	-6.00	1.45	1.52
2	N	109	HIS	CB-CG	5.99	1.58	1.50
2	Z	33	LYS	N-CA	-5.99	1.38	1.46
2	M	178	ILE	C-N	5.99	1.41	1.33
2	2	109	HIS	CB-CG	5.99	1.58	1.50
2	I	33	LYS	N-CA	-5.99	1.38	1.46
2	W	178	ILE	C-N	5.99	1.41	1.33
2	2	33	LYS	N-CA	-5.99	1.38	1.46
2	J	109	HIS	CB-CG	5.99	1.58	1.50
2	K	33	LYS	N-CA	-5.99	1.38	1.46
2	N	178	ILE	C-N	5.98	1.41	1.33
2	X	178	ILE	C-N	5.98	1.41	1.33
1	E	57	ARG	NE-CZ	5.98	1.39	1.33
2	Z	178	ILE	C-N	5.98	1.41	1.33
2	I	178	ILE	C-N	5.98	1.41	1.33
1	D	57	ARG	NE-CZ	5.98	1.39	1.33
1	O	135	SER	CA-C	-5.98	1.45	1.52
1	E	135	SER	CA-C	-5.98	1.45	1.52
1	S	135	SER	CA-C	-5.98	1.45	1.52
1	B	135	SER	CA-C	-5.98	1.45	1.52
1	A	135	SER	CA-C	-5.97	1.45	1.52
1	R	135	SER	CA-C	-5.97	1.45	1.52
1	O	109	ILE	C-N	5.97	1.41	1.33
2	J	178	ILE	C-N	5.97	1.41	1.33
2	V	33	LYS	N-CA	-5.97	1.38	1.46
2	K	178	ILE	C-N	5.97	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	163	LYS	CA-C	-5.96	1.45	1.52
1	D	135	SER	CA-C	-5.96	1.45	1.52
2	M	163	LYS	CA-C	-5.96	1.45	1.52
1	T	57	ARG	NE-CZ	5.96	1.39	1.33
1	T	135	SER	CA-C	-5.96	1.45	1.52
1	C	57	ARG	NE-CZ	5.96	1.39	1.33
1	C	135	SER	CA-C	-5.96	1.45	1.52
2	H	163	LYS	CA-C	-5.96	1.45	1.52
2	Y	163	LYS	CA-C	-5.96	1.45	1.52
2	N	163	LYS	CA-C	-5.96	1.45	1.52
2	2	163	LYS	CA-C	-5.96	1.45	1.52
2	X	163	LYS	CA-C	-5.96	1.45	1.52
2	K	163	LYS	CA-C	-5.96	1.45	1.52
2	Z	163	LYS	CA-C	-5.96	1.45	1.52
2	I	163	LYS	CA-C	-5.96	1.45	1.52
2	1	163	LYS	CA-C	-5.95	1.45	1.52
2	2	178	ILE	C-N	5.95	1.41	1.33
2	V	163	LYS	CA-C	-5.95	1.45	1.52
2	J	163	LYS	CA-C	-5.94	1.45	1.52
1	Q	226	GLN	C-N	5.94	1.42	1.33
2	L	163	LYS	CA-C	-5.94	1.45	1.52
1	S	57	ARG	NE-CZ	5.93	1.39	1.33
1	B	57	ARG	NE-CZ	5.93	1.39	1.33
2	N	33	LYS	N-CA	-5.93	1.39	1.46
2	X	33	LYS	N-CA	-5.93	1.39	1.46
1	A	57	ARG	NE-CZ	5.93	1.39	1.33
1	R	57	ARG	NE-CZ	5.93	1.39	1.33
1	S	226	GLN	C-N	5.92	1.42	1.33
1	B	226	GLN	C-N	5.92	1.42	1.33
1	F	226	GLN	C-N	5.92	1.42	1.33
1	P	226	GLN	C-N	5.92	1.42	1.33
2	W	45	ILE	CA-CB	-5.92	1.47	1.54
1	T	226	GLN	C-N	5.92	1.42	1.33
1	C	226	GLN	C-N	5.92	1.42	1.33
1	F	57	ARG	NE-CZ	5.92	1.39	1.33
1	P	57	ARG	NE-CZ	5.92	1.39	1.33
1	U	226	GLN	C-N	5.92	1.42	1.33
1	D	226	GLN	C-N	5.92	1.42	1.33
1	G	57	ARG	NE-CZ	5.91	1.39	1.33
1	O	226	GLN	C-N	5.91	1.42	1.33
1	Q	57	ARG	NE-CZ	5.91	1.39	1.33
2	K	45	ILE	CA-CB	-5.91	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	45	ILE	CA-CB	-5.91	1.47	1.54
2	M	45	ILE	CA-CB	-5.91	1.47	1.54
1	U	57	ARG	NE-CZ	5.91	1.39	1.33
2	2	60	LYS	C-N	5.91	1.41	1.33
1	O	57	ARG	NE-CZ	5.91	1.39	1.33
1	A	226	GLN	C-N	5.90	1.42	1.33
1	G	226	GLN	C-N	5.89	1.42	1.33
1	R	226	GLN	C-N	5.89	1.42	1.33
1	E	226	GLN	C-N	5.89	1.42	1.33
2	H	45	ILE	CA-CB	-5.89	1.47	1.54
2	Y	45	ILE	CA-CB	-5.89	1.47	1.54
2	Z	45	ILE	CA-CB	-5.88	1.47	1.54
2	I	45	ILE	CA-CB	-5.88	1.47	1.54
2	V	45	ILE	CA-CB	-5.88	1.47	1.54
2	L	45	ILE	CA-CB	-5.88	1.47	1.54
2	1	45	ILE	CA-CB	-5.88	1.47	1.54
2	2	185	VAL	CA-C	-5.88	1.45	1.52
2	J	45	ILE	CA-CB	-5.88	1.47	1.54
2	M	175	VAL	N-CA	-5.88	1.39	1.46
2	W	175	VAL	N-CA	-5.87	1.39	1.46
2	1	60	LYS	C-N	5.87	1.41	1.33
2	1	185	VAL	CA-C	-5.87	1.45	1.52
2	J	185	VAL	CA-C	-5.87	1.45	1.52
2	2	175	VAL	N-CA	-5.86	1.39	1.46
2	K	175	VAL	N-CA	-5.86	1.39	1.46
2	M	185	VAL	CA-C	-5.86	1.45	1.52
2	N	185	VAL	CA-C	-5.86	1.45	1.52
2	W	185	VAL	CA-C	-5.86	1.45	1.52
2	X	185	VAL	CA-C	-5.86	1.45	1.52
2	Z	185	VAL	CA-C	-5.86	1.45	1.52
2	I	185	VAL	CA-C	-5.86	1.45	1.52
2	K	185	VAL	CA-C	-5.86	1.45	1.52
2	K	60	LYS	C-N	5.86	1.41	1.33
1	F	113	VAL	N-CA	-5.86	1.39	1.46
2	H	175	VAL	N-CA	-5.86	1.39	1.46
1	O	113	VAL	N-CA	-5.86	1.39	1.46
1	P	113	VAL	N-CA	-5.86	1.39	1.46
2	Y	175	VAL	N-CA	-5.86	1.39	1.46
1	G	113	VAL	N-CA	-5.85	1.39	1.46
2	Y	185	VAL	CA-C	-5.85	1.45	1.52
1	S	113	VAL	N-CA	-5.85	1.39	1.46
2	Z	175	VAL	N-CA	-5.85	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	113	VAL	N-CA	-5.85	1.39	1.46
1	B	113	VAL	N-CA	-5.85	1.39	1.46
2	I	175	VAL	N-CA	-5.85	1.39	1.46
1	R	113	VAL	N-CA	-5.85	1.39	1.46
1	U	113	VAL	N-CA	-5.85	1.39	1.46
1	D	113	VAL	N-CA	-5.85	1.39	1.46
2	N	45	ILE	CA-CB	-5.85	1.47	1.54
1	Q	113	VAL	N-CA	-5.85	1.39	1.46
2	N	175	VAL	N-CA	-5.85	1.39	1.46
2	V	185	VAL	CA-C	-5.85	1.45	1.52
2	X	175	VAL	N-CA	-5.85	1.39	1.46
2	L	185	VAL	CA-C	-5.85	1.45	1.52
2	2	45	ILE	CA-CB	-5.84	1.47	1.54
1	A	113	VAL	N-CA	-5.84	1.39	1.46
1	C	113	VAL	N-CA	-5.84	1.39	1.46
1	E	113	VAL	N-CA	-5.84	1.39	1.46
2	H	185	VAL	CA-C	-5.84	1.45	1.52
2	Y	157	ARG	NE-CZ	5.84	1.39	1.33
2	M	60	LYS	C-N	5.84	1.41	1.33
2	W	60	LYS	C-N	5.84	1.41	1.33
2	L	157	ARG	NE-CZ	5.84	1.39	1.33
2	V	175	VAL	N-CA	-5.83	1.39	1.46
2	L	175	VAL	N-CA	-5.83	1.39	1.46
2	Z	60	LYS	C-N	5.83	1.41	1.33
2	1	175	VAL	N-CA	-5.83	1.39	1.46
2	I	60	LYS	C-N	5.83	1.41	1.33
2	J	175	VAL	N-CA	-5.83	1.39	1.46
2	H	104	ILE	CA-C	-5.83	1.45	1.52
2	V	104	ILE	CA-C	-5.82	1.45	1.52
2	Z	104	ILE	CA-C	-5.82	1.45	1.52
2	1	157	ARG	NE-CZ	5.82	1.39	1.33
2	I	104	ILE	CA-C	-5.82	1.45	1.52
2	M	104	ILE	CA-C	-5.82	1.45	1.52
2	2	104	ILE	CA-C	-5.82	1.45	1.52
2	W	104	ILE	CA-C	-5.82	1.45	1.52
2	K	104	ILE	CA-C	-5.82	1.45	1.52
2	Y	104	ILE	CA-C	-5.82	1.45	1.52
2	N	104	ILE	CA-C	-5.81	1.45	1.52
2	X	104	ILE	CA-C	-5.81	1.45	1.52
2	Z	157	ARG	NE-CZ	5.81	1.39	1.33
2	1	104	ILE	CA-C	-5.81	1.45	1.52
2	I	157	ARG	NE-CZ	5.81	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	104	ILE	CA-C	-5.81	1.45	1.52
2	L	104	ILE	CA-C	-5.81	1.45	1.52
2	H	157	ARG	NE-CZ	5.81	1.39	1.33
2	Y	60	LYS	C-N	5.80	1.41	1.33
2	M	157	ARG	NE-CZ	5.80	1.39	1.33
2	W	157	ARG	NE-CZ	5.80	1.39	1.33
2	J	157	ARG	NE-CZ	5.80	1.39	1.33
2	N	157	ARG	NE-CZ	5.80	1.39	1.33
2	N	60	LYS	C-N	5.80	1.41	1.33
2	V	157	ARG	NE-CZ	5.80	1.39	1.33
2	X	60	LYS	C-N	5.80	1.41	1.33
2	X	157	ARG	NE-CZ	5.80	1.39	1.33
2	J	60	LYS	C-N	5.79	1.41	1.33
2	2	157	ARG	NE-CZ	5.79	1.39	1.33
2	V	60	LYS	C-N	5.79	1.41	1.33
2	K	157	ARG	NE-CZ	5.79	1.39	1.33
2	L	60	LYS	C-N	5.79	1.41	1.33
2	X	4	VAL	N-CA	-5.79	1.39	1.46
2	H	60	LYS	C-N	5.79	1.41	1.33
2	J	196	ILE	CA-C	-5.79	1.46	1.52
1	U	57	ARG	N-CA	-5.79	1.38	1.46
2	Y	164	GLN	N-CA	-5.78	1.39	1.46
2	L	164	GLN	N-CA	-5.78	1.39	1.46
2	J	164	GLN	N-CA	-5.78	1.39	1.46
2	1	164	GLN	N-CA	-5.78	1.39	1.46
2	X	164	GLN	N-CA	-5.77	1.39	1.46
2	M	196	ILE	CA-C	-5.77	1.46	1.52
1	G	57	ARG	N-CA	-5.77	1.38	1.46
2	N	196	ILE	CA-C	-5.77	1.46	1.52
2	W	196	ILE	CA-C	-5.77	1.46	1.52
2	Z	164	GLN	N-CA	-5.77	1.39	1.46
2	H	164	GLN	N-CA	-5.77	1.39	1.46
2	I	164	GLN	N-CA	-5.77	1.39	1.46
2	N	164	GLN	N-CA	-5.77	1.39	1.46
2	V	164	GLN	N-CA	-5.77	1.39	1.46
2	W	4	VAL	N-CA	-5.77	1.39	1.46
2	M	164	GLN	N-CA	-5.76	1.39	1.46
2	W	164	GLN	N-CA	-5.76	1.39	1.46
2	2	164	GLN	N-CA	-5.76	1.39	1.46
2	K	164	GLN	N-CA	-5.76	1.39	1.46
1	F	179	GLU	C-N	5.76	1.41	1.33
1	D	57	ARG	N-CA	-5.76	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	196	ILE	CA-C	-5.75	1.46	1.52
2	2	4	VAL	N-CA	-5.75	1.39	1.46
2	I	196	ILE	CA-C	-5.75	1.46	1.52
2	2	196	ILE	CA-C	-5.75	1.46	1.52
2	K	196	ILE	CA-C	-5.75	1.46	1.52
1	F	57	ARG	N-CA	-5.75	1.38	1.46
1	P	57	ARG	N-CA	-5.75	1.38	1.46
2	X	196	ILE	CA-C	-5.75	1.46	1.52
2	V	196	ILE	CA-C	-5.74	1.46	1.52
2	L	196	ILE	CA-C	-5.74	1.46	1.52
2	1	196	ILE	CA-C	-5.74	1.46	1.52
2	H	196	ILE	CA-C	-5.74	1.46	1.52
2	Y	196	ILE	CA-C	-5.74	1.46	1.52
1	S	57	ARG	N-CA	-5.74	1.38	1.46
1	A	57	ARG	N-CA	-5.74	1.38	1.46
1	B	57	ARG	N-CA	-5.74	1.38	1.46
1	R	57	ARG	N-CA	-5.74	1.38	1.46
2	M	4	VAL	N-CA	-5.74	1.39	1.46
2	1	4	VAL	N-CA	-5.73	1.39	1.46
2	J	4	VAL	N-CA	-5.73	1.39	1.46
2	2	19	ARG	N-CA	-5.73	1.38	1.46
2	K	19	ARG	N-CA	-5.73	1.38	1.46
1	T	57	ARG	N-CA	-5.73	1.38	1.46
1	C	57	ARG	N-CA	-5.73	1.38	1.46
1	G	179	GLU	C-N	5.73	1.41	1.33
1	Q	57	ARG	N-CA	-5.73	1.38	1.46
2	Z	4	VAL	N-CA	-5.73	1.39	1.46
2	I	4	VAL	N-CA	-5.73	1.39	1.46
1	R	179	GLU	C-N	5.72	1.41	1.33
1	U	179	GLU	C-N	5.72	1.41	1.33
2	H	4	VAL	N-CA	-5.72	1.39	1.46
2	Y	4	VAL	N-CA	-5.72	1.39	1.46
1	E	57	ARG	N-CA	-5.71	1.38	1.46
2	N	4	VAL	N-CA	-5.71	1.39	1.46
1	A	179	GLU	C-N	5.71	1.41	1.33
2	V	8	LEU	N-CA	-5.71	1.39	1.46
2	L	8	LEU	N-CA	-5.71	1.39	1.46
2	L	19	ARG	N-CA	-5.71	1.38	1.46
2	V	19	ARG	N-CA	-5.71	1.38	1.46
2	V	4	VAL	N-CA	-5.70	1.39	1.46
1	P	179	GLU	C-N	5.70	1.41	1.33
2	L	4	VAL	N-CA	-5.70	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	8	LEU	N-CA	-5.70	1.39	1.46
1	S	179	GLU	C-N	5.70	1.41	1.33
1	O	57	ARG	N-CA	-5.70	1.38	1.46
1	B	179	GLU	C-N	5.70	1.41	1.33
2	Z	19	ARG	N-CA	-5.69	1.38	1.46
2	N	19	ARG	N-CA	-5.69	1.38	1.46
2	I	19	ARG	N-CA	-5.69	1.38	1.46
2	X	19	ARG	N-CA	-5.69	1.38	1.46
1	O	179	GLU	C-N	5.69	1.41	1.33
1	E	179	GLU	C-N	5.69	1.41	1.33
1	T	179	GLU	C-N	5.69	1.41	1.33
1	C	179	GLU	C-N	5.69	1.41	1.33
2	H	19	ARG	N-CA	-5.68	1.38	1.46
2	Y	19	ARG	N-CA	-5.68	1.38	1.46
2	1	19	ARG	N-CA	-5.68	1.38	1.46
2	J	19	ARG	N-CA	-5.68	1.38	1.46
1	D	179	GLU	C-N	5.68	1.41	1.33
1	Q	179	GLU	C-N	5.67	1.41	1.33
2	K	4	VAL	N-CA	-5.67	1.39	1.46
2	M	19	ARG	N-CA	-5.67	1.38	1.46
2	W	19	ARG	N-CA	-5.67	1.38	1.46
2	Z	8	LEU	N-CA	-5.66	1.39	1.46
2	I	8	LEU	N-CA	-5.66	1.39	1.46
2	Y	103	GLY	CA-C	-5.66	1.44	1.51
1	E	188	GLU	C-O	-5.66	1.17	1.24
2	2	103	GLY	CA-C	-5.65	1.44	1.51
1	S	188	GLU	C-O	-5.65	1.17	1.24
1	G	188	GLU	C-O	-5.65	1.17	1.24
1	B	188	GLU	C-O	-5.65	1.17	1.24
1	Q	188	GLU	C-O	-5.65	1.17	1.24
1	T	188	GLU	C-O	-5.65	1.17	1.24
2	2	8	LEU	N-CA	-5.65	1.39	1.46
2	2	57	ARG	CA-C	-5.65	1.45	1.52
1	C	188	GLU	C-O	-5.65	1.17	1.24
2	K	8	LEU	N-CA	-5.65	1.39	1.46
2	1	8	LEU	N-CA	-5.65	1.39	1.46
1	A	188	GLU	C-O	-5.65	1.17	1.24
1	P	188	GLU	C-O	-5.65	1.17	1.24
2	J	8	LEU	N-CA	-5.65	1.39	1.46
1	R	188	GLU	C-O	-5.65	1.17	1.24
1	U	188	GLU	C-O	-5.64	1.17	1.24
1	D	188	GLU	C-O	-5.64	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	8	LEU	N-CA	-5.64	1.39	1.46
1	O	188	GLU	C-O	-5.64	1.17	1.24
2	1	153	ASP	N-CA	-5.64	1.39	1.46
2	J	153	ASP	N-CA	-5.64	1.39	1.46
1	F	188	GLU	C-O	-5.63	1.17	1.24
2	V	153	ASP	N-CA	-5.63	1.39	1.46
1	T	198	LYS	CA-C	-5.63	1.45	1.52
2	N	103	GLY	CA-C	-5.62	1.44	1.51
2	X	103	GLY	CA-C	-5.62	1.44	1.51
2	Z	153	ASP	N-CA	-5.62	1.39	1.46
2	N	8	LEU	N-CA	-5.62	1.39	1.46
2	I	153	ASP	N-CA	-5.62	1.39	1.46
2	Y	8	LEU	N-CA	-5.62	1.39	1.46
2	M	153	ASP	N-CA	-5.62	1.39	1.46
2	H	153	ASP	N-CA	-5.62	1.39	1.46
2	V	57	ARG	CA-C	-5.62	1.45	1.52
2	Y	153	ASP	N-CA	-5.62	1.39	1.46
2	M	103	GLY	CA-C	-5.62	1.44	1.51
2	W	103	GLY	CA-C	-5.62	1.44	1.51
2	K	153	ASP	N-CA	-5.62	1.39	1.46
1	A	198	LYS	CA-C	-5.61	1.45	1.52
2	L	153	ASP	N-CA	-5.61	1.39	1.46
2	N	57	ARG	CA-C	-5.61	1.45	1.52
2	X	57	ARG	CA-C	-5.61	1.45	1.52
1	S	198	LYS	CA-C	-5.61	1.45	1.52
2	N	153	ASP	N-CA	-5.61	1.39	1.46
1	B	198	LYS	CA-C	-5.61	1.45	1.52
2	X	153	ASP	N-CA	-5.61	1.39	1.46
2	Z	103	GLY	CA-C	-5.61	1.44	1.51
2	I	103	GLY	CA-C	-5.61	1.44	1.51
2	M	8	LEU	N-CA	-5.61	1.39	1.46
1	G	198	LYS	CA-C	-5.61	1.45	1.52
2	2	153	ASP	N-CA	-5.61	1.39	1.46
2	W	8	LEU	N-CA	-5.61	1.39	1.46
1	Q	198	LYS	CA-C	-5.61	1.45	1.52
1	F	198	LYS	CA-C	-5.60	1.45	1.52
1	O	198	LYS	CA-C	-5.60	1.45	1.52
1	P	198	LYS	CA-C	-5.60	1.45	1.52
2	W	153	ASP	N-CA	-5.60	1.39	1.46
2	K	57	ARG	CA-C	-5.60	1.45	1.52
1	U	198	LYS	CA-C	-5.60	1.45	1.52
1	D	198	LYS	CA-C	-5.60	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	103	GLY	CA-C	-5.60	1.44	1.51
2	J	103	GLY	CA-C	-5.60	1.44	1.51
1	E	198	LYS	CA-C	-5.60	1.45	1.52
2	H	103	GLY	CA-C	-5.60	1.44	1.51
1	C	198	LYS	CA-C	-5.60	1.45	1.52
1	P	11	ALA	CA-C	-5.60	1.45	1.52
1	R	198	LYS	CA-C	-5.60	1.45	1.52
1	C	11	ALA	CA-C	-5.59	1.45	1.52
1	A	11	ALA	CA-C	-5.59	1.45	1.52
1	R	11	ALA	CA-C	-5.59	1.45	1.52
1	G	11	ALA	CA-C	-5.59	1.45	1.52
2	W	57	ARG	CA-C	-5.59	1.45	1.52
1	O	11	ALA	CA-C	-5.59	1.45	1.52
1	E	11	ALA	CA-C	-5.59	1.45	1.52
1	S	11	ALA	CA-C	-5.59	1.45	1.52
2	Z	57	ARG	CA-C	-5.59	1.45	1.52
1	F	11	ALA	CA-C	-5.59	1.45	1.52
2	V	103	GLY	CA-C	-5.59	1.44	1.51
1	B	11	ALA	CA-C	-5.59	1.45	1.52
2	I	57	ARG	CA-C	-5.59	1.45	1.52
2	L	103	GLY	CA-C	-5.59	1.44	1.51
1	F	114	LYS	C-O	-5.58	1.17	1.24
1	P	114	LYS	C-O	-5.58	1.17	1.24
1	T	11	ALA	CA-C	-5.58	1.45	1.52
1	U	11	ALA	CA-C	-5.58	1.45	1.52
2	H	57	ARG	CA-C	-5.58	1.45	1.52
1	Q	11	ALA	CA-C	-5.58	1.45	1.52
1	D	11	ALA	CA-C	-5.58	1.45	1.52
2	Y	57	ARG	CA-C	-5.58	1.45	1.52
2	K	103	GLY	CA-C	-5.58	1.45	1.51
1	S	114	LYS	C-O	-5.57	1.17	1.24
2	M	172	MET	N-CA	5.57	1.53	1.46
1	T	114	LYS	C-O	-5.57	1.17	1.24
1	B	114	LYS	C-O	-5.57	1.17	1.24
2	W	172	MET	N-CA	5.57	1.53	1.46
1	C	114	LYS	C-O	-5.57	1.17	1.24
2	1	57	ARG	CA-C	-5.57	1.45	1.52
2	J	57	ARG	CA-C	-5.57	1.45	1.52
2	N	172	MET	N-CA	5.57	1.53	1.46
2	X	172	MET	N-CA	5.57	1.53	1.46
2	M	57	ARG	CA-C	-5.56	1.45	1.52
2	1	172	MET	N-CA	5.56	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	172	MET	N-CA	5.56	1.53	1.46
1	E	114	LYS	C-O	-5.56	1.17	1.24
2	L	57	ARG	CA-C	-5.56	1.45	1.52
1	G	114	LYS	C-O	-5.55	1.17	1.24
1	Q	114	LYS	C-O	-5.55	1.17	1.24
2	K	172	MET	N-CA	5.55	1.53	1.46
1	D	114	LYS	C-O	-5.54	1.17	1.24
1	A	114	LYS	C-O	-5.54	1.17	1.24
2	V	172	MET	N-CA	5.54	1.53	1.46
2	Y	172	MET	N-CA	5.54	1.53	1.46
1	U	114	LYS	C-O	-5.53	1.17	1.24
2	Z	172	MET	N-CA	5.53	1.53	1.46
2	I	172	MET	N-CA	5.53	1.53	1.46
1	R	114	LYS	C-O	-5.53	1.17	1.24
2	L	172	MET	N-CA	5.52	1.53	1.46
1	P	113	VAL	CA-CB	-5.52	1.47	1.54
2	H	172	MET	N-CA	5.52	1.53	1.46
1	O	114	LYS	C-O	-5.52	1.17	1.24
2	2	172	MET	N-CA	5.51	1.53	1.46
1	T	113	VAL	CA-CB	-5.50	1.47	1.54
1	R	113	VAL	CA-CB	-5.50	1.47	1.54
1	G	113	VAL	CA-CB	-5.49	1.47	1.54
2	1	173	ILE	CB-CG1	5.49	1.64	1.53
2	M	77	GLU	N-CA	-5.49	1.39	1.46
2	W	77	GLU	N-CA	-5.49	1.39	1.46
1	O	113	VAL	CA-CB	-5.49	1.47	1.54
2	K	173	ILE	CB-CG1	5.49	1.64	1.53
1	E	95	SER	CA-C	-5.49	1.45	1.52
1	O	142	ASP	CA-C	-5.49	1.45	1.52
2	N	173	ILE	CB-CG1	5.48	1.64	1.53
1	A	95	SER	CA-C	-5.48	1.45	1.52
1	R	95	SER	CA-C	-5.48	1.45	1.52
2	Z	77	GLU	N-CA	-5.48	1.39	1.46
1	G	95	SER	CA-C	-5.48	1.45	1.52
2	I	77	GLU	N-CA	-5.48	1.39	1.46
1	Q	95	SER	CA-C	-5.48	1.45	1.52
1	U	142	ASP	CA-C	-5.48	1.45	1.52
2	H	77	GLU	N-CA	-5.48	1.39	1.46
2	Y	77	GLU	N-CA	-5.48	1.39	1.46
1	F	142	ASP	CA-C	-5.48	1.45	1.52
1	T	95	SER	CA-C	-5.47	1.45	1.52
1	Q	113	VAL	CA-CB	-5.47	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	77	GLU	N-CA	-5.47	1.39	1.46
2	H	71	ARG	CD-NE	5.47	1.53	1.46
2	J	77	GLU	N-CA	-5.47	1.39	1.46
1	S	113	VAL	CA-CB	-5.47	1.47	1.54
2	V	114	ASP	C-O	5.47	1.30	1.23
1	B	113	VAL	CA-CB	-5.47	1.47	1.54
2	J	173	ILE	CB-CG1	5.47	1.64	1.53
2	L	173	ILE	CB-CG1	5.47	1.64	1.53
2	V	77	GLU	N-CA	-5.47	1.39	1.46
2	L	77	GLU	N-CA	-5.47	1.39	1.46
1	C	61	GLN	CA-C	-5.47	1.45	1.52
1	F	95	SER	CA-C	-5.46	1.45	1.52
2	H	114	ASP	C-O	5.46	1.30	1.23
1	P	95	SER	CA-C	-5.46	1.45	1.52
1	F	113	VAL	CA-CB	-5.46	1.47	1.54
2	N	114	ASP	C-O	5.46	1.30	1.23
2	H	173	ILE	CB-CG1	5.46	1.64	1.53
1	C	113	VAL	CA-CB	-5.46	1.47	1.54
1	Q	61	GLN	CA-C	-5.46	1.45	1.52
2	X	114	ASP	C-O	5.46	1.30	1.23
2	Y	173	ILE	CB-CG1	5.46	1.64	1.53
1	A	113	VAL	CA-CB	-5.46	1.47	1.54
2	V	71	ARG	CD-NE	5.46	1.53	1.46
2	L	71	ARG	CD-NE	5.46	1.53	1.46
1	F	61	GLN	CA-C	-5.46	1.45	1.52
2	2	114	ASP	C-O	5.46	1.30	1.23
1	P	61	GLN	CA-C	-5.46	1.45	1.52
2	K	114	ASP	C-O	5.46	1.30	1.23
2	Z	173	ILE	CB-CG1	5.46	1.64	1.53
2	I	173	ILE	CB-CG1	5.46	1.64	1.53
2	Z	114	ASP	C-O	5.46	1.30	1.23
2	I	114	ASP	C-O	5.46	1.30	1.23
1	S	95	SER	CA-C	-5.45	1.45	1.52
2	1	71	ARG	CD-NE	5.45	1.53	1.46
1	G	100	LYS	N-CA	5.45	1.52	1.46
2	H	32	LYS	CA-C	-5.45	1.45	1.52
1	B	95	SER	CA-C	-5.45	1.45	1.52
2	Y	32	LYS	CA-C	-5.45	1.45	1.52
2	1	114	ASP	C-O	5.45	1.30	1.23
1	U	113	VAL	CA-CB	-5.45	1.47	1.54
1	A	61	GLN	CA-C	-5.45	1.45	1.52
2	J	114	ASP	C-O	5.45	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	114	ASP	C-O	5.45	1.30	1.23
1	G	142	ASP	CA-C	-5.45	1.45	1.52
1	U	95	SER	CA-C	-5.45	1.45	1.52
1	Q	142	ASP	CA-C	-5.45	1.45	1.52
2	X	173	ILE	CB-CG1	5.45	1.64	1.53
1	D	95	SER	CA-C	-5.45	1.45	1.52
1	S	142	ASP	CA-C	-5.45	1.45	1.52
1	B	142	ASP	CA-C	-5.45	1.45	1.52
1	P	142	ASP	CA-C	-5.45	1.45	1.52
2	W	114	ASP	C-O	5.45	1.30	1.23
2	J	32	LYS	CA-C	-5.45	1.45	1.52
2	Y	114	ASP	C-O	5.45	1.30	1.23
2	2	173	ILE	CB-CG1	5.45	1.64	1.53
1	A	142	ASP	CA-C	-5.45	1.45	1.52
1	R	142	ASP	CA-C	-5.45	1.45	1.52
1	U	61	GLN	CA-C	-5.45	1.45	1.52
2	K	77	GLU	N-CA	-5.45	1.39	1.46
2	M	32	LYS	CA-C	-5.44	1.45	1.52
2	V	165	ARG	CZ-NH1	5.44	1.40	1.32
2	W	32	LYS	CA-C	-5.44	1.45	1.52
1	Q	74	VAL	CA-C	-5.44	1.45	1.52
2	L	165	ARG	CZ-NH1	5.44	1.40	1.32
2	N	32	LYS	CA-C	-5.44	1.45	1.52
2	2	32	LYS	CA-C	-5.44	1.45	1.52
2	J	165	ARG	CZ-NH1	5.44	1.40	1.32
2	X	32	LYS	CA-C	-5.44	1.45	1.52
1	D	113	VAL	CA-CB	-5.44	1.47	1.54
2	M	114	ASP	C-O	5.44	1.30	1.23
1	A	100	LYS	N-CA	5.44	1.52	1.46
2	V	173	ILE	CB-CG1	5.44	1.64	1.53
1	R	100	LYS	N-CA	5.44	1.52	1.46
1	E	61	GLN	CA-C	-5.44	1.45	1.52
2	1	124	TYR	CA-CB	5.44	1.62	1.53
2	Z	32	LYS	CA-C	-5.44	1.45	1.52
2	I	32	LYS	CA-C	-5.44	1.45	1.52
1	C	95	SER	CA-C	-5.44	1.45	1.52
2	K	125	ALA	CA-C	-5.44	1.45	1.52
2	X	71	ARG	CD-NE	5.43	1.53	1.46
2	Z	71	ARG	CD-NE	5.43	1.53	1.46
2	1	32	LYS	CA-C	-5.43	1.45	1.52
2	I	71	ARG	CD-NE	5.43	1.53	1.46
1	E	113	VAL	CA-CB	-5.43	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	71	ARG	CD-NE	5.43	1.53	1.46
1	D	142	ASP	CA-C	-5.43	1.45	1.52
2	K	71	ARG	CD-NE	5.43	1.53	1.46
1	S	61	GLN	CA-C	-5.43	1.45	1.52
2	M	173	ILE	CB-CG1	5.43	1.64	1.53
1	B	61	GLN	CA-C	-5.43	1.45	1.52
2	W	173	ILE	CB-CG1	5.43	1.64	1.53
1	T	61	GLN	CA-C	-5.43	1.45	1.52
2	H	165	ARG	CZ-NH1	5.43	1.40	1.32
2	V	124	TYR	CA-CB	5.43	1.62	1.53
2	L	124	TYR	CA-CB	5.43	1.62	1.53
2	M	124	TYR	CA-CB	5.42	1.62	1.53
1	O	95	SER	CA-C	-5.42	1.45	1.52
2	W	124	TYR	CA-CB	5.42	1.62	1.53
1	E	142	ASP	CA-C	-5.42	1.45	1.52
2	N	124	TYR	CA-CB	5.42	1.62	1.53
1	F	100	LYS	N-CA	5.42	1.52	1.46
2	M	71	ARG	CD-NE	5.42	1.53	1.46
2	2	77	GLU	N-CA	-5.42	1.39	1.46
1	P	100	LYS	N-CA	5.42	1.52	1.46
2	V	32	LYS	CA-C	-5.42	1.45	1.52
2	Y	165	ARG	CZ-NH1	5.42	1.40	1.32
2	L	32	LYS	CA-C	-5.42	1.45	1.52
2	Z	124	TYR	CA-CB	5.42	1.62	1.53
1	T	142	ASP	CA-C	-5.42	1.45	1.52
2	N	77	GLU	N-CA	-5.42	1.39	1.46
2	N	165	ARG	CZ-NH1	5.42	1.40	1.32
1	O	61	GLN	CA-C	-5.42	1.45	1.52
2	I	124	TYR	CA-CB	5.42	1.62	1.53
1	C	142	ASP	CA-C	-5.42	1.45	1.52
2	X	77	GLU	N-CA	-5.42	1.39	1.46
2	X	165	ARG	CZ-NH1	5.42	1.40	1.32
1	D	100	LYS	N-CA	5.42	1.52	1.46
2	J	71	ARG	CD-NE	5.41	1.53	1.46
2	N	125	ALA	CA-C	-5.41	1.45	1.52
1	S	100	LYS	N-CA	5.41	1.52	1.46
1	G	61	GLN	CA-C	-5.41	1.45	1.52
1	O	100	LYS	N-CA	5.41	1.52	1.46
1	B	100	LYS	N-CA	5.41	1.52	1.46
2	J	124	TYR	CA-CB	5.41	1.62	1.53
1	A	74	VAL	CA-C	-5.41	1.45	1.52
1	O	74	VAL	CA-C	-5.41	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	71	ARG	CD-NE	5.41	1.53	1.46
2	X	124	TYR	CA-CB	5.41	1.62	1.53
1	R	61	GLN	CA-C	-5.41	1.45	1.52
1	E	74	VAL	CA-C	-5.41	1.45	1.52
2	Y	71	ARG	CD-NE	5.41	1.53	1.46
1	Q	100	LYS	N-CA	5.40	1.52	1.46
2	Z	165	ARG	CZ-NH1	5.40	1.40	1.32
2	I	165	ARG	CZ-NH1	5.40	1.40	1.32
1	P	74	VAL	CA-C	-5.40	1.45	1.52
2	M	165	ARG	CZ-NH1	5.40	1.40	1.32
1	G	74	VAL	CA-C	-5.40	1.45	1.52
2	W	165	ARG	CZ-NH1	5.40	1.40	1.32
1	S	74	VAL	CA-C	-5.40	1.45	1.52
1	B	74	VAL	CA-C	-5.40	1.45	1.52
2	J	125	ALA	CA-C	-5.40	1.45	1.52
2	2	165	ARG	CZ-NH1	5.39	1.40	1.32
1	D	61	GLN	CA-C	-5.39	1.45	1.52
2	K	165	ARG	CZ-NH1	5.39	1.40	1.32
1	T	100	LYS	N-CA	5.39	1.52	1.46
1	C	100	LYS	N-CA	5.39	1.52	1.46
2	K	32	LYS	CA-C	-5.39	1.45	1.52
1	E	100	LYS	N-CA	5.39	1.52	1.46
2	H	125	ALA	CA-C	-5.39	1.45	1.52
2	Y	125	ALA	CA-C	-5.39	1.45	1.52
1	F	74	VAL	CA-C	-5.39	1.45	1.52
2	1	182	ASP	N-CA	-5.39	1.39	1.46
2	Y	124	TYR	CA-CB	5.39	1.62	1.53
2	1	28	HIS	ND1-CE1	5.39	1.38	1.32
2	1	178	ILE	N-CA	-5.39	1.39	1.46
2	2	178	ILE	N-CA	-5.39	1.39	1.46
2	J	178	ILE	N-CA	-5.39	1.39	1.46
2	K	178	ILE	N-CA	-5.39	1.39	1.46
2	M	125	ALA	CA-C	-5.39	1.45	1.52
2	2	124	TYR	CA-CB	5.39	1.62	1.53
2	H	178	ILE	N-CA	-5.39	1.39	1.46
2	V	125	ALA	CA-C	-5.39	1.45	1.52
2	W	125	ALA	CA-C	-5.39	1.45	1.52
2	K	124	TYR	CA-CB	5.39	1.62	1.53
2	L	125	ALA	CA-C	-5.39	1.45	1.52
1	U	74	VAL	CA-C	-5.38	1.45	1.52
1	U	100	LYS	N-CA	5.38	1.52	1.46
2	V	178	ILE	N-CA	-5.38	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	74	VAL	CA-C	-5.38	1.45	1.52
2	L	178	ILE	N-CA	-5.38	1.39	1.46
2	Z	125	ALA	CA-C	-5.38	1.45	1.52
2	I	125	ALA	CA-C	-5.38	1.45	1.52
2	Z	178	ILE	N-CA	-5.38	1.39	1.46
2	M	182	ASP	N-CA	-5.38	1.39	1.46
2	I	178	ILE	N-CA	-5.38	1.39	1.46
2	W	182	ASP	N-CA	-5.38	1.39	1.46
2	1	165	ARG	CZ-NH1	5.38	1.40	1.32
2	M	178	ILE	N-CA	-5.38	1.39	1.46
2	N	28	HIS	ND1-CE1	5.38	1.38	1.32
2	W	178	ILE	N-CA	-5.38	1.39	1.46
2	X	28	HIS	ND1-CE1	5.38	1.38	1.32
1	T	74	VAL	CA-C	-5.37	1.45	1.52
1	C	74	VAL	CA-C	-5.37	1.45	1.52
2	N	71	ARG	CD-NE	5.37	1.53	1.46
2	N	178	ILE	N-CA	-5.37	1.39	1.46
2	X	178	ILE	N-CA	-5.37	1.39	1.46
2	H	124	TYR	CA-CB	5.37	1.62	1.53
2	1	125	ALA	CA-C	-5.37	1.45	1.52
2	K	28	HIS	ND1-CE1	5.37	1.38	1.32
2	Y	178	ILE	N-CA	-5.37	1.39	1.46
2	2	125	ALA	CA-C	-5.36	1.45	1.52
2	L	28	HIS	ND1-CE1	5.36	1.38	1.32
2	J	182	ASP	N-CA	-5.36	1.39	1.46
2	K	50	GLY	CA-C	-5.36	1.44	1.51
2	X	125	ALA	CA-C	-5.35	1.45	1.52
2	N	50	GLY	CA-C	-5.35	1.44	1.51
2	2	182	ASP	N-CA	-5.35	1.39	1.46
2	X	50	GLY	CA-C	-5.35	1.44	1.51
2	K	182	ASP	N-CA	-5.35	1.39	1.46
2	Z	28	HIS	ND1-CE1	5.35	1.37	1.32
2	I	28	HIS	ND1-CE1	5.35	1.37	1.32
2	2	92	TYR	CG-CD1	5.34	1.50	1.39
2	Z	92	TYR	CG-CD1	5.34	1.50	1.39
2	M	92	TYR	CG-CD1	5.34	1.50	1.39
2	1	92	TYR	CG-CD1	5.34	1.50	1.39
2	I	92	TYR	CG-CD1	5.34	1.50	1.39
2	J	67	ARG	CZ-NH1	5.34	1.40	1.32
1	R	74	VAL	CA-C	-5.34	1.45	1.52
2	N	92	TYR	CG-CD1	5.34	1.50	1.39
2	H	92	TYR	CG-CD1	5.34	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	92	TYR	CG-CD1	5.34	1.50	1.39
2	X	92	TYR	CG-CD1	5.34	1.50	1.39
2	Y	92	TYR	CG-CD1	5.34	1.50	1.39
2	V	92	TYR	CG-CD1	5.34	1.50	1.39
2	L	92	TYR	CG-CD1	5.34	1.50	1.39
2	Z	50	GLY	CA-C	-5.34	1.44	1.51
1	A	107	VAL	CA-C	-5.34	1.46	1.52
2	I	50	GLY	CA-C	-5.34	1.44	1.51
2	J	50	GLY	CA-C	-5.34	1.44	1.51
2	J	92	TYR	CG-CD1	5.34	1.50	1.39
2	K	72	VAL	C-N	5.34	1.40	1.33
2	K	92	TYR	CG-CD1	5.34	1.50	1.39
2	V	28	HIS	ND1-CE1	5.33	1.37	1.32
1	E	107	VAL	CA-C	-5.33	1.46	1.52
1	G	107	VAL	CA-C	-5.33	1.46	1.52
2	H	50	GLY	CA-C	-5.33	1.44	1.51
2	Y	50	GLY	CA-C	-5.33	1.44	1.51
2	1	67	ARG	CZ-NH1	5.33	1.40	1.32
2	2	72	VAL	C-N	5.33	1.40	1.33
2	N	72	VAL	C-N	5.33	1.40	1.33
2	X	72	VAL	C-N	5.33	1.40	1.33
1	S	107	VAL	CA-C	-5.32	1.46	1.52
2	M	28	HIS	ND1-CE1	5.32	1.37	1.32
2	M	72	VAL	C-N	5.32	1.40	1.33
1	B	107	VAL	CA-C	-5.32	1.46	1.52
2	W	28	HIS	ND1-CE1	5.32	1.37	1.32
2	W	72	VAL	C-N	5.32	1.40	1.33
2	Z	72	VAL	C-N	5.32	1.40	1.33
1	U	107	VAL	CA-C	-5.32	1.46	1.52
2	I	72	VAL	C-N	5.32	1.40	1.33
1	D	107	VAL	CA-C	-5.32	1.46	1.52
1	T	107	VAL	CA-C	-5.32	1.46	1.52
2	2	67	ARG	CZ-NH1	5.32	1.40	1.32
1	C	107	VAL	CA-C	-5.32	1.46	1.52
2	M	50	GLY	CA-C	-5.32	1.44	1.51
2	V	72	VAL	C-N	5.32	1.40	1.33
2	L	72	VAL	C-N	5.32	1.40	1.33
2	1	50	GLY	CA-C	-5.32	1.44	1.51
2	Z	182	ASP	N-CA	-5.31	1.39	1.46
2	I	182	ASP	N-CA	-5.31	1.39	1.46
2	W	50	GLY	CA-C	-5.31	1.44	1.51
2	2	28	HIS	ND1-CE1	5.31	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	107	VAL	CA-C	-5.31	1.46	1.52
2	V	50	GLY	CA-C	-5.31	1.44	1.51
1	P	107	VAL	CA-C	-5.31	1.46	1.52
2	L	50	GLY	CA-C	-5.31	1.44	1.51
1	F	107	VAL	CA-C	-5.31	1.46	1.52
1	Q	107	VAL	CA-C	-5.31	1.46	1.52
2	M	124	TYR	CA-C	-5.31	1.45	1.52
2	H	72	VAL	C-N	5.31	1.40	1.33
1	R	107	VAL	CA-C	-5.31	1.46	1.52
2	Y	72	VAL	C-N	5.31	1.40	1.33
2	N	182	ASP	N-CA	-5.31	1.39	1.46
2	H	182	ASP	N-CA	-5.31	1.39	1.46
2	X	182	ASP	N-CA	-5.31	1.39	1.46
2	Y	182	ASP	N-CA	-5.31	1.39	1.46
2	1	72	VAL	C-N	5.30	1.40	1.33
2	J	72	VAL	C-N	5.30	1.40	1.33
2	X	67	ARG	CZ-NH1	5.30	1.40	1.32
2	2	50	GLY	CA-C	-5.30	1.44	1.51
2	Z	67	ARG	CZ-NH1	5.29	1.40	1.32
2	1	125	ALA	N-CA	-5.29	1.39	1.46
2	I	67	ARG	CZ-NH1	5.29	1.40	1.32
2	2	125	ALA	N-CA	-5.29	1.39	1.46
2	J	28	HIS	ND1-CE1	5.29	1.37	1.32
2	K	125	ALA	N-CA	-5.29	1.39	1.46
2	V	125	ALA	N-CA	-5.29	1.39	1.46
2	H	28	HIS	ND1-CE1	5.28	1.37	1.32
2	H	67	ARG	CZ-NH1	5.28	1.40	1.32
2	Y	28	HIS	ND1-CE1	5.28	1.37	1.32
2	Y	67	ARG	CZ-NH1	5.28	1.40	1.32
2	1	80	ALA	N-CA	-5.28	1.40	1.46
2	V	67	ARG	CZ-NH1	5.28	1.40	1.32
2	L	67	ARG	CZ-NH1	5.28	1.40	1.32
2	K	67	ARG	CZ-NH1	5.27	1.40	1.32
2	M	67	ARG	CZ-NH1	5.27	1.40	1.32
2	W	67	ARG	CZ-NH1	5.27	1.40	1.32
2	N	67	ARG	CZ-NH1	5.27	1.40	1.32
2	L	125	ALA	N-CA	-5.26	1.39	1.46
2	V	182	ASP	N-CA	-5.26	1.39	1.46
2	X	125	ALA	N-CA	-5.26	1.39	1.46
2	L	182	ASP	N-CA	-5.26	1.39	1.46
2	1	15	ALA	CA-C	-5.26	1.46	1.52
2	M	80	ALA	N-CA	-5.26	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	80	ALA	N-CA	-5.26	1.40	1.46
2	J	80	ALA	N-CA	-5.26	1.40	1.46
2	K	80	ALA	N-CA	-5.26	1.40	1.46
2	L	124	TYR	CA-C	-5.26	1.45	1.52
2	Z	80	ALA	N-CA	-5.25	1.40	1.46
2	Z	125	ALA	N-CA	-5.25	1.39	1.46
2	V	80	ALA	N-CA	-5.25	1.40	1.46
2	I	80	ALA	N-CA	-5.25	1.40	1.46
2	I	125	ALA	N-CA	-5.25	1.39	1.46
2	K	124	TYR	CA-C	-5.25	1.45	1.52
2	L	80	ALA	N-CA	-5.25	1.40	1.46
1	O	74	VAL	CA-CB	-5.25	1.47	1.54
1	E	74	VAL	CA-CB	-5.25	1.47	1.54
2	Z	124	TYR	CA-C	-5.25	1.45	1.52
2	I	124	TYR	CA-C	-5.25	1.45	1.52
1	G	159	GLU	C-N	5.25	1.41	1.33
2	M	125	ALA	N-CA	-5.25	1.39	1.46
2	N	124	TYR	CA-C	-5.25	1.45	1.52
1	A	133	GLY	CA-C	-5.25	1.44	1.51
2	H	80	ALA	N-CA	-5.25	1.40	1.46
2	W	125	ALA	N-CA	-5.25	1.39	1.46
2	X	124	TYR	CA-C	-5.25	1.45	1.52
1	R	133	GLY	CA-C	-5.25	1.44	1.51
2	Y	80	ALA	N-CA	-5.25	1.40	1.46
2	1	124	TYR	CA-C	-5.25	1.45	1.52
2	2	80	ALA	N-CA	-5.25	1.40	1.46
2	J	124	TYR	CA-C	-5.25	1.45	1.52
2	N	80	ALA	N-CA	-5.24	1.40	1.46
2	X	80	ALA	N-CA	-5.24	1.40	1.46
1	T	74	VAL	CA-CB	-5.24	1.47	1.54
1	C	74	VAL	CA-CB	-5.24	1.47	1.54
2	W	124	TYR	CA-C	-5.24	1.45	1.52
2	Y	125	ALA	N-CA	-5.23	1.39	1.46
1	S	74	VAL	CA-CB	-5.23	1.47	1.54
1	T	133	GLY	CA-C	-5.23	1.44	1.51
1	G	74	VAL	CA-CB	-5.23	1.47	1.54
2	V	124	TYR	CA-C	-5.23	1.45	1.52
1	B	74	VAL	CA-CB	-5.23	1.47	1.54
1	P	74	VAL	CA-CB	-5.23	1.47	1.54
1	C	133	GLY	CA-C	-5.23	1.44	1.51
1	Q	74	VAL	CA-CB	-5.23	1.47	1.54
1	F	133	GLY	CA-C	-5.22	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	125	ALA	N-CA	-5.22	1.39	1.46
1	P	133	GLY	CA-C	-5.22	1.44	1.51
1	U	74	VAL	CA-CB	-5.22	1.47	1.54
1	D	74	VAL	CA-CB	-5.22	1.47	1.54
1	G	216	THR	CB-OG1	-5.22	1.35	1.43
1	O	133	GLY	CA-C	-5.22	1.44	1.51
1	C	216	THR	CB-OG1	-5.22	1.35	1.43
2	J	125	ALA	N-CA	-5.22	1.39	1.46
1	E	133	GLY	CA-C	-5.22	1.44	1.51
1	U	133	GLY	CA-C	-5.22	1.44	1.51
2	2	124	TYR	CA-C	-5.22	1.45	1.52
1	D	133	GLY	CA-C	-5.22	1.44	1.51
2	2	15	ALA	CA-C	-5.22	1.46	1.52
2	M	15	ALA	CA-C	-5.21	1.46	1.52
1	S	133	GLY	CA-C	-5.21	1.44	1.51
2	M	96	MET	CA-C	-5.21	1.47	1.53
1	B	133	GLY	CA-C	-5.21	1.44	1.51
1	F	159	GLU	C-N	5.21	1.40	1.33
1	P	159	GLU	C-N	5.21	1.40	1.33
1	A	74	VAL	CA-CB	-5.21	1.47	1.54
1	R	74	VAL	CA-CB	-5.21	1.47	1.54
2	Y	96	MET	CA-C	-5.21	1.47	1.53
1	F	216	THR	CB-OG1	-5.20	1.35	1.43
1	P	216	THR	CB-OG1	-5.20	1.35	1.43
1	T	159	GLU	C-N	5.20	1.40	1.33
1	G	133	GLY	CA-C	-5.20	1.44	1.51
1	Q	133	GLY	CA-C	-5.20	1.44	1.51
1	A	159	GLU	C-N	5.20	1.40	1.33
2	H	124	TYR	CA-C	-5.20	1.45	1.52
1	R	159	GLU	C-N	5.20	1.40	1.33
1	T	229	VAL	N-CA	-5.20	1.40	1.46
1	A	216	THR	CB-OG1	-5.20	1.35	1.43
2	X	112	SER	CA-C	-5.20	1.46	1.52
1	R	216	THR	CB-OG1	-5.20	1.35	1.43
2	N	125	ALA	N-CA	-5.20	1.39	1.46
2	Y	124	TYR	CA-C	-5.20	1.45	1.52
1	G	229	VAL	N-CA	-5.20	1.40	1.46
2	N	15	ALA	CA-C	-5.20	1.46	1.52
1	O	159	GLU	C-N	5.20	1.40	1.33
2	X	15	ALA	CA-C	-5.20	1.46	1.52
1	D	216	THR	CB-OG1	-5.20	1.35	1.43
2	Z	15	ALA	CA-C	-5.19	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	15	ALA	CA-C	-5.19	1.46	1.52
1	S	159	GLU	C-N	5.19	1.40	1.33
2	2	28	HIS	CE1-NE2	-5.19	1.27	1.32
2	V	165	ARG	CZ-NH2	5.19	1.40	1.33
1	B	159	GLU	C-N	5.19	1.40	1.33
1	D	218	GLY	CA-C	5.19	1.58	1.51
1	R	229	VAL	N-CA	-5.19	1.40	1.46
2	2	165	ARG	CZ-NH2	5.19	1.40	1.33
2	K	165	ARG	CZ-NH2	5.19	1.40	1.33
1	E	159	GLU	C-N	5.19	1.40	1.33
2	J	15	ALA	CA-C	-5.19	1.46	1.52
2	1	165	ARG	CZ-NH2	5.19	1.40	1.33
1	G	218	GLY	CA-C	5.19	1.58	1.51
2	N	28	HIS	CE1-NE2	-5.19	1.27	1.32
2	2	113	ILE	CA-CB	-5.19	1.48	1.54
2	H	15	ALA	CA-C	-5.19	1.46	1.52
2	J	165	ARG	CZ-NH2	5.19	1.40	1.33
1	Q	218	GLY	CA-C	5.19	1.58	1.51
2	Z	165	ARG	CZ-NH2	5.19	1.40	1.33
2	M	113	ILE	CA-CB	-5.19	1.48	1.54
1	O	216	THR	CB-OG1	-5.19	1.35	1.43
2	I	165	ARG	CZ-NH2	5.19	1.40	1.33
2	W	113	ILE	CA-CB	-5.19	1.48	1.54
1	E	216	THR	CB-OG1	-5.19	1.35	1.43
1	U	159	GLU	C-N	5.18	1.40	1.33
2	H	165	ARG	CZ-NH2	5.18	1.40	1.33
2	V	96	MET	CA-C	-5.18	1.47	1.53
2	Y	15	ALA	CA-C	-5.18	1.46	1.52
1	S	216	THR	CB-OG1	-5.18	1.35	1.43
1	B	216	THR	CB-OG1	-5.18	1.35	1.43
1	Q	159	GLU	C-N	5.18	1.40	1.33
2	K	15	ALA	CA-C	-5.18	1.46	1.52
2	L	15	ALA	CA-C	-5.18	1.46	1.52
2	L	165	ARG	CZ-NH2	5.18	1.40	1.33
2	N	113	ILE	CA-CB	-5.18	1.48	1.54
2	H	113	ILE	CA-CB	-5.18	1.48	1.54
2	Y	113	ILE	CA-CB	-5.18	1.48	1.54
1	T	216	THR	CB-OG1	-5.18	1.35	1.43
2	N	165	ARG	CZ-NH2	5.18	1.40	1.33
2	X	28	HIS	CE1-NE2	-5.18	1.27	1.32
2	X	165	ARG	CZ-NH2	5.18	1.40	1.33
1	F	218	GLY	CA-C	5.17	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	96	MET	CA-C	-5.17	1.47	1.53
1	P	218	GLY	CA-C	5.17	1.58	1.51
2	Z	96	MET	CA-C	-5.17	1.47	1.53
2	I	96	MET	CA-C	-5.17	1.47	1.53
2	Y	165	ARG	CZ-NH2	5.17	1.40	1.33
2	L	112	SER	CA-C	-5.17	1.46	1.52
1	F	74	VAL	CA-CB	-5.17	1.47	1.54
1	O	229	VAL	N-CA	-5.17	1.40	1.46
2	M	28	HIS	CE1-NE2	-5.17	1.27	1.32
1	G	103	TYR	CA-C	-5.17	1.45	1.52
2	V	113	ILE	CA-CB	-5.17	1.48	1.54
1	S	218	GLY	CA-C	5.17	1.58	1.51
2	Z	113	ILE	CA-CB	-5.17	1.48	1.54
2	M	165	ARG	CZ-NH2	5.17	1.40	1.33
2	1	96	MET	CA-C	-5.17	1.47	1.53
2	1	113	ILE	CA-CB	-5.17	1.48	1.54
1	B	218	GLY	CA-C	5.17	1.58	1.51
2	I	113	ILE	CA-CB	-5.17	1.48	1.54
2	W	165	ARG	CZ-NH2	5.17	1.40	1.33
2	J	96	MET	CA-C	-5.17	1.47	1.53
2	J	113	ILE	CA-CB	-5.17	1.48	1.54
1	Q	216	THR	CB-OG1	-5.17	1.35	1.43
1	T	218	GLY	CA-C	5.16	1.58	1.51
1	A	218	GLY	CA-C	5.16	1.58	1.51
1	C	218	GLY	CA-C	5.16	1.58	1.51
1	R	218	GLY	CA-C	5.16	1.58	1.51
2	N	96	MET	CA-C	-5.16	1.47	1.53
1	A	229	VAL	N-CA	-5.16	1.40	1.46
1	E	229	VAL	N-CA	-5.16	1.40	1.46
1	F	229	VAL	N-CA	-5.16	1.40	1.46
1	O	218	GLY	CA-C	5.16	1.58	1.51
1	U	229	VAL	N-CA	-5.16	1.40	1.46
1	D	229	VAL	N-CA	-5.16	1.40	1.46
2	V	15	ALA	CA-C	-5.15	1.46	1.52
1	S	229	VAL	N-CA	-5.15	1.40	1.46
1	B	229	VAL	N-CA	-5.15	1.40	1.46
1	Q	131	PRO	C-N	5.15	1.40	1.33
2	N	112	SER	CA-C	-5.15	1.46	1.52
1	C	229	VAL	N-CA	-5.15	1.40	1.46
2	K	113	ILE	CA-CB	-5.15	1.48	1.54
2	X	113	ILE	CA-CB	-5.15	1.48	1.54
2	W	15	ALA	CA-C	-5.14	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	229	VAL	N-CA	-5.14	1.40	1.46
2	L	113	ILE	CA-CB	-5.14	1.48	1.54
2	Z	112	SER	CA-C	-5.14	1.46	1.52
1	G	131	PRO	C-N	5.14	1.40	1.33
2	I	112	SER	CA-C	-5.14	1.46	1.52
2	K	28	HIS	CE1-NE2	-5.14	1.27	1.32
2	Y	112	SER	CA-C	-5.14	1.46	1.52
1	U	216	THR	CB-OG1	-5.14	1.35	1.43
1	A	165	ILE	CA-C	-5.14	1.46	1.52
2	K	112	SER	CA-C	-5.14	1.46	1.52
1	C	159	GLU	C-N	5.14	1.40	1.33
2	M	167	SER	CA-CB	5.13	1.62	1.53
2	J	167	SER	CA-CB	5.13	1.62	1.53
2	N	108	PRO	N-CA	-5.13	1.41	1.46
2	N	167	SER	CA-CB	5.13	1.62	1.53
1	A	131	PRO	C-N	5.13	1.40	1.33
2	H	167	SER	CA-CB	5.13	1.62	1.53
1	D	159	GLU	C-N	5.13	1.40	1.33
1	R	131	PRO	C-N	5.13	1.40	1.33
2	Z	28	HIS	CE1-NE2	-5.13	1.27	1.32
1	O	131	PRO	C-N	5.13	1.40	1.33
2	I	28	HIS	CE1-NE2	-5.13	1.27	1.32
2	W	96	MET	CA-C	-5.13	1.47	1.53
1	E	131	PRO	C-N	5.13	1.40	1.33
1	P	229	VAL	N-CA	-5.12	1.40	1.46
1	F	103	TYR	CA-C	-5.12	1.45	1.52
2	2	112	SER	CA-C	-5.12	1.46	1.52
1	P	103	TYR	CA-C	-5.12	1.45	1.52
2	L	96	MET	CA-C	-5.12	1.47	1.53
1	T	131	PRO	C-N	5.12	1.40	1.33
1	U	218	GLY	CA-C	5.12	1.58	1.51
1	C	131	PRO	C-N	5.12	1.40	1.33
2	X	96	MET	CA-C	-5.12	1.47	1.53
1	G	86	ARG	CD-NE	5.12	1.53	1.46
2	V	112	SER	CA-C	-5.12	1.46	1.52
1	Q	86	ARG	CD-NE	5.12	1.53	1.46
2	M	112	SER	CA-C	-5.12	1.46	1.52
2	H	112	SER	CA-C	-5.12	1.46	1.52
2	W	112	SER	CA-C	-5.12	1.46	1.52
1	S	103	TYR	CA-C	-5.12	1.45	1.52
2	Z	167	SER	CA-CB	5.12	1.62	1.53
2	1	112	SER	CA-C	-5.12	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	96	MET	CA-C	-5.12	1.47	1.53
2	2	167	SER	CA-CB	5.12	1.62	1.53
1	B	103	TYR	CA-C	-5.12	1.45	1.52
2	I	167	SER	CA-CB	5.12	1.62	1.53
2	J	112	SER	CA-C	-5.12	1.46	1.52
1	Q	103	TYR	CA-C	-5.12	1.45	1.52
2	K	96	MET	CA-C	-5.12	1.47	1.53
2	K	167	SER	CA-CB	5.12	1.62	1.53
2	J	108	PRO	N-CA	-5.11	1.41	1.46
1	T	220	LYS	CA-CB	5.11	1.61	1.53
1	C	220	LYS	CA-CB	5.11	1.61	1.53
1	F	131	PRO	C-N	5.11	1.40	1.33
1	T	103	TYR	CA-C	-5.11	1.45	1.52
1	P	131	PRO	C-N	5.11	1.40	1.33
1	C	103	TYR	CA-C	-5.11	1.45	1.52
2	Y	167	SER	CA-CB	5.11	1.62	1.53
1	S	131	PRO	C-N	5.11	1.40	1.33
1	U	131	PRO	C-N	5.11	1.40	1.33
1	B	131	PRO	C-N	5.11	1.40	1.33
1	D	131	PRO	C-N	5.11	1.40	1.33
1	F	220	LYS	CA-CB	5.11	1.61	1.53
2	V	28	HIS	CE1-NE2	-5.11	1.27	1.32
2	K	162	ALA	C-N	5.11	1.40	1.33
2	L	28	HIS	CE1-NE2	-5.11	1.27	1.32
2	N	162	ALA	C-N	5.10	1.40	1.33
1	U	165	ILE	CA-C	-5.10	1.46	1.52
1	D	165	ILE	CA-C	-5.10	1.46	1.52
1	E	218	GLY	CA-C	5.10	1.58	1.51
2	M	108	PRO	N-CA	-5.10	1.41	1.46
1	T	165	ILE	CA-C	-5.10	1.46	1.52
2	1	28	HIS	CE1-NE2	-5.10	1.27	1.32
1	O	165	ILE	CA-C	-5.10	1.46	1.52
2	W	108	PRO	N-CA	-5.10	1.41	1.46
1	C	165	ILE	CA-C	-5.10	1.46	1.52
2	J	28	HIS	CE1-NE2	-5.10	1.27	1.32
2	W	167	SER	CA-CB	5.10	1.62	1.53
1	A	103	TYR	CA-C	-5.10	1.45	1.52
1	P	86	ARG	CD-NE	5.10	1.53	1.46
1	P	220	LYS	CA-CB	5.10	1.61	1.53
2	W	28	HIS	CE1-NE2	-5.10	1.27	1.32
1	R	103	TYR	CA-C	-5.10	1.45	1.52
2	1	162	ALA	C-N	5.09	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	165	ILE	CA-C	-5.09	1.46	1.52
2	J	162	ALA	C-N	5.09	1.40	1.33
1	Q	165	ILE	CA-C	-5.09	1.46	1.52
1	E	103	TYR	CA-C	-5.09	1.45	1.52
2	X	162	ALA	C-N	5.09	1.40	1.33
1	S	165	ILE	CA-C	-5.09	1.46	1.52
2	1	167	SER	CA-CB	5.09	1.62	1.53
1	G	220	LYS	CA-CB	5.09	1.61	1.53
2	2	108	PRO	N-CA	-5.09	1.41	1.46
1	B	165	ILE	CA-C	-5.09	1.46	1.52
2	K	108	PRO	N-CA	-5.09	1.41	1.46
2	V	162	ALA	C-N	5.09	1.40	1.33
1	P	12	ILE	C-N	5.09	1.40	1.33
2	X	167	SER	CA-CB	5.09	1.62	1.53
2	L	162	ALA	C-N	5.09	1.40	1.33
1	U	103	TYR	CA-C	-5.09	1.46	1.52
2	V	167	SER	CA-CB	5.09	1.62	1.53
1	D	103	TYR	CA-C	-5.09	1.46	1.52
1	A	12	ILE	C-N	5.09	1.40	1.33
2	L	167	SER	CA-CB	5.09	1.62	1.53
1	U	220	LYS	CA-CB	5.08	1.61	1.53
1	A	86	ARG	CD-NE	5.08	1.53	1.46
1	O	220	LYS	CA-CB	5.08	1.61	1.53
1	D	220	LYS	CA-CB	5.08	1.61	1.53
1	R	86	ARG	CD-NE	5.08	1.53	1.46
1	E	220	LYS	CA-CB	5.08	1.61	1.53
1	S	220	LYS	CA-CB	5.08	1.61	1.53
1	T	86	ARG	CD-NE	5.08	1.53	1.46
1	U	86	ARG	CD-NE	5.08	1.53	1.46
1	B	220	LYS	CA-CB	5.08	1.61	1.53
1	D	86	ARG	CD-NE	5.08	1.53	1.46
1	A	220	LYS	CA-CB	5.08	1.61	1.53
1	R	220	LYS	CA-CB	5.08	1.61	1.53
1	R	165	ILE	CA-C	-5.08	1.46	1.52
2	Z	162	ALA	C-N	5.07	1.40	1.33
2	V	36	GLN	CA-C	-5.07	1.46	1.52
2	I	162	ALA	C-N	5.07	1.40	1.33
1	S	12	ILE	C-N	5.07	1.40	1.33
1	B	12	ILE	C-N	5.07	1.40	1.33
2	H	28	HIS	CE1-NE2	-5.07	1.27	1.32
2	Y	28	HIS	CE1-NE2	-5.07	1.27	1.32
1	S	86	ARG	CD-NE	5.07	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	12	ILE	C-N	5.07	1.40	1.33
1	T	12	ILE	C-N	5.07	1.40	1.33
1	O	12	ILE	C-N	5.07	1.40	1.33
1	B	86	ARG	CD-NE	5.07	1.53	1.46
1	P	78	THR	CA-C	-5.07	1.46	1.52
1	C	12	ILE	C-N	5.07	1.40	1.33
1	E	12	ILE	C-N	5.07	1.40	1.33
2	Z	108	PRO	N-CA	-5.07	1.41	1.46
1	U	12	ILE	C-N	5.07	1.40	1.33
2	I	108	PRO	N-CA	-5.07	1.41	1.46
1	D	12	ILE	C-N	5.07	1.40	1.33
1	G	12	ILE	C-N	5.07	1.40	1.33
2	2	162	ALA	C-N	5.07	1.40	1.33
1	Q	12	ILE	C-N	5.07	1.40	1.33
1	R	12	ILE	C-N	5.07	1.40	1.33
1	O	103	TYR	CA-C	-5.06	1.46	1.52
1	F	172	VAL	C-O	-5.06	1.18	1.24
1	G	78	THR	CA-C	-5.06	1.46	1.52
1	O	86	ARG	CD-NE	5.06	1.53	1.46
1	E	86	ARG	CD-NE	5.06	1.53	1.46
1	F	78	THR	CA-C	-5.06	1.46	1.52
1	F	165	ILE	CA-C	-5.06	1.46	1.52
1	Q	220	LYS	CA-CB	5.06	1.61	1.53
2	H	162	ALA	C-N	5.05	1.40	1.33
2	Y	162	ALA	C-N	5.05	1.40	1.33
1	E	165	ILE	CA-C	-5.05	1.46	1.52
1	U	78	THR	CA-C	-5.05	1.46	1.52
1	P	165	ILE	CA-C	-5.05	1.46	1.52
2	X	108	PRO	N-CA	-5.05	1.41	1.46
1	D	78	THR	CA-C	-5.05	1.46	1.52
2	1	108	PRO	N-CA	-5.05	1.41	1.46
2	H	108	PRO	N-CA	-5.05	1.41	1.46
1	P	73	TYR	C-N	5.05	1.39	1.33
1	Q	27	ALA	CA-CB	5.05	1.61	1.53
2	Y	108	PRO	N-CA	-5.05	1.41	1.46
1	S	78	THR	CA-C	-5.05	1.46	1.52
1	T	27	ALA	CA-CB	5.05	1.61	1.53
1	O	27	ALA	CA-CB	5.05	1.61	1.53
1	B	78	THR	CA-C	-5.05	1.46	1.52
1	E	27	ALA	CA-CB	5.05	1.61	1.53
2	M	36	GLN	CA-C	-5.04	1.46	1.52
2	1	36	GLN	CA-C	-5.04	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	27	ALA	CA-CB	5.04	1.61	1.53
2	2	4	VAL	C-N	5.04	1.40	1.33
2	W	36	GLN	CA-C	-5.04	1.46	1.52
2	J	36	GLN	CA-C	-5.04	1.46	1.52
2	K	4	VAL	C-N	5.04	1.40	1.33
1	O	51	ASP	N-CA	-5.04	1.39	1.45
1	Q	80	GLY	C-N	5.04	1.40	1.33
2	M	162	ALA	C-N	5.04	1.40	1.33
1	T	78	THR	CA-C	-5.04	1.46	1.52
2	W	162	ALA	C-N	5.04	1.40	1.33
1	C	78	THR	CA-C	-5.04	1.46	1.52
1	G	23	GLN	CA-C	-5.04	1.46	1.52
2	Z	36	GLN	CA-C	-5.04	1.46	1.52
2	M	4	VAL	C-N	5.04	1.40	1.33
1	U	51	ASP	N-CA	-5.04	1.39	1.45
1	A	27	ALA	CA-CB	5.04	1.61	1.53
2	H	36	GLN	CA-C	-5.04	1.46	1.52
2	V	108	PRO	N-CA	-5.04	1.41	1.46
2	I	36	GLN	CA-C	-5.04	1.46	1.52
2	W	4	VAL	C-N	5.04	1.40	1.33
2	J	4	VAL	C-N	5.04	1.40	1.33
1	R	27	ALA	CA-CB	5.04	1.61	1.53
2	Y	36	GLN	CA-C	-5.04	1.46	1.52
1	Q	78	THR	CA-C	-5.03	1.46	1.52
1	F	86	ARG	CD-NE	5.03	1.53	1.46
1	O	78	THR	CA-C	-5.03	1.46	1.52
1	E	78	THR	CA-C	-5.03	1.46	1.52
2	L	36	GLN	CA-C	-5.03	1.46	1.52
1	S	27	ALA	CA-CB	5.03	1.61	1.53
1	A	78	THR	CA-C	-5.03	1.46	1.52
1	B	27	ALA	CA-CB	5.03	1.61	1.53
1	C	86	ARG	CD-NE	5.03	1.53	1.46
1	R	78	THR	CA-C	-5.03	1.46	1.52
1	F	27	ALA	CA-CB	5.03	1.61	1.53
1	O	172	VAL	C-O	-5.03	1.18	1.24
1	P	27	ALA	CA-CB	5.03	1.61	1.53
2	K	42	GLY	CA-C	-5.02	1.48	1.52
1	U	80	GLY	C-N	5.02	1.40	1.33
1	D	80	GLY	C-N	5.02	1.40	1.33
1	C	27	ALA	CA-CB	5.02	1.61	1.53
1	F	13	THR	CA-CB	5.02	1.59	1.52
2	M	83	LEU	N-CA	5.02	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	4	VAL	C-N	5.02	1.40	1.33
2	W	83	LEU	N-CA	5.02	1.52	1.46
1	G	27	ALA	CA-CB	5.02	1.61	1.53
1	U	172	VAL	C-O	-5.02	1.18	1.24
1	D	172	VAL	C-O	-5.02	1.18	1.24
1	F	51	ASP	N-CA	-5.01	1.39	1.45
2	1	4	VAL	C-N	5.01	1.40	1.33
1	G	99	GLU	CA-C	-5.01	1.45	1.52
1	P	51	ASP	N-CA	-5.01	1.39	1.45
2	J	83	LEU	N-CA	5.01	1.52	1.46
1	Q	99	GLU	CA-C	-5.01	1.45	1.52
1	D	27	ALA	CA-CB	5.01	1.61	1.53
1	U	30	ALA	C-N	5.01	1.40	1.33
1	D	30	ALA	C-N	5.01	1.40	1.33
1	T	80	GLY	C-N	5.01	1.40	1.33
1	U	71	ASP	CA-CB	5.01	1.62	1.53
1	C	80	GLY	C-N	5.01	1.40	1.33
1	D	71	ASP	CA-CB	5.01	1.62	1.53
2	L	108	PRO	N-CA	-5.01	1.41	1.46
2	N	4	VAL	C-N	5.01	1.40	1.33
2	2	42	GLY	CA-C	-5.01	1.48	1.52
1	A	96	ALA	CA-C	-5.01	1.46	1.52
2	L	4	VAL	C-N	5.01	1.40	1.33
2	Z	4	VAL	C-N	5.01	1.40	1.33
1	F	99	GLU	CA-C	-5.01	1.45	1.52
1	A	30	ALA	C-N	5.01	1.40	1.33
2	I	4	VAL	C-N	5.01	1.40	1.33
1	R	30	ALA	C-N	5.01	1.40	1.33
1	S	80	GLY	C-N	5.01	1.40	1.33
1	T	51	ASP	N-CA	-5.01	1.39	1.45
2	N	36	GLN	CA-C	-5.01	1.46	1.52
1	B	80	GLY	C-N	5.01	1.40	1.33
1	P	96	ALA	CA-C	-5.01	1.46	1.52
1	C	51	ASP	N-CA	-5.01	1.39	1.45
1	C	172	VAL	C-O	-5.01	1.18	1.24
1	Q	23	GLN	CA-C	-5.01	1.46	1.52
2	X	36	GLN	CA-C	-5.01	1.46	1.52
2	2	36	GLN	CA-C	-5.00	1.46	1.52
1	G	80	GLY	C-N	5.00	1.40	1.33
2	H	83	LEU	N-CA	5.00	1.52	1.46
1	Q	71	ASP	CA-CB	5.00	1.62	1.53
1	D	13	THR	CA-CB	5.00	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	96	ALA	CA-C	-5.00	1.46	1.52
1	O	96	ALA	CA-C	-5.00	1.46	1.52
1	E	51	ASP	N-CA	-5.00	1.39	1.45
1	E	96	ALA	CA-C	-5.00	1.46	1.52

All (3253) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	200	SER	CA-C-N	9.66	136.05	120.60
1	G	200	SER	C-N-CA	9.66	136.05	120.60
1	U	200	SER	CA-C-N	9.66	136.05	120.60
1	U	200	SER	C-N-CA	9.66	136.05	120.60
1	Q	200	SER	CA-C-N	9.66	136.05	120.60
1	Q	200	SER	C-N-CA	9.66	136.05	120.60
1	S	200	SER	CA-C-N	9.65	136.03	120.60
1	S	200	SER	C-N-CA	9.65	136.03	120.60
1	F	200	SER	CA-C-N	9.65	136.04	120.60
1	F	200	SER	C-N-CA	9.65	136.04	120.60
1	O	200	SER	CA-C-N	9.65	136.03	120.60
1	O	200	SER	C-N-CA	9.65	136.03	120.60
1	B	200	SER	CA-C-N	9.65	136.03	120.60
1	B	200	SER	C-N-CA	9.65	136.03	120.60
1	R	200	SER	CA-C-N	9.65	136.03	120.60
1	R	200	SER	C-N-CA	9.65	136.03	120.60
1	A	200	SER	CA-C-N	9.64	136.03	120.60
1	A	200	SER	C-N-CA	9.64	136.03	120.60
1	E	200	SER	CA-C-N	9.64	136.03	120.60
1	E	200	SER	C-N-CA	9.64	136.03	120.60
1	D	200	SER	CA-C-N	9.64	136.02	120.60
1	D	200	SER	C-N-CA	9.64	136.02	120.60
1	P	200	SER	CA-C-N	9.64	136.02	120.60
1	P	200	SER	C-N-CA	9.64	136.02	120.60
1	T	200	SER	CA-C-N	9.63	136.01	120.60
1	T	200	SER	C-N-CA	9.63	136.01	120.60
1	C	200	SER	CA-C-N	9.63	136.01	120.60
1	C	200	SER	C-N-CA	9.63	136.01	120.60
1	F	232	PHE	CA-CB-CG	-9.56	104.24	113.80
1	G	232	PHE	CA-CB-CG	-9.54	104.26	113.80
1	Q	232	PHE	CA-CB-CG	-9.53	104.27	113.80
1	S	232	PHE	CA-CB-CG	-9.53	104.27	113.80
1	T	232	PHE	CA-CB-CG	-9.53	104.27	113.80
1	B	232	PHE	CA-CB-CG	-9.53	104.27	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	232	PHE	CA-CB-CG	-9.52	104.28	113.80
1	R	232	PHE	CA-CB-CG	-9.51	104.29	113.80
1	C	232	PHE	CA-CB-CG	-9.51	104.29	113.80
1	O	232	PHE	CA-CB-CG	-9.50	104.30	113.80
1	P	232	PHE	CA-CB-CG	-9.50	104.30	113.80
1	A	232	PHE	CA-CB-CG	-9.50	104.30	113.80
1	U	232	PHE	CA-CB-CG	-9.50	104.30	113.80
1	D	232	PHE	CA-CB-CG	-9.49	104.31	113.80
2	N	107	ALA	N-CA-C	-9.40	99.76	108.22
2	L	107	ALA	N-CA-C	-9.38	99.78	108.22
2	K	107	ALA	N-CA-C	-9.38	99.78	108.22
2	1	107	ALA	N-CA-C	-9.38	99.78	108.22
2	J	107	ALA	N-CA-C	-9.38	99.78	108.22
2	Z	107	ALA	N-CA-C	-9.37	99.79	108.22
2	I	107	ALA	N-CA-C	-9.37	99.79	108.22
2	V	107	ALA	N-CA-C	-9.36	99.79	108.22
2	M	107	ALA	N-CA-C	-9.36	99.80	108.22
2	W	107	ALA	N-CA-C	-9.36	99.80	108.22
2	H	107	ALA	N-CA-C	-9.36	99.80	108.22
2	Y	107	ALA	N-CA-C	-9.36	99.80	108.22
2	X	107	ALA	N-CA-C	-9.35	99.80	108.22
2	2	107	ALA	N-CA-C	-9.32	99.83	108.22
1	Q	170	ASP	O-C-N	9.19	131.86	122.12
1	R	170	ASP	O-C-N	9.18	131.85	122.12
1	E	170	ASP	O-C-N	9.18	131.85	122.12
1	P	170	ASP	O-C-N	9.17	131.84	122.12
1	D	170	ASP	O-C-N	9.17	131.84	122.12
1	T	170	ASP	O-C-N	9.16	131.83	122.12
1	A	170	ASP	O-C-N	9.16	131.83	122.12
1	G	170	ASP	O-C-N	9.15	131.82	122.12
1	S	170	ASP	O-C-N	9.14	131.81	122.12
1	B	170	ASP	O-C-N	9.14	131.81	122.12
1	U	170	ASP	O-C-N	9.14	131.81	122.12
1	O	170	ASP	O-C-N	9.14	131.81	122.12
1	F	170	ASP	O-C-N	9.13	131.80	122.12
1	C	170	ASP	O-C-N	9.09	131.76	122.12
2	K	81	THR	CA-C-N	9.01	132.16	120.44
2	K	81	THR	C-N-CA	9.01	132.16	120.44
2	W	81	THR	CA-C-N	9.01	132.15	120.44
2	W	81	THR	C-N-CA	9.01	132.15	120.44
2	1	81	THR	CA-C-N	9.00	132.14	120.44
2	1	81	THR	C-N-CA	9.00	132.14	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	81	THR	CA-C-N	9.00	132.14	120.44
2	V	81	THR	C-N-CA	9.00	132.14	120.44
2	H	81	THR	CA-C-N	8.99	132.13	120.44
2	H	81	THR	C-N-CA	8.99	132.13	120.44
2	Y	81	THR	CA-C-N	8.99	132.13	120.44
2	Y	81	THR	C-N-CA	8.99	132.13	120.44
2	Z	81	THR	CA-C-N	8.99	132.13	120.44
2	Z	81	THR	C-N-CA	8.99	132.13	120.44
2	2	81	THR	CA-C-N	8.99	132.13	120.44
2	2	81	THR	C-N-CA	8.99	132.13	120.44
2	I	81	THR	CA-C-N	8.99	132.13	120.44
2	I	81	THR	C-N-CA	8.99	132.13	120.44
2	N	81	THR	CA-C-N	8.99	132.12	120.44
2	N	81	THR	C-N-CA	8.99	132.12	120.44
2	X	81	THR	CA-C-N	8.99	132.12	120.44
2	X	81	THR	C-N-CA	8.99	132.12	120.44
2	M	81	THR	CA-C-N	8.98	132.12	120.44
2	M	81	THR	C-N-CA	8.98	132.12	120.44
2	J	81	THR	CA-C-N	8.98	132.12	120.44
2	J	81	THR	C-N-CA	8.98	132.12	120.44
2	L	81	THR	CA-C-N	8.98	132.11	120.44
2	L	81	THR	C-N-CA	8.98	132.11	120.44
2	K	21	THR	CA-C-N	8.66	137.29	121.70
2	K	21	THR	C-N-CA	8.66	137.29	121.70
2	H	21	THR	CA-C-N	8.66	137.28	121.70
2	H	21	THR	C-N-CA	8.66	137.28	121.70
2	N	21	THR	CA-C-N	8.65	137.28	121.70
2	N	21	THR	C-N-CA	8.65	137.28	121.70
2	X	21	THR	CA-C-N	8.65	137.28	121.70
2	X	21	THR	C-N-CA	8.65	137.28	121.70
2	M	21	THR	CA-C-N	8.64	137.26	121.70
2	M	21	THR	C-N-CA	8.64	137.26	121.70
2	2	21	THR	CA-C-N	8.64	137.26	121.70
2	2	21	THR	C-N-CA	8.64	137.26	121.70
2	L	21	THR	CA-C-N	8.64	137.25	121.70
2	L	21	THR	C-N-CA	8.64	137.25	121.70
2	Z	21	THR	CA-C-N	8.64	137.25	121.70
2	Z	21	THR	C-N-CA	8.64	137.25	121.70
2	I	21	THR	CA-C-N	8.64	137.25	121.70
2	I	21	THR	C-N-CA	8.64	137.25	121.70
2	Y	21	THR	CA-C-N	8.63	137.24	121.70
2	Y	21	THR	C-N-CA	8.63	137.24	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	21	THR	CA-C-N	8.62	137.22	121.70
2	V	21	THR	C-N-CA	8.62	137.22	121.70
2	W	21	THR	CA-C-N	8.62	137.22	121.70
2	W	21	THR	C-N-CA	8.62	137.22	121.70
2	J	21	THR	CA-C-N	8.61	137.19	121.70
2	J	21	THR	C-N-CA	8.61	137.19	121.70
2	1	21	THR	CA-C-N	8.60	137.19	121.70
2	1	21	THR	C-N-CA	8.60	137.19	121.70
2	W	170	GLY	O-C-N	-8.59	115.22	123.81
2	N	170	GLY	O-C-N	-8.59	115.22	123.81
2	1	170	GLY	O-C-N	-8.59	115.22	123.81
2	J	170	GLY	O-C-N	-8.59	115.22	123.81
2	H	170	GLY	O-C-N	-8.58	115.23	123.81
2	X	170	GLY	O-C-N	-8.57	115.23	123.81
2	Z	170	GLY	O-C-N	-8.57	115.24	123.81
2	I	170	GLY	O-C-N	-8.57	115.24	123.81
2	2	170	GLY	O-C-N	-8.57	115.24	123.81
2	M	170	GLY	O-C-N	-8.56	115.25	123.81
2	V	170	GLY	O-C-N	-8.56	115.25	123.81
2	L	170	GLY	O-C-N	-8.56	115.25	123.81
2	K	170	GLY	O-C-N	-8.54	115.27	123.81
2	Y	170	GLY	O-C-N	-8.54	115.27	123.81
1	T	94	ILE	CA-C-O	-8.36	112.26	120.95
1	A	94	ILE	CA-C-O	-8.35	112.26	120.95
1	R	94	ILE	CA-C-O	-8.35	112.26	120.95
1	U	94	ILE	CA-C-O	-8.35	112.27	120.95
2	X	93	MET	N-CA-C	-8.35	96.44	109.79
1	D	94	ILE	CA-C-O	-8.35	112.27	120.95
2	2	93	MET	N-CA-C	-8.34	96.44	109.79
1	Q	94	ILE	CA-C-O	-8.34	112.28	120.95
2	V	93	MET	N-CA-C	-8.33	96.46	109.79
1	S	94	ILE	CA-C-O	-8.33	112.29	120.95
2	Z	93	MET	N-CA-C	-8.33	96.46	109.79
1	B	94	ILE	CA-C-O	-8.33	112.29	120.95
2	I	93	MET	N-CA-C	-8.33	96.46	109.79
2	W	93	MET	N-CA-C	-8.33	96.46	109.79
1	P	94	ILE	CA-C-O	-8.33	112.29	120.95
1	C	94	ILE	CA-C-O	-8.33	112.29	120.95
1	E	94	ILE	CA-C-O	-8.33	112.29	120.95
2	N	93	MET	N-CA-C	-8.33	96.47	109.79
2	H	93	MET	N-CA-C	-8.33	96.47	109.79
1	F	94	ILE	CA-C-O	-8.33	112.29	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	93	MET	N-CA-C	-8.31	96.49	109.79
2	K	93	MET	N-CA-C	-8.31	96.50	109.79
2	M	93	MET	N-CA-C	-8.31	96.50	109.79
2	J	134	VAL	CA-C-N	8.31	132.24	120.28
2	J	134	VAL	C-N-CA	8.31	132.24	120.28
2	Y	93	MET	N-CA-C	-8.30	96.50	109.79
2	1	93	MET	N-CA-C	-8.30	96.50	109.79
2	J	93	MET	N-CA-C	-8.30	96.50	109.79
2	L	134	VAL	CA-C-N	8.30	132.23	120.28
2	L	134	VAL	C-N-CA	8.30	132.23	120.28
1	O	94	ILE	CA-C-O	-8.30	112.32	120.95
1	G	94	ILE	CA-C-O	-8.30	112.32	120.95
2	V	134	VAL	CA-C-N	8.29	132.22	120.28
2	V	134	VAL	C-N-CA	8.29	132.22	120.28
1	Q	42	PHE	CA-CB-CG	8.29	122.09	113.80
2	W	134	VAL	CA-C-N	8.29	132.21	120.28
2	W	134	VAL	C-N-CA	8.29	132.21	120.28
2	1	134	VAL	CA-C-N	8.28	132.20	120.28
2	1	134	VAL	C-N-CA	8.28	132.20	120.28
2	X	134	VAL	CA-C-N	8.28	132.20	120.28
2	X	134	VAL	C-N-CA	8.28	132.20	120.28
1	T	42	PHE	CA-CB-CG	8.27	122.07	113.80
2	Y	134	VAL	CA-C-N	8.27	132.19	120.28
2	Y	134	VAL	C-N-CA	8.27	132.19	120.28
2	M	134	VAL	CA-C-N	8.27	132.19	120.28
2	M	134	VAL	C-N-CA	8.27	132.19	120.28
1	E	42	PHE	CA-CB-CG	8.27	122.07	113.80
2	Z	134	VAL	CA-C-N	8.26	132.18	120.28
2	Z	134	VAL	C-N-CA	8.26	132.18	120.28
1	A	42	PHE	CA-CB-CG	8.26	122.06	113.80
2	I	134	VAL	CA-C-N	8.26	132.18	120.28
2	I	134	VAL	C-N-CA	8.26	132.18	120.28
1	D	42	PHE	CA-CB-CG	8.26	122.06	113.80
1	R	42	PHE	CA-CB-CG	8.26	122.06	113.80
1	G	42	PHE	CA-CB-CG	8.25	122.05	113.80
2	H	134	VAL	CA-C-N	8.25	132.16	120.28
2	H	134	VAL	C-N-CA	8.25	132.16	120.28
1	F	42	PHE	CA-CB-CG	8.24	122.05	113.80
1	P	42	PHE	CA-CB-CG	8.24	122.05	113.80
1	S	42	PHE	CA-CB-CG	8.24	122.04	113.80
1	B	42	PHE	CA-CB-CG	8.24	122.04	113.80
1	O	42	PHE	CA-CB-CG	8.24	122.04	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	42	PHE	CA-CB-CG	8.24	122.04	113.80
2	2	134	VAL	CA-C-N	8.24	132.14	120.28
2	2	134	VAL	C-N-CA	8.24	132.14	120.28
2	K	134	VAL	CA-C-N	8.24	132.14	120.28
2	K	134	VAL	C-N-CA	8.24	132.14	120.28
1	C	42	PHE	CA-CB-CG	8.23	122.03	113.80
2	N	134	VAL	CA-C-N	8.23	132.13	120.28
2	N	134	VAL	C-N-CA	8.23	132.13	120.28
1	Q	126	TYR	CA-C-N	8.21	131.76	122.15
1	Q	126	TYR	C-N-CA	8.21	131.76	122.15
1	T	126	TYR	CA-C-N	8.20	131.75	122.15
1	T	126	TYR	C-N-CA	8.20	131.75	122.15
2	W	149	ASP	CA-CB-CG	-8.19	104.41	112.60
1	G	126	TYR	CA-C-N	8.19	131.73	122.15
1	G	126	TYR	C-N-CA	8.19	131.73	122.15
1	U	126	TYR	CA-C-N	8.19	131.73	122.15
1	U	126	TYR	C-N-CA	8.19	131.73	122.15
2	L	149	ASP	CA-CB-CG	-8.19	104.41	112.60
1	O	126	TYR	CA-C-N	8.19	131.73	122.15
1	O	126	TYR	C-N-CA	8.19	131.73	122.15
1	E	126	TYR	CA-C-N	8.19	131.73	122.15
1	E	126	TYR	C-N-CA	8.19	131.73	122.15
1	S	126	TYR	CA-C-N	8.18	131.72	122.15
1	S	126	TYR	C-N-CA	8.18	131.72	122.15
1	B	126	TYR	CA-C-N	8.18	131.72	122.15
2	N	149	ASP	CA-CB-CG	-8.18	104.42	112.60
2	V	149	ASP	CA-CB-CG	-8.18	104.42	112.60
1	B	126	TYR	C-N-CA	8.18	131.72	122.15
1	P	126	TYR	CA-C-N	8.18	131.72	122.15
1	P	126	TYR	C-N-CA	8.18	131.72	122.15
2	X	149	ASP	CA-CB-CG	-8.18	104.42	112.60
1	A	126	TYR	CA-C-N	8.17	131.71	122.15
1	A	126	TYR	C-N-CA	8.17	131.71	122.15
1	R	126	TYR	CA-C-N	8.17	131.71	122.15
1	R	126	TYR	C-N-CA	8.17	131.71	122.15
2	1	149	ASP	CA-CB-CG	-8.17	104.43	112.60
1	C	126	TYR	CA-C-N	8.17	131.71	122.15
1	C	126	TYR	C-N-CA	8.17	131.71	122.15
2	Z	149	ASP	CA-CB-CG	-8.16	104.44	112.60
2	I	149	ASP	CA-CB-CG	-8.16	104.44	112.60
2	H	149	ASP	CA-CB-CG	-8.16	104.44	112.60
2	M	149	ASP	CA-CB-CG	-8.16	104.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	149	ASP	CA-CB-CG	-8.16	104.44	112.60
2	Y	149	ASP	CA-CB-CG	-8.15	104.44	112.60
1	F	126	TYR	CA-C-N	8.15	131.68	122.15
1	F	126	TYR	C-N-CA	8.15	131.68	122.15
2	2	149	ASP	CA-CB-CG	-8.15	104.45	112.60
1	D	126	TYR	CA-C-N	8.15	131.68	122.15
1	D	126	TYR	C-N-CA	8.15	131.68	122.15
2	J	149	ASP	CA-CB-CG	-8.14	104.46	112.60
2	L	88	ASN	OD1-CG-ND2	8.07	130.67	122.60
2	W	88	ASN	OD1-CG-ND2	8.05	130.65	122.60
2	1	88	ASN	OD1-CG-ND2	8.04	130.64	122.60
2	V	88	ASN	OD1-CG-ND2	8.03	130.63	122.60
2	J	88	ASN	OD1-CG-ND2	8.04	130.63	122.60
2	Y	88	ASN	OD1-CG-ND2	8.03	130.63	122.60
1	A	209	ALA	CA-C-N	8.02	127.91	120.21
1	A	209	ALA	C-N-CA	8.02	127.91	120.21
2	Z	88	ASN	OD1-CG-ND2	8.01	130.61	122.60
2	I	88	ASN	OD1-CG-ND2	8.01	130.61	122.60
1	U	209	ALA	CA-C-N	8.01	127.90	120.21
1	U	209	ALA	C-N-CA	8.01	127.90	120.21
1	E	209	ALA	CA-C-N	8.01	127.90	120.21
1	E	209	ALA	C-N-CA	8.01	127.90	120.21
1	F	209	ALA	CA-C-N	8.00	127.89	120.21
1	F	209	ALA	C-N-CA	8.00	127.89	120.21
1	R	209	ALA	CA-C-N	8.00	127.89	120.21
1	R	209	ALA	C-N-CA	8.00	127.89	120.21
2	H	88	ASN	OD1-CG-ND2	8.00	130.60	122.60
1	S	209	ALA	CA-C-N	8.00	127.89	120.21
1	S	209	ALA	C-N-CA	8.00	127.89	120.21
1	T	209	ALA	CA-C-N	8.00	127.89	120.21
1	T	209	ALA	C-N-CA	8.00	127.89	120.21
1	B	209	ALA	CA-C-N	8.00	127.89	120.21
1	B	209	ALA	C-N-CA	8.00	127.89	120.21
1	C	209	ALA	CA-C-N	8.00	127.89	120.21
1	C	209	ALA	C-N-CA	8.00	127.89	120.21
2	M	88	ASN	OD1-CG-ND2	7.99	130.59	122.60
2	K	88	ASN	OD1-CG-ND2	7.98	130.58	122.60
1	D	209	ALA	CA-C-N	7.98	127.87	120.21
1	D	209	ALA	C-N-CA	7.98	127.87	120.21
2	X	88	ASN	OD1-CG-ND2	7.98	130.58	122.60
1	Q	209	ALA	CA-C-N	7.97	127.86	120.21
1	Q	209	ALA	C-N-CA	7.97	127.86	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	88	ASN	OD1-CG-ND2	7.97	130.57	122.60
2	2	88	ASN	OD1-CG-ND2	7.97	130.57	122.60
1	O	209	ALA	CA-C-N	7.97	127.86	120.21
1	O	209	ALA	C-N-CA	7.97	127.86	120.21
1	G	209	ALA	CA-C-N	7.96	127.85	120.21
1	G	209	ALA	C-N-CA	7.96	127.85	120.21
1	Q	58	LEU	N-CA-C	-7.95	103.37	113.23
1	P	209	ALA	CA-C-N	7.95	127.84	120.21
1	P	209	ALA	C-N-CA	7.95	127.84	120.21
1	U	58	LEU	N-CA-C	-7.94	103.38	113.23
2	M	62	GLU	O-C-N	-7.94	113.71	122.12
1	A	58	LEU	N-CA-C	-7.93	103.39	113.23
1	R	58	LEU	N-CA-C	-7.93	103.39	113.23
1	S	58	LEU	N-CA-C	-7.93	103.40	113.23
1	B	58	LEU	N-CA-C	-7.93	103.40	113.23
1	E	58	LEU	N-CA-C	-7.93	103.40	113.23
1	T	58	LEU	N-CA-C	-7.93	103.40	113.23
1	C	58	LEU	N-CA-C	-7.93	103.40	113.23
1	G	58	LEU	N-CA-C	-7.92	103.40	113.23
2	W	62	GLU	O-C-N	-7.92	113.72	122.12
2	V	62	GLU	O-C-N	-7.92	113.72	122.12
2	L	62	GLU	O-C-N	-7.92	113.72	122.12
1	D	58	LEU	N-CA-C	-7.92	103.41	113.23
1	O	58	LEU	N-CA-C	-7.91	103.42	113.23
2	X	62	GLU	O-C-N	-7.90	113.74	122.12
1	P	58	LEU	N-CA-C	-7.90	103.44	113.23
1	F	58	LEU	N-CA-C	-7.89	103.44	113.23
2	Z	62	GLU	O-C-N	-7.89	113.76	122.12
2	1	62	GLU	O-C-N	-7.89	113.76	122.12
2	I	62	GLU	O-C-N	-7.89	113.76	122.12
2	J	62	GLU	O-C-N	-7.89	113.76	122.12
2	N	62	GLU	O-C-N	-7.87	113.78	122.12
2	H	62	GLU	O-C-N	-7.86	113.79	122.12
2	Y	62	GLU	O-C-N	-7.86	113.79	122.12
2	2	62	GLU	O-C-N	-7.86	113.79	122.12
2	Y	86	MET	N-CA-C	7.85	120.53	111.11
2	K	62	GLU	O-C-N	-7.84	113.81	122.12
2	K	86	MET	N-CA-C	7.84	120.51	111.11
2	M	86	MET	N-CA-C	7.83	120.51	111.11
2	W	86	MET	N-CA-C	7.83	120.50	111.11
2	L	86	MET	N-CA-C	7.83	120.50	111.11
2	J	86	MET	N-CA-C	7.83	120.50	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	86	MET	N-CA-C	7.82	120.50	111.11
2	I	86	MET	N-CA-C	7.82	120.50	111.11
2	H	86	MET	N-CA-C	7.82	120.49	111.11
2	1	86	MET	N-CA-C	7.82	120.49	111.11
2	N	86	MET	N-CA-C	7.81	120.48	111.11
2	2	86	MET	N-CA-C	7.81	120.48	111.11
2	V	86	MET	N-CA-C	7.81	120.48	111.11
2	X	86	MET	N-CA-C	7.81	120.48	111.11
2	J	119	SER	CA-C-O	7.66	128.36	120.24
2	V	119	SER	CA-C-O	7.64	128.34	120.24
2	K	119	SER	CA-C-O	7.63	128.33	120.24
2	M	119	SER	CA-C-O	7.62	128.32	120.24
2	Z	119	SER	CA-C-O	7.62	128.32	120.24
2	1	119	SER	CA-C-O	7.62	128.32	120.24
2	I	119	SER	CA-C-O	7.62	128.32	120.24
2	L	119	SER	CA-C-O	7.62	128.31	120.24
2	N	119	SER	CA-C-O	7.61	128.30	120.24
2	X	119	SER	CA-C-O	7.61	128.30	120.24
2	2	119	SER	CA-C-O	7.60	128.30	120.24
2	N	24	ASN	O-C-N	-7.60	111.78	122.04
2	H	119	SER	CA-C-O	7.60	128.30	120.24
2	Y	119	SER	CA-C-O	7.60	128.30	120.24
2	W	119	SER	CA-C-O	7.59	128.29	120.24
2	X	24	ASN	O-C-N	-7.58	111.80	122.04
1	Q	124	THR	N-CA-C	-7.58	104.26	113.97
2	V	24	ASN	O-C-N	-7.58	111.81	122.04
1	G	124	THR	N-CA-C	-7.58	104.27	113.97
1	F	124	THR	N-CA-C	-7.58	104.27	113.97
2	H	24	ASN	O-C-N	-7.58	111.81	122.04
2	W	24	ASN	O-C-N	-7.58	111.81	122.04
2	Y	24	ASN	O-C-N	-7.58	111.81	122.04
1	R	124	THR	N-CA-C	-7.57	104.28	113.97
2	Z	24	ASN	O-C-N	-7.57	111.82	122.04
2	I	24	ASN	O-C-N	-7.57	111.82	122.04
2	L	24	ASN	O-C-N	-7.57	111.82	122.04
1	S	124	THR	N-CA-C	-7.57	104.28	113.97
1	B	124	THR	N-CA-C	-7.57	104.28	113.97
1	A	124	THR	N-CA-C	-7.57	104.28	113.97
1	E	124	THR	N-CA-C	-7.57	104.28	113.97
1	T	124	THR	N-CA-C	-7.56	104.29	113.97
1	C	124	THR	N-CA-C	-7.56	104.29	113.97
1	O	124	THR	N-CA-C	-7.56	104.29	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	24	ASN	O-C-N	-7.56	111.84	122.04
1	P	158	ASN	CA-CB-CG	-7.56	105.04	112.60
2	2	24	ASN	O-C-N	-7.56	111.84	122.04
2	K	24	ASN	O-C-N	-7.56	111.84	122.04
2	1	24	ASN	O-C-N	-7.55	111.85	122.04
1	U	124	THR	N-CA-C	-7.55	104.31	113.97
1	D	124	THR	N-CA-C	-7.55	104.31	113.97
1	C	158	ASN	CA-CB-CG	-7.55	105.05	112.60
2	J	24	ASN	O-C-N	-7.55	111.85	122.04
1	G	158	ASN	CA-CB-CG	-7.55	105.05	112.60
1	A	158	ASN	CA-CB-CG	-7.55	105.05	112.60
1	Q	158	ASN	CA-CB-CG	-7.55	105.05	112.60
1	Q	81	LEU	CA-C-N	7.54	130.33	120.60
1	Q	81	LEU	C-N-CA	7.54	130.33	120.60
1	R	158	ASN	CA-CB-CG	-7.54	105.06	112.60
2	N	165	ARG	NE-CZ-NH2	7.54	125.99	119.20
1	P	124	THR	N-CA-C	-7.54	104.32	113.97
1	P	81	LEU	CA-C-N	7.54	130.33	120.60
1	P	81	LEU	C-N-CA	7.54	130.33	120.60
1	U	158	ASN	CA-CB-CG	-7.54	105.06	112.60
1	D	158	ASN	CA-CB-CG	-7.54	105.06	112.60
1	O	81	LEU	CA-C-N	7.53	130.32	120.60
1	O	81	LEU	C-N-CA	7.53	130.32	120.60
1	S	158	ASN	CA-CB-CG	-7.53	105.07	112.60
1	F	81	LEU	CA-C-N	7.53	130.31	120.60
1	F	81	LEU	C-N-CA	7.53	130.31	120.60
1	B	158	ASN	CA-CB-CG	-7.53	105.07	112.60
1	S	81	LEU	CA-C-N	7.53	130.31	120.60
1	S	81	LEU	C-N-CA	7.53	130.31	120.60
1	U	81	LEU	CA-C-N	7.53	130.31	120.60
1	U	81	LEU	C-N-CA	7.53	130.31	120.60
1	B	81	LEU	CA-C-N	7.53	130.31	120.60
1	B	81	LEU	C-N-CA	7.53	130.31	120.60
1	F	158	ASN	CA-CB-CG	-7.53	105.07	112.60
2	H	165	ARG	NE-CZ-NH2	7.53	125.97	119.20
2	W	165	ARG	NE-CZ-NH2	7.53	125.97	119.20
1	E	81	LEU	CA-C-N	7.53	130.31	120.60
1	E	81	LEU	C-N-CA	7.53	130.31	120.60
1	D	81	LEU	CA-C-N	7.52	130.30	120.60
1	D	81	LEU	C-N-CA	7.52	130.30	120.60
2	Y	165	ARG	NE-CZ-NH2	7.52	125.97	119.20
1	T	81	LEU	CA-C-N	7.52	130.30	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	81	LEU	C-N-CA	7.52	130.30	120.60
1	G	81	LEU	CA-C-N	7.52	130.30	120.60
1	G	81	LEU	C-N-CA	7.52	130.30	120.60
1	A	81	LEU	CA-C-N	7.52	130.30	120.60
1	A	81	LEU	C-N-CA	7.52	130.30	120.60
1	C	81	LEU	CA-C-N	7.52	130.30	120.60
1	C	81	LEU	C-N-CA	7.52	130.30	120.60
1	R	81	LEU	CA-C-N	7.52	130.30	120.60
1	R	81	LEU	C-N-CA	7.52	130.30	120.60
2	L	165	ARG	NE-CZ-NH2	7.51	125.96	119.20
2	1	165	ARG	NE-CZ-NH2	7.51	125.96	119.20
2	J	165	ARG	NE-CZ-NH2	7.51	125.96	119.20
1	O	158	ASN	CA-CB-CG	-7.50	105.09	112.60
1	E	158	ASN	CA-CB-CG	-7.50	105.09	112.60
2	X	165	ARG	NE-CZ-NH2	7.50	125.95	119.20
2	Z	165	ARG	NE-CZ-NH2	7.50	125.95	119.20
2	I	165	ARG	NE-CZ-NH2	7.50	125.95	119.20
1	T	158	ASN	CA-CB-CG	-7.49	105.11	112.60
2	V	165	ARG	NE-CZ-NH2	7.49	125.94	119.20
2	M	165	ARG	NE-CZ-NH2	7.48	125.93	119.20
2	2	165	ARG	NE-CZ-NH2	7.48	125.93	119.20
2	K	165	ARG	NE-CZ-NH2	7.48	125.93	119.20
1	F	175	PHE	CA-C-N	7.27	130.03	120.28
1	F	175	PHE	C-N-CA	7.27	130.03	120.28
1	R	175	PHE	CA-C-N	7.27	130.02	120.28
1	R	175	PHE	C-N-CA	7.27	130.02	120.28
1	U	175	PHE	CA-C-N	7.26	130.01	120.28
1	U	175	PHE	C-N-CA	7.26	130.01	120.28
1	D	175	PHE	CA-C-N	7.26	130.01	120.28
1	D	175	PHE	C-N-CA	7.26	130.01	120.28
1	O	175	PHE	CA-C-N	7.25	130.00	120.28
1	O	175	PHE	C-N-CA	7.25	130.00	120.28
1	P	175	PHE	CA-C-N	7.25	130.00	120.28
1	P	175	PHE	C-N-CA	7.25	130.00	120.28
1	S	175	PHE	CA-C-N	7.25	129.99	120.28
1	S	175	PHE	C-N-CA	7.25	129.99	120.28
1	B	175	PHE	CA-C-N	7.25	129.99	120.28
1	B	175	PHE	C-N-CA	7.25	129.99	120.28
1	C	175	PHE	CA-C-N	7.24	129.98	120.28
1	C	175	PHE	C-N-CA	7.24	129.98	120.28
1	G	175	PHE	CA-C-N	7.24	129.97	120.28
1	G	175	PHE	C-N-CA	7.24	129.97	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	203	LEU	N-CA-CB	7.23	122.79	110.50
1	Q	175	PHE	CA-C-N	7.23	129.97	120.28
1	Q	175	PHE	C-N-CA	7.23	129.97	120.28
2	1	203	LEU	N-CA-CB	7.23	122.79	110.50
1	E	175	PHE	CA-C-N	7.23	129.96	120.28
1	E	175	PHE	C-N-CA	7.23	129.96	120.28
1	T	175	PHE	CA-C-N	7.22	129.96	120.28
1	T	175	PHE	C-N-CA	7.22	129.96	120.28
1	A	175	PHE	CA-C-N	7.22	129.96	120.28
1	A	175	PHE	C-N-CA	7.22	129.96	120.28
2	2	203	LEU	N-CA-CB	7.22	122.77	110.50
2	1	110	VAL	N-CA-CB	7.21	123.13	111.23
2	2	12	VAL	N-CA-C	-7.21	98.10	108.42
2	J	110	VAL	N-CA-CB	7.21	123.13	111.23
2	L	203	LEU	N-CA-CB	7.21	122.76	110.50
2	H	133	PHE	CA-CB-CG	-7.21	106.59	113.80
2	M	12	VAL	N-CA-C	-7.21	98.11	108.42
2	H	110	VAL	N-CA-CB	7.20	123.11	111.23
2	H	203	LEU	N-CA-CB	7.20	122.74	110.50
2	Z	203	LEU	N-CA-CB	7.20	122.74	110.50
2	I	203	LEU	N-CA-CB	7.20	122.74	110.50
2	Y	12	VAL	N-CA-C	-7.20	98.12	108.42
2	Y	110	VAL	N-CA-CB	7.20	123.11	111.23
2	Z	110	VAL	N-CA-CB	7.20	123.11	111.23
2	1	12	VAL	N-CA-C	-7.20	98.12	108.42
2	I	110	VAL	N-CA-CB	7.20	123.11	111.23
2	W	12	VAL	N-CA-C	-7.20	98.12	108.42
2	W	110	VAL	N-CA-CB	7.20	123.11	111.23
2	J	12	VAL	N-CA-C	-7.20	98.12	108.42
2	N	133	PHE	CA-CB-CG	-7.20	106.61	113.80
2	H	177	VAL	CA-C-O	7.20	128.92	120.72
2	W	203	LEU	N-CA-CB	7.20	122.73	110.50
2	X	133	PHE	CA-CB-CG	-7.20	106.61	113.80
2	M	177	VAL	CA-C-O	7.19	128.92	120.72
2	K	12	VAL	N-CA-C	-7.19	98.13	108.42
2	Z	12	VAL	N-CA-C	-7.19	98.13	108.42
2	1	177	VAL	CA-C-O	7.19	128.92	120.72
2	N	110	VAL	N-CA-CB	7.19	123.10	111.23
2	2	110	VAL	N-CA-CB	7.19	123.10	111.23
2	I	12	VAL	N-CA-C	-7.19	98.13	108.42
2	J	177	VAL	CA-C-O	7.19	128.92	120.72
2	L	110	VAL	N-CA-CB	7.19	123.10	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	12	VAL	N-CA-C	-7.19	98.14	108.42
2	V	203	LEU	N-CA-CB	7.19	122.72	110.50
2	J	133	PHE	CA-CB-CG	-7.19	106.61	113.80
2	X	203	LEU	N-CA-CB	7.19	122.72	110.50
2	L	12	VAL	N-CA-C	-7.19	98.14	108.42
2	K	203	LEU	N-CA-CB	7.19	122.72	110.50
2	K	110	VAL	N-CA-CB	7.19	123.09	111.23
2	N	203	LEU	N-CA-CB	7.18	122.71	110.50
2	V	110	VAL	N-CA-CB	7.18	123.08	111.23
2	X	12	VAL	N-CA-C	-7.18	98.15	108.42
2	M	203	LEU	N-CA-CB	7.18	122.71	110.50
2	Y	203	LEU	N-CA-CB	7.18	122.71	110.50
2	M	110	VAL	N-CA-CB	7.18	123.08	111.23
2	N	12	VAL	N-CA-C	-7.18	98.15	108.42
2	2	133	PHE	CA-CB-CG	-7.18	106.62	113.80
2	W	133	PHE	CA-CB-CG	-7.18	106.62	113.80
2	W	177	VAL	CA-C-O	7.18	128.90	120.72
2	2	177	VAL	CA-C-O	7.18	128.90	120.72
2	Z	177	VAL	CA-C-O	7.17	128.90	120.72
2	H	12	VAL	N-CA-C	-7.17	98.17	108.42
2	I	177	VAL	CA-C-O	7.17	128.90	120.72
2	K	133	PHE	CA-CB-CG	-7.17	106.63	113.80
2	Y	6	ILE	N-CA-C	-7.17	97.70	108.17
2	Y	133	PHE	CA-CB-CG	-7.17	106.63	113.80
2	Z	133	PHE	CA-CB-CG	-7.17	106.63	113.80
2	I	133	PHE	CA-CB-CG	-7.17	106.63	113.80
2	N	177	VAL	CA-C-O	7.17	128.89	120.72
2	X	177	VAL	CA-C-O	7.17	128.89	120.72
2	1	133	PHE	CA-CB-CG	-7.16	106.64	113.80
2	N	6	ILE	N-CA-C	-7.16	97.72	108.17
2	L	6	ILE	N-CA-C	-7.16	97.72	108.17
2	H	6	ILE	N-CA-C	-7.16	97.72	108.17
2	X	110	VAL	N-CA-CB	7.16	123.04	111.23
2	1	6	ILE	N-CA-C	-7.16	97.72	108.17
2	V	6	ILE	N-CA-C	-7.16	97.72	108.17
2	J	6	ILE	N-CA-C	-7.16	97.72	108.17
2	M	6	ILE	N-CA-C	-7.15	97.73	108.17
2	Z	6	ILE	N-CA-C	-7.15	97.73	108.17
2	I	6	ILE	N-CA-C	-7.15	97.73	108.17
2	K	177	VAL	CA-C-O	7.15	128.87	120.72
2	Y	124	TYR	N-CA-CB	7.15	122.61	111.24
2	V	133	PHE	CA-CB-CG	-7.15	106.65	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	177	VAL	CA-C-O	7.15	128.87	120.72
2	L	133	PHE	CA-CB-CG	-7.15	106.65	113.80
2	L	177	VAL	CA-C-O	7.15	128.87	120.72
2	2	6	ILE	N-CA-C	-7.15	97.73	108.17
2	K	6	ILE	N-CA-C	-7.15	97.73	108.17
2	X	6	ILE	N-CA-C	-7.14	97.74	108.17
2	X	124	TYR	N-CA-CB	7.14	122.60	111.24
2	J	124	TYR	N-CA-CB	7.14	122.59	111.24
2	W	6	ILE	N-CA-C	-7.14	97.75	108.17
2	V	124	TYR	N-CA-CB	7.14	122.59	111.24
2	M	133	PHE	CA-CB-CG	-7.14	106.66	113.80
2	2	124	TYR	N-CA-CB	7.14	122.59	111.24
2	Y	177	VAL	CA-C-O	7.14	128.85	120.72
2	L	124	TYR	N-CA-CB	7.13	122.58	111.24
2	H	124	TYR	N-CA-CB	7.13	122.57	111.24
2	Z	124	TYR	N-CA-CB	7.13	122.57	111.24
2	1	124	TYR	N-CA-CB	7.13	122.57	111.24
2	2	56	VAL	N-CA-C	7.13	117.23	110.53
2	I	124	TYR	N-CA-CB	7.13	122.57	111.24
2	K	124	TYR	N-CA-CB	7.12	122.57	111.24
2	M	124	TYR	N-CA-CB	7.12	122.56	111.24
2	W	124	TYR	N-CA-CB	7.12	122.56	111.24
2	H	56	VAL	N-CA-C	7.12	117.22	110.53
2	M	186	GLN	CB-CG-CD	-7.11	100.51	112.60
2	Y	56	VAL	N-CA-C	7.11	117.21	110.53
2	W	186	GLN	CB-CG-CD	-7.11	100.52	112.60
2	1	56	VAL	N-CA-C	7.11	117.21	110.53
2	N	124	TYR	N-CA-CB	7.11	122.54	111.24
2	J	56	VAL	N-CA-C	7.11	117.21	110.53
2	2	186	GLN	CB-CG-CD	-7.10	100.52	112.60
2	V	186	GLN	CB-CG-CD	-7.10	100.53	112.60
2	J	135	TYR	N-CA-CB	7.10	121.16	110.22
2	N	56	VAL	N-CA-C	7.10	117.20	110.53
2	J	186	GLN	CB-CG-CD	-7.10	100.53	112.60
2	K	56	VAL	N-CA-C	7.10	117.20	110.53
2	M	56	VAL	N-CA-C	7.10	117.20	110.53
2	L	135	TYR	N-CA-CB	7.10	121.15	110.22
2	Z	186	GLN	CB-CG-CD	-7.10	100.53	112.60
2	N	186	GLN	CB-CG-CD	-7.10	100.53	112.60
2	I	186	GLN	CB-CG-CD	-7.10	100.53	112.60
2	X	186	GLN	CB-CG-CD	-7.10	100.53	112.60
2	H	186	GLN	CB-CG-CD	-7.10	100.54	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	56	VAL	N-CA-C	7.10	117.20	110.53
2	K	186	GLN	CB-CG-CD	-7.09	100.54	112.60
2	L	186	GLN	CB-CG-CD	-7.09	100.54	112.60
2	X	135	TYR	N-CA-CB	7.09	121.14	110.22
2	Z	56	VAL	N-CA-C	7.09	117.19	110.53
2	I	56	VAL	N-CA-C	7.09	117.19	110.53
2	V	135	TYR	N-CA-CB	7.09	121.13	110.22
2	Y	186	GLN	CB-CG-CD	-7.09	100.55	112.60
2	M	135	TYR	N-CA-CB	7.08	121.13	110.22
2	W	135	TYR	N-CA-CB	7.08	121.13	110.22
2	1	186	GLN	CB-CG-CD	-7.08	100.56	112.60
2	1	135	TYR	N-CA-CB	7.08	121.12	110.22
2	H	135	TYR	N-CA-CB	7.08	121.12	110.22
2	Y	135	TYR	N-CA-CB	7.08	121.12	110.22
2	Z	135	TYR	N-CA-CB	7.08	121.12	110.22
2	I	135	TYR	N-CA-CB	7.08	121.12	110.22
2	V	56	VAL	N-CA-C	7.07	117.18	110.53
2	W	56	VAL	N-CA-C	7.06	117.17	110.53
2	2	135	TYR	N-CA-CB	7.05	121.08	110.22
2	X	56	VAL	N-CA-C	7.05	117.16	110.53
2	K	135	TYR	N-CA-CB	7.05	121.08	110.22
1	E	149	PHE	CA-CB-CG	-7.05	106.75	113.80
2	N	135	TYR	N-CA-CB	7.05	121.07	110.22
1	T	149	PHE	CA-CB-CG	-7.03	106.77	113.80
1	A	149	PHE	CA-CB-CG	-7.03	106.77	113.80
1	R	149	PHE	CA-CB-CG	-7.03	106.77	113.80
1	S	149	PHE	CA-CB-CG	-7.03	106.77	113.80
1	B	149	PHE	CA-CB-CG	-7.03	106.77	113.80
1	O	149	PHE	CA-CB-CG	-7.02	106.78	113.80
1	Q	222	ARG	NE-CZ-NH2	7.02	125.52	119.20
1	F	149	PHE	CA-CB-CG	-7.02	106.78	113.80
1	Q	149	PHE	CA-CB-CG	-7.01	106.79	113.80
1	C	149	PHE	CA-CB-CG	-7.01	106.79	113.80
1	P	222	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	T	222	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	U	149	PHE	CA-CB-CG	-7.00	106.80	113.80
1	P	149	PHE	CA-CB-CG	-7.00	106.80	113.80
1	C	222	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	D	149	PHE	CA-CB-CG	-7.00	106.80	113.80
1	G	149	PHE	CA-CB-CG	-7.00	106.80	113.80
1	U	222	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	D	222	ARG	NE-CZ-NH2	7.00	125.50	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	82	LEU	CA-C-N	7.00	129.53	120.44
2	2	82	LEU	C-N-CA	7.00	129.53	120.44
2	K	82	LEU	CA-C-N	7.00	129.53	120.44
2	K	82	LEU	C-N-CA	7.00	129.53	120.44
1	G	222	ARG	NE-CZ-NH2	6.99	125.49	119.20
1	F	222	ARG	NE-CZ-NH2	6.99	125.49	119.20
1	S	222	ARG	NE-CZ-NH2	6.99	125.49	119.20
1	B	222	ARG	NE-CZ-NH2	6.99	125.49	119.20
2	V	82	LEU	CA-C-N	6.98	129.51	120.44
2	V	82	LEU	C-N-CA	6.98	129.51	120.44
2	L	82	LEU	CA-C-N	6.98	129.51	120.44
2	L	82	LEU	C-N-CA	6.98	129.51	120.44
1	O	222	ARG	NE-CZ-NH2	6.97	125.48	119.20
1	E	222	ARG	NE-CZ-NH2	6.97	125.48	119.20
2	H	82	LEU	CA-C-N	6.97	129.50	120.44
2	H	82	LEU	C-N-CA	6.97	129.50	120.44
2	Z	82	LEU	CA-C-N	6.97	129.50	120.44
2	Z	82	LEU	C-N-CA	6.97	129.50	120.44
2	1	82	LEU	CA-C-N	6.97	129.50	120.44
2	1	82	LEU	C-N-CA	6.97	129.50	120.44
2	I	82	LEU	CA-C-N	6.97	129.50	120.44
2	I	82	LEU	C-N-CA	6.97	129.50	120.44
2	Y	82	LEU	CA-C-N	6.97	129.50	120.44
2	Y	82	LEU	C-N-CA	6.97	129.50	120.44
2	X	82	LEU	CA-C-N	6.96	129.49	120.44
2	X	82	LEU	C-N-CA	6.96	129.49	120.44
1	A	222	ARG	NE-CZ-NH2	6.96	125.46	119.20
1	R	222	ARG	NE-CZ-NH2	6.96	125.46	119.20
2	M	82	LEU	CA-C-N	6.96	129.48	120.44
2	M	82	LEU	C-N-CA	6.96	129.48	120.44
2	W	82	LEU	CA-C-N	6.96	129.48	120.44
2	W	82	LEU	C-N-CA	6.96	129.48	120.44
2	H	191	GLN	N-CA-C	6.95	119.70	111.71
2	Y	191	GLN	N-CA-C	6.95	119.70	111.71
2	J	82	LEU	CA-C-N	6.94	129.46	120.44
2	J	82	LEU	C-N-CA	6.94	129.46	120.44
2	N	191	GLN	N-CA-C	6.94	119.69	111.71
2	K	191	GLN	N-CA-C	6.94	119.69	111.71
2	W	191	GLN	N-CA-C	6.94	119.69	111.71
2	N	82	LEU	CA-C-N	6.93	129.45	120.44
2	N	82	LEU	C-N-CA	6.93	129.45	120.44
2	1	191	GLN	N-CA-C	6.93	119.68	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	191	GLN	N-CA-C	6.93	119.68	111.71
1	F	220	LYS	CA-C-N	6.93	130.55	120.71
1	F	220	LYS	C-N-CA	6.93	130.55	120.71
2	Z	191	GLN	N-CA-C	6.93	119.68	111.71
2	I	191	GLN	N-CA-C	6.93	119.68	111.71
1	G	220	LYS	CA-C-N	6.92	130.54	120.71
1	G	220	LYS	C-N-CA	6.92	130.54	120.71
1	A	220	LYS	CA-C-N	6.92	130.53	120.71
1	A	220	LYS	C-N-CA	6.92	130.53	120.71
2	2	191	GLN	N-CA-C	6.91	119.66	111.71
1	P	220	LYS	CA-C-N	6.91	130.52	120.71
1	P	220	LYS	C-N-CA	6.91	130.52	120.71
2	V	191	GLN	N-CA-C	6.91	119.65	111.71
1	Q	220	LYS	CA-C-N	6.91	130.51	120.71
1	Q	220	LYS	C-N-CA	6.91	130.51	120.71
2	L	191	GLN	N-CA-C	6.91	119.65	111.71
1	S	220	LYS	CA-C-N	6.90	130.51	120.71
1	S	220	LYS	C-N-CA	6.90	130.51	120.71
1	B	220	LYS	CA-C-N	6.90	130.51	120.71
1	B	220	LYS	C-N-CA	6.90	130.51	120.71
1	R	220	LYS	CA-C-N	6.90	130.51	120.71
1	R	220	LYS	C-N-CA	6.90	130.51	120.71
2	M	191	GLN	N-CA-C	6.90	119.64	111.71
1	D	220	LYS	CA-C-N	6.90	130.50	120.71
1	D	220	LYS	C-N-CA	6.90	130.50	120.71
1	T	220	LYS	CA-C-N	6.90	130.50	120.71
1	T	220	LYS	C-N-CA	6.90	130.50	120.71
2	W	177	VAL	CA-CB-CG1	6.90	122.12	110.40
2	X	191	GLN	N-CA-C	6.89	119.64	111.71
2	H	187	LEU	CA-C-O	-6.89	112.91	119.80
2	Y	187	LEU	CA-C-O	-6.89	112.91	119.80
2	M	177	VAL	CA-CB-CG1	6.89	122.11	110.40
1	E	220	LYS	CA-C-N	6.89	130.50	120.71
1	E	220	LYS	C-N-CA	6.89	130.50	120.71
1	U	220	LYS	CA-C-N	6.89	130.49	120.71
1	U	220	LYS	C-N-CA	6.89	130.49	120.71
2	X	177	VAL	CA-CB-CG1	6.89	122.11	110.40
2	V	177	VAL	CA-CB-CG1	6.89	122.11	110.40
2	L	177	VAL	CA-CB-CG1	6.89	122.11	110.40
2	2	177	VAL	CA-CB-CG1	6.88	122.11	110.40
2	2	187	LEU	CA-C-O	-6.88	112.92	119.80
2	K	177	VAL	CA-CB-CG1	6.88	122.11	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	177	VAL	CA-CB-CG1	6.88	122.10	110.40
2	J	177	VAL	CA-CB-CG1	6.88	122.09	110.40
2	Z	177	VAL	CA-CB-CG1	6.88	122.09	110.40
2	I	177	VAL	CA-CB-CG1	6.88	122.09	110.40
1	C	220	LYS	CA-C-N	6.88	130.47	120.71
1	C	220	LYS	C-N-CA	6.88	130.47	120.71
2	Z	187	LEU	CA-C-O	-6.87	112.93	119.80
2	I	187	LEU	CA-C-O	-6.87	112.93	119.80
2	K	35	PHE	CA-CB-CG	-6.87	106.93	113.80
2	H	177	VAL	CA-CB-CG1	6.86	122.06	110.40
2	Y	177	VAL	CA-CB-CG1	6.86	122.06	110.40
2	1	177	VAL	CA-CB-CG1	6.86	122.06	110.40
2	V	187	LEU	CA-C-O	-6.86	112.94	119.80
2	J	35	PHE	CA-CB-CG	-6.86	106.94	113.80
2	L	187	LEU	CA-C-O	-6.86	112.94	119.80
1	O	220	LYS	CA-C-N	6.86	130.45	120.71
1	O	220	LYS	C-N-CA	6.86	130.45	120.71
2	X	187	LEU	CA-C-O	-6.86	112.94	119.80
2	L	35	PHE	CA-CB-CG	-6.85	106.95	113.80
2	K	187	LEU	CA-C-O	-6.84	112.95	119.80
2	1	35	PHE	CA-CB-CG	-6.84	106.96	113.80
2	1	187	LEU	CA-C-O	-6.84	112.96	119.80
2	2	35	PHE	CA-CB-CG	-6.84	106.96	113.80
2	Y	35	PHE	CA-CB-CG	-6.84	106.96	113.80
1	G	77	VAL	N-CA-C	-6.84	98.27	108.46
2	J	187	LEU	CA-C-O	-6.84	112.96	119.80
2	M	187	LEU	CA-C-O	-6.83	112.97	119.80
2	N	187	LEU	CA-C-O	-6.83	112.97	119.80
2	W	187	LEU	CA-C-O	-6.83	112.97	119.80
2	Z	35	PHE	CA-CB-CG	-6.83	106.97	113.80
2	H	35	PHE	CA-CB-CG	-6.83	106.97	113.80
2	I	35	PHE	CA-CB-CG	-6.83	106.97	113.80
2	V	35	PHE	CA-CB-CG	-6.83	106.97	113.80
1	T	77	VAL	N-CA-C	-6.82	98.29	108.46
1	A	77	VAL	N-CA-C	-6.82	98.29	108.46
1	O	77	VAL	N-CA-C	-6.82	98.29	108.46
2	W	35	PHE	CA-CB-CG	-6.82	106.98	113.80
1	R	77	VAL	N-CA-C	-6.82	98.30	108.46
1	F	85	ALA	CA-C-O	-6.82	113.66	120.82
1	U	77	VAL	N-CA-C	-6.82	98.30	108.46
1	P	85	ALA	CA-C-O	-6.82	113.66	120.82
2	X	35	PHE	CA-CB-CG	-6.82	106.98	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	77	VAL	N-CA-C	-6.82	98.30	108.46
1	E	77	VAL	N-CA-C	-6.82	98.30	108.46
1	S	77	VAL	N-CA-C	-6.81	98.31	108.46
1	B	77	VAL	N-CA-C	-6.81	98.31	108.46
1	D	85	ALA	CA-C-O	-6.81	113.67	120.82
2	N	35	PHE	CA-CB-CG	-6.81	106.99	113.80
1	F	27	ALA	CA-C-N	6.81	129.40	120.28
1	F	27	ALA	C-N-CA	6.81	129.40	120.28
1	P	27	ALA	CA-C-N	6.81	129.40	120.28
1	P	27	ALA	C-N-CA	6.81	129.40	120.28
1	P	77	VAL	N-CA-C	-6.81	98.32	108.46
1	O	85	ALA	CA-C-O	-6.80	113.68	120.82
1	O	117	ALA	CA-C-N	6.80	129.40	120.28
1	O	117	ALA	C-N-CA	6.80	129.40	120.28
1	E	117	ALA	CA-C-N	6.80	129.40	120.28
1	E	117	ALA	C-N-CA	6.80	129.40	120.28
2	M	35	PHE	CA-CB-CG	-6.80	107.00	113.80
1	A	85	ALA	CA-C-O	-6.80	113.69	120.82
1	C	27	ALA	CA-C-N	6.80	129.39	120.28
1	C	27	ALA	C-N-CA	6.80	129.39	120.28
1	Q	77	VAL	N-CA-C	-6.80	98.33	108.46
1	R	85	ALA	CA-C-O	-6.80	113.69	120.82
1	R	117	ALA	CA-C-N	6.80	129.39	120.28
1	R	117	ALA	C-N-CA	6.80	129.39	120.28
1	S	85	ALA	CA-C-O	-6.79	113.69	120.82
1	G	27	ALA	CA-C-N	6.79	129.39	120.28
1	G	27	ALA	C-N-CA	6.79	129.39	120.28
1	B	85	ALA	CA-C-O	-6.79	113.69	120.82
1	G	85	ALA	CA-C-O	-6.79	113.69	120.82
1	C	117	ALA	CA-C-N	6.79	129.38	120.28
1	C	117	ALA	C-N-CA	6.79	129.38	120.28
1	A	117	ALA	CA-C-N	6.79	129.38	120.28
1	A	117	ALA	C-N-CA	6.79	129.38	120.28
1	F	117	ALA	CA-C-N	6.79	129.37	120.28
1	F	117	ALA	C-N-CA	6.79	129.37	120.28
1	G	117	ALA	CA-C-N	6.79	129.37	120.28
1	G	117	ALA	C-N-CA	6.79	129.37	120.28
1	P	117	ALA	CA-C-N	6.79	129.37	120.28
1	P	117	ALA	C-N-CA	6.79	129.37	120.28
1	C	77	VAL	N-CA-C	-6.79	98.35	108.46
1	Q	117	ALA	CA-C-N	6.79	129.37	120.28
1	Q	117	ALA	C-N-CA	6.79	129.37	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	85	ALA	CA-C-O	-6.78	113.70	120.82
1	D	117	ALA	CA-C-N	6.78	129.37	120.28
1	D	117	ALA	C-N-CA	6.78	129.37	120.28
1	S	117	ALA	CA-C-N	6.78	129.36	120.28
1	S	117	ALA	C-N-CA	6.78	129.36	120.28
1	B	117	ALA	CA-C-N	6.78	129.36	120.28
1	B	117	ALA	C-N-CA	6.78	129.36	120.28
1	F	77	VAL	N-CA-C	-6.78	98.36	108.46
1	U	117	ALA	CA-C-N	6.78	129.36	120.28
1	U	117	ALA	C-N-CA	6.78	129.36	120.28
2	2	149	ASP	CA-C-N	6.78	129.36	120.28
2	2	149	ASP	C-N-CA	6.78	129.36	120.28
1	C	85	ALA	CA-C-O	-6.78	113.70	120.82
1	E	85	ALA	CA-C-O	-6.77	113.71	120.82
1	Q	85	ALA	CA-C-O	-6.77	113.71	120.82
1	S	27	ALA	CA-C-N	6.77	129.35	120.28
1	S	27	ALA	C-N-CA	6.77	129.35	120.28
1	B	27	ALA	CA-C-N	6.77	129.35	120.28
1	B	27	ALA	C-N-CA	6.77	129.35	120.28
1	T	85	ALA	CA-C-O	-6.77	113.72	120.82
2	X	149	ASP	CA-C-N	6.77	129.35	120.28
2	X	149	ASP	C-N-CA	6.77	129.35	120.28
1	T	27	ALA	CA-C-N	6.77	129.35	120.28
1	T	27	ALA	C-N-CA	6.77	129.35	120.28
1	T	117	ALA	CA-C-N	6.77	129.35	120.28
1	T	117	ALA	C-N-CA	6.77	129.35	120.28
2	H	149	ASP	CA-C-N	6.76	129.34	120.28
2	H	149	ASP	C-N-CA	6.76	129.34	120.28
2	Y	149	ASP	CA-C-N	6.76	129.34	120.28
2	Y	149	ASP	C-N-CA	6.76	129.34	120.28
2	Z	149	ASP	CA-C-N	6.76	129.34	120.28
2	Z	149	ASP	C-N-CA	6.76	129.34	120.28
1	O	27	ALA	CA-C-N	6.76	129.34	120.28
1	O	27	ALA	C-N-CA	6.76	129.34	120.28
2	I	149	ASP	CA-C-N	6.76	129.34	120.28
2	I	149	ASP	C-N-CA	6.76	129.34	120.28
1	R	37	ALA	N-CA-C	-6.76	98.45	108.79
1	E	27	ALA	CA-C-N	6.76	129.34	120.28
1	E	27	ALA	C-N-CA	6.76	129.34	120.28
2	M	149	ASP	CA-C-N	6.76	129.33	120.28
2	M	149	ASP	C-N-CA	6.76	129.33	120.28
2	V	149	ASP	CA-C-N	6.76	129.33	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	149	ASP	C-N-CA	6.76	129.33	120.28
2	W	149	ASP	CA-C-N	6.76	129.33	120.28
2	W	149	ASP	C-N-CA	6.76	129.33	120.28
2	L	149	ASP	CA-C-N	6.76	129.33	120.28
2	L	149	ASP	C-N-CA	6.76	129.33	120.28
1	D	27	ALA	CA-C-N	6.75	129.33	120.28
1	D	27	ALA	C-N-CA	6.75	129.33	120.28
1	T	37	ALA	N-CA-C	-6.74	98.47	108.79
1	A	27	ALA	CA-C-N	6.74	129.31	120.28
1	A	27	ALA	C-N-CA	6.74	129.31	120.28
1	P	37	ALA	N-CA-C	-6.74	98.47	108.79
1	C	37	ALA	N-CA-C	-6.74	98.47	108.79
1	R	27	ALA	CA-C-N	6.74	129.31	120.28
1	R	27	ALA	C-N-CA	6.74	129.31	120.28
2	N	149	ASP	CA-C-N	6.74	129.31	120.28
2	N	149	ASP	C-N-CA	6.74	129.31	120.28
1	U	37	ALA	N-CA-C	-6.74	98.48	108.79
1	Q	27	ALA	CA-C-N	6.74	129.31	120.28
1	Q	27	ALA	C-N-CA	6.74	129.31	120.28
1	D	37	ALA	N-CA-C	-6.74	98.48	108.79
2	J	149	ASP	CA-C-N	6.74	129.31	120.28
2	J	149	ASP	C-N-CA	6.74	129.31	120.28
1	U	27	ALA	CA-C-N	6.74	129.31	120.28
1	U	27	ALA	C-N-CA	6.74	129.31	120.28
1	S	37	ALA	N-CA-C	-6.74	98.48	108.79
1	B	37	ALA	N-CA-C	-6.74	98.48	108.79
2	K	149	ASP	CA-C-N	6.74	129.31	120.28
2	K	149	ASP	C-N-CA	6.74	129.31	120.28
1	E	37	ALA	N-CA-C	-6.74	98.48	108.79
1	F	37	ALA	N-CA-C	-6.73	98.49	108.79
1	A	37	ALA	N-CA-C	-6.73	98.49	108.79
1	Q	37	ALA	N-CA-C	-6.73	98.50	108.79
1	R	115	ARG	CA-C-N	6.72	129.67	120.46
1	R	115	ARG	C-N-CA	6.72	129.67	120.46
2	1	149	ASP	CA-C-N	6.72	129.28	120.28
2	1	149	ASP	C-N-CA	6.72	129.28	120.28
1	G	37	ALA	N-CA-C	-6.72	98.51	108.79
1	O	37	ALA	N-CA-C	-6.71	98.52	108.79
1	C	115	ARG	CA-C-N	6.70	129.64	120.46
1	C	115	ARG	C-N-CA	6.70	129.64	120.46
1	A	115	ARG	CA-C-N	6.70	129.64	120.46
1	A	115	ARG	C-N-CA	6.70	129.64	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	115	ARG	CA-C-N	6.70	129.63	120.46
1	G	115	ARG	C-N-CA	6.70	129.63	120.46
1	Q	115	ARG	CA-C-N	6.70	129.63	120.46
1	Q	115	ARG	C-N-CA	6.70	129.63	120.46
1	U	115	ARG	CA-C-N	6.69	129.63	120.46
1	U	115	ARG	C-N-CA	6.69	129.63	120.46
1	D	115	ARG	CA-C-N	6.69	129.63	120.46
1	D	115	ARG	C-N-CA	6.69	129.63	120.46
1	S	115	ARG	CA-C-N	6.69	129.62	120.46
1	S	115	ARG	C-N-CA	6.69	129.62	120.46
1	B	115	ARG	CA-C-N	6.69	129.62	120.46
1	B	115	ARG	C-N-CA	6.69	129.62	120.46
1	P	115	ARG	CA-C-N	6.69	129.62	120.46
1	P	115	ARG	C-N-CA	6.69	129.62	120.46
1	O	115	ARG	CA-C-N	6.68	129.61	120.46
1	O	115	ARG	C-N-CA	6.68	129.61	120.46
1	F	115	ARG	CA-C-N	6.67	129.60	120.46
1	F	115	ARG	C-N-CA	6.67	129.60	120.46
2	M	54	VAL	CA-C-N	6.67	129.21	120.28
2	M	54	VAL	C-N-CA	6.67	129.21	120.28
1	T	115	ARG	CA-C-N	6.67	129.59	120.46
1	T	115	ARG	C-N-CA	6.67	129.59	120.46
2	W	54	VAL	CA-C-N	6.67	129.21	120.28
2	W	54	VAL	C-N-CA	6.67	129.21	120.28
2	K	54	VAL	CA-C-N	6.66	129.21	120.28
2	K	54	VAL	C-N-CA	6.66	129.21	120.28
1	Q	188	GLU	N-CA-C	-6.66	104.10	111.36
2	H	54	VAL	CA-C-N	6.66	129.21	120.28
2	H	54	VAL	C-N-CA	6.66	129.21	120.28
2	Y	54	VAL	CA-C-N	6.66	129.21	120.28
2	Y	54	VAL	C-N-CA	6.66	129.21	120.28
1	G	188	GLU	N-CA-C	-6.66	104.11	111.36
1	O	188	GLU	N-CA-C	-6.66	104.11	111.36
2	Z	54	VAL	CA-C-N	6.65	129.20	120.28
2	Z	54	VAL	C-N-CA	6.65	129.20	120.28
2	I	54	VAL	CA-C-N	6.65	129.20	120.28
2	I	54	VAL	C-N-CA	6.65	129.20	120.28
2	J	151	GLY	CA-C-N	6.65	129.57	120.46
2	J	151	GLY	C-N-CA	6.65	129.57	120.46
2	1	54	VAL	CA-C-N	6.65	129.19	120.28
2	1	54	VAL	C-N-CA	6.65	129.19	120.28
2	N	54	VAL	CA-C-N	6.65	129.19	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	54	VAL	C-N-CA	6.65	129.19	120.28
2	V	54	VAL	CA-C-N	6.65	129.19	120.28
2	V	54	VAL	C-N-CA	6.65	129.19	120.28
2	J	54	VAL	CA-C-N	6.65	129.19	120.28
2	J	54	VAL	C-N-CA	6.65	129.19	120.28
2	X	54	VAL	CA-C-N	6.65	129.19	120.28
2	X	54	VAL	C-N-CA	6.65	129.19	120.28
1	S	188	GLU	N-CA-C	-6.65	104.12	111.36
1	B	188	GLU	N-CA-C	-6.65	104.12	111.36
2	2	54	VAL	CA-C-N	6.64	129.18	120.28
2	2	54	VAL	C-N-CA	6.64	129.18	120.28
1	P	170	ASP	CA-CB-CG	-6.64	105.96	112.60
2	L	54	VAL	CA-C-N	6.64	129.18	120.28
2	L	54	VAL	C-N-CA	6.64	129.18	120.28
2	M	151	GLY	CA-C-N	6.64	129.56	120.46
2	M	151	GLY	C-N-CA	6.64	129.56	120.46
1	T	170	ASP	CA-CB-CG	-6.64	105.96	112.60
1	D	170	ASP	CA-CB-CG	-6.64	105.96	112.60
1	R	188	GLU	N-CA-C	-6.64	104.12	111.36
1	A	170	ASP	CA-CB-CG	-6.64	105.96	112.60
1	R	170	ASP	CA-CB-CG	-6.64	105.96	112.60
1	U	170	ASP	CA-CB-CG	-6.64	105.96	112.60
1	S	170	ASP	CA-CB-CG	-6.64	105.96	112.60
1	B	170	ASP	CA-CB-CG	-6.64	105.96	112.60
1	E	115	ARG	CA-C-N	6.64	129.55	120.46
1	E	115	ARG	C-N-CA	6.64	129.55	120.46
1	F	188	GLU	N-CA-C	-6.63	104.13	111.36
1	O	170	ASP	CA-CB-CG	-6.63	105.97	112.60
1	P	188	GLU	N-CA-C	-6.63	104.13	111.36
1	G	170	ASP	CA-CB-CG	-6.63	105.97	112.60
1	A	188	GLU	N-CA-C	-6.63	104.13	111.36
1	T	188	GLU	N-CA-C	-6.63	104.13	111.36
1	C	188	GLU	N-CA-C	-6.63	104.14	111.36
1	E	188	GLU	N-CA-C	-6.63	104.14	111.36
1	Q	170	ASP	CA-CB-CG	-6.63	105.97	112.60
2	Y	143	SER	N-CA-C	-6.63	98.58	108.99
2	W	151	GLY	CA-C-N	6.62	129.54	120.46
2	W	151	GLY	C-N-CA	6.62	129.54	120.46
2	H	143	SER	N-CA-C	-6.62	98.60	108.99
2	W	143	SER	N-CA-C	-6.62	98.60	108.99
2	2	143	SER	N-CA-C	-6.62	98.60	108.99
2	N	151	GLY	CA-C-N	6.62	129.53	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	151	GLY	C-N-CA	6.62	129.53	120.46
2	X	151	GLY	CA-C-N	6.62	129.53	120.46
2	X	151	GLY	C-N-CA	6.62	129.53	120.46
2	Z	151	GLY	CA-C-N	6.62	129.52	120.46
2	Z	151	GLY	C-N-CA	6.62	129.52	120.46
2	I	151	GLY	CA-C-N	6.62	129.52	120.46
2	I	151	GLY	C-N-CA	6.62	129.52	120.46
1	C	170	ASP	CA-CB-CG	-6.62	105.98	112.60
2	L	151	GLY	CA-C-N	6.61	129.52	120.46
2	L	151	GLY	C-N-CA	6.61	129.52	120.46
2	1	143	SER	N-CA-C	-6.61	98.61	108.99
2	J	143	SER	N-CA-C	-6.61	98.61	108.99
2	V	143	SER	N-CA-C	-6.61	98.61	108.99
2	L	143	SER	N-CA-C	-6.61	98.61	108.99
1	F	170	ASP	CA-CB-CG	-6.61	105.99	112.60
2	1	151	GLY	CA-C-N	6.61	129.51	120.46
2	1	151	GLY	C-N-CA	6.61	129.51	120.46
2	N	143	SER	N-CA-C	-6.61	98.61	108.99
2	X	143	SER	N-CA-C	-6.61	98.61	108.99
2	Z	143	SER	N-CA-C	-6.61	98.61	108.99
2	I	143	SER	N-CA-C	-6.61	98.61	108.99
1	E	170	ASP	CA-CB-CG	-6.61	105.99	112.60
2	M	143	SER	N-CA-C	-6.61	98.62	108.99
1	U	188	GLU	N-CA-C	-6.61	104.16	111.36
2	2	151	GLY	CA-C-N	6.61	129.51	120.46
2	2	151	GLY	C-N-CA	6.61	129.51	120.46
1	D	188	GLU	N-CA-C	-6.60	104.16	111.36
2	H	151	GLY	CA-C-N	6.60	129.50	120.46
2	H	151	GLY	C-N-CA	6.60	129.50	120.46
2	Y	151	GLY	CA-C-N	6.60	129.50	120.46
2	Y	151	GLY	C-N-CA	6.60	129.50	120.46
2	V	151	GLY	CA-C-N	6.60	129.50	120.46
2	V	151	GLY	C-N-CA	6.60	129.50	120.46
2	K	143	SER	N-CA-C	-6.59	98.64	108.99
2	K	151	GLY	CA-C-N	6.59	129.48	120.46
2	K	151	GLY	C-N-CA	6.59	129.48	120.46
1	P	62	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	G	147	ARG	CD-NE-CZ	-6.56	115.21	124.40
1	Q	147	ARG	CD-NE-CZ	-6.56	115.21	124.40
1	E	62	ASN	OD1-CG-ND2	-6.56	116.04	122.60
1	P	147	ARG	CD-NE-CZ	-6.56	115.22	124.40
1	R	147	ARG	CD-NE-CZ	-6.56	115.22	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	147	ARG	CD-NE-CZ	-6.55	115.22	124.40
1	D	147	ARG	CD-NE-CZ	-6.55	115.23	124.40
1	S	147	ARG	CD-NE-CZ	-6.55	115.23	124.40
1	T	147	ARG	CD-NE-CZ	-6.55	115.23	124.40
1	B	147	ARG	CD-NE-CZ	-6.55	115.23	124.40
1	O	147	ARG	CD-NE-CZ	-6.55	115.23	124.40
1	A	147	ARG	CD-NE-CZ	-6.54	115.24	124.40
2	L	122	ASP	N-CA-C	-6.54	99.39	109.14
1	U	147	ARG	CD-NE-CZ	-6.54	115.24	124.40
1	C	147	ARG	CD-NE-CZ	-6.54	115.24	124.40
2	Y	122	ASP	N-CA-C	-6.54	99.40	109.14
1	F	147	ARG	CD-NE-CZ	-6.53	115.25	124.40
2	X	122	ASP	N-CA-C	-6.53	99.40	109.14
2	2	122	ASP	N-CA-C	-6.53	99.41	109.14
1	Q	62	ASN	OD1-CG-ND2	-6.53	116.07	122.60
1	D	62	ASN	OD1-CG-ND2	-6.53	116.07	122.60
1	S	62	ASN	OD1-CG-ND2	-6.53	116.07	122.60
2	M	122	ASP	N-CA-C	-6.53	99.41	109.14
2	N	122	ASP	N-CA-C	-6.53	99.42	109.14
1	O	62	ASN	OD1-CG-ND2	-6.53	116.07	122.60
1	B	62	ASN	OD1-CG-ND2	-6.53	116.07	122.60
2	Z	122	ASP	N-CA-C	-6.52	99.42	109.14
2	I	122	ASP	N-CA-C	-6.52	99.42	109.14
2	1	122	ASP	N-CA-C	-6.52	99.42	109.14
2	J	122	ASP	N-CA-C	-6.52	99.42	109.14
1	A	62	ASN	OD1-CG-ND2	-6.52	116.08	122.60
2	K	122	ASP	N-CA-C	-6.52	99.43	109.14
1	R	62	ASN	OD1-CG-ND2	-6.52	116.08	122.60
2	V	122	ASP	N-CA-C	-6.52	99.43	109.14
2	W	191	GLN	CA-C-O	6.52	127.46	120.10
1	R	23	GLN	CA-C-N	6.52	129.39	120.46
1	R	23	GLN	C-N-CA	6.52	129.39	120.46
1	T	62	ASN	OD1-CG-ND2	-6.51	116.09	122.60
1	U	62	ASN	OD1-CG-ND2	-6.51	116.08	122.60
2	H	122	ASP	N-CA-C	-6.51	99.43	109.14
2	H	191	GLN	CA-C-O	6.51	127.46	120.10
1	C	23	GLN	CA-C-N	6.51	129.38	120.46
1	C	23	GLN	C-N-CA	6.51	129.38	120.46
2	W	153	ASP	CA-C-N	6.51	129.33	120.54
2	W	153	ASP	C-N-CA	6.51	129.33	120.54
1	F	62	ASN	OD1-CG-ND2	-6.51	116.09	122.60
1	G	23	GLN	CA-C-N	6.51	129.37	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	23	GLN	C-N-CA	6.51	129.37	120.46
2	N	191	GLN	CA-C-O	6.51	127.45	120.10
2	J	153	ASP	CA-C-N	6.51	129.32	120.54
2	J	153	ASP	C-N-CA	6.51	129.32	120.54
1	D	23	GLN	CA-C-N	6.51	129.37	120.46
1	D	23	GLN	C-N-CA	6.51	129.37	120.46
2	K	191	GLN	CA-C-O	6.51	127.45	120.10
2	Y	191	GLN	CA-C-O	6.50	127.45	120.10
2	L	153	ASP	CA-C-N	6.50	129.32	120.54
2	L	153	ASP	C-N-CA	6.50	129.32	120.54
2	W	122	ASP	N-CA-C	-6.50	99.45	109.14
1	S	23	GLN	CA-C-N	6.50	129.37	120.46
1	S	23	GLN	C-N-CA	6.50	129.37	120.46
2	V	153	ASP	CA-C-N	6.50	129.32	120.54
2	V	153	ASP	C-N-CA	6.50	129.32	120.54
1	B	23	GLN	CA-C-N	6.50	129.37	120.46
1	B	23	GLN	C-N-CA	6.50	129.37	120.46
2	Z	191	GLN	CA-C-O	6.50	127.44	120.10
1	F	23	GLN	CA-C-N	6.50	129.36	120.46
1	F	23	GLN	C-N-CA	6.50	129.36	120.46
2	1	191	GLN	CA-C-O	6.50	127.44	120.10
2	2	153	ASP	CA-C-N	6.50	129.31	120.54
2	2	153	ASP	C-N-CA	6.50	129.31	120.54
2	I	191	GLN	CA-C-O	6.50	127.44	120.10
2	J	191	GLN	CA-C-O	6.50	127.44	120.10
1	A	23	GLN	CA-C-N	6.50	129.36	120.46
1	A	23	GLN	C-N-CA	6.50	129.36	120.46
1	E	23	GLN	CA-C-N	6.50	129.36	120.46
1	E	23	GLN	C-N-CA	6.50	129.36	120.46
2	N	153	ASP	CA-C-N	6.49	129.31	120.54
2	N	153	ASP	C-N-CA	6.49	129.31	120.54
2	Z	153	ASP	CA-C-N	6.49	129.30	120.54
2	Z	153	ASP	C-N-CA	6.49	129.30	120.54
1	T	23	GLN	CA-C-N	6.49	129.35	120.46
1	T	23	GLN	C-N-CA	6.49	129.35	120.46
1	U	23	GLN	CA-C-N	6.49	129.35	120.46
1	U	23	GLN	C-N-CA	6.49	129.35	120.46
2	H	153	ASP	CA-C-N	6.49	129.30	120.54
2	H	153	ASP	C-N-CA	6.49	129.30	120.54
2	I	153	ASP	CA-C-N	6.49	129.30	120.54
2	I	153	ASP	C-N-CA	6.49	129.30	120.54
2	Y	153	ASP	CA-C-N	6.49	129.30	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	153	ASP	C-N-CA	6.49	129.30	120.54
1	G	62	ASN	OD1-CG-ND2	-6.49	116.11	122.60
1	O	23	GLN	CA-C-N	6.48	129.34	120.46
1	O	23	GLN	C-N-CA	6.48	129.34	120.46
2	K	153	ASP	CA-C-N	6.48	129.29	120.54
2	K	153	ASP	C-N-CA	6.48	129.29	120.54
1	Q	23	GLN	CA-C-N	6.48	129.34	120.46
1	Q	23	GLN	C-N-CA	6.48	129.34	120.46
2	1	153	ASP	CA-C-N	6.48	129.29	120.54
2	1	153	ASP	C-N-CA	6.48	129.29	120.54
2	M	153	ASP	CA-C-N	6.48	129.28	120.54
2	M	153	ASP	C-N-CA	6.48	129.28	120.54
2	2	191	GLN	CA-C-O	6.48	127.42	120.10
2	X	191	GLN	CA-C-O	6.47	127.42	120.10
2	2	28	HIS	ND1-CE1-NE2	6.47	114.87	108.40
1	C	62	ASN	OD1-CG-ND2	-6.47	116.13	122.60
2	H	28	HIS	ND1-CE1-NE2	6.47	114.87	108.40
2	X	153	ASP	CA-C-N	6.47	129.27	120.54
2	X	153	ASP	C-N-CA	6.47	129.27	120.54
2	Y	28	HIS	ND1-CE1-NE2	6.47	114.87	108.40
2	N	28	HIS	ND1-CE1-NE2	6.47	114.87	108.40
2	V	191	GLN	CA-C-O	6.46	127.40	120.10
2	W	28	HIS	ND1-CE1-NE2	6.46	114.86	108.40
2	L	191	GLN	CA-C-O	6.46	127.40	120.10
2	M	191	GLN	CA-C-O	6.45	127.39	120.10
2	L	28	HIS	ND1-CE1-NE2	6.45	114.85	108.40
1	P	23	GLN	CA-C-N	6.45	129.30	120.46
1	P	23	GLN	C-N-CA	6.45	129.30	120.46
2	J	28	HIS	ND1-CE1-NE2	6.44	114.84	108.40
2	1	28	HIS	ND1-CE1-NE2	6.44	114.84	108.40
1	E	161	LYS	N-CA-C	-6.43	106.01	114.31
2	Z	28	HIS	ND1-CE1-NE2	6.43	114.83	108.40
1	A	161	LYS	N-CA-C	-6.43	106.01	114.31
2	I	28	HIS	ND1-CE1-NE2	6.43	114.83	108.40
2	M	28	HIS	ND1-CE1-NE2	6.43	114.83	108.40
1	G	154	ALA	N-CA-C	-6.43	105.48	113.38
2	X	28	HIS	ND1-CE1-NE2	6.42	114.82	108.40
1	F	154	ALA	N-CA-C	-6.42	105.48	113.38
1	T	161	LYS	N-CA-C	-6.42	106.03	114.31
1	U	154	ALA	N-CA-C	-6.42	105.49	113.38
1	Q	161	LYS	N-CA-C	-6.42	106.03	114.31
1	D	154	ALA	N-CA-C	-6.42	105.49	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	28	HIS	ND1-CE1-NE2	6.42	114.81	108.40
1	S	154	ALA	N-CA-C	-6.41	105.50	113.38
1	S	161	LYS	N-CA-C	-6.41	106.05	114.31
1	O	154	ALA	N-CA-C	-6.41	105.50	113.38
1	B	154	ALA	N-CA-C	-6.41	105.50	113.38
1	B	161	LYS	N-CA-C	-6.41	106.05	114.31
1	G	161	LYS	N-CA-C	-6.40	106.05	114.31
1	T	154	ALA	N-CA-C	-6.40	105.50	113.38
1	C	154	ALA	N-CA-C	-6.40	105.50	113.38
1	C	161	LYS	N-CA-C	-6.40	106.05	114.31
2	K	28	HIS	ND1-CE1-NE2	6.40	114.80	108.40
1	F	161	LYS	N-CA-C	-6.40	106.06	114.31
2	N	45	ILE	CA-C-O	-6.40	113.43	120.72
1	A	154	ALA	N-CA-C	-6.40	105.51	113.38
1	R	154	ALA	N-CA-C	-6.40	105.51	113.38
1	Q	154	ALA	N-CA-C	-6.40	105.51	113.38
1	O	161	LYS	N-CA-C	-6.39	106.06	114.31
1	P	161	LYS	N-CA-C	-6.39	106.06	114.31
1	R	161	LYS	N-CA-C	-6.39	106.06	114.31
1	U	161	LYS	N-CA-C	-6.39	106.06	114.31
1	D	161	LYS	N-CA-C	-6.39	106.06	114.31
1	E	154	ALA	N-CA-C	-6.39	105.52	113.38
1	P	154	ALA	N-CA-C	-6.39	105.52	113.38
2	M	45	ILE	CA-C-O	-6.38	113.44	120.72
1	Q	166	GLY	CA-C-N	6.38	128.73	120.44
1	Q	166	GLY	C-N-CA	6.38	128.73	120.44
2	X	45	ILE	CA-C-O	-6.38	113.45	120.72
2	1	45	ILE	CA-C-O	-6.37	113.46	120.72
2	J	45	ILE	CA-C-O	-6.37	113.46	120.72
1	U	166	GLY	CA-C-N	6.37	128.72	120.44
1	U	166	GLY	C-N-CA	6.37	128.72	120.44
1	P	166	GLY	CA-C-N	6.37	128.72	120.44
1	P	166	GLY	C-N-CA	6.37	128.72	120.44
1	E	166	GLY	CA-C-N	6.37	128.72	120.44
1	E	166	GLY	C-N-CA	6.37	128.72	120.44
1	G	166	GLY	CA-C-N	6.36	128.71	120.44
1	G	166	GLY	C-N-CA	6.36	128.71	120.44
2	V	45	ILE	CA-C-O	-6.36	113.47	120.72
2	Z	45	ILE	CA-C-O	-6.36	113.47	120.72
2	I	45	ILE	CA-C-O	-6.36	113.47	120.72
1	F	166	GLY	CA-C-N	6.36	128.70	120.44
1	F	166	GLY	C-N-CA	6.36	128.70	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	166	GLY	CA-C-N	6.36	128.71	120.44
1	T	166	GLY	C-N-CA	6.36	128.71	120.44
1	S	166	GLY	CA-C-N	6.36	128.70	120.44
1	S	166	GLY	C-N-CA	6.36	128.70	120.44
1	B	166	GLY	CA-C-N	6.36	128.70	120.44
1	B	166	GLY	C-N-CA	6.36	128.70	120.44
2	V	62	GLU	N-CA-C	6.35	119.02	111.33
1	R	92	ALA	N-CA-C	6.35	118.20	111.28
2	W	45	ILE	CA-C-O	-6.35	113.48	120.72
2	W	62	GLU	N-CA-C	6.35	119.01	111.33
1	C	166	GLY	CA-C-N	6.35	128.69	120.44
1	C	166	GLY	C-N-CA	6.35	128.69	120.44
1	D	166	GLY	CA-C-N	6.35	128.69	120.44
1	D	166	GLY	C-N-CA	6.35	128.69	120.44
2	L	45	ILE	CA-C-O	-6.35	113.48	120.72
2	Y	45	ILE	CA-C-O	-6.35	113.48	120.72
1	E	92	ALA	N-CA-C	6.34	118.20	111.28
1	A	166	GLY	CA-C-N	6.34	128.69	120.44
1	A	166	GLY	C-N-CA	6.34	128.69	120.44
1	R	166	GLY	CA-C-N	6.34	128.69	120.44
1	R	166	GLY	C-N-CA	6.34	128.69	120.44
2	N	62	GLU	N-CA-C	6.34	119.00	111.33
1	O	166	GLY	CA-C-N	6.34	128.68	120.44
1	O	166	GLY	C-N-CA	6.34	128.68	120.44
2	Z	62	GLU	N-CA-C	6.33	118.99	111.33
2	I	62	GLU	N-CA-C	6.33	118.99	111.33
2	2	62	GLU	N-CA-C	6.33	118.99	111.33
1	A	92	ALA	N-CA-C	6.33	118.18	111.28
2	H	45	ILE	CA-C-O	-6.33	113.50	120.72
1	C	92	ALA	N-CA-C	6.33	118.18	111.28
2	X	62	GLU	N-CA-C	6.33	118.99	111.33
2	K	62	GLU	N-CA-C	6.33	118.99	111.33
1	F	92	ALA	N-CA-C	6.33	118.18	111.28
2	K	45	ILE	CA-C-O	-6.33	113.50	120.72
1	T	92	ALA	N-CA-C	6.33	118.18	111.28
2	1	62	GLU	N-CA-C	6.33	118.99	111.33
2	2	45	ILE	CA-C-O	-6.33	113.51	120.72
1	U	92	ALA	N-CA-C	6.33	118.17	111.28
2	Y	62	GLU	N-CA-C	6.32	118.98	111.33
1	Q	92	ALA	N-CA-C	6.32	118.17	111.28
1	S	92	ALA	N-CA-C	6.32	118.17	111.28
2	M	62	GLU	N-CA-C	6.32	118.97	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	ALA	N-CA-C	6.32	118.17	111.28
1	P	92	ALA	N-CA-C	6.31	118.16	111.28
1	O	92	ALA	N-CA-C	6.31	118.16	111.28
1	G	92	ALA	N-CA-C	6.31	118.16	111.28
2	L	62	GLU	N-CA-C	6.30	118.96	111.33
1	D	92	ALA	N-CA-C	6.30	118.15	111.28
2	H	62	GLU	N-CA-C	6.29	118.95	111.33
1	C	223	ILE	N-CA-C	-6.29	99.36	108.36
1	T	223	ILE	N-CA-C	-6.29	99.37	108.36
2	J	62	GLU	N-CA-C	6.29	118.94	111.33
1	D	223	ILE	N-CA-C	-6.28	99.38	108.36
1	S	223	ILE	N-CA-C	-6.28	99.38	108.36
1	F	223	ILE	N-CA-C	-6.28	99.38	108.36
1	A	223	ILE	N-CA-C	-6.28	99.38	108.36
1	B	223	ILE	N-CA-C	-6.28	99.38	108.36
1	P	223	ILE	N-CA-C	-6.28	99.38	108.36
1	R	223	ILE	N-CA-C	-6.28	99.38	108.36
1	O	223	ILE	N-CA-C	-6.28	99.39	108.36
1	G	223	ILE	N-CA-C	-6.27	99.39	108.36
1	Q	223	ILE	N-CA-C	-6.27	99.39	108.36
1	U	223	ILE	N-CA-C	-6.27	99.39	108.36
1	E	223	ILE	N-CA-C	-6.27	99.39	108.36
1	U	117	ALA	N-CA-C	6.26	118.10	111.28
1	T	117	ALA	N-CA-C	6.26	118.10	111.28
1	C	117	ALA	N-CA-C	6.26	118.10	111.28
1	D	117	ALA	N-CA-C	6.24	118.08	111.28
2	1	23	GLU	N-CA-CB	6.24	121.04	110.49
2	V	23	GLU	N-CA-CB	6.24	121.04	110.49
2	Y	23	GLU	N-CA-CB	6.24	121.04	110.49
2	2	23	GLU	N-CA-CB	6.24	121.03	110.49
1	P	117	ALA	N-CA-C	6.24	118.08	111.28
2	J	23	GLU	N-CA-CB	6.24	121.03	110.49
2	L	23	GLU	N-CA-CB	6.24	121.03	110.49
1	F	117	ALA	N-CA-C	6.23	118.07	111.28
1	P	188	GLU	O-C-N	6.23	129.26	122.15
2	V	131	SER	CA-C-N	6.23	125.72	119.24
2	V	131	SER	C-N-CA	6.23	125.72	119.24
1	O	117	ALA	N-CA-C	6.23	118.07	111.28
1	E	117	ALA	N-CA-C	6.23	118.07	111.28
2	W	131	SER	CA-C-N	6.23	125.72	119.24
2	W	131	SER	C-N-CA	6.23	125.72	119.24
2	Z	23	GLU	N-CA-CB	6.22	121.01	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	144	GLU	CA-C-N	6.22	132.31	122.60
2	N	144	GLU	C-N-CA	6.22	132.31	122.60
2	I	23	GLU	N-CA-CB	6.22	121.01	110.49
1	E	188	GLU	O-C-N	6.22	129.24	122.15
1	S	117	ALA	N-CA-C	6.22	118.06	111.28
1	B	117	ALA	N-CA-C	6.22	118.06	111.28
2	L	131	SER	CA-C-N	6.22	125.71	119.24
2	L	131	SER	C-N-CA	6.22	125.71	119.24
1	S	188	GLU	O-C-N	6.22	129.24	122.15
2	M	23	GLU	N-CA-CB	6.22	121.00	110.49
1	G	117	ALA	N-CA-C	6.22	118.06	111.28
1	G	188	GLU	O-C-N	6.22	129.24	122.15
1	A	117	ALA	N-CA-C	6.22	118.06	111.28
2	H	23	GLU	N-CA-CB	6.22	121.00	110.49
1	B	188	GLU	O-C-N	6.22	129.24	122.15
1	Q	117	ALA	N-CA-C	6.22	118.06	111.28
1	R	117	ALA	N-CA-C	6.22	118.06	111.28
1	T	188	GLU	O-C-N	6.21	129.23	122.15
1	C	188	GLU	O-C-N	6.21	129.23	122.15
2	J	144	GLU	CA-C-N	6.21	132.29	122.60
2	J	144	GLU	C-N-CA	6.21	132.29	122.60
2	K	23	GLU	N-CA-CB	6.21	120.99	110.49
1	T	64	ILE	N-CA-C	-6.21	98.04	107.73
2	N	23	GLU	N-CA-CB	6.21	120.99	110.49
2	H	144	GLU	CA-C-N	6.21	132.29	122.60
2	H	144	GLU	C-N-CA	6.21	132.29	122.60
2	W	23	GLU	N-CA-CB	6.21	120.99	110.49
2	X	23	GLU	N-CA-CB	6.21	120.99	110.49
2	V	144	GLU	CA-C-N	6.21	132.29	122.60
2	V	144	GLU	C-N-CA	6.21	132.29	122.60
2	Z	144	GLU	CA-C-N	6.21	132.29	122.60
2	Z	144	GLU	C-N-CA	6.21	132.29	122.60
2	M	144	GLU	CA-C-N	6.21	132.28	122.60
2	M	144	GLU	C-N-CA	6.21	132.28	122.60
1	G	64	ILE	N-CA-C	-6.21	98.05	107.73
2	I	144	GLU	CA-C-N	6.21	132.29	122.60
2	I	144	GLU	C-N-CA	6.21	132.29	122.60
2	X	144	GLU	CA-C-N	6.21	132.28	122.60
2	X	144	GLU	C-N-CA	6.21	132.28	122.60
2	L	144	GLU	CA-C-N	6.21	132.28	122.60
2	L	144	GLU	C-N-CA	6.21	132.28	122.60
2	K	131	SER	CA-C-N	6.20	125.69	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	131	SER	C-N-CA	6.20	125.69	119.24
2	Y	144	GLU	CA-C-N	6.20	132.28	122.60
2	Y	144	GLU	C-N-CA	6.20	132.28	122.60
1	E	64	ILE	N-CA-C	-6.20	98.05	107.73
2	W	144	GLU	CA-C-N	6.20	132.28	122.60
2	W	144	GLU	C-N-CA	6.20	132.28	122.60
2	1	144	GLU	CA-C-N	6.20	132.27	122.60
2	1	144	GLU	C-N-CA	6.20	132.27	122.60
2	2	144	GLU	CA-C-N	6.20	132.27	122.60
2	2	144	GLU	C-N-CA	6.20	132.27	122.60
1	A	188	GLU	O-C-N	6.20	129.22	122.15
2	K	144	GLU	CA-C-N	6.20	132.27	122.60
2	K	144	GLU	C-N-CA	6.20	132.27	122.60
1	R	89	VAL	N-CA-CB	6.20	118.50	110.57
2	L	110	VAL	CA-CB-CG1	6.20	120.94	110.40
2	Y	110	VAL	CA-CB-CG1	6.20	120.93	110.40
2	Z	131	SER	CA-C-N	6.19	125.68	119.24
2	Z	131	SER	C-N-CA	6.19	125.68	119.24
2	I	131	SER	CA-C-N	6.19	125.68	119.24
2	I	131	SER	C-N-CA	6.19	125.68	119.24
2	N	131	SER	CA-C-N	6.19	125.68	119.24
2	N	131	SER	C-N-CA	6.19	125.68	119.24
1	D	89	VAL	N-CA-CB	6.19	118.50	110.57
1	R	188	GLU	O-C-N	6.19	129.21	122.15
2	1	131	SER	CA-C-N	6.19	125.68	119.24
2	1	131	SER	C-N-CA	6.19	125.68	119.24
2	2	110	VAL	CA-CB-CG1	6.19	120.92	110.40
1	C	64	ILE	N-CA-C	-6.19	98.07	107.73
2	J	131	SER	CA-C-N	6.19	125.68	119.24
2	J	131	SER	C-N-CA	6.19	125.68	119.24
2	W	110	VAL	CA-CB-CG1	6.19	120.92	110.40
1	Q	64	ILE	N-CA-C	-6.19	98.08	107.73
2	Y	131	SER	CA-C-N	6.19	125.67	119.24
2	Y	131	SER	C-N-CA	6.19	125.67	119.24
2	Z	110	VAL	CA-CB-CG1	6.19	120.92	110.40
1	U	188	GLU	O-C-N	6.19	129.20	122.15
2	I	110	VAL	CA-CB-CG1	6.19	120.92	110.40
1	D	188	GLU	O-C-N	6.19	129.20	122.15
1	Q	188	GLU	O-C-N	6.18	129.20	122.15
1	F	64	ILE	N-CA-C	-6.18	98.08	107.73
1	O	188	GLU	O-C-N	6.18	129.20	122.15
1	T	89	VAL	N-CA-CB	6.18	118.48	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	110	VAL	CA-CB-CG1	6.18	120.91	110.40
2	V	110	VAL	CA-CB-CG1	6.18	120.91	110.40
1	C	89	VAL	N-CA-CB	6.18	118.48	110.57
2	J	110	VAL	CA-CB-CG1	6.18	120.91	110.40
2	H	110	VAL	CA-CB-CG1	6.18	120.90	110.40
1	O	64	ILE	N-CA-C	-6.18	98.09	107.73
2	X	110	VAL	CA-CB-CG1	6.18	120.91	110.40
2	M	110	VAL	CA-CB-CG1	6.18	120.90	110.40
2	V	158	ALA	O-C-N	-6.18	115.47	122.08
2	L	158	ALA	O-C-N	-6.18	115.47	122.08
1	S	64	ILE	N-CA-C	-6.18	98.10	107.73
1	B	64	ILE	N-CA-C	-6.18	98.10	107.73
2	K	110	VAL	CA-CB-CG1	6.18	120.90	110.40
1	P	89	VAL	N-CA-CB	6.17	118.47	110.57
2	K	158	ALA	O-C-N	-6.17	115.47	122.08
1	O	89	VAL	N-CA-CB	6.17	118.47	110.57
1	A	89	VAL	N-CA-CB	6.17	118.47	110.57
1	P	64	ILE	N-CA-C	-6.17	98.11	107.73
1	S	89	VAL	N-CA-CB	6.17	118.47	110.57
2	M	131	SER	CA-C-N	6.17	125.66	119.24
2	M	131	SER	C-N-CA	6.17	125.66	119.24
1	B	89	VAL	N-CA-CB	6.17	118.47	110.57
1	D	64	ILE	N-CA-C	-6.17	98.11	107.73
1	R	64	ILE	N-CA-C	-6.17	98.11	107.73
1	G	89	VAL	N-CA-CB	6.17	118.46	110.57
1	U	64	ILE	N-CA-C	-6.17	98.11	107.73
2	X	131	SER	CA-C-N	6.17	125.65	119.24
2	X	131	SER	C-N-CA	6.17	125.65	119.24
1	E	89	VAL	N-CA-CB	6.17	118.46	110.57
1	Q	89	VAL	N-CA-CB	6.17	118.46	110.57
1	F	188	GLU	O-C-N	6.16	129.18	122.15
2	N	110	VAL	CA-CB-CG1	6.16	120.88	110.40
1	U	89	VAL	N-CA-CB	6.16	118.46	110.57
2	H	131	SER	CA-C-N	6.16	125.65	119.24
2	H	131	SER	C-N-CA	6.16	125.65	119.24
1	F	89	VAL	N-CA-CB	6.16	118.45	110.57
2	J	158	ALA	O-C-N	-6.16	115.49	122.08
1	G	185	PRO	N-CA-CB	6.15	109.05	103.33
2	2	131	SER	CA-C-N	6.15	125.64	119.24
2	2	131	SER	C-N-CA	6.15	125.64	119.24
1	A	64	ILE	N-CA-C	-6.15	98.13	107.73
2	M	158	ALA	O-C-N	-6.14	115.51	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	158	ALA	O-C-N	-6.14	115.51	122.08
2	Y	158	ALA	O-C-N	-6.14	115.51	122.08
2	Z	158	ALA	O-C-N	-6.14	115.51	122.08
2	I	158	ALA	O-C-N	-6.14	115.51	122.08
1	U	224	TYR	CA-CB-CG	6.14	124.95	113.90
1	P	185	PRO	N-CA-CB	6.14	109.04	103.33
2	1	158	ALA	O-C-N	-6.13	115.52	122.08
1	D	185	PRO	N-CA-CB	6.13	109.03	103.33
1	C	224	TYR	CA-CB-CG	6.13	124.94	113.90
1	Q	185	PRO	N-CA-CB	6.13	109.03	103.33
1	D	224	TYR	CA-CB-CG	6.13	124.94	113.90
2	N	158	ALA	O-C-N	-6.13	115.52	122.08
1	O	224	TYR	CA-CB-CG	6.13	124.93	113.90
2	X	158	ALA	O-C-N	-6.13	115.52	122.08
1	S	224	TYR	CA-CB-CG	6.13	124.93	113.90
1	T	185	PRO	N-CA-CB	6.13	109.03	103.33
1	B	224	TYR	CA-CB-CG	6.13	124.93	113.90
1	R	123	TYR	CA-C-N	6.13	132.16	122.11
1	R	123	TYR	C-N-CA	6.13	132.16	122.11
1	F	224	TYR	CA-CB-CG	6.12	124.92	113.90
1	G	224	TYR	CA-CB-CG	6.12	124.92	113.90
1	P	224	TYR	CA-CB-CG	6.12	124.92	113.90
1	Q	224	TYR	CA-CB-CG	6.12	124.92	113.90
1	T	224	TYR	CA-CB-CG	6.12	124.92	113.90
1	C	185	PRO	N-CA-CB	6.12	109.03	103.33
1	A	224	TYR	CA-CB-CG	6.12	124.92	113.90
1	R	224	TYR	CA-CB-CG	6.12	124.92	113.90
1	F	123	TYR	CA-C-N	6.12	132.15	122.11
1	F	123	TYR	C-N-CA	6.12	132.15	122.11
1	E	123	TYR	CA-C-N	6.12	132.14	122.11
1	E	123	TYR	C-N-CA	6.12	132.14	122.11
1	E	224	TYR	CA-CB-CG	6.12	124.91	113.90
1	S	123	TYR	CA-C-N	6.11	132.14	122.11
1	S	123	TYR	C-N-CA	6.11	132.14	122.11
1	T	123	TYR	CA-C-N	6.11	132.13	122.11
1	T	123	TYR	C-N-CA	6.11	132.13	122.11
1	B	123	TYR	CA-C-N	6.11	132.14	122.11
1	B	123	TYR	C-N-CA	6.11	132.14	122.11
1	P	123	TYR	CA-C-N	6.11	132.14	122.11
1	P	123	TYR	C-N-CA	6.11	132.14	122.11
1	C	123	TYR	CA-C-N	6.11	132.13	122.11
1	C	123	TYR	C-N-CA	6.11	132.13	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	176	LEU	CA-C-O	-6.11	114.07	120.55
1	U	123	TYR	CA-C-N	6.11	132.13	122.11
1	U	123	TYR	C-N-CA	6.11	132.13	122.11
1	G	123	TYR	CA-C-N	6.11	132.13	122.11
1	G	123	TYR	C-N-CA	6.11	132.13	122.11
1	U	185	PRO	N-CA-CB	6.11	109.01	103.33
1	Q	123	TYR	CA-C-N	6.11	132.13	122.11
1	Q	123	TYR	C-N-CA	6.11	132.13	122.11
1	O	185	PRO	N-CA-CB	6.11	109.01	103.33
1	D	123	TYR	CA-C-N	6.11	132.13	122.11
1	D	123	TYR	C-N-CA	6.11	132.13	122.11
1	E	185	PRO	N-CA-CB	6.11	109.01	103.33
2	2	158	ALA	O-C-N	-6.11	115.55	122.08
1	A	123	TYR	CA-C-N	6.11	132.13	122.11
1	A	123	TYR	C-N-CA	6.11	132.13	122.11
1	C	176	LEU	CA-C-O	-6.11	114.08	120.55
1	S	185	PRO	N-CA-CB	6.11	109.01	103.33
1	A	185	PRO	N-CA-CB	6.11	109.01	103.33
1	B	185	PRO	N-CA-CB	6.11	109.01	103.33
1	R	185	PRO	N-CA-CB	6.11	109.01	103.33
1	O	123	TYR	CA-C-N	6.10	132.11	122.11
1	O	123	TYR	C-N-CA	6.10	132.11	122.11
1	A	176	LEU	CA-C-O	-6.10	114.09	120.55
1	P	176	LEU	CA-C-O	-6.10	114.09	120.55
1	R	225	ASP	CA-C-N	6.09	129.96	120.82
1	R	225	ASP	C-N-CA	6.09	129.96	120.82
1	T	225	ASP	CA-C-N	6.09	129.96	120.82
1	T	225	ASP	C-N-CA	6.09	129.96	120.82
1	C	225	ASP	CA-C-N	6.09	129.96	120.82
1	C	225	ASP	C-N-CA	6.09	129.96	120.82
2	H	158	ALA	O-C-N	-6.09	115.56	122.08
1	E	225	ASP	CA-C-N	6.09	129.96	120.82
1	E	225	ASP	C-N-CA	6.09	129.96	120.82
1	F	185	PRO	N-CA-CB	6.09	108.99	103.33
1	O	176	LEU	CA-C-O	-6.09	114.10	120.55
1	P	225	ASP	CA-C-N	6.08	129.94	120.82
1	P	225	ASP	C-N-CA	6.08	129.94	120.82
2	1	134	VAL	N-CA-C	-6.08	104.58	110.72
2	L	134	VAL	N-CA-C	-6.08	104.58	110.72
1	S	176	LEU	CA-C-O	-6.08	114.11	120.55
1	T	176	LEU	CA-C-O	-6.08	114.11	120.55
1	B	176	LEU	CA-C-O	-6.08	114.11	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	134	VAL	N-CA-C	-6.07	104.59	110.72
1	D	225	ASP	CA-C-N	6.07	129.93	120.82
1	D	225	ASP	C-N-CA	6.07	129.93	120.82
1	E	176	LEU	CA-C-O	-6.07	114.12	120.55
1	S	225	ASP	CA-C-N	6.07	129.92	120.82
1	S	225	ASP	C-N-CA	6.07	129.92	120.82
1	F	225	ASP	CA-C-N	6.07	129.92	120.82
1	F	225	ASP	C-N-CA	6.07	129.92	120.82
1	B	225	ASP	CA-C-N	6.07	129.92	120.82
1	B	225	ASP	C-N-CA	6.07	129.92	120.82
1	G	225	ASP	CA-C-N	6.07	129.92	120.82
1	G	225	ASP	C-N-CA	6.07	129.92	120.82
1	R	176	LEU	CA-C-O	-6.07	114.12	120.55
1	U	225	ASP	CA-C-N	6.07	129.92	120.82
1	U	225	ASP	C-N-CA	6.07	129.92	120.82
1	C	91	PHE	CA-C-O	6.07	127.19	120.82
1	Q	176	LEU	CA-C-O	-6.07	114.12	120.55
1	Q	225	ASP	CA-C-N	6.07	129.92	120.82
1	Q	225	ASP	C-N-CA	6.07	129.92	120.82
1	A	225	ASP	CA-C-N	6.06	129.91	120.82
1	A	225	ASP	C-N-CA	6.06	129.91	120.82
1	D	91	PHE	CA-C-O	6.06	127.18	120.82
1	D	176	LEU	CA-C-O	-6.06	114.13	120.55
1	F	176	LEU	CA-C-O	-6.05	114.13	120.55
1	A	91	PHE	CA-C-O	6.05	127.18	120.82
1	O	225	ASP	CA-C-N	6.05	129.90	120.82
1	O	225	ASP	C-N-CA	6.05	129.90	120.82
2	N	134	VAL	N-CA-C	-6.05	104.61	110.72
2	M	134	VAL	N-CA-C	-6.05	104.61	110.72
2	W	134	VAL	N-CA-C	-6.05	104.61	110.72
1	D	84	ASP	CA-CB-CG	-6.05	106.55	112.60
2	H	134	VAL	N-CA-C	-6.04	104.61	110.72
1	O	91	PHE	CA-C-O	6.04	127.17	120.82
2	Z	134	VAL	N-CA-C	-6.04	104.62	110.72
1	T	91	PHE	CA-C-O	6.04	127.17	120.82
1	U	91	PHE	CA-C-O	6.04	127.17	120.82
1	O	141	ILE	N-CA-CB	6.04	119.75	111.41
2	V	134	VAL	N-CA-C	-6.04	104.62	110.72
2	I	134	VAL	N-CA-C	-6.04	104.62	110.72
1	Q	84	ASP	CA-CB-CG	-6.04	106.56	112.60
2	X	134	VAL	N-CA-C	-6.04	104.61	110.72
2	Y	134	VAL	N-CA-C	-6.04	104.62	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	91	PHE	CA-C-O	6.04	127.16	120.82
1	U	84	ASP	CA-CB-CG	-6.04	106.56	112.60
1	U	171	ALA	CA-C-N	6.04	128.73	120.46
1	U	171	ALA	C-N-CA	6.04	128.73	120.46
2	2	134	VAL	N-CA-C	-6.04	104.62	110.72
1	B	91	PHE	CA-C-O	6.04	127.16	120.82
1	O	84	ASP	CA-CB-CG	-6.03	106.57	112.60
1	F	91	PHE	CA-C-O	6.03	127.15	120.82
1	E	91	PHE	CA-C-O	6.03	127.15	120.82
1	G	91	PHE	CA-C-O	6.03	127.15	120.82
1	E	141	ILE	N-CA-CB	6.03	119.73	111.41
1	F	84	ASP	CA-CB-CG	-6.03	106.57	112.60
1	G	27	ALA	N-CA-CB	6.03	118.75	110.01
1	G	84	ASP	CA-CB-CG	-6.03	106.57	112.60
1	C	27	ALA	N-CA-CB	6.03	118.75	110.01
1	F	27	ALA	N-CA-CB	6.02	118.75	110.01
1	U	176	LEU	CA-C-O	-6.02	114.17	120.55
1	D	27	ALA	N-CA-CB	6.02	118.74	110.01
1	D	171	ALA	CA-C-N	6.02	128.71	120.46
1	D	171	ALA	C-N-CA	6.02	128.71	120.46
1	T	168	GLY	O-C-N	-6.02	114.88	122.70
1	T	171	ALA	CA-C-N	6.02	128.71	120.46
1	T	171	ALA	C-N-CA	6.02	128.71	120.46
1	A	171	ALA	CA-C-N	6.02	128.71	120.46
1	A	171	ALA	C-N-CA	6.02	128.71	120.46
1	C	171	ALA	CA-C-N	6.02	128.71	120.46
1	C	171	ALA	C-N-CA	6.02	128.71	120.46
1	D	141	ILE	N-CA-CB	6.02	119.72	111.41
1	R	171	ALA	CA-C-N	6.02	128.71	120.46
1	R	171	ALA	C-N-CA	6.02	128.71	120.46
1	A	168	GLY	O-C-N	-6.02	114.88	122.70
1	R	91	PHE	CA-C-O	6.02	127.14	120.82
1	P	171	ALA	CA-C-N	6.01	128.70	120.46
1	P	171	ALA	C-N-CA	6.01	128.70	120.46
1	Q	91	PHE	CA-C-O	6.01	127.14	120.82
1	Q	171	ALA	CA-C-N	6.01	128.70	120.46
1	Q	171	ALA	C-N-CA	6.01	128.70	120.46
1	O	171	ALA	CA-C-N	6.01	128.70	120.46
1	O	171	ALA	C-N-CA	6.01	128.70	120.46
1	T	84	ASP	CA-CB-CG	-6.01	106.59	112.60
1	C	84	ASP	CA-CB-CG	-6.01	106.59	112.60
1	S	171	ALA	CA-C-N	6.01	128.69	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	171	ALA	C-N-CA	6.01	128.69	120.46
1	B	171	ALA	CA-C-N	6.01	128.69	120.46
1	B	171	ALA	C-N-CA	6.01	128.69	120.46
1	S	27	ALA	N-CA-CB	6.01	118.72	110.01
1	B	27	ALA	N-CA-CB	6.01	118.72	110.01
1	F	141	ILE	N-CA-CB	6.01	119.70	111.41
1	G	171	ALA	CA-C-N	6.01	128.69	120.46
1	G	171	ALA	C-N-CA	6.01	128.69	120.46
1	A	84	ASP	CA-CB-CG	-6.01	106.59	112.60
1	P	27	ALA	N-CA-CB	6.01	118.72	110.01
1	R	84	ASP	CA-CB-CG	-6.01	106.59	112.60
1	S	84	ASP	CA-CB-CG	-6.00	106.60	112.60
1	G	141	ILE	N-CA-CB	6.00	119.70	111.41
1	B	84	ASP	CA-CB-CG	-6.00	106.60	112.60
1	Q	141	ILE	N-CA-CB	6.00	119.70	111.41
2	1	181	LYS	O-C-N	-6.00	115.89	122.07
2	J	181	LYS	O-C-N	-6.00	115.89	122.07
2	K	134	VAL	N-CA-C	-6.00	104.66	110.72
1	S	141	ILE	N-CA-CB	6.00	119.69	111.41
2	2	181	LYS	O-C-N	-6.00	115.89	122.07
1	A	141	ILE	N-CA-CB	6.00	119.69	111.41
1	B	141	ILE	N-CA-CB	6.00	119.69	111.41
1	R	141	ILE	N-CA-CB	6.00	119.69	111.41
1	E	84	ASP	CA-CB-CG	-6.00	106.60	112.60
1	S	168	GLY	O-C-N	-6.00	114.91	122.70
1	T	141	ILE	N-CA-CB	6.00	119.69	111.41
1	U	204	GLY	N-CA-C	-6.00	106.31	115.66
1	A	27	ALA	N-CA-CB	6.00	118.71	110.01
1	B	168	GLY	O-C-N	-6.00	114.91	122.70
1	P	168	GLY	O-C-N	-6.00	114.91	122.70
1	P	204	GLY	N-CA-C	-6.00	106.31	115.66
2	W	15	ALA	O-C-N	6.00	130.43	123.17
1	C	141	ILE	N-CA-CB	6.00	119.69	111.41
1	U	141	ILE	N-CA-CB	6.00	119.68	111.41
1	E	204	GLY	N-CA-C	-6.00	106.31	115.66
1	P	84	ASP	CA-CB-CG	-5.99	106.61	112.60
1	P	91	PHE	CA-C-O	5.99	127.11	120.82
2	J	15	ALA	O-C-N	5.99	130.42	123.17
1	O	27	ALA	N-CA-CB	5.99	118.70	110.01
1	E	27	ALA	N-CA-CB	5.99	118.70	110.01
2	N	15	ALA	O-C-N	5.99	130.42	123.17
1	O	168	GLY	O-C-N	-5.99	114.91	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	204	GLY	N-CA-C	-5.99	106.31	115.66
1	E	168	GLY	O-C-N	-5.99	114.91	122.70
1	U	27	ALA	N-CA-CB	5.99	118.69	110.01
2	V	181	LYS	O-C-N	-5.99	115.90	122.07
1	R	27	ALA	N-CA-CB	5.99	118.69	110.01
2	H	15	ALA	O-C-N	5.98	130.41	123.17
1	Q	27	ALA	N-CA-CB	5.98	118.69	110.01
2	Y	15	ALA	O-C-N	5.98	130.41	123.17
1	E	171	ALA	CA-C-N	5.98	128.66	120.46
1	E	171	ALA	C-N-CA	5.98	128.66	120.46
2	K	15	ALA	O-C-N	5.98	130.41	123.17
1	T	27	ALA	N-CA-CB	5.98	118.68	110.01
1	C	168	GLY	O-C-N	-5.98	114.92	122.70
1	R	204	GLY	N-CA-C	-5.98	106.33	115.66
1	F	168	GLY	O-C-N	-5.98	114.93	122.70
1	F	171	ALA	CA-C-N	5.98	128.65	120.46
1	F	171	ALA	C-N-CA	5.98	128.65	120.46
2	V	15	ALA	O-C-N	5.98	130.40	123.17
2	Z	15	ALA	O-C-N	5.98	130.40	123.17
2	I	15	ALA	O-C-N	5.98	130.40	123.17
1	D	204	GLY	N-CA-C	-5.97	106.34	115.66
1	U	168	GLY	O-C-N	-5.97	114.94	122.70
1	U	199	SER	CA-C-N	5.97	132.95	121.54
1	U	199	SER	C-N-CA	5.97	132.95	121.54
1	P	141	ILE	N-CA-CB	5.97	119.65	111.41
1	D	168	GLY	O-C-N	-5.97	114.94	122.70
1	E	199	SER	CA-C-N	5.97	132.95	121.54
1	E	199	SER	C-N-CA	5.97	132.95	121.54
1	F	204	GLY	N-CA-C	-5.97	106.34	115.66
1	S	204	GLY	N-CA-C	-5.97	106.35	115.66
1	G	168	GLY	O-C-N	-5.97	114.94	122.70
1	G	199	SER	CA-C-N	5.97	132.94	121.54
1	G	199	SER	C-N-CA	5.97	132.94	121.54
1	O	199	SER	CA-C-N	5.97	132.94	121.54
1	O	199	SER	C-N-CA	5.97	132.94	121.54
1	B	204	GLY	N-CA-C	-5.97	106.35	115.66
1	C	199	SER	CA-C-N	5.97	132.94	121.54
1	C	199	SER	C-N-CA	5.97	132.94	121.54
1	Q	168	GLY	O-C-N	-5.97	114.94	122.70
1	Q	199	SER	CA-C-N	5.97	132.94	121.54
1	Q	199	SER	C-N-CA	5.97	132.94	121.54
1	R	168	GLY	O-C-N	-5.97	114.94	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	204	GLY	N-CA-C	-5.97	106.35	115.66
1	S	199	SER	CA-C-N	5.97	132.94	121.54
1	S	199	SER	C-N-CA	5.97	132.94	121.54
2	1	15	ALA	O-C-N	5.97	130.39	123.17
1	B	199	SER	CA-C-N	5.97	132.94	121.54
1	B	199	SER	C-N-CA	5.97	132.94	121.54
2	M	15	ALA	O-C-N	5.96	130.39	123.17
1	C	183	ASN	CA-CB-CG	-5.96	106.64	112.60
1	Q	62	ASN	CA-CB-CG	-5.96	106.64	112.60
2	X	181	LYS	O-C-N	-5.96	115.93	122.07
1	O	62	ASN	CA-CB-CG	-5.96	106.64	112.60
1	T	199	SER	CA-C-N	5.96	132.93	121.54
1	T	199	SER	C-N-CA	5.96	132.93	121.54
1	F	199	SER	CA-C-N	5.96	132.92	121.54
1	F	199	SER	C-N-CA	5.96	132.92	121.54
1	G	204	GLY	N-CA-C	-5.96	106.36	115.66
1	A	199	SER	CA-C-N	5.96	132.92	121.54
1	A	199	SER	C-N-CA	5.96	132.92	121.54
1	Q	204	GLY	N-CA-C	-5.96	106.36	115.66
1	R	199	SER	CA-C-N	5.96	132.92	121.54
1	R	199	SER	C-N-CA	5.96	132.92	121.54
2	Y	181	LYS	O-C-N	-5.96	115.93	122.07
1	A	183	ASN	CA-CB-CG	-5.96	106.64	112.60
1	A	204	GLY	N-CA-C	-5.96	106.37	115.66
1	O	204	GLY	N-CA-C	-5.96	106.37	115.66
1	P	199	SER	CA-C-N	5.96	132.91	121.54
1	P	199	SER	C-N-CA	5.96	132.91	121.54
1	E	183	ASN	CA-CB-CG	-5.96	106.64	112.60
2	L	15	ALA	O-C-N	5.96	130.38	123.17
1	D	199	SER	CA-C-N	5.96	132.91	121.54
1	D	199	SER	C-N-CA	5.96	132.91	121.54
2	X	15	ALA	O-C-N	5.95	130.37	123.17
1	D	150	ASP	N-CA-C	-5.95	100.29	109.52
2	Z	181	LYS	O-C-N	-5.95	115.94	122.07
2	I	181	LYS	O-C-N	-5.95	115.94	122.07
1	S	183	ASN	CA-CB-CG	-5.95	106.65	112.60
2	2	15	ALA	O-C-N	5.95	130.37	123.17
1	B	183	ASN	CA-CB-CG	-5.95	106.65	112.60
1	T	150	ASP	N-CA-C	-5.95	100.30	109.52
1	G	183	ASN	CA-CB-CG	-5.95	106.65	112.60
1	U	150	ASP	N-CA-C	-5.95	100.30	109.52
1	G	62	ASN	CA-CB-CG	-5.95	106.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	62	ASN	CA-CB-CG	-5.95	106.65	112.60
1	R	62	ASN	CA-CB-CG	-5.95	106.66	112.60
1	E	62	ASN	CA-CB-CG	-5.95	106.66	112.60
2	N	181	LYS	O-C-N	-5.94	115.95	122.07
1	F	183	ASN	CA-CB-CG	-5.94	106.66	112.60
1	P	183	ASN	CA-CB-CG	-5.94	106.66	112.60
1	S	62	ASN	CA-CB-CG	-5.94	106.66	112.60
1	B	62	ASN	CA-CB-CG	-5.94	106.66	112.60
1	A	62	ASN	CA-CB-CG	-5.94	106.66	112.60
1	P	150	ASP	N-CA-C	-5.94	100.32	109.52
1	E	150	ASP	N-CA-C	-5.94	100.32	109.52
2	W	181	LYS	O-C-N	-5.93	115.96	122.07
1	T	62	ASN	CA-CB-CG	-5.93	106.67	112.60
1	U	183	ASN	CA-CB-CG	-5.93	106.67	112.60
1	C	62	ASN	CA-CB-CG	-5.93	106.67	112.60
1	D	183	ASN	CA-CB-CG	-5.93	106.67	112.60
1	R	183	ASN	CA-CB-CG	-5.93	106.67	112.60
2	L	181	LYS	O-C-N	-5.93	115.96	122.07
1	F	62	ASN	CA-CB-CG	-5.93	106.67	112.60
1	T	183	ASN	CA-CB-CG	-5.93	106.67	112.60
1	U	62	ASN	CA-CB-CG	-5.93	106.67	112.60
1	D	62	ASN	CA-CB-CG	-5.93	106.67	112.60
1	S	150	ASP	N-CA-C	-5.93	100.33	109.52
1	B	150	ASP	N-CA-C	-5.93	100.33	109.52
2	K	181	LYS	O-C-N	-5.93	115.96	122.07
2	M	181	LYS	O-C-N	-5.92	115.97	122.07
1	O	150	ASP	N-CA-C	-5.92	100.34	109.52
2	H	181	LYS	O-C-N	-5.92	115.97	122.07
1	Q	183	ASN	CA-CB-CG	-5.92	106.68	112.60
1	C	150	ASP	N-CA-C	-5.92	100.34	109.52
1	F	150	ASP	N-CA-C	-5.91	100.35	109.52
1	G	150	ASP	N-CA-C	-5.91	100.35	109.52
1	G	221	TYR	N-CA-C	-5.91	101.66	110.23
1	Q	150	ASP	N-CA-C	-5.91	100.35	109.52
1	F	221	TYR	N-CA-C	-5.91	101.66	110.23
1	T	221	TYR	N-CA-C	-5.91	101.66	110.23
1	A	150	ASP	N-CA-C	-5.91	100.36	109.52
1	O	183	ASN	CA-CB-CG	-5.91	106.69	112.60
1	P	221	TYR	N-CA-C	-5.91	101.66	110.23
1	C	221	TYR	N-CA-C	-5.91	101.66	110.23
1	Q	221	TYR	N-CA-C	-5.91	101.66	110.23
1	R	221	TYR	N-CA-C	-5.91	101.66	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	150	ASP	N-CA-C	-5.91	100.36	109.52
1	S	221	TYR	N-CA-C	-5.90	101.67	110.23
1	B	221	TYR	N-CA-C	-5.90	101.67	110.23
1	A	221	TYR	N-CA-C	-5.90	101.67	110.23
2	H	69	GLN	CA-C-O	-5.90	114.17	120.42
2	J	69	GLN	CA-C-O	-5.90	114.17	120.42
1	U	221	TYR	N-CA-C	-5.90	101.68	110.23
1	D	221	TYR	N-CA-C	-5.90	101.68	110.23
2	X	120	VAL	N-CA-C	-5.89	99.73	108.45
2	N	180	ARG	NE-CZ-NH1	5.88	127.38	121.50
1	O	221	TYR	N-CA-C	-5.88	101.70	110.23
1	E	221	TYR	N-CA-C	-5.88	101.70	110.23
2	Y	69	GLN	CA-C-O	-5.88	114.19	120.42
2	Y	120	VAL	N-CA-C	-5.88	99.75	108.45
2	N	69	GLN	CA-C-O	-5.87	114.19	120.42
2	V	59	MET	N-CA-C	5.87	117.68	111.28
2	X	69	GLN	CA-C-O	-5.87	114.19	120.42
2	X	180	ARG	NE-CZ-NH1	5.87	127.37	121.50
2	K	69	GLN	CA-C-O	-5.87	114.19	120.42
2	Z	69	GLN	CA-C-O	-5.87	114.20	120.42
2	N	59	MET	N-CA-C	5.87	117.68	111.28
2	N	120	VAL	N-CA-C	-5.87	99.76	108.45
2	I	69	GLN	CA-C-O	-5.87	114.20	120.42
2	Y	180	ARG	NE-CZ-NH1	5.87	127.37	121.50
2	V	180	ARG	NE-CZ-NH1	5.87	127.37	121.50
2	H	59	MET	N-CA-C	5.87	117.67	111.28
2	V	120	VAL	N-CA-C	-5.87	99.77	108.45
1	T	25	GLU	N-CA-CB	5.86	118.57	110.07
2	Z	120	VAL	N-CA-C	-5.86	99.77	108.45
2	M	69	GLN	CA-C-O	-5.86	114.21	120.42
2	I	120	VAL	N-CA-C	-5.86	99.77	108.45
2	W	69	GLN	CA-C-O	-5.86	114.21	120.42
2	1	69	GLN	CA-C-O	-5.86	114.21	120.42
2	W	180	ARG	NE-CZ-NH1	5.86	127.36	121.50
2	H	120	VAL	N-CA-C	-5.86	99.78	108.45
2	L	59	MET	N-CA-C	5.86	117.66	111.28
2	Z	59	MET	N-CA-C	5.86	117.66	111.28
2	1	180	ARG	NE-CZ-NH1	5.86	127.36	121.50
2	2	59	MET	N-CA-C	5.86	117.66	111.28
2	I	59	MET	N-CA-C	5.86	117.66	111.28
2	J	180	ARG	NE-CZ-NH1	5.86	127.36	121.50
2	K	59	MET	N-CA-C	5.86	117.66	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	25	GLU	N-CA-CB	5.86	118.56	110.07
2	Z	180	ARG	NE-CZ-NH1	5.85	127.35	121.50
1	F	25	GLU	N-CA-CB	5.85	118.56	110.07
1	A	25	GLU	N-CA-CB	5.85	118.56	110.07
2	I	180	ARG	NE-CZ-NH1	5.85	127.35	121.50
2	J	120	VAL	N-CA-C	-5.85	99.79	108.45
2	M	180	ARG	NE-CZ-NH1	5.85	127.35	121.50
2	2	180	ARG	NE-CZ-NH1	5.85	127.35	121.50
2	K	180	ARG	NE-CZ-NH1	5.85	127.35	121.50
2	M	120	VAL	N-CA-C	-5.85	99.79	108.45
2	V	69	GLN	CA-C-O	-5.85	114.22	120.42
2	L	69	GLN	CA-C-O	-5.85	114.22	120.42
2	M	23	GLU	CA-C-O	-5.85	112.15	120.51
2	W	23	GLU	CA-C-O	-5.85	112.15	120.51
2	1	23	GLU	CA-C-O	-5.84	112.15	120.51
2	1	59	MET	N-CA-C	5.84	117.65	111.28
2	N	23	GLU	CA-C-O	-5.84	112.15	120.51
2	M	59	MET	N-CA-C	5.84	117.65	111.28
2	2	120	VAL	N-CA-C	-5.84	99.81	108.45
1	O	25	GLU	N-CA-CB	5.84	118.54	110.07
1	C	25	GLU	N-CA-CB	5.84	118.54	110.07
2	K	120	VAL	N-CA-C	-5.84	99.81	108.45
1	E	25	GLU	N-CA-CB	5.84	118.54	110.07
2	L	120	VAL	N-CA-C	-5.84	99.81	108.45
2	L	180	ARG	NE-CZ-NH1	5.84	127.34	121.50
1	G	25	GLU	N-CA-CB	5.84	118.54	110.07
1	Q	25	GLU	N-CA-CB	5.84	118.54	110.07
2	X	59	MET	N-CA-C	5.84	117.64	111.28
2	Y	59	MET	N-CA-C	5.84	117.65	111.28
1	S	25	GLU	N-CA-CB	5.84	118.54	110.07
1	B	25	GLU	N-CA-CB	5.84	118.54	110.07
1	U	25	GLU	N-CA-CB	5.84	118.53	110.07
1	U	83	ALA	N-CA-C	5.84	118.14	111.02
1	D	25	GLU	N-CA-CB	5.84	118.53	110.07
2	1	120	VAL	N-CA-C	-5.83	99.81	108.45
2	W	59	MET	N-CA-C	5.83	117.64	111.28
2	2	69	GLN	CA-C-O	-5.83	114.24	120.42
2	X	23	GLU	CA-C-O	-5.83	112.17	120.51
2	H	23	GLU	CA-C-O	-5.83	112.18	120.51
2	H	180	ARG	NE-CZ-NH1	5.83	127.33	121.50
2	J	23	GLU	CA-C-O	-5.83	112.18	120.51
2	K	23	GLU	CA-C-O	-5.83	112.17	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	23	GLU	CA-C-O	-5.83	112.18	120.51
2	I	23	GLU	CA-C-O	-5.83	112.18	120.51
2	Y	23	GLU	CA-C-O	-5.83	112.18	120.51
2	W	120	VAL	N-CA-C	-5.83	99.83	108.45
2	J	59	MET	N-CA-C	5.83	117.63	111.28
2	2	23	GLU	CA-C-O	-5.82	112.19	120.51
2	M	102	GLY	CA-C-O	-5.81	115.77	121.76
2	V	23	GLU	CA-C-O	-5.81	112.20	120.51
2	W	102	GLY	CA-C-O	-5.81	115.77	121.76
2	L	23	GLU	CA-C-O	-5.81	112.20	120.51
1	P	25	GLU	N-CA-CB	5.81	118.50	110.07
1	F	83	ALA	N-CA-C	5.81	118.11	111.02
1	P	83	ALA	N-CA-C	5.81	118.11	111.02
1	D	83	ALA	N-CA-C	5.80	118.10	111.02
2	M	183	GLY	CA-C-N	5.80	130.13	121.72
2	M	183	GLY	C-N-CA	5.80	130.13	121.72
2	N	183	GLY	CA-C-N	5.80	130.13	121.72
2	N	183	GLY	C-N-CA	5.80	130.13	121.72
1	A	83	ALA	N-CA-C	5.80	118.10	111.02
2	W	183	GLY	CA-C-N	5.80	130.13	121.72
2	W	183	GLY	C-N-CA	5.80	130.13	121.72
1	S	83	ALA	N-CA-C	5.80	118.09	111.02
2	N	102	GLY	CA-C-O	-5.80	115.79	121.76
1	B	83	ALA	N-CA-C	5.80	118.09	111.02
2	J	183	GLY	CA-C-N	5.80	130.13	121.72
2	J	183	GLY	C-N-CA	5.80	130.13	121.72
2	X	102	GLY	CA-C-O	-5.80	115.79	121.76
2	1	183	GLY	CA-C-N	5.79	130.12	121.72
2	1	183	GLY	C-N-CA	5.79	130.12	121.72
2	2	183	GLY	CA-C-N	5.79	130.12	121.72
2	2	183	GLY	C-N-CA	5.79	130.12	121.72
2	1	79	VAL	CA-CB-CG1	5.79	120.25	110.40
2	2	102	GLY	CA-C-O	-5.79	115.80	121.76
2	Z	183	GLY	CA-C-N	5.79	130.12	121.72
2	Z	183	GLY	C-N-CA	5.79	130.12	121.72
2	I	183	GLY	CA-C-N	5.79	130.12	121.72
2	I	183	GLY	C-N-CA	5.79	130.12	121.72
2	M	79	VAL	CA-CB-CG1	5.79	120.24	110.40
2	Y	183	GLY	CA-C-N	5.79	130.11	121.72
2	Y	183	GLY	C-N-CA	5.79	130.11	121.72
1	O	83	ALA	N-CA-C	5.79	118.08	111.02
1	E	83	ALA	N-CA-C	5.79	118.08	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	183	GLY	CA-C-N	5.78	130.10	121.72
2	H	183	GLY	C-N-CA	5.78	130.10	121.72
2	X	183	GLY	CA-C-N	5.78	130.10	121.72
2	X	183	GLY	C-N-CA	5.78	130.10	121.72
2	K	183	GLY	CA-C-N	5.78	130.10	121.72
2	K	183	GLY	C-N-CA	5.78	130.10	121.72
1	R	83	ALA	N-CA-C	5.78	118.07	111.02
1	G	83	ALA	N-CA-C	5.78	118.07	111.02
2	N	157	ARG	CA-C-N	5.78	128.82	120.79
2	N	157	ARG	C-N-CA	5.78	128.82	120.79
2	V	79	VAL	CA-CB-CG1	5.78	120.22	110.40
2	W	79	VAL	CA-CB-CG1	5.78	120.22	110.40
2	L	183	GLY	CA-C-N	5.78	130.10	121.72
2	L	183	GLY	C-N-CA	5.78	130.10	121.72
2	Z	102	GLY	CA-C-O	-5.77	115.81	121.76
2	I	102	GLY	CA-C-O	-5.77	115.81	121.76
1	Q	83	ALA	N-CA-C	5.77	118.06	111.02
1	T	83	ALA	N-CA-C	5.77	118.06	111.02
1	G	200	SER	O-C-N	-5.77	114.91	122.59
1	U	200	SER	O-C-N	-5.77	114.91	122.59
2	V	183	GLY	CA-C-N	5.77	130.09	121.72
2	V	183	GLY	C-N-CA	5.77	130.09	121.72
1	C	83	ALA	N-CA-C	5.77	118.06	111.02
2	J	79	VAL	CA-CB-CG1	5.77	120.21	110.40
2	2	79	VAL	CA-CB-CG1	5.77	120.21	110.40
2	X	79	VAL	CA-CB-CG1	5.77	120.21	110.40
2	K	79	VAL	CA-CB-CG1	5.77	120.21	110.40
2	L	79	VAL	CA-CB-CG1	5.77	120.21	110.40
2	H	157	ARG	CA-C-N	5.77	128.81	120.79
2	H	157	ARG	C-N-CA	5.77	128.81	120.79
2	Z	79	VAL	CA-CB-CG1	5.77	120.20	110.40
2	I	79	VAL	CA-CB-CG1	5.77	120.20	110.40
2	H	79	VAL	CA-CB-CG1	5.76	120.20	110.40
2	Y	79	VAL	CA-CB-CG1	5.76	120.20	110.40
2	N	79	VAL	CA-CB-CG1	5.76	120.19	110.40
2	W	157	ARG	CA-C-N	5.76	128.79	120.79
2	W	157	ARG	C-N-CA	5.76	128.79	120.79
2	H	102	GLY	CA-C-O	-5.75	115.83	121.76
2	Y	102	GLY	CA-C-O	-5.75	115.83	121.76
2	M	157	ARG	CA-C-N	5.75	128.79	120.79
2	M	157	ARG	C-N-CA	5.75	128.79	120.79
2	V	90	VAL	CA-C-O	5.75	127.97	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	SER	O-C-N	-5.75	114.94	122.59
1	R	200	SER	O-C-N	-5.75	114.94	122.59
2	Y	157	ARG	CA-C-N	5.75	128.78	120.79
2	Y	157	ARG	C-N-CA	5.75	128.78	120.79
2	L	157	ARG	CA-C-N	5.75	128.78	120.79
2	L	157	ARG	C-N-CA	5.75	128.78	120.79
1	O	200	SER	O-C-N	-5.75	114.94	122.59
2	J	157	ARG	CA-C-N	5.75	128.78	120.79
2	J	157	ARG	C-N-CA	5.75	128.78	120.79
1	E	200	SER	O-C-N	-5.75	114.94	122.59
2	Z	157	ARG	CA-C-N	5.75	128.78	120.79
2	Z	157	ARG	C-N-CA	5.75	128.78	120.79
2	I	157	ARG	CA-C-N	5.75	128.78	120.79
2	I	157	ARG	C-N-CA	5.75	128.78	120.79
1	Q	200	SER	O-C-N	-5.75	114.94	122.59
1	S	200	SER	O-C-N	-5.75	114.95	122.59
1	B	200	SER	O-C-N	-5.75	114.95	122.59
1	F	200	SER	O-C-N	-5.74	114.95	122.59
2	2	90	VAL	CA-C-O	5.74	127.96	120.78
2	V	157	ARG	CA-C-N	5.74	128.77	120.79
2	V	157	ARG	C-N-CA	5.74	128.77	120.79
2	L	102	GLY	CA-C-O	-5.74	115.85	121.76
2	K	102	GLY	CA-C-O	-5.74	115.85	121.76
2	1	102	GLY	CA-C-O	-5.74	115.85	121.76
2	1	157	ARG	CA-C-N	5.74	128.76	120.79
2	1	157	ARG	C-N-CA	5.74	128.76	120.79
2	J	102	GLY	CA-C-O	-5.74	115.85	121.76
1	P	200	SER	O-C-N	-5.74	114.96	122.59
2	K	157	ARG	CA-C-N	5.74	128.76	120.79
2	K	157	ARG	C-N-CA	5.74	128.76	120.79
2	X	157	ARG	CA-C-N	5.73	128.76	120.79
2	X	157	ARG	C-N-CA	5.73	128.76	120.79
2	1	90	VAL	CA-C-O	5.73	127.95	120.78
2	Z	90	VAL	CA-C-O	5.73	127.94	120.78
2	H	90	VAL	CA-C-O	5.73	127.94	120.78
2	I	90	VAL	CA-C-O	5.73	127.94	120.78
2	Y	90	VAL	CA-C-O	5.73	127.94	120.78
2	X	90	VAL	CA-C-O	5.73	127.94	120.78
2	J	90	VAL	CA-C-O	5.73	127.94	120.78
2	K	90	VAL	CA-C-O	5.72	127.94	120.78
2	2	157	ARG	CA-C-N	5.72	128.74	120.79
2	2	157	ARG	C-N-CA	5.72	128.74	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	102	GLY	CA-C-O	-5.72	115.87	121.76
2	L	90	VAL	CA-C-O	5.72	127.93	120.78
1	T	200	SER	O-C-N	-5.72	114.98	122.59
1	T	186	GLU	CA-C-N	5.72	128.26	120.54
1	T	186	GLU	C-N-CA	5.72	128.26	120.54
1	C	186	GLU	CA-C-N	5.72	128.26	120.54
1	C	186	GLU	C-N-CA	5.72	128.26	120.54
1	D	200	SER	O-C-N	-5.72	114.98	122.59
1	C	200	SER	O-C-N	-5.71	115.00	122.59
1	Q	176	LEU	CA-C-N	5.71	128.72	120.38
1	Q	176	LEU	C-N-CA	5.71	128.72	120.38
1	F	186	GLU	CA-C-N	5.71	128.25	120.54
1	F	186	GLU	C-N-CA	5.71	128.25	120.54
1	U	186	GLU	CA-C-N	5.71	128.24	120.54
1	U	186	GLU	C-N-CA	5.71	128.24	120.54
1	O	186	GLU	CA-C-N	5.70	128.24	120.54
1	O	186	GLU	C-N-CA	5.70	128.24	120.54
1	D	186	GLU	CA-C-N	5.70	128.24	120.54
1	D	186	GLU	C-N-CA	5.70	128.24	120.54
2	M	90	VAL	CA-C-O	5.70	127.91	120.78
1	P	186	GLU	CA-C-N	5.70	128.24	120.54
1	P	186	GLU	C-N-CA	5.70	128.24	120.54
2	W	90	VAL	CA-C-O	5.70	127.91	120.78
2	N	90	VAL	CA-C-O	5.70	127.90	120.78
1	S	186	GLU	CA-C-N	5.70	128.23	120.54
1	S	186	GLU	C-N-CA	5.70	128.23	120.54
1	G	176	LEU	CA-C-N	5.70	128.70	120.38
1	G	176	LEU	C-N-CA	5.70	128.70	120.38
1	B	186	GLU	CA-C-N	5.70	128.23	120.54
1	B	186	GLU	C-N-CA	5.70	128.23	120.54
1	R	186	GLU	CA-C-N	5.70	128.23	120.54
1	R	186	GLU	C-N-CA	5.70	128.23	120.54
2	L	153	ASP	CA-C-O	-5.70	114.83	120.70
1	C	176	LEU	CA-C-N	5.69	128.69	120.38
1	C	176	LEU	C-N-CA	5.69	128.69	120.38
1	D	176	LEU	CA-C-N	5.69	128.69	120.38
1	D	176	LEU	C-N-CA	5.69	128.69	120.38
2	H	153	ASP	CA-C-O	-5.69	114.84	120.70
1	O	176	LEU	CA-C-N	5.69	128.68	120.38
1	O	176	LEU	C-N-CA	5.69	128.68	120.38
1	P	176	LEU	CA-C-N	5.69	128.69	120.38
1	P	176	LEU	C-N-CA	5.69	128.69	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	176	LEU	CA-C-N	5.69	128.68	120.38
1	E	176	LEU	C-N-CA	5.69	128.68	120.38
1	S	176	LEU	CA-C-N	5.68	128.68	120.38
1	S	176	LEU	C-N-CA	5.68	128.68	120.38
1	T	176	LEU	CA-C-N	5.68	128.68	120.38
1	T	176	LEU	C-N-CA	5.68	128.68	120.38
1	U	176	LEU	CA-C-N	5.68	128.68	120.38
1	U	176	LEU	C-N-CA	5.68	128.68	120.38
1	A	176	LEU	CA-C-N	5.68	128.68	120.38
1	A	176	LEU	C-N-CA	5.68	128.68	120.38
1	B	176	LEU	CA-C-N	5.68	128.68	120.38
1	B	176	LEU	C-N-CA	5.68	128.68	120.38
1	E	186	GLU	CA-C-N	5.68	128.22	120.54
1	E	186	GLU	C-N-CA	5.68	128.22	120.54
1	A	186	GLU	CA-C-N	5.68	128.21	120.54
1	A	186	GLU	C-N-CA	5.68	128.21	120.54
1	F	176	LEU	CA-C-N	5.68	128.67	120.38
1	F	176	LEU	C-N-CA	5.68	128.67	120.38
2	N	107	ALA	O-C-N	-5.67	116.55	121.71
2	V	153	ASP	CA-C-O	-5.67	114.86	120.70
1	G	186	GLU	CA-C-N	5.67	128.20	120.54
1	G	186	GLU	C-N-CA	5.67	128.20	120.54
1	Q	186	GLU	CA-C-N	5.67	128.20	120.54
1	Q	186	GLU	C-N-CA	5.67	128.20	120.54
1	R	176	LEU	CA-C-N	5.67	128.66	120.38
1	R	176	LEU	C-N-CA	5.67	128.66	120.38
2	M	153	ASP	CA-C-O	-5.67	114.86	120.70
2	2	153	ASP	CA-C-O	-5.67	114.86	120.70
2	X	153	ASP	CA-C-O	-5.67	114.86	120.70
2	1	107	ALA	O-C-N	-5.66	116.56	121.71
2	2	107	ALA	O-C-N	-5.66	116.56	121.71
2	V	87	LEU	O-C-N	5.66	128.20	122.09
2	J	107	ALA	O-C-N	-5.66	116.56	121.71
2	1	135	TYR	CB-CG-CD1	-5.65	112.32	120.80
2	X	135	TYR	CB-CG-CD1	-5.65	112.33	120.80
2	Z	153	ASP	CA-C-O	-5.65	114.88	120.70
2	I	153	ASP	CA-C-O	-5.65	114.88	120.70
2	2	87	LEU	O-C-N	5.65	128.19	122.09
2	W	107	ALA	O-C-N	-5.65	116.57	121.71
2	K	87	LEU	O-C-N	5.65	128.19	122.09
2	1	153	ASP	CA-C-O	-5.64	114.89	120.70
2	W	135	TYR	CB-CG-CD1	-5.64	112.33	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	153	ASP	CA-C-O	-5.64	114.89	120.70
2	1	87	LEU	O-C-N	5.64	128.18	122.09
1	G	200	SER	N-CA-CB	-5.64	100.95	110.49
1	C	200	SER	N-CA-CB	-5.64	100.95	110.49
2	Y	107	ALA	O-C-N	-5.64	116.58	121.71
2	N	155	VAL	CA-C-N	5.64	128.19	120.46
2	N	155	VAL	C-N-CA	5.64	128.19	120.46
2	N	153	ASP	CA-C-O	-5.64	114.89	120.70
2	2	135	TYR	CB-CG-CD1	-5.64	112.35	120.80
2	J	153	ASP	CA-C-O	-5.64	114.89	120.70
1	Q	200	SER	N-CA-CB	-5.64	100.96	110.49
1	D	200	SER	N-CA-CB	-5.64	100.97	110.49
2	K	135	TYR	CB-CG-CD1	-5.64	112.35	120.80
2	Y	155	VAL	CA-C-N	5.64	128.18	120.46
2	Y	155	VAL	C-N-CA	5.64	128.18	120.46
1	F	200	SER	N-CA-CB	-5.63	100.97	110.49
1	T	200	SER	N-CA-CB	-5.63	100.97	110.49
2	Y	87	LEU	O-C-N	5.63	128.18	122.09
2	Z	107	ALA	O-C-N	-5.63	116.58	121.71
2	V	155	VAL	CA-C-N	5.63	128.18	120.46
2	V	155	VAL	C-N-CA	5.63	128.18	120.46
2	I	107	ALA	O-C-N	-5.63	116.58	121.71
2	1	155	VAL	CA-C-N	5.63	128.17	120.46
2	1	155	VAL	C-N-CA	5.63	128.17	120.46
2	N	87	LEU	O-C-N	5.63	128.17	122.09
2	H	155	VAL	CA-C-N	5.63	128.17	120.46
2	H	155	VAL	C-N-CA	5.63	128.17	120.46
2	X	87	LEU	O-C-N	5.63	128.17	122.09
2	X	107	ALA	O-C-N	-5.63	116.59	121.71
1	S	200	SER	N-CA-CB	-5.63	100.98	110.49
1	B	200	SER	N-CA-CB	-5.63	100.98	110.49
2	L	155	VAL	CA-C-N	5.63	128.17	120.46
2	L	155	VAL	C-N-CA	5.63	128.17	120.46
2	Z	87	LEU	O-C-N	5.62	128.16	122.09
2	Z	155	VAL	CA-C-N	5.62	128.16	120.46
2	Z	155	VAL	C-N-CA	5.62	128.16	120.46
1	U	200	SER	N-CA-CB	-5.62	100.99	110.49
2	I	87	LEU	O-C-N	5.62	128.16	122.09
2	I	155	VAL	CA-C-N	5.62	128.16	120.46
2	I	155	VAL	C-N-CA	5.62	128.16	120.46
2	Z	135	TYR	CB-CG-CD1	-5.62	112.37	120.80
2	M	155	VAL	CA-C-N	5.62	128.16	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	155	VAL	C-N-CA	5.62	128.16	120.46
2	H	87	LEU	O-C-N	5.62	128.16	122.09
2	V	107	ALA	O-C-N	-5.62	116.59	121.71
2	I	135	TYR	CB-CG-CD1	-5.62	112.37	120.80
1	A	200	SER	N-CA-CB	-5.62	100.99	110.49
1	O	200	SER	N-CA-CB	-5.62	100.99	110.49
2	K	107	ALA	O-C-N	-5.62	116.59	121.71
1	R	200	SER	N-CA-CB	-5.62	100.99	110.49
1	P	200	SER	N-CA-CB	-5.62	101.00	110.49
2	Y	153	ASP	CA-C-O	-5.62	114.91	120.70
2	J	135	TYR	CB-CG-CD1	-5.62	112.38	120.80
2	X	155	VAL	CA-C-N	5.62	128.15	120.46
2	X	155	VAL	C-N-CA	5.62	128.15	120.46
1	E	200	SER	N-CA-CB	-5.62	101.00	110.49
2	L	87	LEU	O-C-N	5.62	128.16	122.09
2	M	135	TYR	CB-CG-CD1	-5.61	112.38	120.80
2	N	135	TYR	CB-CG-CD1	-5.61	112.38	120.80
2	2	155	VAL	CA-C-N	5.61	128.15	120.46
2	2	155	VAL	C-N-CA	5.61	128.15	120.46
2	H	107	ALA	O-C-N	-5.61	116.60	121.71
2	V	98	GLN	CA-C-O	-5.61	114.51	120.40
2	M	87	LEU	O-C-N	5.61	128.15	122.09
2	M	107	ALA	O-C-N	-5.61	116.60	121.71
2	W	87	LEU	O-C-N	5.61	128.15	122.09
2	H	135	TYR	CB-CG-CD1	-5.61	112.39	120.80
2	Y	135	TYR	CB-CG-CD1	-5.61	112.39	120.80
2	J	87	LEU	O-C-N	5.61	128.15	122.09
2	J	155	VAL	CA-C-N	5.61	128.14	120.46
2	J	155	VAL	C-N-CA	5.61	128.14	120.46
2	K	155	VAL	CA-C-N	5.61	128.14	120.46
2	K	155	VAL	C-N-CA	5.61	128.14	120.46
2	V	135	TYR	CB-CG-CD1	-5.61	112.39	120.80
2	K	153	ASP	CA-C-O	-5.61	114.93	120.70
2	L	98	GLN	CA-C-O	-5.61	114.52	120.40
2	L	135	TYR	CB-CG-CD1	-5.60	112.39	120.80
2	L	165	ARG	CA-C-O	5.60	125.90	119.35
2	J	98	GLN	CA-C-O	-5.60	114.52	120.40
2	L	107	ALA	O-C-N	-5.60	116.61	121.71
2	V	165	ARG	CA-C-O	5.60	125.90	119.35
2	J	25	PHE	CB-CG-CD1	5.60	130.22	120.70
2	W	98	GLN	CA-C-O	-5.60	114.53	120.40
2	W	165	ARG	CA-C-O	5.60	125.90	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	165	ARG	CA-C-O	5.59	125.90	119.35
2	W	155	VAL	CA-C-N	5.59	128.12	120.46
2	W	155	VAL	C-N-CA	5.59	128.12	120.46
2	2	165	ARG	CA-C-O	5.59	125.89	119.35
2	K	165	ARG	CA-C-O	5.59	125.89	119.35
2	Z	98	GLN	CA-C-O	-5.59	114.53	120.40
2	Z	165	ARG	CA-C-O	5.59	125.89	119.35
2	M	98	GLN	CA-C-O	-5.59	114.53	120.40
2	I	98	GLN	CA-C-O	-5.59	114.53	120.40
2	I	165	ARG	CA-C-O	5.59	125.89	119.35
2	1	165	ARG	CA-C-O	5.58	125.89	119.35
2	J	165	ARG	CA-C-O	5.58	125.89	119.35
1	G	210	PRO	CA-C-O	-5.58	114.44	122.31
2	2	98	GLN	CA-C-O	-5.58	114.54	120.40
2	1	13	ILE	CB-CG1-CD1	-5.58	102.08	113.80
2	N	25	PHE	CB-CG-CD1	5.58	130.19	120.70
2	X	13	ILE	CB-CG1-CD1	-5.58	102.08	113.80
2	Y	165	ARG	CA-C-O	5.58	125.88	119.35
2	M	165	ARG	CA-C-O	5.58	125.88	119.35
2	1	25	PHE	CB-CG-CD1	5.58	130.18	120.70
2	V	25	PHE	CB-CG-CD1	5.58	130.18	120.70
1	D	210	PRO	CA-C-O	-5.58	114.45	122.31
2	K	13	ILE	CB-CG1-CD1	-5.58	102.09	113.80
2	K	38	ASP	CA-CB-CG	5.58	118.18	112.60
2	Y	25	PHE	CB-CG-CD1	5.58	130.18	120.70
2	Z	25	PHE	CB-CG-CD1	5.57	130.18	120.70
2	M	25	PHE	CB-CG-CD1	5.57	130.18	120.70
2	I	25	PHE	CB-CG-CD1	5.57	130.18	120.70
2	W	25	PHE	CB-CG-CD1	5.57	130.18	120.70
1	C	210	PRO	CA-C-O	-5.57	114.45	122.31
2	V	13	ILE	CB-CG1-CD1	-5.57	102.10	113.80
2	X	165	ARG	CA-C-O	5.57	125.87	119.35
2	Z	13	ILE	CB-CG1-CD1	-5.57	102.10	113.80
2	H	13	ILE	CB-CG1-CD1	-5.57	102.10	113.80
1	O	210	PRO	CA-C-O	-5.57	114.46	122.31
2	I	13	ILE	CB-CG1-CD1	-5.57	102.10	113.80
2	Y	13	ILE	CB-CG1-CD1	-5.57	102.10	113.80
1	E	210	PRO	CA-C-O	-5.57	114.46	122.31
2	N	13	ILE	CB-CG1-CD1	-5.57	102.11	113.80
2	M	13	ILE	CB-CG1-CD1	-5.57	102.11	113.80
2	N	165	ARG	CA-C-O	5.57	125.86	119.35
2	W	13	ILE	CB-CG1-CD1	-5.57	102.11	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	13	ILE	CB-CG1-CD1	-5.57	102.11	113.80
2	J	13	ILE	CB-CG1-CD1	-5.57	102.11	113.80
2	N	98	GLN	CA-C-O	-5.56	114.56	120.40
2	H	98	GLN	CA-C-O	-5.56	114.56	120.40
2	X	98	GLN	CA-C-O	-5.56	114.56	120.40
2	Y	98	GLN	CA-C-O	-5.56	114.56	120.40
2	L	25	PHE	CB-CG-CD1	5.56	130.16	120.70
1	F	210	PRO	CA-C-O	-5.56	114.47	122.31
2	2	13	ILE	CB-CG1-CD1	-5.56	102.12	113.80
2	2	25	PHE	CB-CG-CD1	5.56	130.16	120.70
2	H	25	PHE	CB-CG-CD1	5.56	130.16	120.70
2	K	25	PHE	CB-CG-CD1	5.56	130.16	120.70
1	S	210	PRO	CA-C-O	-5.56	114.47	122.31
1	T	210	PRO	CA-C-O	-5.56	114.47	122.31
2	1	98	GLN	CA-C-O	-5.56	114.56	120.40
1	B	210	PRO	CA-C-O	-5.56	114.47	122.31
1	U	210	PRO	CA-C-O	-5.56	114.47	122.31
2	J	88	ASN	O-C-N	-5.56	116.23	122.12
1	Q	210	PRO	CA-C-O	-5.55	114.48	122.31
1	A	210	PRO	CA-C-O	-5.55	114.48	122.31
2	V	38	ASP	CA-CB-CG	5.55	118.15	112.60
2	L	38	ASP	CA-CB-CG	5.55	118.15	112.60
2	2	38	ASP	CA-CB-CG	5.55	118.15	112.60
1	F	113	VAL	O-C-N	-5.55	116.12	121.83
2	V	33	LYS	N-CA-C	-5.55	107.76	114.75
1	Q	160	TYR	CA-CB-CG	-5.55	103.92	113.90
2	X	25	PHE	CB-CG-CD1	5.55	130.13	120.70
1	R	210	PRO	CA-C-O	-5.55	114.49	122.31
2	H	38	ASP	CA-CB-CG	5.54	118.14	112.60
2	Y	38	ASP	CA-CB-CG	5.54	118.14	112.60
2	X	33	LYS	N-CA-C	-5.54	107.77	114.75
2	N	33	LYS	N-CA-C	-5.54	107.77	114.75
2	N	88	ASN	O-C-N	-5.54	116.25	122.12
2	V	88	ASN	O-C-N	-5.54	116.25	122.12
1	Q	113	VAL	O-C-N	-5.54	116.12	121.83
1	D	194	ILE	CA-C-N	5.54	127.64	120.44
1	D	194	ILE	C-N-CA	5.54	127.64	120.44
2	L	88	ASN	O-C-N	-5.54	116.25	122.12
1	P	210	PRO	CA-C-O	-5.54	114.50	122.31
2	Z	38	ASP	CA-CB-CG	5.54	118.14	112.60
2	I	38	ASP	CA-CB-CG	5.54	118.14	112.60
2	K	98	GLN	CA-C-O	-5.54	114.59	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	33	LYS	N-CA-C	-5.53	107.78	114.75
1	A	194	ILE	CA-C-N	5.53	127.63	120.44
1	A	194	ILE	C-N-CA	5.53	127.63	120.44
2	J	38	ASP	CA-CB-CG	5.53	118.13	112.60
2	M	88	ASN	O-C-N	-5.53	116.26	122.12
1	U	160	TYR	CA-CB-CG	-5.53	103.95	113.90
1	D	160	TYR	CA-CB-CG	-5.53	103.95	113.90
2	Z	33	LYS	N-CA-C	-5.53	107.78	114.75
1	F	160	TYR	CA-CB-CG	-5.53	103.95	113.90
2	I	33	LYS	N-CA-C	-5.53	107.78	114.75
1	F	48	LEU	N-CA-C	-5.53	100.01	109.24
1	T	194	ILE	CA-C-N	5.53	127.62	120.44
1	T	194	ILE	C-N-CA	5.53	127.62	120.44
2	N	38	ASP	CA-CB-CG	5.53	118.13	112.60
2	2	33	LYS	N-CA-C	-5.53	107.79	114.75
2	X	38	ASP	CA-CB-CG	5.53	118.13	112.60
2	K	33	LYS	N-CA-C	-5.53	107.79	114.75
1	R	194	ILE	CA-C-N	5.53	127.62	120.44
1	R	194	ILE	C-N-CA	5.53	127.62	120.44
1	S	160	TYR	CA-CB-CG	-5.52	103.96	113.90
2	1	38	ASP	CA-CB-CG	5.52	118.12	112.60
1	B	160	TYR	CA-CB-CG	-5.52	103.96	113.90
1	C	194	ILE	CA-C-N	5.52	127.62	120.44
1	C	194	ILE	C-N-CA	5.52	127.62	120.44
1	Q	13	THR	CA-C-O	5.52	127.37	121.02
1	E	194	ILE	CA-C-N	5.52	127.62	120.44
1	E	194	ILE	C-N-CA	5.52	127.62	120.44
1	F	13	THR	CA-C-O	5.52	127.37	121.02
1	T	160	TYR	CA-CB-CG	-5.52	103.96	113.90
1	G	194	ILE	CA-C-N	5.52	127.62	120.44
1	G	194	ILE	C-N-CA	5.52	127.62	120.44
2	H	33	LYS	N-CA-C	-5.52	107.79	114.75
1	P	13	THR	CA-C-O	5.52	127.37	121.02
2	W	33	LYS	N-CA-C	-5.52	107.79	114.75
1	C	160	TYR	CA-CB-CG	-5.52	103.96	113.90
1	U	48	LEU	N-CA-C	-5.52	100.02	109.24
2	H	88	ASN	O-C-N	-5.52	116.27	122.12
1	T	48	LEU	N-CA-C	-5.52	100.02	109.24
1	G	13	THR	CA-C-O	5.52	127.37	121.02
1	G	48	LEU	N-CA-C	-5.52	100.02	109.24
2	X	88	ASN	O-C-N	-5.52	116.27	122.12
1	D	113	VAL	O-C-N	-5.52	116.15	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	13	THR	CA-C-O	5.52	127.36	121.02
1	U	113	VAL	O-C-N	-5.52	116.15	121.83
1	U	194	ILE	CA-C-N	5.52	127.61	120.44
1	U	194	ILE	C-N-CA	5.52	127.61	120.44
1	C	13	THR	CA-C-O	5.52	127.36	121.02
2	L	33	LYS	N-CA-C	-5.52	107.80	114.75
1	S	48	LEU	N-CA-C	-5.52	100.03	109.24
1	F	194	ILE	CA-C-N	5.52	127.61	120.44
1	F	194	ILE	C-N-CA	5.52	127.61	120.44
1	B	48	LEU	N-CA-C	-5.52	100.03	109.24
1	C	113	VAL	O-C-N	-5.52	116.15	121.83
1	G	160	TYR	CA-CB-CG	-5.51	103.97	113.90
1	O	73	TYR	CB-CA-C	-5.51	101.40	110.72
1	P	113	VAL	O-C-N	-5.51	116.15	121.83
1	S	194	ILE	CA-C-N	5.51	127.61	120.44
1	S	194	ILE	C-N-CA	5.51	127.61	120.44
2	M	38	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	160	TYR	CA-CB-CG	-5.51	103.98	113.90
1	B	194	ILE	CA-C-N	5.51	127.61	120.44
1	B	194	ILE	C-N-CA	5.51	127.61	120.44
2	W	38	ASP	CA-CB-CG	5.51	118.11	112.60
1	R	160	TYR	CA-CB-CG	-5.51	103.98	113.90
2	Z	88	ASN	O-C-N	-5.51	116.28	122.12
1	A	113	VAL	O-C-N	-5.51	116.15	121.83
2	I	88	ASN	O-C-N	-5.51	116.28	122.12
1	P	48	LEU	N-CA-C	-5.51	100.04	109.24
1	P	194	ILE	CA-C-N	5.51	127.61	120.44
1	P	194	ILE	C-N-CA	5.51	127.61	120.44
1	Q	194	ILE	CA-C-N	5.51	127.61	120.44
1	Q	194	ILE	C-N-CA	5.51	127.61	120.44
2	Y	88	ASN	O-C-N	-5.51	116.28	122.12
2	V	134	VAL	CA-C-O	-5.51	115.01	120.85
2	L	134	VAL	CA-C-O	-5.51	115.01	120.85
1	A	48	LEU	N-CA-C	-5.51	100.04	109.24
1	P	160	TYR	CA-CB-CG	-5.51	103.99	113.90
1	R	48	LEU	N-CA-C	-5.51	100.04	109.24
1	S	13	THR	CA-C-O	5.51	127.35	121.02
1	B	13	THR	CA-C-O	5.51	127.35	121.02
2	K	88	ASN	O-C-N	-5.51	116.28	122.12
1	D	73	TYR	CB-CA-C	-5.50	101.42	110.72
1	S	113	VAL	O-C-N	-5.50	116.16	121.83
1	B	113	VAL	O-C-N	-5.50	116.16	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	33	LYS	N-CA-C	-5.50	107.82	114.75
1	U	13	THR	CA-C-O	5.50	127.35	121.02
1	O	48	LEU	N-CA-C	-5.50	100.05	109.24
1	O	160	TYR	CA-CB-CG	-5.50	104.00	113.90
1	D	13	THR	CA-C-O	5.50	127.35	121.02
1	D	48	LEU	N-CA-C	-5.50	100.05	109.24
1	E	73	TYR	CB-CA-C	-5.50	101.42	110.72
2	1	88	ASN	O-C-N	-5.50	116.29	122.12
2	H	134	VAL	CA-C-O	-5.50	115.02	120.85
1	C	48	LEU	N-CA-C	-5.50	100.06	109.24
2	Y	33	LYS	N-CA-C	-5.50	107.82	114.75
1	E	48	LEU	N-CA-C	-5.50	100.06	109.24
1	O	113	VAL	O-C-N	-5.50	116.17	121.83
1	O	194	ILE	CA-C-N	5.50	127.58	120.44
1	O	194	ILE	C-N-CA	5.50	127.58	120.44
1	C	73	TYR	CB-CA-C	-5.50	101.43	110.72
2	J	33	LYS	N-CA-C	-5.50	107.83	114.75
1	Q	48	LEU	N-CA-C	-5.50	100.06	109.24
1	E	113	VAL	O-C-N	-5.50	116.17	121.83
2	2	88	ASN	O-C-N	-5.50	116.30	122.12
1	O	112	LEU	CA-C-N	5.50	128.22	120.42
1	O	112	LEU	C-N-CA	5.50	128.22	120.42
1	F	112	LEU	CA-C-N	5.49	128.22	120.42
1	F	112	LEU	C-N-CA	5.49	128.22	120.42
1	U	73	TYR	CB-CA-C	-5.49	101.44	110.72
1	O	13	THR	CA-C-O	5.49	127.34	121.02
1	O	118	ASP	N-CA-CB	5.49	118.20	110.12
1	P	112	LEU	CA-C-N	5.49	128.22	120.42
1	P	112	LEU	C-N-CA	5.49	128.22	120.42
2	W	131	SER	N-CA-CB	5.49	120.15	110.37
1	E	13	THR	CA-C-O	5.49	127.34	121.02
1	E	160	TYR	CA-CB-CG	-5.49	104.01	113.90
2	1	134	VAL	CA-C-O	-5.49	115.03	120.85
1	A	73	TYR	CB-CA-C	-5.49	101.44	110.72
2	2	131	SER	N-CA-CB	5.49	120.14	110.37
1	A	13	THR	CA-C-O	5.49	127.33	121.02
1	P	118	ASP	N-CA-CB	5.49	118.19	110.12
2	J	134	VAL	CA-C-O	-5.49	115.03	120.85
2	K	131	SER	N-CA-CB	5.49	120.14	110.37
1	R	13	THR	CA-C-O	5.49	127.33	121.02
1	S	73	TYR	CB-CA-C	-5.49	101.44	110.72
2	Z	134	VAL	CA-C-O	-5.49	115.03	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	131	SER	N-CA-CB	5.49	120.14	110.37
1	B	73	TYR	CB-CA-C	-5.49	101.44	110.72
2	I	134	VAL	CA-C-O	-5.49	115.03	120.85
2	X	131	SER	N-CA-CB	5.49	120.14	110.37
1	Q	112	LEU	CA-C-N	5.49	128.21	120.42
1	Q	112	LEU	C-N-CA	5.49	128.21	120.42
1	R	113	VAL	O-C-N	-5.49	116.18	121.83
1	T	113	VAL	O-C-N	-5.49	116.18	121.83
1	G	112	LEU	CA-C-N	5.49	128.21	120.42
1	G	112	LEU	C-N-CA	5.49	128.21	120.42
1	T	73	TYR	CB-CA-C	-5.48	101.45	110.72
2	2	134	VAL	CA-C-O	-5.48	115.04	120.85
2	K	134	VAL	CA-C-O	-5.48	115.04	120.85
1	P	73	TYR	CB-CA-C	-5.48	101.45	110.72
1	G	73	TYR	CB-CA-C	-5.48	101.46	110.72
1	Q	73	TYR	CB-CA-C	-5.48	101.46	110.72
2	X	134	VAL	CA-C-O	-5.48	115.04	120.85
1	R	118	ASP	N-CA-CB	5.48	118.18	110.12
2	L	86	MET	CA-C-N	5.48	127.89	120.44
2	L	86	MET	C-N-CA	5.48	127.89	120.44
1	S	112	LEU	CA-C-N	5.48	128.20	120.42
1	S	112	LEU	C-N-CA	5.48	128.20	120.42
1	G	113	VAL	O-C-N	-5.48	116.19	121.83
1	B	112	LEU	CA-C-N	5.48	128.20	120.42
1	B	112	LEU	C-N-CA	5.48	128.20	120.42
2	Y	131	SER	N-CA-CB	5.48	120.12	110.37
1	S	118	ASP	N-CA-CB	5.48	118.17	110.12
1	B	118	ASP	N-CA-CB	5.48	118.17	110.12
1	D	112	LEU	CA-C-N	5.48	128.20	120.42
1	D	112	LEU	C-N-CA	5.48	128.20	120.42
1	E	118	ASP	N-CA-CB	5.48	118.17	110.12
1	T	112	LEU	CA-C-N	5.48	128.20	120.42
1	T	112	LEU	C-N-CA	5.48	128.20	120.42
1	G	73	TYR	CB-CG-CD1	-5.48	112.59	120.80
1	P	73	TYR	CB-CG-CD1	-5.48	112.59	120.80
1	Q	73	TYR	CB-CG-CD1	-5.48	112.59	120.80
1	R	112	LEU	CA-C-N	5.48	128.20	120.42
1	R	112	LEU	C-N-CA	5.48	128.20	120.42
1	E	73	TYR	CB-CG-CD1	-5.48	112.58	120.80
2	V	86	MET	CA-C-N	5.47	127.89	120.44
2	V	86	MET	C-N-CA	5.47	127.89	120.44
2	W	88	ASN	O-C-N	-5.47	116.32	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	73	TYR	CB-CA-C	-5.47	101.47	110.72
1	F	73	TYR	CB-CG-CD1	-5.47	112.59	120.80
1	C	73	TYR	CB-CG-CD1	-5.47	112.59	120.80
1	C	118	ASP	N-CA-CB	5.47	118.16	110.12
2	M	134	VAL	CA-C-O	-5.47	115.05	120.85
2	W	134	VAL	CA-C-O	-5.47	115.05	120.85
2	Z	131	SER	N-CA-CB	5.47	120.11	110.37
1	T	118	ASP	N-CA-CB	5.47	118.16	110.12
1	G	118	ASP	N-CA-CB	5.47	118.16	110.12
1	U	73	TYR	CB-CG-CD1	-5.47	112.60	120.80
1	U	112	LEU	CA-C-N	5.47	128.19	120.42
1	U	112	LEU	C-N-CA	5.47	128.19	120.42
2	V	24	ASN	CB-CA-C	-5.47	100.62	110.35
2	I	131	SER	N-CA-CB	5.47	120.11	110.37
1	Q	118	ASP	N-CA-CB	5.47	118.16	110.12
2	N	86	MET	CA-C-N	5.47	127.88	120.44
2	N	86	MET	C-N-CA	5.47	127.88	120.44
2	H	131	SER	N-CA-CB	5.47	120.10	110.37
1	O	73	TYR	CB-CG-CD1	-5.47	112.60	120.80
2	X	86	MET	CA-C-N	5.47	127.88	120.44
2	X	86	MET	C-N-CA	5.47	127.88	120.44
1	R	73	TYR	CB-CA-C	-5.47	101.48	110.72
2	L	55	LEU	N-CA-C	-5.47	105.32	111.28
2	L	131	SER	N-CA-CB	5.47	120.10	110.37
1	F	118	ASP	N-CA-CB	5.47	118.15	110.12
1	A	118	ASP	N-CA-CB	5.47	118.16	110.12
1	O	149	PHE	N-CA-CB	5.47	121.06	111.55
2	J	131	SER	N-CA-CB	5.47	120.10	110.37
1	D	73	TYR	CB-CG-CD1	-5.47	112.60	120.80
1	E	149	PHE	N-CA-CB	5.47	121.06	111.55
1	S	73	TYR	CB-CG-CD1	-5.46	112.60	120.80
1	F	149	PHE	N-CA-CB	5.46	121.06	111.55
2	M	24	ASN	CB-CA-C	-5.46	100.62	110.35
2	1	86	MET	CA-C-N	5.46	127.87	120.44
2	1	86	MET	C-N-CA	5.46	127.87	120.44
1	B	73	TYR	CB-CG-CD1	-5.46	112.60	120.80
1	C	112	LEU	CA-C-N	5.46	128.18	120.42
1	C	112	LEU	C-N-CA	5.46	128.18	120.42
2	X	24	ASN	CB-CA-C	-5.46	100.62	110.35
2	Z	24	ASN	CB-CA-C	-5.46	100.63	110.35
1	G	149	PHE	N-CA-CB	5.46	121.06	111.55
2	V	131	SER	N-CA-CB	5.46	120.09	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	24	ASN	CB-CA-C	-5.46	100.63	110.35
1	D	149	PHE	N-CA-CB	5.46	121.06	111.55
2	K	24	ASN	CB-CA-C	-5.46	100.62	110.35
1	S	149	PHE	N-CA-CB	5.46	121.05	111.55
2	M	131	SER	N-CA-CB	5.46	120.09	110.37
1	U	149	PHE	N-CA-CB	5.46	121.05	111.55
1	B	149	PHE	N-CA-CB	5.46	121.05	111.55
2	1	24	ASN	CB-CA-C	-5.46	100.63	110.35
2	N	24	ASN	CB-CA-C	-5.46	100.63	110.35
2	2	24	ASN	CB-CA-C	-5.46	100.63	110.35
2	W	24	ASN	CB-CA-C	-5.46	100.63	110.35
1	R	149	PHE	N-CA-CB	5.46	121.05	111.55
1	T	149	PHE	N-CA-CB	5.46	121.05	111.55
1	P	149	PHE	N-CA-CB	5.46	121.05	111.55
1	D	118	ASP	N-CA-CB	5.46	118.14	110.12
2	N	134	VAL	CA-C-O	-5.46	115.07	120.85
1	R	73	TYR	CB-CG-CD1	-5.46	112.62	120.80
2	M	86	MET	CA-C-N	5.46	127.86	120.44
2	M	86	MET	C-N-CA	5.46	127.86	120.44
1	A	149	PHE	N-CA-CB	5.46	121.04	111.55
2	L	24	ASN	CB-CA-C	-5.46	100.64	110.35
1	U	118	ASP	N-CA-CB	5.45	118.14	110.12
2	2	86	MET	CA-C-N	5.45	127.86	120.44
2	2	86	MET	C-N-CA	5.45	127.86	120.44
1	A	112	LEU	CA-C-N	5.45	128.16	120.42
1	A	112	LEU	C-N-CA	5.45	128.16	120.42
2	H	24	ASN	CB-CA-C	-5.45	100.64	110.35
2	J	24	ASN	CB-CA-C	-5.45	100.64	110.35
2	Y	24	ASN	CB-CA-C	-5.45	100.64	110.35
1	T	73	TYR	CB-CG-CD1	-5.45	112.62	120.80
1	C	149	PHE	N-CA-CB	5.45	121.03	111.55
1	Q	149	PHE	N-CA-CB	5.45	121.04	111.55
2	Y	134	VAL	CA-C-O	-5.45	115.07	120.85
2	M	55	LEU	N-CA-C	-5.45	105.34	111.28
2	1	131	SER	N-CA-CB	5.45	120.07	110.37
1	A	73	TYR	CB-CG-CD1	-5.45	112.63	120.80
2	Y	86	MET	CA-C-N	5.45	127.85	120.44
2	Y	86	MET	C-N-CA	5.45	127.85	120.44
2	Z	86	MET	CA-C-N	5.45	127.85	120.44
2	Z	86	MET	C-N-CA	5.45	127.85	120.44
2	I	86	MET	CA-C-N	5.45	127.85	120.44
2	I	86	MET	C-N-CA	5.45	127.85	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	112	LEU	CA-C-N	5.45	128.15	120.42
1	E	112	LEU	C-N-CA	5.45	128.15	120.42
2	M	162	ALA	CB-CA-C	-5.44	101.42	110.68
2	W	162	ALA	CB-CA-C	-5.44	101.42	110.68
2	1	75	PRO	N-CA-CB	-5.44	98.75	103.32
2	H	55	LEU	N-CA-C	-5.44	105.35	111.28
2	J	75	PRO	N-CA-CB	-5.44	98.75	103.32
2	K	55	LEU	N-CA-C	-5.44	105.35	111.28
2	K	162	ALA	CB-CA-C	-5.44	101.43	110.68
2	Y	55	LEU	N-CA-C	-5.44	105.35	111.28
2	H	86	MET	CA-C-N	5.44	127.84	120.44
2	H	86	MET	C-N-CA	5.44	127.84	120.44
2	Z	55	LEU	N-CA-C	-5.44	105.35	111.28
2	Z	162	ALA	CB-CA-C	-5.44	101.44	110.68
2	I	55	LEU	N-CA-C	-5.44	105.35	111.28
2	I	162	ALA	CB-CA-C	-5.44	101.44	110.68
2	K	86	MET	CA-C-N	5.44	127.83	120.44
2	K	86	MET	C-N-CA	5.44	127.83	120.44
2	1	162	ALA	CB-CA-C	-5.43	101.44	110.68
2	J	162	ALA	CB-CA-C	-5.43	101.44	110.68
2	X	162	ALA	CB-CA-C	-5.43	101.44	110.68
1	U	189	ALA	CA-C-O	-5.43	115.11	120.82
2	W	86	MET	CA-C-N	5.43	127.83	120.44
2	W	86	MET	C-N-CA	5.43	127.83	120.44
2	N	162	ALA	CB-CA-C	-5.43	101.45	110.68
2	H	162	ALA	CB-CA-C	-5.43	101.45	110.68
2	Y	162	ALA	CB-CA-C	-5.43	101.45	110.68
2	L	162	ALA	CB-CA-C	-5.43	101.45	110.68
2	N	55	LEU	N-CA-C	-5.43	105.36	111.28
2	V	162	ALA	CB-CA-C	-5.43	101.45	110.68
2	X	55	LEU	N-CA-C	-5.43	105.36	111.28
1	U	14	VAL	N-CA-C	-5.42	100.39	107.88
1	C	189	ALA	CA-C-O	-5.42	115.12	120.82
1	D	14	VAL	N-CA-C	-5.42	100.39	107.88
2	1	55	LEU	N-CA-C	-5.42	105.37	111.28
2	J	55	LEU	N-CA-C	-5.42	105.37	111.28
2	N	75	PRO	N-CA-CB	-5.42	98.77	103.32
2	2	162	ALA	CB-CA-C	-5.42	101.46	110.68
1	F	189	ALA	CA-C-O	-5.42	115.13	120.82
2	W	55	LEU	N-CA-C	-5.42	105.37	111.28
1	Q	189	ALA	CA-C-O	-5.42	115.13	120.82
2	M	75	PRO	N-CA-CB	-5.42	98.77	103.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	189	ALA	CA-C-O	-5.42	115.13	120.82
2	Z	75	PRO	N-CA-CB	-5.42	98.77	103.32
2	H	75	PRO	N-CA-CB	-5.42	98.77	103.32
1	O	14	VAL	N-CA-C	-5.42	100.40	107.88
1	O	189	ALA	CA-C-O	-5.42	115.13	120.82
2	I	75	PRO	N-CA-CB	-5.42	98.77	103.32
1	D	187	LYS	N-CA-CB	5.42	118.01	109.94
1	E	14	VAL	N-CA-C	-5.42	100.40	107.88
1	E	189	ALA	CA-C-O	-5.42	115.13	120.82
1	T	187	LYS	N-CA-CB	5.41	118.00	109.94
2	L	145	LYS	O-C-N	5.41	128.69	122.25
1	S	189	ALA	CA-C-O	-5.41	115.14	120.82
1	F	187	LYS	N-CA-CB	5.41	118.00	109.94
1	T	14	VAL	N-CA-C	-5.41	100.41	107.88
2	V	55	LEU	N-CA-C	-5.41	105.38	111.28
1	B	189	ALA	CA-C-O	-5.41	115.14	120.82
1	P	187	LYS	N-CA-CB	5.41	118.00	109.94
1	C	14	VAL	N-CA-C	-5.41	100.41	107.88
1	S	14	VAL	N-CA-C	-5.41	100.41	107.88
1	B	14	VAL	N-CA-C	-5.41	100.41	107.88
2	J	86	MET	CA-C-N	5.41	127.80	120.44
2	J	86	MET	C-N-CA	5.41	127.80	120.44
2	Y	145	LYS	O-C-N	5.41	128.69	122.25
1	F	14	VAL	N-CA-C	-5.41	100.42	107.88
2	1	134	VAL	N-CA-CB	5.41	118.69	110.58
1	P	14	VAL	N-CA-C	-5.41	100.42	107.88
2	2	55	LEU	N-CA-C	-5.41	105.39	111.28
2	V	75	PRO	N-CA-CB	-5.41	98.78	103.32
1	P	189	ALA	CA-C-O	-5.41	115.14	120.82
2	W	75	PRO	N-CA-CB	-5.41	98.78	103.32
1	C	187	LYS	N-CA-CB	5.41	118.00	109.94
1	Q	137	ILE	N-CA-C	-5.41	100.41	108.46
2	K	145	LYS	O-C-N	5.41	128.68	122.25
2	L	75	PRO	N-CA-CB	-5.41	98.78	103.32
1	U	187	LYS	N-CA-CB	5.40	117.99	109.94
1	G	14	VAL	N-CA-C	-5.40	100.43	107.88
2	H	134	VAL	N-CA-CB	5.40	118.68	110.58
2	W	37	ILE	O-C-N	5.40	128.94	122.03
1	Q	14	VAL	N-CA-C	-5.40	100.43	107.88
2	X	75	PRO	N-CA-CB	-5.40	98.78	103.32
1	R	14	VAL	N-CA-C	-5.40	100.42	107.88
2	Y	134	VAL	N-CA-CB	5.40	118.68	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	187	LYS	N-CA-CB	5.40	117.99	109.94
2	2	134	VAL	N-CA-CB	5.40	118.68	110.58
1	B	187	LYS	N-CA-CB	5.40	117.99	109.94
1	G	189	ALA	CA-C-O	-5.40	115.15	120.82
1	A	187	LYS	N-CA-CB	5.40	117.98	109.94
1	O	187	LYS	N-CA-CB	5.40	117.98	109.94
2	X	37	ILE	O-C-N	5.40	128.94	122.03
2	L	134	VAL	N-CA-CB	5.40	118.68	110.58
1	F	137	ILE	N-CA-C	-5.39	100.42	108.46
1	G	137	ILE	N-CA-C	-5.39	100.42	108.46
2	2	75	PRO	N-CA-CB	-5.39	98.79	103.32
1	O	137	ILE	N-CA-C	-5.39	100.42	108.46
2	K	75	PRO	N-CA-CB	-5.39	98.79	103.32
2	V	134	VAL	N-CA-CB	5.39	118.67	110.58
2	M	145	LYS	O-C-N	5.39	128.66	122.25
1	T	189	ALA	CA-C-O	-5.39	115.16	120.82
2	1	145	LYS	O-C-N	5.39	128.66	122.25
1	U	137	ILE	N-CA-C	-5.39	100.43	108.46
2	W	145	LYS	O-C-N	5.39	128.66	122.25
2	J	145	LYS	O-C-N	5.39	128.66	122.25
1	D	137	ILE	N-CA-C	-5.39	100.43	108.46
1	R	137	ILE	N-CA-C	-5.39	100.43	108.46
2	N	134	VAL	N-CA-CB	5.39	118.66	110.58
1	E	137	ILE	N-CA-C	-5.39	100.43	108.46
2	Z	134	VAL	N-CA-CB	5.39	118.66	110.58
2	N	201	LEU	N-CA-C	-5.39	105.41	112.41
1	A	14	VAL	N-CA-C	-5.39	100.45	107.88
2	I	134	VAL	N-CA-CB	5.39	118.66	110.58
1	P	137	ILE	N-CA-C	-5.39	100.44	108.46
2	Y	37	ILE	O-C-N	5.39	128.92	122.03
1	T	137	ILE	N-CA-C	-5.38	100.44	108.46
1	G	187	LYS	N-CA-CB	5.38	117.96	109.94
2	2	37	ILE	O-C-N	5.38	128.92	122.03
1	C	137	ILE	N-CA-C	-5.38	100.44	108.46
2	K	37	ILE	O-C-N	5.38	128.92	122.03
1	R	187	LYS	N-CA-CB	5.38	117.96	109.94
1	S	137	ILE	N-CA-C	-5.38	100.44	108.46
2	1	201	LEU	N-CA-C	-5.38	105.41	112.41
1	B	137	ILE	N-CA-C	-5.38	100.44	108.46
2	Z	37	ILE	O-C-N	5.38	128.92	122.03
2	V	37	ILE	O-C-N	5.38	128.92	122.03
2	I	37	ILE	O-C-N	5.38	128.92	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	201	LEU	N-CA-C	-5.38	105.41	112.41
1	E	187	LYS	N-CA-CB	5.38	117.96	109.94
2	M	37	ILE	O-C-N	5.38	128.91	122.03
2	H	201	LEU	N-CA-C	-5.38	105.42	112.41
2	V	145	LYS	O-C-N	5.38	128.65	122.25
2	Y	201	LEU	N-CA-C	-5.38	105.42	112.41
2	L	37	ILE	O-C-N	5.38	128.91	122.03
2	M	134	VAL	N-CA-CB	5.38	118.65	110.58
2	H	37	ILE	O-C-N	5.38	128.91	122.03
2	W	134	VAL	N-CA-CB	5.38	118.65	110.58
2	Y	75	PRO	N-CA-CB	-5.38	98.81	103.32
2	M	201	LEU	N-CA-C	-5.37	105.42	112.41
2	1	37	ILE	O-C-N	5.37	128.91	122.03
1	A	189	ALA	CA-C-O	-5.37	115.18	120.82
2	W	201	LEU	N-CA-C	-5.37	105.42	112.41
2	J	201	LEU	N-CA-C	-5.37	105.42	112.41
1	Q	187	LYS	N-CA-CB	5.37	117.95	109.94
2	Z	145	LYS	O-C-N	5.37	128.64	122.25
2	N	37	ILE	O-C-N	5.37	128.91	122.03
2	I	145	LYS	O-C-N	5.37	128.64	122.25
2	J	37	ILE	O-C-N	5.37	128.91	122.03
2	X	16	THR	N-CA-C	-5.37	100.91	109.07
1	D	189	ALA	CA-C-O	-5.37	115.18	120.82
2	N	145	LYS	O-C-N	5.37	128.64	122.25
1	Q	150	ASP	CA-CB-CG	5.37	117.97	112.60
2	X	145	LYS	O-C-N	5.37	128.64	122.25
2	1	16	THR	N-CA-C	-5.37	100.91	109.07
2	V	201	LEU	N-CA-C	-5.37	105.43	112.41
1	P	150	ASP	CA-CB-CG	5.37	117.97	112.60
2	J	16	THR	N-CA-C	-5.37	100.91	109.07
2	J	134	VAL	N-CA-CB	5.37	118.63	110.58
2	K	201	LEU	N-CA-C	-5.37	105.43	112.41
2	Y	16	THR	N-CA-C	-5.37	100.91	109.07
2	K	134	VAL	N-CA-CB	5.37	118.63	110.58
2	2	16	THR	N-CA-C	-5.37	100.91	109.07
2	K	16	THR	N-CA-C	-5.37	100.91	109.07
1	E	150	ASP	CA-CB-CG	5.37	117.97	112.60
2	Z	201	LEU	N-CA-C	-5.36	105.44	112.41
1	U	150	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	218	GLY	O-C-N	-5.36	115.58	122.39
2	I	201	LEU	N-CA-C	-5.36	105.44	112.41
1	D	150	ASP	CA-CB-CG	5.36	117.96	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ASP	CA-CB-CG	5.36	117.96	112.60
1	P	218	GLY	O-C-N	-5.36	115.58	122.39
2	N	16	THR	N-CA-C	-5.36	100.93	109.07
1	S	150	ASP	CA-CB-CG	5.36	117.95	112.60
1	B	150	ASP	CA-CB-CG	5.36	117.95	112.60
2	J	44	THR	CA-C-N	5.36	130.01	123.10
2	J	44	THR	C-N-CA	5.36	130.01	123.10
2	L	16	THR	N-CA-C	-5.36	100.93	109.07
1	A	137	ILE	N-CA-C	-5.35	100.48	108.46
2	Z	16	THR	N-CA-C	-5.35	100.93	109.07
1	F	218	GLY	O-C-N	-5.35	115.59	122.39
2	I	16	THR	N-CA-C	-5.35	100.93	109.07
2	2	145	LYS	O-C-N	5.35	128.62	122.25
2	H	16	THR	N-CA-C	-5.35	100.94	109.07
1	D	164	ALA	N-CA-C	-5.35	100.99	108.96
2	L	201	LEU	N-CA-C	-5.35	105.46	112.41
2	M	16	THR	N-CA-C	-5.35	100.94	109.07
2	V	16	THR	N-CA-C	-5.35	100.94	109.07
1	C	164	ALA	N-CA-C	-5.35	100.99	108.96
2	X	134	VAL	N-CA-CB	5.35	118.60	110.58
2	2	201	LEU	N-CA-C	-5.34	105.46	112.41
2	W	44	THR	CA-C-N	5.34	129.99	123.10
2	W	44	THR	C-N-CA	5.34	129.99	123.10
1	S	164	ALA	N-CA-C	-5.34	101.00	108.96
2	H	145	LYS	O-C-N	5.34	128.61	122.25
1	B	164	ALA	N-CA-C	-5.34	101.00	108.96
1	G	150	ASP	CA-CB-CG	5.34	117.94	112.60
2	Y	31	GLY	N-CA-C	-5.34	104.40	112.41
1	P	164	ALA	N-CA-C	-5.34	101.00	108.96
1	R	218	GLY	O-C-N	-5.34	115.61	122.39
1	F	150	ASP	CA-CB-CG	5.34	117.94	112.60
1	T	150	ASP	CA-CB-CG	5.34	117.94	112.60
1	U	218	GLY	O-C-N	-5.34	115.61	122.39
1	C	150	ASP	CA-CB-CG	5.34	117.94	112.60
2	Y	44	THR	CA-C-N	5.34	129.99	123.10
2	Y	44	THR	C-N-CA	5.34	129.99	123.10
1	C	218	GLY	O-C-N	-5.34	115.61	122.39
1	Q	68	GLN	CB-CG-CD	-5.34	103.53	112.60
1	E	218	GLY	O-C-N	-5.34	115.61	122.39
2	2	44	THR	CA-C-N	5.33	129.98	123.10
2	2	44	THR	C-N-CA	5.33	129.98	123.10
2	K	44	THR	CA-C-N	5.33	129.98	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	44	THR	C-N-CA	5.33	129.98	123.10
1	S	218	GLY	O-C-N	-5.33	115.62	122.39
1	G	164	ALA	N-CA-C	-5.33	101.01	108.96
2	H	31	GLY	N-CA-C	-5.33	104.41	112.41
1	B	218	GLY	O-C-N	-5.33	115.62	122.39
2	W	31	GLY	N-CA-C	-5.33	104.41	112.41
1	C	68	GLN	CB-CG-CD	-5.33	103.53	112.60
1	Q	164	ALA	N-CA-C	-5.33	101.01	108.96
2	X	44	THR	CA-C-N	5.33	129.98	123.10
2	X	44	THR	C-N-CA	5.33	129.98	123.10
2	1	44	THR	CA-C-N	5.33	129.98	123.10
2	1	44	THR	C-N-CA	5.33	129.98	123.10
1	O	150	ASP	CA-CB-CG	5.33	117.93	112.60
1	Q	218	GLY	O-C-N	-5.33	115.62	122.39
1	T	164	ALA	N-CA-C	-5.33	101.02	108.96
1	R	150	ASP	CA-CB-CG	5.33	117.93	112.60
2	2	31	GLY	N-CA-C	-5.33	104.42	112.41
2	V	44	THR	CA-C-N	5.33	129.97	123.10
2	V	44	THR	C-N-CA	5.33	129.97	123.10
2	K	31	GLY	N-CA-C	-5.33	104.42	112.41
1	F	68	GLN	CB-CG-CD	-5.33	103.55	112.60
1	U	164	ALA	N-CA-C	-5.33	101.02	108.96
1	P	68	GLN	CB-CG-CD	-5.33	103.55	112.60
2	W	16	THR	N-CA-C	-5.33	100.97	109.07
2	Z	31	GLY	N-CA-C	-5.32	104.43	112.41
1	T	68	GLN	CB-CG-CD	-5.32	103.55	112.60
2	I	31	GLY	N-CA-C	-5.32	104.43	112.41
1	R	68	GLN	CB-CG-CD	-5.32	103.55	112.60
1	O	218	GLY	O-C-N	-5.32	115.63	122.39
2	N	31	GLY	N-CA-C	-5.32	104.43	112.41
1	A	164	ALA	N-CA-C	-5.32	101.03	108.96
2	X	31	GLY	N-CA-C	-5.32	104.43	112.41
1	D	68	GLN	CB-CG-CD	-5.32	103.55	112.60
2	N	44	THR	CA-C-N	5.32	129.96	123.10
2	N	44	THR	C-N-CA	5.32	129.96	123.10
1	S	68	GLN	CB-CG-CD	-5.32	103.56	112.60
2	Z	44	THR	CA-C-N	5.32	129.96	123.10
2	Z	44	THR	C-N-CA	5.32	129.96	123.10
1	B	68	GLN	CB-CG-CD	-5.32	103.56	112.60
2	I	44	THR	CA-C-N	5.32	129.96	123.10
2	I	44	THR	C-N-CA	5.32	129.96	123.10
1	E	164	ALA	N-CA-C	-5.32	101.04	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	68	GLN	CB-CG-CD	-5.32	103.56	112.60
2	M	44	THR	CA-C-N	5.31	129.95	123.10
2	M	44	THR	C-N-CA	5.31	129.95	123.10
2	1	31	GLY	N-CA-C	-5.31	104.44	112.41
2	J	31	GLY	N-CA-C	-5.31	104.44	112.41
1	R	164	ALA	N-CA-C	-5.31	101.05	108.96
1	T	218	GLY	O-C-N	-5.31	115.65	122.39
1	A	68	GLN	CB-CG-CD	-5.31	103.57	112.60
2	H	44	THR	CA-C-N	5.31	129.95	123.10
2	H	44	THR	C-N-CA	5.31	129.95	123.10
1	O	68	GLN	CB-CG-CD	-5.31	103.57	112.60
1	O	164	ALA	N-CA-C	-5.31	101.05	108.96
1	D	218	GLY	O-C-N	-5.31	115.65	122.39
1	U	68	GLN	CB-CG-CD	-5.31	103.58	112.60
1	F	164	ALA	N-CA-C	-5.30	101.06	108.96
2	V	31	GLY	N-CA-C	-5.30	104.45	112.41
1	G	218	GLY	O-C-N	-5.30	115.66	122.39
2	L	44	THR	CA-C-N	5.30	129.94	123.10
2	L	44	THR	C-N-CA	5.30	129.94	123.10
2	M	31	GLY	N-CA-C	-5.30	104.47	112.41
1	E	68	GLN	CB-CG-CD	-5.29	103.60	112.60
2	L	31	GLY	N-CA-C	-5.29	104.47	112.41
1	T	222	ARG	CB-CA-C	-5.29	101.39	110.16
1	R	222	ARG	CB-CA-C	-5.29	101.39	110.16
1	D	222	ARG	CB-CA-C	-5.28	101.39	110.16
1	A	222	ARG	CB-CA-C	-5.28	101.40	110.16
1	S	222	ARG	CB-CA-C	-5.28	101.40	110.16
1	B	222	ARG	CB-CA-C	-5.28	101.40	110.16
1	F	222	ARG	CB-CA-C	-5.28	101.40	110.16
1	U	222	ARG	CB-CA-C	-5.28	101.40	110.16
1	O	222	ARG	CB-CA-C	-5.28	101.40	110.16
2	V	12	VAL	CA-C-O	5.28	126.62	121.19
1	P	222	ARG	CB-CA-C	-5.28	101.40	110.16
1	E	222	ARG	CB-CA-C	-5.28	101.40	110.16
2	K	12	VAL	CA-C-O	5.27	126.62	121.19
2	M	12	VAL	CA-C-O	5.27	126.62	121.19
1	G	222	ARG	CB-CA-C	-5.27	101.41	110.16
2	W	12	VAL	CA-C-O	5.27	126.62	121.19
1	C	222	ARG	CB-CA-C	-5.27	101.41	110.16
1	Q	222	ARG	CB-CA-C	-5.27	101.41	110.16
2	H	12	VAL	CA-C-O	5.26	126.61	121.19
2	Y	12	VAL	CA-C-O	5.26	126.61	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	12	VAL	CA-C-O	5.26	126.61	121.19
1	A	132	TYR	CB-CG-CD1	-5.26	112.91	120.80
1	R	132	TYR	CB-CG-CD1	-5.26	112.91	120.80
2	N	12	VAL	CA-C-O	5.26	126.61	121.19
2	Z	12	VAL	CA-C-O	5.25	126.60	121.19
1	G	132	TYR	CB-CG-CD1	-5.25	112.92	120.80
1	U	101	VAL	CA-CB-CG1	5.25	119.33	110.40
2	I	12	VAL	CA-C-O	5.25	126.60	121.19
2	L	12	VAL	CA-C-O	5.25	126.60	121.19
1	A	10	ARG	NH1-CZ-NH2	5.25	126.12	119.30
1	P	101	VAL	CA-CB-CG1	5.25	119.32	110.40
1	R	10	ARG	NH1-CZ-NH2	5.25	126.12	119.30
1	D	10	ARG	NH1-CZ-NH2	5.25	126.12	119.30
1	A	101	VAL	CA-CB-CG1	5.24	119.31	110.40
1	O	132	TYR	CB-CG-CD1	-5.24	112.93	120.80
2	J	12	VAL	CA-C-O	5.24	126.59	121.19
2	2	12	VAL	CA-C-O	5.24	126.59	121.19
1	T	101	VAL	CA-CB-CG1	5.24	119.31	110.40
1	O	101	VAL	CA-CB-CG1	5.24	119.31	110.40
1	C	101	VAL	CA-CB-CG1	5.24	119.31	110.40
1	C	132	TYR	CB-CG-CD1	-5.24	112.94	120.80
1	E	101	VAL	CA-CB-CG1	5.24	119.31	110.40
1	F	101	VAL	CA-CB-CG1	5.24	119.31	110.40
1	F	132	TYR	CB-CG-CD1	-5.24	112.94	120.80
2	2	194	SER	N-CA-C	-5.24	105.46	111.07
1	P	132	TYR	CB-CG-CD1	-5.24	112.94	120.80
1	Q	101	VAL	CA-CB-CG1	5.24	119.31	110.40
1	D	101	VAL	CA-CB-CG1	5.24	119.31	110.40
1	E	132	TYR	CB-CG-CD1	-5.24	112.94	120.80
1	S	101	VAL	CA-CB-CG1	5.24	119.30	110.40
1	B	101	VAL	CA-CB-CG1	5.24	119.30	110.40
1	T	10	ARG	NH1-CZ-NH2	5.23	126.10	119.30
1	C	10	ARG	NH1-CZ-NH2	5.23	126.10	119.30
1	S	132	TYR	CB-CG-CD1	-5.23	112.95	120.80
1	B	132	TYR	CB-CG-CD1	-5.23	112.95	120.80
2	X	80	ALA	CA-C-N	5.23	127.24	120.44
2	X	80	ALA	C-N-CA	5.23	127.24	120.44
1	G	101	VAL	CA-CB-CG1	5.23	119.29	110.40
2	W	194	SER	N-CA-C	-5.23	105.47	111.07
2	X	12	VAL	CA-C-O	5.23	126.58	121.19
2	Y	80	ALA	CA-C-N	5.23	127.24	120.44
2	Y	80	ALA	C-N-CA	5.23	127.24	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	132	TYR	CB-CG-CD1	-5.23	112.96	120.80
1	R	101	VAL	CA-CB-CG1	5.23	119.28	110.40
1	U	10	ARG	NH1-CZ-NH2	5.22	126.09	119.30
2	W	80	ALA	CA-C-N	5.22	127.23	120.44
2	W	80	ALA	C-N-CA	5.22	127.23	120.44
2	J	80	ALA	CA-C-N	5.22	127.23	120.44
2	J	80	ALA	C-N-CA	5.22	127.23	120.44
2	H	80	ALA	CA-C-N	5.22	127.23	120.44
2	H	80	ALA	C-N-CA	5.22	127.23	120.44
2	X	194	SER	N-CA-C	-5.22	105.48	111.07
1	F	10	ARG	NH1-CZ-NH2	5.22	126.08	119.30
1	U	132	TYR	CB-CG-CD1	-5.22	112.97	120.80
1	P	10	ARG	NH1-CZ-NH2	5.22	126.08	119.30
2	M	2	THR	O-C-N	-5.22	117.53	123.48
1	T	132	TYR	CB-CG-CD1	-5.22	112.97	120.80
2	W	2	THR	O-C-N	-5.22	117.53	123.48
2	Z	80	ALA	CA-C-N	5.22	127.22	120.44
2	Z	80	ALA	C-N-CA	5.22	127.22	120.44
2	V	194	SER	N-CA-C	-5.22	105.49	111.07
2	I	80	ALA	CA-C-N	5.22	127.22	120.44
2	I	80	ALA	C-N-CA	5.22	127.22	120.44
2	J	152	VAL	N-CA-CB	5.22	117.63	110.54
1	Q	10	ARG	NH1-CZ-NH2	5.22	126.08	119.30
2	K	194	SER	N-CA-C	-5.21	105.49	111.07
2	1	2	THR	O-C-N	-5.21	117.54	123.48
2	V	80	ALA	CA-C-N	5.21	127.21	120.44
2	V	80	ALA	C-N-CA	5.21	127.21	120.44
2	J	2	THR	O-C-N	-5.21	117.54	123.48
2	L	80	ALA	CA-C-N	5.21	127.21	120.44
2	L	80	ALA	C-N-CA	5.21	127.21	120.44
1	S	10	ARG	NH1-CZ-NH2	5.21	126.07	119.30
2	N	80	ALA	CA-C-N	5.21	127.21	120.44
2	N	80	ALA	C-N-CA	5.21	127.21	120.44
2	N	194	SER	N-CA-C	-5.21	105.50	111.07
1	B	10	ARG	NH1-CZ-NH2	5.21	126.07	119.30
2	K	2	THR	O-C-N	-5.21	117.54	123.48
2	L	2	THR	O-C-N	-5.21	117.54	123.48
2	K	80	ALA	CA-C-N	5.21	127.21	120.44
2	K	80	ALA	C-N-CA	5.21	127.21	120.44
1	G	22	PHE	CB-CG-CD2	-5.21	111.85	120.70
1	O	10	ARG	NH1-CZ-NH2	5.20	126.06	119.30
2	W	152	VAL	N-CA-CB	5.20	117.62	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	152	VAL	N-CA-CB	5.20	117.62	110.54
2	J	194	SER	N-CA-C	-5.20	105.50	111.07
2	Z	2	THR	O-C-N	-5.20	117.55	123.48
2	Z	194	SER	N-CA-C	-5.20	105.51	111.07
2	2	80	ALA	CA-C-N	5.20	127.20	120.44
2	2	80	ALA	C-N-CA	5.20	127.20	120.44
2	H	194	SER	N-CA-C	-5.20	105.50	111.07
2	I	2	THR	O-C-N	-5.20	117.55	123.48
2	I	194	SER	N-CA-C	-5.20	105.51	111.07
2	Y	194	SER	N-CA-C	-5.20	105.50	111.07
2	1	80	ALA	CA-C-N	5.20	127.20	120.44
2	1	80	ALA	C-N-CA	5.20	127.20	120.44
2	2	75	PRO	CA-C-O	-5.20	115.61	121.43
1	D	132	TYR	CB-CG-CD1	-5.20	113.00	120.80
1	E	10	ARG	NH1-CZ-NH2	5.20	126.06	119.30
2	M	194	SER	N-CA-C	-5.20	105.51	111.07
2	N	2	THR	O-C-N	-5.20	117.56	123.48
2	2	2	THR	O-C-N	-5.20	117.56	123.48
2	H	75	PRO	CA-C-O	-5.20	115.61	121.43
2	Y	75	PRO	CA-C-O	-5.20	115.61	121.43
1	G	10	ARG	NH1-CZ-NH2	5.19	126.05	119.30
1	C	22	PHE	CB-CG-CD2	-5.19	111.87	120.70
2	X	2	THR	O-C-N	-5.19	117.56	123.48
2	M	152	VAL	N-CA-CB	5.19	117.60	110.54
1	T	22	PHE	CB-CG-CD2	-5.19	111.88	120.70
1	O	22	PHE	CB-CG-CD2	-5.19	111.88	120.70
1	O	193	GLY	CA-C-N	5.19	127.57	120.46
1	O	193	GLY	C-N-CA	5.19	127.57	120.46
2	V	2	THR	O-C-N	-5.19	117.56	123.48
1	Q	22	PHE	CB-CG-CD2	-5.19	111.88	120.70
1	D	193	GLY	CA-C-N	5.19	127.57	120.46
1	D	193	GLY	C-N-CA	5.19	127.57	120.46
1	E	22	PHE	CB-CG-CD2	-5.19	111.88	120.70
2	Z	152	VAL	N-CA-CB	5.19	117.60	110.54
2	2	152	VAL	N-CA-CB	5.19	117.60	110.54
2	I	152	VAL	N-CA-CB	5.19	117.60	110.54
1	U	193	GLY	CA-C-N	5.19	127.57	120.46
1	U	193	GLY	C-N-CA	5.19	127.57	120.46
1	A	193	GLY	CA-C-N	5.19	127.57	120.46
1	A	193	GLY	C-N-CA	5.19	127.57	120.46
2	V	75	PRO	CA-C-O	-5.19	115.62	121.43
1	R	193	GLY	CA-C-N	5.19	127.57	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	193	GLY	C-N-CA	5.19	127.57	120.46
2	L	75	PRO	CA-C-O	-5.19	115.62	121.43
1	S	22	PHE	CB-CG-CD2	-5.19	111.88	120.70
1	B	22	PHE	CB-CG-CD2	-5.19	111.88	120.70
1	Q	115	ARG	N-CA-CB	5.19	117.53	110.01
2	N	152	VAL	N-CA-CB	5.18	117.59	110.54
2	H	2	THR	O-C-N	-5.18	117.57	123.48
2	H	152	VAL	N-CA-CB	5.18	117.59	110.54
1	C	115	ARG	N-CA-CB	5.18	117.53	110.01
2	X	152	VAL	N-CA-CB	5.18	117.59	110.54
2	Y	2	THR	O-C-N	-5.18	117.57	123.48
2	1	75	PRO	CA-C-O	-5.18	115.63	121.43
2	1	152	VAL	N-CA-CB	5.18	117.59	110.54
2	N	75	PRO	CA-C-O	-5.18	115.62	121.43
2	J	75	PRO	CA-C-O	-5.18	115.63	121.43
2	Z	75	PRO	CA-C-O	-5.18	115.63	121.43
2	I	75	PRO	CA-C-O	-5.18	115.63	121.43
1	D	202	GLU	N-CA-CB	5.18	119.25	110.49
2	M	80	ALA	CA-C-N	5.18	127.17	120.44
2	M	80	ALA	C-N-CA	5.18	127.17	120.44
1	U	22	PHE	CB-CG-CD2	-5.18	111.89	120.70
1	A	22	PHE	CB-CG-CD2	-5.18	111.89	120.70
1	O	115	ARG	N-CA-CB	5.18	117.52	110.01
1	D	22	PHE	CB-CG-CD2	-5.18	111.89	120.70
1	R	22	PHE	CB-CG-CD2	-5.18	111.89	120.70
1	E	115	ARG	N-CA-CB	5.18	117.52	110.01
2	L	152	VAL	N-CA-CB	5.18	117.58	110.54
1	S	193	GLY	CA-C-N	5.18	127.55	120.46
1	S	193	GLY	C-N-CA	5.18	127.55	120.46
1	B	193	GLY	CA-C-N	5.18	127.55	120.46
1	B	193	GLY	C-N-CA	5.18	127.55	120.46
2	W	75	PRO	CA-C-O	-5.18	115.63	121.43
2	K	75	PRO	CA-C-O	-5.18	115.63	121.43
1	F	115	ARG	N-CA-CB	5.18	117.52	110.01
2	M	75	PRO	CA-C-O	-5.18	115.63	121.43
1	T	193	GLY	CA-C-N	5.18	127.55	120.46
1	T	193	GLY	C-N-CA	5.18	127.55	120.46
1	G	115	ARG	N-CA-CB	5.17	117.51	110.01
1	A	115	ARG	N-CA-CB	5.17	117.51	110.01
1	S	115	ARG	N-CA-CB	5.17	117.51	110.01
2	V	152	VAL	N-CA-CB	5.17	117.57	110.54
1	B	115	ARG	N-CA-CB	5.17	117.51	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	22	PHE	CB-CG-CD2	-5.17	111.91	120.70
1	E	193	GLY	CA-C-N	5.17	127.54	120.46
1	E	193	GLY	C-N-CA	5.17	127.54	120.46
1	P	193	GLY	CA-C-N	5.17	127.54	120.46
1	P	193	GLY	C-N-CA	5.17	127.54	120.46
1	T	115	ARG	N-CA-CB	5.17	117.50	110.01
2	1	194	SER	N-CA-C	-5.17	105.54	111.07
1	U	202	GLU	N-CA-CB	5.17	119.22	110.49
1	O	205	GLU	N-CA-CB	5.17	120.57	112.46
1	D	115	ARG	N-CA-CB	5.17	117.50	110.01
2	K	152	VAL	N-CA-CB	5.17	117.57	110.54
2	L	194	SER	N-CA-C	-5.17	105.54	111.07
1	G	193	GLY	CA-C-N	5.17	127.54	120.46
1	G	193	GLY	C-N-CA	5.17	127.54	120.46
1	G	202	GLU	N-CA-CB	5.17	119.22	110.49
1	U	115	ARG	N-CA-CB	5.17	117.50	110.01
1	Q	193	GLY	CA-C-N	5.17	127.54	120.46
1	Q	193	GLY	C-N-CA	5.17	127.54	120.46
1	Q	202	GLU	N-CA-CB	5.17	119.22	110.49
1	R	202	GLU	N-CA-CB	5.17	119.22	110.49
1	S	202	GLU	N-CA-CB	5.16	119.22	110.49
1	T	205	GLU	N-CA-CB	5.16	120.57	112.46
1	U	200	SER	CA-C-O	5.16	127.89	120.51
1	B	202	GLU	N-CA-CB	5.16	119.22	110.49
1	F	22	PHE	CB-CG-CD2	-5.16	111.92	120.70
2	X	75	PRO	CA-C-O	-5.16	115.65	121.43
1	F	193	GLY	CA-C-N	5.16	127.53	120.46
1	F	193	GLY	C-N-CA	5.16	127.53	120.46
1	G	205	GLU	N-CA-CB	5.16	120.56	112.46
1	Q	205	GLU	N-CA-CB	5.16	120.56	112.46
1	D	205	GLU	N-CA-CB	5.16	120.56	112.46
1	R	205	GLU	N-CA-CB	5.16	120.56	112.46
1	E	202	GLU	N-CA-CB	5.16	119.21	110.49
1	G	200	SER	CA-C-O	5.16	127.89	120.51
1	T	202	GLU	N-CA-CB	5.16	119.21	110.49
1	R	115	ARG	N-CA-CB	5.16	117.49	110.01
1	F	202	GLU	N-CA-CB	5.16	119.20	110.49
1	U	205	GLU	N-CA-CB	5.16	120.56	112.46
1	A	200	SER	CA-C-O	5.16	127.88	120.51
1	A	205	GLU	N-CA-CB	5.16	120.55	112.46
1	P	202	GLU	N-CA-CB	5.16	119.20	110.49
1	P	205	GLU	N-CA-CB	5.16	120.55	112.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	205	GLU	N-CA-CB	5.15	120.55	112.46
1	O	200	SER	CA-C-O	5.15	127.88	120.51
1	O	202	GLU	N-CA-CB	5.15	119.20	110.49
1	B	205	GLU	N-CA-CB	5.15	120.55	112.46
1	P	115	ARG	N-CA-CB	5.15	117.48	110.01
1	C	193	GLY	CA-C-N	5.15	127.52	120.46
1	C	193	GLY	C-N-CA	5.15	127.52	120.46
1	R	200	SER	CA-C-O	5.15	127.88	120.51
1	E	200	SER	CA-C-O	5.15	127.88	120.51
1	E	205	GLU	N-CA-CB	5.15	120.55	112.46
2	L	48	LEU	N-CA-CB	-5.15	102.48	110.57
1	T	200	SER	CA-C-O	5.15	127.87	120.51
1	A	202	GLU	N-CA-CB	5.15	119.19	110.49
1	P	200	SER	CA-C-O	5.15	127.87	120.51
2	K	48	LEU	N-CA-CB	-5.15	102.49	110.57
1	C	205	GLU	N-CA-CB	5.15	120.54	112.46
1	S	200	SER	CA-C-O	5.14	127.87	120.51
1	B	200	SER	CA-C-O	5.14	127.87	120.51
1	C	202	GLU	N-CA-CB	5.14	119.19	110.49
2	2	48	LEU	N-CA-CB	-5.14	102.50	110.57
1	T	46	VAL	N-CA-C	-5.14	100.47	108.44
1	F	200	SER	CA-C-O	5.14	127.86	120.51
1	F	205	GLU	N-CA-CB	5.14	120.52	112.46
1	Q	200	SER	CA-C-O	5.13	127.85	120.51
1	F	46	VAL	N-CA-C	-5.13	100.49	108.44
2	M	48	LEU	N-CA-CB	-5.13	102.51	110.57
1	T	13	THR	CA-C-N	5.13	128.84	121.96
1	T	13	THR	C-N-CA	5.13	128.84	121.96
2	1	48	LEU	N-CA-CB	-5.13	102.51	110.57
1	P	46	VAL	N-CA-C	-5.13	100.49	108.44
2	J	48	LEU	N-CA-CB	-5.13	102.51	110.57
1	D	200	SER	CA-C-O	5.13	127.85	120.51
1	U	46	VAL	N-CA-C	-5.13	100.49	108.44
1	D	46	VAL	N-CA-C	-5.13	100.49	108.44
1	R	46	VAL	N-CA-C	-5.13	100.49	108.44
1	G	46	VAL	N-CA-C	-5.13	100.49	108.44
1	S	46	VAL	N-CA-C	-5.13	100.49	108.44
2	Z	48	LEU	N-CA-CB	-5.13	102.52	110.57
1	A	46	VAL	N-CA-C	-5.13	100.49	108.44
1	B	46	VAL	N-CA-C	-5.13	100.49	108.44
2	I	48	LEU	N-CA-CB	-5.13	102.52	110.57
1	U	219	ASN	N-CA-C	5.12	115.81	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	152	ASP	N-CA-CB	-5.12	100.82	110.09
1	O	219	ASN	N-CA-C	5.12	115.81	108.74
1	C	200	SER	CA-C-O	5.12	127.84	120.51
1	F	219	ASN	N-CA-C	5.12	115.81	108.74
2	M	150	GLU	CB-CG-CD	-5.12	103.89	112.60
1	P	219	ASN	N-CA-C	5.12	115.81	108.74
2	W	150	GLU	CB-CG-CD	-5.12	103.89	112.60
1	Q	13	THR	CA-C-N	5.12	128.82	121.96
1	Q	13	THR	C-N-CA	5.12	128.82	121.96
1	Q	46	VAL	N-CA-C	-5.12	100.50	108.44
2	H	48	LEU	N-CA-CB	-5.12	102.53	110.57
1	C	219	ASN	N-CA-C	5.12	115.80	108.74
2	Y	48	LEU	N-CA-CB	-5.12	102.53	110.57
1	S	219	ASN	N-CA-C	5.12	115.80	108.74
1	B	219	ASN	N-CA-C	5.12	115.80	108.74
1	A	152	ASP	N-CA-CB	-5.12	100.83	110.09
2	N	134	VAL	CA-CB-CG2	5.11	119.09	110.40
1	O	152	ASP	N-CA-CB	-5.11	100.84	110.09
2	V	48	LEU	N-CA-CB	-5.11	102.54	110.57
1	P	170	ASP	CA-C-O	-5.11	115.11	120.63
1	D	170	ASP	CA-C-O	-5.11	115.11	120.63
1	O	13	THR	CA-C-N	5.11	128.81	121.96
1	O	13	THR	C-N-CA	5.11	128.81	121.96
2	X	48	LEU	N-CA-CB	-5.11	102.54	110.57
2	Y	150	GLU	CB-CG-CD	-5.11	103.91	112.60
1	E	13	THR	CA-C-N	5.11	128.81	121.96
1	E	13	THR	C-N-CA	5.11	128.81	121.96
2	1	150	GLU	CB-CG-CD	-5.11	103.91	112.60
2	2	150	GLU	CB-CG-CD	-5.11	103.91	112.60
1	A	170	ASP	CA-C-O	-5.11	115.11	120.63
2	W	132	PRO	CA-C-N	5.11	127.08	120.44
2	W	132	PRO	C-N-CA	5.11	127.08	120.44
1	C	46	VAL	N-CA-C	-5.11	100.52	108.44
2	J	150	GLU	CB-CG-CD	-5.11	103.91	112.60
1	R	13	THR	CA-C-N	5.11	128.81	121.96
1	R	13	THR	C-N-CA	5.11	128.81	121.96
1	E	219	ASN	N-CA-C	5.11	115.79	108.74
2	W	48	LEU	N-CA-CB	-5.11	102.55	110.57
1	E	46	VAL	N-CA-C	-5.11	100.52	108.44
1	S	152	ASP	N-CA-CB	-5.11	100.85	110.09
2	N	48	LEU	N-CA-CB	-5.11	102.55	110.57
1	A	13	THR	CA-C-N	5.11	128.80	121.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	THR	C-N-CA	5.11	128.80	121.96
2	V	134	VAL	CA-CB-CG2	5.11	119.08	110.40
1	B	152	ASP	N-CA-CB	-5.11	100.85	110.09
2	N	150	GLU	CB-CG-CD	-5.11	103.92	112.60
2	V	150	GLU	CB-CG-CD	-5.11	103.92	112.60
1	Q	152	ASP	N-CA-CB	-5.11	100.85	110.09
2	X	134	VAL	CA-CB-CG2	5.11	119.08	110.40
2	L	150	GLU	CB-CG-CD	-5.11	103.92	112.60
1	F	152	ASP	N-CA-CB	-5.10	100.85	110.09
1	O	46	VAL	N-CA-C	-5.10	100.53	108.44
1	P	152	ASP	N-CA-CB	-5.10	100.85	110.09
2	J	134	VAL	CA-CB-CG2	5.10	119.08	110.40
1	S	13	THR	CA-C-N	5.10	128.80	121.96
1	S	13	THR	C-N-CA	5.10	128.80	121.96
1	G	215	ILE	N-CA-C	-5.10	100.54	108.81
1	B	13	THR	CA-C-N	5.10	128.80	121.96
1	B	13	THR	C-N-CA	5.10	128.80	121.96
1	Q	170	ASP	CA-C-O	-5.10	115.12	120.63
1	D	152	ASP	N-CA-CB	-5.10	100.85	110.09
1	R	219	ASN	N-CA-C	5.10	115.78	108.74
2	Z	150	GLU	CB-CG-CD	-5.10	103.93	112.60
2	I	150	GLU	CB-CG-CD	-5.10	103.93	112.60
1	C	13	THR	CA-C-N	5.10	128.79	121.96
1	C	13	THR	C-N-CA	5.10	128.79	121.96
1	F	13	THR	CA-C-N	5.10	128.79	121.96
1	F	13	THR	C-N-CA	5.10	128.79	121.96
1	F	84	ASP	CB-CA-C	-5.10	102.33	110.79
1	F	215	ILE	N-CA-C	-5.10	100.55	108.81
1	T	219	ASN	N-CA-C	5.10	115.78	108.74
1	P	13	THR	CA-C-N	5.10	128.79	121.96
1	P	13	THR	C-N-CA	5.10	128.79	121.96
1	Q	84	ASP	CB-CA-C	-5.10	102.32	110.79
1	D	219	ASN	N-CA-C	5.10	115.78	108.74
1	T	152	ASP	N-CA-CB	-5.10	100.86	110.09
1	G	84	ASP	CB-CA-C	-5.10	102.33	110.79
1	U	152	ASP	N-CA-CB	-5.10	100.86	110.09
1	A	219	ASN	N-CA-C	5.10	115.78	108.74
1	Q	215	ILE	N-CA-C	-5.10	100.55	108.81
1	D	84	ASP	CB-CA-C	-5.10	102.33	110.79
2	K	150	GLU	CB-CG-CD	-5.10	103.93	112.60
1	G	219	ASN	N-CA-C	5.10	115.77	108.74
1	O	215	ILE	N-CA-C	-5.10	100.56	108.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	219	ASN	N-CA-C	5.10	115.77	108.74
1	E	215	ILE	N-CA-C	-5.10	100.56	108.81
2	1	134	VAL	CA-CB-CG2	5.09	119.06	110.40
2	X	150	GLU	CB-CG-CD	-5.09	103.94	112.60
1	R	152	ASP	N-CA-CB	-5.09	100.87	110.09
1	G	13	THR	CA-C-N	5.09	128.78	121.96
1	G	13	THR	C-N-CA	5.09	128.78	121.96
1	U	13	THR	CA-C-N	5.09	128.78	121.96
1	U	13	THR	C-N-CA	5.09	128.78	121.96
1	D	13	THR	CA-C-N	5.09	128.78	121.96
1	D	13	THR	C-N-CA	5.09	128.78	121.96
2	2	134	VAL	CA-CB-CG2	5.09	119.06	110.40
2	L	134	VAL	CA-CB-CG2	5.09	119.06	110.40
1	S	215	ILE	N-CA-C	-5.09	100.57	108.81
2	H	132	PRO	CA-C-N	5.09	127.06	120.44
2	H	132	PRO	C-N-CA	5.09	127.06	120.44
1	B	215	ILE	N-CA-C	-5.09	100.57	108.81
1	R	215	ILE	N-CA-C	-5.09	100.57	108.81
1	O	84	ASP	CB-CA-C	-5.09	102.34	110.79
1	C	152	ASP	N-CA-CB	-5.09	100.88	110.09
2	Z	134	VAL	CA-CB-CG2	5.09	119.05	110.40
1	T	84	ASP	CB-CA-C	-5.09	102.35	110.79
1	A	215	ILE	N-CA-C	-5.09	100.57	108.81
2	H	150	GLU	CB-CG-CD	-5.09	103.95	112.60
1	O	184	LEU	CA-C-O	-5.09	114.54	120.03
2	I	134	VAL	CA-CB-CG2	5.09	119.05	110.40
1	C	84	ASP	CB-CA-C	-5.09	102.35	110.79
1	E	152	ASP	N-CA-CB	-5.08	100.89	110.09
1	T	170	ASP	CA-C-O	-5.08	115.14	120.63
2	N	132	PRO	CA-C-N	5.08	127.05	120.44
2	N	132	PRO	C-N-CA	5.08	127.05	120.44
2	2	132	PRO	CA-C-N	5.08	127.05	120.44
2	2	132	PRO	C-N-CA	5.08	127.05	120.44
2	H	28	HIS	CE1-NE2-CD2	-5.08	103.92	109.00
1	P	84	ASP	CB-CA-C	-5.08	102.35	110.79
2	X	132	PRO	CA-C-N	5.08	127.05	120.44
2	X	132	PRO	C-N-CA	5.08	127.05	120.44
2	M	134	VAL	CA-CB-CG2	5.08	119.04	110.40
1	U	184	LEU	CA-C-O	-5.08	114.54	120.03
1	U	215	ILE	N-CA-C	-5.08	100.58	108.81
2	W	134	VAL	CA-CB-CG2	5.08	119.04	110.40
1	D	184	LEU	CA-C-O	-5.08	114.54	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	215	ILE	N-CA-C	-5.08	100.58	108.81
1	P	215	ILE	N-CA-C	-5.08	100.58	108.81
1	C	184	LEU	CA-C-O	-5.08	114.54	120.03
2	Y	134	VAL	CA-CB-CG2	5.08	119.04	110.40
1	S	84	ASP	CB-CA-C	-5.08	102.36	110.79
1	B	84	ASP	CB-CA-C	-5.08	102.36	110.79
1	S	170	ASP	CA-C-O	-5.08	115.15	120.63
2	M	132	PRO	CA-C-N	5.08	127.04	120.44
2	M	132	PRO	C-N-CA	5.08	127.04	120.44
1	A	84	ASP	CB-CA-C	-5.08	102.36	110.79
1	A	184	LEU	CA-C-O	-5.08	114.55	120.03
1	O	170	ASP	CA-C-O	-5.08	115.15	120.63
1	B	170	ASP	CA-C-O	-5.08	115.15	120.63
1	R	84	ASP	CB-CA-C	-5.08	102.36	110.79
1	E	170	ASP	CA-C-O	-5.08	115.15	120.63
1	C	215	ILE	N-CA-C	-5.07	100.59	108.81
1	F	170	ASP	CA-C-O	-5.07	115.15	120.63
1	T	215	ILE	N-CA-C	-5.07	100.60	108.81
1	U	84	ASP	CB-CA-C	-5.07	102.38	110.79
2	K	134	VAL	CA-CB-CG2	5.07	119.02	110.40
2	Z	132	PRO	CA-C-N	5.07	127.03	120.44
2	Z	132	PRO	C-N-CA	5.07	127.03	120.44
2	I	132	PRO	CA-C-N	5.07	127.03	120.44
2	I	132	PRO	C-N-CA	5.07	127.03	120.44
1	R	138	PHE	CA-CB-CG	-5.07	108.73	113.80
1	R	170	ASP	CA-C-O	-5.07	115.16	120.63
1	E	84	ASP	CB-CA-C	-5.07	102.38	110.79
1	G	170	ASP	CA-C-O	-5.07	115.16	120.63
1	F	184	LEU	CA-C-O	-5.06	114.56	120.03
2	H	134	VAL	CA-CB-CG2	5.06	119.01	110.40
1	E	184	LEU	CA-C-O	-5.06	114.56	120.03
1	G	36	THR	O-C-N	-5.06	116.72	122.89
1	Q	36	THR	O-C-N	-5.06	116.72	122.89
1	Q	138	PHE	CA-CB-CG	-5.06	108.74	113.80
2	Y	71	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	Q	184	LEU	CA-C-O	-5.06	114.57	120.03
1	R	184	LEU	CA-C-O	-5.06	114.57	120.03
2	Y	28	HIS	CE1-NE2-CD2	-5.06	103.94	109.00
1	S	184	LEU	CA-C-O	-5.05	114.57	120.03
1	F	36	THR	O-C-N	-5.05	116.72	122.89
1	A	185	PRO	CA-C-O	-5.05	115.50	121.67
1	B	184	LEU	CA-C-O	-5.05	114.57	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	162	ALA	CA-C-N	5.05	127.05	120.28
2	J	162	ALA	C-N-CA	5.05	127.05	120.28
2	K	132	PRO	CA-C-N	5.05	127.01	120.44
2	K	132	PRO	C-N-CA	5.05	127.01	120.44
2	Y	132	PRO	CA-C-N	5.05	127.01	120.44
2	Y	132	PRO	C-N-CA	5.05	127.01	120.44
1	E	36	THR	O-C-N	-5.05	116.72	122.89
1	U	170	ASP	CA-C-O	-5.05	115.17	120.63
1	O	185	PRO	CA-C-O	-5.05	115.50	121.67
2	W	28	HIS	CE1-NE2-CD2	-5.05	103.95	109.00
1	E	138	PHE	CA-CB-CG	-5.05	108.75	113.80
1	F	185	PRO	CA-C-O	-5.05	115.51	121.67
2	N	162	ALA	CA-C-N	5.05	127.05	120.28
2	N	162	ALA	C-N-CA	5.05	127.05	120.28
2	J	71	ARG	NE-CZ-NH2	5.05	123.75	119.20
2	J	132	PRO	CA-C-N	5.05	127.01	120.44
2	J	132	PRO	C-N-CA	5.05	127.01	120.44
2	L	28	HIS	CE1-NE2-CD2	-5.05	103.95	109.00
1	T	184	LEU	CA-C-O	-5.05	114.58	120.03
1	D	138	PHE	CA-CB-CG	-5.05	108.75	113.80
1	S	36	THR	O-C-N	-5.05	116.73	122.89
2	V	132	PRO	CA-C-N	5.05	127.00	120.44
2	V	132	PRO	C-N-CA	5.05	127.00	120.44
1	B	36	THR	O-C-N	-5.05	116.73	122.89
1	C	36	THR	O-C-N	-5.05	116.73	122.89
2	M	71	ARG	NE-CZ-NH2	5.04	123.74	119.20
2	V	162	ALA	CA-C-N	5.04	127.04	120.28
2	V	162	ALA	C-N-CA	5.04	127.04	120.28
2	K	162	ALA	CA-C-N	5.04	127.04	120.28
2	K	162	ALA	C-N-CA	5.04	127.04	120.28
2	L	162	ALA	CA-C-N	5.04	127.04	120.28
2	L	162	ALA	C-N-CA	5.04	127.04	120.28
2	Z	162	ALA	CA-C-N	5.04	127.04	120.28
2	Z	162	ALA	C-N-CA	5.04	127.04	120.28
2	M	162	ALA	CA-C-N	5.04	127.04	120.28
2	M	162	ALA	C-N-CA	5.04	127.04	120.28
2	I	162	ALA	CA-C-N	5.04	127.04	120.28
2	I	162	ALA	C-N-CA	5.04	127.04	120.28
2	W	71	ARG	NE-CZ-NH2	5.04	123.74	119.20
2	W	162	ALA	CA-C-N	5.04	127.04	120.28
2	W	162	ALA	C-N-CA	5.04	127.04	120.28
1	T	36	THR	O-C-N	-5.04	116.74	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	28	HIS	CE1-NE2-CD2	-5.04	103.96	109.00
2	1	28	HIS	CE1-NE2-CD2	-5.04	103.96	109.00
1	A	36	THR	O-C-N	-5.04	116.74	122.89
1	D	185	PRO	CA-C-O	-5.04	115.52	121.67
1	S	185	PRO	CA-C-O	-5.04	115.53	121.67
1	B	185	PRO	CA-C-O	-5.04	115.53	121.67
1	C	185	PRO	CA-C-O	-5.04	115.53	121.67
1	S	138	PHE	CA-CB-CG	-5.04	108.77	113.80
2	1	71	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	G	184	LEU	CA-C-O	-5.04	114.59	120.03
1	B	138	PHE	CA-CB-CG	-5.04	108.77	113.80
2	K	71	ARG	NE-CZ-NH2	5.04	123.73	119.20
2	1	132	PRO	CA-C-N	5.03	126.98	120.44
2	1	132	PRO	C-N-CA	5.03	126.98	120.44
2	1	162	ALA	CA-C-N	5.03	127.03	120.28
2	1	162	ALA	C-N-CA	5.03	127.03	120.28
2	H	162	ALA	CA-C-N	5.03	127.03	120.28
2	H	162	ALA	C-N-CA	5.03	127.03	120.28
1	O	36	THR	O-C-N	-5.03	116.75	122.89
1	U	36	THR	O-C-N	-5.03	116.75	122.89
1	P	36	THR	O-C-N	-5.03	116.75	122.89
1	P	185	PRO	CA-C-O	-5.03	115.53	121.67
1	D	36	THR	O-C-N	-5.03	116.75	122.89
1	R	36	THR	O-C-N	-5.03	116.75	122.89
1	P	184	LEU	CA-C-O	-5.03	114.60	120.03
1	T	185	PRO	CA-C-O	-5.03	115.54	121.67
1	U	138	PHE	CA-CB-CG	-5.03	108.77	113.80
2	L	132	PRO	CA-C-N	5.03	126.98	120.44
2	L	132	PRO	C-N-CA	5.03	126.98	120.44
1	F	138	PHE	CA-CB-CG	-5.02	108.78	113.80
1	G	138	PHE	CA-CB-CG	-5.02	108.78	113.80
1	C	170	ASP	CA-C-O	-5.02	115.20	120.63
2	Y	162	ALA	CA-C-N	5.02	127.01	120.28
2	Y	162	ALA	C-N-CA	5.02	127.01	120.28
2	2	162	ALA	CA-C-N	5.02	127.01	120.28
2	2	162	ALA	C-N-CA	5.02	127.01	120.28
2	Z	71	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	G	185	PRO	CA-C-O	-5.02	115.55	121.67
2	N	28	HIS	CE1-NE2-CD2	-5.02	103.98	109.00
2	N	71	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	A	138	PHE	CA-CB-CG	-5.02	108.78	113.80
2	I	71	ARG	NE-CZ-NH2	5.02	123.72	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	138	PHE	CA-CB-CG	-5.02	108.78	113.80
1	Q	185	PRO	CA-C-O	-5.02	115.55	121.67
2	X	71	ARG	NE-CZ-NH2	5.02	123.72	119.20
2	J	28	HIS	CE1-NE2-CD2	-5.02	103.98	109.00
1	R	185	PRO	CA-C-O	-5.02	115.55	121.67
2	Z	28	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
2	H	71	ARG	NE-CZ-NH2	5.01	123.71	119.20
2	V	28	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
2	I	28	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
1	U	34	GLY	CA-C-O	5.01	127.18	121.92
1	U	185	PRO	CA-C-O	-5.01	115.56	121.67
1	O	138	PHE	CA-CB-CG	-5.01	108.79	113.80
2	X	162	ALA	CA-C-N	5.01	126.99	120.28
2	X	162	ALA	C-N-CA	5.01	126.99	120.28
2	N	6	ILE	CA-C-O	5.01	125.89	120.43
1	E	185	PRO	CA-C-O	-5.01	115.56	121.67
1	F	34	GLY	CA-C-O	5.00	127.17	121.92
2	V	40	TYR	N-CA-C	-5.00	104.93	112.99
2	X	40	TYR	N-CA-C	-5.00	104.93	112.99
2	L	40	TYR	N-CA-C	-5.00	104.93	112.99
2	1	6	ILE	CA-C-O	5.00	125.88	120.43
2	K	28	HIS	CE1-NE2-CD2	-5.00	104.00	109.00
1	T	138	PHE	CA-CB-CG	-5.00	108.80	113.80
2	2	6	ILE	CA-C-O	5.00	125.88	120.43
1	C	138	PHE	CA-CB-CG	-5.00	108.80	113.80
2	Y	6	ILE	CA-C-O	5.00	125.88	120.43
2	L	6	ILE	CA-C-O	5.00	125.88	120.43

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

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Mol	Chain	Res	Type	Group
2	2	180	ARG	Sidechain
2	2	24	ASN	Peptide
2	2	28	HIS	Sidechain
2	2	66	TYR	Sidechain
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

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Mol	Chain	Res	Type	Group
2	I	124	TYR	Sidechain
2	I	165	ARG	Sidechain
2	I	180	ARG	Sidechain
2	I	24	ASN	Peptide
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

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Mol	Chain	Res	Type	Group
2	N	180	ARG	Sidechain
2	N	24	ASN	Peptide
2	N	28	HIS	Sidechain
2	N	66	TYR	Sidechain
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

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Mol	Chain	Res	Type	Group
2	W	124	TYR	Sidechain
2	W	165	ARG	Sidechain
2	W	180	ARG	Sidechain
2	W	24	ASN	Peptide
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 ⓘ

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1744	0	1782	24	0
1	C	1744	0	1782	24	0
1	D	1744	0	1782	24	0
1	E	1744	0	1782	24	0
1	F	1744	0	1782	25	0
1	G	1744	0	1782	24	0
1	O	1744	0	1782	24	0
1	P	1744	0	1782	25	0
1	Q	1744	0	1782	24	0
1	R	1744	0	1782	24	0
1	S	1744	0	1782	24	0
1	T	1744	0	1782	24	0
1	U	1744	0	1782	24	0
2	1	1558	0	1609	35	0
2	2	1558	0	1609	35	0
2	H	1558	0	1609	36	0
2	I	1558	0	1609	35	0
2	J	1558	0	1609	35	0
2	K	1558	0	1609	35	0
2	L	1558	0	1609	35	0
2	M	1558	0	1609	34	0
2	N	1558	0	1609	34	0
2	V	1558	0	1609	36	0
2	W	1558	0	1609	34	0
2	X	1558	0	1609	34	0
2	Y	1558	0	1609	36	0
2	Z	1558	0	1609	35	0
All	All	46228	0	47474	532	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 6.

All (532) 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:S:10:ARG:CZ	1:R:11:ALA:CB	1.95	1.43
1:A:11:ALA:CB	1:B:10:ARG:CZ	1.95	1.43
1:C:11:ALA:CB	1:D:10:ARG:CZ	1.95	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:ALA:CB	1:A: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
1:Q:11:ALA:CB	1:R:10:ARG:CZ	1.95	1.42
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:S:10:ARG:NH1	1:R:11:ALA:HB1	1.03	1.36
1:A:11:ALA:HB1	1:B:10:ARG:NH1	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: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:Q:11:ALA:HB1	1:R: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:11:ALA:HB2	1:G:10:ARG:NH2	1.65	1.12
1:U:11:ALA:HB2	1:O:10:ARG:NH2	1.65	1.12
1:P:11:ALA:HB2	1:Q: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: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:G:11:ALA:HB2	1:A:10:ARG:NH2	1.65	1.09
1:B:11:ALA:HB2	1:C: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:1:167:SER:HB2	2:L:167:SER:O	1.64	0.97
2:N:167:SER:O	2:Y:167:SER:HB2	1.64	0.97
2:Z:167:SER:O	2:M:167:SER:HB2	1.64	0.97
2:Z:167:SER:HB2	2:M:167:SER:O	1.64	0.97
2:H:167:SER:HB2	2:X:167:SER:O	1.64	0.97
2:H:167:SER:O	2:X:167:SER:HB2	1.64	0.97
2:V:167:SER:HB2	2:J:167:SER:O	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: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
2:2:167: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: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:Z:28:HIS:CD2	2:1:120:VAL:HG11	2.02	0.94
2:I:28:HIS:CD2	2:J: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:N:203:LEU:OXT	2:Y:203:LEU:OXT	1.92	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:203:LEU:OXT	2:X: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
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
2:M:28:HIS:CD2	2:N:120:VAL:CG1	2.62	0.83
1:T:11:ALA:CB	1:U:10:ARG:NH2	2.32	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:M:120:VAL:CG1	2:L:28:HIS:CD2	2.62	0.83
2:2:28:HIS:CD2	2:V:120:VAL:CG1	2.62	0.83
2:V:28:HIS:CD2	2:W:120:VAL:CG1	2.62	0.83
2:K:28:HIS:CD2	2:L: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:F:54:VAL:O	1:F:55:ARG:NH1	2.29	0.65
1:E:54:VAL:O	1:E: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
2:Z:22:MET:HE3	2:1:114:ASP:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:22:MET:HE3	2:J:114:ASP:HB3	1.79	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:R:54:VAL:O	1:R:55:ARG:NH1	2.29	0.65
1:T:54:VAL:O	1:T:55:ARG:NH1	2.29	0.65
2:1:22:MET:HE3	2:2:114:ASP:HB3	1.79	0.65
1:G:54:VAL:O	1:G:55:ARG:NH1	2.29	0.65
2:H:22:MET:HE3	2:I:114:ASP:HB3	1.79	0.65
1:Q:54:VAL:O	1:Q:55:ARG:NH1	2.29	0.65
2:Z:114:ASP:HB3	2:Y:22:MET:HE3	1.79	0.65
2:J:22:MET:HE3	2:K:114:ASP:HB3	1.79	0.65
2:N:22:MET:HE3	2:H:114:ASP:HB3	1.79	0.64
2:X:22:MET:HE3	2:Y:114:ASP:HB3	1.79	0.64
2:K:22:MET:HE3	2:L:114:ASP:HB3	1.79	0.64
2:2:22:MET:HE3	2:V:114:ASP:HB3	1.79	0.64
2:M:114:ASP:HB3	2:L:22:MET:HE3	1.79	0.63
2:M:22:MET:HE3	2:N:114:ASP:HB3	1.79	0.63
2:V:22:MET:HE3	2:W:114:ASP:HB3	1.79	0.63
2:W:22:MET:HE3	2:X:114:ASP:HB3	1.79	0.63
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
2:1:167: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
2:1:167: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
2:1:28: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:Z:6:ILE:HD12	2:Z:155:VAL:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:6:ILE:HD12	2:M:155:VAL:HG23	1.89	0.55
2:1:6:ILE:HD12	2:1:155: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:J:6:ILE:HD12	2:J:155:VAL:HG23	1.89	0.55
2:K:28:HIS:CD2	2:L:120:VAL:HG13	2.41	0.55
2:Z:28:HIS:CD2	2:1:120:VAL:HG13	2.41	0.54
2:M:120:VAL:HG13	2:L:28:HIS:CD2	2.41	0.54
2:V:6:ILE:HD12	2:V:155:VAL:HG23	1.89	0.54
2:V:28:HIS:CD2	2:W:120:VAL:HG13	2.41	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:Z:93:MET:HB3	2:1:92:TYR:CE2	2.43	0.54
2:H:28:HIS:CD2	2:I:120:VAL:HG13	2.41	0.54
2:Z:92:TYR:CE2	2:Y:93:MET:HB3	2.43	0.54
2:Z:120:VAL:HG13	2:Y:28:HIS:CD2	2.41	0.54
2:H:93:MET:HB3	2:I:92:TYR:CE2	2.43	0.54
2:I:93:MET:HB3	2:J: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
2:N:93:MET:HB3	2:H:92:TYR:CE2	2.43	0.53
1:D:36:THR:HB	1:D:168:GLY:H	1.73	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
2:M:93:MET:HB3	2:N:92:TYR:CE2	2.43	0.53
2:V:93:MET:HB3	2:W:92:TYR:CE2	2.43	0.53
1:P:36:THR:HB	1:P:168:GLY:H	1.73	0.53
2:W:93:MET:HB3	2:X: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:M:28:HIS:CD2	2:N:120:VAL:HG13	2.41	0.53
2:N:28:HIS:CD2	2:H: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:36:THR:HB	1:B:168:GLY:H	1.73	0.52
1:R:35:SER:HB2	1:R:53:LYS:HG2	1.91	0.52
2:L:141:GLN:HE22	2:L:157:ARG:HE	1.58	0.52
2:2:141:GLN:HE22	2:2:157:ARG:HE	1.58	0.51
1:B:35:SER:HB2	1:B:53:LYS:HG2	1.91	0.51
1:S:35:SER:HB2	1:S:53:LYS:HG2	1.91	0.51
1:S:36:THR:HB	1:S:168:GLY:H	1.73	0.51
2:M:141:GLN:HE22	2:M:157:ARG:HE	1.58	0.51
1:A:35:SER:HB2	1:A:53:LYS:HG2	1.91	0.51
1:O:36:THR:HB	1:O:168:GLY:H	1.73	0.51
1:P:35:SER:HB2	1:P:53:LYS:HG2	1.91	0.51
2:K:141:GLN:HE22	2:K: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
1:U:35:SER:HB2	1:U:53:LYS:HG2	1.92	0.51
2:X:141:GLN:HE22	2:X:157:ARG:HE	1.58	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
2:2:139: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:W:165:ARG:HD3	2:J:139:GLU:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:28:HIS:HD2	2:1:120:VAL:HG11	1.72	0.48
2:Z:139:GLU:OE1	2:N:165:ARG:HD3	2.14	0.48
2:I:28:HIS:HD2	2:J:120:VAL:HG11	1.72	0.48
2:I:139:GLU:OE1	2:X:165:ARG:HD3	2.14	0.48
2:2:165:ARG:HD3	2:L:139:GLU:OE1	2.14	0.48
2:V:139:GLU:OE1	2:K:165:ARG:HD3	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
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:W:139:GLU:OE1	2:J:165:ARG:HD3	2.14	0.47
2:M:120:VAL:HG13	2:L:28:HIS:NE2	2.30	0.47
1:U:121:GLN:HE21	1:O:87:VAL:HG21	1.79	0.47
2:H:139:GLU:OE1	2:Y:165:ARG:HD3	2.14	0.47
1:B:121:GLN:HE21	1:C:87:VAL:HG21	1.79	0.47
1:D:121:GLN:HE21	1:E:87:VAL:HG21	1.79	0.47
1:S:87:VAL:HG21	1:R:121:GLN:HE21	1.79	0.47
2:Z:165:ARG:HD3	2:N:139:GLU:OE1	2.14	0.47
2:1:28:HIS:NE2	2:2:120:VAL:HG13	2.30	0.47
2:2:28:HIS:NE2	2:V:120:VAL:HG13	2.30	0.47
2:H:165:ARG:HD3	2:Y:139:GLU:OE1	2.14	0.47
2:V:28:HIS:NE2	2:W:120:VAL:HG13	2.30	0.47
2:W:7:THR:HG23	2:W:108:PRO:HB2	1.97	0.47
2:J:28:HIS:NE2	2:K:120:VAL:HG13	2.30	0.47
2:M:7:THR:HG23	2:M:108:PRO:HB2	1.97	0.47
1:A:121:GLN:HE21	1:B:87:VAL:HG21	1.79	0.47
2:I:165:ARG:HD3	2:X:139:GLU:OE1	2.14	0.47
2:X:159:ILE:HB	2:X:173:ILE:HD12	1.97	0.47
2:K:28:HIS:NE2	2:L:120:VAL:HG13	2.30	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:Z:120:VAL:HG11	2:Y:28:HIS:HD2	1.72	0.47
2:Z:120:VAL:HG13	2:Y:28:HIS:NE2	2.30	0.47
1:F:87:VAL:HG21	1:E:121:GLN:HE21	1.79	0.47
2:1:7:THR:HG23	2:1:108:PRO:HB2	1.97	0.47
2:1:159:ILE:HB	2:1:173:ILE:HD12	1.97	0.47
1:G:121:GLN:HE21	1:A:87:VAL:HG21	1.79	0.47
2:N:7:THR:HG23	2:N:108:PRO:HB2	1.97	0.47
2:N:28:HIS:NE2	2:H:120:VAL:HG13	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:159:ILE:HB	2:N:173:ILE:HD12	1.97	0.47
2:2:7:THR:HG23	2:2:108:PRO:HB2	1.97	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
1:O:121:GLN:HE21	1:P:87:VAL:HG21	1.79	0.47
2:I:159:ILE:HB	2:I:173:ILE:HD12	1.97	0.47
1:P:121:GLN:HE21	1:Q:87:VAL:HG21	1.79	0.47
2:J:159:ILE:HB	2:J:173:ILE:HD12	1.97	0.47
1:Q:121:GLN:HE21	1:R:87:VAL:HG21	1.79	0.47
2:X:7:THR:HG23	2:X:108:PRO:HB2	1.97	0.47
2:X:28:HIS:NE2	2:Y:120:VAL:HG13	2.30	0.47
2:K:7:THR:HG23	2:K: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:Z:28:HIS:NE2	2:1:120:VAL:HG13	2.30	0.47
2:M:28:HIS:NE2	2:N:120:VAL:HG13	2.30	0.47
2:M:159:ILE:HB	2:M:173:ILE:HD12	1.97	0.47
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
2:2:159:ILE:HB	2:2:173:ILE:HD12	1.97	0.46
2:I:28:HIS:NE2	2:J:120:VAL:HG13	2.30	0.46
2:W:28:HIS:NE2	2:X:120:VAL:HG13	2.30	0.46
2:Y:7:THR:HG23	2:Y:108:PRO:HB2	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:V:7:THR:HG23	2:V:108:PRO:HB2	1.97	0.46
2:I:7:THR:HG23	2:I:108:PRO:HB2	1.97	0.46
2:Z:7:THR:HG23	2:Z:108:PRO:HB2	1.97	0.46
2:L:7:THR:HG23	2:L:108:PRO:HB2	1.97	0.46
1:U:70:ILE:HG21	1:U:112:LEU:HD21	1.98	0.45
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
2:2:87:LEU:HD23	2:2:95:TYR:CD2	2.52	0.45
2:Z:87:LEU:HD23	2:Z:95:TYR:CD2	2.52	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
1:D:70:ILE:HG21	1:D:112:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:1:87:LEU:HD23	2:1:95:TYR:CD2	2.52	0.45
1:E:70:ILE:HG21	1:E:112:LEU:HD21	1.98	0.45
2:M:87:LEU:HD23	2:M:95:TYR:CD2	2.52	0.44
1:A:70:ILE:HG21	1:A:112:LEU:HD21	1.98	0.44
2:W:87:LEU:HD23	2:W:95:TYR:CD2	2.52	0.44
1:R:70:ILE:HG21	1:R:112:LEU:HD21	1.98	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
1:B:70:ILE:HG21	1:B:112:LEU:HD21	1.98	0.44
2:X:87:LEU:HD23	2:X:95:TYR:CD2	2.52	0.44
2:N:131:SER:HB3	2:N:132:PRO:HD3	2.00	0.43
2:W:131:SER:HB3	2:W:132:PRO:HD3	2.00	0.43
2:X:131:SER:HB3	2:X:132:PRO:HD3	2.00	0.43
2:M:131:SER:HB3	2:M:132:PRO:HD3	2.00	0.43
2:1:3:THR:HG22	2:1:16:THR:HG22	1.99	0.43
2:1:131:SER:HB3	2:1:132:PRO:HD3	2.00	0.43
2:2:131:SER:HB3	2:2:132:PRO:HD3	2.00	0.43
2:H:132:PRO:HB2	2:Y:132:PRO:HB2	2.01	0.43
2:Z:3:THR:HG22	2:Z:16:THR:HG22	1.99	0.43
2:V:131:SER:HB3	2:V:132:PRO:HD3	2.00	0.43
2:I:3:THR:HG22	2:I:16:THR:HG22	1.99	0.43
2:J:131:SER:HB3	2:J:132:PRO:HD3	2.00	0.43
2:X:3:THR:HG22	2:X:16:THR:HG22	1.99	0.43
2:K:131:SER:HB3	2:K:132:PRO:HD3	2.00	0.43
1:S:54:VAL:O	1:S:54:VAL:HG13	2.19	0.43
2:Z:132:PRO:HB2	2:N:132:PRO:HB2	2.01	0.43
2:Z:203:LEU:HD13	2:Z:203:LEU:C	2.44	0.43
2:M:203:LEU:C	2:M:203:LEU:HD13	2.44	0.43
2:N:3:THR:HG22	2:N:16:THR:HG22	1.99	0.43
1:B:54:VAL:O	1:B:54:VAL:HG13	2.19	0.43
2:I:203:LEU:HD13	2:I:203:LEU:C	2.44	0.43
2:W:203:LEU:C	2:W:203:LEU:HD13	2.44	0.43
2:J:3:THR:HG22	2:J:16:THR:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:54:VAL:O	1:R:54:VAL:HG13	2.19	0.43
2:Y:203:LEU:C	2:Y:203:LEU:HD13	2.44	0.43
2:L:131:SER:HB3	2:L:132:PRO:HD3	2.00	0.43
2:N:203:LEU:HD13	2:N:203:LEU:C	2.44	0.43
1:A:54:VAL:O	1:A:54:VAL:HG13	2.19	0.43
2:H:131:SER:HB3	2:H:132:PRO:HD3	2.00	0.43
2:H:203:LEU:C	2:H:203:LEU:HD13	2.44	0.43
2:I:132:PRO:HB2	2:X:132:PRO:HB2	2.01	0.43
2:W:3:THR:HG22	2:W:16:THR:HG22	1.99	0.43
2:X:203:LEU:HD13	2:X:203:LEU:C	2.44	0.43
2:K:203:LEU:C	2:K:203:LEU:HD13	2.44	0.43
2:L:3:THR:HG22	2:L:16:THR:HG22	1.99	0.43
2:M:3:THR:HG22	2:M:16:THR:HG22	1.99	0.43
1:T:54:VAL:O	1:T:54:VAL:HG13	2.19	0.43
2:2:203:LEU:C	2:2:203:LEU:HD13	2.44	0.43
2:Y:131:SER:HB3	2:Y:132:PRO:HD3	2.00	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:V:203:LEU:HD13	2:V:203:LEU:C	2.44	0.43
2:Y:3:THR:HG22	2:Y:16:THR:HG22	1.99	0.43
2:M:132:PRO:HB2	2:1:132:PRO:CB	2.49	0.43
2:W:132:PRO:HB2	2:J:132:PRO:CB	2.49	0.43
2:W:132:PRO:CB	2:J:132:PRO:HB2	2.49	0.43
1:C:54:VAL:O	1:C:54:VAL:HG13	2.19	0.43
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
2:1:203:LEU:HD13	2:1:203:LEU:C	2.44	0.42
1:D:54:VAL:O	1:D:54:VAL:HG13	2.19	0.42
2:L:203:LEU:HD13	2:L:203:LEU:C	2.44	0.42
1:F:53:LYS:HD3	1:F:53:LYS:HA	1.78	0.42
2:H:3:THR:HG22	2:H:16:THR:HG22	1.99	0.42
2:J:203:LEU:HD13	2:J:203:LEU:C	2.44	0.42
2:2:3:THR:HG22	2:2:16:THR:HG22	1.99	0.42
2:I:132:PRO:CB	2:X:132:PRO:HB2	2.49	0.42
1:P:53:LYS:HD3	1:P:53:LYS:HA	1.78	0.42
2:K:3:THR:HG22	2:K: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: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:I:132:PRO:HB2	2:X:132:PRO:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:144:GLU:CD	2:K:144:GLU:H	2.28	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
2:2:144:GLU:CD	2:2:144:GLU:H	2.28	0.42
2:M:144:GLU:CD	2:M:144:GLU:H	2.28	0.42
2:H:132:PRO:HB2	2:Y:132:PRO:CB	2.49	0.42
2:I:131:SER:HB3	2:I:132:PRO:HD3	2.00	0.42
1:E:54:VAL:O	1:E:54:VAL:HG13	2.19	0.42
1:F:54:VAL:O	1:F:54:VAL:HG13	2.19	0.42
2:M:21:THR:HG23	2:M:21:THR:O	2.20	0.42
1:G:54:VAL:O	1:G:54:VAL:HG13	2.19	0.42
2:H:132:PRO:CB	2:Y:132:PRO:HB2	2.49	0.42
1:O:54:VAL:O	1:O:54:VAL:HG13	2.19	0.42
2:W:21:THR:HG23	2:W:21:THR:O	2.20	0.42
1:Q:54:VAL:O	1:Q:54:VAL:HG13	2.19	0.42
2:2:132:PRO:HB2	2:L:132:PRO:HB2	2.00	0.42
1:P:54:VAL:O	1:P:54:VAL:HG13	2.19	0.42
2:W:144:GLU:CD	2:W:144:GLU:H	2.28	0.42
2:H:144:GLU:CD	2:H:144:GLU:H	2.28	0.41
2:Y:144:GLU:CD	2:Y:144:GLU:H	2.28	0.41
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:H:21:THR:HG23	2:H:21:THR:O	2.20	0.41
1:B:54:VAL:C	1:B:55:ARG:HG2	2.46	0.41
2:Y:21:THR:HG23	2:Y:21:THR:O	2.20	0.41
2:L:21:THR:HG23	2:L:21:THR:O	2.20	0.41
2:M:132:PRO:HB2	2:1:132:PRO:HB2	2.01	0.41
1:T:54:VAL:C	1:T:55:ARG:HG2	2.46	0.41
2:V:28:HIS:HD2	2:W:120:VAL:HG11	1.72	0.41
2:V:144:GLU:CD	2:V:144:GLU:H	2.28	0.41
2:Y:20:VAL:HG23	2:Y:31:GLY:HA3	2.03	0.41
1:S:54:VAL:C	1:S:55:ARG:HG2	2.46	0.41
2:N:21:THR:O	2:N:21:THR:HG23	2.20	0.41
2:V:21:THR:HG23	2:V:21:THR:O	2.20	0.41
1:C:54:VAL:C	1:C:55:ARG:HG2	2.46	0.41
2:X:21:THR:O	2:X:21:THR:HG23	2.20	0.41
2:K:20:VAL:HG23	2:K:31:GLY:HA3	2.03	0.41
2:Z:144:GLU:H	2:Z:144:GLU:CD	2.28	0.41
2:2:20:VAL:HG23	2:2:31:GLY:HA3	2.03	0.41
2:H:20:VAL:HG23	2:H:31:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:20:VAL:HG23	2:V:31:GLY:HA3	2.03	0.41
2:I:144:GLU:H	2:I:144:GLU:CD	2.28	0.41
1:P:54:VAL:C	1:P:55:ARG:HG2	2.46	0.41
2:K:21:THR:HG23	2:K:21:THR:O	2.20	0.41
2:L:20:VAL:HG23	2:L:31:GLY:HA3	2.03	0.41
2:L:144:GLU:H	2:L:144:GLU:CD	2.28	0.41
1:U:54:VAL:C	1:U:55:ARG:HG2	2.46	0.41
2:1:144:GLU:H	2:1:144:GLU:CD	2.28	0.41
1:G:54:VAL:C	1:G:55:ARG:HG2	2.46	0.41
2:N:20:VAL:HG23	2:N:31:GLY:HA3	2.03	0.41
2:2:21:THR:HG23	2:2:21:THR:O	2.20	0.41
2:J:21:THR:HG23	2:J:21:THR:O	2.20	0.41
2:J:144:GLU:H	2:J:144:GLU:CD	2.28	0.41
1:Q:54:VAL:C	1:Q:55:ARG:HG2	2.46	0.41
2:X:20:VAL:HG23	2:X:31:GLY:HA3	2.03	0.41
1:D:54:VAL:C	1:D:55:ARG:HG2	2.46	0.41
2:K:28:HIS:HD2	2:L:120:VAL:HG11	1.72	0.41
1:E:54:VAL:C	1:E:55:ARG:HG2	2.46	0.41
2:Z:20:VAL:HG23	2:Z:31:GLY:HA3	2.03	0.41
2:Z:21:THR:O	2:Z:21:THR:HG23	2.20	0.41
2:M:20:VAL:HG23	2:M:31:GLY:HA3	2.03	0.41
2:1:21:THR:HG23	2:1:21:THR:O	2.20	0.41
2:2:28:HIS:HD2	2:V:120:VAL:HG11	1.72	0.41
1:O:54:VAL:C	1:O:55:ARG:HG2	2.46	0.41
2:I:21:THR:O	2:I:21:THR:HG23	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
1:F:54:VAL:C	1:F:55:ARG:HG2	2.46	0.40
2:H:167:SER:HB3	2:X:26:ILE:HG21	2.04	0.40
1:R:54:VAL:C	1:R:55:ARG:HG2	2.46	0.40
2:1:20:VAL:HG23	2:1:31:GLY:HA3	2.03	0.40
2:N:26:ILE:HG21	2:Y:167:SER:HB3	2.04	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	14	43
1	B	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	14	43
1	C	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	14	43
1	D	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	14	43
1	E	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	14	43
1	F	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	14	43
1	G	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	14	43
1	O	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	14	43
1	P	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	14	43
1	Q	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	14	43
1	R	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	14	43
1	S	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	14	43
1	T	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	14	43
1	U	222/224 (99%)	199 (90%)	21 (10%)	2 (1%)	14	43
2	1	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	3	20
2	2	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	3	20
2	H	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	3	20
2	I	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	3	20
2	J	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	3	20
2	K	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	3	20
2	L	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	3	20
2	M	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	3	20
2	N	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	3	20
2	V	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	3	20
2	W	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	X	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	3	20
2	Y	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	3	20
2	Z	201/203 (99%)	182 (90%)	13 (6%)	6 (3%)	3	20
All	All	5922/5978 (99%)	5334 (90%)	476 (8%)	112 (2%)	8	28

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	171 (92%)	15 (8%)	11	36
1	B	186/186 (100%)	171 (92%)	15 (8%)	11	36
1	C	186/186 (100%)	171 (92%)	15 (8%)	11	36
1	D	186/186 (100%)	171 (92%)	15 (8%)	11	36
1	E	186/186 (100%)	171 (92%)	15 (8%)	11	36
1	F	186/186 (100%)	171 (92%)	15 (8%)	11	36
1	G	186/186 (100%)	171 (92%)	15 (8%)	11	36
1	O	186/186 (100%)	171 (92%)	15 (8%)	11	36
1	P	186/186 (100%)	171 (92%)	15 (8%)	11	36
1	Q	186/186 (100%)	171 (92%)	15 (8%)	11	36
1	R	186/186 (100%)	171 (92%)	15 (8%)	11	36
1	S	186/186 (100%)	171 (92%)	15 (8%)	11	36
1	T	186/186 (100%)	171 (92%)	15 (8%)	11	36
1	U	186/186 (100%)	171 (92%)	15 (8%)	11	36
2	1	170/170 (100%)	152 (89%)	18 (11%)	6	24
2	2	170/170 (100%)	152 (89%)	18 (11%)	6	24
2	H	170/170 (100%)	152 (89%)	18 (11%)	6	24
2	I	170/170 (100%)	152 (89%)	18 (11%)	6	24
2	J	170/170 (100%)	152 (89%)	18 (11%)	6	24
2	K	170/170 (100%)	152 (89%)	18 (11%)	6	24
2	L	170/170 (100%)	152 (89%)	18 (11%)	6	24
2	M	170/170 (100%)	152 (89%)	18 (11%)	6	24
2	N	170/170 (100%)	152 (89%)	18 (11%)	6	24
2	V	170/170 (100%)	152 (89%)	18 (11%)	6	24
2	W	170/170 (100%)	152 (89%)	18 (11%)	6	24
2	X	170/170 (100%)	152 (89%)	18 (11%)	6	24
2	Y	170/170 (100%)	152 (89%)	18 (11%)	6	24
2	Z	170/170 (100%)	152 (89%)	18 (11%)	6	24
All	All	4984/4984 (100%)	4522 (91%)	462 (9%)	11	30

All (462) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	38	LEU
1	S	47	LEU
1	S	53	LYS
1	S	74	VAL
1	S	77	VAL
1	S	136	LEU
1	S	137	ILE
1	S	141	ILE
1	S	177	GLU
1	S	212	ILE
1	S	216	THR
1	S	221	TYR
1	S	224	TYR
1	S	225	ASP
1	S	229	VAL
2	Z	12	VAL
2	Z	17	GLU
2	Z	26	ILE
2	Z	30	ASN
2	Z	37	ILE
2	Z	45	ILE
2	Z	49	VAL
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
2	Z	198	LYS
2	Z	203	LEU
1	F	38	LEU
1	F	47	LEU
1	F	53	LYS
1	F	74	VAL
1	F	77	VAL
1	F	136	LEU
1	F	137	ILE
1	F	141	ILE
1	F	177	GLU

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Mol	Chain	Res	Type
1	F	212	ILE
1	F	216	THR
1	F	221	TYR
1	F	224	TYR
1	F	225	ASP
1	F	229	VAL
2	M	12	VAL
2	M	17	GLU
2	M	26	ILE
2	M	30	ASN
2	M	37	ILE
2	M	45	ILE
2	M	49	VAL
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
2	M	198	LYS
2	M	203	LEU
1	T	38	LEU
1	T	47	LEU
1	T	53	LYS
1	T	74	VAL
1	T	77	VAL
1	T	136	LEU
1	T	137	ILE
1	T	141	ILE
1	T	177	GLU
1	T	212	ILE
1	T	216	THR
1	T	221	TYR
1	T	224	TYR
1	T	225	ASP
1	T	229	VAL
2	1	12	VAL
2	1	17	GLU
2	1	26	ILE

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Mol	Chain	Res	Type
2	1	30	ASN
2	1	37	ILE
2	1	45	ILE
2	1	49	VAL
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
2	1	198	LYS
2	1	203	LEU
1	G	38	LEU
1	G	47	LEU
1	G	53	LYS
1	G	74	VAL
1	G	77	VAL
1	G	136	LEU
1	G	137	ILE
1	G	141	ILE
1	G	177	GLU
1	G	212	ILE
1	G	216	THR
1	G	221	TYR
1	G	224	TYR
1	G	225	ASP
1	G	229	VAL
2	N	12	VAL
2	N	17	GLU
2	N	26	ILE
2	N	30	ASN
2	N	37	ILE
2	N	45	ILE
2	N	49	VAL
2	N	68	LEU
2	N	79	VAL
2	N	100	LEU
2	N	120	VAL
2	N	137	VAL

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Mol	Chain	Res	Type
2	N	144	GLU
2	N	175	VAL
2	N	178	ILE
2	N	179	THR
2	N	198	LYS
2	N	203	LEU
1	U	38	LEU
1	U	47	LEU
1	U	53	LYS
1	U	74	VAL
1	U	77	VAL
1	U	136	LEU
1	U	137	ILE
1	U	141	ILE
1	U	177	GLU
1	U	212	ILE
1	U	216	THR
1	U	221	TYR
1	U	224	TYR
1	U	225	ASP
1	U	229	VAL
2	2	12	VAL
2	2	17	GLU
2	2	26	ILE
2	2	30	ASN
2	2	37	ILE
2	2	45	ILE
2	2	49	VAL
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
2	2	198	LYS
2	2	203	LEU
1	A	38	LEU
1	A	47	LEU
1	A	53	LYS

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Mol	Chain	Res	Type
1	A	74	VAL
1	A	77	VAL
1	A	136	LEU
1	A	137	ILE
1	A	141	ILE
1	A	177	GLU
1	A	212	ILE
1	A	216	THR
1	A	221	TYR
1	A	224	TYR
1	A	225	ASP
1	A	229	VAL
2	H	12	VAL
2	H	17	GLU
2	H	26	ILE
2	H	30	ASN
2	H	37	ILE
2	H	45	ILE
2	H	49	VAL
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
2	H	178	ILE
2	H	179	THR
2	H	198	LYS
2	H	203	LEU
1	O	38	LEU
1	O	47	LEU
1	O	53	LYS
1	O	74	VAL
1	O	77	VAL
1	O	136	LEU
1	O	137	ILE
1	O	141	ILE
1	O	177	GLU
1	O	212	ILE
1	O	216	THR
1	O	221	TYR

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Mol	Chain	Res	Type
1	O	224	TYR
1	O	225	ASP
1	O	229	VAL
2	V	12	VAL
2	V	17	GLU
2	V	26	ILE
2	V	30	ASN
2	V	37	ILE
2	V	45	ILE
2	V	49	VAL
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
2	V	198	LYS
2	V	203	LEU
1	B	38	LEU
1	B	47	LEU
1	B	53	LYS
1	B	74	VAL
1	B	77	VAL
1	B	136	LEU
1	B	137	ILE
1	B	141	ILE
1	B	177	GLU
1	B	212	ILE
1	B	216	THR
1	B	221	TYR
1	B	224	TYR
1	B	225	ASP
1	B	229	VAL
2	I	12	VAL
2	I	17	GLU
2	I	26	ILE
2	I	30	ASN
2	I	37	ILE
2	I	45	ILE

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Mol	Chain	Res	Type
2	I	49	VAL
2	I	68	LEU
2	I	79	VAL
2	I	100	LEU
2	I	120	VAL
2	I	137	VAL
2	I	144	GLU
2	I	175	VAL
2	I	178	ILE
2	I	179	THR
2	I	198	LYS
2	I	203	LEU
1	P	38	LEU
1	P	47	LEU
1	P	53	LYS
1	P	74	VAL
1	P	77	VAL
1	P	136	LEU
1	P	137	ILE
1	P	141	ILE
1	P	177	GLU
1	P	212	ILE
1	P	216	THR
1	P	221	TYR
1	P	224	TYR
1	P	225	ASP
1	P	229	VAL
2	W	12	VAL
2	W	17	GLU
2	W	26	ILE
2	W	30	ASN
2	W	37	ILE
2	W	45	ILE
2	W	49	VAL
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

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Mol	Chain	Res	Type
2	W	179	THR
2	W	198	LYS
2	W	203	LEU
1	C	38	LEU
1	C	47	LEU
1	C	53	LYS
1	C	74	VAL
1	C	77	VAL
1	C	136	LEU
1	C	137	ILE
1	C	141	ILE
1	C	177	GLU
1	C	212	ILE
1	C	216	THR
1	C	221	TYR
1	C	224	TYR
1	C	225	ASP
1	C	229	VAL
2	J	12	VAL
2	J	17	GLU
2	J	26	ILE
2	J	30	ASN
2	J	37	ILE
2	J	45	ILE
2	J	49	VAL
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
2	J	198	LYS
2	J	203	LEU
1	Q	38	LEU
1	Q	47	LEU
1	Q	53	LYS
1	Q	74	VAL
1	Q	77	VAL
1	Q	136	LEU

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Mol	Chain	Res	Type
1	Q	137	ILE
1	Q	141	ILE
1	Q	177	GLU
1	Q	212	ILE
1	Q	216	THR
1	Q	221	TYR
1	Q	224	TYR
1	Q	225	ASP
1	Q	229	VAL
2	X	12	VAL
2	X	17	GLU
2	X	26	ILE
2	X	30	ASN
2	X	37	ILE
2	X	45	ILE
2	X	49	VAL
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
2	X	198	LYS
2	X	203	LEU
1	D	38	LEU
1	D	47	LEU
1	D	53	LYS
1	D	74	VAL
1	D	77	VAL
1	D	136	LEU
1	D	137	ILE
1	D	141	ILE
1	D	177	GLU
1	D	212	ILE
1	D	216	THR
1	D	221	TYR
1	D	224	TYR
1	D	225	ASP
1	D	229	VAL

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Mol	Chain	Res	Type
2	K	12	VAL
2	K	17	GLU
2	K	26	ILE
2	K	30	ASN
2	K	37	ILE
2	K	45	ILE
2	K	49	VAL
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
2	K	198	LYS
2	K	203	LEU
1	R	38	LEU
1	R	47	LEU
1	R	53	LYS
1	R	74	VAL
1	R	77	VAL
1	R	136	LEU
1	R	137	ILE
1	R	141	ILE
1	R	177	GLU
1	R	212	ILE
1	R	216	THR
1	R	221	TYR
1	R	224	TYR
1	R	225	ASP
1	R	229	VAL
2	Y	12	VAL
2	Y	17	GLU
2	Y	26	ILE
2	Y	30	ASN
2	Y	37	ILE
2	Y	45	ILE
2	Y	49	VAL
2	Y	68	LEU
2	Y	79	VAL

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Mol	Chain	Res	Type
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
2	Y	198	LYS
2	Y	203	LEU
1	E	38	LEU
1	E	47	LEU
1	E	53	LYS
1	E	74	VAL
1	E	77	VAL
1	E	136	LEU
1	E	137	ILE
1	E	141	ILE
1	E	177	GLU
1	E	212	ILE
1	E	216	THR
1	E	221	TYR
1	E	224	TYR
1	E	225	ASP
1	E	229	VAL
2	L	12	VAL
2	L	17	GLU
2	L	26	ILE
2	L	30	ASN
2	L	37	ILE
2	L	45	ILE
2	L	49	VAL
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
2	L	198	LYS
2	L	203	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	97	GLN
1	S	111	ASN
1	S	121	GLN
1	S	158	ASN
2	Z	30	ASN
2	Z	85	ASN
2	Z	89	GLN
2	Z	98	GLN
2	Z	164	GLN
2	Z	191	GLN
1	F	97	GLN
1	F	111	ASN
1	F	121	GLN
2	M	30	ASN
2	M	85	ASN
2	M	89	GLN
2	M	164	GLN
2	M	191	GLN
1	T	97	GLN
1	T	111	ASN
1	T	121	GLN
1	T	158	ASN
2	1	30	ASN
2	1	85	ASN
2	1	89	GLN
2	1	164	GLN
2	1	191	GLN
1	G	97	GLN
1	G	111	ASN
1	G	121	GLN
1	G	158	ASN
2	N	30	ASN
2	N	85	ASN
2	N	89	GLN
2	N	164	GLN
2	N	191	GLN
1	U	97	GLN
1	U	111	ASN
1	U	121	GLN
2	2	30	ASN
2	2	85	ASN

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Mol	Chain	Res	Type
2	2	89	GLN
2	2	164	GLN
2	2	191	GLN
1	A	97	GLN
1	A	111	ASN
1	A	121	GLN
1	A	158	ASN
2	H	30	ASN
2	H	85	ASN
2	H	89	GLN
2	H	164	GLN
2	H	191	GLN
1	O	97	GLN
1	O	111	ASN
1	O	121	GLN
1	O	158	ASN
2	V	30	ASN
2	V	85	ASN
2	V	89	GLN
2	V	164	GLN
2	V	191	GLN
1	B	97	GLN
1	B	111	ASN
1	B	121	GLN
2	I	30	ASN
2	I	85	ASN
2	I	89	GLN
2	I	164	GLN
2	I	191	GLN
1	P	97	GLN
1	P	111	ASN
1	P	121	GLN
2	W	30	ASN
2	W	85	ASN
2	W	89	GLN
2	W	164	GLN
2	W	191	GLN
1	C	97	GLN
1	C	111	ASN
1	C	121	GLN
2	J	30	ASN
2	J	85	ASN

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Mol	Chain	Res	Type
2	J	89	GLN
2	J	164	GLN
2	J	191	GLN
1	Q	97	GLN
1	Q	111	ASN
1	Q	121	GLN
2	X	30	ASN
2	X	85	ASN
2	X	89	GLN
2	X	164	GLN
2	X	191	GLN
1	D	97	GLN
1	D	111	ASN
1	D	121	GLN
2	K	30	ASN
2	K	85	ASN
2	K	89	GLN
2	K	164	GLN
2	K	191	GLN
1	R	97	GLN
1	R	111	ASN
1	R	121	GLN
1	R	158	ASN
2	Y	30	ASN
2	Y	85	ASN
2	Y	89	GLN
2	Y	164	GLN
2	Y	191	GLN
1	E	97	GLN
1	E	111	ASN
1	E	121	GLN
1	E	158	ASN
2	L	30	ASN
2	L	85	ASN
2	L	89	GLN
2	L	164	GLN
2	L	191	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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.

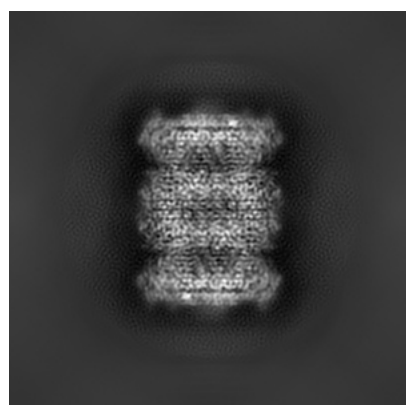
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5623. These allow visual inspection of the internal detail of the map and identification of artifacts.

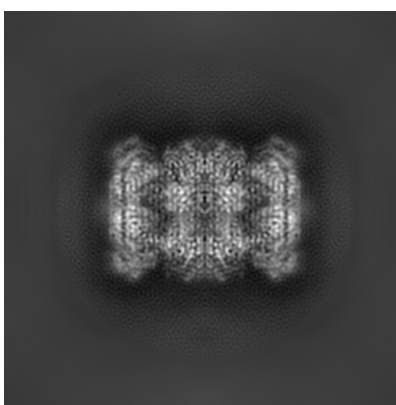
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

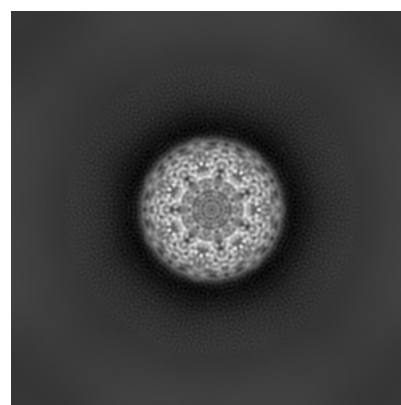
6.1.1 Primary map



X



Y

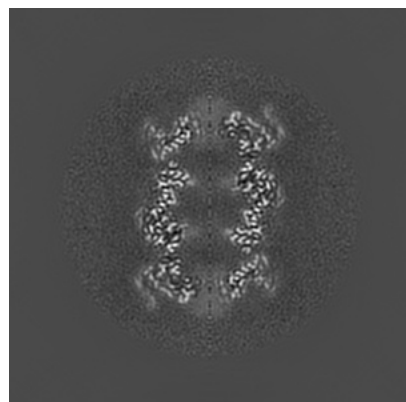


Z

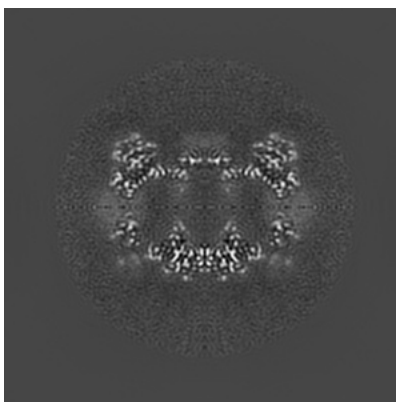
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

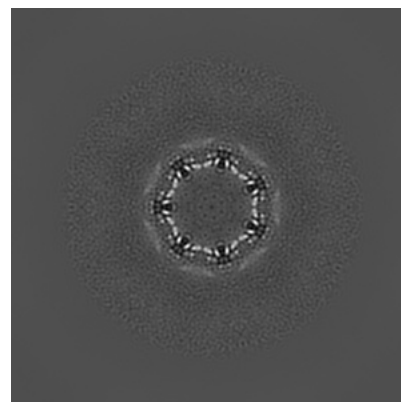
6.2.1 Primary map



X Index: 128



Y Index: 128

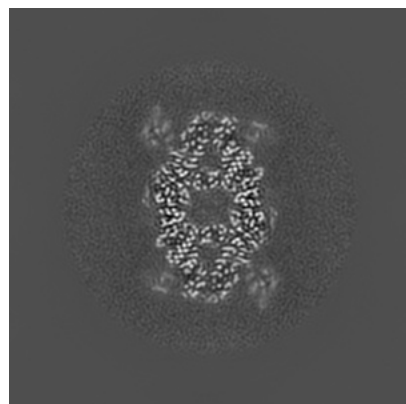


Z Index: 128

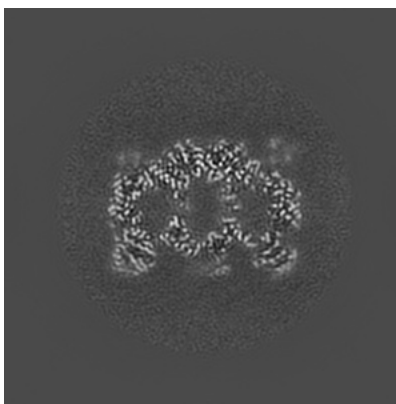
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

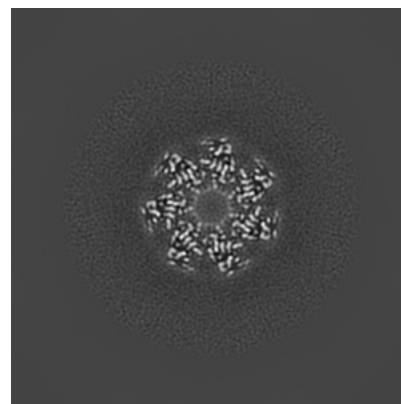
6.3.1 Primary map



X Index: 109



Y Index: 113

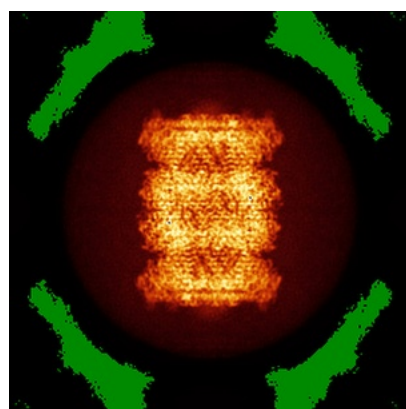


Z Index: 142

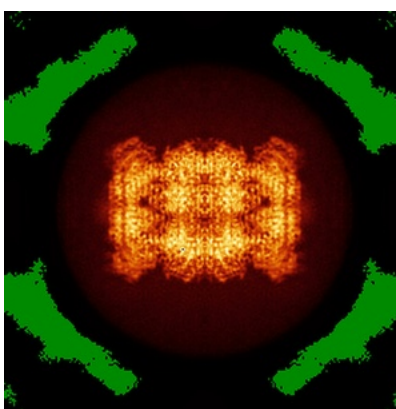
The images above show the largest variance slices of the map in three orthogonal directions.

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

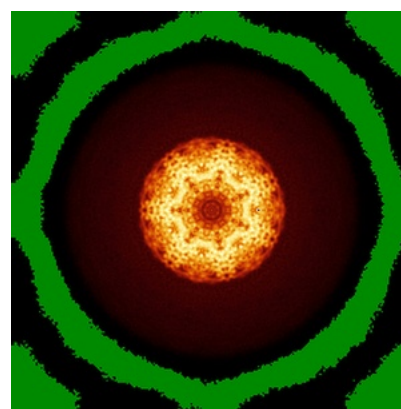
6.4.1 Primary map



X



Y

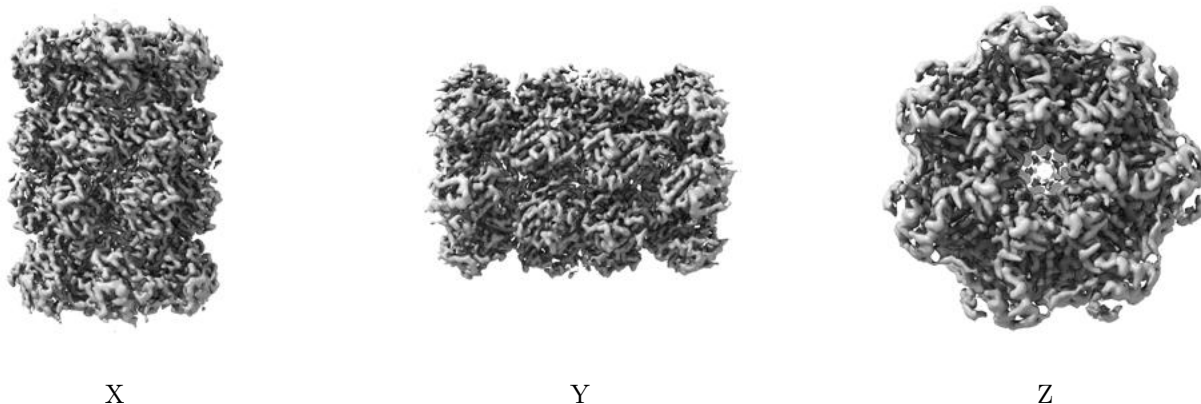


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

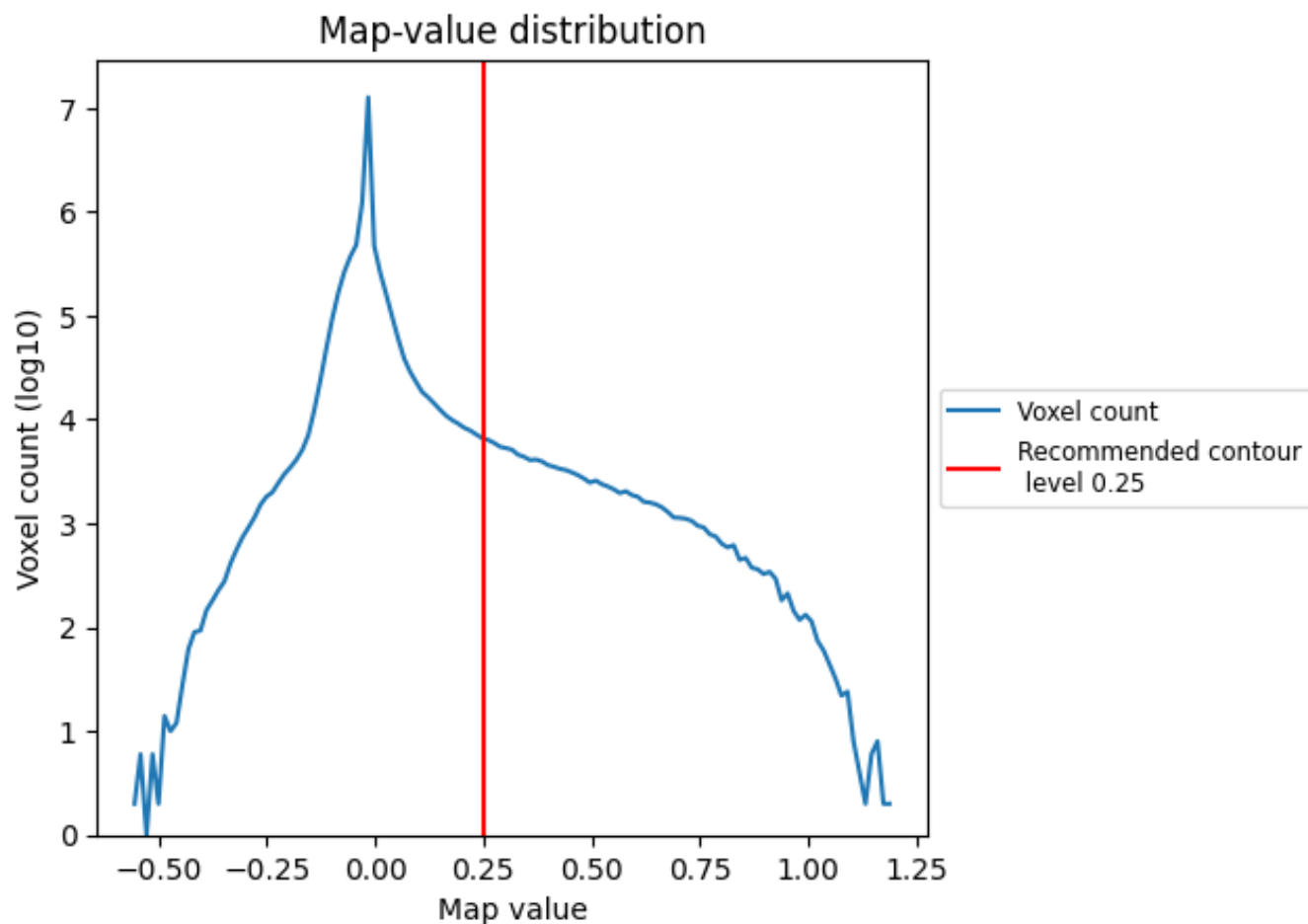
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

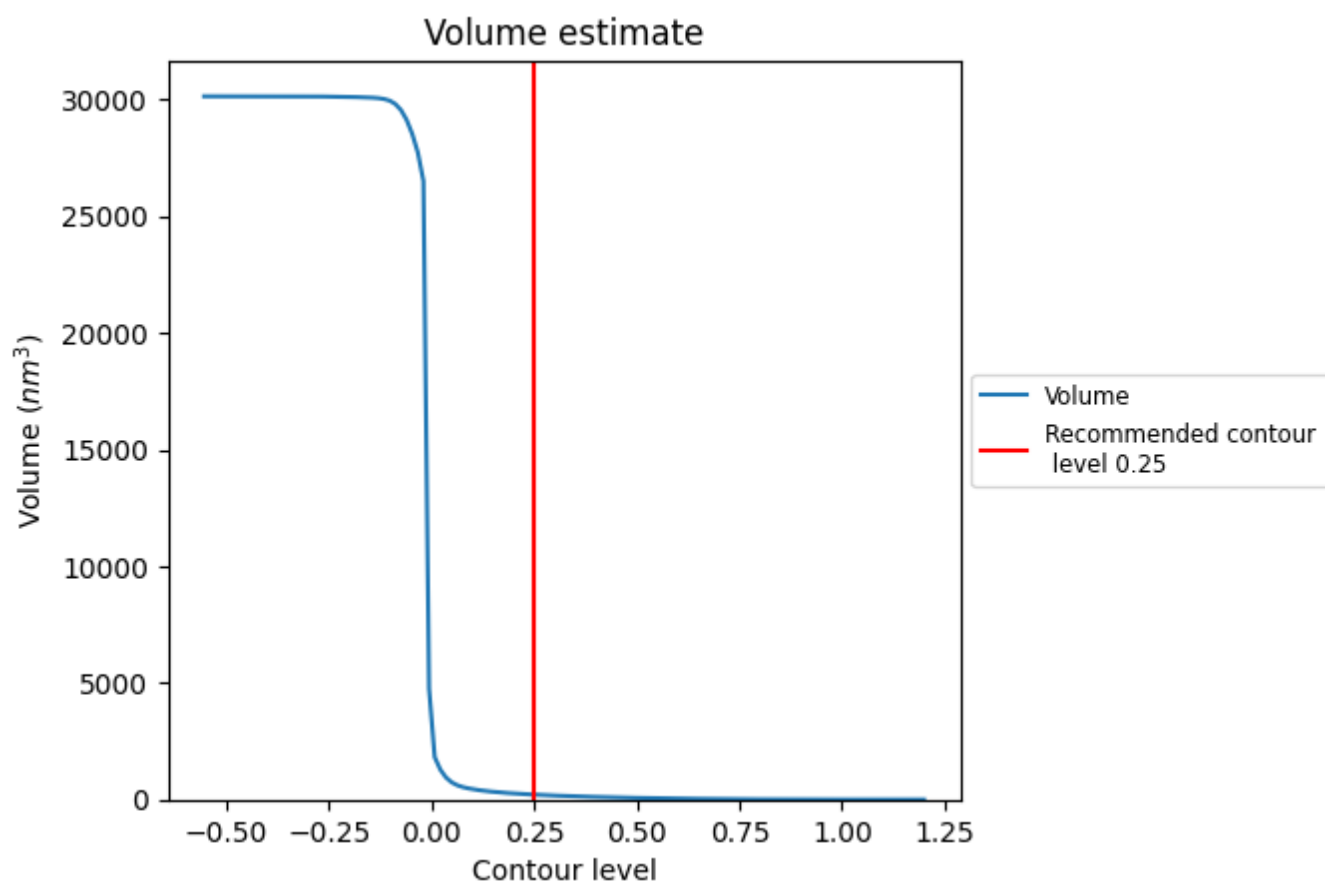
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

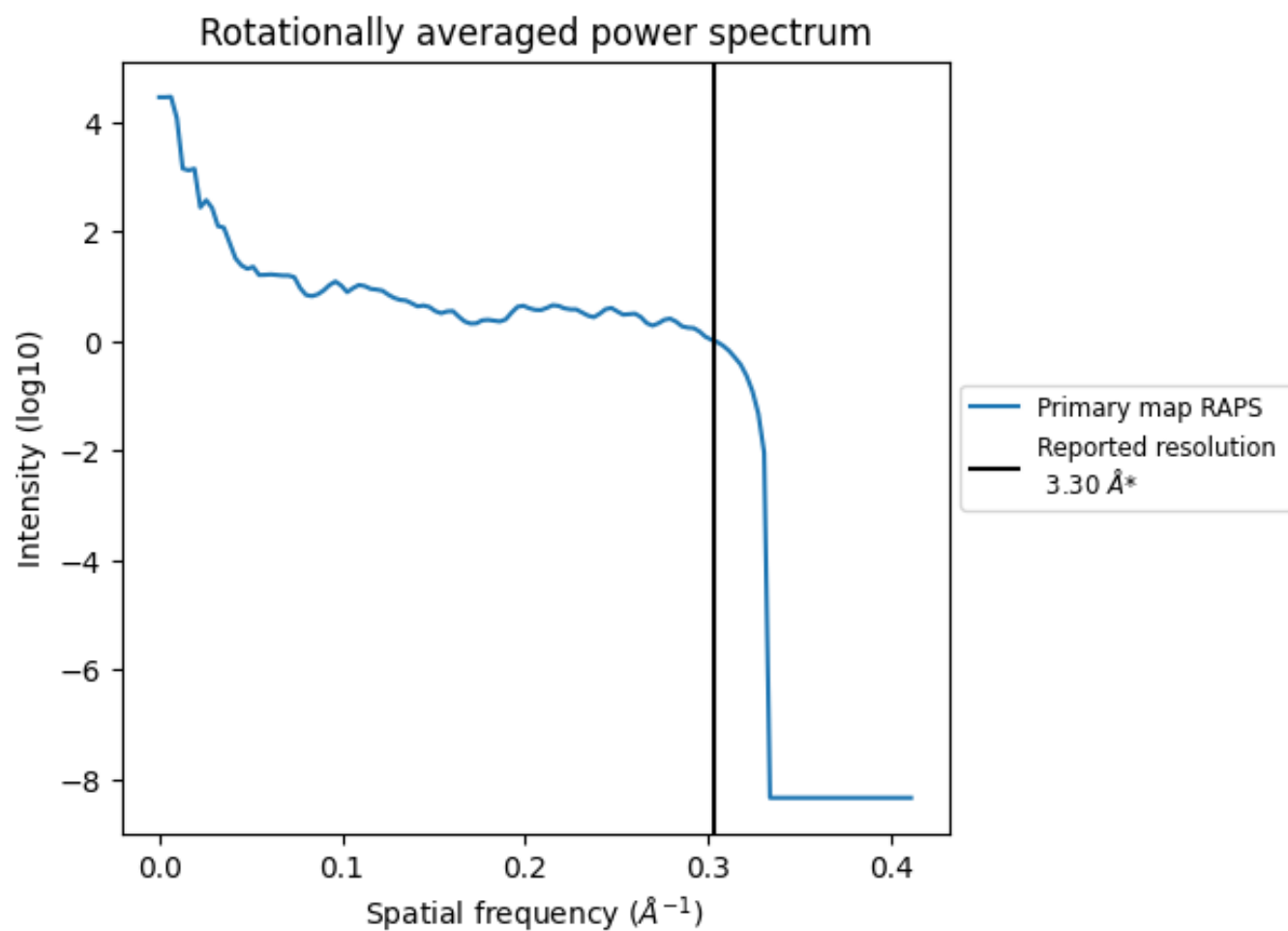
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 211 nm³; this corresponds to an approximate mass of 191 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

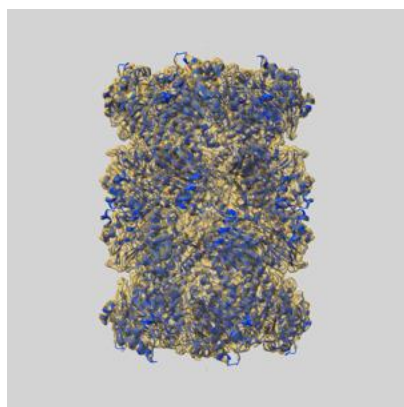
8 Fourier-Shell correlation ⓘ

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

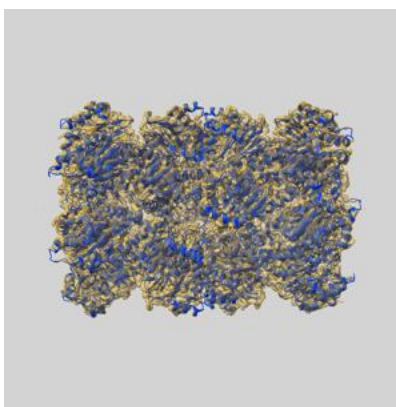
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5623 and PDB model 3J9I. Per-residue inclusion information can be found in section [3](#) on page [6](#).

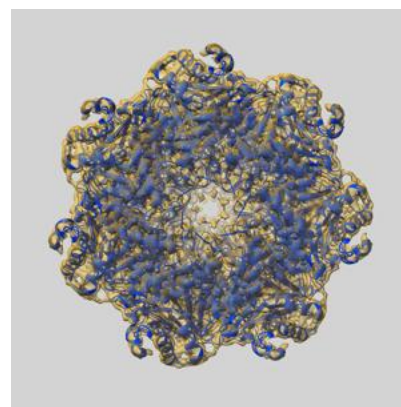
9.1 Map-model overlay [i](#)



X



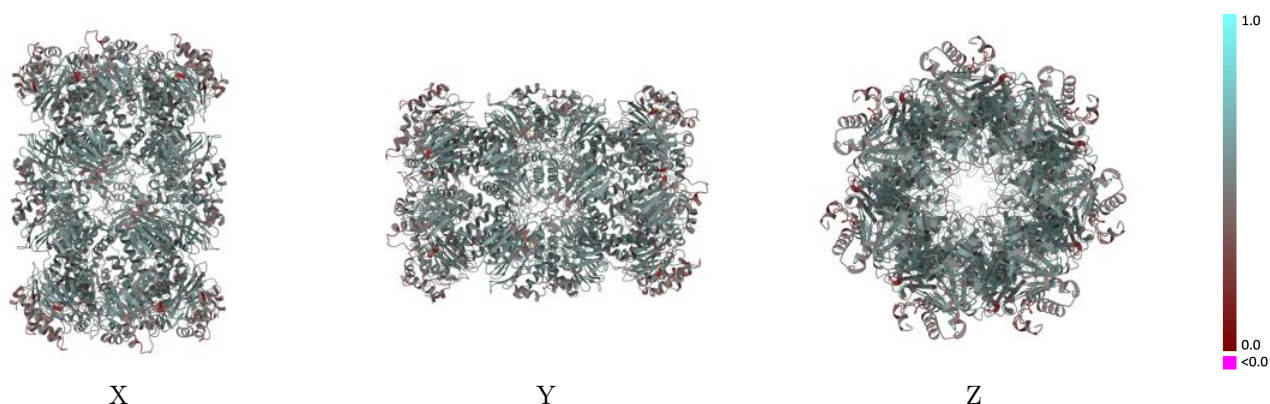
Y



Z

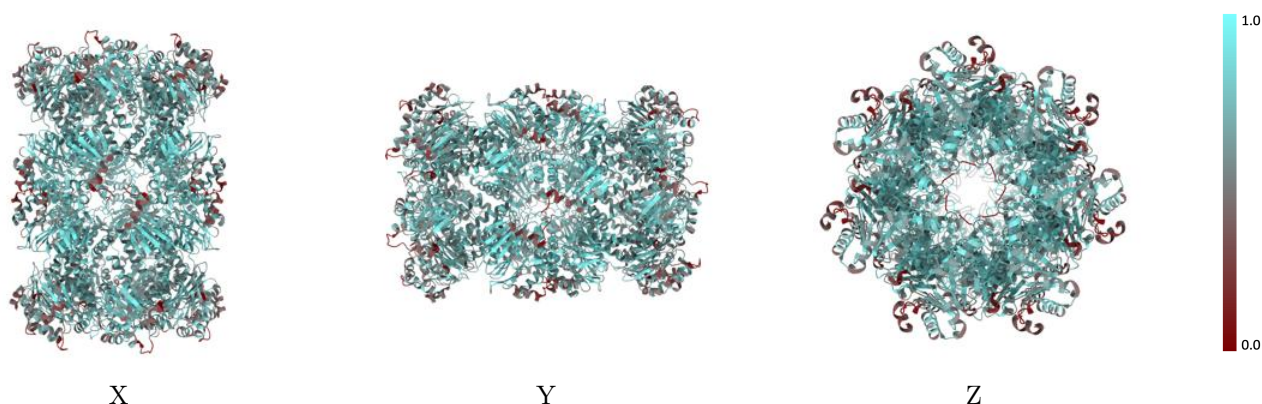
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



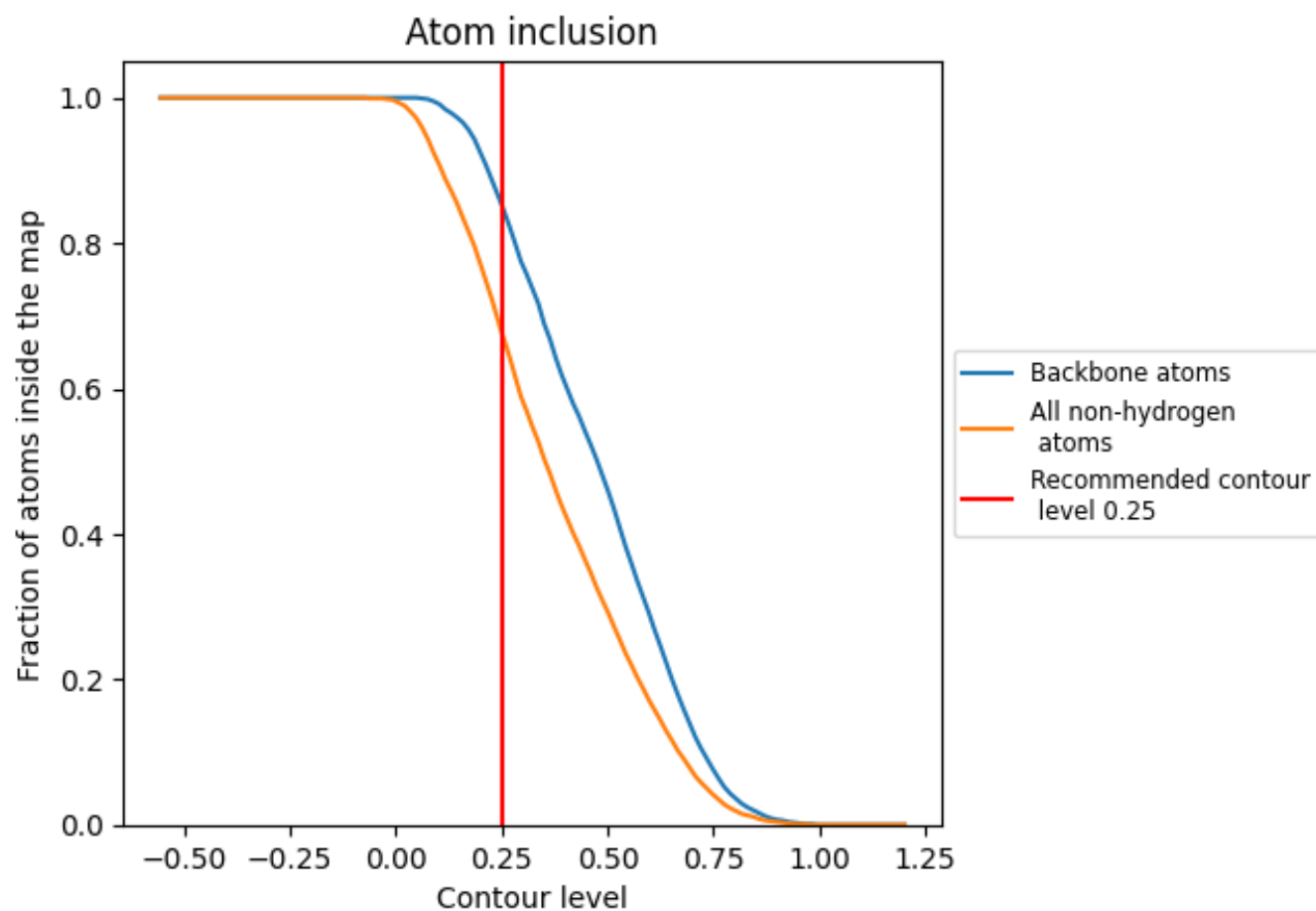
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6770	 0.5100
1	 0.7270	 0.5330
2	 0.7340	 0.5360
A	 0.6230	 0.4860
B	 0.6250	 0.4860
C	 0.6290	 0.4860
D	 0.6310	 0.4850
E	 0.6250	 0.4870
F	 0.6280	 0.4880
G	 0.6310	 0.4880
H	 0.7350	 0.5340
I	 0.7390	 0.5370
J	 0.7280	 0.5310
K	 0.7340	 0.5350
L	 0.7320	 0.5340
M	 0.7320	 0.5360
N	 0.7320	 0.5340
O	 0.6250	 0.4860
P	 0.6280	 0.4860
Q	 0.6310	 0.4870
R	 0.6230	 0.4860
S	 0.6240	 0.4890
T	 0.6290	 0.4890
U	 0.6310	 0.4870
V	 0.7320	 0.5340
W	 0.7320	 0.5360
X	 0.7320	 0.5350
Y	 0.7350	 0.5350
Z	 0.7390	 0.5380

