



Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 07:33 pm BST

PDB ID : 6YL3 / pdb_00006yl3
EMDB ID : EMD-10835
Title : High resolution cryo-EM structure of urease from the pathogen *Yersinia enterocolitica*
Authors : Righetto, R.D.; Anton, L.; Adaixo, R.; Jakob, R.; Zivanov, J.; Mahi, M.A.; Ringler, P.; Schwede, T.; Maier, T.; Stahlberg, H.
Deposited on : 2020-04-06
Resolution : 1.98 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

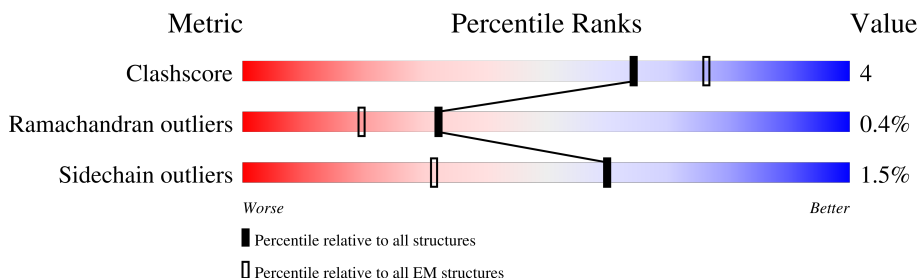
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.











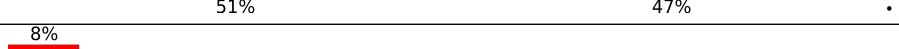
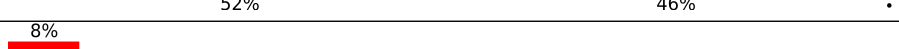



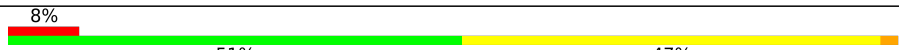
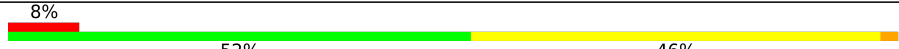










Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	2	100	
1	5	100	
1	8	100	
1	A	100	
1	D	100	
1	G	100	
1	J	100	
1	M	100	



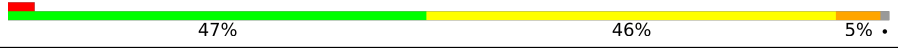
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Mol	Chain	Length	Quality of chain
1	P	100	
1	S	100	
1	W	100	
1	Z	100	
2	0	132	
2	3	132	
2	6	132	
2	9	132	
2	B	132	
2	E	132	
2	H	132	
2	K	132	
2	N	132	
2	Q	132	
2	T	132	
2	X	132	
3	1	571	
3	4	571	
3	7	571	
3	C	571	
3	F	571	
3	I	571	
3	L	571	
3	O	571	
3	R	571	

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Mol	Chain	Length	Quality of chain
3	U	571	
3	V	571	
3	Y	571	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 150276 atoms, of which 73164 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 Urease subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	D	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	G	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	J	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	M	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	P	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	S	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	W	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	Z	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	2	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	5	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		
1	8	100	Total	C	H	N	O	S	8	0
			1661	509	856	136	154	6		

- Molecule 2 is a protein called Urease subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	132	Total	C	H	N	O	S	2	0
			2061	654	1019	190	197	1		
2	E	132	Total	C	H	N	O	S	2	0
			2061	654	1019	190	197	1		
2	H	132	Total	C	H	N	O	S	2	0
			2061	654	1019	190	197	1		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	K	132	Total 2061	C 654	H 1019	N 190	O 197	S 1	2	0
2	N	132	Total 2061	C 654	H 1019	N 190	O 197	S 1	2	0
2	Q	132	Total 2061	C 654	H 1019	N 190	O 197	S 1	2	0
2	T	132	Total 2061	C 654	H 1019	N 190	O 197	S 1	2	0
2	X	132	Total 2061	C 654	H 1019	N 190	O 197	S 1	2	0
2	0	132	Total 2061	C 654	H 1019	N 190	O 197	S 1	2	0
2	3	132	Total 2061	C 654	H 1019	N 190	O 197	S 1	2	0
2	6	132	Total 2061	C 654	H 1019	N 190	O 197	S 1	2	0
2	9	132	Total 2061	C 654	H 1019	N 190	O 197	S 1	2	0

- Molecule 3 is a protein called Urease subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	564	Total 8493	C 2669	H 4222	N 756	O 818	S 28	10	0
3	F	564	Total 8493	C 2669	H 4222	N 756	O 818	S 28	10	0
3	I	564	Total 8493	C 2669	H 4222	N 756	O 818	S 28	10	0
3	L	564	Total 8493	C 2669	H 4222	N 756	O 818	S 28	10	0
3	O	564	Total 8493	C 2669	H 4222	N 756	O 818	S 28	10	0
3	R	564	Total 8493	C 2669	H 4222	N 756	O 818	S 28	10	0
3	V	564	Total 8493	C 2669	H 4222	N 756	O 818	S 28	10	0
3	Y	564	Total 8493	C 2669	H 4222	N 756	O 818	S 28	10	0
3	1	564	Total 8493	C 2669	H 4222	N 756	O 818	S 28	10	0
3	4	564	Total 8493	C 2669	H 4222	N 756	O 818	S 28	10	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
3	7	564	Total	C	H	N	O	S	10	0
			8493	2669	4222	756	818	28		
3	U	564	Total	C	H	N	O	S	10	0
			8493	2669	4222	756	818	28		

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		AltConf
4	C	2	Total	Ni	0
			2	2	
4	F	2	Total	Ni	0
			2	2	
4	I	2	Total	Ni	0
			2	2	
4	L	2	Total	Ni	0
			2	2	
4	O	2	Total	Ni	0
			2	2	
4	R	2	Total	Ni	0
			2	2	
4	V	2	Total	Ni	0
			2	2	
4	Y	2	Total	Ni	0
			2	2	
4	1	2	Total	Ni	0
			2	2	
4	4	2	Total	Ni	0
			2	2	
4	7	2	Total	Ni	0
			2	2	
4	U	2	Total	Ni	0
			2	2	

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	25	Total	O	0
			25	25	
5	B	59	Total	O	0
			59	59	
5	C	224	Total	O	0
			224	224	

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Mol	Chain	Residues	Atoms		AltConf
5	D	25	Total 25	O 25	0
5	E	59	Total 59	O 59	0
5	F	225	Total 225	O 225	0
5	G	27	Total 27	O 27	0
5	H	58	Total 58	O 58	0
5	I	227	Total 227	O 227	0
5	J	25	Total 25	O 25	0
5	K	59	Total 59	O 59	0
5	L	227	Total 227	O 227	0
5	M	25	Total 25	O 25	0
5	N	57	Total 57	O 57	0
5	O	222	Total 222	O 222	0
5	P	25	Total 25	O 25	0
5	Q	57	Total 57	O 57	0
5	R	216	Total 216	O 216	0
5	S	25	Total 25	O 25	0
5	T	58	Total 58	O 58	0
5	V	227	Total 227	O 227	0
5	W	25	Total 25	O 25	0
5	X	58	Total 58	O 58	0
5	Y	226	Total 226	O 226	0

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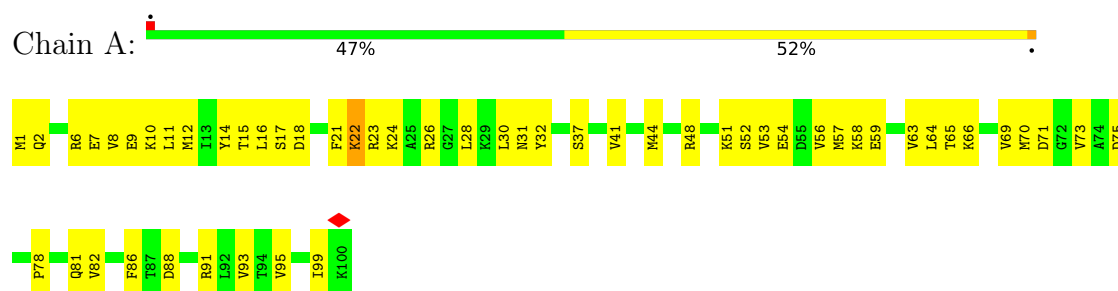
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Mol	Chain	Residues	Atoms		AltConf
5	Z	26	Total 26	O 26	0
5	0	57	Total 57	O 57	0
5	1	224	Total 224	O 224	0
5	2	25	Total 25	O 25	0
5	3	57	Total 57	O 57	0
5	4	216	Total 216	O 216	0
5	5	25	Total 25	O 25	0
5	6	57	Total 57	O 57	0
5	7	220	Total 220	O 220	0
5	8	25	Total 25	O 25	0
5	9	56	Total 56	O 56	0
5	U	223	Total 223	O 223	0

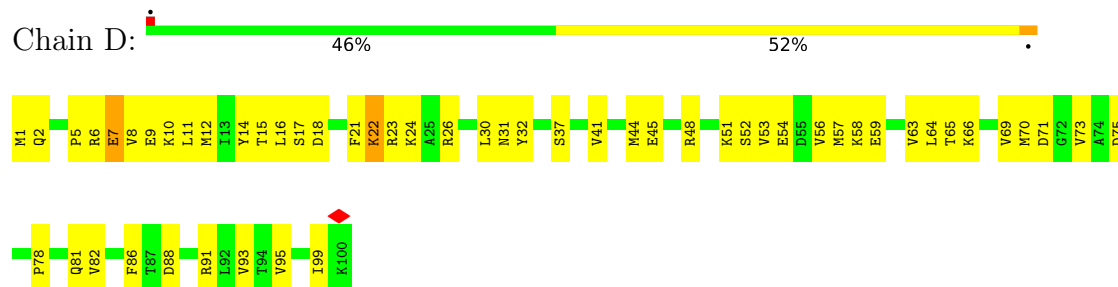
3 Residue-property plots

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

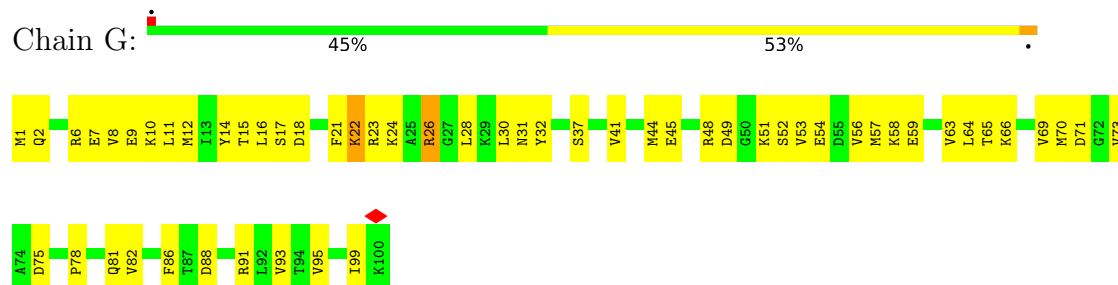
• Molecule 1: Urease subunit gamma



• Molecule 1: Urease subunit gamma

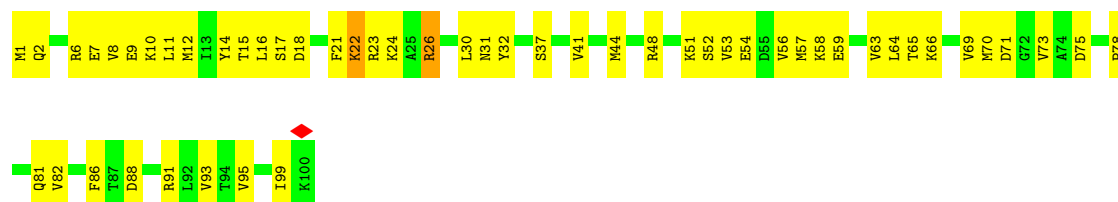


• Molecule 1: Urease subunit gamma

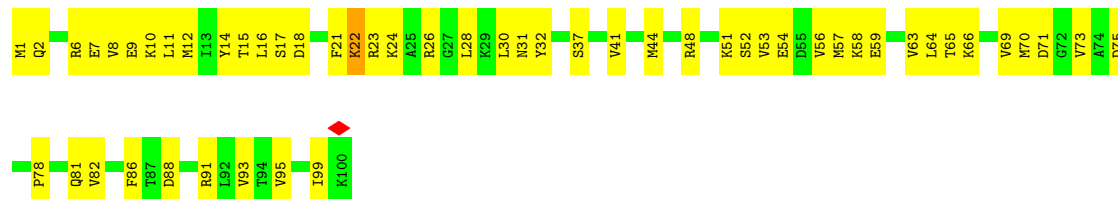


• Molecule 1: Urease subunit gamma

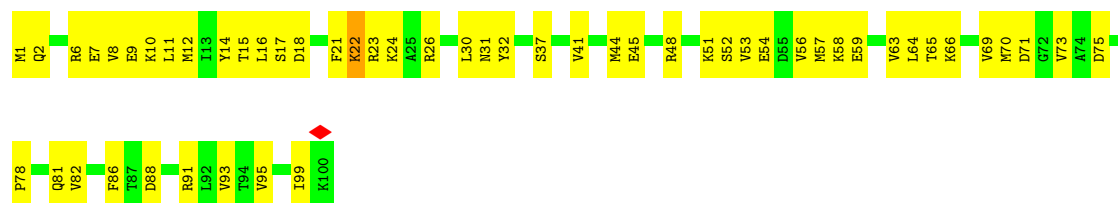




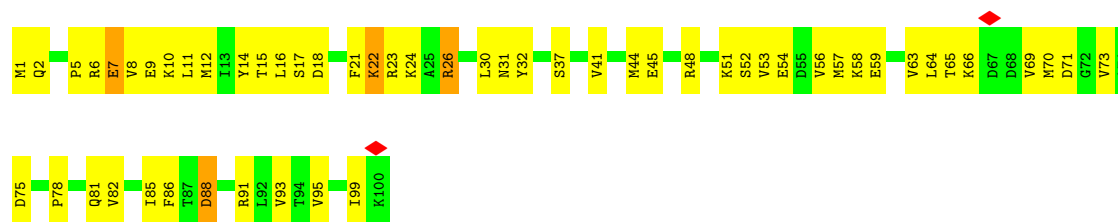
- Molecule 1: Urease subunit gamma



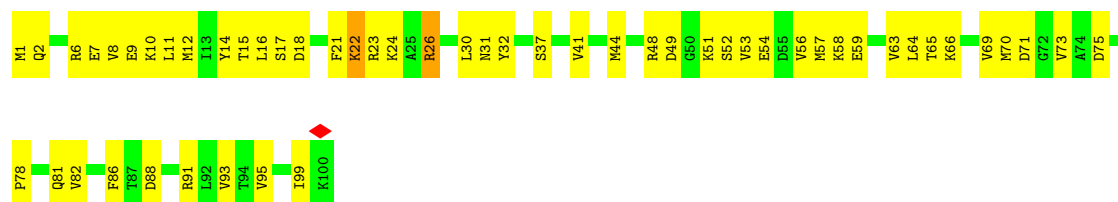
- Molecule 1: Urease subunit gamma



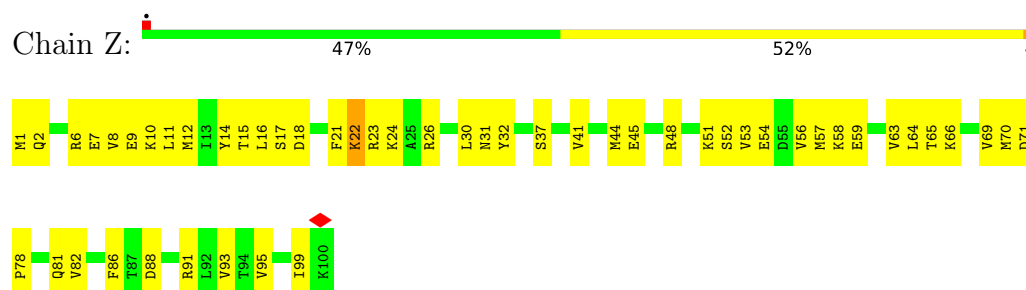
- Molecule 1: Urease subunit gamma



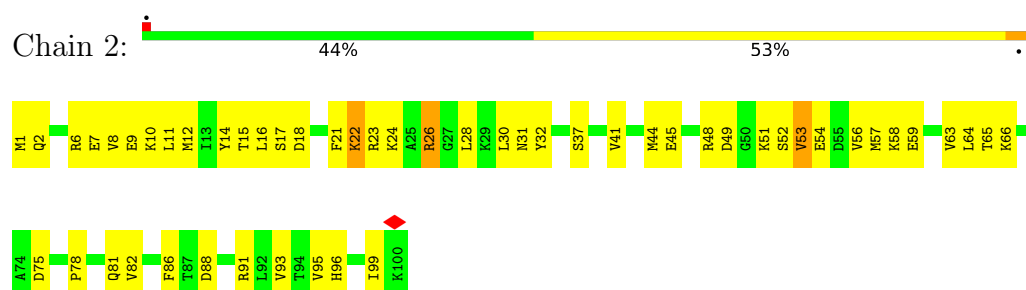
- Molecule 1: Urease subunit gamma



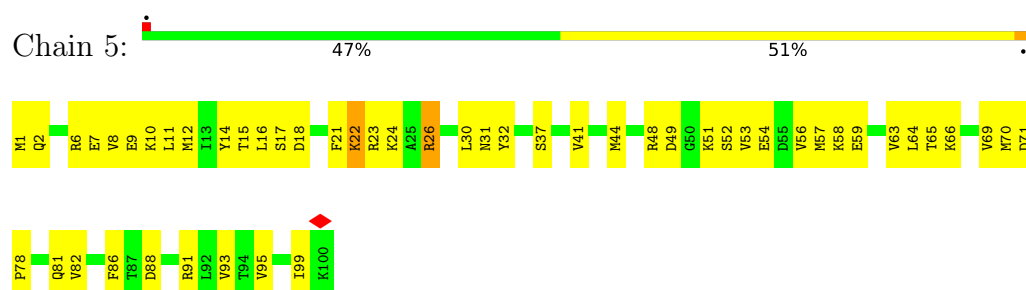
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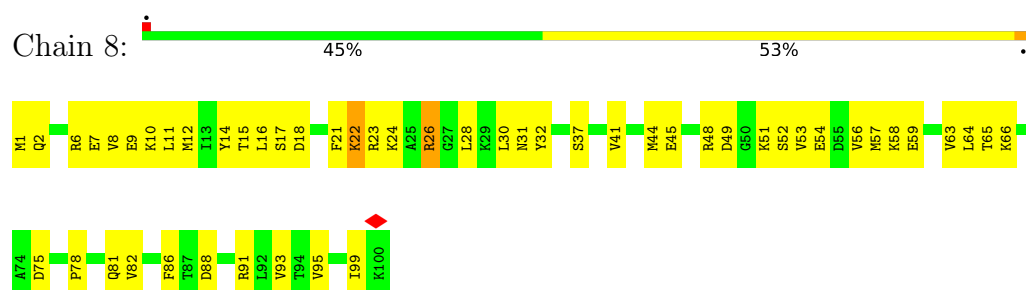
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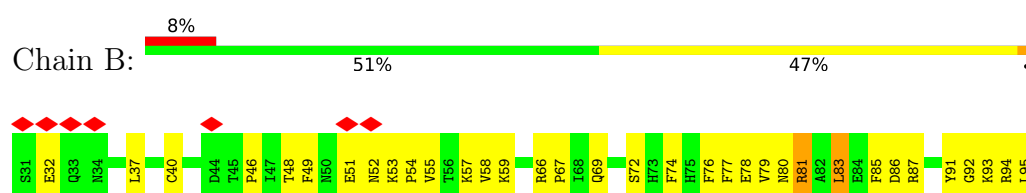
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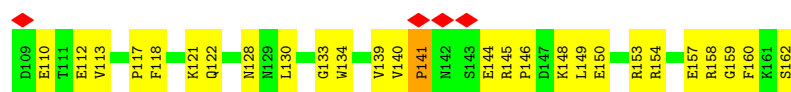


- Molecule 1: Urease subunit gamma

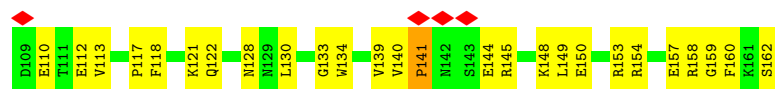


- Molecule 2: Urease subunit beta

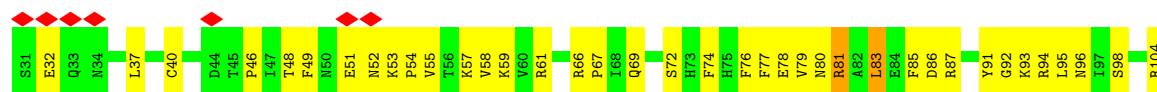




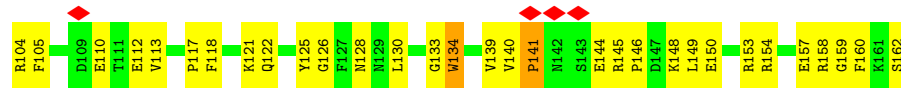
• Molecule 2: Urease subunit beta



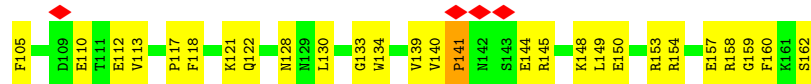
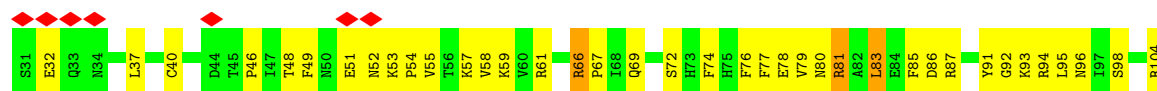
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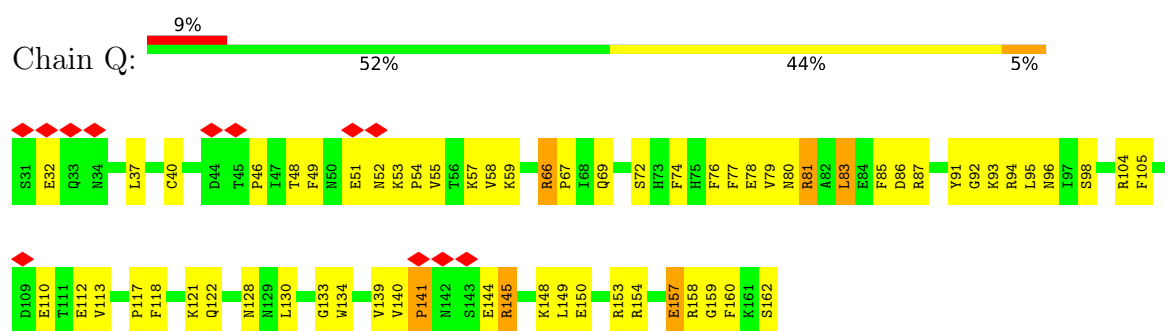
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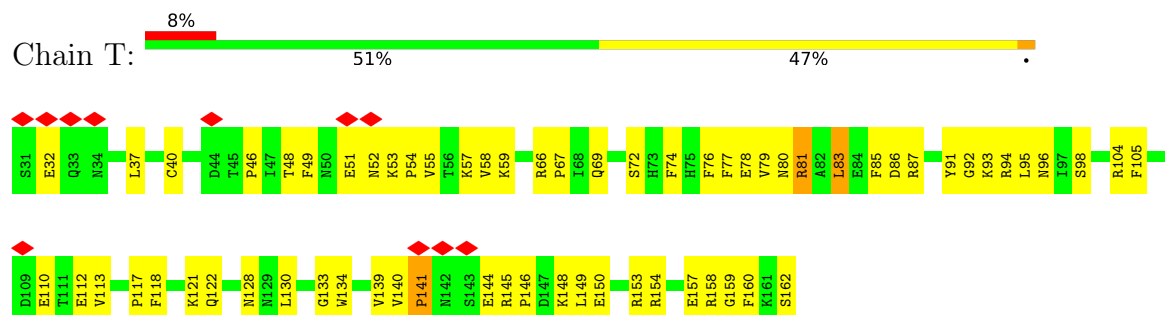
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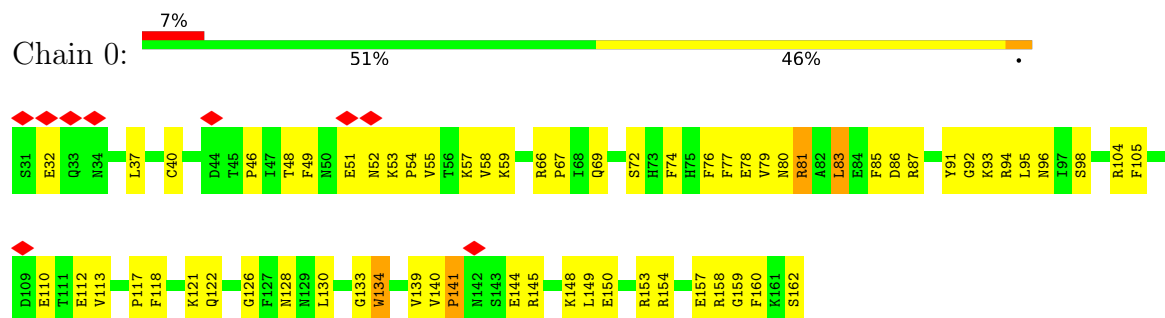
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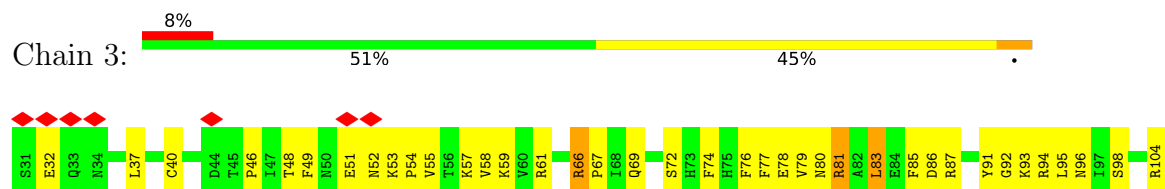
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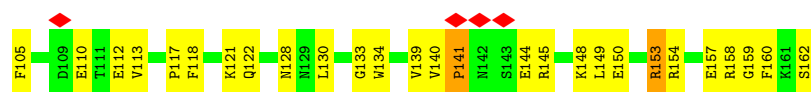


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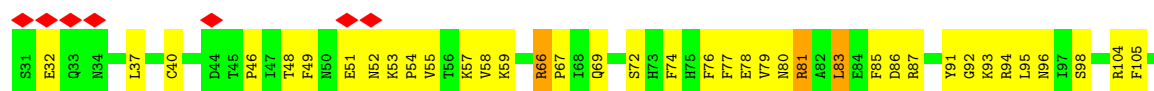


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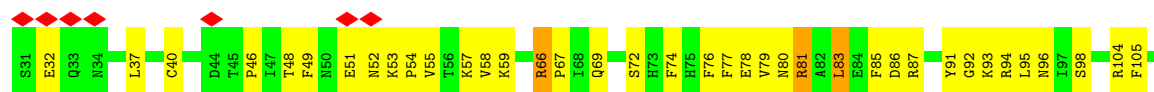




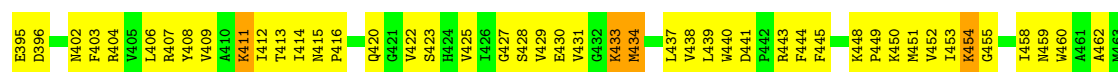
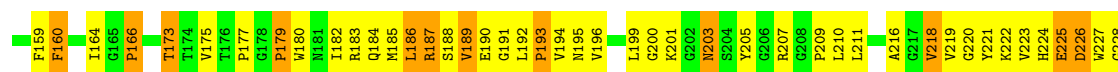
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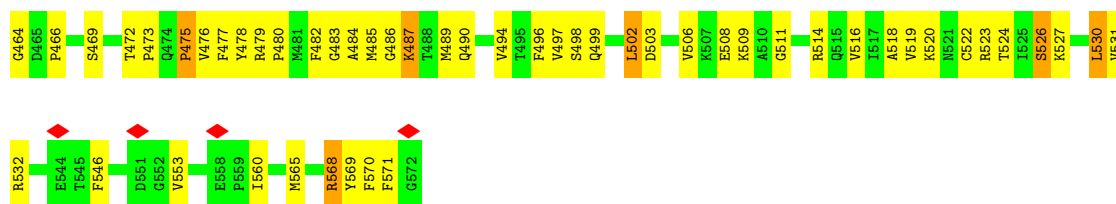


• Molecule 2: Urease subunit beta

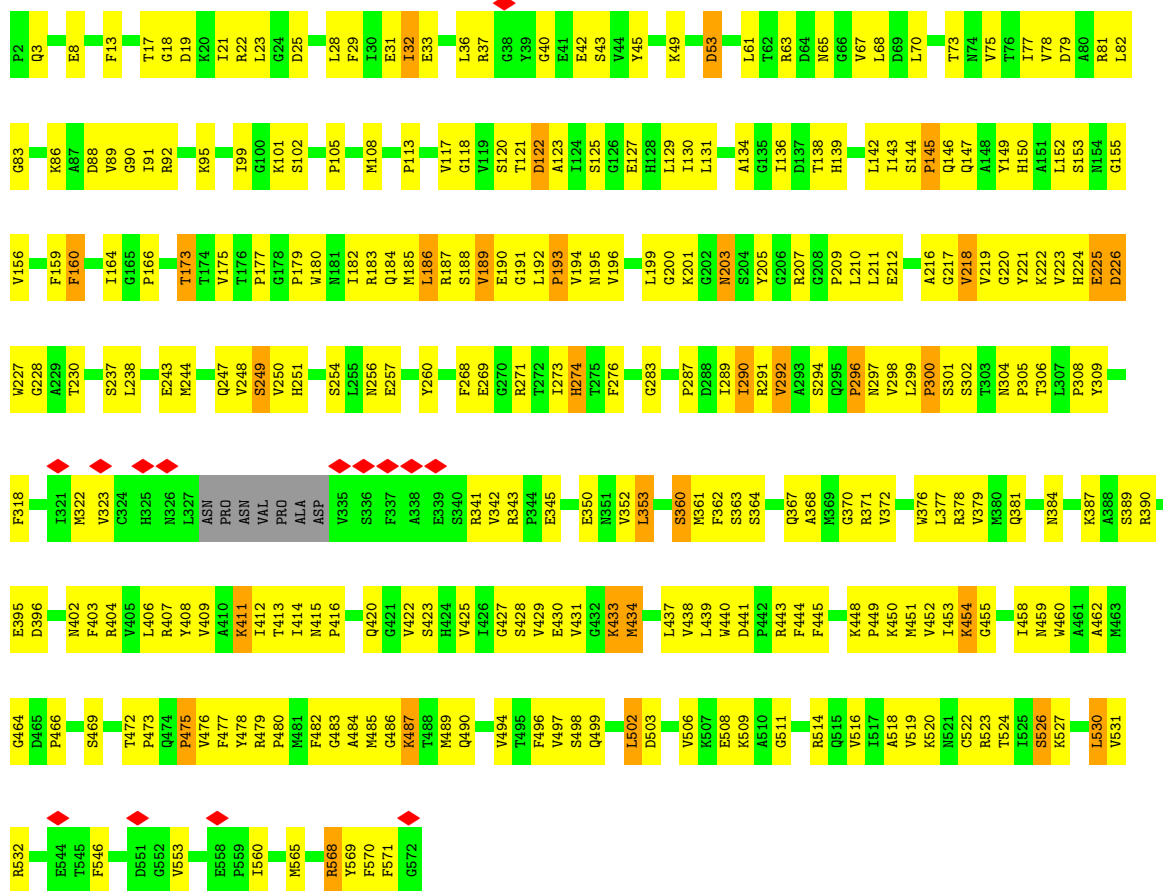


• Molecule 3: Urease subunit alpha

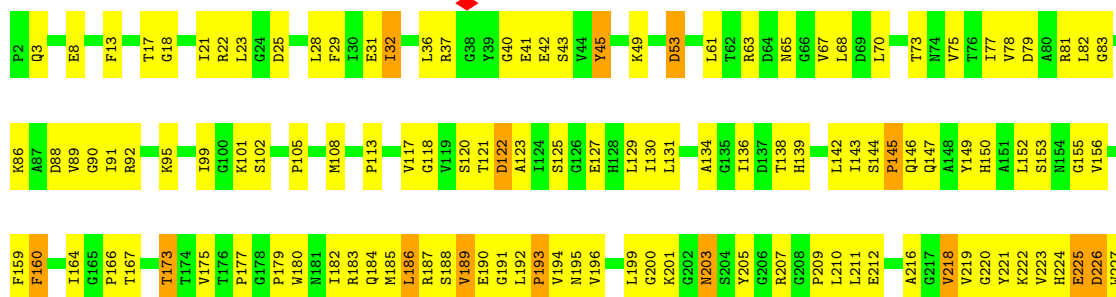


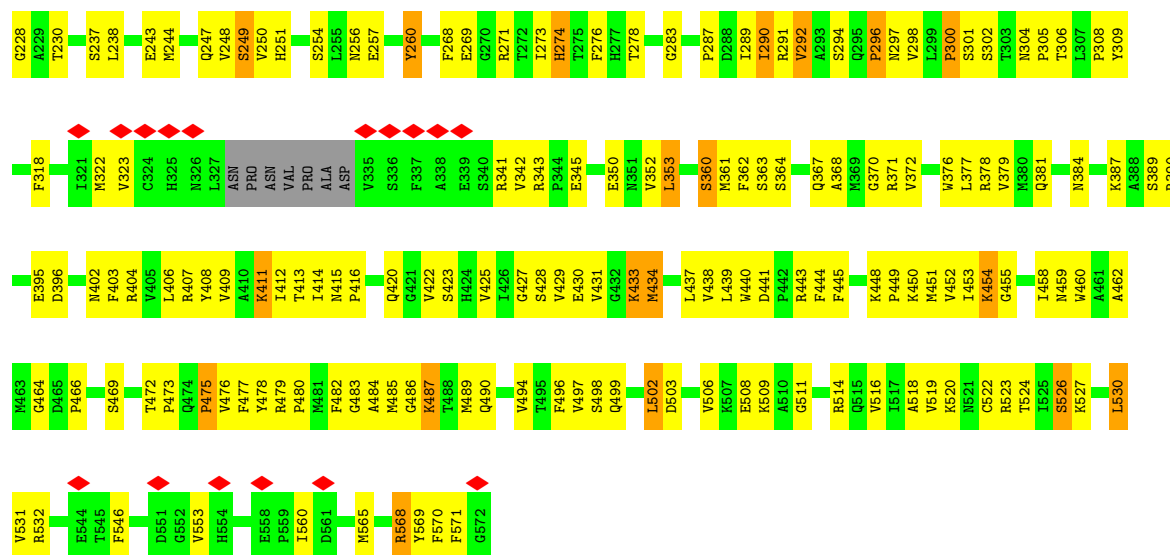


• Molecule 3: Urease subunit alpha

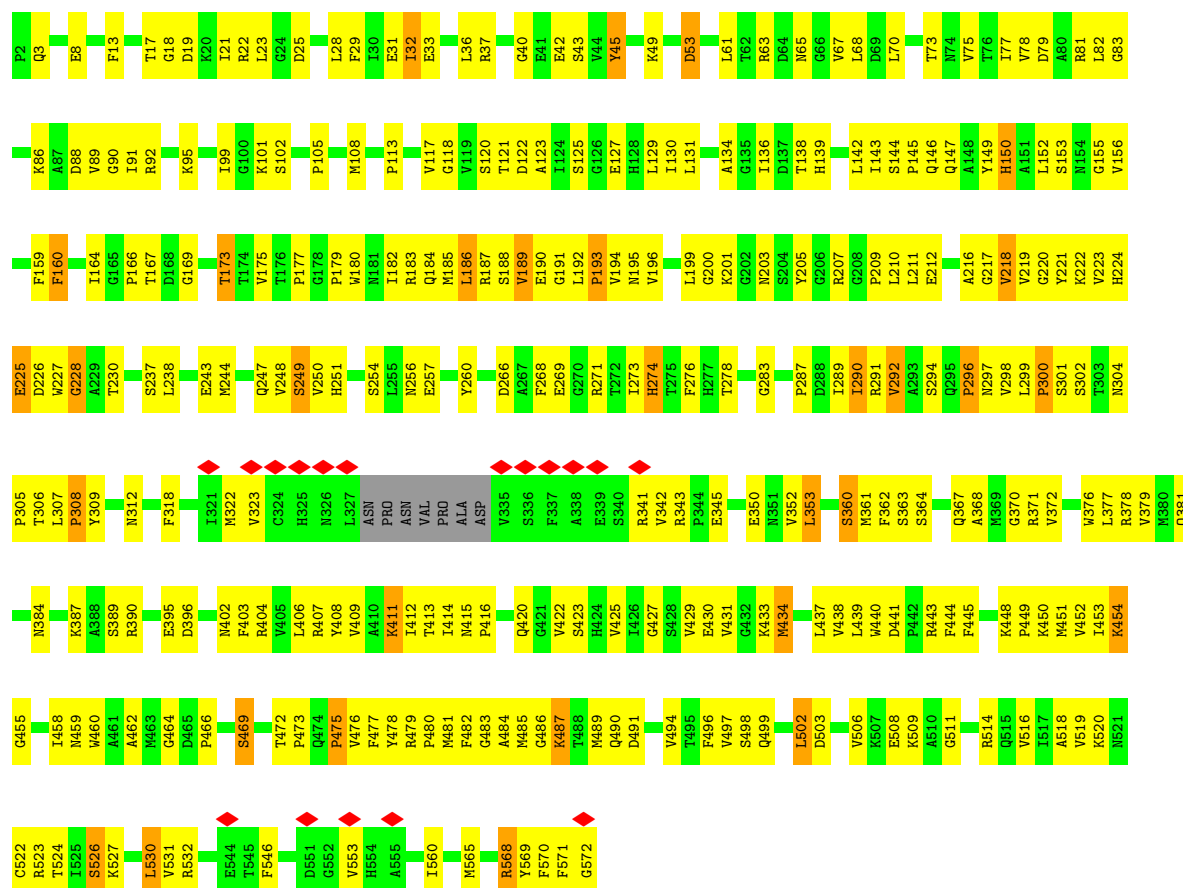


• Molecule 3: Urease subunit alpha



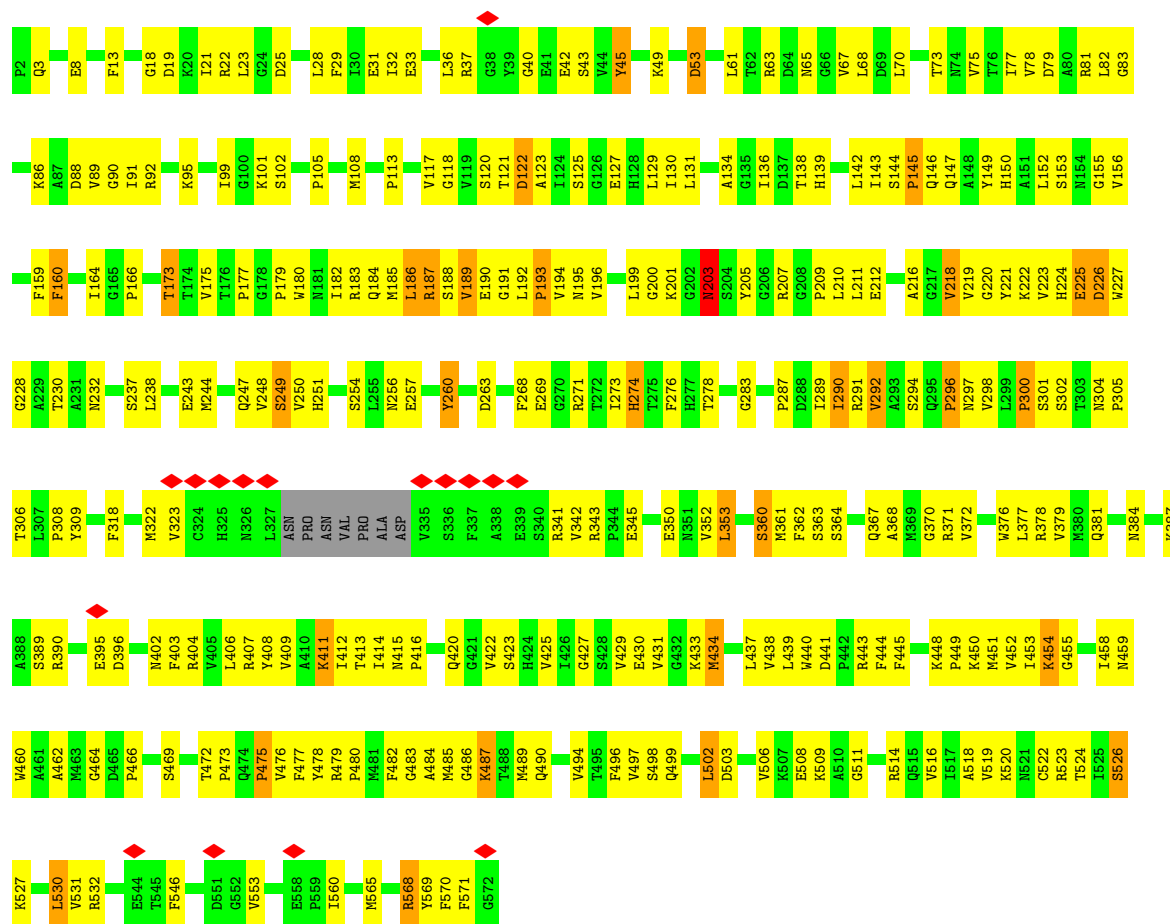


• Molecule 3: Urease subunit alpha



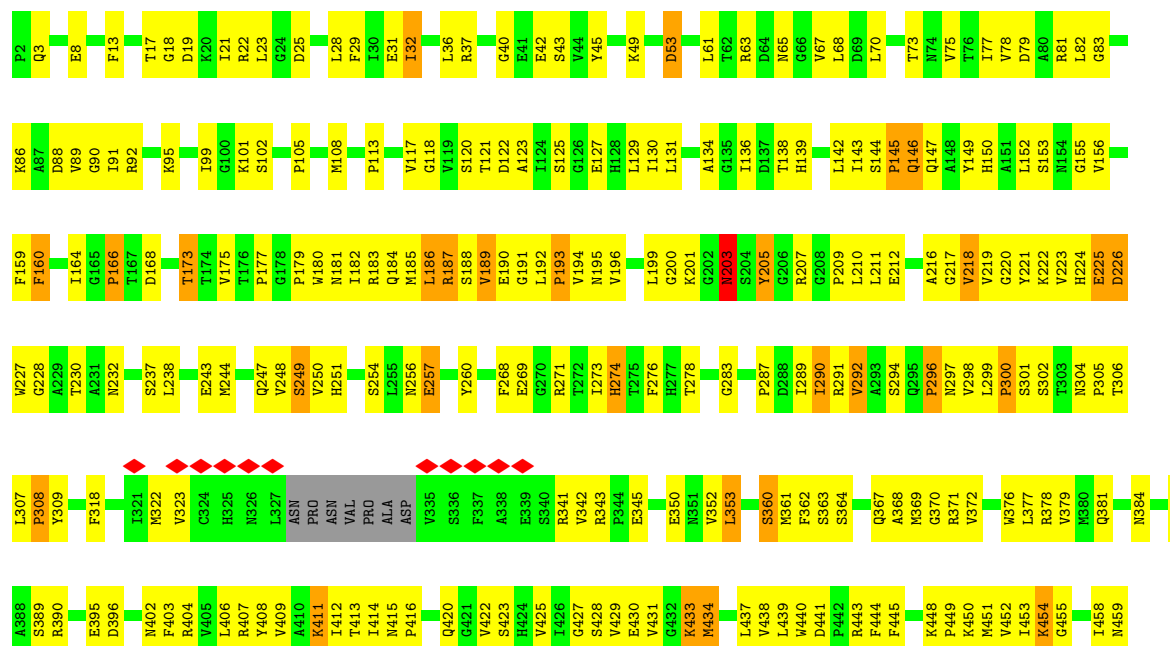
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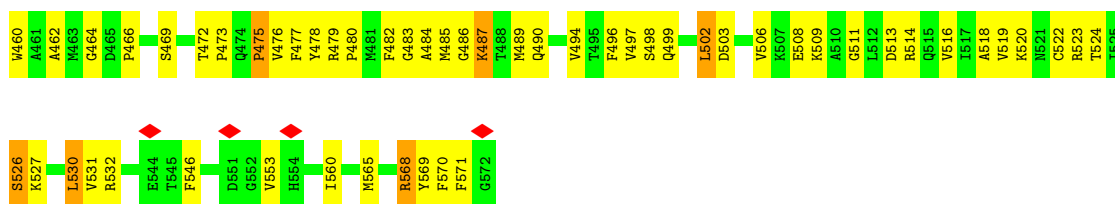




• Molecule 3: Urease subunit alpha

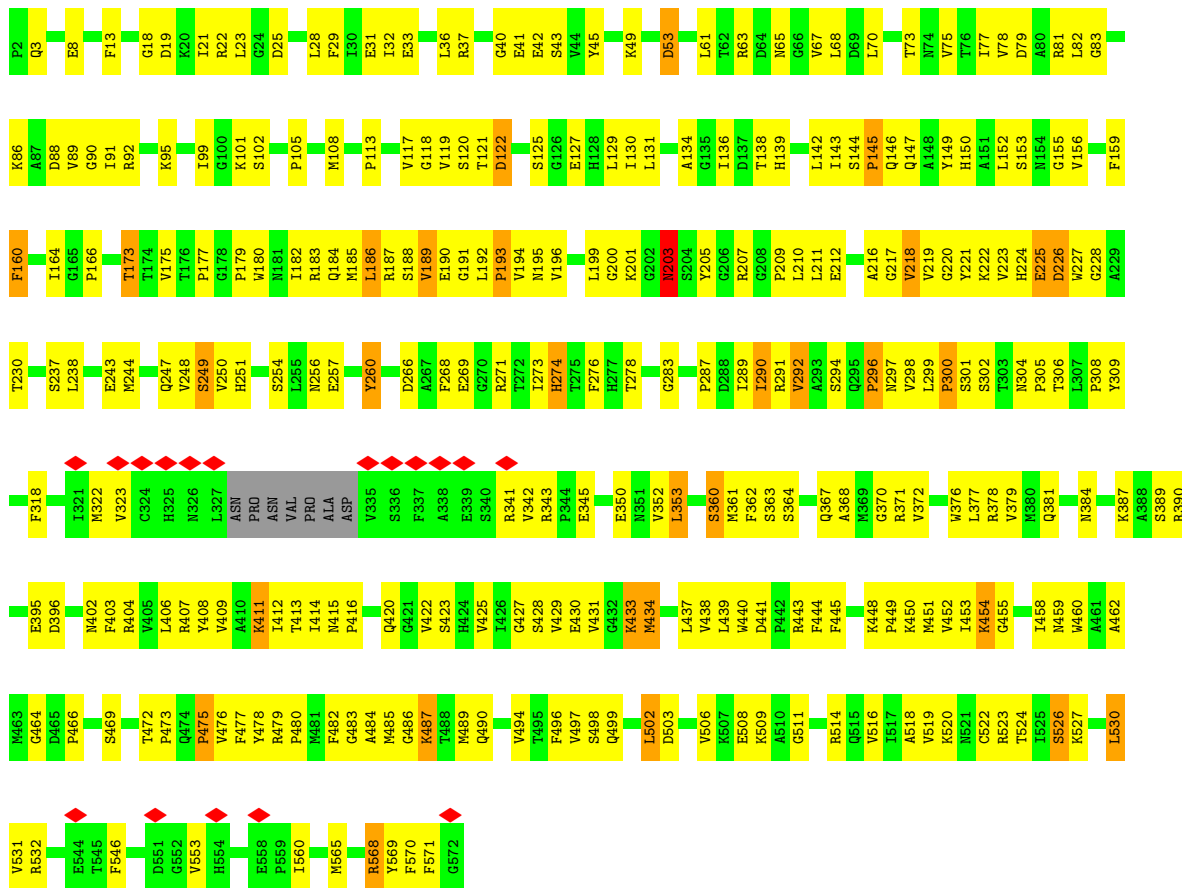
Chain R: 47% 45% 6%





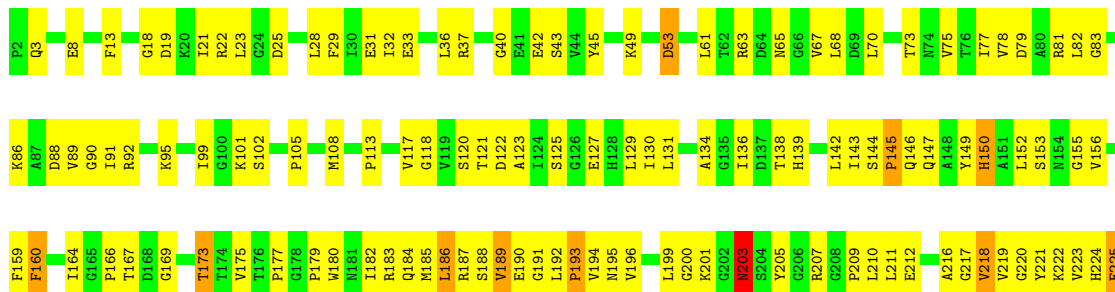
• Molecule 3: Urease subunit alpha

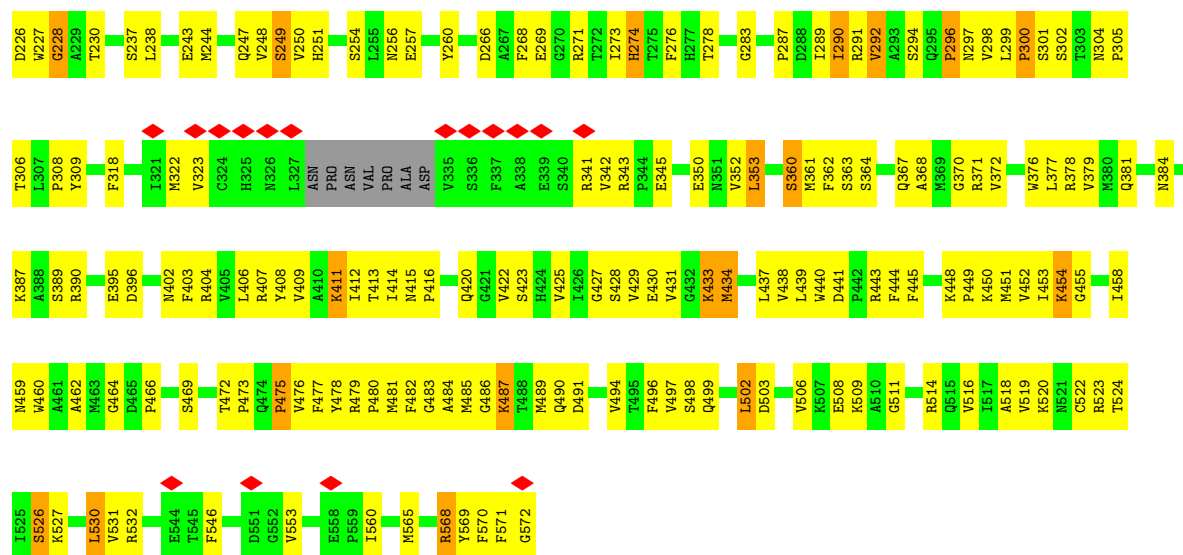
Chain V: 48% 46% 5% .



• Molecule 3: Urease subunit alpha

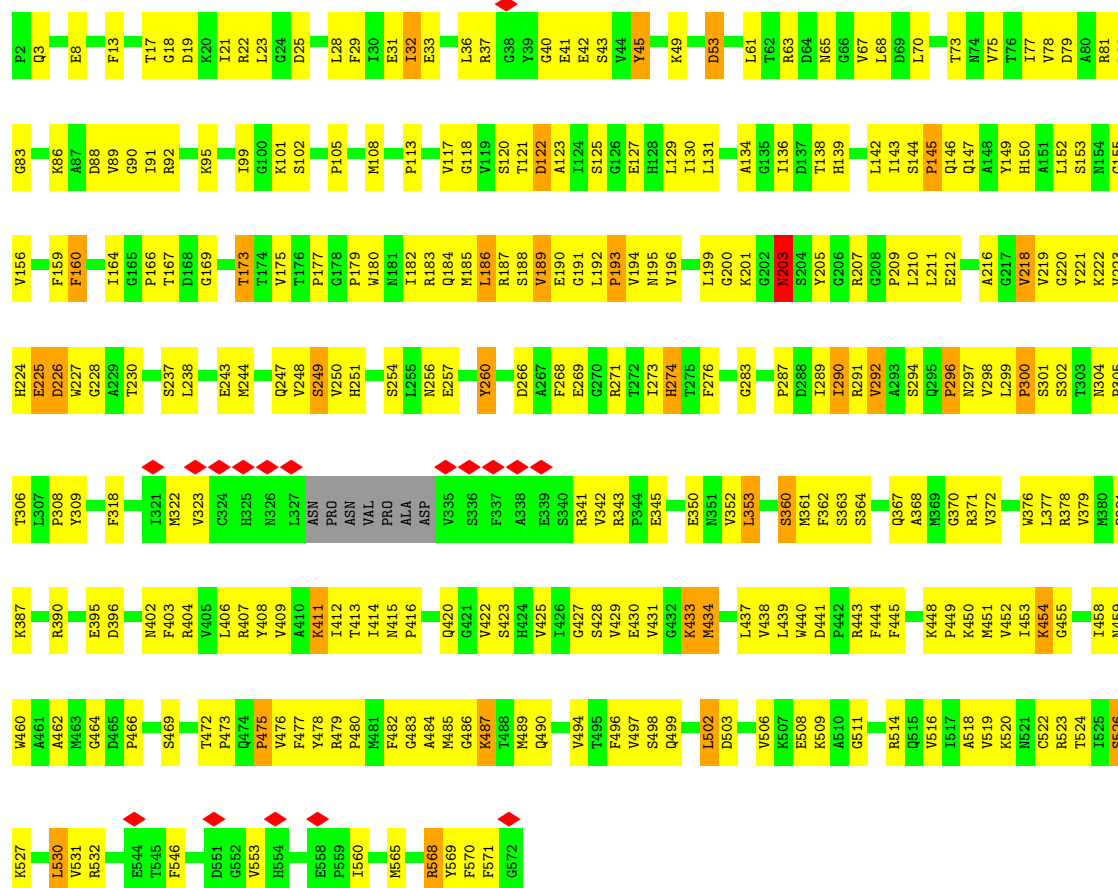
Chain Y: 47% 46% 5% .





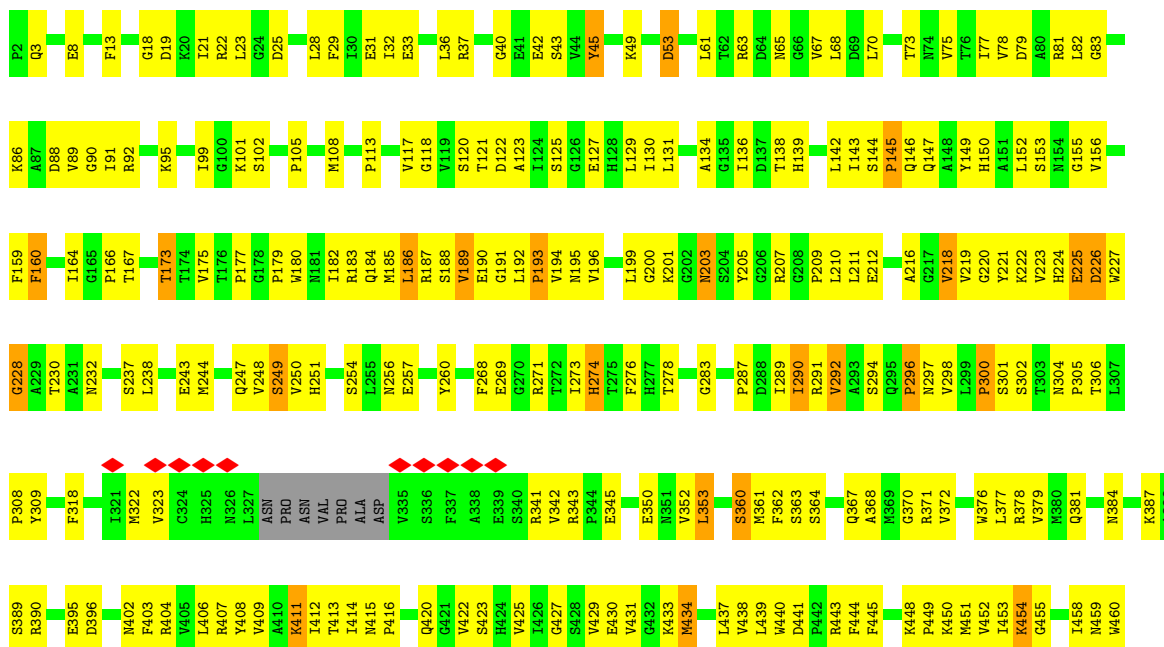
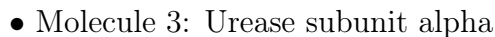
• Molecule 3: Urease subunit alpha

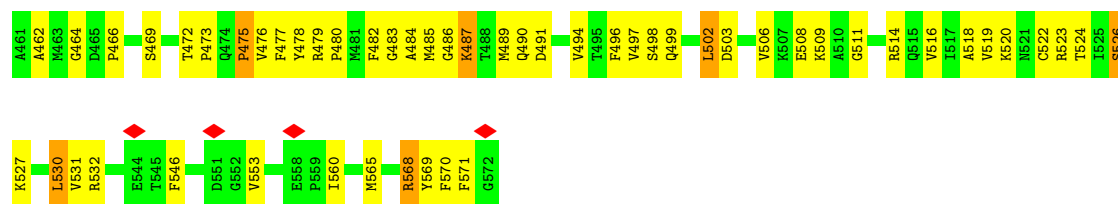
Chain 1: 48% 45% 6%



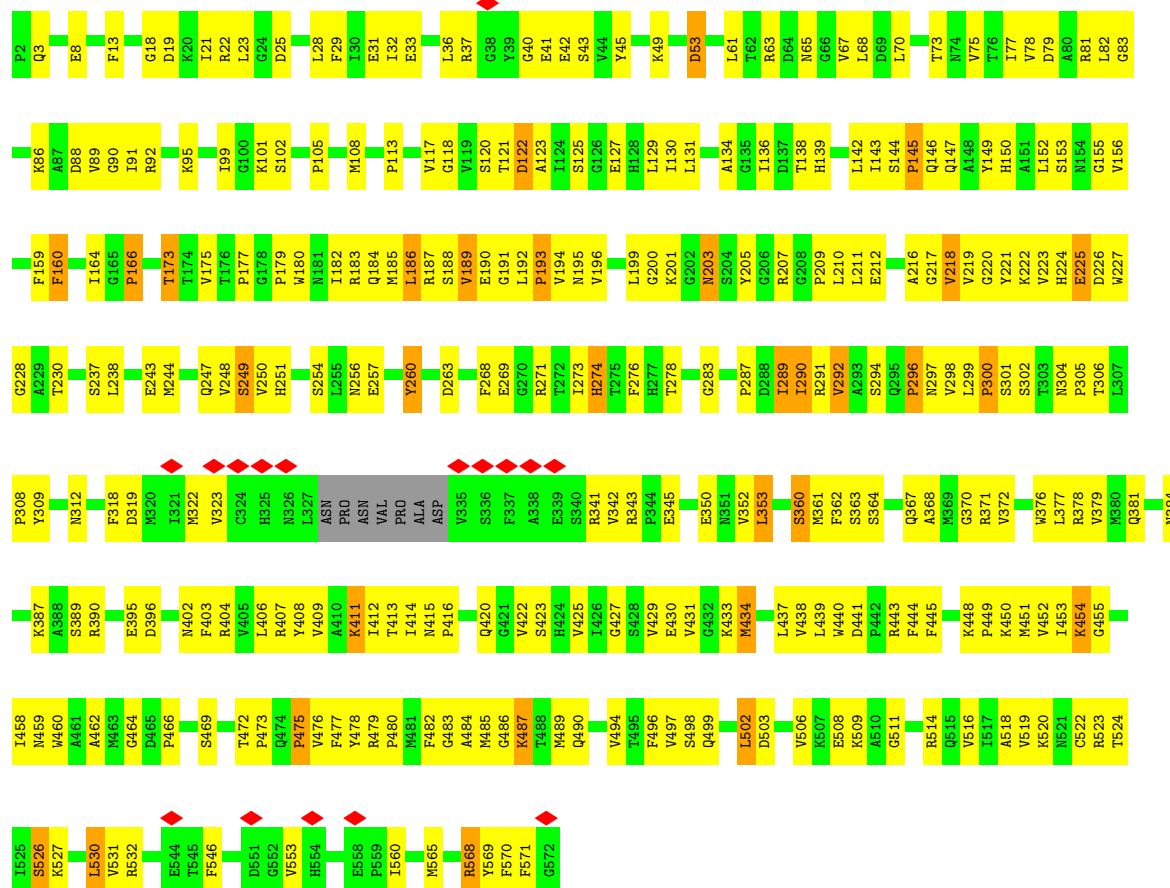
• Molecule 3: Urease subunit alpha

Chain 4: 48% 46% 6%





• Molecule 3: Urease subunit alpha



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, T	Depositor
Number of particles used	97627	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.248	Depositor
Minimum map value	-0.146	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	327.168, 327.168, 327.168	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.639, 0.639, 0.639	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	2	2.72	69/844 (8.2%)	1.66	20/1135 (1.8%)
1	5	2.72	69/844 (8.2%)	1.66	20/1135 (1.8%)
1	8	2.72	70/844 (8.3%)	1.66	19/1135 (1.7%)
1	A	2.72	70/844 (8.3%)	1.66	20/1135 (1.8%)
1	D	2.72	70/844 (8.3%)	1.66	20/1135 (1.8%)
1	G	2.72	70/844 (8.3%)	1.66	19/1135 (1.7%)
1	J	2.72	70/844 (8.3%)	1.66	19/1135 (1.7%)
1	M	2.72	68/844 (8.1%)	1.66	20/1135 (1.8%)
1	P	2.72	69/844 (8.2%)	1.66	19/1135 (1.7%)
1	S	2.72	69/844 (8.2%)	1.66	20/1135 (1.8%)
1	W	2.72	69/844 (8.2%)	1.66	20/1135 (1.8%)
1	Z	2.72	69/844 (8.2%)	1.66	20/1135 (1.8%)
2	0	2.83	88/1076 (8.2%)	1.91	29/1455 (2.0%)
2	3	2.83	88/1076 (8.2%)	1.91	30/1455 (2.1%)
2	6	2.83	87/1076 (8.1%)	1.91	29/1455 (2.0%)
2	9	2.83	87/1076 (8.1%)	1.91	29/1455 (2.0%)
2	B	2.83	87/1076 (8.1%)	1.91	29/1455 (2.0%)
2	E	2.83	88/1076 (8.2%)	1.91	29/1455 (2.0%)
2	H	2.83	89/1076 (8.3%)	1.91	30/1455 (2.1%)
2	K	2.83	87/1076 (8.1%)	1.91	30/1455 (2.1%)
2	N	2.83	87/1076 (8.1%)	1.91	30/1455 (2.1%)
2	Q	2.83	87/1076 (8.1%)	1.91	29/1455 (2.0%)
2	T	2.83	87/1076 (8.1%)	1.91	29/1455 (2.0%)
2	X	2.83	88/1076 (8.2%)	1.91	29/1455 (2.0%)
3	1	2.99	405/4377 (9.3%)	1.91	135/5934 (2.3%)
3	4	2.99	407/4377 (9.3%)	1.91	136/5934 (2.3%)
3	7	2.99	402/4377 (9.2%)	1.91	135/5934 (2.3%)
3	C	2.97	403/4377 (9.2%)	1.91	136/5934 (2.3%)
3	F	2.99	407/4377 (9.3%)	1.91	138/5934 (2.3%)
3	I	2.99	405/4377 (9.3%)	1.91	132/5934 (2.2%)
3	L	2.99	405/4377 (9.3%)	1.91	135/5934 (2.3%)
3	O	2.99	406/4377 (9.3%)	1.91	137/5934 (2.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	R	2.99	408/4377 (9.3%)	1.91	135/5934 (2.3%)
3	U	2.99	406/4377 (9.3%)	1.91	136/5934 (2.3%)
3	V	2.99	408/4377 (9.3%)	1.91	137/5934 (2.3%)
3	Y	2.99	406/4377 (9.3%)	1.91	139/5934 (2.3%)
All	All	2.93	6750/75564 (8.9%)	1.88	2219/102288 (2.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	2
1	5	0	2
1	8	0	2
1	A	0	2
1	D	0	2
1	G	0	2
1	J	0	2
1	M	0	2
1	P	0	2
1	S	0	2
1	W	0	2
1	Z	0	2
3	1	0	1
3	4	0	1
3	7	0	1
3	C	0	1
3	F	0	1
3	I	0	1
3	L	0	1
3	O	0	1
3	R	0	1
3	U	0	1
3	V	0	1
3	Y	0	1
All	All	0	36

All (6750) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	212	GLU	CB-CG	-19.23	1.15	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	212	GLU	CB-CG	-19.21	1.15	1.52
3	O	212	GLU	CB-CG	-19.21	1.15	1.52
3	4	212	GLU	CB-CG	-19.21	1.15	1.52
3	L	212	GLU	CB-CG	-19.21	1.15	1.52
3	U	212	GLU	CB-CG	-19.20	1.15	1.52
3	1	212	GLU	CB-CG	-19.19	1.15	1.52
3	V	212	GLU	CB-CG	-19.19	1.15	1.52
3	F	212	GLU	CB-CG	-19.19	1.15	1.52
3	7	212	GLU	CB-CG	-19.18	1.15	1.52
3	I	212	GLU	CB-CG	-19.18	1.15	1.52
2	9	134	TRP	CB-CG	-16.16	1.21	1.50
2	K	134	TRP	CB-CG	-16.15	1.21	1.50
2	0	134	TRP	CB-CG	-16.14	1.21	1.50
2	3	134	TRP	CB-CG	-16.14	1.21	1.50
2	T	134	TRP	CB-CG	-16.13	1.21	1.50
2	E	134	TRP	CB-CG	-16.13	1.21	1.50
2	B	134	TRP	CB-CG	-16.12	1.21	1.50
2	Q	134	TRP	CB-CG	-16.12	1.21	1.50
2	X	134	TRP	CB-CG	-16.12	1.21	1.50
2	N	134	TRP	CB-CG	-16.11	1.21	1.50
2	H	134	TRP	CB-CG	-16.07	1.21	1.50
2	6	134	TRP	CB-CG	-16.07	1.21	1.50
3	4	478	TYR	CD2-CE2	-15.43	1.16	1.39
3	U	478	TYR	CD2-CE2	-15.41	1.16	1.39
3	1	478	TYR	CD2-CE2	-15.40	1.16	1.39
3	O	478	TYR	CD2-CE2	-15.39	1.16	1.39
3	R	478	TYR	CD2-CE2	-15.39	1.16	1.39
3	V	478	TYR	CD2-CE2	-15.39	1.16	1.39
3	C	478	TYR	CD2-CE2	-15.36	1.16	1.39
3	L	478	TYR	CD2-CE2	-15.36	1.16	1.39
3	Y	478	TYR	CD2-CE2	-15.35	1.16	1.39
3	7	478	TYR	CD2-CE2	-15.34	1.16	1.39
3	I	478	TYR	CD2-CE2	-15.33	1.16	1.39
3	F	478	TYR	CD2-CE2	-15.32	1.16	1.39
3	I	440	TRP	CZ3-CH2	-15.27	1.15	1.40
3	Y	440	TRP	CZ3-CH2	-15.27	1.15	1.40
3	V	440	TRP	CZ3-CH2	-15.27	1.15	1.40
3	1	440	TRP	CZ3-CH2	-15.27	1.15	1.40
3	O	440	TRP	CZ3-CH2	-15.26	1.15	1.40
3	R	440	TRP	CZ3-CH2	-15.26	1.15	1.40
3	C	440	TRP	CZ3-CH2	-15.26	1.15	1.40
3	U	440	TRP	CZ3-CH2	-15.25	1.15	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	440	TRP	CZ3-CH2	-15.24	1.15	1.40
3	F	440	TRP	CZ3-CH2	-15.24	1.15	1.40
3	4	440	TRP	CZ3-CH2	-15.23	1.15	1.40
2	N	91	TYR	CE2-CZ	-15.21	1.18	1.38
3	7	440	TRP	CZ3-CH2	-15.20	1.15	1.40
2	E	91	TYR	CE2-CZ	-15.17	1.18	1.38
2	K	91	TYR	CE2-CZ	-15.17	1.18	1.38
2	Q	91	TYR	CE2-CZ	-15.16	1.18	1.38
2	6	91	TYR	CE2-CZ	-15.16	1.18	1.38
2	3	91	TYR	CE2-CZ	-15.16	1.18	1.38
2	0	91	TYR	CE2-CZ	-15.15	1.18	1.38
2	B	91	TYR	CE2-CZ	-15.15	1.18	1.38
2	T	91	TYR	CE2-CZ	-15.15	1.18	1.38
3	Y	257	GLU	CD-OE2	-15.15	1.08	1.25
2	H	91	TYR	CE2-CZ	-15.14	1.18	1.38
2	9	91	TYR	CE2-CZ	-15.14	1.18	1.38
3	L	257	GLU	CD-OE2	-15.12	1.09	1.25
3	V	257	GLU	CD-OE2	-15.10	1.09	1.25
2	X	91	TYR	CE2-CZ	-15.10	1.19	1.38
3	F	257	GLU	CD-OE2	-15.09	1.09	1.25
3	4	257	GLU	CD-OE2	-15.09	1.09	1.25
3	I	257	GLU	CD-OE2	-15.08	1.09	1.25
3	C	257	GLU	CD-OE2	-15.07	1.09	1.25
3	7	257	GLU	CD-OE2	-15.06	1.09	1.25
3	1	257	GLU	CD-OE2	-15.06	1.09	1.25
3	R	257	GLU	CD-OE2	-15.04	1.09	1.25
3	U	257	GLU	CD-OE2	-15.04	1.09	1.25
3	O	86	LYS	CE-NZ	-15.03	1.11	1.49
3	U	86	LYS	CE-NZ	-15.03	1.11	1.49
3	O	257	GLU	CD-OE2	-15.03	1.09	1.25
3	C	86	LYS	CE-NZ	-15.01	1.11	1.49
3	L	86	LYS	CE-NZ	-15.01	1.11	1.49
3	4	86	LYS	CE-NZ	-15.00	1.11	1.49
3	V	86	LYS	CE-NZ	-15.00	1.11	1.49
3	1	86	LYS	CE-NZ	-15.00	1.11	1.49
3	R	86	LYS	CE-NZ	-15.00	1.11	1.49
3	7	86	LYS	CE-NZ	-15.00	1.11	1.49
3	I	86	LYS	CE-NZ	-14.99	1.11	1.49
3	Y	86	LYS	CE-NZ	-14.99	1.11	1.49
3	F	86	LYS	CE-NZ	-14.97	1.11	1.49
1	2	32	TYR	CD1-CE1	-14.34	1.17	1.39
1	W	32	TYR	CD1-CE1	-14.30	1.17	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	32	TYR	CD1-CE1	-14.30	1.18	1.39
1	J	32	TYR	CD1-CE1	-14.29	1.18	1.39
1	Z	32	TYR	CD1-CE1	-14.29	1.18	1.39
1	G	32	TYR	CD1-CE1	-14.28	1.18	1.39
1	M	32	TYR	CD1-CE1	-14.28	1.18	1.39
1	8	32	TYR	CD1-CE1	-14.27	1.18	1.39
1	D	32	TYR	CD1-CE1	-14.27	1.18	1.39
1	A	32	TYR	CD1-CE1	-14.27	1.18	1.39
1	P	32	TYR	CD1-CE1	-14.23	1.18	1.39
1	S	32	TYR	CD1-CE1	-14.23	1.18	1.39
3	U	523	ARG	CG-CD	-13.96	1.17	1.51
3	V	523	ARG	CG-CD	-13.95	1.17	1.51
3	1	523	ARG	CG-CD	-13.95	1.17	1.51
3	I	523	ARG	CG-CD	-13.94	1.17	1.51
3	7	523	ARG	CG-CD	-13.94	1.17	1.51
3	C	523	ARG	CG-CD	-13.93	1.17	1.51
3	Y	523	ARG	CG-CD	-13.93	1.17	1.51
3	4	523	ARG	CG-CD	-13.93	1.17	1.51
3	L	523	ARG	CG-CD	-13.92	1.17	1.51
3	F	523	ARG	CG-CD	-13.92	1.17	1.51
3	R	523	ARG	CG-CD	-13.91	1.17	1.51
3	O	523	ARG	CG-CD	-13.91	1.17	1.51
3	R	523	ARG	CZ-NH1	-13.70	1.15	1.33
3	O	523	ARG	CZ-NH1	-13.70	1.15	1.33
3	Y	523	ARG	CZ-NH1	-13.70	1.15	1.33
3	V	523	ARG	CZ-NH1	-13.69	1.15	1.33
3	C	523	ARG	CZ-NH1	-13.68	1.15	1.33
3	I	523	ARG	CZ-NH1	-13.68	1.15	1.33
3	L	523	ARG	CZ-NH1	-13.68	1.15	1.33
3	7	523	ARG	CZ-NH1	-13.66	1.15	1.33
3	U	523	ARG	CZ-NH1	-13.65	1.15	1.33
3	F	523	ARG	CZ-NH1	-13.65	1.15	1.33
3	4	523	ARG	CZ-NH1	-13.64	1.15	1.33
3	1	523	ARG	CZ-NH1	-13.61	1.15	1.33
2	N	134	TRP	CZ3-CH2	-13.51	1.18	1.40
2	Q	141	PRO	N-CA	13.51	1.70	1.47
2	0	141	PRO	N-CA	13.49	1.70	1.47
2	0	134	TRP	CZ3-CH2	-13.47	1.18	1.40
2	3	141	PRO	N-CA	13.47	1.70	1.47
2	E	85	PHE	CE1-CZ	-13.46	1.11	1.37
2	B	141	PRO	N-CA	13.46	1.70	1.47
2	Q	134	TRP	CZ3-CH2	-13.46	1.18	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	141	PRO	N-CA	13.46	1.70	1.47
2	X	141	PRO	N-CA	13.46	1.70	1.47
2	K	141	PRO	N-CA	13.46	1.70	1.47
2	T	134	TRP	CZ3-CH2	-13.46	1.18	1.40
2	6	134	TRP	CZ3-CH2	-13.45	1.18	1.40
2	6	141	PRO	N-CA	13.45	1.70	1.47
2	0	85	PHE	CE1-CZ	-13.45	1.11	1.37
2	9	134	TRP	CZ3-CH2	-13.45	1.18	1.40
2	B	134	TRP	CZ3-CH2	-13.44	1.18	1.40
2	9	141	PRO	N-CA	13.45	1.70	1.47
2	3	134	TRP	CZ3-CH2	-13.44	1.18	1.40
2	3	85	PHE	CE1-CZ	-13.44	1.11	1.37
2	E	141	PRO	N-CA	13.43	1.70	1.47
2	H	141	PRO	N-CA	13.43	1.70	1.47
2	T	85	PHE	CE1-CZ	-13.43	1.11	1.37
2	K	85	PHE	CE1-CZ	-13.43	1.11	1.37
2	B	85	PHE	CE1-CZ	-13.43	1.11	1.37
2	K	134	TRP	CZ3-CH2	-13.43	1.18	1.40
2	9	85	PHE	CE1-CZ	-13.43	1.11	1.37
2	E	134	TRP	CZ3-CH2	-13.42	1.18	1.40
2	H	85	PHE	CE1-CZ	-13.42	1.11	1.37
2	X	134	TRP	CZ3-CH2	-13.42	1.18	1.40
1	P	32	TYR	CE1-CZ	-13.42	1.21	1.38
2	H	134	TRP	CZ3-CH2	-13.42	1.18	1.40
2	N	141	PRO	N-CA	13.42	1.70	1.47
1	D	32	TYR	CE1-CZ	-13.41	1.21	1.38
2	Q	85	PHE	CE1-CZ	-13.41	1.11	1.37
2	X	85	PHE	CE1-CZ	-13.40	1.11	1.37
2	6	85	PHE	CE1-CZ	-13.38	1.11	1.37
2	N	85	PHE	CE1-CZ	-13.38	1.11	1.37
3	F	159	PHE	CE2-CZ	-13.37	1.11	1.37
3	O	159	PHE	CE2-CZ	-13.37	1.11	1.37
1	S	32	TYR	CE1-CZ	-13.37	1.21	1.38
1	J	32	TYR	CE1-CZ	-13.35	1.21	1.38
3	I	159	PHE	CE2-CZ	-13.35	1.11	1.37
3	4	159	PHE	CE2-CZ	-13.35	1.11	1.37
2	T	77	PHE	CD2-CE2	-13.35	1.12	1.39
1	G	32	TYR	CE1-CZ	-13.34	1.21	1.38
3	V	159	PHE	CE2-CZ	-13.34	1.11	1.37
1	A	32	TYR	CE1-CZ	-13.34	1.21	1.38
1	Z	32	TYR	CE1-CZ	-13.34	1.21	1.38
3	7	159	PHE	CE2-CZ	-13.34	1.12	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	32	TYR	CE1-CZ	-13.34	1.21	1.38
3	C	159	PHE	CE2-CZ	-13.33	1.12	1.37
3	R	159	PHE	CE2-CZ	-13.33	1.12	1.37
2	3	77	PHE	CD2-CE2	-13.33	1.12	1.39
2	B	77	PHE	CD2-CE2	-13.32	1.12	1.39
2	E	77	PHE	CD2-CE2	-13.32	1.12	1.39
2	Q	77	PHE	CD2-CE2	-13.32	1.12	1.39
2	K	77	PHE	CD2-CE2	-13.32	1.12	1.39
3	1	159	PHE	CE2-CZ	-13.32	1.12	1.37
3	L	159	PHE	CE2-CZ	-13.32	1.12	1.37
2	0	77	PHE	CD2-CE2	-13.31	1.12	1.39
1	8	32	TYR	CE1-CZ	-13.31	1.21	1.38
2	6	77	PHE	CD2-CE2	-13.31	1.12	1.39
2	H	77	PHE	CD2-CE2	-13.30	1.12	1.39
3	Y	159	PHE	CE2-CZ	-13.30	1.12	1.37
1	2	32	TYR	CE1-CZ	-13.30	1.21	1.38
2	9	77	PHE	CD2-CE2	-13.30	1.12	1.39
3	U	159	PHE	CE2-CZ	-13.30	1.12	1.37
2	X	77	PHE	CD2-CE2	-13.30	1.12	1.39
1	M	32	TYR	CE1-CZ	-13.29	1.21	1.38
3	O	514	ARG	CZ-NH1	-13.29	1.15	1.33
2	N	77	PHE	CD2-CE2	-13.28	1.12	1.39
3	R	376	TRP	CG-CD1	-13.28	1.18	1.36
1	5	32	TYR	CE1-CZ	-13.28	1.21	1.38
3	7	376	TRP	CG-CD1	-13.28	1.18	1.36
3	1	376	TRP	CG-CD1	-13.27	1.18	1.36
3	O	376	TRP	CG-CD1	-13.26	1.18	1.36
3	4	514	ARG	CZ-NH1	-13.26	1.15	1.33
3	U	514	ARG	CZ-NH1	-13.24	1.15	1.33
3	F	376	TRP	CG-CD1	-13.24	1.18	1.36
3	Y	514	ARG	CZ-NH1	-13.24	1.15	1.33
3	C	376	TRP	CG-CD1	-13.23	1.18	1.36
3	C	514	ARG	CZ-NH1	-13.23	1.15	1.33
3	L	376	TRP	CG-CD1	-13.23	1.18	1.36
3	1	514	ARG	CZ-NH1	-13.23	1.15	1.33
3	F	514	ARG	CZ-NH1	-13.23	1.15	1.33
3	Y	376	TRP	CG-CD1	-13.23	1.18	1.36
3	L	514	ARG	CZ-NH1	-13.22	1.15	1.33
3	7	514	ARG	CZ-NH1	-13.22	1.15	1.33
3	V	376	TRP	CG-CD1	-13.21	1.18	1.36
3	4	376	TRP	CG-CD1	-13.21	1.18	1.36
3	I	376	TRP	CG-CD1	-13.21	1.18	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	514	ARG	CZ-NH1	-13.20	1.15	1.33
3	I	514	ARG	CZ-NH1	-13.19	1.15	1.33
3	R	514	ARG	CZ-NH1	-13.20	1.15	1.33
3	U	376	TRP	CG-CD1	-13.19	1.18	1.36
3	I	376	TRP	CE3-CZ3	-13.11	1.16	1.38
3	L	376	TRP	CE3-CZ3	-13.11	1.16	1.38
3	O	376	TRP	CE3-CZ3	-13.10	1.16	1.38
3	1	376	TRP	CE3-CZ3	-13.09	1.16	1.38
3	7	376	TRP	CE3-CZ3	-13.09	1.16	1.38
3	U	376	TRP	CE3-CZ3	-13.09	1.16	1.38
3	V	376	TRP	CE3-CZ3	-13.08	1.16	1.38
3	C	376	TRP	CE3-CZ3	-13.07	1.16	1.38
3	4	376	TRP	CE3-CZ3	-13.07	1.16	1.38
3	Y	376	TRP	CE3-CZ3	-13.06	1.16	1.38
3	F	376	TRP	CE3-CZ3	-13.06	1.16	1.38
3	R	376	TRP	CE3-CZ3	-13.04	1.16	1.38
2	T	94	ARG	CZ-NH1	-12.98	1.16	1.33
2	H	94	ARG	CZ-NH1	-12.98	1.16	1.33
2	X	94	ARG	CZ-NH1	-12.97	1.16	1.33
2	3	94	ARG	CZ-NH1	-12.97	1.16	1.33
2	9	94	ARG	CZ-NH1	-12.97	1.16	1.33
2	0	94	ARG	CZ-NH1	-12.97	1.16	1.33
2	K	94	ARG	CZ-NH1	-12.96	1.16	1.33
2	B	94	ARG	CZ-NH1	-12.96	1.16	1.33
2	N	94	ARG	CZ-NH1	-12.96	1.16	1.33
2	Q	94	ARG	CZ-NH1	-12.92	1.16	1.33
2	6	94	ARG	CZ-NH1	-12.91	1.16	1.33
2	E	94	ARG	CZ-NH1	-12.91	1.16	1.33
1	G	14	TYR	CD1-CE1	-12.63	1.20	1.39
1	J	14	TYR	CD1-CE1	-12.60	1.20	1.39
1	Z	14	TYR	CD1-CE1	-12.59	1.20	1.39
1	D	14	TYR	CD1-CE1	-12.58	1.20	1.39
1	2	14	TYR	CD1-CE1	-12.58	1.20	1.39
1	A	14	TYR	CD1-CE1	-12.57	1.20	1.39
1	S	14	TYR	CD1-CE1	-12.57	1.20	1.39
1	P	14	TYR	CD1-CE1	-12.56	1.20	1.39
1	8	14	TYR	CD1-CE1	-12.56	1.20	1.39
1	5	14	TYR	CD1-CE1	-12.55	1.20	1.39
1	M	14	TYR	CD1-CE1	-12.54	1.20	1.39
1	W	14	TYR	CD1-CE1	-12.54	1.20	1.39
2	E	58	VAL	CB-CG2	-12.52	1.26	1.52
2	N	58	VAL	CB-CG2	-12.51	1.26	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	58	VAL	CB-CG2	-12.49	1.26	1.52
3	1	221	TYR	CE2-CZ	-12.49	1.22	1.38
2	3	58	VAL	CB-CG2	-12.49	1.26	1.52
2	B	58	VAL	CB-CG2	-12.48	1.26	1.52
2	6	58	VAL	CB-CG2	-12.48	1.26	1.52
2	K	58	VAL	CB-CG2	-12.47	1.26	1.52
2	Q	58	VAL	CB-CG2	-12.47	1.26	1.52
2	X	58	VAL	CB-CG2	-12.47	1.26	1.52
3	7	221	TYR	CE2-CZ	-12.46	1.22	1.38
3	R	496	PHE	CE2-CZ	-12.46	1.13	1.37
3	Y	221	TYR	CE2-CZ	-12.46	1.22	1.38
3	R	221	TYR	CE2-CZ	-12.46	1.22	1.38
2	T	58	VAL	CB-CG2	-12.46	1.26	1.52
2	H	58	VAL	CB-CG2	-12.46	1.26	1.52
3	C	496	PHE	CE2-CZ	-12.46	1.13	1.37
3	I	496	PHE	CE2-CZ	-12.46	1.13	1.37
3	V	496	PHE	CE2-CZ	-12.45	1.13	1.37
3	4	221	TYR	CE2-CZ	-12.45	1.22	1.38
3	F	496	PHE	CE2-CZ	-12.45	1.13	1.37
3	O	496	PHE	CE2-CZ	-12.45	1.13	1.37
3	4	496	PHE	CE2-CZ	-12.45	1.13	1.37
2	9	58	VAL	CB-CG2	-12.45	1.26	1.52
3	L	496	PHE	CE2-CZ	-12.44	1.13	1.37
3	O	221	TYR	CE2-CZ	-12.44	1.22	1.38
3	7	496	PHE	CE2-CZ	-12.44	1.13	1.37
3	C	221	TYR	CE2-CZ	-12.44	1.22	1.38
3	U	496	PHE	CE2-CZ	-12.44	1.13	1.37
3	1	496	PHE	CE2-CZ	-12.43	1.13	1.37
3	I	221	TYR	CE2-CZ	-12.43	1.22	1.38
3	L	221	TYR	CE2-CZ	-12.43	1.22	1.38
3	Y	496	PHE	CE2-CZ	-12.43	1.13	1.37
3	V	221	TYR	CE2-CZ	-12.41	1.22	1.38
3	U	221	TYR	CE2-CZ	-12.40	1.22	1.38
3	F	221	TYR	CE2-CZ	-12.40	1.22	1.38
3	4	425	VAL	CB-CG2	-12.31	1.26	1.52
3	I	425	VAL	CB-CG2	-12.31	1.26	1.52
3	O	425	VAL	CB-CG2	-12.31	1.26	1.52
3	Y	425	VAL	CB-CG2	-12.29	1.27	1.52
3	F	425	VAL	CB-CG2	-12.29	1.27	1.52
3	1	425	VAL	CB-CG2	-12.28	1.27	1.52
3	U	188	SER	CB-OG	-12.28	1.26	1.42
3	R	188	SER	CB-OG	-12.28	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	425	VAL	CB-CG2	-12.28	1.27	1.52
3	I	188	SER	CB-OG	-12.28	1.26	1.42
3	L	425	VAL	CB-CG2	-12.28	1.27	1.52
3	R	425	VAL	CB-CG2	-12.27	1.27	1.52
3	V	425	VAL	CB-CG2	-12.27	1.27	1.52
3	U	425	VAL	CB-CG2	-12.27	1.27	1.52
3	O	188	SER	CB-OG	-12.27	1.26	1.42
3	F	188	SER	CB-OG	-12.26	1.26	1.42
3	1	188	SER	CB-OG	-12.25	1.26	1.42
3	7	188	SER	CB-OG	-12.24	1.26	1.42
3	C	188	SER	CB-OG	-12.24	1.26	1.42
3	L	188	SER	CB-OG	-12.23	1.26	1.42
3	7	425	VAL	CB-CG2	-12.23	1.27	1.52
3	V	188	SER	CB-OG	-12.23	1.26	1.42
3	C	179	PRO	N-CA	12.23	1.68	1.47
3	Y	188	SER	CB-OG	-12.22	1.26	1.42
3	U	149	TYR	CD1-CE1	-12.21	1.21	1.39
3	I	407[A]	ARG	CZ-NH1	-12.21	1.17	1.33
3	I	407[B]	ARG	CZ-NH1	-12.21	1.17	1.33
3	R	407[A]	ARG	CZ-NH1	-12.21	1.17	1.33
3	R	407[B]	ARG	CZ-NH1	-12.21	1.17	1.33
3	7	407[A]	ARG	CZ-NH1	-12.20	1.17	1.33
3	7	407[B]	ARG	CZ-NH1	-12.20	1.17	1.33
3	O	149	TYR	CD1-CE1	-12.20	1.21	1.39
3	L	149	TYR	CD1-CE1	-12.20	1.21	1.39
3	F	407[A]	ARG	CZ-NH1	-12.19	1.17	1.33
3	F	407[B]	ARG	CZ-NH1	-12.19	1.17	1.33
3	Y	407[A]	ARG	CZ-NH1	-12.20	1.17	1.33
3	Y	407[B]	ARG	CZ-NH1	-12.20	1.17	1.33
3	4	188	SER	CB-OG	-12.19	1.26	1.42
3	U	407[A]	ARG	CZ-NH1	-12.19	1.17	1.33
3	U	407[B]	ARG	CZ-NH1	-12.19	1.17	1.33
3	O	407[A]	ARG	CZ-NH1	-12.19	1.17	1.33
3	O	407[B]	ARG	CZ-NH1	-12.19	1.17	1.33
3	V	149	TYR	CD1-CE1	-12.19	1.21	1.39
3	L	407[A]	ARG	CZ-NH1	-12.18	1.17	1.33
3	L	407[B]	ARG	CZ-NH1	-12.18	1.17	1.33
3	I	149	TYR	CD1-CE1	-12.18	1.21	1.39
3	R	149	TYR	CD1-CE1	-12.18	1.21	1.39
3	Y	149	TYR	CD1-CE1	-12.17	1.21	1.39
3	1	149	TYR	CD1-CE1	-12.17	1.21	1.39
3	F	149	TYR	CD1-CE1	-12.17	1.21	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	149	TYR	CD1-CE1	-12.16	1.21	1.39
3	C	407[A]	ARG	CZ-NH1	-12.16	1.17	1.33
3	C	407[B]	ARG	CZ-NH1	-12.16	1.17	1.33
3	1	407[A]	ARG	CZ-NH1	-12.15	1.17	1.33
3	1	407[B]	ARG	CZ-NH1	-12.15	1.17	1.33
3	V	407[A]	ARG	CZ-NH1	-12.14	1.17	1.33
3	V	407[B]	ARG	CZ-NH1	-12.14	1.17	1.33
3	4	149	TYR	CD1-CE1	-12.13	1.21	1.39
3	7	149	TYR	CD1-CE1	-12.13	1.21	1.39
3	4	407[A]	ARG	CZ-NH1	-12.13	1.17	1.33
3	4	407[B]	ARG	CZ-NH1	-12.13	1.17	1.33
3	U	431	VAL	CB-CG1	-11.99	1.27	1.52
3	L	431	VAL	CB-CG1	-11.99	1.27	1.52
3	7	431	VAL	CB-CG1	-11.98	1.27	1.52
3	Y	431	VAL	CB-CG1	-11.98	1.27	1.52
3	1	431	VAL	CB-CG1	-11.97	1.27	1.52
3	V	431	VAL	CB-CG1	-11.97	1.27	1.52
3	C	431	VAL	CB-CG1	-11.96	1.27	1.52
3	F	431	VAL	CB-CG1	-11.96	1.27	1.52
3	L	221	TYR	CE1-CZ	-11.95	1.23	1.38
3	O	431	VAL	CB-CG1	-11.95	1.27	1.52
3	4	431	VAL	CB-CG1	-11.95	1.27	1.52
3	V	221	TYR	CD2-CE2	-11.95	1.21	1.39
3	1	221	TYR	CE1-CZ	-11.94	1.23	1.38
3	I	221	TYR	CD2-CE2	-11.94	1.21	1.39
3	I	431	VAL	CB-CG1	-11.94	1.27	1.52
3	1	221	TYR	CD2-CE2	-11.94	1.21	1.39
3	4	221	TYR	CE1-CZ	-11.93	1.23	1.38
3	R	221	TYR	CE1-CZ	-11.92	1.23	1.38
3	U	221	TYR	CE1-CZ	-11.92	1.23	1.38
3	R	431	VAL	CB-CG1	-11.92	1.27	1.52
3	C	221	TYR	CD2-CE2	-11.92	1.21	1.39
3	Y	221	TYR	CE1-CZ	-11.92	1.23	1.38
3	4	221	TYR	CD2-CE2	-11.91	1.21	1.39
3	U	221	TYR	CD2-CE2	-11.91	1.21	1.39
3	F	221	TYR	CD2-CE2	-11.90	1.21	1.39
3	C	221	TYR	CE1-CZ	-11.89	1.23	1.38
3	I	221	TYR	CE1-CZ	-11.89	1.23	1.38
3	Y	221	TYR	CD2-CE2	-11.89	1.21	1.39
3	O	221	TYR	CE1-CZ	-11.88	1.23	1.38
3	7	221	TYR	CE1-CZ	-11.88	1.23	1.38
3	R	221	TYR	CD2-CE2	-11.88	1.21	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7	221	TYR	CD2-CE2	-11.88	1.21	1.39
3	7	45	TYR	CE2-CZ	-11.87	1.23	1.38
3	F	221	TYR	CE1-CZ	-11.87	1.23	1.38
3	L	221	TYR	CD2-CE2	-11.87	1.21	1.39
3	O	221	TYR	CD2-CE2	-11.86	1.21	1.39
3	V	221	TYR	CE1-CZ	-11.85	1.23	1.38
1	2	41	VAL	CB-CG1	-11.85	1.27	1.52
1	D	41	VAL	CB-CG1	-11.85	1.27	1.52
1	A	41	VAL	CB-CG1	-11.83	1.28	1.52
1	8	41	VAL	CB-CG1	-11.83	1.28	1.52
3	L	45	TYR	CE2-CZ	-11.83	1.23	1.38
1	M	41	VAL	CB-CG1	-11.83	1.28	1.52
3	1	43	SER	CB-OG	-11.83	1.26	1.42
3	O	45	TYR	CE2-CZ	-11.82	1.23	1.38
1	W	41	VAL	CB-CG1	-11.82	1.28	1.52
3	C	45	TYR	CE2-CZ	-11.82	1.23	1.38
1	G	41	VAL	CB-CG1	-11.82	1.28	1.52
3	R	45	TYR	CE2-CZ	-11.82	1.23	1.38
1	5	41	VAL	CB-CG1	-11.82	1.28	1.52
1	P	41	VAL	CB-CG1	-11.81	1.28	1.52
1	S	41	VAL	CB-CG1	-11.81	1.28	1.52
1	J	41	VAL	CB-CG1	-11.81	1.28	1.52
3	1	45	TYR	CE2-CZ	-11.81	1.23	1.38
3	Y	45	TYR	CE2-CZ	-11.80	1.23	1.38
1	Z	41	VAL	CB-CG1	-11.80	1.28	1.52
3	4	45	TYR	CE2-CZ	-11.80	1.23	1.38
3	U	45	TYR	CE2-CZ	-11.80	1.23	1.38
3	I	45	TYR	CE2-CZ	-11.79	1.23	1.38
3	V	43	SER	CB-OG	-11.79	1.26	1.42
3	V	45	TYR	CE2-CZ	-11.79	1.23	1.38
3	L	43	SER	CB-OG	-11.78	1.26	1.42
3	O	43	SER	CB-OG	-11.78	1.26	1.42
3	1	444	PHE	CD1-CE1	-11.78	1.15	1.39
3	I	43	SER	CB-OG	-11.77	1.26	1.42
3	4	444	PHE	CD1-CE1	-11.77	1.15	1.39
3	R	43	SER	CB-OG	-11.77	1.26	1.42
3	U	444	PHE	CD1-CE1	-11.77	1.15	1.39
3	C	43	SER	CB-OG	-11.76	1.26	1.42
3	F	45	TYR	CE2-CZ	-11.76	1.23	1.38
3	7	444	PHE	CD1-CE1	-11.76	1.15	1.39
3	R	444	PHE	CD1-CE1	-11.75	1.15	1.39
3	V	444	PHE	CD1-CE1	-11.75	1.15	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	444	PHE	CD1-CE1	-11.75	1.15	1.39
3	Y	444	PHE	CD1-CE1	-11.75	1.15	1.39
3	4	43	SER	CB-OG	-11.75	1.26	1.42
3	F	444	PHE	CD1-CE1	-11.74	1.15	1.39
3	O	444	PHE	CD1-CE1	-11.74	1.15	1.39
3	C	444	PHE	CD1-CE1	-11.74	1.15	1.39
3	F	43	SER	CB-OG	-11.74	1.26	1.42
3	7	43	SER	CB-OG	-11.74	1.26	1.42
3	L	444	PHE	CD1-CE1	-11.73	1.15	1.39
3	U	43	SER	CB-OG	-11.71	1.27	1.42
3	Y	43	SER	CB-OG	-11.71	1.27	1.42
3	F	485	MET	CB-CG	-11.56	1.14	1.51
3	U	485	MET	CB-CG	-11.55	1.14	1.51
3	Y	485	MET	CB-CG	-11.55	1.14	1.51
3	4	485	MET	CB-CG	-11.55	1.14	1.51
3	V	485	MET	CB-CG	-11.54	1.14	1.51
3	C	485	MET	CB-CG	-11.54	1.14	1.51
3	L	485	MET	CB-CG	-11.54	1.14	1.51
3	7	485	MET	CB-CG	-11.54	1.14	1.51
3	O	485	MET	CB-CG	-11.53	1.14	1.51
3	I	485	MET	CB-CG	-11.53	1.14	1.51
3	1	485	MET	CB-CG	-11.53	1.14	1.51
3	R	485	MET	CB-CG	-11.52	1.14	1.51
3	I	445	PHE	CD1-CE1	-11.48	1.16	1.39
3	U	445	PHE	CD1-CE1	-11.47	1.16	1.39
3	1	445	PHE	CD1-CE1	-11.45	1.16	1.39
3	L	445	PHE	CD1-CE1	-11.45	1.16	1.39
3	C	445	PHE	CD1-CE1	-11.45	1.16	1.39
3	4	445	PHE	CD1-CE1	-11.45	1.16	1.39
3	O	445	PHE	CD1-CE1	-11.44	1.16	1.39
3	R	445	PHE	CD1-CE1	-11.44	1.16	1.39
3	V	445	PHE	CD1-CE1	-11.44	1.16	1.39
3	F	445	PHE	CD1-CE1	-11.44	1.16	1.39
3	Y	445	PHE	CD1-CE1	-11.43	1.16	1.39
3	7	445	PHE	CD1-CE1	-11.41	1.16	1.39
3	I	257	GLU	CD-OE1	-11.39	1.13	1.25
3	4	257	GLU	CD-OE1	-11.36	1.13	1.25
3	O	257	GLU	CD-OE1	-11.35	1.13	1.25
3	7	257	GLU	CD-OE1	-11.35	1.13	1.25
3	L	257	GLU	CD-OE1	-11.34	1.13	1.25
3	R	257	GLU	CD-OE1	-11.33	1.13	1.25
3	V	257	GLU	CD-OE1	-11.33	1.13	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	257	GLU	CD-OE1	-11.32	1.13	1.25
3	U	257	GLU	CD-OE1	-11.31	1.13	1.25
3	1	102	SER	CB-OG	-11.29	1.27	1.42
3	O	102	SER	CB-OG	-11.29	1.27	1.42
3	U	102	SER	CB-OG	-11.29	1.27	1.42
3	F	257	GLU	CD-OE1	-11.29	1.13	1.25
3	F	102	SER	CB-OG	-11.27	1.27	1.42
3	1	257	GLU	CD-OE1	-11.27	1.13	1.25
3	Y	257	GLU	CD-OE1	-11.26	1.13	1.25
3	Y	102	SER	CB-OG	-11.26	1.27	1.42
3	I	102	SER	CB-OG	-11.25	1.27	1.42
3	R	102	SER	CB-OG	-11.24	1.27	1.42
3	7	102	SER	CB-OG	-11.24	1.27	1.42
3	C	102	SER	CB-OG	-11.24	1.27	1.42
3	V	102	SER	CB-OG	-11.23	1.27	1.42
3	I	423	SER	CB-OG	-11.21	1.27	1.42
3	4	102	SER	CB-OG	-11.21	1.27	1.42
3	L	102	SER	CB-OG	-11.20	1.27	1.42
1	S	93	VAL	CB-CG2	-11.19	1.29	1.52
1	P	93	VAL	CB-CG2	-11.18	1.29	1.52
1	2	93	VAL	CB-CG2	-11.18	1.29	1.52
3	R	423	SER	CB-OG	-11.18	1.27	1.42
3	V	423	SER	CB-OG	-11.18	1.27	1.42
3	1	423	SER	CB-OG	-11.18	1.27	1.42
1	D	93	VAL	CB-CG2	-11.17	1.29	1.52
1	M	93	VAL	CB-CG2	-11.17	1.29	1.52
1	A	93	VAL	CB-CG2	-11.16	1.29	1.52
1	8	93	VAL	CB-CG2	-11.16	1.29	1.52
1	5	93	VAL	CB-CG2	-11.16	1.29	1.52
3	7	423	SER	CB-OG	-11.16	1.27	1.42
1	G	93	VAL	CB-CG2	-11.15	1.29	1.52
3	O	423	SER	CB-OG	-11.15	1.27	1.42
3	Y	423	SER	CB-OG	-11.15	1.27	1.42
3	L	423	SER	CB-OG	-11.15	1.27	1.42
3	C	423	SER	CB-OG	-11.15	1.27	1.42
2	0	85	PHE	CD2-CE2	-11.14	1.17	1.39
3	F	423	SER	CB-OG	-11.14	1.27	1.42
1	Z	93	VAL	CB-CG2	-11.14	1.29	1.52
1	W	93	VAL	CB-CG2	-11.13	1.29	1.52
1	J	93	VAL	CB-CG2	-11.12	1.29	1.52
2	K	85	PHE	CD2-CE2	-11.12	1.17	1.39
2	6	85	PHE	CD2-CE2	-11.12	1.17	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	195	ASN	CG-ND2	-11.11	1.05	1.32
2	Q	85	PHE	CD2-CE2	-11.11	1.17	1.39
2	X	85	PHE	CD2-CE2	-11.11	1.17	1.39
3	R	195	ASN	CG-ND2	-11.10	1.05	1.32
3	Y	195	ASN	CG-ND2	-11.10	1.05	1.32
3	1	195	ASN	CG-ND2	-11.10	1.05	1.32
3	U	423	SER	CB-OG	-11.10	1.27	1.42
2	B	85	PHE	CD2-CE2	-11.10	1.17	1.39
2	H	85	PHE	CD2-CE2	-11.09	1.17	1.39
3	L	438	VAL	CB-CG2	-11.09	1.29	1.52
3	4	195	ASN	CG-ND2	-11.09	1.05	1.32
2	9	85	PHE	CD2-CE2	-11.09	1.17	1.39
2	E	85	PHE	CD2-CE2	-11.09	1.17	1.39
2	T	85	PHE	CD2-CE2	-11.09	1.17	1.39
2	3	85	PHE	CD2-CE2	-11.09	1.17	1.39
3	U	438	VAL	CB-CG2	-11.09	1.29	1.52
3	V	195	ASN	CG-ND2	-11.09	1.05	1.32
3	4	423	SER	CB-OG	-11.09	1.27	1.42
3	C	195	ASN	CG-ND2	-11.09	1.05	1.32
3	I	195	ASN	CG-ND2	-11.09	1.05	1.32
3	U	195	ASN	CG-ND2	-11.09	1.05	1.32
2	N	85	PHE	CD2-CE2	-11.08	1.17	1.39
3	R	438	VAL	CB-CG2	-11.08	1.29	1.52
3	7	195	ASN	CG-ND2	-11.07	1.05	1.32
3	O	438	VAL	CB-CG2	-11.07	1.29	1.52
3	Y	438	VAL	CB-CG2	-11.07	1.29	1.52
3	7	438	VAL	CB-CG2	-11.07	1.29	1.52
3	C	438	VAL	CB-CG2	-11.06	1.29	1.52
3	F	195	ASN	CG-ND2	-11.06	1.05	1.32
3	O	195	ASN	CG-ND2	-11.06	1.05	1.32
3	4	438	VAL	CB-CG2	-11.06	1.29	1.52
3	I	438	VAL	CB-CG2	-11.05	1.29	1.52
3	I	301	SER	CB-OG	-11.05	1.27	1.42
3	1	438	VAL	CB-CG2	-11.05	1.29	1.52
3	U	301	SER	CB-OG	-11.05	1.27	1.42
3	F	438	VAL	CB-CG2	-11.05	1.29	1.52
3	O	301	SER	CB-OG	-11.05	1.27	1.42
3	4	460	TRP	CE3-CZ3	-11.04	1.19	1.38
3	V	438	VAL	CB-CG2	-11.04	1.29	1.52
3	R	460	TRP	CE3-CZ3	-11.04	1.19	1.38
3	L	301	SER	CB-OG	-11.03	1.27	1.42
3	4	301	SER	CB-OG	-11.03	1.27	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	460	TRP	CE3-CZ3	-11.02	1.19	1.38
3	C	301	SER	CB-OG	-11.02	1.27	1.42
3	O	460	TRP	CE3-CZ3	-11.02	1.19	1.38
3	R	301	SER	CB-OG	-11.01	1.27	1.42
3	Y	460	TRP	CE3-CZ3	-11.01	1.19	1.38
3	7	301	SER	CB-OG	-11.01	1.27	1.42
3	F	301	SER	CB-OG	-11.01	1.27	1.42
3	1	460	TRP	CE3-CZ3	-11.01	1.19	1.38
3	7	460	TRP	CE3-CZ3	-11.01	1.19	1.38
3	C	460	TRP	CE3-CZ3	-11.00	1.19	1.38
3	1	301	SER	CB-OG	-10.99	1.27	1.42
3	U	460	TRP	CE3-CZ3	-10.99	1.19	1.38
3	V	460	TRP	CE3-CZ3	-10.98	1.19	1.38
3	I	460	TRP	CE3-CZ3	-10.97	1.19	1.38
3	L	460	TRP	CE3-CZ3	-10.97	1.19	1.38
3	Y	301	SER	CB-OG	-10.97	1.27	1.42
3	U	45	TYR	CD1-CE1	-10.96	1.23	1.39
3	V	301	SER	CB-OG	-10.96	1.28	1.42
3	I	45	TYR	CD1-CE1	-10.95	1.23	1.39
3	7	384	ASN	CG-ND2	-10.93	1.05	1.32
3	Y	45	TYR	CD1-CE1	-10.93	1.23	1.39
3	F	45	TYR	CD1-CE1	-10.92	1.23	1.39
3	4	384	ASN	CG-ND2	-10.92	1.05	1.32
3	1	384	ASN	CG-ND2	-10.92	1.05	1.32
3	7	45	TYR	CD1-CE1	-10.92	1.23	1.39
3	R	45	TYR	CD1-CE1	-10.91	1.23	1.39
3	I	384	ASN	CG-ND2	-10.91	1.05	1.32
3	R	384	ASN	CG-ND2	-10.91	1.05	1.32
3	4	45	TYR	CD1-CE1	-10.91	1.23	1.39
3	V	45	TYR	CD1-CE1	-10.91	1.23	1.39
3	Y	384	ASN	CG-ND2	-10.91	1.05	1.32
3	O	45	TYR	CD1-CE1	-10.90	1.23	1.39
3	O	384	ASN	CG-ND2	-10.90	1.05	1.32
3	C	45	TYR	CD1-CE1	-10.89	1.23	1.39
3	V	384	ASN	CG-ND2	-10.89	1.05	1.32
3	U	384	ASN	CG-ND2	-10.89	1.05	1.32
3	C	384	ASN	CG-ND2	-10.89	1.05	1.32
3	F	384	ASN	CG-ND2	-10.89	1.05	1.32
3	L	45	TYR	CD1-CE1	-10.87	1.23	1.39
3	L	384	ASN	CG-ND2	-10.87	1.05	1.32
3	1	45	TYR	CD1-CE1	-10.85	1.23	1.39
1	5	14	TYR	CE1-CZ	-10.84	1.24	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	520	LYS	C-O	-10.82	1.02	1.23
1	P	14	TYR	CE1-CZ	-10.82	1.24	1.38
3	R	520	LYS	C-O	-10.81	1.02	1.23
3	Y	520	LYS	C-O	-10.81	1.02	1.23
1	A	14	TYR	CE1-CZ	-10.80	1.24	1.38
3	O	520	LYS	C-O	-10.80	1.02	1.23
3	U	160	PHE	CD2-CE2	-10.80	1.17	1.39
3	I	160	PHE	CD2-CE2	-10.79	1.17	1.39
1	W	14	TYR	CE1-CZ	-10.79	1.24	1.38
1	Z	14	TYR	CE1-CZ	-10.79	1.24	1.38
1	J	14	TYR	CE1-CZ	-10.79	1.24	1.38
3	C	520	LYS	C-O	-10.78	1.02	1.23
3	Y	160	PHE	CD2-CE2	-10.79	1.17	1.39
3	L	160	PHE	CD2-CE2	-10.78	1.17	1.39
1	D	14	TYR	CE1-CZ	-10.78	1.24	1.38
3	L	520	LYS	C-O	-10.78	1.02	1.23
1	S	14	TYR	CE1-CZ	-10.78	1.24	1.38
3	4	520	LYS	C-O	-10.78	1.02	1.23
3	V	160	PHE	CD2-CE2	-10.78	1.17	1.39
3	R	160	PHE	CD2-CE2	-10.77	1.17	1.39
3	V	520	LYS	C-O	-10.77	1.02	1.23
3	4	160	PHE	CD2-CE2	-10.77	1.17	1.39
1	G	14	TYR	CE1-CZ	-10.77	1.24	1.38
3	U	520	LYS	C-O	-10.77	1.02	1.23
3	C	160	PHE	CD2-CE2	-10.76	1.17	1.39
3	1	520	LYS	C-O	-10.76	1.02	1.23
1	2	14	TYR	CE1-CZ	-10.76	1.24	1.38
3	F	160	PHE	CD2-CE2	-10.76	1.17	1.39
3	7	520	LYS	C-O	-10.76	1.02	1.23
3	I	520	LYS	C-O	-10.76	1.02	1.23
3	V	144	SER	CB-OG	-10.76	1.28	1.42
3	1	160	PHE	CD2-CE2	-10.75	1.17	1.39
3	7	160	PHE	CD2-CE2	-10.75	1.17	1.39
3	F	144	SER	CB-OG	-10.75	1.28	1.42
3	O	160	PHE	CD2-CE2	-10.75	1.17	1.39
1	8	14	TYR	CE1-CZ	-10.75	1.24	1.38
3	U	144	SER	CB-OG	-10.74	1.28	1.42
3	O	144	SER	CB-OG	-10.74	1.28	1.42
3	L	144	SER	CB-OG	-10.74	1.28	1.42
3	7	73	THR	CB-CG2	-10.74	1.17	1.52
3	Y	144	SER	CB-OG	-10.73	1.28	1.42
3	O	73	THR	CB-CG2	-10.73	1.17	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	532	ARG	CZ-NH1	-10.73	1.19	1.33
1	M	14	TYR	CE1-CZ	-10.73	1.24	1.38
3	U	73	THR	CB-CG2	-10.72	1.17	1.52
3	R	73	THR	CB-CG2	-10.72	1.17	1.52
3	L	73	THR	CB-CG2	-10.72	1.17	1.52
3	4	144	SER	CB-OG	-10.72	1.28	1.42
3	U	159	PHE	CD2-CE2	-10.71	1.17	1.39
3	C	73	THR	CB-CG2	-10.71	1.17	1.52
3	C	144	SER	CB-OG	-10.71	1.28	1.42
3	1	144	SER	CB-OG	-10.71	1.28	1.42
3	1	159	PHE	CD2-CE2	-10.71	1.17	1.39
3	1	73	THR	CB-CG2	-10.71	1.17	1.52
3	4	379	VAL	CB-CG1	-10.71	1.30	1.52
3	F	379	VAL	CB-CG1	-10.71	1.30	1.52
3	R	144	SER	CB-OG	-10.71	1.28	1.42
3	V	73	THR	CB-CG2	-10.71	1.17	1.52
3	V	379	VAL	CB-CG1	-10.70	1.30	1.52
3	F	73	THR	CB-CG2	-10.70	1.17	1.52
3	I	73	THR	CB-CG2	-10.70	1.17	1.52
3	O	29	PHE	CD1-CE1	-10.70	1.17	1.39
3	4	29	PHE	CD1-CE1	-10.70	1.17	1.39
3	O	159	PHE	CD2-CE2	-10.70	1.17	1.39
3	L	379	VAL	CB-CG1	-10.70	1.30	1.52
3	Y	73	THR	CB-CG2	-10.70	1.17	1.52
3	Y	379	VAL	CB-CG1	-10.69	1.30	1.52
3	4	73	THR	CB-CG2	-10.69	1.17	1.52
3	4	147	GLN	CD-NE2	-10.69	1.06	1.32
3	4	159	PHE	CD2-CE2	-10.69	1.17	1.39
3	7	144	SER	CB-OG	-10.69	1.28	1.42
3	C	379	VAL	CB-CG1	-10.69	1.30	1.52
3	I	379	VAL	CB-CG1	-10.69	1.30	1.52
3	C	159	PHE	CD2-CE2	-10.69	1.17	1.39
3	L	159	PHE	CD2-CE2	-10.69	1.17	1.39
3	U	379	VAL	CB-CG1	-10.69	1.30	1.52
3	1	379	VAL	CB-CG1	-10.68	1.30	1.52
3	I	147	GLN	CD-NE2	-10.68	1.06	1.32
3	L	147	GLN	CD-NE2	-10.68	1.06	1.32
3	O	532	ARG	CZ-NH1	-10.68	1.19	1.33
3	Y	147	GLN	CD-NE2	-10.68	1.06	1.32
3	U	147	GLN	CD-NE2	-10.68	1.06	1.32
3	7	379	VAL	CB-CG1	-10.68	1.30	1.52
3	F	159	PHE	CD2-CE2	-10.68	1.17	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	159	PHE	CD2-CE2	-10.68	1.17	1.39
3	7	159	PHE	CD2-CE2	-10.68	1.17	1.39
3	C	147	GLN	CD-NE2	-10.68	1.06	1.32
3	R	147	GLN	CD-NE2	-10.68	1.06	1.32
3	R	379	VAL	CB-CG1	-10.68	1.30	1.52
3	Y	477	PHE	CE2-CZ	-10.68	1.17	1.37
3	L	29	PHE	CD1-CE1	-10.67	1.18	1.39
3	O	147	GLN	CD-NE2	-10.67	1.06	1.32
3	V	159	PHE	CD2-CE2	-10.67	1.18	1.39
3	V	29	PHE	CD1-CE1	-10.67	1.18	1.39
3	1	147	GLN	CD-NE2	-10.67	1.06	1.32
3	U	477	PHE	CE2-CZ	-10.67	1.17	1.37
3	7	147	GLN	CD-NE2	-10.67	1.06	1.32
3	F	147	GLN	CD-NE2	-10.67	1.06	1.32
3	I	159	PHE	CD2-CE2	-10.67	1.18	1.39
3	O	379	VAL	CB-CG1	-10.67	1.30	1.52
3	1	29	PHE	CD1-CE1	-10.67	1.18	1.39
3	C	29	PHE	CD1-CE1	-10.66	1.18	1.39
3	I	144	SER	CB-OG	-10.66	1.28	1.42
3	F	29	PHE	CD1-CE1	-10.66	1.18	1.39
3	U	29	PHE	CD1-CE1	-10.66	1.18	1.39
3	L	477	PHE	CE2-CZ	-10.66	1.17	1.37
3	7	29	PHE	CD1-CE1	-10.66	1.18	1.39
3	V	147	GLN	CD-NE2	-10.66	1.06	1.32
3	C	532	ARG	CZ-NH1	-10.65	1.19	1.33
3	O	477	PHE	CE2-CZ	-10.65	1.17	1.37
3	Y	532	ARG	CZ-NH1	-10.65	1.19	1.33
3	4	477	PHE	CE2-CZ	-10.65	1.17	1.37
3	I	29	PHE	CD1-CE1	-10.64	1.18	1.39
3	Y	29	PHE	CD1-CE1	-10.64	1.18	1.39
3	4	532	ARG	CZ-NH1	-10.64	1.19	1.33
3	7	532	ARG	CZ-NH1	-10.64	1.19	1.33
3	L	532	ARG	CZ-NH1	-10.64	1.19	1.33
3	R	477	PHE	CE2-CZ	-10.64	1.17	1.37
3	V	477	PHE	CE2-CZ	-10.64	1.17	1.37
3	F	477	PHE	CE2-CZ	-10.64	1.17	1.37
3	C	477	PHE	CE2-CZ	-10.63	1.17	1.37
3	R	29	PHE	CD1-CE1	-10.63	1.18	1.39
3	R	159	PHE	CD2-CE2	-10.63	1.18	1.39
3	R	532	ARG	CZ-NH1	-10.64	1.19	1.33
3	1	477	PHE	CE2-CZ	-10.63	1.17	1.37
3	I	532	ARG	CZ-NH1	-10.62	1.19	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	532	ARG	CZ-NH1	-10.62	1.19	1.33
3	7	477	PHE	CE2-CZ	-10.62	1.17	1.37
3	I	477	PHE	CE2-CZ	-10.62	1.17	1.37
3	F	532	ARG	CZ-NH1	-10.61	1.19	1.33
3	U	532	ARG	CZ-NH1	-10.61	1.19	1.33
2	0	93	LYS	CE-NZ	-10.60	1.22	1.49
2	H	93	LYS	CE-NZ	-10.59	1.22	1.49
2	9	93	LYS	CE-NZ	-10.59	1.22	1.49
2	E	93	LYS	CE-NZ	-10.59	1.22	1.49
2	B	93	LYS	CE-NZ	-10.58	1.22	1.49
2	T	93	LYS	CE-NZ	-10.58	1.22	1.49
2	X	93	LYS	CE-NZ	-10.58	1.22	1.49
2	Q	93	LYS	CE-NZ	-10.57	1.22	1.49
2	K	93	LYS	CE-NZ	-10.57	1.22	1.49
2	N	93	LYS	CE-NZ	-10.57	1.22	1.49
2	3	93	LYS	CE-NZ	-10.57	1.22	1.49
2	6	93	LYS	CE-NZ	-10.56	1.22	1.49
3	Y	482	PHE	CE2-CZ	-10.51	1.17	1.37
3	R	482	PHE	CE2-CZ	-10.51	1.17	1.37
3	1	230	THR	CB-CG2	-10.51	1.17	1.52
3	V	199	LEU	C-N	-10.50	1.14	1.33
3	I	230	THR	CB-CG2	-10.50	1.17	1.52
3	Y	230	THR	CB-CG2	-10.50	1.17	1.52
3	7	482	PHE	CE2-CZ	-10.50	1.17	1.37
3	7	230	THR	CB-CG2	-10.50	1.17	1.52
3	V	230	THR	CB-CG2	-10.50	1.17	1.52
3	I	460	TRP	CG-CD1	-10.49	1.22	1.36
3	U	460	TRP	CG-CD1	-10.49	1.22	1.36
3	R	460	TRP	CG-CD1	-10.49	1.22	1.36
3	4	230	THR	CB-CG2	-10.49	1.17	1.52
3	U	482	PHE	CE2-CZ	-10.49	1.17	1.37
3	C	482	PHE	CE2-CZ	-10.49	1.17	1.37
3	O	460	TRP	CG-CD1	-10.49	1.22	1.36
3	R	230	THR	CB-CG2	-10.49	1.17	1.52
3	C	230	THR	CB-CG2	-10.49	1.17	1.52
3	O	482	PHE	CE2-CZ	-10.49	1.17	1.37
3	U	230	THR	CB-CG2	-10.49	1.17	1.52
3	V	460	TRP	CG-CD1	-10.48	1.22	1.36
3	F	230	THR	CB-CG2	-10.48	1.17	1.52
3	L	230	THR	CB-CG2	-10.48	1.17	1.52
3	L	482	PHE	CE2-CZ	-10.48	1.17	1.37
3	R	199	LEU	C-N	-10.48	1.14	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	482	PHE	CE2-CZ	-10.48	1.17	1.37
3	4	460	TRP	CG-CD1	-10.48	1.22	1.36
3	4	482	PHE	CE2-CZ	-10.48	1.17	1.37
3	C	460	TRP	CG-CD1	-10.47	1.22	1.36
3	1	482	PHE	CE2-CZ	-10.47	1.17	1.37
3	U	199	LEU	C-N	-10.47	1.14	1.33
3	L	199	LEU	C-N	-10.47	1.14	1.33
3	O	230	THR	CB-CG2	-10.47	1.17	1.52
3	O	199	LEU	C-N	-10.46	1.14	1.33
3	F	482	PHE	CE2-CZ	-10.46	1.17	1.37
3	I	482	PHE	CE2-CZ	-10.46	1.17	1.37
3	F	199	LEU	C-N	-10.46	1.14	1.33
3	7	460	TRP	CG-CD1	-10.46	1.22	1.36
3	1	199	LEU	C-N	-10.45	1.14	1.33
3	C	199	LEU	C-N	-10.45	1.14	1.33
3	1	460	TRP	CG-CD1	-10.45	1.22	1.36
3	7	199	LEU	C-N	-10.45	1.14	1.33
3	Y	460	TRP	CG-CD1	-10.44	1.22	1.36
3	4	199	LEU	C-N	-10.44	1.14	1.33
3	F	460	TRP	CG-CD1	-10.43	1.22	1.36
3	I	199	LEU	C-N	-10.43	1.14	1.33
3	Y	199	LEU	C-N	-10.43	1.14	1.33
3	L	460	TRP	CG-CD1	-10.42	1.22	1.36
3	U	364	SER	C-O	-10.26	1.03	1.23
3	L	364	SER	C-O	-10.26	1.03	1.23
3	F	364	SER	C-O	-10.25	1.03	1.23
3	I	364	SER	C-O	-10.24	1.03	1.23
3	V	190	GLU	CB-CG	-10.23	1.32	1.52
3	C	364	SER	C-O	-10.23	1.03	1.23
3	O	190	GLU	CB-CG	-10.23	1.32	1.52
3	Y	553	VAL	CB-CG1	-10.23	1.31	1.52
3	4	364	SER	C-O	-10.22	1.03	1.23
3	V	364	SER	C-O	-10.22	1.03	1.23
3	R	364	SER	C-O	-10.21	1.03	1.23
3	Y	190	GLU	CB-CG	-10.21	1.32	1.52
3	1	364	SER	C-O	-10.21	1.03	1.23
3	4	190	GLU	CB-CG	-10.21	1.32	1.52
3	7	553	VAL	CB-CG1	-10.21	1.31	1.52
3	L	49	LYS	CE-NZ	-10.21	1.23	1.49
3	1	411	LYS	CE-NZ	-10.20	1.23	1.49
3	7	190	GLU	CB-CG	-10.20	1.32	1.52
3	Y	364	SER	C-O	-10.20	1.03	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	49	LYS	CE-NZ	-10.20	1.23	1.49
3	1	190	GLU	CB-CG	-10.20	1.32	1.52
3	U	190	GLU	CB-CG	-10.20	1.32	1.52
3	C	190	GLU	CB-CG	-10.20	1.32	1.52
3	I	190	GLU	CB-CG	-10.20	1.32	1.52
3	I	553	VAL	CB-CG1	-10.20	1.31	1.52
3	R	411	LYS	CE-NZ	-10.20	1.23	1.49
3	R	190	GLU	CB-CG	-10.19	1.32	1.52
3	U	553	VAL	CB-CG1	-10.19	1.31	1.52
3	L	190	GLU	CB-CG	-10.19	1.32	1.52
3	L	553	VAL	CB-CG1	-10.19	1.31	1.52
3	O	364	SER	C-O	-10.19	1.03	1.23
3	1	49	LYS	CE-NZ	-10.19	1.23	1.49
3	F	553	VAL	CB-CG1	-10.19	1.31	1.52
3	C	553	VAL	CB-CG1	-10.18	1.31	1.52
3	I	49	LYS	CE-NZ	-10.18	1.23	1.49
3	V	49	LYS	CE-NZ	-10.18	1.23	1.49
3	C	411	LYS	CE-NZ	-10.18	1.23	1.49
3	F	190	GLU	CB-CG	-10.18	1.32	1.52
3	I	411	LYS	CE-NZ	-10.18	1.23	1.49
3	7	49	LYS	CE-NZ	-10.18	1.23	1.49
3	7	364	SER	C-O	-10.18	1.04	1.23
3	Y	411	LYS	CE-NZ	-10.18	1.23	1.49
3	U	49	LYS	CE-NZ	-10.18	1.23	1.49
3	C	49	LYS	CE-NZ	-10.17	1.23	1.49
3	4	553	VAL	CB-CG1	-10.17	1.31	1.52
3	U	411	LYS	CE-NZ	-10.17	1.23	1.49
3	7	411	LYS	CE-NZ	-10.17	1.23	1.49
3	O	411	LYS	CE-NZ	-10.17	1.23	1.49
3	Y	49	LYS	CE-NZ	-10.17	1.23	1.49
2	H	118	PHE	CE2-CZ	-10.16	1.18	1.37
3	L	411	LYS	CE-NZ	-10.16	1.23	1.49
3	O	49	LYS	CE-NZ	-10.16	1.23	1.49
3	R	49	LYS	CE-NZ	-10.16	1.23	1.49
3	R	553	VAL	CB-CG1	-10.16	1.31	1.52
3	F	160	PHE	CE1-CZ	-10.16	1.18	1.37
3	O	160	PHE	CE1-CZ	-10.16	1.18	1.37
3	O	553	VAL	CB-CG1	-10.16	1.31	1.52
3	4	160	PHE	CE1-CZ	-10.16	1.18	1.37
3	4	411	LYS	CE-NZ	-10.16	1.23	1.49
2	Q	118	PHE	CE2-CZ	-10.15	1.18	1.37
3	V	411	LYS	CE-NZ	-10.15	1.23	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	553	VAL	CB-CG1	-10.15	1.31	1.52
3	I	160	PHE	CE1-CZ	-10.15	1.18	1.37
3	F	411	LYS	CE-NZ	-10.15	1.23	1.49
3	4	49	LYS	CE-NZ	-10.15	1.23	1.49
2	E	118	PHE	CE2-CZ	-10.15	1.18	1.37
2	0	118	PHE	CE2-CZ	-10.15	1.18	1.37
3	1	553	VAL	CB-CG1	-10.15	1.31	1.52
2	9	118	PHE	CE2-CZ	-10.14	1.18	1.37
2	B	118	PHE	CE2-CZ	-10.14	1.18	1.37
2	K	118	PHE	CE2-CZ	-10.14	1.18	1.37
1	G	63	VAL	CB-CG2	-10.14	1.31	1.52
2	6	118	PHE	CE2-CZ	-10.13	1.18	1.37
3	1	160	PHE	CE1-CZ	-10.13	1.18	1.37
2	T	118	PHE	CE2-CZ	-10.13	1.18	1.37
1	D	63	VAL	CB-CG2	-10.13	1.31	1.52
3	C	160	PHE	CE1-CZ	-10.12	1.18	1.37
1	J	63	VAL	CB-CG2	-10.13	1.31	1.52
3	U	160	PHE	CE1-CZ	-10.12	1.18	1.37
2	N	118	PHE	CE2-CZ	-10.12	1.18	1.37
3	V	160	PHE	CE1-CZ	-10.12	1.18	1.37
3	7	160	PHE	CE1-CZ	-10.12	1.18	1.37
3	L	160	PHE	CE1-CZ	-10.11	1.18	1.37
1	P	63	VAL	CB-CG2	-10.11	1.31	1.52
2	3	118	PHE	CE2-CZ	-10.11	1.18	1.37
1	A	63	VAL	CB-CG2	-10.11	1.31	1.52
3	R	160	PHE	CE1-CZ	-10.10	1.18	1.37
1	M	63	VAL	CB-CG2	-10.10	1.31	1.52
1	S	63	VAL	CB-CG2	-10.10	1.31	1.52
2	X	118	PHE	CE2-CZ	-10.10	1.18	1.37
1	5	63	VAL	CB-CG2	-10.10	1.31	1.52
1	8	63	VAL	CB-CG2	-10.10	1.31	1.52
1	2	63	VAL	CB-CG2	-10.09	1.31	1.52
3	4	237	SER	CB-OG	-10.09	1.29	1.42
3	I	180	TRP	CE3-CZ3	-10.09	1.21	1.38
1	Z	63	VAL	CB-CG2	-10.08	1.31	1.52
3	4	180	TRP	CE3-CZ3	-10.08	1.21	1.38
1	W	63	VAL	CB-CG2	-10.08	1.31	1.52
3	Y	160	PHE	CE1-CZ	-10.08	1.18	1.37
3	1	180	TRP	CE3-CZ3	-10.08	1.21	1.38
3	I	223	VAL	CB-CG2	-10.07	1.31	1.52
3	R	223	VAL	CB-CG2	-10.07	1.31	1.52
3	V	180	TRP	CE3-CZ3	-10.07	1.21	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	223	VAL	CB-CG2	-10.07	1.31	1.52
3	F	180	TRP	CE3-CZ3	-10.06	1.21	1.38
3	Y	180	TRP	CE3-CZ3	-10.06	1.21	1.38
3	Y	402	ASN	CG-ND2	-10.06	1.07	1.32
3	L	180	TRP	CE3-CZ3	-10.06	1.21	1.38
3	C	180	TRP	CE3-CZ3	-10.05	1.21	1.38
3	I	402	ASN	CG-ND2	-10.05	1.07	1.32
3	1	223	VAL	CB-CG2	-10.05	1.31	1.52
3	I	404	ARG	CZ-NH1	-10.05	1.20	1.33
3	C	223	VAL	CB-CG2	-10.05	1.31	1.52
3	F	223	VAL	CB-CG2	-10.05	1.31	1.52
3	O	180	TRP	CE3-CZ3	-10.05	1.21	1.38
3	1	402	ASN	CG-ND2	-10.05	1.07	1.32
3	V	402	ASN	CG-ND2	-10.05	1.07	1.32
3	Y	237	SER	CB-OG	-10.04	1.29	1.42
3	4	402	ASN	CG-ND2	-10.04	1.07	1.32
3	U	223	VAL	CB-CG2	-10.04	1.31	1.52
3	L	404	ARG	CZ-NH1	-10.04	1.20	1.33
3	Y	223	VAL	CB-CG2	-10.04	1.31	1.52
3	C	402	ASN	CG-ND2	-10.03	1.07	1.32
3	L	402	ASN	CG-ND2	-10.04	1.07	1.32
3	1	404	ARG	CZ-NH1	-10.03	1.20	1.33
3	4	223	VAL	CB-CG2	-10.03	1.31	1.52
3	7	223	VAL	CB-CG2	-10.03	1.31	1.52
3	7	402	ASN	CG-ND2	-10.03	1.07	1.32
3	F	402	ASN	CG-ND2	-10.03	1.07	1.32
3	1	237	SER	CB-OG	-10.03	1.29	1.42
3	U	180	TRP	CE3-CZ3	-10.02	1.21	1.38
3	O	223	VAL	CB-CG2	-10.02	1.31	1.52
3	O	402	ASN	CG-ND2	-10.02	1.07	1.32
3	R	402	ASN	CG-ND2	-10.02	1.07	1.32
3	L	223	VAL	CB-CG2	-10.02	1.31	1.52
3	R	404	ARG	CZ-NH1	-10.02	1.20	1.33
3	R	180	TRP	CE3-CZ3	-10.02	1.21	1.38
3	V	404	ARG	CZ-NH1	-10.02	1.20	1.33
3	7	180	TRP	CE3-CZ3	-10.02	1.21	1.38
3	U	402	ASN	CG-ND2	-10.02	1.07	1.32
3	U	237	SER	CB-OG	-10.01	1.29	1.42
3	O	404	ARG	CZ-NH1	-10.01	1.20	1.33
3	C	237	SER	CB-OG	-10.01	1.29	1.42
3	4	404	ARG	CZ-NH1	-10.00	1.20	1.33
3	7	404	ARG	CZ-NH1	-10.00	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	237	SER	CB-OG	-10.00	1.29	1.42
3	C	404	ARG	CZ-NH1	-10.00	1.20	1.33
3	R	237	SER	CB-OG	-9.99	1.29	1.42
3	U	404	ARG	CZ-NH1	-9.99	1.20	1.33
3	L	237	SER	CB-OG	-9.99	1.29	1.42
3	O	237	SER	CB-OG	-9.99	1.29	1.42
3	V	237	SER	CB-OG	-9.98	1.29	1.42
3	F	404	ARG	CZ-NH1	-9.97	1.20	1.33
3	7	29	PHE	C-N	-9.97	1.11	1.34
3	7	237	SER	CB-OG	-9.97	1.29	1.42
3	U	29	PHE	C-N	-9.96	1.11	1.34
3	F	29	PHE	C-N	-9.95	1.11	1.34
3	Y	404	ARG	CZ-NH1	-9.94	1.20	1.33
3	C	29	PHE	C-N	-9.94	1.11	1.34
3	R	29	PHE	C-N	-9.94	1.11	1.34
3	I	29	PHE	C-N	-9.94	1.11	1.34
3	L	29	PHE	C-N	-9.94	1.11	1.34
3	F	237	SER	CB-OG	-9.94	1.29	1.42
3	Y	29	PHE	C-N	-9.93	1.11	1.34
3	1	29	PHE	C-N	-9.93	1.11	1.34
3	O	29	PHE	C-N	-9.93	1.11	1.34
3	4	29	PHE	C-N	-9.93	1.11	1.34
3	V	29	PHE	C-N	-9.90	1.11	1.34
3	Y	221	TYR	CG-CD1	-9.88	1.26	1.39
3	Y	569	TYR	CD2-CE2	-9.88	1.24	1.39
3	1	221	TYR	CG-CD1	-9.88	1.26	1.39
3	I	125	SER	CB-OG	-9.87	1.29	1.42
3	I	569	TYR	CD2-CE2	-9.87	1.24	1.39
3	4	221	TYR	CG-CD1	-9.85	1.26	1.39
3	7	221	TYR	CG-CD1	-9.85	1.26	1.39
3	C	221	TYR	CG-CD1	-9.85	1.26	1.39
3	L	569	TYR	CD2-CE2	-9.85	1.24	1.39
3	V	221	TYR	CG-CD1	-9.84	1.26	1.39
3	F	221	TYR	CG-CD1	-9.83	1.26	1.39
3	O	569	TYR	CD2-CE2	-9.83	1.24	1.39
3	7	125	SER	CB-OG	-9.83	1.29	1.42
3	F	125	SER	CB-OG	-9.82	1.29	1.42
3	R	221	TYR	CG-CD1	-9.82	1.26	1.39
3	C	569	TYR	CD2-CE2	-9.82	1.24	1.39
3	O	125	SER	CB-OG	-9.82	1.29	1.42
3	O	221	TYR	CG-CD1	-9.82	1.26	1.39
3	V	125	SER	CB-OG	-9.82	1.29	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	569	TYR	CD2-CE2	-9.82	1.24	1.39
3	U	125	SER	CB-OG	-9.81	1.29	1.42
3	R	569	TYR	CD2-CE2	-9.81	1.24	1.39
3	V	569	TYR	CD2-CE2	-9.81	1.24	1.39
1	W	8	VAL	CB-CG1	-9.81	1.32	1.52
3	4	569	TYR	CD2-CE2	-9.80	1.24	1.39
3	F	569	TYR	CD2-CE2	-9.80	1.24	1.39
3	C	125	SER	CB-OG	-9.80	1.29	1.42
3	1	569	TYR	CD2-CE2	-9.79	1.24	1.39
1	D	8	VAL	CB-CG1	-9.79	1.32	1.52
1	G	8	VAL	CB-CG1	-9.79	1.32	1.52
3	I	221	TYR	CG-CD1	-9.79	1.26	1.39
3	L	125	SER	CB-OG	-9.79	1.29	1.42
3	L	221	TYR	CG-CD1	-9.79	1.26	1.39
1	M	8	VAL	CB-CG1	-9.78	1.32	1.52
3	R	125	SER	CB-OG	-9.78	1.29	1.42
3	1	125	SER	CB-OG	-9.78	1.29	1.42
3	U	221	TYR	CG-CD1	-9.78	1.26	1.39
1	A	8	VAL	CB-CG1	-9.78	1.32	1.52
3	7	569	TYR	CD2-CE2	-9.78	1.24	1.39
1	8	8	VAL	CB-CG1	-9.77	1.32	1.52
1	2	8	VAL	CB-CG1	-9.77	1.32	1.52
3	4	125	SER	CB-OG	-9.77	1.29	1.42
1	Z	8	VAL	CB-CG1	-9.76	1.32	1.52
1	P	8	VAL	CB-CG1	-9.76	1.32	1.52
3	Y	125	SER	CB-OG	-9.76	1.29	1.42
1	S	8	VAL	CB-CG1	-9.75	1.32	1.52
1	5	8	VAL	CB-CG1	-9.75	1.32	1.52
1	J	8	VAL	CB-CG1	-9.74	1.32	1.52
3	L	193	PRO	CB-CG	-9.72	1.01	1.50
1	G	14	TYR	CD2-CE2	-9.72	1.24	1.39
3	O	193	PRO	CB-CG	-9.72	1.01	1.50
3	Y	193	PRO	CB-CG	-9.72	1.01	1.50
3	F	341	ARG	CZ-NH2	-9.71	1.20	1.33
3	1	193	PRO	CB-CG	-9.71	1.01	1.50
3	1	341	ARG	CZ-NH2	-9.71	1.20	1.33
1	5	14	TYR	CD2-CE2	-9.71	1.24	1.39
3	I	193	PRO	CB-CG	-9.71	1.01	1.50
3	V	341	ARG	CZ-NH2	-9.71	1.20	1.33
3	C	193	PRO	CB-CG	-9.71	1.01	1.50
1	D	14	TYR	CD2-CE2	-9.71	1.24	1.39
1	W	14	TYR	CD2-CE2	-9.71	1.24	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	193	PRO	CB-CG	-9.71	1.01	1.50
3	V	193	PRO	CB-CG	-9.71	1.01	1.50
3	7	193	PRO	CB-CG	-9.70	1.01	1.50
3	U	193	PRO	CB-CG	-9.70	1.01	1.50
1	8	14	TYR	CD2-CE2	-9.70	1.24	1.39
3	F	193	PRO	CB-CG	-9.70	1.01	1.50
1	A	14	TYR	CD2-CE2	-9.70	1.24	1.39
3	I	341	ARG	CZ-NH2	-9.70	1.20	1.33
1	J	14	TYR	CD2-CE2	-9.70	1.24	1.39
1	P	14	TYR	CD2-CE2	-9.70	1.24	1.39
3	4	193	PRO	CB-CG	-9.70	1.01	1.50
1	2	14	TYR	CD2-CE2	-9.69	1.24	1.39
3	Y	341	ARG	CZ-NH2	-9.69	1.20	1.33
3	4	341	ARG	CZ-NH2	-9.69	1.20	1.33
1	S	14	TYR	CD2-CE2	-9.68	1.24	1.39
3	U	341	ARG	CZ-NH2	-9.68	1.20	1.33
1	M	14	TYR	CZ-OH	-9.68	1.21	1.37
1	Z	14	TYR	CD2-CE2	-9.68	1.24	1.39
3	C	341	ARG	CZ-NH2	-9.67	1.20	1.33
3	7	341	ARG	CZ-NH2	-9.67	1.20	1.33
3	O	341	ARG	CZ-NH2	-9.67	1.20	1.33
3	7	268	PHE	CE1-CZ	-9.66	1.19	1.37
1	M	14	TYR	CD2-CE2	-9.66	1.24	1.39
3	I	350	GLU	CD-OE1	-9.66	1.15	1.25
3	O	268	PHE	CE1-CZ	-9.66	1.19	1.37
3	Y	268	PHE	CE1-CZ	-9.65	1.19	1.37
3	U	570	PHE	CE2-CZ	-9.65	1.19	1.37
3	I	570	PHE	CE2-CZ	-9.64	1.19	1.37
3	O	570	PHE	CE2-CZ	-9.64	1.19	1.37
3	R	268	PHE	CE1-CZ	-9.64	1.19	1.37
3	V	570	PHE	CE2-CZ	-9.64	1.19	1.37
1	2	14	TYR	CZ-OH	-9.64	1.21	1.37
1	W	14	TYR	CZ-OH	-9.64	1.21	1.37
3	R	350	GLU	CD-OE1	-9.64	1.15	1.25
1	D	14	TYR	CZ-OH	-9.64	1.21	1.37
3	C	268	PHE	CE1-CZ	-9.63	1.19	1.37
1	G	14	TYR	CZ-OH	-9.63	1.21	1.37
3	I	268	PHE	CE1-CZ	-9.63	1.19	1.37
3	L	268	PHE	CE1-CZ	-9.63	1.19	1.37
1	Z	14	TYR	CZ-OH	-9.63	1.21	1.37
3	L	341	ARG	CZ-NH2	-9.63	1.20	1.33
3	C	570	PHE	CE2-CZ	-9.62	1.19	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	268	PHE	CE1-CZ	-9.62	1.19	1.37
3	R	570	PHE	CE2-CZ	-9.62	1.19	1.37
1	S	14	TYR	CZ-OH	-9.62	1.21	1.37
3	V	268	PHE	CE1-CZ	-9.62	1.19	1.37
3	4	268	PHE	CE1-CZ	-9.62	1.19	1.37
3	4	570	PHE	CE2-CZ	-9.63	1.19	1.37
1	A	14	TYR	CZ-OH	-9.62	1.21	1.37
1	J	14	TYR	CZ-OH	-9.62	1.21	1.37
3	1	570	PHE	CE2-CZ	-9.62	1.19	1.37
3	R	341	ARG	CZ-NH2	-9.62	1.20	1.33
1	8	14	TYR	CZ-OH	-9.62	1.21	1.37
3	U	350	GLU	CD-OE1	-9.62	1.15	1.25
3	F	570	PHE	CE2-CZ	-9.62	1.19	1.37
3	7	570	PHE	CE2-CZ	-9.62	1.19	1.37
2	Q	98	SER	CB-OG	-9.61	1.29	1.42
1	P	14	TYR	CZ-OH	-9.61	1.21	1.37
3	1	268	PHE	CE1-CZ	-9.61	1.19	1.37
3	L	570	PHE	CE2-CZ	-9.61	1.19	1.37
2	9	98	SER	CB-OG	-9.60	1.29	1.42
3	Y	570	PHE	CE2-CZ	-9.60	1.19	1.37
3	U	268	PHE	CE1-CZ	-9.60	1.19	1.37
3	L	350	GLU	CD-OE1	-9.60	1.15	1.25
3	1	350	GLU	CD-OE1	-9.60	1.15	1.25
3	V	350	GLU	CD-OE1	-9.59	1.15	1.25
3	C	350	GLU	CD-OE1	-9.59	1.15	1.25
3	F	350	GLU	CD-OE1	-9.59	1.15	1.25
2	T	98	SER	CB-OG	-9.58	1.29	1.42
3	4	350	GLU	CD-OE1	-9.58	1.15	1.25
2	6	98	SER	CB-OG	-9.58	1.29	1.42
3	7	350	GLU	CD-OE1	-9.58	1.15	1.25
2	K	98	SER	CB-OG	-9.58	1.29	1.42
2	X	98	SER	CB-OG	-9.58	1.29	1.42
1	D	53	VAL	CB-CG1	-9.57	1.32	1.52
2	B	98	SER	CB-OG	-9.56	1.29	1.42
3	F	403	PHE	CD1-CE1	-9.56	1.20	1.39
3	I	403	PHE	CD1-CE1	-9.56	1.20	1.39
1	5	14	TYR	CZ-OH	-9.56	1.21	1.37
2	0	98	SER	CB-OG	-9.56	1.29	1.42
3	L	403	PHE	CD1-CE1	-9.56	1.20	1.39
3	7	403	PHE	CD1-CE1	-9.56	1.20	1.39
1	Z	53	VAL	CB-CG1	-9.55	1.32	1.52
3	U	403	PHE	CD1-CE1	-9.56	1.20	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	98	SER	CB-OG	-9.55	1.29	1.42
3	Y	403	PHE	CD1-CE1	-9.55	1.20	1.39
3	1	403	PHE	CD1-CE1	-9.55	1.20	1.39
3	4	403	PHE	CD1-CE1	-9.55	1.20	1.39
3	C	403	PHE	CD1-CE1	-9.55	1.20	1.39
2	3	98	SER	CB-OG	-9.54	1.29	1.42
3	4	45	TYR	CG-CD2	-9.54	1.26	1.39
3	O	350	GLU	CD-OE1	-9.54	1.15	1.25
1	M	53	VAL	CB-CG1	-9.54	1.32	1.52
1	S	53	VAL	CB-CG1	-9.54	1.32	1.52
3	V	403	PHE	CD1-CE1	-9.54	1.20	1.39
3	Y	350	GLU	CD-OE1	-9.54	1.15	1.25
1	5	53	VAL	CB-CG1	-9.54	1.32	1.52
1	8	53	VAL	CB-CG1	-9.54	1.32	1.52
3	I	45	TYR	CG-CD2	-9.54	1.26	1.39
3	O	45	TYR	CG-CD2	-9.53	1.26	1.39
3	O	403	PHE	CD1-CE1	-9.53	1.20	1.39
1	J	53	VAL	CB-CG1	-9.53	1.32	1.52
3	R	45	TYR	CG-CD2	-9.53	1.26	1.39
3	V	45	TYR	CG-CD2	-9.53	1.26	1.39
3	U	45	TYR	CG-CD2	-9.53	1.26	1.39
1	A	53	VAL	CB-CG1	-9.53	1.32	1.52
1	W	53	VAL	CB-CG1	-9.53	1.32	1.52
1	P	53	VAL	CB-CG1	-9.52	1.32	1.52
3	R	403	PHE	CD1-CE1	-9.52	1.20	1.39
3	C	45	TYR	CG-CD2	-9.52	1.26	1.39
1	2	53	VAL	CB-CG1	-9.52	1.32	1.52
3	7	45	TYR	CG-CD2	-9.52	1.26	1.39
3	Y	45	TYR	CG-CD2	-9.51	1.26	1.39
2	N	98	SER	CB-OG	-9.51	1.29	1.42
2	E	98	SER	CB-OG	-9.50	1.29	1.42
3	F	45	TYR	CG-CD2	-9.50	1.26	1.39
3	I	150	HIS	C-O	-9.50	1.05	1.23
3	U	150	HIS	C-O	-9.49	1.05	1.23
1	G	53	VAL	CB-CG1	-9.49	1.32	1.52
3	1	45	TYR	CG-CD2	-9.49	1.26	1.39
3	4	150	HIS	C-O	-9.49	1.05	1.23
3	F	150	HIS	C-O	-9.48	1.05	1.23
3	F	514	ARG	CB-CG	-9.48	1.26	1.52
3	O	364	SER	C-N	-9.48	1.12	1.34
3	1	150	HIS	C-O	-9.48	1.05	1.23
3	7	364	SER	C-N	-9.48	1.12	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	422	VAL	CB-CG1	-9.48	1.32	1.52
3	O	150	HIS	C-O	-9.48	1.05	1.23
3	I	376	TRP	CD1-NE1	-9.47	1.21	1.38
3	I	514	ARG	CB-CG	-9.47	1.26	1.52
3	O	422	VAL	CB-CG1	-9.47	1.32	1.52
3	R	422	VAL	CB-CG1	-9.47	1.32	1.52
2	6	74	PHE	CD2-CE2	-9.47	1.20	1.39
3	V	422	VAL	CB-CG1	-9.47	1.32	1.52
3	C	150	HIS	C-O	-9.46	1.05	1.23
3	F	376	TRP	CD1-NE1	-9.47	1.21	1.38
3	L	150	HIS	C-O	-9.46	1.05	1.23
3	L	422	VAL	CB-CG1	-9.46	1.32	1.52
3	R	514	ARG	CB-CG	-9.47	1.26	1.52
3	Y	422	VAL	CB-CG1	-9.46	1.32	1.52
3	7	514	ARG	CB-CG	-9.46	1.26	1.52
3	V	150	HIS	C-O	-9.46	1.05	1.23
3	U	364	SER	C-N	-9.46	1.12	1.34
3	O	514	ARG	CB-CG	-9.46	1.27	1.52
3	U	415	ASN	CG-ND2	-9.46	1.09	1.32
3	U	514	ARG	CB-CG	-9.46	1.27	1.52
3	C	514	ARG	CB-CG	-9.46	1.27	1.52
3	L	45	TYR	CG-CD2	-9.46	1.26	1.39
3	L	514	ARG	CB-CG	-9.46	1.27	1.52
3	V	364	SER	C-N	-9.46	1.12	1.34
3	Y	514	ARG	CB-CG	-9.46	1.27	1.52
3	1	422	VAL	CB-CG1	-9.46	1.32	1.52
2	E	74	PHE	CD2-CE2	-9.46	1.20	1.39
3	1	514	ARG	CB-CG	-9.46	1.27	1.52
3	I	364	SER	C-N	-9.45	1.12	1.34
3	Y	150	HIS	C-O	-9.45	1.05	1.23
3	4	364	SER	C-N	-9.45	1.12	1.34
3	C	422	VAL	CB-CG1	-9.45	1.33	1.52
3	R	150	HIS	C-O	-9.45	1.05	1.23
3	4	514	ARG	CB-CG	-9.45	1.27	1.52
3	L	364	SER	C-N	-9.45	1.12	1.34
3	L	376	TRP	CD1-NE1	-9.45	1.21	1.38
3	R	376	TRP	CD1-NE1	-9.45	1.21	1.38
3	V	514	ARG	CB-CG	-9.45	1.27	1.52
3	C	364	SER	C-N	-9.45	1.12	1.34
3	F	422	VAL	CB-CG1	-9.44	1.33	1.52
3	V	415	ASN	CG-ND2	-9.45	1.09	1.32
3	Y	364	SER	C-N	-9.44	1.12	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	74	PHE	CD2-CE2	-9.44	1.20	1.39
3	7	150	HIS	C-O	-9.44	1.05	1.23
3	7	415	ASN	CG-ND2	-9.44	1.09	1.32
2	B	74	PHE	CD2-CE2	-9.44	1.20	1.39
2	T	74	PHE	CD2-CE2	-9.44	1.20	1.39
3	1	364	SER	C-N	-9.44	1.12	1.34
3	7	376	TRP	CD1-NE1	-9.44	1.22	1.38
3	F	364	SER	C-N	-9.44	1.12	1.34
3	F	415	ASN	CG-ND2	-9.44	1.09	1.32
2	N	74	PHE	CD2-CE2	-9.44	1.20	1.39
3	R	415	ASN	CG-ND2	-9.44	1.09	1.32
3	C	415	ASN	CG-ND2	-9.43	1.09	1.32
3	7	422	VAL	CB-CG1	-9.43	1.33	1.52
3	Y	415	ASN	CG-ND2	-9.43	1.09	1.32
1	Z	86	PHE	CD2-CE2	-9.43	1.20	1.39
2	H	74	PHE	CD2-CE2	-9.43	1.20	1.39
2	K	74	PHE	CD2-CE2	-9.43	1.20	1.39
3	R	364	SER	C-N	-9.43	1.12	1.34
3	1	415	ASN	CG-ND2	-9.43	1.09	1.32
3	4	376	TRP	CD1-NE1	-9.43	1.22	1.38
3	C	376	TRP	CD1-NE1	-9.43	1.22	1.38
3	O	415	ASN	CG-ND2	-9.43	1.09	1.32
1	S	86	PHE	CD2-CE2	-9.43	1.20	1.39
1	2	86	PHE	CD2-CE2	-9.43	1.20	1.39
3	4	422	VAL	CB-CG1	-9.43	1.33	1.52
3	7	407[A]	ARG	CZ-NH2	-9.43	1.20	1.33
3	7	407[B]	ARG	CZ-NH2	-9.43	1.20	1.33
1	8	86	PHE	CD2-CE2	-9.43	1.20	1.39
3	4	415	ASN	CG-ND2	-9.42	1.09	1.32
3	L	415	ASN	CG-ND2	-9.42	1.09	1.32
3	I	415	ASN	CG-ND2	-9.42	1.09	1.32
1	G	86	PHE	CD2-CE2	-9.42	1.20	1.39
1	5	86	PHE	CD2-CE2	-9.42	1.20	1.39
2	9	74	PHE	CD2-CE2	-9.42	1.20	1.39
3	O	376	TRP	CD1-NE1	-9.42	1.22	1.38
3	V	376	TRP	CD1-NE1	-9.42	1.22	1.38
3	7	268	PHE	CD2-CE2	-9.41	1.20	1.39
3	F	407[A]	ARG	CZ-NH2	-9.41	1.20	1.33
3	F	407[B]	ARG	CZ-NH2	-9.41	1.20	1.33
2	0	74	PHE	CD2-CE2	-9.41	1.20	1.39
3	U	376	TRP	CD1-NE1	-9.41	1.22	1.38
1	A	86	PHE	CD2-CE2	-9.41	1.20	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	268	PHE	CD2-CE2	-9.41	1.20	1.39
1	W	86	PHE	CD2-CE2	-9.41	1.20	1.39
2	Q	74	PHE	CD2-CE2	-9.40	1.20	1.39
3	V	407[A]	ARG	CZ-NH2	-9.40	1.20	1.33
3	V	407[B]	ARG	CZ-NH2	-9.40	1.20	1.33
2	X	74	PHE	CD2-CE2	-9.40	1.20	1.39
3	U	422	VAL	CB-CG1	-9.40	1.33	1.52
3	Y	376	TRP	CD1-NE1	-9.40	1.22	1.38
3	1	376	TRP	CD1-NE1	-9.40	1.22	1.38
1	D	86	PHE	CD2-CE2	-9.40	1.20	1.39
1	J	86	PHE	CD2-CE2	-9.40	1.20	1.39
3	I	407[A]	ARG	CZ-NH2	-9.40	1.20	1.33
3	I	407[B]	ARG	CZ-NH2	-9.40	1.20	1.33
1	M	86	PHE	CD2-CE2	-9.39	1.20	1.39
3	L	81	ARG	CZ-NH1	-9.39	1.20	1.33
3	C	407[A]	ARG	CZ-NH2	-9.38	1.20	1.33
3	C	407[B]	ARG	CZ-NH2	-9.38	1.20	1.33
3	L	268	PHE	CD2-CE2	-9.38	1.20	1.39
3	O	407[A]	ARG	CZ-NH2	-9.38	1.20	1.33
3	O	407[B]	ARG	CZ-NH2	-9.38	1.20	1.33
3	R	81	ARG	CZ-NH1	-9.38	1.20	1.33
3	4	407[A]	ARG	CZ-NH2	-9.38	1.20	1.33
3	4	407[B]	ARG	CZ-NH2	-9.38	1.20	1.33
3	I	268	PHE	CD2-CE2	-9.38	1.20	1.39
3	R	268	PHE	CD2-CE2	-9.38	1.20	1.39
3	V	81	ARG	CZ-NH1	-9.38	1.20	1.33
3	Y	407[A]	ARG	CZ-NH2	-9.37	1.20	1.33
3	Y	407[B]	ARG	CZ-NH2	-9.37	1.20	1.33
3	1	407[A]	ARG	CZ-NH2	-9.37	1.20	1.33
3	1	407[B]	ARG	CZ-NH2	-9.37	1.20	1.33
3	U	81	ARG	CZ-NH1	-9.37	1.20	1.33
3	C	268	PHE	CD2-CE2	-9.37	1.20	1.39
3	F	81	ARG	CZ-NH1	-9.37	1.20	1.33
3	C	81	ARG	CZ-NH1	-9.36	1.20	1.33
1	P	86	PHE	CD2-CE2	-9.36	1.20	1.39
3	V	268	PHE	CD2-CE2	-9.36	1.20	1.39
3	Y	81	ARG	CZ-NH1	-9.36	1.20	1.33
3	Y	268	PHE	CD2-CE2	-9.36	1.20	1.39
2	X	105	PHE	CE1-CZ	-9.36	1.19	1.37
3	4	81	ARG	CZ-NH1	-9.36	1.20	1.33
3	O	81	ARG	CZ-NH1	-9.36	1.20	1.33
3	F	268	PHE	CD2-CE2	-9.36	1.20	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	105	PHE	CE1-CZ	-9.35	1.19	1.37
3	7	81	ARG	CZ-NH1	-9.35	1.20	1.33
3	U	268	PHE	CD2-CE2	-9.35	1.20	1.39
3	L	407[A]	ARG	CZ-NH2	-9.35	1.20	1.33
3	L	407[B]	ARG	CZ-NH2	-9.35	1.20	1.33
3	1	268	PHE	CD2-CE2	-9.35	1.20	1.39
3	F	152	LEU	CG-CD2	-9.35	1.17	1.51
2	N	105	PHE	CE1-CZ	-9.35	1.19	1.37
2	E	105	PHE	CE1-CZ	-9.34	1.19	1.37
2	K	105	PHE	CE1-CZ	-9.34	1.19	1.37
2	0	105	PHE	CE1-CZ	-9.34	1.19	1.37
3	1	152	LEU	CG-CD2	-9.34	1.17	1.51
3	U	407[A]	ARG	CZ-NH2	-9.34	1.21	1.33
3	U	407[B]	ARG	CZ-NH2	-9.34	1.21	1.33
3	R	407[A]	ARG	CZ-NH2	-9.34	1.21	1.33
3	R	407[B]	ARG	CZ-NH2	-9.34	1.21	1.33
3	V	152	LEU	CG-CD2	-9.34	1.17	1.51
3	4	268	PHE	CD2-CE2	-9.34	1.20	1.39
2	B	105	PHE	CE1-CZ	-9.33	1.19	1.37
3	I	81	ARG	CZ-NH1	-9.33	1.21	1.33
2	3	105	PHE	CE1-CZ	-9.33	1.19	1.37
3	C	152	LEU	CG-CD2	-9.33	1.17	1.51
3	Y	152	LEU	CG-CD2	-9.33	1.17	1.51
2	9	105	PHE	CE1-CZ	-9.33	1.19	1.37
3	4	152	LEU	CG-CD2	-9.33	1.17	1.51
3	I	152	LEU	CG-CD2	-9.32	1.17	1.51
3	1	81	ARG	CZ-NH1	-9.32	1.21	1.33
2	6	105	PHE	CE1-CZ	-9.32	1.19	1.37
3	R	152	LEU	CG-CD2	-9.32	1.17	1.51
3	U	152	LEU	CG-CD2	-9.32	1.17	1.51
3	L	152	LEU	CG-CD2	-9.32	1.17	1.51
2	Q	105	PHE	CE1-CZ	-9.32	1.19	1.37
2	T	105	PHE	CE1-CZ	-9.31	1.19	1.37
3	7	152	LEU	CG-CD2	-9.31	1.17	1.51
3	O	152	LEU	CG-CD2	-9.31	1.17	1.51
3	F	460	TRP	CB-CG	-9.30	1.33	1.50
3	O	460	TRP	CB-CG	-9.29	1.33	1.50
3	V	460	TRP	CB-CG	-9.29	1.33	1.50
3	L	460	TRP	CB-CG	-9.29	1.33	1.50
2	Q	148	LYS	CE-NZ	-9.29	1.25	1.49
3	7	460	TRP	CB-CG	-9.29	1.33	1.50
3	4	120	SER	CB-OG	-9.29	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	460	TRP	CB-CG	-9.28	1.33	1.50
3	R	460	TRP	CB-CG	-9.28	1.33	1.50
1	S	7	GLU	CD-OE2	-9.28	1.15	1.25
2	X	148	LYS	CE-NZ	-9.28	1.25	1.49
2	B	148	LYS	CE-NZ	-9.27	1.25	1.49
3	C	460	TRP	CB-CG	-9.27	1.33	1.50
2	E	148	LYS	CE-NZ	-9.27	1.25	1.49
2	6	148	LYS	CE-NZ	-9.27	1.25	1.49
3	7	120	SER	CB-OG	-9.27	1.30	1.42
3	I	460	TRP	CB-CG	-9.27	1.33	1.50
2	9	148	LYS	CE-NZ	-9.27	1.25	1.49
3	Y	460	TRP	CB-CG	-9.26	1.33	1.50
2	3	148	LYS	CE-NZ	-9.26	1.25	1.49
3	U	460	TRP	CB-CG	-9.26	1.33	1.50
2	N	148	LYS	CE-NZ	-9.26	1.25	1.49
2	H	148	LYS	CE-NZ	-9.26	1.25	1.49
2	K	148	LYS	CE-NZ	-9.26	1.25	1.49
2	T	148	LYS	CE-NZ	-9.26	1.25	1.49
3	V	120	SER	CB-OG	-9.25	1.30	1.42
2	0	148	LYS	CE-NZ	-9.25	1.25	1.49
1	D	7	GLU	CD-OE2	-9.25	1.15	1.25
3	1	120	SER	CB-OG	-9.25	1.30	1.42
3	4	460	TRP	CB-CG	-9.25	1.33	1.50
3	F	302	SER	CA-CB	-9.25	1.39	1.52
3	R	367	GLN	CD-NE2	-9.24	1.09	1.32
1	2	7	GLU	CD-OE2	-9.24	1.15	1.25
3	V	367	GLN	CD-NE2	-9.24	1.09	1.32
3	I	367	GLN	CD-NE2	-9.24	1.09	1.32
1	M	7	GLU	CD-OE2	-9.24	1.15	1.25
3	L	120	SER	CB-OG	-9.23	1.30	1.42
3	V	302	SER	CA-CB	-9.23	1.39	1.52
3	Y	120	SER	CB-OG	-9.23	1.30	1.42
3	R	480	PRO	CB-CG	-9.23	1.03	1.50
3	4	367	GLN	CD-NE2	-9.23	1.09	1.32
1	5	7	GLU	CD-OE2	-9.23	1.15	1.25
1	Z	7	GLU	CD-OE2	-9.23	1.15	1.25
3	C	120	SER	CB-OG	-9.23	1.30	1.42
3	L	480	PRO	CB-CG	-9.23	1.03	1.50
3	Y	480	PRO	CB-CG	-9.22	1.03	1.50
3	V	480	PRO	CB-CG	-9.22	1.03	1.50
3	C	480	PRO	CB-CG	-9.22	1.03	1.50
3	L	367	GLN	CD-NE2	-9.22	1.09	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	7	GLU	CD-OE2	-9.22	1.15	1.25
3	Y	367	GLN	CD-NE2	-9.22	1.09	1.32
3	U	120	SER	CB-OG	-9.22	1.30	1.42
1	A	7	GLU	CD-OE2	-9.22	1.15	1.25
3	O	367	GLN	CD-NE2	-9.22	1.09	1.32
3	O	480	PRO	CB-CG	-9.22	1.03	1.50
3	7	480	PRO	CB-CG	-9.22	1.03	1.50
3	C	367	GLN	CD-NE2	-9.21	1.09	1.32
3	I	302	SER	CA-CB	-9.21	1.39	1.52
3	1	480	PRO	CB-CG	-9.21	1.03	1.50
1	8	7	GLU	CD-OE2	-9.21	1.15	1.25
3	F	480	PRO	CB-CG	-9.21	1.03	1.50
3	I	480	PRO	CB-CG	-9.21	1.03	1.50
3	F	367	GLN	CD-NE2	-9.21	1.09	1.32
3	U	480	PRO	CB-CG	-9.21	1.03	1.50
3	O	120	SER	CB-OG	-9.20	1.30	1.42
1	W	7	GLU	CD-OE2	-9.21	1.15	1.25
3	7	367	GLN	CD-NE2	-9.20	1.09	1.32
3	F	120	SER	CB-OG	-9.20	1.30	1.42
3	4	480	PRO	CB-CG	-9.20	1.03	1.50
3	U	302	SER	CA-CB	-9.20	1.39	1.52
3	U	367	GLN	CD-NE2	-9.20	1.09	1.32
3	1	367	GLN	CD-NE2	-9.20	1.09	1.32
3	L	302	SER	CA-CB	-9.19	1.39	1.52
3	7	302	SER	CA-CB	-9.19	1.39	1.52
3	R	302	SER	CA-CB	-9.18	1.39	1.52
3	Y	302	SER	CA-CB	-9.18	1.39	1.52
3	O	302	SER	CA-CB	-9.18	1.39	1.52
3	R	120	SER	CB-OG	-9.18	1.30	1.42
3	C	302	SER	CA-CB	-9.17	1.39	1.52
1	P	7	GLU	CD-OE2	-9.17	1.15	1.25
3	I	120	SER	CB-OG	-9.17	1.30	1.42
3	4	302	SER	CA-CB	-9.17	1.39	1.52
1	G	7	GLU	CD-OE2	-9.16	1.15	1.25
3	R	89	VAL	CB-CG2	-9.16	1.33	1.52
3	L	89	VAL	CB-CG2	-9.15	1.33	1.52
3	C	89	VAL	CB-CG2	-9.15	1.33	1.52
3	O	89	VAL	CB-CG2	-9.15	1.33	1.52
3	7	89	VAL	CB-CG2	-9.15	1.33	1.52
3	F	89	VAL	CB-CG2	-9.15	1.33	1.52
3	1	89	VAL	CB-CG2	-9.15	1.33	1.52
3	4	89	VAL	CB-CG2	-9.15	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	89	VAL	CB-CG2	-9.14	1.33	1.52
3	V	89	VAL	CB-CG2	-9.14	1.33	1.52
3	Y	89	VAL	CB-CG2	-9.13	1.33	1.52
3	I	89	VAL	CB-CG2	-9.13	1.33	1.52
3	L	497	VAL	CB-CG2	-9.12	1.33	1.52
3	1	302	SER	CA-CB	-9.11	1.39	1.52
1	8	56	VAL	CB-CG2	-9.11	1.33	1.52
3	Y	29	PHE	CE1-CZ	-9.10	1.20	1.37
3	1	29	PHE	CE1-CZ	-9.10	1.20	1.37
3	7	497	VAL	CB-CG2	-9.10	1.33	1.52
1	G	56	VAL	CB-CG2	-9.10	1.33	1.52
3	R	29	PHE	CE1-CZ	-9.10	1.20	1.37
1	S	56	VAL	CB-CG2	-9.10	1.33	1.52
3	O	497	VAL	CB-CG2	-9.09	1.33	1.52
3	Y	497	VAL	CB-CG2	-9.09	1.33	1.52
1	W	56	VAL	CB-CG2	-9.09	1.33	1.52
1	M	56	VAL	CB-CG2	-9.09	1.33	1.52
3	O	29	PHE	CE1-CZ	-9.09	1.20	1.37
1	5	56	VAL	CB-CG2	-9.09	1.33	1.52
1	A	56	VAL	CB-CG2	-9.08	1.33	1.52
3	R	497	VAL	CB-CG2	-9.08	1.33	1.52
3	1	497	VAL	CB-CG2	-9.08	1.33	1.52
3	C	497	VAL	CB-CG2	-9.08	1.33	1.52
1	D	56	VAL	CB-CG2	-9.08	1.33	1.52
3	C	29	PHE	CE1-CZ	-9.07	1.20	1.37
3	F	29	PHE	CE1-CZ	-9.07	1.20	1.37
1	P	56	VAL	CB-CG2	-9.07	1.33	1.52
1	Z	56	VAL	CB-CG2	-9.07	1.33	1.52
3	7	29	PHE	CE1-CZ	-9.07	1.20	1.37
3	4	497	VAL	CB-CG2	-9.07	1.33	1.52
3	U	29	PHE	CE1-CZ	-9.07	1.20	1.37
3	L	29	PHE	CE1-CZ	-9.06	1.20	1.37
1	5	73	VAL	CB-CG1	-9.06	1.33	1.52
1	2	56	VAL	CB-CG2	-9.06	1.33	1.52
3	I	497	VAL	CB-CG2	-9.05	1.33	1.52
3	V	29	PHE	CE1-CZ	-9.05	1.20	1.37
3	4	29	PHE	CE1-CZ	-9.05	1.20	1.37
3	F	444	PHE	CG-CD1	-9.05	1.25	1.38
3	I	29	PHE	CE1-CZ	-9.05	1.20	1.37
3	V	497	VAL	CB-CG2	-9.05	1.33	1.52
1	Z	73	VAL	CB-CG1	-9.05	1.33	1.52
3	F	497	VAL	CB-CG2	-9.05	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	497	VAL	CB-CG2	-9.05	1.33	1.52
3	I	444	PHE	CG-CD1	-9.04	1.25	1.38
1	8	73	VAL	CB-CG1	-9.04	1.33	1.52
1	A	73	VAL	CB-CG1	-9.04	1.33	1.52
1	D	73	VAL	CB-CG1	-9.04	1.33	1.52
1	J	56	VAL	CB-CG2	-9.04	1.33	1.52
1	2	73	VAL	CB-CG1	-9.03	1.33	1.52
3	F	496	PHE	CE1-CZ	-9.03	1.20	1.37
1	G	73	VAL	CB-CG1	-9.03	1.33	1.52
3	1	496	PHE	CE1-CZ	-9.03	1.20	1.37
1	M	73	VAL	CB-CG1	-9.02	1.33	1.52
1	S	73	VAL	CB-CG1	-9.02	1.33	1.52
3	4	496	PHE	CE1-CZ	-9.02	1.20	1.37
3	7	496	PHE	CE1-CZ	-9.02	1.20	1.37
3	Y	444	PHE	CG-CD1	-9.02	1.25	1.38
3	V	444	PHE	CG-CD1	-9.02	1.25	1.38
3	Y	496	PHE	CE1-CZ	-9.02	1.20	1.37
1	J	73	VAL	CB-CG1	-9.02	1.33	1.52
1	W	73	VAL	CB-CG1	-9.01	1.33	1.52
3	L	496	PHE	CE1-CZ	-9.01	1.20	1.37
3	R	159	PHE	CG-CD1	-9.01	1.25	1.38
1	P	73	VAL	CB-CG1	-9.00	1.33	1.52
3	R	444	PHE	CG-CD1	-9.00	1.25	1.38
3	U	496	PHE	CE1-CZ	-9.00	1.20	1.37
3	C	496	PHE	CE1-CZ	-8.99	1.20	1.37
3	1	159	PHE	CG-CD1	-8.99	1.25	1.38
3	O	444	PHE	CG-CD1	-8.99	1.25	1.38
3	C	444	PHE	CG-CD1	-8.99	1.25	1.38
3	V	496	PHE	CE1-CZ	-8.99	1.20	1.37
3	4	444	PHE	CG-CD1	-8.99	1.25	1.38
3	U	477	PHE	CG-CD1	-8.99	1.25	1.38
3	I	496	PHE	CE1-CZ	-8.98	1.20	1.37
3	O	477	PHE	CG-CD1	-8.98	1.25	1.38
3	R	477	PHE	CG-CD1	-8.98	1.25	1.38
3	4	477	PHE	CG-CD1	-8.98	1.25	1.38
3	F	477	PHE	CG-CD1	-8.97	1.25	1.38
3	L	477	PHE	CG-CD1	-8.97	1.25	1.38
3	R	496	PHE	CE1-CZ	-8.97	1.20	1.37
3	O	496	PHE	CE1-CZ	-8.97	1.20	1.37
3	Y	159	PHE	CG-CD1	-8.97	1.25	1.38
3	C	159	PHE	CG-CD1	-8.96	1.25	1.38
3	F	478	TYR	CG-CD2	-8.96	1.27	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	159	PHE	CG-CD1	-8.96	1.25	1.38
1	J	78	PRO	CB-CG	-8.96	1.05	1.50
3	U	444	PHE	CG-CD1	-8.96	1.25	1.38
3	1	477	PHE	CG-CD1	-8.96	1.25	1.38
1	8	78	PRO	CB-CG	-8.96	1.05	1.50
3	I	477	PHE	CG-CD1	-8.96	1.25	1.38
3	R	527	LYS	CB-CG	-8.96	1.28	1.52
3	V	477	PHE	CG-CD1	-8.95	1.25	1.38
3	V	159	PHE	CG-CD1	-8.95	1.25	1.38
1	5	78	PRO	CB-CG	-8.95	1.05	1.50
3	U	478	TYR	CG-CD2	-8.95	1.27	1.39
1	D	78	PRO	CB-CG	-8.95	1.05	1.50
3	1	527	LYS	CB-CG	-8.95	1.28	1.52
3	I	159	PHE	CG-CD1	-8.95	1.25	1.38
3	V	478	TYR	CG-CD2	-8.95	1.27	1.39
3	Y	527	LYS	CB-CG	-8.95	1.28	1.52
3	7	159	PHE	CG-CD1	-8.95	1.25	1.38
1	S	78	PRO	CB-CG	-8.95	1.05	1.50
1	Z	78	PRO	CB-CG	-8.95	1.05	1.50
1	2	78	PRO	CB-CG	-8.95	1.05	1.50
1	A	78	PRO	CB-CG	-8.94	1.05	1.50
3	F	159	PHE	CG-CD1	-8.94	1.25	1.38
3	I	403	PHE	CE2-CZ	-8.95	1.20	1.37
1	W	78	PRO	CB-CG	-8.94	1.05	1.50
3	1	444	PHE	CG-CD1	-8.95	1.25	1.38
3	C	477	PHE	CG-CD1	-8.94	1.25	1.38
1	G	78	PRO	CB-CG	-8.94	1.05	1.50
3	O	298	VAL	CB-CG1	-8.94	1.34	1.52
1	P	78	PRO	CB-CG	-8.94	1.05	1.50
3	7	444	PHE	CG-CD1	-8.94	1.25	1.38
3	O	478	TYR	CG-CD2	-8.94	1.27	1.39
1	M	78	PRO	CB-CG	-8.94	1.05	1.50
3	O	478	TYR	CE1-CZ	-8.94	1.26	1.38
3	7	403	PHE	CE2-CZ	-8.94	1.20	1.37
3	7	478	TYR	CE1-CZ	-8.94	1.26	1.38
3	F	527	LYS	CB-CG	-8.94	1.28	1.52
3	L	444	PHE	CG-CD1	-8.94	1.25	1.38
3	Y	477	PHE	CG-CD1	-8.94	1.25	1.38
3	7	478	TYR	CG-CD2	-8.94	1.27	1.39
3	C	527	LYS	CB-CG	-8.93	1.28	1.52
3	L	449	PRO	CG-CD	-8.93	1.21	1.50
3	O	159	PHE	CG-CD1	-8.93	1.25	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	298	VAL	CB-CG1	-8.93	1.34	1.52
3	Y	298	VAL	CB-CG1	-8.93	1.34	1.52
3	Y	478	TYR	CE1-CZ	-8.93	1.26	1.38
3	4	403	PHE	CE2-CZ	-8.93	1.20	1.37
3	V	527	LYS	CB-CG	-8.93	1.28	1.52
3	7	298	VAL	CB-CG1	-8.93	1.34	1.52
3	I	527	LYS	CB-CG	-8.93	1.28	1.52
3	F	478	TYR	CE1-CZ	-8.93	1.26	1.38
3	I	478	TYR	CE1-CZ	-8.93	1.26	1.38
3	L	527	LYS	CB-CG	-8.93	1.28	1.52
3	R	449	PRO	CG-CD	-8.93	1.21	1.50
3	4	527	LYS	CB-CG	-8.93	1.28	1.52
3	U	527	LYS	CB-CG	-8.93	1.28	1.52
3	C	478	TYR	CE1-CZ	-8.92	1.26	1.38
3	C	403	PHE	CE2-CZ	-8.92	1.20	1.37
3	I	449	PRO	CG-CD	-8.92	1.21	1.50
3	L	298	VAL	CB-CG1	-8.92	1.34	1.52
3	O	449	PRO	CG-CD	-8.92	1.21	1.50
3	V	449	PRO	CG-CD	-8.92	1.21	1.50
3	7	449	PRO	CG-CD	-8.92	1.21	1.50
3	7	527	LYS	CB-CG	-8.92	1.28	1.52
3	Y	449	PRO	CG-CD	-8.92	1.21	1.50
3	1	478	TYR	CE1-CZ	-8.92	1.26	1.38
3	C	298	VAL	CB-CG1	-8.92	1.34	1.52
3	C	478	TYR	CG-CD2	-8.92	1.27	1.39
3	F	449	PRO	CG-CD	-8.92	1.21	1.50
3	L	478	TYR	CE1-CZ	-8.92	1.26	1.38
3	C	449	PRO	CG-CD	-8.91	1.21	1.50
3	I	478	TYR	CG-CD2	-8.91	1.27	1.39
3	1	449	PRO	CG-CD	-8.91	1.21	1.50
3	4	449	PRO	CG-CD	-8.91	1.21	1.50
3	7	477	PHE	CG-CD1	-8.91	1.25	1.38
3	I	298	VAL	CB-CG1	-8.91	1.34	1.52
3	R	478	TYR	CG-CD2	-8.91	1.27	1.39
3	V	298	VAL	CB-CG1	-8.91	1.34	1.52
3	4	478	TYR	CE1-CZ	-8.91	1.26	1.38
3	R	478	TYR	CE1-CZ	-8.91	1.26	1.38
3	U	159	PHE	CG-CD1	-8.91	1.25	1.38
3	L	159	PHE	CG-CD1	-8.90	1.25	1.38
3	O	527	LYS	CB-CG	-8.90	1.28	1.52
3	R	403	PHE	CE2-CZ	-8.90	1.20	1.37
3	1	298	VAL	CB-CG1	-8.90	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	449	PRO	CG-CD	-8.90	1.21	1.50
3	1	403	PHE	CE2-CZ	-8.90	1.20	1.37
3	4	298	VAL	CB-CG1	-8.90	1.34	1.52
3	4	478	TYR	CG-CD2	-8.90	1.27	1.39
3	L	403	PHE	CE2-CZ	-8.90	1.20	1.37
3	L	478	TYR	CG-CD2	-8.90	1.27	1.39
3	V	403	PHE	CE2-CZ	-8.90	1.20	1.37
3	F	403	PHE	CE2-CZ	-8.90	1.20	1.37
3	U	298	VAL	CB-CG1	-8.90	1.34	1.52
3	U	478	TYR	CE1-CZ	-8.89	1.26	1.38
3	Y	403	PHE	CE2-CZ	-8.89	1.20	1.37
3	F	298	VAL	CB-CG1	-8.88	1.34	1.52
3	O	403	PHE	CE2-CZ	-8.88	1.20	1.37
3	U	403	PHE	CE2-CZ	-8.88	1.20	1.37
3	Y	478	TYR	CG-CD2	-8.88	1.27	1.39
3	1	478	TYR	CG-CD2	-8.86	1.27	1.39
3	V	478	TYR	CE1-CZ	-8.86	1.27	1.38
2	H	157	GLU	CB-CG	-8.83	1.35	1.52
2	T	134	TRP	CG-CD1	-8.82	1.24	1.36
2	6	158	ARG	CG-CD	-8.82	1.29	1.51
2	9	157	GLU	CB-CG	-8.82	1.35	1.52
2	Q	157	GLU	CB-CG	-8.82	1.35	1.52
2	X	134	TRP	CG-CD1	-8.81	1.24	1.36
2	T	157	GLU	CB-CG	-8.81	1.35	1.52
2	3	134	TRP	CG-CD1	-8.81	1.24	1.36
2	N	157	GLU	CB-CG	-8.80	1.35	1.52
3	O	445	PHE	CD2-CE2	-8.80	1.21	1.39
2	3	157	GLU	CB-CG	-8.80	1.35	1.52
2	Q	158	ARG	CG-CD	-8.80	1.29	1.51
2	6	134	TRP	CG-CD1	-8.80	1.24	1.36
2	H	158	ARG	CG-CD	-8.79	1.29	1.51
2	B	157	GLU	CB-CG	-8.79	1.35	1.52
3	L	445	PHE	CD2-CE2	-8.79	1.21	1.39
2	N	134	TRP	CG-CD1	-8.79	1.24	1.36
3	7	445	PHE	CD2-CE2	-8.79	1.21	1.39
3	Y	445	PHE	CD2-CE2	-8.79	1.21	1.39
2	Q	134	TRP	CG-CD1	-8.78	1.24	1.36
3	F	445	PHE	CD2-CE2	-8.78	1.21	1.39
3	I	445	PHE	CD2-CE2	-8.78	1.21	1.39
2	N	158	ARG	CG-CD	-8.78	1.29	1.51
2	0	157	GLU	CB-CG	-8.78	1.35	1.52
2	9	134	TRP	CG-CD1	-8.78	1.24	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	445	PHE	CD2-CE2	-8.78	1.21	1.39
2	3	158	ARG	CG-CD	-8.78	1.30	1.51
2	B	134	TRP	CG-CD1	-8.77	1.24	1.36
2	B	158	ARG	CG-CD	-8.77	1.30	1.51
2	E	134	TRP	CG-CD1	-8.77	1.24	1.36
2	X	158	ARG	CG-CD	-8.77	1.30	1.51
3	C	445	PHE	CD2-CE2	-8.77	1.21	1.39
2	E	157	GLU	CB-CG	-8.77	1.35	1.52
2	6	157	GLU	CB-CG	-8.77	1.35	1.52
2	K	157	GLU	CB-CG	-8.76	1.35	1.52
3	1	445	PHE	CD2-CE2	-8.76	1.21	1.39
3	4	445	PHE	CD2-CE2	-8.76	1.21	1.39
3	7	420	GLN	CB-CG	-8.76	1.28	1.52
2	E	158	ARG	CG-CD	-8.76	1.30	1.51
2	K	158	ARG	CG-CD	-8.76	1.30	1.51
3	R	445	PHE	CD2-CE2	-8.76	1.21	1.39
2	T	158	ARG	CG-CD	-8.76	1.30	1.51
2	0	134	TRP	CG-CD1	-8.76	1.24	1.36
2	0	158	ARG	CG-CD	-8.76	1.30	1.51
2	H	134	TRP	CG-CD1	-8.76	1.24	1.36
3	V	420	GLN	CB-CG	-8.76	1.28	1.52
3	4	420	GLN	CB-CG	-8.76	1.28	1.52
3	U	420	GLN	CB-CG	-8.76	1.28	1.52
3	U	445	PHE	CD2-CE2	-8.76	1.21	1.39
3	O	420	GLN	CB-CG	-8.75	1.28	1.52
3	I	420	GLN	CB-CG	-8.75	1.28	1.52
2	K	74	PHE	CE2-CZ	-8.75	1.20	1.37
1	M	32	TYR	CZ-OH	-8.75	1.23	1.37
3	R	420	GLN	CB-CG	-8.75	1.28	1.52
3	C	420	GLN	CB-CG	-8.75	1.28	1.52
2	9	158	ARG	CG-CD	-8.75	1.30	1.51
3	I	352	VAL	CB-CG2	-8.75	1.34	1.52
2	X	157	GLU	CB-CG	-8.75	1.35	1.52
2	K	134	TRP	CD2-CE2	-8.75	1.30	1.41
3	Y	352	VAL	CB-CG2	-8.75	1.34	1.52
3	L	420	GLN	CB-CG	-8.74	1.28	1.52
3	R	352	VAL	CB-CG2	-8.74	1.34	1.52
3	F	420	GLN	CB-CG	-8.74	1.28	1.52
2	N	74	PHE	CE2-CZ	-8.74	1.20	1.37
3	Y	420	GLN	CB-CG	-8.74	1.28	1.52
2	E	134	TRP	CD2-CE2	-8.73	1.30	1.41
3	L	352	VAL	CB-CG2	-8.73	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	134	TRP	CD2-CE2	-8.73	1.30	1.41
3	7	352	VAL	CB-CG2	-8.73	1.34	1.52
2	H	134	TRP	CD2-CE2	-8.73	1.30	1.41
2	Q	134	TRP	CD2-CE2	-8.73	1.30	1.41
1	Z	32	TYR	CZ-OH	-8.73	1.23	1.37
3	1	352	VAL	CB-CG2	-8.73	1.34	1.52
1	5	32	TYR	CZ-OH	-8.72	1.23	1.37
3	C	352	VAL	CB-CG2	-8.72	1.34	1.52
3	1	420	GLN	CB-CG	-8.72	1.29	1.52
2	B	134	TRP	CD2-CE2	-8.72	1.30	1.41
2	Q	91	TYR	CG-CD2	-8.72	1.27	1.39
3	V	352	VAL	CB-CG2	-8.72	1.34	1.52
2	9	91	TYR	CG-CD2	-8.72	1.27	1.39
2	E	74	PHE	CE2-CZ	-8.72	1.20	1.37
2	H	74	PHE	CE2-CZ	-8.72	1.20	1.37
1	J	32	TYR	CZ-OH	-8.72	1.23	1.37
2	K	134	TRP	CG-CD1	-8.71	1.24	1.36
2	N	91	TYR	CG-CD2	-8.71	1.27	1.39
2	0	74	PHE	CE2-CZ	-8.71	1.20	1.37
2	T	74	PHE	CE2-CZ	-8.71	1.20	1.37
2	T	91	TYR	CG-CD2	-8.71	1.27	1.39
2	6	74	PHE	CE2-CZ	-8.71	1.20	1.37
2	B	74	PHE	CE2-CZ	-8.71	1.20	1.37
3	F	352	VAL	CB-CG2	-8.70	1.34	1.52
1	2	32	TYR	CZ-OH	-8.71	1.23	1.37
2	3	74	PHE	CE2-CZ	-8.70	1.20	1.37
3	4	352	VAL	CB-CG2	-8.70	1.34	1.52
2	N	134	TRP	CD2-CE2	-8.70	1.30	1.41
1	A	32	TYR	CZ-OH	-8.70	1.23	1.37
2	3	134	TRP	CD2-CE2	-8.70	1.30	1.41
2	H	91	TYR	CG-CD2	-8.70	1.27	1.39
2	T	134	TRP	CD2-CE2	-8.70	1.30	1.41
1	G	32	TYR	CZ-OH	-8.70	1.23	1.37
1	S	32	TYR	CZ-OH	-8.69	1.23	1.37
1	W	32	TYR	CZ-OH	-8.69	1.23	1.37
2	0	91	TYR	CG-CD2	-8.69	1.27	1.39
1	D	32	TYR	CZ-OH	-8.69	1.23	1.37
2	X	91	TYR	CG-CD2	-8.69	1.27	1.39
2	Q	74	PHE	CE2-CZ	-8.69	1.20	1.37
3	O	352	VAL	CB-CG2	-8.69	1.34	1.52
3	U	352	VAL	CB-CG2	-8.68	1.34	1.52
1	8	32	TYR	CZ-OH	-8.68	1.23	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	260	TYR	CE2-CZ	-8.68	1.27	1.38
3	1	23	LEU	C-O	-8.68	1.06	1.23
2	E	91	TYR	CG-CD2	-8.68	1.27	1.39
2	6	134	TRP	CD2-CE2	-8.68	1.30	1.41
2	B	91	TYR	CG-CD2	-8.67	1.27	1.39
2	X	74	PHE	CE2-CZ	-8.67	1.20	1.37
2	9	74	PHE	CE2-CZ	-8.67	1.20	1.37
3	7	23	LEU	C-O	-8.67	1.06	1.23
2	9	134	TRP	CD2-CE2	-8.67	1.30	1.41
3	F	23	LEU	C-O	-8.67	1.06	1.23
1	P	32	TYR	CZ-OH	-8.67	1.23	1.37
3	L	23	LEU	C-O	-8.66	1.06	1.23
2	X	134	TRP	CD2-CE2	-8.66	1.30	1.41
3	C	23	LEU	C-O	-8.66	1.06	1.23
3	O	23	LEU	C-O	-8.66	1.06	1.23
3	4	23	LEU	C-O	-8.66	1.06	1.23
3	F	260	TYR	CE2-CZ	-8.65	1.27	1.38
3	R	23	LEU	C-O	-8.65	1.06	1.23
2	3	91	TYR	CG-CD2	-8.65	1.27	1.39
3	Y	23	LEU	C-O	-8.65	1.06	1.23
3	V	23	LEU	C-O	-8.64	1.06	1.23
3	U	260	TYR	CE2-CZ	-8.64	1.27	1.38
2	K	91	TYR	CG-CD2	-8.63	1.27	1.39
3	7	260	TYR	CE2-CZ	-8.64	1.27	1.38
3	I	23	LEU	C-O	-8.62	1.06	1.23
3	I	260	TYR	CE2-CZ	-8.63	1.27	1.38
3	1	260	TYR	CE2-CZ	-8.62	1.27	1.38
3	U	23	LEU	C-O	-8.61	1.06	1.23
3	L	260	TYR	CE2-CZ	-8.61	1.27	1.38
3	V	32	ILE	CB-CG2	-8.61	1.26	1.52
3	C	260	TYR	CE2-CZ	-8.61	1.27	1.38
2	6	91	TYR	CG-CD2	-8.61	1.27	1.39
3	Y	414	ILE	CB-CG2	-8.60	1.26	1.52
3	V	414	ILE	CB-CG2	-8.60	1.26	1.52
3	I	482	PHE	CE1-CZ	-8.60	1.21	1.37
3	U	482	PHE	CE1-CZ	-8.60	1.21	1.37
3	F	414	ILE	CB-CG2	-8.60	1.26	1.52
3	F	482	PHE	CE1-CZ	-8.60	1.21	1.37
3	Y	395	GLU	CB-CG	-8.60	1.35	1.52
3	R	414	ILE	CB-CG2	-8.60	1.26	1.52
3	4	414	ILE	CB-CG2	-8.59	1.26	1.52
3	L	32	ILE	CB-CG2	-8.59	1.26	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	414	ILE	CB-CG2	-8.59	1.26	1.52
3	L	414	ILE	CB-CG2	-8.59	1.26	1.52
3	O	482	PHE	CE1-CZ	-8.59	1.21	1.37
3	I	32	ILE	CB-CG2	-8.59	1.26	1.52
2	X	134	TRP	CE3-CZ3	-8.59	1.23	1.38
2	T	134	TRP	CE3-CZ3	-8.59	1.23	1.38
3	V	260	TYR	CE2-CZ	-8.58	1.27	1.38
3	C	414	ILE	CB-CG2	-8.58	1.26	1.52
3	V	482	PHE	CE1-CZ	-8.58	1.21	1.37
2	6	134	TRP	CE3-CZ3	-8.58	1.23	1.38
3	U	32	ILE	CB-CG2	-8.58	1.26	1.52
2	E	134	TRP	CE3-CZ3	-8.58	1.23	1.38
3	O	260	TYR	CE2-CZ	-8.58	1.27	1.38
3	7	395	GLU	CB-CG	-8.58	1.35	1.52
2	3	134	TRP	CE3-CZ3	-8.58	1.23	1.38
3	C	32	ILE	CB-CG2	-8.58	1.26	1.52
3	4	260	TYR	CE2-CZ	-8.58	1.27	1.38
3	L	482	PHE	CE1-CZ	-8.58	1.21	1.37
3	R	179	PRO	CB-CG	-8.58	1.07	1.50
3	4	32	ILE	CB-CG2	-8.58	1.26	1.52
3	R	32	ILE	CB-CG2	-8.57	1.26	1.52
3	7	414	ILE	CB-CG2	-8.57	1.26	1.52
3	1	414	ILE	CB-CG2	-8.57	1.26	1.52
3	C	482	PHE	CE1-CZ	-8.57	1.21	1.37
3	7	32	ILE	CB-CG2	-8.57	1.26	1.52
3	7	179	PRO	CB-CG	-8.57	1.07	1.50
3	7	482	PHE	CE1-CZ	-8.57	1.21	1.37
3	1	482	PHE	CE1-CZ	-8.57	1.21	1.37
3	O	32	ILE	CB-CG2	-8.57	1.26	1.52
3	I	179	PRO	CB-CG	-8.56	1.07	1.50
2	0	134	TRP	CE3-CZ3	-8.56	1.23	1.38
3	L	179	PRO	CB-CG	-8.56	1.07	1.50
3	I	414	ILE	CB-CG2	-8.56	1.26	1.52
3	Y	32	ILE	CB-CG2	-8.56	1.26	1.52
3	Y	179	PRO	CB-CG	-8.56	1.07	1.50
2	9	134	TRP	CE3-CZ3	-8.56	1.23	1.38
3	U	414	ILE	CB-CG2	-8.56	1.26	1.52
3	U	179	PRO	CB-CG	-8.56	1.07	1.50
2	B	134	TRP	CE3-CZ3	-8.56	1.24	1.38
3	L	372	VAL	CB-CG2	-8.56	1.34	1.52
3	O	179	PRO	CB-CG	-8.56	1.07	1.50
3	V	179	PRO	CB-CG	-8.56	1.07	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	32	ILE	CB-CG2	-8.56	1.26	1.52
3	F	395	GLU	CB-CG	-8.55	1.35	1.52
3	I	395	GLU	CB-CG	-8.55	1.35	1.52
2	K	134	TRP	CE3-CZ3	-8.55	1.24	1.38
3	F	32	ILE	CB-CG2	-8.55	1.26	1.52
3	Y	482	PHE	CE1-CZ	-8.55	1.21	1.37
3	1	179	PRO	CB-CG	-8.55	1.07	1.50
3	4	482	PHE	CE1-CZ	-8.55	1.21	1.37
3	4	395	GLU	CB-CG	-8.55	1.35	1.52
2	Q	134	TRP	CE3-CZ3	-8.55	1.24	1.38
3	V	395	GLU	CB-CG	-8.55	1.35	1.52
3	C	395	GLU	CB-CG	-8.55	1.35	1.52
3	Y	372	VAL	CB-CG2	-8.54	1.34	1.52
3	F	179	PRO	CB-CG	-8.54	1.07	1.50
3	4	179	PRO	CB-CG	-8.54	1.07	1.50
3	V	372	VAL	CB-CG2	-8.54	1.34	1.52
3	4	372	VAL	CB-CG2	-8.54	1.34	1.52
3	7	372	VAL	CB-CG2	-8.54	1.34	1.52
3	U	395	GLU	CB-CG	-8.54	1.35	1.52
2	H	134	TRP	CE3-CZ3	-8.54	1.24	1.38
3	C	372	VAL	CB-CG2	-8.53	1.34	1.52
3	F	372	VAL	CB-CG2	-8.54	1.34	1.52
3	I	372	VAL	CB-CG2	-8.54	1.34	1.52
3	R	372	VAL	CB-CG2	-8.54	1.34	1.52
3	R	482	PHE	CE1-CZ	-8.54	1.21	1.37
3	R	395	GLU	CB-CG	-8.53	1.35	1.52
3	O	372	VAL	CB-CG2	-8.53	1.34	1.52
3	O	395	GLU	CB-CG	-8.53	1.35	1.52
3	R	260	TYR	CE2-CZ	-8.53	1.27	1.38
3	1	395	GLU	CB-CG	-8.52	1.35	1.52
3	L	395	GLU	CB-CG	-8.52	1.35	1.52
2	N	134	TRP	CE3-CZ3	-8.51	1.24	1.38
3	1	372	VAL	CB-CG2	-8.51	1.34	1.52
1	S	26	ARG	CB-CG	-8.50	1.29	1.52
3	U	372	VAL	CB-CG2	-8.50	1.34	1.52
1	8	26	ARG	CB-CG	-8.49	1.29	1.52
1	2	26	ARG	CB-CG	-8.48	1.29	1.52
1	M	26	ARG	CB-CG	-8.48	1.29	1.52
3	F	460	TRP	CD2-CE2	-8.48	1.31	1.41
1	A	26	ARG	CB-CG	-8.47	1.29	1.52
3	L	183	ARG	CG-CD	-8.47	1.30	1.51
1	Z	26	ARG	CB-CG	-8.47	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7	440	TRP	CG-CD1	-8.47	1.24	1.36
1	D	26	ARG	CB-CG	-8.47	1.29	1.52
1	J	26	ARG	CB-CG	-8.47	1.29	1.52
3	U	532	ARG	CZ-NH2	-8.46	1.22	1.33
3	F	221	TYR	CG-CD2	-8.46	1.28	1.39
1	P	26	ARG	CB-CG	-8.46	1.29	1.52
3	O	183	ARG	CG-CD	-8.46	1.30	1.51
1	5	26	ARG	CB-CG	-8.46	1.29	1.52
3	F	183	ARG	CG-CD	-8.46	1.30	1.51
3	I	183	ARG	CG-CD	-8.46	1.30	1.51
3	R	429	VAL	CB-CG2	-8.46	1.35	1.52
3	U	221	TYR	CG-CD2	-8.45	1.28	1.39
3	F	429	VAL	CB-CG2	-8.45	1.35	1.52
3	Y	532	ARG	CZ-NH2	-8.45	1.22	1.33
3	O	440	TRP	CG-CD1	-8.45	1.25	1.36
3	7	429	VAL	CB-CG2	-8.45	1.35	1.52
3	V	429	VAL	CB-CG2	-8.45	1.35	1.52
3	Y	440	TRP	CG-CD1	-8.45	1.25	1.36
3	1	429	VAL	CB-CG2	-8.45	1.35	1.52
1	G	26	ARG	CB-CG	-8.45	1.29	1.52
1	W	26	ARG	CB-CG	-8.45	1.29	1.52
3	Y	183	ARG	CG-CD	-8.45	1.30	1.51
3	C	183	ARG	CG-CD	-8.44	1.30	1.51
3	I	429	VAL	CB-CG2	-8.44	1.35	1.52
3	1	440	TRP	CG-CD1	-8.44	1.25	1.36
3	C	429	VAL	CB-CG2	-8.44	1.35	1.52
3	I	460	TRP	CD2-CE2	-8.44	1.31	1.41
3	R	297	ASN	CG-ND2	-8.44	1.11	1.32
3	4	183	ARG	CG-CD	-8.44	1.30	1.51
3	4	429	VAL	CB-CG2	-8.44	1.35	1.52
3	4	297	ASN	CG-ND2	-8.44	1.11	1.32
3	U	429	VAL	CB-CG2	-8.44	1.35	1.52
3	L	460	TRP	CD2-CE2	-8.44	1.31	1.41
3	1	183	ARG	CG-CD	-8.44	1.30	1.51
3	1	297	ASN	CG-ND2	-8.44	1.11	1.32
3	V	183	ARG	CG-CD	-8.43	1.30	1.51
3	7	183	ARG	CG-CD	-8.43	1.30	1.51
3	7	297	ASN	CG-ND2	-8.43	1.11	1.32
3	O	429	VAL	CB-CG2	-8.43	1.35	1.52
3	I	297	ASN	CG-ND2	-8.43	1.11	1.32
3	L	297	ASN	CG-ND2	-8.43	1.11	1.32
3	4	460	TRP	CD2-CE2	-8.43	1.31	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	440	TRP	CG-CD1	-8.43	1.25	1.36
3	U	297	ASN	CG-ND2	-8.43	1.11	1.32
3	V	297	ASN	CG-ND2	-8.42	1.11	1.32
3	4	221	TYR	CG-CD2	-8.42	1.28	1.39
3	V	221	TYR	CG-CD2	-8.42	1.28	1.39
3	R	183	ARG	CG-CD	-8.42	1.30	1.51
3	Y	429	VAL	CB-CG2	-8.42	1.35	1.52
3	C	297	ASN	CG-ND2	-8.42	1.11	1.32
3	C	440	TRP	CG-CD1	-8.42	1.25	1.36
3	F	297	ASN	CG-ND2	-8.42	1.11	1.32
3	R	244	MET	CB-CG	-8.42	1.24	1.51
3	R	440	TRP	CG-CD1	-8.42	1.25	1.36
3	4	361	MET	CB-CG	-8.41	1.24	1.51
3	7	460	TRP	CD2-CE2	-8.41	1.31	1.41
3	R	221	TYR	CG-CD2	-8.41	1.28	1.39
3	R	361	MET	CB-CG	-8.41	1.24	1.51
3	Y	297	ASN	CG-ND2	-8.41	1.11	1.32
3	Y	460	TRP	CD2-CE2	-8.41	1.31	1.41
3	L	429	VAL	CB-CG2	-8.41	1.35	1.52
3	O	297	ASN	CG-ND2	-8.41	1.11	1.32
3	4	438	VAL	CB-CG1	-8.41	1.35	1.52
3	I	440	TRP	CG-CD1	-8.41	1.25	1.36
3	U	244	MET	CB-CG	-8.41	1.24	1.51
3	C	460	TRP	CD2-CE2	-8.41	1.31	1.41
3	L	221	TYR	CG-CD2	-8.41	1.28	1.39
3	1	244	MET	CB-CG	-8.41	1.24	1.51
3	7	532	ARG	CZ-NH2	-8.41	1.22	1.33
3	4	244	MET	CB-CG	-8.41	1.24	1.51
3	I	244	MET	CB-CG	-8.40	1.24	1.51
3	I	361	MET	CB-CG	-8.40	1.24	1.51
3	1	361	MET	CB-CG	-8.40	1.24	1.51
3	1	460	TRP	CD2-CE2	-8.40	1.31	1.41
3	U	183	ARG	CG-CD	-8.40	1.30	1.51
3	C	221	TYR	CG-CD2	-8.40	1.28	1.39
3	V	532	ARG	CZ-NH2	-8.40	1.22	1.33
3	7	244	MET	CB-CG	-8.40	1.24	1.51
3	V	440	TRP	CG-CD1	-8.40	1.25	1.36
3	F	361	MET	CB-CG	-8.40	1.24	1.51
3	V	361	MET	CB-CG	-8.40	1.24	1.51
3	Y	221	TYR	CG-CD2	-8.40	1.28	1.39
3	1	221	TYR	CG-CD2	-8.40	1.28	1.39
3	F	244	MET	CB-CG	-8.39	1.24	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	460	TRP	CD2-CE2	-8.39	1.31	1.41
3	V	438	VAL	CB-CG1	-8.39	1.35	1.52
3	Y	244	MET	CB-CG	-8.39	1.24	1.51
3	U	361	MET	CB-CG	-8.39	1.24	1.51
3	C	244	MET	CB-CG	-8.39	1.24	1.51
3	C	361	MET	CB-CG	-8.39	1.24	1.51
3	L	244	MET	CB-CG	-8.39	1.24	1.51
3	O	361	MET	CB-CG	-8.39	1.24	1.51
3	F	532	ARG	CZ-NH2	-8.38	1.22	1.33
3	1	438	VAL	CB-CG1	-8.38	1.35	1.52
3	U	440	TRP	CG-CD1	-8.38	1.25	1.36
3	Y	29	PHE	CD2-CE2	-8.38	1.22	1.39
3	Y	438	VAL	CB-CG1	-8.38	1.35	1.52
3	C	532	ARG	CZ-NH2	-8.38	1.22	1.33
3	V	244	MET	CB-CG	-8.38	1.24	1.51
3	Y	361	MET	CB-CG	-8.38	1.24	1.51
3	7	221	TYR	CG-CD2	-8.38	1.28	1.39
3	L	440	TRP	CG-CD1	-8.38	1.25	1.36
3	O	244	MET	CB-CG	-8.38	1.24	1.51
3	7	361	MET	CB-CG	-8.38	1.24	1.51
3	I	532	ARG	CZ-NH2	-8.37	1.22	1.33
3	7	29	PHE	CD2-CE2	-8.37	1.22	1.39
3	F	29	PHE	CD2-CE2	-8.37	1.22	1.39
3	F	440	TRP	CG-CD1	-8.37	1.25	1.36
3	I	221	TYR	CG-CD2	-8.37	1.28	1.39
3	L	29	PHE	CD2-CE2	-8.37	1.22	1.39
3	L	361	MET	CB-CG	-8.37	1.24	1.51
3	O	221	TYR	CG-CD2	-8.37	1.28	1.39
3	R	486	GLY	N-CA	-8.37	1.33	1.46
3	R	532	ARG	CZ-NH2	-8.37	1.22	1.33
3	1	29	PHE	CD2-CE2	-8.37	1.22	1.39
3	4	29	PHE	CD2-CE2	-8.37	1.22	1.39
3	I	438	VAL	CB-CG1	-8.37	1.35	1.52
3	R	29	PHE	CD2-CE2	-8.36	1.22	1.39
3	U	460	TRP	CD2-CE2	-8.36	1.31	1.41
3	C	438	VAL	CB-CG1	-8.36	1.35	1.52
3	F	479	ARG	CZ-NH2	-8.36	1.22	1.33
3	I	29	PHE	CD2-CE2	-8.36	1.22	1.39
3	V	460	TRP	CD2-CE2	-8.36	1.31	1.41
3	U	438	VAL	CB-CG1	-8.36	1.35	1.52
3	C	29	PHE	CD2-CE2	-8.36	1.22	1.39
3	F	438	VAL	CB-CG1	-8.36	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	192	LEU	CG-CD2	-8.36	1.21	1.51
3	V	479	ARG	CZ-NH2	-8.35	1.22	1.33
3	Y	192	LEU	CG-CD2	-8.35	1.21	1.51
3	O	438	VAL	CB-CG1	-8.35	1.35	1.52
3	U	479	ARG	CZ-NH2	-8.35	1.22	1.33
3	R	438	VAL	CB-CG1	-8.35	1.35	1.52
3	Y	486	GLY	N-CA	-8.35	1.33	1.46
3	7	486	GLY	N-CA	-8.35	1.33	1.46
3	U	192	LEU	CG-CD2	-8.35	1.21	1.51
3	C	486	GLY	N-CA	-8.34	1.33	1.46
3	I	479	ARG	CZ-NH2	-8.34	1.22	1.33
3	V	486	GLY	N-CA	-8.34	1.33	1.46
3	1	221	TYR	CB-CG	-8.34	1.39	1.51
3	1	486	GLY	N-CA	-8.34	1.33	1.46
3	V	29	PHE	CD2-CE2	-8.34	1.22	1.39
3	C	192	LEU	CG-CD2	-8.34	1.21	1.51
3	R	192	LEU	CG-CD2	-8.34	1.21	1.51
3	U	29	PHE	CD2-CE2	-8.34	1.22	1.39
3	4	209	PRO	CG-CD	-8.34	1.23	1.50
3	4	479	ARG	CB-CG	-8.34	1.30	1.52
3	7	192	LEU	CG-CD2	-8.34	1.21	1.51
3	F	192	LEU	CG-CD2	-8.33	1.21	1.51
3	I	486	GLY	N-CA	-8.33	1.33	1.46
3	L	192	LEU	CG-CD2	-8.33	1.21	1.51
3	L	438	VAL	CB-CG1	-8.33	1.35	1.52
3	L	209	PRO	CG-CD	-8.33	1.23	1.50
3	L	479	ARG	CB-CG	-8.33	1.30	1.52
3	V	209	PRO	CG-CD	-8.33	1.23	1.50
3	7	438	VAL	CB-CG1	-8.33	1.35	1.52
3	U	209	PRO	CG-CD	-8.33	1.23	1.50
3	O	29	PHE	CD2-CE2	-8.33	1.22	1.39
3	C	479	ARG	CZ-NH2	-8.33	1.22	1.33
3	L	486	GLY	N-CA	-8.33	1.33	1.46
3	O	532	ARG	CZ-NH2	-8.33	1.22	1.33
3	I	192	LEU	CG-CD2	-8.32	1.21	1.51
3	O	192	LEU	CG-CD2	-8.32	1.21	1.51
3	V	192	LEU	CG-CD2	-8.32	1.21	1.51
3	4	192	LEU	CG-CD2	-8.32	1.21	1.51
3	O	486	GLY	N-CA	-8.32	1.33	1.46
3	7	479	ARG	CZ-NH2	-8.32	1.22	1.33
3	C	209	PRO	CG-CD	-8.32	1.23	1.50
3	R	479	ARG	CZ-NH2	-8.32	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	486	GLY	N-CA	-8.32	1.33	1.46
3	I	209	PRO	CG-CD	-8.32	1.23	1.50
3	O	13	PHE	CE2-CZ	-8.32	1.21	1.37
3	4	13	PHE	CE2-CZ	-8.32	1.21	1.37
3	4	479	ARG	CZ-NH2	-8.32	1.22	1.33
3	L	532	ARG	CZ-NH2	-8.32	1.22	1.33
3	O	460	TRP	CD2-CE2	-8.32	1.31	1.41
3	F	479	ARG	CB-CG	-8.31	1.30	1.52
3	I	479	ARG	CB-CG	-8.31	1.30	1.52
3	1	209	PRO	CG-CD	-8.31	1.23	1.50
3	4	532	ARG	CZ-NH2	-8.31	1.22	1.33
3	Y	209	PRO	CG-CD	-8.31	1.23	1.50
3	1	532	ARG	CZ-NH2	-8.31	1.22	1.33
3	F	13	PHE	CE2-CZ	-8.31	1.21	1.37
3	I	221	TYR	CB-CG	-8.31	1.39	1.51
3	L	479	ARG	CZ-NH2	-8.31	1.22	1.33
3	7	13	PHE	CE2-CZ	-8.31	1.21	1.37
3	C	479	ARG	CB-CG	-8.31	1.30	1.52
3	F	209	PRO	CG-CD	-8.31	1.23	1.50
3	F	486	GLY	N-CA	-8.31	1.33	1.46
3	Y	479	ARG	CB-CG	-8.31	1.30	1.52
3	O	209	PRO	CG-CD	-8.31	1.23	1.50
3	R	479	ARG	CB-CG	-8.31	1.30	1.52
3	1	479	ARG	CB-CG	-8.31	1.30	1.52
3	O	479	ARG	CB-CG	-8.30	1.30	1.52
3	O	479	ARG	CZ-NH2	-8.30	1.22	1.33
3	U	479	ARG	CB-CG	-8.30	1.30	1.52
3	1	13	PHE	CE2-CZ	-8.30	1.21	1.37
3	C	13	PHE	CE2-CZ	-8.30	1.21	1.37
3	U	486	GLY	N-CA	-8.30	1.33	1.46
3	7	209	PRO	CG-CD	-8.30	1.23	1.50
3	L	13	PHE	CE2-CZ	-8.30	1.21	1.37
3	I	571	PHE	CG-CD1	-8.29	1.26	1.38
3	R	209	PRO	CG-CD	-8.29	1.23	1.50
3	Y	479	ARG	CZ-NH2	-8.29	1.22	1.33
3	U	13	PHE	CE2-CZ	-8.29	1.21	1.37
3	R	13	PHE	CE2-CZ	-8.29	1.21	1.37
3	V	479	ARG	CB-CG	-8.29	1.30	1.52
3	L	221	TYR	CB-CG	-8.29	1.39	1.51
3	O	221	TYR	CB-CG	-8.28	1.39	1.51
3	R	221	TYR	CB-CG	-8.28	1.39	1.51
3	7	479	ARG	CB-CG	-8.28	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	221	TYR	CB-CG	-8.28	1.39	1.51
3	Y	13	PHE	CE2-CZ	-8.28	1.21	1.37
3	V	13	PHE	CE2-CZ	-8.28	1.21	1.37
3	C	221	TYR	CB-CG	-8.27	1.39	1.51
3	1	499	GLN	CD-NE2	-8.27	1.12	1.32
3	R	186	LEU	CG-CD2	-8.27	1.21	1.51
3	I	13	PHE	CE2-CZ	-8.27	1.21	1.37
3	V	184	GLN	CB-CG	-8.27	1.30	1.52
3	Y	184	GLN	CB-CG	-8.27	1.30	1.52
3	V	499	GLN	CD-NE2	-8.27	1.12	1.32
3	4	221	TYR	CB-CG	-8.27	1.39	1.51
3	I	451	MET	CB-CG	-8.26	1.25	1.51
3	U	451	MET	CB-CG	-8.26	1.25	1.51
3	O	452	VAL	CB-CG2	-8.26	1.35	1.52
3	R	219	VAL	CB-CG2	-8.26	1.35	1.52
3	R	506	VAL	CB-CG1	-8.26	1.35	1.52
3	Y	221	TYR	CB-CG	-8.26	1.39	1.51
3	Y	452	VAL	CB-CG2	-8.26	1.35	1.52
3	1	479	ARG	CZ-NH2	-8.26	1.22	1.33
3	4	184	GLN	CB-CG	-8.26	1.30	1.52
3	7	184	GLN	CB-CG	-8.26	1.30	1.52
3	F	184	GLN	CB-CG	-8.25	1.30	1.52
3	O	499	GLN	CD-NE2	-8.25	1.12	1.32
3	V	219	VAL	CB-CG2	-8.25	1.35	1.52
3	Y	186	LEU	CG-CD2	-8.25	1.21	1.51
3	Y	499	GLN	CD-NE2	-8.25	1.12	1.32
3	F	571	PHE	CG-CD1	-8.25	1.26	1.38
3	4	499	GLN	CD-NE2	-8.25	1.12	1.32
3	7	221	TYR	CB-CG	-8.25	1.39	1.51
3	L	186	LEU	CG-CD2	-8.25	1.21	1.51
3	O	219	VAL	CB-CG2	-8.25	1.35	1.52
3	V	186	LEU	CG-CD2	-8.25	1.21	1.51
3	V	571	PHE	CG-CD1	-8.25	1.26	1.38
3	Y	451	MET	CB-CG	-8.25	1.25	1.51
3	U	571	PHE	CG-CD1	-8.25	1.26	1.38
3	7	506	VAL	CB-CG1	-8.25	1.35	1.52
3	C	186	LEU	CG-CD2	-8.24	1.21	1.51
3	L	184	GLN	CB-CG	-8.24	1.30	1.52
3	C	184	GLN	CB-CG	-8.24	1.30	1.52
3	C	499	GLN	CD-NE2	-8.24	1.12	1.32
3	F	186	LEU	CG-CD2	-8.24	1.21	1.51
3	L	451	MET	CB-CG	-8.24	1.25	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	452	VAL	CB-CG2	-8.24	1.35	1.52
3	O	186	LEU	CG-CD2	-8.24	1.21	1.51
3	R	184	GLN	CB-CG	-8.24	1.30	1.52
3	V	221	TYR	CB-CG	-8.24	1.39	1.51
3	F	221	TYR	CB-CG	-8.24	1.39	1.51
3	I	156	VAL	CB-CG2	-8.24	1.35	1.52
3	O	184	GLN	CB-CG	-8.24	1.30	1.52
3	1	186	LEU	CG-CD2	-8.24	1.21	1.51
3	V	451	MET	CB-CG	-8.24	1.25	1.51
3	V	452	VAL	CB-CG2	-8.24	1.35	1.52
3	1	451	MET	CB-CG	-8.24	1.25	1.51
3	7	186	LEU	CG-CD2	-8.24	1.21	1.51
3	U	184	GLN	CB-CG	-8.24	1.30	1.52
3	I	506	VAL	CB-CG1	-8.24	1.35	1.52
3	L	219	VAL	CB-CG2	-8.24	1.35	1.52
3	O	451	MET	CB-CG	-8.24	1.25	1.51
3	4	571	PHE	CG-CD1	-8.24	1.26	1.38
3	7	451	MET	CB-CG	-8.24	1.25	1.51
3	C	219	VAL	CB-CG2	-8.23	1.35	1.52
3	F	499	GLN	CD-NE2	-8.23	1.12	1.32
3	I	452	VAL	CB-CG2	-8.23	1.35	1.52
3	R	499	GLN	CD-NE2	-8.23	1.12	1.32
3	4	451	MET	CB-CG	-8.23	1.25	1.51
3	7	499	GLN	CD-NE2	-8.23	1.12	1.32
3	U	499	GLN	CD-NE2	-8.23	1.12	1.32
3	C	451	MET	CB-CG	-8.23	1.25	1.51
3	F	451	MET	CB-CG	-8.23	1.25	1.51
3	U	506	VAL	CB-CG1	-8.23	1.35	1.52
3	C	571	PHE	CG-CD1	-8.23	1.26	1.38
3	F	506	VAL	CB-CG1	-8.23	1.35	1.52
3	O	571	PHE	CG-CD1	-8.23	1.26	1.38
3	1	506	VAL	CB-CG1	-8.23	1.35	1.52
3	F	219	VAL	CB-CG2	-8.23	1.35	1.52
3	O	506	VAL	CB-CG1	-8.23	1.35	1.52
3	R	452	VAL	CB-CG2	-8.23	1.35	1.52
3	1	184	GLN	CB-CG	-8.23	1.30	1.52
3	4	186	LEU	CG-CD2	-8.23	1.21	1.51
3	U	186	LEU	CG-CD2	-8.23	1.21	1.51
3	I	499	GLN	CD-NE2	-8.22	1.12	1.32
3	R	451	MET	CB-CG	-8.22	1.25	1.51
3	1	156	VAL	CB-CG2	-8.22	1.35	1.52
3	C	452	VAL	CB-CG2	-8.22	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	184	GLN	CB-CG	-8.22	1.30	1.52
3	O	156	VAL	CB-CG2	-8.22	1.35	1.52
3	V	506	VAL	CB-CG1	-8.22	1.35	1.52
3	7	219	VAL	CB-CG2	-8.22	1.35	1.52
3	U	219	VAL	CB-CG2	-8.22	1.35	1.52
3	C	506	VAL	CB-CG1	-8.21	1.35	1.52
3	I	186	LEU	CG-CD2	-8.21	1.21	1.51
3	L	499	GLN	CD-NE2	-8.22	1.12	1.32
3	V	156	VAL	CB-CG2	-8.21	1.35	1.52
3	1	571	PHE	CG-CD1	-8.22	1.26	1.38
3	4	219	VAL	CB-CG2	-8.21	1.35	1.52
3	4	452	VAL	CB-CG2	-8.21	1.35	1.52
3	I	219	VAL	CB-CG2	-8.21	1.35	1.52
3	L	506	VAL	CB-CG1	-8.20	1.35	1.52
3	R	156	VAL	CB-CG2	-8.20	1.35	1.52
3	4	156	VAL	CB-CG2	-8.20	1.35	1.52
3	C	156	VAL	CB-CG2	-8.20	1.35	1.52
3	F	156	VAL	CB-CG2	-8.20	1.35	1.52
3	7	452	VAL	CB-CG2	-8.20	1.35	1.52
3	U	156	VAL	CB-CG2	-8.20	1.35	1.52
3	R	571	PHE	CG-CD1	-8.20	1.26	1.38
3	Y	156	VAL	CB-CG2	-8.20	1.35	1.52
3	Y	219	VAL	CB-CG2	-8.20	1.35	1.52
3	7	156	VAL	CB-CG2	-8.20	1.35	1.52
3	U	452	VAL	CB-CG2	-8.20	1.35	1.52
3	L	571	PHE	CG-CD1	-8.19	1.26	1.38
3	F	452	VAL	CB-CG2	-8.19	1.35	1.52
2	X	118	PHE	CD1-CE1	-8.19	1.22	1.39
3	4	506	VAL	CB-CG1	-8.19	1.35	1.52
3	1	452	VAL	CB-CG2	-8.19	1.35	1.52
2	Q	55	VAL	CB-CG1	-8.19	1.35	1.52
3	L	156	VAL	CB-CG2	-8.18	1.35	1.52
3	1	219	VAL	CB-CG2	-8.18	1.35	1.52
3	Y	506	VAL	CB-CG1	-8.18	1.35	1.52
2	K	55	VAL	CB-CG1	-8.18	1.35	1.52
2	H	55	VAL	CB-CG1	-8.18	1.35	1.52
2	N	55	VAL	CB-CG1	-8.18	1.35	1.52
3	Y	571	PHE	CG-CD1	-8.18	1.26	1.38
2	H	118	PHE	CD1-CE1	-8.17	1.23	1.39
2	X	55	VAL	CB-CG1	-8.17	1.35	1.52
2	0	55	VAL	CB-CG1	-8.17	1.35	1.52
3	7	571	PHE	CG-CD1	-8.17	1.26	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	118	PHE	CD1-CE1	-8.17	1.23	1.39
2	9	55	VAL	CB-CG1	-8.17	1.35	1.52
3	U	498	SER	CB-OG	-8.17	1.31	1.42
2	B	55	VAL	CB-CG1	-8.16	1.35	1.52
2	3	55	VAL	CB-CG1	-8.16	1.35	1.52
2	N	118	PHE	CD1-CE1	-8.16	1.23	1.39
2	T	118	PHE	CD1-CE1	-8.16	1.23	1.39
3	I	304	ASN	C-N	8.15	1.49	1.34
2	E	55	VAL	CB-CG1	-8.15	1.35	1.52
2	9	118	PHE	CD1-CE1	-8.15	1.23	1.39
2	T	55	VAL	CB-CG1	-8.15	1.35	1.52
3	1	460	TRP	CD1-NE1	-8.15	1.24	1.38
2	3	118	PHE	CD1-CE1	-8.15	1.23	1.39
2	B	118	PHE	CD1-CE1	-8.14	1.23	1.39
3	7	460	TRP	CD1-NE1	-8.14	1.24	1.38
3	R	460	TRP	CD1-NE1	-8.14	1.24	1.38
2	0	118	PHE	CD1-CE1	-8.14	1.23	1.39
3	F	460	TRP	CD1-NE1	-8.14	1.24	1.38
3	V	304	ASN	C-N	8.13	1.49	1.34
3	Y	460	TRP	CD1-NE1	-8.13	1.24	1.38
2	6	118	PHE	CD1-CE1	-8.13	1.23	1.39
2	Q	153[A]	ARG	C-N	-8.13	1.15	1.34
2	Q	153[B]	ARG	C-N	-8.13	1.15	1.34
2	6	55	VAL	CB-CG1	-8.13	1.35	1.52
2	K	118	PHE	CD1-CE1	-8.13	1.23	1.39
3	L	460	TRP	CD1-NE1	-8.13	1.24	1.38
3	F	304	ASN	C-N	8.12	1.49	1.34
3	I	460	TRP	CD1-NE1	-8.13	1.24	1.38
3	7	304	ASN	C-N	8.13	1.49	1.34
2	H	153[A]	ARG	C-N	-8.12	1.15	1.34
2	H	153[B]	ARG	C-N	-8.12	1.15	1.34
2	6	153[A]	ARG	C-N	-8.12	1.15	1.34
2	6	153[B]	ARG	C-N	-8.12	1.15	1.34
3	L	498	SER	CB-OG	-8.12	1.31	1.42
2	B	153[A]	ARG	C-N	-8.11	1.15	1.34
2	B	153[B]	ARG	C-N	-8.11	1.15	1.34
2	3	153[A]	ARG	C-N	-8.11	1.15	1.34
2	3	153[B]	ARG	C-N	-8.11	1.15	1.34
3	U	460	TRP	CD1-NE1	-8.11	1.24	1.38
3	4	460	TRP	CD1-NE1	-8.11	1.24	1.38
3	C	304	ASN	C-N	8.11	1.49	1.34
2	E	118	PHE	CD1-CE1	-8.11	1.23	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	498	SER	CB-OG	-8.11	1.31	1.42
2	T	153[A]	ARG	C-N	-8.11	1.15	1.34
2	T	153[B]	ARG	C-N	-8.11	1.15	1.34
3	1	304	ASN	C-N	8.11	1.49	1.34
3	U	304	ASN	C-N	8.11	1.49	1.34
3	C	460	TRP	CD1-NE1	-8.10	1.24	1.38
3	I	526	SER	CB-OG	-8.10	1.31	1.42
3	O	304	ASN	C-N	8.10	1.49	1.34
3	O	498	SER	CB-OG	-8.10	1.31	1.42
2	X	153[A]	ARG	C-N	-8.10	1.15	1.34
2	X	153[B]	ARG	C-N	-8.10	1.15	1.34
3	4	304	ASN	C-N	8.10	1.49	1.34
2	E	153[A]	ARG	C-N	-8.10	1.15	1.34
2	E	153[B]	ARG	C-N	-8.10	1.15	1.34
3	7	498	SER	CB-OG	-8.10	1.31	1.42
3	R	304	ASN	C-N	8.10	1.49	1.34
3	R	498	SER	CB-OG	-8.10	1.31	1.42
2	0	153[A]	ARG	C-N	-8.10	1.15	1.34
2	0	153[B]	ARG	C-N	-8.10	1.15	1.34
3	F	526	SER	CB-OG	-8.09	1.31	1.42
2	K	153[A]	ARG	C-N	-8.09	1.15	1.34
2	K	153[B]	ARG	C-N	-8.09	1.15	1.34
3	L	304	ASN	C-N	8.09	1.49	1.34
3	Y	304	ASN	C-N	8.09	1.49	1.34
3	C	498	SER	CB-OG	-8.09	1.31	1.42
3	V	460	TRP	CD1-NE1	-8.09	1.24	1.38
3	7	526	SER	CB-OG	-8.09	1.31	1.42
3	O	460	TRP	CD1-NE1	-8.09	1.24	1.38
3	1	498	SER	CB-OG	-8.08	1.31	1.42
3	4	308	PRO	CB-CG	-8.08	1.09	1.50
2	9	153[A]	ARG	C-N	-8.08	1.15	1.34
2	9	153[B]	ARG	C-N	-8.08	1.15	1.34
2	N	153[A]	ARG	C-N	-8.07	1.15	1.34
2	N	153[B]	ARG	C-N	-8.07	1.15	1.34
3	V	526	SER	CB-OG	-8.07	1.31	1.42
3	Y	498	SER	CB-OG	-8.07	1.31	1.42
3	F	271	ARG	CG-CD	-8.07	1.31	1.51
3	F	498	SER	CB-OG	-8.07	1.31	1.42
3	R	271	ARG	CG-CD	-8.07	1.31	1.51
3	4	526	SER	CB-OG	-8.07	1.31	1.42
3	I	308	PRO	CB-CG	-8.07	1.09	1.50
3	R	308	PRO	CB-CG	-8.07	1.09	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	271	ARG	CG-CD	-8.07	1.31	1.51
3	C	308	PRO	CB-CG	-8.06	1.09	1.50
3	F	308	PRO	CB-CG	-8.06	1.09	1.50
3	O	526	SER	CB-OG	-8.06	1.31	1.42
3	I	271	ARG	CG-CD	-8.06	1.31	1.51
3	I	571	PHE	CD1-CE1	-8.06	1.23	1.39
3	V	308	PRO	CB-CG	-8.06	1.09	1.50
3	V	498	SER	CB-OG	-8.06	1.31	1.42
3	L	271	ARG	CG-CD	-8.06	1.31	1.51
3	L	308	PRO	CB-CG	-8.06	1.09	1.50
3	7	308	PRO	CB-CG	-8.06	1.09	1.50
3	L	526	SER	CB-OG	-8.06	1.31	1.42
3	O	308	PRO	CB-CG	-8.06	1.09	1.50
2	Q	77	PHE	CE1-CZ	-8.06	1.22	1.37
3	U	271	ARG	CG-CD	-8.06	1.31	1.51
3	U	526	SER	CB-OG	-8.06	1.31	1.42
3	C	271	ARG	CG-CD	-8.06	1.31	1.51
3	Y	308	PRO	CB-CG	-8.05	1.09	1.50
3	4	498	SER	CB-OG	-8.05	1.31	1.42
3	U	308	PRO	CB-CG	-8.05	1.09	1.50
3	1	308	PRO	CB-CG	-8.05	1.09	1.50
3	L	571	PHE	CD1-CE1	-8.05	1.23	1.39
3	C	526	SER	CB-OG	-8.05	1.31	1.42
3	Y	271	ARG	CG-CD	-8.05	1.31	1.51
2	0	77	PHE	CE1-CZ	-8.04	1.22	1.37
3	Y	571	PHE	CD1-CE1	-8.04	1.23	1.39
3	7	445	PHE	CG-CD1	-8.04	1.26	1.38
2	K	77	PHE	CE1-CZ	-8.04	1.22	1.37
3	R	571	PHE	CD1-CE1	-8.04	1.23	1.39
3	V	271	ARG	CG-CD	-8.04	1.31	1.51
3	1	271	ARG	CG-CD	-8.04	1.31	1.51
3	1	571	PHE	CD1-CE1	-8.04	1.23	1.39
3	F	376	TRP	CD2-CE3	-8.04	1.28	1.40
3	O	271	ARG	CG-CD	-8.04	1.31	1.51
2	T	105	PHE	CB-CG	-8.04	1.37	1.51
2	H	105	PHE	CB-CG	-8.03	1.37	1.51
3	7	571	PHE	CD1-CE1	-8.03	1.23	1.39
3	4	571	PHE	CD1-CE1	-8.03	1.23	1.39
2	N	77	PHE	CE1-CZ	-8.03	1.22	1.37
3	V	445	PHE	CG-CD1	-8.03	1.26	1.38
3	7	271	ARG	CG-CD	-8.03	1.31	1.51
3	U	445	PHE	CG-CD1	-8.03	1.26	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	571	PHE	CD1-CE1	-8.03	1.23	1.39
2	X	77	PHE	CE1-CZ	-8.03	1.22	1.37
2	E	77	PHE	CE1-CZ	-8.02	1.22	1.37
2	6	105	PHE	CB-CG	-8.02	1.37	1.51
2	B	77	PHE	CE1-CZ	-8.02	1.22	1.37
3	C	571	PHE	CD1-CE1	-8.02	1.23	1.39
3	L	445	PHE	CG-CD1	-8.02	1.26	1.38
2	Q	105	PHE	CB-CG	-8.02	1.37	1.51
3	R	526	SER	CB-OG	-8.02	1.31	1.42
2	T	77	PHE	CE1-CZ	-8.02	1.22	1.37
3	C	445	PHE	CG-CD1	-8.01	1.26	1.38
2	3	105	PHE	CB-CG	-8.01	1.37	1.51
2	9	77	PHE	CE1-CZ	-8.01	1.22	1.37
3	R	445	PHE	CG-CD1	-8.01	1.26	1.38
2	E	105	PHE	CB-CG	-8.01	1.37	1.51
3	4	445	PHE	CG-CD1	-8.01	1.26	1.38
3	I	445	PHE	CG-CD1	-8.01	1.26	1.38
3	1	376	TRP	CD2-CE3	-8.01	1.28	1.40
3	1	445	PHE	CG-CD1	-8.01	1.26	1.38
3	1	526	SER	CB-OG	-8.01	1.31	1.42
3	Y	526	SER	CB-OG	-8.00	1.31	1.42
3	O	571	PHE	CD1-CE1	-8.00	1.23	1.39
3	U	571	PHE	CD1-CE1	-8.00	1.23	1.39
2	0	105	PHE	CB-CG	-8.00	1.37	1.51
3	4	78	VAL	CB-CG2	-8.00	1.36	1.52
2	B	105	PHE	CB-CG	-8.00	1.37	1.51
2	3	77	PHE	CE1-CZ	-8.00	1.22	1.37
3	F	571	PHE	CD1-CE1	-8.00	1.23	1.39
3	I	210	LEU	CG-CD2	-8.00	1.22	1.51
3	Y	445	PHE	CG-CD1	-8.00	1.26	1.38
3	F	210	LEU	CG-CD2	-7.99	1.22	1.51
3	U	210	LEU	CG-CD2	-7.99	1.22	1.51
2	H	77	PHE	CE1-CZ	-7.99	1.22	1.37
3	R	376	TRP	CD2-CE3	-7.99	1.28	1.40
3	Y	466	PRO	C-O	-7.99	1.07	1.23
2	6	77	PHE	CE1-CZ	-7.99	1.22	1.37
2	9	105	PHE	CB-CG	-7.99	1.37	1.51
3	R	210	LEU	CG-CD2	-7.98	1.22	1.51
2	X	105	PHE	CB-CG	-7.98	1.37	1.51
3	O	376	TRP	CD2-CE3	-7.98	1.28	1.40
3	C	376	TRP	CD2-CE3	-7.98	1.28	1.40
3	V	376	TRP	CD2-CE3	-7.98	1.28	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	210	LEU	CG-CD2	-7.98	1.22	1.51
3	7	210	LEU	CG-CD2	-7.98	1.22	1.51
3	U	376	TRP	CD2-CE3	-7.98	1.28	1.40
3	C	210	LEU	CG-CD2	-7.98	1.22	1.51
3	F	445	PHE	CG-CD1	-7.97	1.26	1.38
3	O	445	PHE	CG-CD1	-7.97	1.26	1.38
3	Y	210	LEU	CG-CD2	-7.97	1.22	1.51
3	1	210	LEU	CG-CD2	-7.97	1.22	1.51
3	O	210	LEU	CG-CD2	-7.97	1.22	1.51
3	V	210	LEU	CG-CD2	-7.97	1.22	1.51
3	V	78	VAL	CB-CG2	-7.97	1.36	1.52
2	N	105	PHE	CB-CG	-7.97	1.37	1.51
3	U	78	VAL	CB-CG2	-7.96	1.36	1.52
1	D	14	TYR	CG-CD2	-7.96	1.28	1.39
1	G	14	TYR	CG-CD2	-7.96	1.28	1.39
1	8	14	TYR	CG-CD2	-7.96	1.28	1.39
3	L	376	TRP	CD2-CE3	-7.96	1.28	1.40
2	K	105	PHE	CB-CG	-7.96	1.37	1.51
3	L	210	LEU	CG-CD2	-7.96	1.22	1.51
3	R	201	LYS	CB-CG	-7.96	1.31	1.52
3	Y	376	TRP	CD2-CE3	-7.96	1.28	1.40
3	4	466	PRO	C-O	-7.95	1.07	1.23
3	O	78	VAL	CB-CG2	-7.95	1.36	1.52
3	C	78	VAL	CB-CG2	-7.95	1.36	1.52
3	I	466	PRO	C-O	-7.95	1.07	1.23
3	L	466	PRO	C-O	-7.95	1.07	1.23
3	R	78	VAL	CB-CG2	-7.95	1.36	1.52
1	A	14	TYR	CG-CD2	-7.94	1.28	1.39
3	7	376	TRP	CD2-CE3	-7.94	1.28	1.40
3	7	466	PRO	C-O	-7.94	1.07	1.23
1	J	14	TYR	CG-CD2	-7.94	1.28	1.39
3	7	78	VAL	CB-CG2	-7.94	1.36	1.52
3	C	466	PRO	C-O	-7.94	1.07	1.23
3	I	78	VAL	CB-CG2	-7.94	1.36	1.52
1	W	14	TYR	CG-CD2	-7.94	1.28	1.39
3	L	78	VAL	CB-CG2	-7.93	1.36	1.52
3	O	466	PRO	C-O	-7.93	1.07	1.23
3	Y	201	LYS	CB-CG	-7.93	1.31	1.52
1	Z	14	TYR	CG-CD2	-7.93	1.28	1.39
1	5	14	TYR	CG-CD2	-7.93	1.28	1.39
3	1	466	PRO	C-O	-7.93	1.07	1.23
3	F	201	LYS	CB-CG	-7.93	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	14	TYR	CG-CD2	-7.93	1.28	1.39
3	U	201	LYS	CB-CG	-7.93	1.31	1.52
3	7	201	LYS	CB-CG	-7.93	1.31	1.52
3	7	342	VAL	CB-CG1	-7.93	1.36	1.52
3	C	201	LYS	CB-CG	-7.92	1.31	1.52
1	J	86	PHE	CE1-CZ	-7.92	1.22	1.37
3	4	149	TYR	CG-CD1	-7.92	1.28	1.39
3	V	466	PRO	C-O	-7.92	1.07	1.23
3	I	376	TRP	CD2-CE3	-7.92	1.28	1.40
1	M	14	TYR	CG-CD2	-7.92	1.28	1.39
1	P	86	PHE	CE1-CZ	-7.92	1.22	1.37
3	V	201	LYS	CB-CG	-7.92	1.31	1.52
3	1	201	LYS	CB-CG	-7.92	1.31	1.52
3	O	342	VAL	CB-CG1	-7.92	1.36	1.52
3	1	78	VAL	CB-CG2	-7.92	1.36	1.52
3	L	342	VAL	CB-CG1	-7.92	1.36	1.52
3	Y	78	VAL	CB-CG2	-7.92	1.36	1.52
3	O	201	LYS	CB-CG	-7.92	1.31	1.52
3	Y	342	VAL	CB-CG1	-7.92	1.36	1.52
3	4	376	TRP	CD2-CE3	-7.92	1.28	1.40
3	L	149	TYR	CG-CD1	-7.91	1.28	1.39
3	I	201	LYS	CB-CG	-7.91	1.31	1.52
1	2	86	PHE	CE1-CZ	-7.91	1.22	1.37
3	F	466	PRO	C-O	-7.91	1.07	1.23
3	R	466	PRO	C-O	-7.91	1.07	1.23
3	U	466	PRO	C-O	-7.91	1.07	1.23
1	M	86	PHE	CE1-CZ	-7.91	1.22	1.37
1	P	14	TYR	CG-CD2	-7.91	1.28	1.39
1	8	86	PHE	CE1-CZ	-7.91	1.22	1.37
3	4	342	VAL	CB-CG1	-7.90	1.36	1.52
1	5	86	PHE	CE1-CZ	-7.90	1.22	1.37
3	F	78	VAL	CB-CG2	-7.90	1.36	1.52
3	I	342	VAL	CB-CG1	-7.90	1.36	1.52
3	L	201	LYS	CB-CG	-7.90	1.31	1.52
3	4	201	LYS	CB-CG	-7.90	1.31	1.52
1	A	86	PHE	CE1-CZ	-7.89	1.22	1.37
3	R	342	VAL	CB-CG1	-7.89	1.36	1.52
3	Y	149	TYR	CG-CD1	-7.89	1.28	1.39
3	C	342	VAL	CB-CG1	-7.89	1.36	1.52
1	G	86	PHE	CE1-CZ	-7.89	1.22	1.37
3	Y	569	TYR	CE1-CZ	-7.89	1.28	1.38
1	D	86	PHE	CE1-CZ	-7.89	1.22	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	342	VAL	CB-CG1	-7.89	1.36	1.52
3	V	342	VAL	CB-CG1	-7.89	1.36	1.52
3	R	201	LYS	C-N	-7.88	1.18	1.33
3	U	149	TYR	CG-CD1	-7.88	1.28	1.39
1	S	14	TYR	CG-CD2	-7.88	1.28	1.39
1	S	86	PHE	CE1-CZ	-7.88	1.22	1.37
3	4	201	LYS	C-N	-7.88	1.18	1.33
1	Z	54	GLU	CB-CG	-7.88	1.37	1.52
1	Z	86	PHE	CE1-CZ	-7.88	1.22	1.37
3	1	201	LYS	C-N	-7.88	1.18	1.33
3	1	342	VAL	CB-CG1	-7.88	1.36	1.52
3	C	149	TYR	CG-CD1	-7.88	1.28	1.39
3	I	201	LYS	C-N	-7.88	1.18	1.33
1	J	54	GLU	CB-CG	-7.88	1.37	1.52
3	U	342	VAL	CB-CG1	-7.87	1.36	1.52
2	E	85	PHE	CG-CD2	-7.87	1.26	1.38
3	R	149	TYR	CG-CD1	-7.87	1.28	1.39
3	I	149	TYR	CG-CD1	-7.87	1.28	1.39
1	8	54	GLU	CB-CG	-7.87	1.37	1.52
2	T	145	ARG	C-N	7.86	1.49	1.34
2	Q	145	ARG	C-N	7.86	1.49	1.34
1	W	86	PHE	CE1-CZ	-7.86	1.22	1.37
3	C	201	LYS	C-N	-7.86	1.19	1.33
3	F	201	LYS	C-N	-7.86	1.19	1.33
3	Y	201	LYS	C-N	-7.86	1.19	1.33
2	K	145	ARG	C-N	7.86	1.49	1.34
3	V	149	TYR	CG-CD1	-7.86	1.28	1.39
3	1	149	TYR	CG-CD1	-7.86	1.28	1.39
3	U	201	LYS	C-N	-7.86	1.19	1.33
3	F	149	TYR	CG-CD1	-7.85	1.28	1.39
3	1	478	TYR	CE2-CZ	-7.85	1.28	1.38
3	F	569	TYR	CE1-CZ	-7.85	1.28	1.38
3	O	201	LYS	C-N	-7.85	1.19	1.33
3	7	569	TYR	CE1-CZ	-7.85	1.28	1.38
3	V	201	LYS	C-N	-7.85	1.19	1.33
3	F	108	MET	CB-CG	-7.85	1.26	1.51
3	L	201	LYS	C-N	-7.85	1.19	1.33
2	3	52	ASN	C-N	-7.85	1.16	1.34
3	7	149	TYR	CG-CD1	-7.85	1.28	1.39
3	L	108	MET	CB-CG	-7.85	1.26	1.51
2	N	52	ASN	C-N	-7.84	1.16	1.34
3	R	108	MET	CB-CG	-7.84	1.26	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	145	ARG	C-N	7.84	1.49	1.34
1	A	54	GLU	CB-CG	-7.84	1.37	1.52
2	N	145	ARG	C-N	7.84	1.49	1.34
3	O	569	TYR	CE1-CZ	-7.84	1.28	1.38
3	R	478	TYR	CE2-CZ	-7.84	1.28	1.38
3	V	108	MET	CB-CG	-7.84	1.26	1.51
1	W	54	GLU	CB-CG	-7.84	1.37	1.52
3	Y	478	TYR	CE2-CZ	-7.84	1.28	1.38
1	2	54	GLU	CB-CG	-7.84	1.37	1.52
1	G	54	GLU	CB-CG	-7.84	1.37	1.52
3	7	108	MET	CB-CG	-7.84	1.26	1.51
3	Y	108	MET	CB-CG	-7.84	1.26	1.51
3	C	108	MET	CB-CG	-7.84	1.26	1.51
2	T	52	ASN	C-N	-7.84	1.16	1.34
3	1	452	VAL	CB-CG1	-7.84	1.36	1.52
3	4	452	VAL	CB-CG1	-7.84	1.36	1.52
3	U	452	VAL	CB-CG1	-7.84	1.36	1.52
3	O	149	TYR	CG-CD1	-7.83	1.28	1.39
1	P	54	GLU	CB-CG	-7.83	1.37	1.52
3	Y	363	SER	CB-OG	-7.83	1.32	1.42
2	6	145	ARG	C-N	7.83	1.49	1.34
3	C	569	TYR	CE1-CZ	-7.83	1.28	1.38
2	H	145	ARG	C-N	7.83	1.49	1.34
3	4	108	MET	CB-CG	-7.83	1.26	1.51
3	7	201	LYS	C-N	-7.83	1.19	1.33
3	7	478	TYR	CE2-CZ	-7.83	1.28	1.38
3	7	452	VAL	CB-CG1	-7.83	1.36	1.52
2	B	145	ARG	C-N	7.83	1.49	1.34
3	1	569	TYR	CE1-CZ	-7.83	1.28	1.38
1	S	54	GLU	CB-CG	-7.83	1.37	1.52
3	F	478	TYR	CE2-CZ	-7.83	1.28	1.38
3	I	452	VAL	CB-CG1	-7.83	1.36	1.52
3	R	569	TYR	CE1-CZ	-7.83	1.28	1.38
3	1	108	MET	CB-CG	-7.83	1.26	1.51
2	3	85	PHE	CG-CD2	-7.83	1.27	1.38
3	4	569	TYR	CE1-CZ	-7.83	1.28	1.38
2	Q	85	PHE	CG-CD2	-7.82	1.27	1.38
2	X	85	PHE	CG-CD2	-7.82	1.27	1.38
3	O	108	MET	CB-CG	-7.82	1.26	1.51
1	D	54	GLU	CB-CG	-7.82	1.37	1.52
2	E	145	ARG	C-N	7.82	1.49	1.34
3	F	452	VAL	CB-CG1	-7.82	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	54	GLU	CB-CG	-7.82	1.37	1.52
2	6	85	PHE	CG-CD2	-7.82	1.27	1.38
3	C	478	TYR	CE2-CZ	-7.82	1.28	1.38
3	I	569	TYR	CE1-CZ	-7.82	1.28	1.38
3	V	452	VAL	CB-CG1	-7.82	1.36	1.52
3	Y	153	SER	CB-OG	-7.82	1.32	1.42
2	9	145	ARG	C-N	7.82	1.49	1.34
3	C	452	VAL	CB-CG1	-7.82	1.36	1.52
3	L	569	TYR	CE1-CZ	-7.82	1.28	1.38
3	V	569	TYR	CE1-CZ	-7.82	1.28	1.38
3	U	108	MET	CB-CG	-7.82	1.26	1.51
3	V	363	SER	CB-OG	-7.81	1.32	1.42
2	B	52	ASN	C-N	-7.81	1.16	1.34
3	I	108	MET	CB-CG	-7.81	1.26	1.51
3	U	363	SER	CB-OG	-7.81	1.32	1.42
3	Y	452	VAL	CB-CG1	-7.81	1.36	1.52
2	K	52	ASN	C-N	-7.81	1.16	1.34
3	L	452	VAL	CB-CG1	-7.81	1.36	1.52
2	6	52	ASN	C-N	-7.81	1.16	1.34
2	H	117	PRO	CG-CD	-7.81	1.24	1.50
3	I	478	TYR	CE2-CZ	-7.81	1.28	1.38
3	R	452	VAL	CB-CG1	-7.81	1.36	1.52
2	X	145	ARG	C-N	7.81	1.49	1.34
3	4	363	SER	CB-OG	-7.81	1.32	1.42
2	E	52	ASN	C-N	-7.80	1.16	1.34
2	N	85	PHE	CG-CD2	-7.80	1.27	1.38
3	O	452	VAL	CB-CG1	-7.80	1.36	1.52
2	0	52	ASN	C-N	-7.80	1.16	1.34
1	M	54	GLU	CB-CG	-7.80	1.37	1.52
2	B	85	PHE	CG-CD2	-7.80	1.27	1.38
2	3	145	ARG	C-N	7.80	1.49	1.34
2	Q	52	ASN	C-N	-7.80	1.16	1.34
2	9	52	ASN	C-N	-7.79	1.16	1.34
3	L	478	TYR	CE2-CZ	-7.79	1.28	1.38
3	R	363	SER	CB-OG	-7.79	1.32	1.42
3	O	478	TYR	CE2-CZ	-7.79	1.28	1.38
3	7	363	SER	CB-OG	-7.79	1.32	1.42
2	E	117	PRO	CG-CD	-7.79	1.25	1.50
3	C	363	SER	CB-OG	-7.79	1.32	1.42
2	H	52	ASN	C-N	-7.79	1.16	1.34
2	H	85	PHE	CG-CD2	-7.79	1.27	1.38
2	K	85	PHE	CG-CD2	-7.79	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	117	PRO	CG-CD	-7.79	1.25	1.50
2	T	117	PRO	CG-CD	-7.79	1.25	1.50
2	9	117	PRO	CG-CD	-7.79	1.25	1.50
2	X	52	ASN	C-N	-7.78	1.16	1.34
3	V	309	TYR	CD2-CE2	-7.78	1.27	1.39
3	V	478	TYR	CE2-CZ	-7.78	1.28	1.38
3	4	478	TYR	CE2-CZ	-7.78	1.28	1.38
3	O	363	SER	CB-OG	-7.78	1.32	1.42
3	V	294	SER	C-N	-7.78	1.16	1.34
2	0	117	PRO	CG-CD	-7.78	1.25	1.50
2	B	117	PRO	CG-CD	-7.78	1.25	1.50
3	I	294	SER	C-N	-7.78	1.16	1.34
3	O	294	SER	C-N	-7.78	1.16	1.34
3	Y	294	SER	C-N	-7.78	1.16	1.34
3	L	363	SER	CB-OG	-7.77	1.32	1.42
3	R	294	SER	C-N	-7.77	1.16	1.34
3	1	153	SER	CB-OG	-7.77	1.32	1.42
3	1	294	SER	C-N	-7.77	1.16	1.34
2	9	85	PHE	CG-CD2	-7.77	1.27	1.38
3	U	309	TYR	CD2-CE2	-7.77	1.27	1.39
3	U	478	TYR	CE2-CZ	-7.77	1.28	1.38
2	0	85	PHE	CG-CD2	-7.77	1.27	1.38
3	1	309	TYR	CD2-CE2	-7.77	1.27	1.39
3	7	294	SER	C-N	-7.77	1.16	1.34
2	Q	117	PRO	CG-CD	-7.76	1.25	1.50
3	1	156	VAL	CB-CG1	-7.76	1.36	1.52
2	3	117	PRO	CG-CD	-7.76	1.25	1.50
2	6	117	PRO	CG-CD	-7.76	1.25	1.50
3	U	569	TYR	CE1-CZ	-7.76	1.28	1.38
3	I	153	SER	CB-OG	-7.76	1.32	1.42
3	L	309	TYR	CD2-CE2	-7.76	1.27	1.39
3	I	309	TYR	CD2-CE2	-7.76	1.27	1.39
3	C	294	SER	C-N	-7.76	1.16	1.34
2	T	85	PHE	CG-CD2	-7.76	1.27	1.38
3	L	156	VAL	CB-CG1	-7.75	1.36	1.52
3	U	153	SER	CB-OG	-7.75	1.32	1.42
3	C	309	TYR	CD2-CE2	-7.75	1.27	1.39
3	F	294	SER	C-N	-7.75	1.16	1.34
2	X	117	PRO	CG-CD	-7.75	1.25	1.50
3	4	294	SER	C-N	-7.75	1.16	1.34
3	F	13	PHE	CE1-CZ	-7.75	1.22	1.37
3	V	13	PHE	CE1-CZ	-7.75	1.22	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	153	SER	CB-OG	-7.75	1.32	1.42
3	R	309	TYR	CD2-CE2	-7.75	1.27	1.39
3	U	294	SER	C-N	-7.75	1.16	1.34
3	C	153	SER	CB-OG	-7.75	1.32	1.42
3	1	13	PHE	CE1-CZ	-7.75	1.22	1.37
3	7	309	TYR	CD2-CE2	-7.75	1.27	1.39
3	1	363	SER	CB-OG	-7.75	1.32	1.42
2	K	117	PRO	CG-CD	-7.74	1.25	1.50
3	7	153	SER	CB-OG	-7.74	1.32	1.42
3	F	363	SER	CB-OG	-7.74	1.32	1.42
3	I	363	SER	CB-OG	-7.74	1.32	1.42
3	C	156	VAL	CB-CG1	-7.74	1.36	1.52
3	L	294	SER	C-N	-7.74	1.16	1.34
3	V	156	VAL	CB-CG1	-7.74	1.36	1.52
3	Y	156	VAL	CB-CG1	-7.74	1.36	1.52
3	1	570	PHE	CD2-CE2	-7.74	1.23	1.39
3	4	570	PHE	CD2-CE2	-7.74	1.23	1.39
3	L	153	SER	CB-OG	-7.74	1.32	1.42
3	O	570	PHE	CD2-CE2	-7.73	1.23	1.39
3	V	153	SER	CB-OG	-7.73	1.32	1.42
3	F	156	VAL	CB-CG1	-7.73	1.36	1.52
3	7	156	VAL	CB-CG1	-7.73	1.36	1.52
3	I	13	PHE	CE1-CZ	-7.73	1.22	1.37
3	O	156	VAL	CB-CG1	-7.73	1.36	1.52
3	4	13	PHE	CE1-CZ	-7.73	1.22	1.37
3	4	156	VAL	CB-CG1	-7.73	1.36	1.52
3	F	153	SER	CB-OG	-7.73	1.32	1.42
3	7	570	PHE	CD2-CE2	-7.73	1.23	1.39
3	U	13	PHE	CE1-CZ	-7.72	1.22	1.37
3	C	13	PHE	CE1-CZ	-7.72	1.22	1.37
3	F	309	TYR	CD2-CE2	-7.72	1.27	1.39
3	R	156	VAL	CB-CG1	-7.72	1.36	1.52
3	Y	13	PHE	CE1-CZ	-7.72	1.22	1.37
3	O	153	SER	CB-OG	-7.72	1.32	1.42
3	L	570	PHE	CD2-CE2	-7.72	1.23	1.39
3	R	13	PHE	CE1-CZ	-7.72	1.22	1.37
3	4	309	TYR	CD2-CE2	-7.72	1.27	1.39
3	F	570	PHE	CD2-CE2	-7.71	1.23	1.39
3	O	309	TYR	CD2-CE2	-7.71	1.27	1.39
3	Y	309	TYR	CD2-CE2	-7.71	1.27	1.39
3	I	156	VAL	CB-CG1	-7.71	1.36	1.52
3	7	13	PHE	CE1-CZ	-7.71	1.22	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	570	PHE	CD2-CE2	-7.71	1.23	1.39
3	R	153	SER	CB-OG	-7.71	1.32	1.42
3	Y	376	TRP	CD2-CE2	-7.71	1.32	1.41
3	L	376	TRP	CD2-CE2	-7.71	1.32	1.41
3	O	13	PHE	CE1-CZ	-7.71	1.22	1.37
3	Y	160	PHE	CD1-CE1	-7.71	1.23	1.39
3	Y	570	PHE	CD2-CE2	-7.70	1.23	1.39
3	U	156	VAL	CB-CG1	-7.70	1.36	1.52
1	J	17[A]	SER	CB-OG	-7.70	1.32	1.42
1	J	17[B]	SER	CB-OG	-7.70	1.32	1.42
3	Y	476	VAL	CB-CG1	-7.70	1.36	1.52
3	V	476	VAL	CB-CG1	-7.70	1.36	1.52
3	V	570	PHE	CD2-CE2	-7.69	1.23	1.39
3	I	570	PHE	CD2-CE2	-7.69	1.23	1.39
3	I	160	PHE	CD1-CE1	-7.69	1.23	1.39
3	R	570	PHE	CD2-CE2	-7.69	1.23	1.39
3	1	460	TRP	CE2-CZ2	-7.69	1.26	1.39
3	L	13	PHE	CE1-CZ	-7.69	1.22	1.37
3	U	476	VAL	CB-CG1	-7.69	1.36	1.52
3	7	376	TRP	CD2-CE2	-7.69	1.32	1.41
3	U	570	PHE	CD2-CE2	-7.68	1.23	1.39
3	O	160	PHE	CD1-CE1	-7.68	1.23	1.39
3	V	160	PHE	CD1-CE1	-7.68	1.23	1.39
3	R	160	PHE	CD1-CE1	-7.68	1.23	1.39
3	C	376	TRP	CD2-CE2	-7.68	1.32	1.41
1	Z	17[A]	SER	CB-OG	-7.68	1.32	1.42
1	Z	17[B]	SER	CB-OG	-7.68	1.32	1.42
3	4	460	TRP	CE2-CZ2	-7.67	1.26	1.39
3	U	460	TRP	CE2-CZ2	-7.67	1.26	1.39
3	1	160	PHE	CD1-CE1	-7.67	1.24	1.39
3	4	376	TRP	CD2-CE2	-7.67	1.32	1.41
3	Y	460	TRP	CE2-CZ2	-7.67	1.26	1.39
3	F	376	TRP	CD2-CE2	-7.67	1.32	1.41
3	O	376	TRP	CD2-CE2	-7.67	1.32	1.41
3	C	160	PHE	CD1-CE1	-7.66	1.24	1.39
3	I	476	VAL	CB-CG1	-7.66	1.36	1.52
3	O	13	PHE	CD1-CE1	-7.66	1.24	1.39
3	7	160	PHE	CD1-CE1	-7.66	1.24	1.39
1	A	17[A]	SER	CB-OG	-7.66	1.32	1.42
1	A	17[B]	SER	CB-OG	-7.66	1.32	1.42
3	I	376	TRP	CD2-CE2	-7.66	1.32	1.41
3	V	376	TRP	CD2-CE2	-7.66	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	476	VAL	CB-CG1	-7.66	1.36	1.52
1	8	17[A]	SER	CB-OG	-7.66	1.32	1.42
1	8	17[B]	SER	CB-OG	-7.66	1.32	1.42
3	F	13	PHE	CD1-CE1	-7.66	1.24	1.39
3	F	476	VAL	CB-CG1	-7.66	1.36	1.52
3	1	13	PHE	CD1-CE1	-7.66	1.24	1.39
3	4	160	PHE	CD1-CE1	-7.66	1.24	1.39
2	T	49	PHE	CD1-CE1	-7.65	1.24	1.39
3	1	476	VAL	CB-CG1	-7.65	1.36	1.52
3	C	460	TRP	CE2-CZ2	-7.65	1.26	1.39
1	D	17[A]	SER	CB-OG	-7.65	1.32	1.42
1	D	17[B]	SER	CB-OG	-7.65	1.32	1.42
3	F	160	PHE	CD1-CE1	-7.65	1.24	1.39
3	1	453	ILE	CB-CG2	-7.65	1.29	1.52
3	I	460	TRP	CE2-CZ2	-7.65	1.26	1.39
3	L	460	TRP	CE2-CZ2	-7.65	1.26	1.39
3	O	460	TRP	CE2-CZ2	-7.65	1.26	1.39
1	P	17[A]	SER	CB-OG	-7.65	1.32	1.42
1	P	17[B]	SER	CB-OG	-7.65	1.32	1.42
3	U	160	PHE	CD1-CE1	-7.65	1.24	1.39
1	M	17[A]	SER	CB-OG	-7.65	1.32	1.42
1	M	17[B]	SER	CB-OG	-7.65	1.32	1.42
3	4	13	PHE	CD1-CE1	-7.65	1.24	1.39
3	L	13	PHE	CD1-CE1	-7.64	1.24	1.39
3	7	13	PHE	CD1-CE1	-7.64	1.24	1.39
3	U	453	ILE	CB-CG2	-7.64	1.29	1.52
3	O	476	VAL	CB-CG1	-7.64	1.36	1.52
3	I	13	PHE	CD1-CE1	-7.64	1.24	1.39
3	L	160	PHE	CD1-CE1	-7.64	1.24	1.39
3	R	460	TRP	CE2-CZ2	-7.64	1.26	1.39
1	S	17[A]	SER	CB-OG	-7.64	1.32	1.42
1	S	17[B]	SER	CB-OG	-7.64	1.32	1.42
3	4	476	VAL	CB-CG1	-7.64	1.36	1.52
3	7	159	PHE	CD1-CE1	-7.64	1.24	1.39
3	7	476	VAL	CB-CG1	-7.64	1.36	1.52
3	U	376	TRP	CD2-CE2	-7.64	1.32	1.41
2	Q	49	PHE	CD1-CE1	-7.64	1.24	1.39
3	C	13	PHE	CD1-CE1	-7.64	1.24	1.39
3	V	460	TRP	CE2-CZ2	-7.64	1.26	1.39
3	7	460	TRP	CE2-CZ2	-7.64	1.26	1.39
3	F	453	ILE	CB-CG2	-7.63	1.29	1.52
3	L	212	GLU	CG-CD	7.63	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	17[A]	SER	CB-OG	-7.63	1.32	1.42
1	W	17[B]	SER	CB-OG	-7.63	1.32	1.42
3	R	13	PHE	CD1-CE1	-7.63	1.24	1.39
3	R	212	GLU	CG-CD	7.63	1.63	1.51
3	F	460	TRP	CE2-CZ2	-7.63	1.26	1.39
3	I	453	ILE	CB-CG2	-7.63	1.29	1.52
3	R	476	VAL	CB-CG1	-7.63	1.36	1.52
3	V	453	ILE	CB-CG2	-7.63	1.29	1.52
3	L	476	VAL	CB-CG1	-7.62	1.36	1.52
3	1	376	TRP	CD2-CE2	-7.62	1.32	1.41
3	U	159	PHE	CD1-CE1	-7.62	1.24	1.39
3	Y	13	PHE	CD1-CE1	-7.62	1.24	1.39
3	Y	453	ILE	CB-CG2	-7.62	1.29	1.52
3	C	453	ILE	CB-CG2	-7.62	1.29	1.52
2	E	49	PHE	CD1-CE1	-7.62	1.24	1.39
3	R	376	TRP	CD2-CE2	-7.62	1.32	1.41
3	4	159	PHE	CD1-CE1	-7.62	1.24	1.39
2	B	49	PHE	CD1-CE1	-7.62	1.24	1.39
3	F	159	PHE	CD1-CE1	-7.62	1.24	1.39
3	O	159	PHE	CD1-CE1	-7.62	1.24	1.39
3	Y	212	GLU	CG-CD	7.62	1.63	1.51
1	2	17[A]	SER	CB-OG	-7.62	1.32	1.42
1	2	17[B]	SER	CB-OG	-7.62	1.32	1.42
2	N	49	PHE	CD1-CE1	-7.61	1.24	1.39
2	3	49	PHE	CD1-CE1	-7.61	1.24	1.39
3	U	13	PHE	CD1-CE1	-7.61	1.24	1.39
1	G	17[A]	SER	CB-OG	-7.61	1.32	1.42
1	G	17[B]	SER	CB-OG	-7.61	1.32	1.42
2	H	49	PHE	CD1-CE1	-7.61	1.24	1.39
3	L	453	ILE	CB-CG2	-7.61	1.29	1.52
2	6	49	PHE	CD1-CE1	-7.61	1.24	1.39
3	7	212	GLU	CG-CD	7.61	1.63	1.51
2	9	49	PHE	CD1-CE1	-7.61	1.24	1.39
3	C	159	PHE	CD1-CE1	-7.61	1.24	1.39
3	I	159	PHE	CD1-CE1	-7.61	1.24	1.39
2	K	49	PHE	CD1-CE1	-7.61	1.24	1.39
3	R	453	ILE	CB-CG2	-7.61	1.29	1.52
3	1	212	GLU	CG-CD	7.61	1.63	1.51
2	X	49	PHE	CD1-CE1	-7.61	1.24	1.39
3	O	453	ILE	CB-CG2	-7.60	1.29	1.52
3	Y	159	PHE	CD1-CE1	-7.60	1.24	1.39
3	4	453	ILE	CB-CG2	-7.60	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7	453	ILE	CB-CG2	-7.60	1.29	1.52
3	V	212	GLU	CG-CD	7.60	1.63	1.51
3	4	212	GLU	CG-CD	7.60	1.63	1.51
2	0	49	PHE	CD1-CE1	-7.59	1.24	1.39
3	V	13	PHE	CD1-CE1	-7.59	1.24	1.39
2	3	140	VAL	CB-CG1	-7.59	1.36	1.52
3	L	159	PHE	CD1-CE1	-7.59	1.24	1.39
3	O	212	GLU	CG-CD	7.59	1.63	1.51
3	I	218	VAL	C-O	-7.58	1.08	1.23
2	Q	140	VAL	CB-CG1	-7.58	1.36	1.52
3	V	159	PHE	CD1-CE1	-7.58	1.24	1.39
1	5	17[A]	SER	CB-OG	-7.58	1.32	1.42
1	5	17[B]	SER	CB-OG	-7.58	1.32	1.42
3	1	159	PHE	CD1-CE1	-7.57	1.24	1.39
2	0	140	VAL	CB-CG1	-7.57	1.36	1.52
3	R	218	VAL	C-O	-7.56	1.08	1.23
3	7	218	VAL	C-O	-7.56	1.08	1.23
3	F	212	GLU	CG-CD	7.56	1.63	1.51
3	R	159	PHE	CD1-CE1	-7.56	1.24	1.39
3	U	212	GLU	CG-CD	7.56	1.63	1.51
3	F	218	VAL	C-O	-7.55	1.08	1.23
2	T	140	VAL	CB-CG1	-7.55	1.36	1.52
2	K	140	VAL	CB-CG1	-7.55	1.36	1.52
2	B	140	VAL	CB-CG1	-7.55	1.36	1.52
2	X	140	VAL	CB-CG1	-7.55	1.36	1.52
3	U	218	VAL	C-O	-7.55	1.09	1.23
2	H	140	VAL	CB-CG1	-7.55	1.36	1.52
2	N	140	VAL	CB-CG1	-7.55	1.37	1.52
3	I	212	GLU	CG-CD	7.55	1.63	1.51
3	Y	218	VAL	C-O	-7.55	1.09	1.23
3	1	218	VAL	C-O	-7.55	1.09	1.23
3	4	218	VAL	C-O	-7.55	1.09	1.23
2	9	140	VAL	CB-CG1	-7.54	1.37	1.52
3	L	218	VAL	C-O	-7.54	1.09	1.23
3	C	218	VAL	C-O	-7.54	1.09	1.23
3	V	218	VAL	C-O	-7.54	1.09	1.23
2	6	140	VAL	CB-CG1	-7.54	1.37	1.52
2	E	140	VAL	CB-CG1	-7.54	1.37	1.52
3	V	67	VAL	CB-CG1	-7.53	1.37	1.52
3	L	430	GLU	CG-CD	7.52	1.63	1.51
3	I	362	PHE	CB-CG	-7.52	1.38	1.51
3	O	218	VAL	C-O	-7.52	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	105	PHE	CD2-CE2	-7.51	1.24	1.39
3	R	67	VAL	CB-CG1	-7.51	1.37	1.52
2	K	105	PHE	CD2-CE2	-7.51	1.24	1.39
3	U	67	VAL	CB-CG1	-7.51	1.37	1.52
3	V	430	GLU	CG-CD	7.51	1.63	1.51
3	V	516	VAL	CB-CG1	-7.51	1.37	1.52
2	3	105	PHE	CD2-CE2	-7.51	1.24	1.39
3	F	430	GLU	CG-CD	7.50	1.63	1.51
3	7	516	VAL	CB-CG1	-7.50	1.37	1.52
2	X	105	PHE	CD2-CE2	-7.50	1.24	1.39
2	H	105	PHE	CD2-CE2	-7.50	1.24	1.39
3	7	430	GLU	CG-CD	7.50	1.63	1.51
3	U	362	PHE	CB-CG	-7.50	1.38	1.51
3	F	67	VAL	CB-CG1	-7.50	1.37	1.52
3	I	67	VAL	CB-CG1	-7.50	1.37	1.52
2	N	105	PHE	CD2-CE2	-7.50	1.24	1.39
2	T	105	PHE	CD2-CE2	-7.50	1.24	1.39
3	7	67	VAL	CB-CG1	-7.50	1.37	1.52
3	7	362	PHE	CB-CG	-7.50	1.38	1.51
3	U	516	VAL	CB-CG1	-7.50	1.37	1.52
3	C	67	VAL	CB-CG1	-7.49	1.37	1.52
3	F	516	VAL	CB-CG1	-7.49	1.37	1.52
2	6	105	PHE	CD2-CE2	-7.49	1.24	1.39
3	O	430	GLU	CG-CD	7.49	1.63	1.51
3	4	67	VAL	CB-CG1	-7.49	1.37	1.52
3	C	430	GLU	CG-CD	7.49	1.63	1.51
3	R	430	GLU	CG-CD	7.49	1.63	1.51
3	V	362	PHE	CB-CG	-7.49	1.38	1.51
3	1	430	GLU	CG-CD	7.49	1.63	1.51
2	E	105	PHE	CD2-CE2	-7.49	1.24	1.39
3	O	67	VAL	CB-CG1	-7.48	1.37	1.52
3	L	362	PHE	CB-CG	-7.48	1.38	1.51
3	O	362	PHE	CB-CG	-7.48	1.38	1.51
3	R	362	PHE	CB-CG	-7.48	1.38	1.51
3	R	496	PHE	CG-CD1	-7.47	1.27	1.38
3	1	67	VAL	CB-CG1	-7.47	1.37	1.52
3	1	362	PHE	CB-CG	-7.47	1.38	1.51
3	C	516	VAL	CB-CG1	-7.47	1.37	1.52
2	H	112	GLU	CB-CG	-7.47	1.38	1.52
3	Y	67	VAL	CB-CG1	-7.47	1.37	1.52
2	0	105	PHE	CD2-CE2	-7.47	1.24	1.39
2	3	112	GLU	CB-CG	-7.47	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	430	GLU	CG-CD	7.47	1.63	1.51
1	P	65	THR	CB-CG2	-7.47	1.27	1.52
3	Y	516	VAL	CB-CG1	-7.47	1.37	1.52
3	F	362	PHE	CB-CG	-7.47	1.38	1.51
1	M	65	THR	CB-CG2	-7.47	1.27	1.52
2	9	105	PHE	CD2-CE2	-7.47	1.24	1.39
3	C	362	PHE	CB-CG	-7.47	1.38	1.51
3	O	516	VAL	CB-CG1	-7.47	1.37	1.52
3	4	362	PHE	CB-CG	-7.47	1.38	1.51
3	I	430	GLU	CG-CD	7.46	1.63	1.51
3	I	496	PHE	CG-CD1	-7.46	1.27	1.38
2	Q	105	PHE	CD2-CE2	-7.46	1.24	1.39
1	2	65	THR	CB-CG2	-7.46	1.27	1.52
1	5	65	THR	CB-CG2	-7.46	1.27	1.52
3	I	516	VAL	CB-CG1	-7.46	1.37	1.52
3	L	67	VAL	CB-CG1	-7.46	1.37	1.52
2	T	112	GLU	CB-CG	-7.46	1.38	1.52
3	Y	430	GLU	CG-CD	7.46	1.63	1.51
3	1	516	VAL	CB-CG1	-7.46	1.37	1.52
1	A	65	THR	CB-CG2	-7.46	1.27	1.52
2	E	112	GLU	CB-CG	-7.46	1.38	1.52
1	W	65	THR	CB-CG2	-7.46	1.27	1.52
1	Z	65	THR	CB-CG2	-7.46	1.27	1.52
2	6	112	GLU	CB-CG	-7.46	1.38	1.52
1	8	65	THR	CB-CG2	-7.46	1.27	1.52
3	U	430	GLU	CG-CD	7.46	1.63	1.51
1	D	65	THR	CB-CG2	-7.46	1.27	1.52
3	L	516	VAL	CB-CG1	-7.45	1.37	1.52
3	4	516	VAL	CB-CG1	-7.45	1.37	1.52
1	S	23	ARG	CZ-NH1	-7.45	1.23	1.33
2	B	112	GLU	CB-CG	-7.45	1.38	1.52
2	N	112	GLU	CB-CG	-7.45	1.38	1.52
3	V	496	PHE	CG-CD1	-7.45	1.27	1.38
2	X	112	GLU	CB-CG	-7.45	1.38	1.52
3	Y	362	PHE	CB-CG	-7.45	1.38	1.51
3	I	149	TYR	CE1-CZ	-7.45	1.28	1.38
3	R	516	VAL	CB-CG1	-7.44	1.37	1.52
1	S	65	THR	CB-CG2	-7.44	1.27	1.52
1	G	23	ARG	CZ-NH1	-7.44	1.23	1.33
1	G	65	THR	CB-CG2	-7.44	1.27	1.52
1	W	23	ARG	CZ-NH1	-7.44	1.23	1.33
1	5	23	ARG	CG-CD	-7.44	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	65	THR	CB-CG2	-7.44	1.27	1.52
3	7	496	PHE	CG-CD1	-7.44	1.27	1.38
1	Z	23	ARG	CG-CD	-7.44	1.33	1.51
3	4	496	PHE	CG-CD1	-7.44	1.27	1.38
3	Y	496	PHE	CG-CD1	-7.44	1.27	1.38
1	Z	23	ARG	CZ-NH1	-7.44	1.23	1.33
1	A	23	ARG	CZ-NH1	-7.43	1.23	1.33
1	D	23	ARG	CZ-NH1	-7.43	1.23	1.33
3	R	225	GLU	CB-CG	-7.43	1.38	1.52
1	2	23	ARG	CZ-NH1	-7.43	1.23	1.33
3	F	496	PHE	CG-CD1	-7.43	1.27	1.38
1	P	23	ARG	CG-CD	-7.43	1.33	1.51
3	C	496	PHE	CG-CD1	-7.43	1.27	1.38
1	5	23	ARG	CZ-NH1	-7.43	1.23	1.33
3	7	225	GLU	CB-CG	-7.43	1.38	1.52
1	J	23	ARG	CZ-NH1	-7.42	1.23	1.33
2	Q	112	GLU	CB-CG	-7.42	1.38	1.52
1	8	23	ARG	CG-CD	-7.42	1.33	1.51
1	Z	9	GLU	CD-OE1	-7.42	1.17	1.25
3	1	136	ILE	CB-CG2	-7.42	1.29	1.52
2	K	112	GLU	CB-CG	-7.42	1.38	1.52
3	1	496	PHE	CG-CD1	-7.42	1.27	1.38
3	L	496	PHE	CG-CD1	-7.42	1.27	1.38
2	0	112	GLU	CB-CG	-7.42	1.38	1.52
1	A	23	ARG	CG-CD	-7.41	1.33	1.51
3	F	225	GLU	CB-CG	-7.41	1.38	1.52
1	G	23	ARG	CG-CD	-7.41	1.33	1.51
3	I	225	GLU	CB-CG	-7.41	1.38	1.52
3	L	136	ILE	CB-CG2	-7.41	1.29	1.52
3	Y	136	ILE	CB-CG2	-7.41	1.29	1.52
1	M	23	ARG	CG-CD	-7.41	1.33	1.51
1	2	23	ARG	CG-CD	-7.41	1.33	1.51
3	F	149	TYR	CE1-CZ	-7.41	1.28	1.38
3	O	225	GLU	CB-CG	-7.41	1.38	1.52
3	O	496	PHE	CG-CD1	-7.41	1.27	1.38
3	R	149	TYR	CE1-CZ	-7.41	1.28	1.38
1	S	23	ARG	CG-CD	-7.41	1.33	1.51
3	F	136	ILE	CB-CG2	-7.41	1.29	1.52
3	O	136	ILE	CB-CG2	-7.41	1.29	1.52
3	O	149	TYR	CE1-CZ	-7.41	1.28	1.38
3	1	149	TYR	CE1-CZ	-7.41	1.28	1.38
3	I	136	ILE	CB-CG2	-7.40	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	148	LYS	CG-CD	-7.40	1.27	1.52
3	U	149	TYR	CE1-CZ	-7.40	1.28	1.38
3	V	225	GLU	CB-CG	-7.40	1.38	1.52
3	4	136	ILE	CB-CG2	-7.40	1.29	1.52
2	9	112	GLU	CB-CG	-7.40	1.38	1.52
3	C	136	ILE	CB-CG2	-7.40	1.29	1.52
3	F	194	VAL	CB-CG1	-7.40	1.37	1.52
1	W	23	ARG	CG-CD	-7.40	1.33	1.51
3	4	194	VAL	CB-CG1	-7.39	1.37	1.52
1	J	9	GLU	CD-OE1	-7.39	1.17	1.25
2	3	148	LYS	CG-CD	-7.39	1.27	1.52
3	7	136	ILE	CB-CG2	-7.39	1.29	1.52
2	9	148	LYS	CG-CD	-7.39	1.27	1.52
2	Q	148	LYS	CG-CD	-7.39	1.27	1.52
1	D	23	ARG	CG-CD	-7.39	1.33	1.51
1	J	23	ARG	CG-CD	-7.39	1.33	1.51
3	U	136	ILE	CB-CG2	-7.39	1.29	1.52
2	E	162	SER	CB-OG	-7.39	1.32	1.42
2	H	148	LYS	CG-CD	-7.38	1.27	1.52
1	M	23	ARG	CZ-NH1	-7.38	1.23	1.33
1	P	23	ARG	CZ-NH1	-7.38	1.23	1.33
3	Y	149	TYR	CE1-CZ	-7.38	1.28	1.38
3	7	149	TYR	CE1-CZ	-7.38	1.28	1.38
2	K	148	LYS	CG-CD	-7.38	1.27	1.52
3	4	225	GLU	CB-CG	-7.38	1.38	1.52
1	8	9	GLU	CD-OE1	-7.38	1.17	1.25
3	U	194	VAL	CB-CG1	-7.38	1.37	1.52
2	N	148	LYS	CG-CD	-7.38	1.27	1.52
3	R	136	ILE	CB-CG2	-7.38	1.29	1.52
3	L	194	VAL	CB-CG1	-7.38	1.37	1.52
2	B	148	LYS	CG-CD	-7.38	1.27	1.52
3	C	225	GLU	CB-CG	-7.38	1.38	1.52
3	L	225	GLU	CB-CG	-7.38	1.38	1.52
3	V	194	VAL	CB-CG1	-7.38	1.37	1.52
2	X	148	LYS	CG-CD	-7.38	1.27	1.52
3	V	136	ILE	CB-CG2	-7.38	1.29	1.52
2	0	148	LYS	CG-CD	-7.38	1.27	1.52
3	1	225	GLU	CB-CG	-7.38	1.38	1.52
1	D	9	GLU	CD-OE1	-7.37	1.17	1.25
3	O	570	PHE	CE1-CZ	-7.37	1.23	1.37
1	P	9	GLU	CD-OE1	-7.37	1.17	1.25
1	8	23	ARG	CZ-NH1	-7.37	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	177	PRO	CB-CG	-7.37	1.13	1.50
3	I	194	VAL	CB-CG1	-7.37	1.37	1.52
3	C	149	TYR	CE1-CZ	-7.37	1.28	1.38
2	E	148	LYS	CG-CD	-7.37	1.27	1.52
3	R	523	ARG	CZ-NH2	-7.37	1.23	1.33
3	U	225	GLU	CB-CG	-7.37	1.38	1.52
1	A	9	GLU	CD-OE1	-7.36	1.17	1.25
3	C	194	VAL	CB-CG1	-7.36	1.37	1.52
1	M	9	GLU	CD-OE1	-7.36	1.17	1.25
2	6	148	LYS	CG-CD	-7.36	1.27	1.52
3	7	194	VAL	CB-CG1	-7.36	1.37	1.52
3	R	194	VAL	CB-CG1	-7.36	1.37	1.52
2	0	162	SER	CB-OG	-7.36	1.32	1.42
3	U	496	PHE	CG-CD1	-7.36	1.27	1.38
3	L	177	PRO	CB-CG	-7.36	1.13	1.50
3	V	149	TYR	CE1-CZ	-7.36	1.28	1.38
3	I	177	PRO	CB-CG	-7.35	1.13	1.50
3	O	194	VAL	CB-CG1	-7.35	1.37	1.52
3	Y	225	GLU	CB-CG	-7.35	1.38	1.52
2	6	160	PHE	CE2-CZ	-7.35	1.23	1.37
2	9	160	PHE	CE2-CZ	-7.35	1.23	1.37
2	E	160	PHE	CE2-CZ	-7.35	1.23	1.37
3	1	177	PRO	CB-CG	-7.35	1.13	1.50
1	5	9	GLU	CD-OE1	-7.35	1.17	1.25
3	V	177	PRO	CB-CG	-7.35	1.13	1.50
3	C	177	PRO	CB-CG	-7.35	1.13	1.50
3	Y	177	PRO	CB-CG	-7.35	1.13	1.50
2	0	160	PHE	CE2-CZ	-7.35	1.23	1.37
3	1	194	VAL	CB-CG1	-7.35	1.37	1.52
3	Y	194	VAL	CB-CG1	-7.35	1.37	1.52
3	F	523	ARG	CZ-NH2	-7.34	1.23	1.33
1	S	9	GLU	CD-OE1	-7.34	1.17	1.25
2	3	162	SER	CB-OG	-7.34	1.32	1.42
3	R	177	PRO	CB-CG	-7.34	1.13	1.50
3	4	177	PRO	CB-CG	-7.34	1.13	1.50
3	U	177	PRO	CB-CG	-7.34	1.13	1.50
2	B	162	SER	CB-OG	-7.34	1.32	1.42
2	Q	162	SER	CB-OG	-7.34	1.32	1.42
3	U	22	ARG	CG-CD	-7.34	1.33	1.51
1	D	23	ARG	CZ-NH2	-7.34	1.23	1.33
3	7	177	PRO	CB-CG	-7.34	1.13	1.50
3	U	523	ARG	CZ-NH2	-7.34	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	220	GLY	N-CA	-7.34	1.35	1.46
2	H	162	SER	CB-OG	-7.34	1.32	1.42
1	J	23	ARG	CZ-NH2	-7.34	1.23	1.33
3	L	149	TYR	CE1-CZ	-7.34	1.29	1.38
3	1	220	GLY	N-CA	-7.34	1.35	1.46
3	O	177	PRO	CB-CG	-7.33	1.13	1.50
2	N	162	SER	CB-OG	-7.33	1.32	1.42
2	9	162	SER	CB-OG	-7.33	1.32	1.42
3	4	149	TYR	CE1-CZ	-7.33	1.29	1.38
2	B	160	PHE	CE2-CZ	-7.33	1.23	1.37
2	T	160	PHE	CE2-CZ	-7.33	1.23	1.37
3	7	220	GLY	N-CA	-7.33	1.35	1.46
3	4	22	ARG	CG-CD	-7.33	1.33	1.51
3	4	220	GLY	N-CA	-7.33	1.35	1.46
3	4	570	PHE	CE1-CZ	-7.33	1.23	1.37
3	L	523	ARG	CZ-NH2	-7.32	1.23	1.33
2	X	162	SER	CB-OG	-7.32	1.32	1.42
3	Y	273	ILE	CB-CG2	-7.32	1.30	1.52
3	Y	570	PHE	CE1-CZ	-7.32	1.23	1.37
3	I	22	ARG	CG-CD	-7.32	1.33	1.51
2	K	160	PHE	CE2-CZ	-7.32	1.23	1.37
1	W	23	ARG	CZ-NH2	-7.32	1.23	1.33
2	X	160	PHE	CE2-CZ	-7.32	1.23	1.37
3	1	273	ILE	CB-CG2	-7.32	1.30	1.52
3	L	22	ARG	CG-CD	-7.32	1.33	1.51
1	W	9	GLU	CD-OE1	-7.32	1.17	1.25
2	3	160	PHE	CE2-CZ	-7.32	1.23	1.37
1	5	23	ARG	CZ-NH2	-7.32	1.23	1.33
3	C	570	PHE	CE1-CZ	-7.32	1.23	1.37
3	R	570	PHE	CE1-CZ	-7.32	1.23	1.37
3	V	22	ARG	CG-CD	-7.32	1.33	1.51
3	Y	22	ARG	CG-CD	-7.32	1.33	1.51
3	C	22	ARG	CG-CD	-7.31	1.33	1.51
2	H	160	PHE	CE2-CZ	-7.31	1.23	1.37
3	I	570	PHE	CG-CD2	-7.31	1.27	1.38
3	O	220	GLY	N-CA	-7.31	1.35	1.46
3	V	273	ILE	CB-CG2	-7.31	1.30	1.52
3	7	22	ARG	CG-CD	-7.31	1.33	1.51
3	7	523	ARG	CZ-NH2	-7.31	1.23	1.33
3	7	570	PHE	CE1-CZ	-7.31	1.23	1.37
3	U	220	GLY	N-CA	-7.31	1.35	1.46
3	F	273	ILE	CB-CG2	-7.31	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	523	ARG	CZ-NH2	-7.31	1.23	1.33
3	L	570	PHE	CE1-CZ	-7.31	1.23	1.37
2	6	162	SER	CB-OG	-7.31	1.32	1.42
3	O	22	ARG	CG-CD	-7.31	1.33	1.51
3	C	273	ILE	CB-CG2	-7.31	1.30	1.52
3	I	570	PHE	CE1-CZ	-7.31	1.23	1.37
3	L	273	ILE	CB-CG2	-7.31	1.30	1.52
2	Q	160	PHE	CE2-CZ	-7.31	1.23	1.37
1	S	23	ARG	CZ-NH2	-7.31	1.23	1.33
3	1	523	ARG	CZ-NH2	-7.30	1.23	1.33
3	1	570	PHE	CE1-CZ	-7.30	1.23	1.37
3	U	273	ILE	CB-CG2	-7.30	1.30	1.52
3	R	22	ARG	CG-CD	-7.30	1.33	1.51
3	F	22	ARG	CG-CD	-7.30	1.33	1.51
3	L	570	PHE	CG-CD2	-7.30	1.27	1.38
3	1	22	ARG	CG-CD	-7.30	1.33	1.51
3	7	273	ILE	CB-CG2	-7.30	1.30	1.52
1	8	23	ARG	CZ-NH2	-7.30	1.23	1.33
2	N	160	PHE	CE2-CZ	-7.30	1.23	1.37
3	O	273	ILE	CB-CG2	-7.30	1.30	1.52
3	C	220	GLY	N-CA	-7.30	1.35	1.46
3	O	523	ARG	CZ-NH2	-7.30	1.23	1.33
1	P	23	ARG	CZ-NH2	-7.30	1.23	1.33
3	R	273	ILE	CB-CG2	-7.30	1.30	1.52
3	V	220	GLY	N-CA	-7.30	1.35	1.46
3	Y	570	PHE	CG-CD2	-7.30	1.27	1.38
3	F	570	PHE	CE1-CZ	-7.29	1.23	1.37
3	O	413	THR	CB-CG2	-7.29	1.28	1.52
3	I	220	GLY	N-CA	-7.29	1.35	1.46
2	K	162	SER	CB-OG	-7.29	1.32	1.42
3	L	220	GLY	N-CA	-7.29	1.35	1.46
1	2	9	GLU	CD-OE1	-7.29	1.17	1.25
1	A	23	ARG	CZ-NH2	-7.29	1.23	1.33
1	2	23	ARG	CZ-NH2	-7.29	1.23	1.33
3	U	570	PHE	CG-CD2	-7.29	1.27	1.38
3	4	273	ILE	CB-CG2	-7.29	1.30	1.52
3	U	570	PHE	CE1-CZ	-7.29	1.23	1.37
1	G	9	GLU	CD-OE1	-7.29	1.17	1.25
3	V	523	ARG	CZ-NH2	-7.29	1.23	1.33
3	U	413	THR	CB-CG2	-7.29	1.28	1.52
3	7	413	THR	CB-CG2	-7.28	1.28	1.52
3	Y	413	THR	CB-CG2	-7.28	1.28	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	523	ARG	CZ-NH2	-7.28	1.23	1.33
2	T	162	SER	CB-OG	-7.28	1.32	1.42
3	I	413	THR	CB-CG2	-7.28	1.28	1.52
3	V	570	PHE	CG-CD2	-7.28	1.27	1.38
1	G	23	ARG	CZ-NH2	-7.28	1.23	1.33
3	I	273	ILE	CB-CG2	-7.28	1.30	1.52
3	L	413	THR	CB-CG2	-7.28	1.28	1.52
3	1	413	THR	CB-CG2	-7.28	1.28	1.52
3	Y	220	GLY	N-CA	-7.27	1.35	1.46
3	V	570	PHE	CE1-CZ	-7.27	1.23	1.37
3	F	413	THR	CB-CG2	-7.27	1.28	1.52
3	C	413	THR	CB-CG2	-7.27	1.28	1.52
3	L	77	ILE	CG1-CD1	-7.27	1.00	1.50
3	V	413	THR	CB-CG2	-7.27	1.28	1.52
3	7	502	LEU	CG-CD1	-7.27	1.25	1.51
3	U	458	ILE	CB-CG2	-7.27	1.30	1.52
3	C	570	PHE	CG-CD2	-7.27	1.27	1.38
3	4	570	PHE	CG-CD2	-7.27	1.27	1.38
3	1	77	ILE	CG1-CD1	-7.27	1.00	1.50
3	I	77	ILE	CG1-CD1	-7.26	1.00	1.50
3	R	77	ILE	CG1-CD1	-7.26	1.00	1.50
3	4	413	THR	CB-CG2	-7.26	1.28	1.52
2	K	78	GLU	CB-CG	-7.26	1.38	1.52
3	4	458	ILE	CB-CG2	-7.26	1.30	1.52
3	O	77	ILE	CG1-CD1	-7.26	1.00	1.50
3	4	77	ILE	CG1-CD1	-7.26	1.00	1.50
3	C	77	ILE	CG1-CD1	-7.26	1.00	1.50
3	R	413	THR	CB-CG2	-7.26	1.28	1.52
3	R	570	PHE	CG-CD2	-7.26	1.27	1.38
3	Y	77	ILE	CG1-CD1	-7.26	1.00	1.50
3	7	77	ILE	CG1-CD1	-7.26	1.00	1.50
3	U	77	ILE	CG1-CD1	-7.26	1.00	1.50
3	V	77	ILE	CG1-CD1	-7.26	1.00	1.50
3	1	458	ILE	CB-CG2	-7.26	1.30	1.52
3	F	77	ILE	CG1-CD1	-7.26	1.00	1.50
2	H	91	TYR	CD1-CE1	-7.26	1.28	1.39
1	M	23	ARG	CZ-NH2	-7.26	1.23	1.33
3	O	570	PHE	CG-CD2	-7.25	1.27	1.38
3	F	458	ILE	CB-CG2	-7.25	1.30	1.52
3	L	458	ILE	CB-CG2	-7.25	1.30	1.52
2	X	91	TYR	CD1-CE1	-7.25	1.28	1.39
3	1	570	PHE	CG-CD2	-7.25	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	458	ILE	CB-CG2	-7.25	1.30	1.52
3	O	458	ILE	CB-CG2	-7.25	1.30	1.52
3	4	523	ARG	CZ-NH2	-7.25	1.23	1.33
3	C	458	ILE	CB-CG2	-7.25	1.30	1.52
2	9	91	TYR	CD1-CE1	-7.25	1.28	1.39
3	R	220	GLY	N-CA	-7.24	1.35	1.46
3	V	502	LEU	CG-CD1	-7.24	1.25	1.51
2	3	78	GLU	CB-CG	-7.24	1.38	1.52
3	U	502	LEU	CG-CD1	-7.24	1.25	1.51
3	Y	458	ILE	CB-CG2	-7.24	1.30	1.52
3	C	502	LEU	CG-CD1	-7.24	1.25	1.51
3	L	502	LEU	CG-CD1	-7.24	1.25	1.51
3	1	502	LEU	CG-CD1	-7.24	1.25	1.51
3	4	502	LEU	CG-CD1	-7.24	1.25	1.51
3	7	458	ILE	CB-CG2	-7.24	1.30	1.52
3	O	502	LEU	CG-CD1	-7.24	1.25	1.51
3	R	502	LEU	CG-CD1	-7.24	1.25	1.51
2	9	78	GLU	CB-CG	-7.24	1.38	1.52
3	F	570	PHE	CG-CD2	-7.24	1.27	1.38
2	N	91	TYR	CD1-CE1	-7.24	1.28	1.39
3	Y	502	LEU	CG-CD1	-7.24	1.25	1.51
2	0	91	TYR	CD1-CE1	-7.24	1.28	1.39
2	3	91	TYR	CD1-CE1	-7.24	1.28	1.39
2	H	78	GLU	CB-CG	-7.23	1.38	1.52
1	Z	23	ARG	CZ-NH2	-7.23	1.23	1.33
3	R	458	ILE	CB-CG2	-7.23	1.30	1.52
3	V	458	ILE	CB-CG2	-7.23	1.30	1.52
2	K	49	PHE	CE1-CZ	-7.23	1.23	1.37
3	I	523	ARG	CZ-NH2	-7.23	1.23	1.33
3	7	570	PHE	CG-CD2	-7.23	1.27	1.38
2	X	78	GLU	CB-CG	-7.22	1.38	1.52
2	B	78	GLU	CB-CG	-7.22	1.38	1.52
3	F	502	LEU	CG-CD1	-7.22	1.25	1.51
2	0	78	GLU	CB-CG	-7.22	1.38	1.52
2	B	91	TYR	CD1-CE1	-7.22	1.28	1.39
3	I	45	TYR	CE1-CZ	-7.22	1.29	1.38
3	I	502	LEU	CG-CD1	-7.22	1.25	1.51
2	Q	91	TYR	CD1-CE1	-7.22	1.28	1.39
3	V	45	TYR	CE1-CZ	-7.22	1.29	1.38
3	1	45	TYR	CE1-CZ	-7.22	1.29	1.38
2	6	49	PHE	CE1-CZ	-7.22	1.23	1.37
2	6	91	TYR	CD1-CE1	-7.22	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	91	TYR	CD1-CE1	-7.21	1.28	1.39
3	F	45	TYR	CE1-CZ	-7.21	1.29	1.38
2	E	49	PHE	CE1-CZ	-7.21	1.23	1.37
2	N	78	GLU	CB-CG	-7.21	1.38	1.52
2	9	49	PHE	CE1-CZ	-7.21	1.23	1.37
2	Q	49	PHE	CE1-CZ	-7.20	1.23	1.37
2	0	49	PHE	CE1-CZ	-7.20	1.23	1.37
2	E	78	GLU	CB-CG	-7.20	1.38	1.52
3	F	343	ARG	CG-CD	-7.20	1.33	1.51
3	V	221	TYR	CD1-CE1	-7.20	1.28	1.39
2	B	49	PHE	CE1-CZ	-7.20	1.23	1.37
3	7	343	ARG	CG-CD	-7.20	1.33	1.51
2	6	78	GLU	CB-CG	-7.19	1.38	1.52
2	T	78	GLU	CB-CG	-7.19	1.38	1.52
2	T	91	TYR	CD1-CE1	-7.19	1.28	1.39
3	U	45	TYR	CE1-CZ	-7.19	1.29	1.38
2	E	91	TYR	CD1-CE1	-7.19	1.28	1.39
3	R	343	ARG	CG-CD	-7.19	1.33	1.51
2	Q	78	GLU	CB-CG	-7.19	1.38	1.52
3	C	45	TYR	CE1-CZ	-7.18	1.29	1.38
3	I	343	ARG	CG-CD	-7.18	1.33	1.51
3	V	343	ARG	CG-CD	-7.18	1.33	1.51
3	4	45	TYR	CE1-CZ	-7.18	1.29	1.38
2	H	49	PHE	CE1-CZ	-7.18	1.23	1.37
2	X	49	PHE	CE1-CZ	-7.18	1.23	1.37
3	1	343	ARG	CG-CD	-7.18	1.33	1.51
3	7	45	TYR	CE1-CZ	-7.18	1.29	1.38
3	4	343	ARG	CG-CD	-7.18	1.33	1.51
3	Y	343	ARG	CG-CD	-7.18	1.34	1.51
3	7	221	TYR	CD1-CE1	-7.18	1.28	1.39
3	7	292	VAL	CB-CG2	-7.18	1.37	1.52
3	F	221	TYR	CD1-CE1	-7.18	1.28	1.39
3	I	221	TYR	CD1-CE1	-7.18	1.28	1.39
3	L	221	TYR	CD1-CE1	-7.18	1.28	1.39
3	C	343	ARG	CG-CD	-7.17	1.34	1.51
3	O	292	VAL	CB-CG2	-7.17	1.37	1.52
3	L	45	TYR	CE1-CZ	-7.17	1.29	1.38
3	O	221	TYR	CD1-CE1	-7.17	1.28	1.39
3	4	292	VAL	CB-CG2	-7.17	1.37	1.52
3	U	343	ARG	CG-CD	-7.17	1.34	1.51
3	V	292	VAL	CB-CG2	-7.17	1.37	1.52
3	L	343	ARG	CG-CD	-7.16	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	45	TYR	CE1-CZ	-7.16	1.29	1.38
3	V	196	VAL	CB-CG2	-7.16	1.37	1.52
2	3	49	PHE	CE1-CZ	-7.16	1.23	1.37
3	O	343	ARG	CG-CD	-7.16	1.34	1.51
3	R	221	TYR	CD1-CE1	-7.16	1.28	1.39
3	F	292	VAL	CB-CG2	-7.16	1.37	1.52
2	N	49	PHE	CE1-CZ	-7.16	1.23	1.37
3	Y	45	TYR	CE1-CZ	-7.16	1.29	1.38
2	T	49	PHE	CE1-CZ	-7.15	1.23	1.37
3	U	292	VAL	CB-CG2	-7.15	1.37	1.52
3	4	221	TYR	CD1-CE1	-7.15	1.28	1.39
3	C	221	TYR	CD1-CE1	-7.15	1.28	1.39
3	I	196	VAL	CB-CG2	-7.15	1.37	1.52
3	C	292	VAL	CB-CG2	-7.15	1.37	1.52
3	1	221	TYR	CD1-CE1	-7.15	1.28	1.39
3	R	45	TYR	CE1-CZ	-7.14	1.29	1.38
3	R	371	ARG	CB-CG	-7.14	1.33	1.52
3	7	371	ARG	CB-CG	-7.14	1.33	1.52
3	U	221	TYR	CD1-CE1	-7.14	1.28	1.39
3	I	292	VAL	CB-CG2	-7.14	1.37	1.52
3	Y	292	VAL	CB-CG2	-7.14	1.37	1.52
3	4	196	VAL	CB-CG2	-7.14	1.37	1.52
3	F	371	ARG	CB-CG	-7.14	1.33	1.52
3	L	371	ARG	CB-CG	-7.14	1.33	1.52
3	Y	221	TYR	CD1-CE1	-7.13	1.28	1.39
3	1	292	VAL	CB-CG2	-7.13	1.37	1.52
3	I	371	ARG	CB-CG	-7.13	1.33	1.52
3	U	371	ARG	CB-CG	-7.13	1.33	1.52
3	V	371	ARG	CB-CG	-7.13	1.33	1.52
3	R	292	VAL	CB-CG2	-7.12	1.37	1.52
3	U	196	VAL	CB-CG2	-7.12	1.37	1.52
3	C	196	VAL	CB-CG2	-7.12	1.37	1.52
3	F	196	VAL	CB-CG2	-7.12	1.37	1.52
3	C	371	ARG	CB-CG	-7.12	1.33	1.52
3	7	376	TRP	CZ2-CH2	-7.12	1.23	1.37
3	L	292	VAL	CB-CG2	-7.12	1.38	1.52
3	O	371	ARG	CB-CG	-7.12	1.33	1.52
3	4	371	ARG	CB-CG	-7.12	1.33	1.52
3	R	376	TRP	CZ2-CH2	-7.12	1.23	1.37
3	Y	371	ARG	CB-CG	-7.12	1.33	1.52
3	F	407[A]	ARG	CD-NE	-7.11	1.34	1.46
3	F	407[B]	ARG	CD-NE	-7.11	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	479	ARG	CD-NE	-7.11	1.34	1.46
3	O	376	TRP	CZ2-CH2	-7.11	1.23	1.37
3	L	196	VAL	CB-CG2	-7.11	1.38	1.52
3	V	376	TRP	CZ2-CH2	-7.11	1.23	1.37
3	O	196	VAL	CB-CG2	-7.11	1.38	1.52
3	R	196	VAL	CB-CG2	-7.11	1.38	1.52
3	Y	376	TRP	CZ2-CH2	-7.11	1.23	1.37
3	1	196	VAL	CB-CG2	-7.11	1.38	1.52
3	R	479	ARG	CD-NE	-7.10	1.34	1.46
3	1	371	ARG	CB-CG	-7.10	1.33	1.52
3	7	196	VAL	CB-CG2	-7.10	1.38	1.52
3	Y	479	ARG	CD-NE	-7.10	1.34	1.46
2	T	91	TYR	CG-CD1	-7.10	1.29	1.39
3	U	376	TRP	CZ2-CH2	-7.10	1.23	1.37
3	C	376	TRP	CZ2-CH2	-7.09	1.23	1.37
3	I	407[A]	ARG	CD-NE	-7.09	1.34	1.46
3	I	407[B]	ARG	CD-NE	-7.09	1.34	1.46
3	F	376	TRP	CZ2-CH2	-7.09	1.23	1.37
3	4	376	TRP	CZ2-CH2	-7.09	1.23	1.37
3	U	450	LYS	CE-NZ	-7.09	1.31	1.49
3	L	376	TRP	CZ2-CH2	-7.09	1.23	1.37
3	Y	407[A]	ARG	CD-NE	-7.09	1.34	1.46
3	Y	407[B]	ARG	CD-NE	-7.09	1.34	1.46
3	L	89	VAL	CB-CG1	-7.09	1.38	1.52
3	V	407[A]	ARG	CD-NE	-7.09	1.34	1.46
3	V	407[B]	ARG	CD-NE	-7.09	1.34	1.46
3	V	450	LYS	CE-NZ	-7.09	1.31	1.49
3	Y	196	VAL	CB-CG2	-7.09	1.38	1.52
3	U	407[A]	ARG	CD-NE	-7.09	1.34	1.46
3	U	407[B]	ARG	CD-NE	-7.09	1.34	1.46
3	O	89	VAL	CB-CG1	-7.08	1.38	1.52
3	V	29	PHE	CB-CG	-7.08	1.39	1.51
3	1	376	TRP	CZ2-CH2	-7.08	1.23	1.37
3	U	479	ARG	CD-NE	-7.08	1.34	1.46
3	O	450	LYS	CE-NZ	-7.08	1.31	1.49
3	I	376	TRP	CZ2-CH2	-7.08	1.24	1.37
3	4	89	VAL	CB-CG1	-7.08	1.38	1.52
3	7	29	PHE	CB-CG	-7.08	1.39	1.51
3	I	450	LYS	CE-NZ	-7.07	1.31	1.49
3	L	29	PHE	CB-CG	-7.07	1.39	1.51
3	R	89	VAL	CB-CG1	-7.07	1.38	1.52
3	7	450	LYS	CE-NZ	-7.07	1.31	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	89	VAL	CB-CG1	-7.07	1.38	1.52
3	C	479	ARG	CD-NE	-7.07	1.34	1.46
3	4	450	LYS	CE-NZ	-7.07	1.31	1.49
3	V	89	VAL	CB-CG1	-7.07	1.38	1.52
3	7	407[A]	ARG	CD-NE	-7.07	1.34	1.46
3	7	407[B]	ARG	CD-NE	-7.07	1.34	1.46
3	F	29	PHE	CB-CG	-7.07	1.39	1.51
3	1	450	LYS	CE-NZ	-7.07	1.31	1.49
3	1	407[A]	ARG	CD-NE	-7.06	1.34	1.46
3	1	407[B]	ARG	CD-NE	-7.06	1.34	1.46
3	C	450	LYS	CE-NZ	-7.06	1.31	1.49
3	Y	89	VAL	CB-CG1	-7.06	1.38	1.52
3	R	407[A]	ARG	CD-NE	-7.06	1.34	1.46
3	R	407[B]	ARG	CD-NE	-7.06	1.34	1.46
3	F	89	VAL	CB-CG1	-7.06	1.38	1.52
3	L	450	LYS	CE-NZ	-7.06	1.31	1.49
3	Y	29	PHE	CB-CG	-7.06	1.39	1.51
1	Z	91	ARG	CG-CD	-7.06	1.34	1.51
1	G	91	ARG	CG-CD	-7.06	1.34	1.51
3	R	450	LYS	CE-NZ	-7.06	1.31	1.49
2	6	91	TYR	CG-CD1	-7.06	1.29	1.39
3	I	89	VAL	CB-CG1	-7.05	1.38	1.52
3	Y	450	LYS	CE-NZ	-7.05	1.31	1.49
3	C	89	VAL	CB-CG1	-7.05	1.38	1.52
3	C	407[A]	ARG	CD-NE	-7.05	1.34	1.46
3	C	407[B]	ARG	CD-NE	-7.05	1.34	1.46
2	X	91	TYR	CG-CD1	-7.05	1.29	1.39
3	I	448	LYS	CE-NZ	-7.05	1.31	1.49
3	O	29	PHE	CB-CG	-7.05	1.39	1.51
3	V	479	ARG	CD-NE	-7.05	1.34	1.46
2	3	91	TYR	CG-CD1	-7.05	1.29	1.39
3	7	89	VAL	CB-CG1	-7.05	1.38	1.52
3	I	29	PHE	CB-CG	-7.05	1.39	1.51
3	4	29	PHE	CB-CG	-7.05	1.39	1.51
3	O	448	LYS	CE-NZ	-7.05	1.31	1.49
3	O	479	ARG	CD-NE	-7.05	1.34	1.46
3	R	29	PHE	CB-CG	-7.05	1.39	1.51
2	Q	91	TYR	CG-CD1	-7.04	1.29	1.39
3	4	479	ARG	CD-NE	-7.04	1.34	1.46
2	B	91	TYR	CG-CD1	-7.04	1.29	1.39
3	F	450	LYS	CE-NZ	-7.04	1.31	1.49
3	O	407[A]	ARG	CD-NE	-7.04	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	407[B]	ARG	CD-NE	-7.04	1.34	1.46
3	U	448	LYS	CE-NZ	-7.04	1.31	1.49
3	C	29	PHE	CB-CG	-7.04	1.39	1.51
3	R	422	VAL	CB-CG2	-7.04	1.38	1.52
2	0	91	TYR	CG-CD1	-7.04	1.29	1.39
3	F	448	LYS	CE-NZ	-7.04	1.31	1.49
3	1	422	VAL	CB-CG2	-7.04	1.38	1.52
3	R	448	LYS	CE-NZ	-7.04	1.31	1.49
1	D	91	ARG	CG-CD	-7.04	1.34	1.51
2	E	91	TYR	CG-CD1	-7.04	1.30	1.39
3	1	448	LYS	CE-NZ	-7.03	1.31	1.49
3	F	479	ARG	CD-NE	-7.03	1.34	1.46
1	5	91	ARG	CG-CD	-7.03	1.34	1.51
3	7	479	ARG	CD-NE	-7.03	1.34	1.46
3	V	448	LYS	CE-NZ	-7.03	1.31	1.49
1	A	91	ARG	CG-CD	-7.03	1.34	1.51
3	7	422	VAL	CB-CG2	-7.03	1.38	1.52
1	8	91	ARG	CG-CD	-7.03	1.34	1.51
3	L	407[A]	ARG	CD-NE	-7.03	1.34	1.46
3	L	407[B]	ARG	CD-NE	-7.03	1.34	1.46
3	V	422	VAL	CB-CG2	-7.03	1.38	1.52
3	1	479	ARG	CD-NE	-7.03	1.34	1.46
1	2	91	ARG	CG-CD	-7.03	1.34	1.51
1	P	91	ARG	CG-CD	-7.03	1.34	1.51
3	Y	422	VAL	CB-CG2	-7.03	1.38	1.52
3	1	29	PHE	CB-CG	-7.03	1.39	1.51
3	7	546	PHE	CD1-CE1	-7.02	1.25	1.39
3	R	184	GLN	CD-NE2	-7.02	1.15	1.32
3	C	448	LYS	CE-NZ	-7.02	1.31	1.49
3	R	8	GLU	CB-CG	-7.02	1.38	1.52
3	1	89	VAL	CB-CG1	-7.02	1.38	1.52
3	4	407[A]	ARG	CD-NE	-7.02	1.34	1.46
3	4	407[B]	ARG	CD-NE	-7.02	1.34	1.46
3	7	448	LYS	CE-NZ	-7.02	1.31	1.49
2	K	91	TYR	CG-CD1	-7.02	1.30	1.39
3	L	479	ARG	CD-NE	-7.02	1.34	1.46
3	1	184	GLN	CD-NE2	-7.02	1.15	1.32
3	4	448	LYS	CE-NZ	-7.02	1.31	1.49
3	U	29	PHE	CB-CG	-7.02	1.39	1.51
3	U	422	VAL	CB-CG2	-7.02	1.38	1.52
3	R	546	PHE	CD1-CE1	-7.01	1.25	1.39
3	7	180	TRP	CD2-CE3	-7.01	1.29	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	180	TRP	CD2-CE3	-7.01	1.29	1.40
3	V	184	GLN	CD-NE2	-7.01	1.15	1.32
1	W	91	ARG	CG-CD	-7.01	1.34	1.51
3	C	422	VAL	CB-CG2	-7.01	1.38	1.52
1	S	91	ARG	CG-CD	-7.01	1.34	1.51
3	Y	448	LYS	CE-NZ	-7.01	1.31	1.49
1	M	91	ARG	CG-CD	-7.01	1.34	1.51
3	V	180	TRP	CD2-CE3	-7.01	1.29	1.40
3	C	184	GLN	CD-NE2	-7.01	1.15	1.32
3	F	184	GLN	CD-NE2	-7.01	1.15	1.32
3	I	184	GLN	CD-NE2	-7.01	1.15	1.32
3	L	546	PHE	CD1-CE1	-7.01	1.25	1.39
3	4	143	ILE	CB-CG2	-7.01	1.31	1.52
3	I	180	TRP	CD2-CE3	-7.00	1.29	1.40
2	N	91	TYR	CG-CD1	-7.00	1.30	1.39
3	Y	180	TRP	CD2-CE3	-7.00	1.29	1.40
3	L	8	GLU	CB-CG	-7.00	1.38	1.52
3	O	180	TRP	CD2-CE3	-7.00	1.29	1.40
3	O	422	VAL	CB-CG2	-7.00	1.38	1.52
3	V	143	ILE	CB-CG2	-7.00	1.31	1.52
3	Y	445	PHE	CB-CG	-7.00	1.39	1.51
3	Y	546	PHE	CD1-CE1	-7.00	1.25	1.39
3	4	184	GLN	CD-NE2	-7.00	1.15	1.32
1	J	91	ARG	CG-CD	-7.00	1.34	1.51
3	R	180	TRP	CD2-CE3	-7.00	1.29	1.40
3	U	184	GLN	CD-NE2	-7.00	1.15	1.32
3	L	143	ILE	CB-CG2	-7.00	1.31	1.52
3	L	448	LYS	CE-NZ	-7.00	1.31	1.49
3	F	143	ILE	CB-CG2	-7.00	1.31	1.52
2	H	91	TYR	CG-CD1	-7.00	1.30	1.39
3	L	184	GLN	CD-NE2	-7.00	1.15	1.32
3	L	422	VAL	CB-CG2	-7.00	1.38	1.52
3	O	184	GLN	CD-NE2	-7.00	1.15	1.32
2	9	91	TYR	CG-CD1	-7.00	1.30	1.39
3	I	143	ILE	CB-CG2	-7.00	1.31	1.52
3	I	422	VAL	CB-CG2	-7.00	1.38	1.52
3	1	180	TRP	CD2-CE3	-6.99	1.29	1.40
3	7	184	GLN	CD-NE2	-6.99	1.15	1.32
3	R	143	ILE	CB-CG2	-6.99	1.31	1.52
3	F	422	VAL	CB-CG2	-6.99	1.38	1.52
3	I	546	PHE	CD1-CE1	-6.99	1.25	1.39
3	O	546	PHE	CD1-CE1	-6.99	1.25	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	184	GLN	CD-NE2	-6.99	1.15	1.32
3	F	8	GLU	CB-CG	-6.98	1.38	1.52
3	F	445	PHE	CB-CG	-6.98	1.39	1.51
3	C	143	ILE	CB-CG2	-6.98	1.31	1.52
3	C	546	PHE	CD1-CE1	-6.98	1.25	1.39
3	O	8	GLU	CB-CG	-6.98	1.38	1.52
3	U	180	TRP	CD2-CE3	-6.98	1.29	1.40
3	U	546	PHE	CD1-CE1	-6.98	1.25	1.39
3	1	546	PHE	CD1-CE1	-6.98	1.25	1.39
3	4	546	PHE	CD1-CE1	-6.98	1.25	1.39
3	I	8	GLU	CB-CG	-6.98	1.38	1.52
3	7	445	PHE	CB-CG	-6.98	1.39	1.51
3	U	8	GLU	CB-CG	-6.98	1.38	1.52
3	O	143	ILE	CB-CG2	-6.98	1.31	1.52
3	V	546	PHE	CD1-CE1	-6.98	1.25	1.39
3	1	143	ILE	CB-CG2	-6.98	1.31	1.52
3	R	445	PHE	CB-CG	-6.97	1.39	1.51
3	4	422	VAL	CB-CG2	-6.97	1.38	1.52
3	F	180	TRP	CD2-CE3	-6.97	1.29	1.40
3	C	8	GLU	CB-CG	-6.97	1.39	1.52
3	L	180	TRP	CD2-CE3	-6.97	1.29	1.40
3	Y	8	GLU	CB-CG	-6.97	1.39	1.52
3	Y	143	ILE	CB-CG2	-6.97	1.31	1.52
3	7	143	ILE	CB-CG2	-6.97	1.31	1.52
3	V	445	PHE	CB-CG	-6.97	1.39	1.51
3	U	143	ILE	CB-CG2	-6.97	1.31	1.52
3	F	546	PHE	CD1-CE1	-6.96	1.25	1.39
3	V	8	GLU	CB-CG	-6.96	1.39	1.52
3	1	8	GLU	CB-CG	-6.96	1.39	1.52
3	4	8	GLU	CB-CG	-6.96	1.39	1.52
3	C	445	PHE	CB-CG	-6.96	1.39	1.51
3	O	445	PHE	CB-CG	-6.96	1.39	1.51
2	E	77	PHE	CD1-CE1	-6.96	1.25	1.39
3	I	445	PHE	CB-CG	-6.96	1.39	1.51
3	4	180	TRP	CD2-CE3	-6.96	1.29	1.40
2	9	77	PHE	CD1-CE1	-6.96	1.25	1.39
2	0	77	PHE	CD1-CE1	-6.96	1.25	1.39
3	L	445	PHE	CB-CG	-6.96	1.39	1.51
3	1	445	PHE	CB-CG	-6.95	1.39	1.51
2	H	77	PHE	CD1-CE1	-6.95	1.25	1.39
3	7	482	PHE	CD2-CE2	-6.95	1.25	1.39
1	5	32	TYR	CB-CG	-6.94	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	77	PHE	CD1-CE1	-6.94	1.25	1.39
2	Q	77	PHE	CD1-CE1	-6.94	1.25	1.39
1	8	32	TYR	CB-CG	-6.94	1.41	1.51
1	2	32	TYR	CB-CG	-6.94	1.41	1.51
1	P	32	TYR	CB-CG	-6.94	1.41	1.51
3	V	482	PHE	CD2-CE2	-6.94	1.25	1.39
3	V	546	PHE	CE2-CZ	-6.94	1.24	1.37
2	3	77	PHE	CD1-CE1	-6.94	1.25	1.39
3	U	445	PHE	CB-CG	-6.94	1.39	1.51
2	B	77	PHE	CD1-CE1	-6.93	1.25	1.39
3	Y	309	TYR	CE2-CZ	-6.93	1.29	1.38
3	4	445	PHE	CB-CG	-6.93	1.39	1.51
1	A	32	TYR	CB-CG	-6.93	1.41	1.51
1	J	32	TYR	CB-CG	-6.93	1.41	1.51
1	Z	32	TYR	CB-CG	-6.93	1.41	1.51
1	G	32	TYR	CD2-CE2	-6.93	1.28	1.39
1	P	32	TYR	CD2-CE2	-6.93	1.28	1.39
3	7	8	GLU	CB-CG	-6.93	1.39	1.52
3	F	546	PHE	CE2-CZ	-6.93	1.24	1.37
1	S	32	TYR	CB-CG	-6.92	1.41	1.51
3	4	482	PHE	CD2-CE2	-6.92	1.25	1.39
1	G	32	TYR	CB-CG	-6.92	1.41	1.51
2	6	77	PHE	CD1-CE1	-6.92	1.25	1.39
3	L	482	PHE	CD2-CE2	-6.92	1.25	1.39
3	1	482	PHE	CD2-CE2	-6.92	1.25	1.39
3	C	482	PHE	CD2-CE2	-6.92	1.25	1.39
3	R	482	PHE	CD2-CE2	-6.92	1.25	1.39
2	N	77	PHE	CD1-CE1	-6.92	1.25	1.39
1	W	32	TYR	CD2-CE2	-6.92	1.28	1.39
2	X	77	PHE	CD1-CE1	-6.91	1.25	1.39
1	5	32	TYR	CD2-CE2	-6.91	1.28	1.39
3	O	482	PHE	CD2-CE2	-6.91	1.25	1.39
1	D	32	TYR	CB-CG	-6.91	1.41	1.51
3	U	482	PHE	CD2-CE2	-6.91	1.25	1.39
3	L	546	PHE	CE2-CZ	-6.91	1.24	1.37
1	M	32	TYR	CB-CG	-6.91	1.41	1.51
1	8	32	TYR	CD2-CE2	-6.91	1.28	1.39
3	R	445	PHE	CE2-CZ	-6.90	1.24	1.37
2	T	77	PHE	CD1-CE1	-6.90	1.25	1.39
3	4	440	TRP	CD1-NE1	-6.90	1.26	1.38
1	A	32	TYR	CD2-CE2	-6.90	1.28	1.39
1	M	32	TYR	CD2-CE2	-6.90	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	445	PHE	CE2-CZ	-6.90	1.24	1.37
3	F	482	PHE	CD2-CE2	-6.90	1.25	1.39
3	V	440	TRP	CD1-NE1	-6.89	1.26	1.38
3	U	546	PHE	CE2-CZ	-6.89	1.24	1.37
3	1	445	PHE	CE2-CZ	-6.89	1.24	1.37
3	F	440	TRP	CD1-NE1	-6.89	1.26	1.38
1	J	32	TYR	CD2-CE2	-6.89	1.29	1.39
3	O	309	TYR	CE2-CZ	-6.89	1.29	1.38
3	C	546	PHE	CE2-CZ	-6.89	1.24	1.37
3	I	309	TYR	CE2-CZ	-6.89	1.29	1.38
1	W	32	TYR	CB-CG	-6.89	1.41	1.51
1	Z	32	TYR	CD2-CE2	-6.89	1.29	1.39
3	I	546	PHE	CE2-CZ	-6.88	1.24	1.37
3	L	309	TYR	CE2-CZ	-6.88	1.29	1.38
3	4	309	TYR	CE2-CZ	-6.88	1.29	1.38
3	U	445	PHE	CE2-CZ	-6.88	1.24	1.37
3	Y	482	PHE	CD2-CE2	-6.88	1.25	1.39
3	4	546	PHE	CE2-CZ	-6.88	1.24	1.37
3	I	482	PHE	CD2-CE2	-6.88	1.25	1.39
3	7	440	TRP	CD1-NE1	-6.88	1.26	1.38
3	7	546	PHE	CE2-CZ	-6.88	1.24	1.37
3	O	546	PHE	CE2-CZ	-6.88	1.24	1.37
3	O	445	PHE	CE2-CZ	-6.88	1.24	1.37
3	R	546	PHE	CE2-CZ	-6.88	1.24	1.37
3	C	445	PHE	CE2-CZ	-6.88	1.24	1.37
3	Y	546	PHE	CE2-CZ	-6.87	1.24	1.37
3	1	546	PHE	CE2-CZ	-6.87	1.24	1.37
3	V	445	PHE	CE2-CZ	-6.87	1.24	1.37
3	U	396	ASP	C-N	-6.87	1.18	1.34
3	I	268	PHE	CE2-CZ	-6.87	1.24	1.37
3	C	309	TYR	CE2-CZ	-6.87	1.29	1.38
2	E	87	ARG	CZ-NH1	-6.86	1.24	1.33
2	X	87	ARG	CZ-NH1	-6.86	1.24	1.33
3	Y	396	ASP	C-N	-6.86	1.18	1.34
1	2	32	TYR	CD2-CE2	-6.86	1.29	1.39
3	F	309	TYR	CE2-CZ	-6.86	1.29	1.38
3	F	396	ASP	C-N	-6.86	1.18	1.34
3	U	268	PHE	CE2-CZ	-6.86	1.24	1.37
2	T	87	ARG	CZ-NH1	-6.86	1.24	1.33
3	1	309	TYR	CE2-CZ	-6.86	1.29	1.38
3	C	440	TRP	CD1-NE1	-6.86	1.26	1.38
3	L	445	PHE	CE2-CZ	-6.85	1.24	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	445	PHE	CE2-CZ	-6.85	1.24	1.37
3	I	445	PHE	CE2-CZ	-6.85	1.24	1.37
3	I	546	PHE	CE1-CZ	-6.85	1.24	1.37
3	O	396	ASP	C-N	-6.85	1.18	1.34
2	Q	87	ARG	CZ-NH1	-6.85	1.24	1.33
1	D	32	TYR	CD2-CE2	-6.85	1.29	1.39
1	S	32	TYR	CD2-CE2	-6.85	1.29	1.39
3	Y	445	PHE	CE2-CZ	-6.85	1.24	1.37
3	1	192	LEU	C-N	-6.85	1.21	1.34
2	9	87	ARG	CZ-NH1	-6.85	1.24	1.33
2	K	87	ARG	CZ-NH1	-6.85	1.24	1.33
3	O	546	PHE	CE1-CZ	-6.85	1.24	1.37
3	1	440	TRP	CD1-NE1	-6.85	1.26	1.38
3	7	445	PHE	CE2-CZ	-6.85	1.24	1.37
2	H	87	ARG	CZ-NH1	-6.84	1.24	1.33
3	U	440	TRP	CD1-NE1	-6.84	1.26	1.38
3	V	268	PHE	CE2-CZ	-6.84	1.24	1.37
3	L	440	TRP	CD1-NE1	-6.84	1.26	1.38
2	6	87	ARG	CZ-NH1	-6.84	1.24	1.33
3	U	546	PHE	CE1-CZ	-6.84	1.24	1.37
3	7	309	TYR	CE2-CZ	-6.84	1.29	1.38
3	C	396	ASP	C-N	-6.83	1.18	1.34
3	I	396	ASP	C-N	-6.83	1.18	1.34
3	7	192	LEU	C-N	-6.83	1.21	1.34
3	L	396	ASP	C-N	-6.83	1.18	1.34
3	R	268	PHE	CE2-CZ	-6.83	1.24	1.37
3	Y	440	TRP	CD1-NE1	-6.83	1.26	1.38
3	C	268	PHE	CE2-CZ	-6.83	1.24	1.37
3	O	440	TRP	CD1-NE1	-6.83	1.26	1.38
3	F	192	LEU	C-N	-6.83	1.21	1.34
3	1	268	PHE	CE2-CZ	-6.83	1.24	1.37
3	U	309	TYR	CE2-CZ	-6.83	1.29	1.38
2	B	87	ARG	CZ-NH1	-6.82	1.24	1.33
3	C	546	PHE	CE1-CZ	-6.82	1.24	1.37
3	I	440	TRP	CD1-NE1	-6.82	1.26	1.38
3	R	440	TRP	CD1-NE1	-6.82	1.26	1.38
3	Y	546	PHE	CE1-CZ	-6.82	1.24	1.37
3	7	396	ASP	C-N	-6.82	1.18	1.34
3	4	546	PHE	CE1-CZ	-6.82	1.24	1.37
3	F	546	PHE	CE1-CZ	-6.82	1.24	1.37
3	R	396	ASP	C-N	-6.82	1.18	1.34
3	O	296	PRO	CB-CG	-6.82	1.15	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	268	PHE	CE2-CZ	-6.81	1.24	1.37
3	Y	296	PRO	CB-CG	-6.81	1.15	1.50
3	7	296	PRO	CB-CG	-6.81	1.15	1.50
3	F	296	PRO	CB-CG	-6.81	1.15	1.50
3	I	296	PRO	CB-CG	-6.81	1.16	1.50
3	Y	268	PHE	CE2-CZ	-6.81	1.24	1.37
3	1	296	PRO	CB-CG	-6.81	1.15	1.50
3	1	546	PHE	CE1-CZ	-6.81	1.24	1.37
3	4	268	PHE	CE2-CZ	-6.81	1.24	1.37
3	7	268	PHE	CE2-CZ	-6.81	1.24	1.37
3	C	296	PRO	CB-CG	-6.81	1.16	1.50
3	R	192	LEU	C-N	-6.81	1.21	1.34
3	V	309	TYR	CE2-CZ	-6.81	1.29	1.38
2	3	87	ARG	CZ-NH1	-6.81	1.24	1.33
3	L	296	PRO	CB-CG	-6.81	1.16	1.50
3	V	296	PRO	CB-CG	-6.81	1.16	1.50
3	1	396	ASP	C-N	-6.81	1.18	1.34
3	Y	192	LEU	C-N	-6.80	1.21	1.34
3	4	396	ASP	C-N	-6.80	1.18	1.34
3	F	268	PHE	CE2-CZ	-6.80	1.24	1.37
3	O	268	PHE	CE2-CZ	-6.80	1.24	1.37
3	C	192	LEU	C-N	-6.80	1.21	1.34
3	F	146	GLN	CD-NE2	-6.80	1.15	1.32
3	V	396	ASP	C-N	-6.80	1.18	1.34
3	U	192	LEU	C-N	-6.80	1.21	1.34
3	L	192	LEU	C-N	-6.79	1.21	1.34
3	R	296	PRO	CB-CG	-6.79	1.16	1.50
3	R	309	TYR	CE2-CZ	-6.79	1.29	1.38
3	U	296	PRO	CB-CG	-6.79	1.16	1.50
2	0	87	ARG	CZ-NH1	-6.79	1.24	1.33
3	4	296	PRO	CB-CG	-6.79	1.16	1.50
3	7	546	PHE	CE1-CZ	-6.79	1.24	1.37
3	R	146	GLN	CD-NE2	-6.79	1.15	1.32
3	L	146	GLN	CD-NE2	-6.79	1.15	1.32
3	V	192	LEU	C-N	-6.79	1.21	1.34
3	O	192	LEU	C-N	-6.79	1.21	1.34
3	V	146	GLN	CD-NE2	-6.78	1.15	1.32
3	V	406[A]	LEU	CG-CD1	-6.78	1.26	1.51
3	V	406[B]	LEU	CG-CD1	-6.78	1.26	1.51
3	1	146	GLN	CD-NE2	-6.78	1.15	1.32
3	I	146	GLN	CD-NE2	-6.78	1.15	1.32
3	V	546	PHE	CE1-CZ	-6.78	1.24	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	546	PHE	CE1-CZ	-6.78	1.24	1.37
3	I	406[A]	LEU	CG-CD1	-6.78	1.26	1.51
3	I	406[B]	LEU	CG-CD1	-6.78	1.26	1.51
3	R	546	PHE	CE1-CZ	-6.78	1.24	1.37
3	7	406[A]	LEU	CG-CD1	-6.78	1.26	1.51
3	7	406[B]	LEU	CG-CD1	-6.78	1.26	1.51
3	7	146	GLN	CD-NE2	-6.77	1.16	1.32
3	Y	146	GLN	CD-NE2	-6.77	1.16	1.32
3	4	192	LEU	C-N	-6.77	1.21	1.34
3	C	146	GLN	CD-NE2	-6.77	1.16	1.32
3	I	192	LEU	C-N	-6.77	1.21	1.34
3	R	406[A]	LEU	CG-CD1	-6.77	1.26	1.51
3	R	406[B]	LEU	CG-CD1	-6.77	1.26	1.51
3	C	406[A]	LEU	CG-CD1	-6.76	1.26	1.51
3	C	406[B]	LEU	CG-CD1	-6.76	1.26	1.51
3	F	406[A]	LEU	CG-CD1	-6.76	1.26	1.51
3	F	406[B]	LEU	CG-CD1	-6.76	1.26	1.51
3	L	406[A]	LEU	CG-CD1	-6.76	1.26	1.51
3	L	406[B]	LEU	CG-CD1	-6.76	1.26	1.51
3	4	406[A]	LEU	CG-CD1	-6.76	1.26	1.51
3	4	406[B]	LEU	CG-CD1	-6.76	1.26	1.51
3	O	146	GLN	CD-NE2	-6.76	1.16	1.32
3	1	406[A]	LEU	CG-CD1	-6.76	1.26	1.51
3	1	406[B]	LEU	CG-CD1	-6.76	1.26	1.51
3	4	146	GLN	CD-NE2	-6.76	1.16	1.32
3	Y	406[A]	LEU	CG-CD1	-6.76	1.26	1.51
3	Y	406[B]	LEU	CG-CD1	-6.76	1.26	1.51
3	U	146	GLN	CD-NE2	-6.76	1.16	1.32
2	N	87	ARG	CZ-NH1	-6.76	1.24	1.33
3	U	406[A]	LEU	CG-CD1	-6.76	1.26	1.51
3	U	406[B]	LEU	CG-CD1	-6.76	1.26	1.51
3	L	444	PHE	CG-CD2	-6.75	1.28	1.38
3	O	406[A]	LEU	CG-CD1	-6.75	1.26	1.51
3	O	406[B]	LEU	CG-CD1	-6.75	1.26	1.51
3	U	404	ARG	CZ-NH2	-6.75	1.24	1.33
3	1	444	PHE	CG-CD2	-6.75	1.28	1.38
3	R	444	PHE	CG-CD2	-6.74	1.28	1.38
2	N	105	PHE	CG-CD1	-6.74	1.28	1.38
3	L	404	ARG	CZ-NH2	-6.73	1.24	1.33
3	Y	444	PHE	CG-CD2	-6.73	1.28	1.38
1	G	8	VAL	CB-CG2	6.73	1.67	1.52
2	K	105	PHE	CG-CD1	-6.73	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	122	GLN	CB-CG	-6.72	1.34	1.52
2	9	122	GLN	CB-CG	-6.72	1.34	1.52
1	2	8	VAL	CB-CG2	6.72	1.67	1.52
1	P	8	VAL	CB-CG2	6.72	1.67	1.52
2	X	105	PHE	CG-CD1	-6.72	1.28	1.38
3	F	444	PHE	CD2-CE2	-6.72	1.25	1.39
2	3	105	PHE	CG-CD1	-6.72	1.28	1.38
1	S	53	VAL	CB-CG2	-6.71	1.38	1.52
2	0	105	PHE	CG-CD1	-6.71	1.28	1.38
2	0	122	GLN	CB-CG	-6.71	1.34	1.52
3	4	444	PHE	CG-CD2	-6.71	1.28	1.38
3	7	444	PHE	CG-CD2	-6.71	1.28	1.38
2	B	105	PHE	CG-CD1	-6.71	1.28	1.38
3	R	404	ARG	CZ-NH2	-6.71	1.24	1.33
2	6	122	GLN	CB-CG	-6.71	1.34	1.52
3	C	444	PHE	CG-CD2	-6.71	1.28	1.38
2	B	122	GLN	CB-CG	-6.71	1.34	1.52
2	E	122	GLN	CB-CG	-6.71	1.34	1.52
2	N	122	GLN	CB-CG	-6.71	1.34	1.52
3	V	404	ARG	CZ-NH2	-6.71	1.24	1.33
1	D	8	VAL	CB-CG2	6.70	1.67	1.52
2	Q	122	GLN	CB-CG	-6.70	1.34	1.52
3	1	404	ARG	CZ-NH2	-6.70	1.24	1.33
2	6	87	ARG	CG-CD	-6.70	1.35	1.51
3	F	404	ARG	CZ-NH2	-6.70	1.24	1.33
2	T	122	GLN	CB-CG	-6.70	1.34	1.52
3	4	117	VAL	CB-CG1	-6.70	1.38	1.52
3	C	404	ARG	CZ-NH2	-6.70	1.24	1.33
1	G	53	VAL	CB-CG2	-6.70	1.38	1.52
3	I	117	VAL	CB-CG1	-6.70	1.38	1.52
3	I	404	ARG	CZ-NH2	-6.70	1.24	1.33
3	L	341	ARG	CB-CG	-6.70	1.34	1.52
2	X	87	ARG	CG-CD	-6.70	1.35	1.51
3	4	341	ARG	CB-CG	-6.70	1.34	1.52
1	W	8	VAL	CB-CG2	6.70	1.67	1.52
1	W	53	VAL	CB-CG2	-6.70	1.38	1.52
1	8	53	VAL	CB-CG2	-6.70	1.38	1.52
2	N	87	ARG	CG-CD	-6.69	1.35	1.51
2	Q	105	PHE	CG-CD1	-6.69	1.28	1.38
1	Z	8	VAL	CB-CG2	6.69	1.67	1.52
1	A	8	VAL	CB-CG2	6.69	1.67	1.52
3	U	444	PHE	CG-CD2	-6.69	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	53	VAL	CB-CG2	-6.69	1.38	1.52
2	H	122	GLN	CB-CG	-6.69	1.34	1.52
2	K	122	GLN	CB-CG	-6.69	1.34	1.52
1	P	53	VAL	CB-CG2	-6.69	1.38	1.52
2	6	105	PHE	CG-CD1	-6.69	1.28	1.38
1	8	8	VAL	CB-CG2	6.69	1.67	1.52
3	F	117	VAL	CB-CG1	-6.69	1.38	1.52
1	M	8	VAL	CB-CG2	6.69	1.66	1.52
1	S	8	VAL	CB-CG2	6.69	1.66	1.52
3	V	117	VAL	CB-CG1	-6.69	1.38	1.52
2	H	105	PHE	CG-CD1	-6.69	1.28	1.38
3	I	362	PHE	CD2-CE2	-6.69	1.25	1.39
3	I	444	PHE	CG-CD2	-6.69	1.28	1.38
1	2	53	VAL	CB-CG2	-6.69	1.38	1.52
2	E	87	ARG	CG-CD	-6.68	1.35	1.51
2	H	87	ARG	CG-CD	-6.68	1.35	1.51
1	5	8	VAL	CB-CG2	6.68	1.66	1.52
1	J	8	VAL	CB-CG2	6.68	1.66	1.52
1	A	53	VAL	CB-CG2	-6.68	1.38	1.52
2	E	105	PHE	CG-CD1	-6.68	1.28	1.38
2	3	122	GLN	CB-CG	-6.68	1.34	1.52
2	9	87	ARG	CG-CD	-6.68	1.35	1.51
2	9	105	PHE	CG-CD1	-6.68	1.28	1.38
3	C	341	ARG	CB-CG	-6.68	1.34	1.52
3	O	117	VAL	CB-CG1	-6.68	1.38	1.52
1	5	53	VAL	CB-CG2	-6.68	1.38	1.52
3	U	341	ARG	CB-CG	-6.68	1.34	1.52
1	Z	53	VAL	CB-CG2	-6.68	1.38	1.52
3	O	341	ARG	CB-CG	-6.68	1.34	1.52
3	O	444	PHE	CD2-CE2	-6.68	1.25	1.39
2	Q	87	ARG	CG-CD	-6.68	1.35	1.51
2	B	87	ARG	CG-CD	-6.67	1.35	1.51
3	V	341	ARG	CB-CG	-6.67	1.34	1.52
2	T	87	ARG	CG-CD	-6.67	1.35	1.51
3	V	444	PHE	CD2-CE2	-6.67	1.25	1.39
3	Y	404	ARG	CZ-NH2	-6.67	1.24	1.33
3	1	260	TYR	CG-CD1	-6.67	1.30	1.39
3	7	117	VAL	CB-CG1	-6.67	1.38	1.52
2	0	87	ARG	CG-CD	-6.67	1.35	1.51
3	7	444	PHE	CD2-CE2	-6.67	1.25	1.39
3	U	117	VAL	CB-CG1	-6.67	1.38	1.52
3	U	362	PHE	CD2-CE2	-6.67	1.25	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	117	VAL	CB-CG1	-6.67	1.38	1.52
3	C	444	PHE	CD2-CE2	-6.67	1.25	1.39
3	O	362	PHE	CD2-CE2	-6.67	1.25	1.39
3	V	260	TYR	CG-CD1	-6.67	1.30	1.39
3	Y	117	VAL	CB-CG1	-6.67	1.38	1.52
3	1	341	ARG	CB-CG	-6.67	1.34	1.52
3	1	371	ARG	CG-CD	-6.67	1.35	1.51
2	T	105	PHE	CG-CD1	-6.67	1.28	1.38
3	I	260	TYR	CG-CD1	-6.66	1.30	1.39
1	J	53	VAL	CB-CG2	-6.66	1.38	1.52
3	L	444	PHE	CD2-CE2	-6.66	1.25	1.39
3	Y	341	ARG	CB-CG	-6.66	1.34	1.52
3	7	404	ARG	CZ-NH2	-6.66	1.24	1.33
1	M	53	VAL	CB-CG2	-6.66	1.38	1.52
3	O	444	PHE	CG-CD2	-6.66	1.28	1.38
3	V	371	ARG	CG-CD	-6.66	1.35	1.51
3	F	371	ARG	CG-CD	-6.66	1.35	1.51
3	F	444	PHE	CG-CD2	-6.66	1.28	1.38
2	3	87	ARG	CG-CD	-6.66	1.35	1.51
3	C	371	ARG	CG-CD	-6.66	1.35	1.51
3	R	362	PHE	CD2-CE2	-6.66	1.25	1.39
3	Y	362	PHE	CD2-CE2	-6.66	1.25	1.39
2	3	91	TYR	CE1-CZ	-6.66	1.29	1.38
3	4	404	ARG	CZ-NH2	-6.66	1.24	1.33
3	7	341	ARG	CB-CG	-6.66	1.34	1.52
2	9	91	TYR	CE1-CZ	-6.66	1.29	1.38
3	F	341	ARG	CB-CG	-6.66	1.34	1.52
2	K	87	ARG	CG-CD	-6.66	1.35	1.51
3	V	444	PHE	CG-CD2	-6.66	1.28	1.38
3	I	371	ARG	CG-CD	-6.65	1.35	1.51
3	F	260	TYR	CG-CD1	-6.65	1.30	1.39
2	H	91	TYR	CE1-CZ	-6.65	1.29	1.38
3	L	362	PHE	CD2-CE2	-6.65	1.25	1.39
3	L	371	ARG	CG-CD	-6.65	1.35	1.51
2	Q	91	TYR	CE1-CZ	-6.65	1.29	1.38
3	1	117	VAL	CB-CG1	-6.65	1.38	1.52
3	1	444	PHE	CD2-CE2	-6.65	1.25	1.39
3	7	362	PHE	CD2-CE2	-6.65	1.25	1.39
3	R	341	ARG	CB-CG	-6.65	1.34	1.52
3	U	444	PHE	CD2-CE2	-6.65	1.25	1.39
3	I	444	PHE	CD2-CE2	-6.65	1.25	1.39
3	Y	260	TYR	CG-CD1	-6.65	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	362	PHE	CD2-CE2	-6.65	1.25	1.39
3	F	362	PHE	CD2-CE2	-6.65	1.25	1.39
3	I	341	ARG	CB-CG	-6.65	1.34	1.52
3	O	404	ARG	CZ-NH2	-6.65	1.24	1.33
2	B	91	TYR	CE1-CZ	-6.64	1.29	1.38
2	6	91	TYR	CE1-CZ	-6.64	1.29	1.38
3	O	371	ARG	CG-CD	-6.64	1.35	1.51
2	N	91	TYR	CE1-CZ	-6.64	1.29	1.38
3	V	362	PHE	CD2-CE2	-6.64	1.25	1.39
1	5	7	GLU	CD-OE1	-6.64	1.18	1.25
3	R	444	PHE	CD2-CE2	-6.64	1.25	1.39
3	1	362	PHE	CD2-CE2	-6.64	1.25	1.39
3	7	409	VAL	CB-CG1	-6.64	1.39	1.52
3	L	117	VAL	CB-CG1	-6.64	1.39	1.52
3	U	371	ARG	CG-CD	-6.64	1.35	1.51
3	Y	409	VAL	CB-CG1	-6.63	1.39	1.52
2	9	92	GLY	CA-C	-6.63	1.41	1.51
3	I	531	VAL	CB-CG1	-6.63	1.39	1.52
2	0	91	TYR	CE1-CZ	-6.63	1.29	1.38
3	4	362	PHE	CD2-CE2	-6.63	1.25	1.39
3	4	444	PHE	CD2-CE2	-6.63	1.25	1.39
2	E	91	TYR	CE1-CZ	-6.63	1.29	1.38
1	G	7	GLU	CD-OE1	-6.63	1.18	1.25
3	L	40	GLY	C-O	-6.63	1.13	1.23
3	R	117	VAL	CB-CG1	-6.63	1.39	1.52
3	R	371	ARG	CG-CD	-6.63	1.35	1.51
3	R	378	ARG	CZ-NH2	-6.63	1.24	1.33
3	C	260	TYR	CG-CD1	-6.63	1.30	1.39
3	Y	444	PHE	CD2-CE2	-6.63	1.25	1.39
3	7	371	ARG	CG-CD	-6.63	1.35	1.51
3	V	40	GLY	C-O	-6.63	1.13	1.23
3	F	531	VAL	CB-CG1	-6.62	1.39	1.52
3	R	260	TYR	CG-CD1	-6.62	1.30	1.39
3	I	378	ARG	CZ-NH2	-6.62	1.24	1.33
3	O	180	TRP	CZ3-CH2	-6.62	1.29	1.40
3	R	531	VAL	CB-CG1	-6.62	1.39	1.52
3	7	531	VAL	CB-CG1	-6.62	1.39	1.52
3	O	40	GLY	C-O	-6.62	1.13	1.23
3	Y	371	ARG	CG-CD	-6.62	1.35	1.51
3	R	40	GLY	C-O	-6.62	1.13	1.23
3	4	371	ARG	CG-CD	-6.62	1.35	1.51
3	C	40	GLY	C-O	-6.62	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	260	TYR	CG-CD1	-6.62	1.30	1.39
1	D	7	GLU	CD-OE1	-6.61	1.18	1.25
3	F	40	GLY	C-O	-6.61	1.13	1.23
3	F	409	VAL	CB-CG1	-6.61	1.39	1.52
3	Y	40	GLY	C-O	-6.61	1.13	1.23
1	M	7	GLU	CD-OE1	-6.61	1.18	1.25
3	O	531	VAL	CB-CG1	-6.61	1.39	1.52
3	U	378	ARG	CZ-NH2	-6.61	1.24	1.33
3	O	260	TYR	CG-CD1	-6.61	1.30	1.39
3	R	409	VAL	CB-CG1	-6.61	1.39	1.52
3	1	409	VAL	CB-CG1	-6.61	1.39	1.52
3	L	409	VAL	CB-CG1	-6.61	1.39	1.52
3	V	531	VAL	CB-CG1	-6.61	1.39	1.52
3	Y	378	ARG	CZ-NH2	-6.60	1.24	1.33
3	U	260	TYR	CG-CD1	-6.60	1.30	1.39
3	C	409	VAL	CB-CG1	-6.60	1.39	1.52
2	T	91	TYR	CE1-CZ	-6.60	1.29	1.38
3	C	531	VAL	CB-CG1	-6.60	1.39	1.52
1	J	7	GLU	CD-OE1	-6.60	1.18	1.25
3	O	409	VAL	CB-CG1	-6.60	1.39	1.52
3	V	409	VAL	CB-CG1	-6.60	1.39	1.52
1	A	7	GLU	CD-OE1	-6.60	1.18	1.25
3	I	40	GLY	C-O	-6.60	1.13	1.23
3	L	531	VAL	CB-CG1	-6.60	1.39	1.52
2	X	92	GLY	CA-C	-6.60	1.41	1.51
3	4	409	VAL	CB-CG1	-6.60	1.39	1.52
3	V	378	ARG	CZ-NH2	-6.60	1.24	1.33
2	0	92	GLY	CA-C	-6.60	1.41	1.51
3	C	378	ARG	CZ-NH2	-6.60	1.24	1.33
3	L	180	TRP	CZ3-CH2	-6.60	1.29	1.40
3	4	40	GLY	C-O	-6.59	1.13	1.23
3	7	260	TYR	CG-CD1	-6.59	1.30	1.39
3	Y	531	VAL	CB-CG1	-6.59	1.39	1.52
1	S	7	GLU	CD-OE1	-6.59	1.18	1.25
3	U	409	VAL	CB-CG1	-6.59	1.39	1.52
3	F	378	ARG	CZ-NH2	-6.59	1.24	1.33
1	P	7	GLU	CD-OE1	-6.59	1.18	1.25
3	V	180	TRP	CZ3-CH2	-6.59	1.29	1.40
3	Y	180	TRP	CZ3-CH2	-6.59	1.29	1.40
3	F	302	SER	CB-OG	-6.58	1.33	1.42
1	W	7	GLU	CD-OE1	-6.58	1.18	1.25
3	F	180	TRP	CZ3-CH2	-6.58	1.29	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	92	GLY	CA-C	-6.58	1.41	1.51
2	T	93	LYS	CG-CD	-6.58	1.30	1.52
2	3	92	GLY	CA-C	-6.58	1.41	1.51
3	U	531	VAL	CB-CG1	-6.58	1.39	1.52
2	K	91	TYR	CE1-CZ	-6.58	1.29	1.38
3	V	145	PRO	CG-CD	-6.58	1.28	1.50
2	X	91	TYR	CE1-CZ	-6.58	1.29	1.38
3	1	40	GLY	C-O	-6.58	1.13	1.23
1	8	7	GLU	CD-OE1	-6.58	1.18	1.25
3	I	145	PRO	CG-CD	-6.58	1.28	1.50
3	I	302	SER	CB-OG	-6.58	1.33	1.42
2	N	92	GLY	CA-C	-6.58	1.41	1.51
3	4	531	VAL	CB-CG1	-6.58	1.39	1.52
2	6	93	LYS	CG-CD	-6.58	1.30	1.52
1	M	24	LYS	CB-CG	-6.58	1.34	1.52
2	6	57	LYS	CB-CG	-6.58	1.34	1.52
2	6	92	GLY	CA-C	-6.58	1.41	1.51
2	B	92	GLY	CA-C	-6.58	1.41	1.51
2	E	92	GLY	CA-C	-6.58	1.41	1.51
3	Y	92	ARG	CZ-NH1	-6.58	1.24	1.33
3	4	378	ARG	CZ-NH2	-6.58	1.24	1.33
3	C	145	PRO	CG-CD	-6.57	1.28	1.50
3	L	260	TYR	CG-CD1	-6.57	1.30	1.39
3	1	145	PRO	CG-CD	-6.57	1.28	1.50
3	1	302	SER	CB-OG	-6.57	1.33	1.42
3	7	145	PRO	CG-CD	-6.57	1.28	1.50
3	L	145	PRO	CG-CD	-6.57	1.28	1.50
3	O	378	ARG	CZ-NH2	-6.57	1.24	1.33
3	R	302	SER	CB-OG	-6.57	1.33	1.42
1	A	24	LYS	CB-CG	-6.57	1.34	1.52
1	D	24	LYS	CB-CG	-6.57	1.34	1.52
3	F	145	PRO	CG-CD	-6.57	1.28	1.50
3	I	409	VAL	CB-CG1	-6.57	1.39	1.52
2	Q	92	GLY	CA-C	-6.57	1.41	1.51
2	9	93	LYS	CG-CD	-6.57	1.30	1.52
3	V	302	SER	CB-OG	-6.57	1.33	1.42
2	B	93	LYS	CG-CD	-6.57	1.30	1.52
3	C	302	SER	CB-OG	-6.57	1.33	1.42
2	K	57	LYS	CB-CG	-6.57	1.34	1.52
2	N	93	LYS	CG-CD	-6.57	1.30	1.52
3	O	145	PRO	CG-CD	-6.57	1.28	1.50
2	X	77	PHE	CG-CD1	-6.57	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	57	LYS	CB-CG	-6.57	1.34	1.52
2	T	92	GLY	CA-C	-6.57	1.41	1.51
3	Y	145	PRO	CG-CD	-6.57	1.28	1.50
2	0	93	LYS	CG-CD	-6.57	1.30	1.52
3	1	531	VAL	CB-CG1	-6.57	1.39	1.52
2	T	57	LYS	CB-CG	-6.56	1.34	1.52
1	5	24	LYS	CB-CG	-6.56	1.34	1.52
3	L	378	ARG	CZ-NH2	-6.56	1.24	1.33
2	T	77	PHE	CG-CD1	-6.56	1.28	1.38
1	W	24	LYS	CB-CG	-6.56	1.34	1.52
3	7	40	GLY	C-O	-6.56	1.13	1.23
3	C	180	TRP	CZ3-CH2	-6.56	1.29	1.40
1	Z	7	GLU	CD-OE1	-6.56	1.18	1.25
3	1	378	ARG	CZ-NH2	-6.56	1.24	1.33
3	7	180	TRP	CZ3-CH2	-6.56	1.29	1.40
2	E	57	LYS	CB-CG	-6.56	1.34	1.52
2	K	93	LYS	CG-CD	-6.56	1.30	1.52
2	3	57	LYS	CB-CG	-6.56	1.34	1.52
3	4	145	PRO	CG-CD	-6.56	1.29	1.50
2	B	57	LYS	CB-CG	-6.56	1.34	1.52
2	H	77	PHE	CG-CD1	-6.56	1.28	1.38
2	H	93	LYS	CG-CD	-6.56	1.30	1.52
1	J	24	LYS	CB-CG	-6.56	1.34	1.52
2	Q	93	LYS	CG-CD	-6.56	1.30	1.52
1	8	24	LYS	CB-CG	-6.56	1.34	1.52
3	U	40	GLY	C-O	-6.56	1.13	1.23
2	Q	77	PHE	CG-CD1	-6.56	1.28	1.38
1	Z	24	LYS	CB-CG	-6.55	1.34	1.52
3	U	469	SER	CB-OG	-6.55	1.33	1.42
3	L	302	SER	CB-OG	-6.55	1.33	1.42
1	2	24	LYS	CB-CG	-6.55	1.34	1.52
3	U	145	PRO	CG-CD	-6.55	1.29	1.50
2	E	93	LYS	CG-CD	-6.55	1.30	1.52
2	K	92	GLY	CA-C	-6.55	1.41	1.51
2	N	57	LYS	CB-CG	-6.55	1.34	1.52
3	R	180	TRP	CZ3-CH2	-6.55	1.29	1.40
1	S	24	LYS	CB-CG	-6.55	1.34	1.52
2	X	93	LYS	CG-CD	-6.55	1.30	1.52
3	7	302	SER	CB-OG	-6.55	1.33	1.42
3	O	469	SER	CB-OG	-6.55	1.33	1.42
3	R	145	PRO	CG-CD	-6.55	1.29	1.50
2	X	57	LYS	CB-CG	-6.55	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	302	SER	CB-OG	-6.55	1.33	1.42
3	7	92	ARG	CZ-NH1	-6.55	1.24	1.33
3	U	302	SER	CB-OG	-6.55	1.33	1.42
2	3	93	LYS	CG-CD	-6.55	1.30	1.52
3	L	469	SER	CB-OG	-6.54	1.33	1.42
3	C	92	ARG	CZ-NH1	-6.54	1.24	1.33
1	G	24	LYS	CB-CG	-6.54	1.34	1.52
1	P	24	LYS	CB-CG	-6.54	1.34	1.52
3	I	180	TRP	CZ3-CH2	-6.54	1.29	1.40
3	U	180	TRP	CZ3-CH2	-6.54	1.29	1.40
2	Q	57	LYS	CB-CG	-6.54	1.34	1.52
2	0	57	LYS	CB-CG	-6.54	1.34	1.52
3	4	180	TRP	CZ3-CH2	-6.54	1.29	1.40
3	4	92	ARG	CZ-NH1	-6.54	1.24	1.33
2	N	77	PHE	CG-CD1	-6.53	1.28	1.38
2	T	113	VAL	CB-CG2	-6.53	1.39	1.52
3	V	268	PHE	CD1-CE1	-6.53	1.26	1.39
3	Y	302	SER	CB-OG	-6.53	1.33	1.42
3	4	302	SER	CB-OG	-6.53	1.33	1.42
3	O	92	ARG	CZ-NH1	-6.53	1.24	1.33
3	1	180	TRP	CZ3-CH2	-6.53	1.29	1.40
2	9	57	LYS	CB-CG	-6.53	1.34	1.52
3	C	469	SER	CB-OG	-6.53	1.33	1.42
3	U	92	ARG	CZ-NH1	-6.53	1.24	1.33
2	B	77	PHE	CG-CD1	-6.53	1.28	1.38
3	V	92	ARG	CZ-NH1	-6.53	1.24	1.33
2	6	77	PHE	CG-CD1	-6.53	1.28	1.38
3	V	469	SER	CB-OG	-6.52	1.33	1.42
1	2	7	GLU	CD-OE1	-6.52	1.18	1.25
2	3	77	PHE	CG-CD1	-6.52	1.28	1.38
3	7	378	ARG	CZ-NH2	-6.52	1.24	1.33
3	L	268	PHE	CD1-CE1	-6.52	1.26	1.39
3	1	92	ARG	CZ-NH1	-6.52	1.24	1.33
3	1	469	SER	CB-OG	-6.52	1.33	1.42
3	R	469	SER	CB-OG	-6.52	1.33	1.42
3	V	180	TRP	CD2-CE2	-6.51	1.33	1.41
3	1	268	PHE	CD1-CE1	-6.51	1.26	1.39
2	E	77	PHE	CG-CD1	-6.51	1.28	1.38
3	L	92	ARG	CZ-NH1	-6.51	1.24	1.33
2	0	77	PHE	CG-CD1	-6.51	1.28	1.38
1	W	1	MET	CB-CG	-6.51	1.30	1.51
3	Y	180	TRP	CD2-CE2	-6.51	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	45	TYR	CD2-CE2	-6.51	1.29	1.39
3	4	268	PHE	CD1-CE1	-6.51	1.26	1.39
3	7	469	SER	CB-OG	-6.51	1.33	1.42
3	R	268	PHE	CD1-CE1	-6.50	1.26	1.39
3	F	45	TYR	CD2-CE2	-6.50	1.29	1.39
3	F	469	SER	CB-OG	-6.50	1.33	1.42
2	9	77	PHE	CG-CD1	-6.50	1.28	1.38
3	F	92	ARG	CZ-NH1	-6.50	1.24	1.33
1	S	1	MET	CB-CG	-6.50	1.30	1.51
3	U	268	PHE	CD1-CE1	-6.50	1.26	1.39
2	K	77	PHE	CG-CD1	-6.50	1.29	1.38
1	P	1	MET	CB-CG	-6.50	1.30	1.51
3	R	92	ARG	CZ-NH1	-6.50	1.24	1.33
2	6	67	PRO	CB-CG	-6.50	1.17	1.50
3	I	92	ARG	CZ-NH1	-6.50	1.24	1.33
2	B	113	VAL	CB-CG2	-6.49	1.39	1.52
3	R	180	TRP	CD2-CE2	-6.49	1.33	1.41
2	X	113	VAL	CB-CG2	-6.49	1.39	1.52
2	0	67	PRO	CB-CG	-6.49	1.17	1.50
3	4	45	TYR	CD2-CE2	-6.49	1.29	1.39
1	A	1	MET	CB-CG	-6.49	1.30	1.51
1	D	1	MET	CB-CG	-6.49	1.30	1.51
1	M	1	MET	CB-CG	-6.49	1.30	1.51
1	8	1	MET	CB-CG	-6.49	1.30	1.51
2	X	67	PRO	CB-CG	-6.49	1.17	1.50
1	2	1	MET	CB-CG	-6.49	1.30	1.51
1	5	1	MET	CB-CG	-6.49	1.30	1.51
2	N	113	VAL	CB-CG2	-6.49	1.39	1.52
3	O	268	PHE	CD1-CE1	-6.49	1.26	1.39
3	I	469	SER	CB-OG	-6.49	1.33	1.42
2	K	67	PRO	CB-CG	-6.49	1.17	1.50
2	K	113	VAL	CB-CG2	-6.49	1.39	1.52
3	Y	469	SER	CB-OG	-6.49	1.33	1.42
2	H	37	LEU	C-O	-6.48	1.11	1.23
2	H	67	PRO	CB-CG	-6.48	1.17	1.50
1	Z	1	MET	CB-CG	-6.48	1.30	1.51
2	0	113	VAL	CB-CG2	-6.48	1.39	1.52
2	B	67	PRO	CB-CG	-6.48	1.17	1.50
3	C	268	PHE	CD1-CE1	-6.48	1.26	1.39
2	H	113	VAL	CB-CG2	-6.48	1.39	1.52
2	N	67	PRO	CB-CG	-6.48	1.17	1.50
1	G	1	MET	CB-CG	-6.48	1.30	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	45	TYR	CD2-CE2	-6.48	1.29	1.39
2	6	113	VAL	CB-CG2	-6.48	1.39	1.52
3	L	180	TRP	CD2-CE2	-6.48	1.33	1.41
3	F	305	PRO	C-O	-6.48	1.10	1.23
3	Y	45	TYR	CD2-CE2	-6.48	1.29	1.39
3	Y	268	PHE	CD1-CE1	-6.48	1.26	1.39
2	3	67	PRO	CB-CG	-6.48	1.17	1.50
3	U	45	TYR	CD2-CE2	-6.48	1.29	1.39
2	Q	67	PRO	CB-CG	-6.48	1.17	1.50
2	Q	113	VAL	CB-CG2	-6.48	1.39	1.52
2	T	67	PRO	CB-CG	-6.48	1.17	1.50
2	E	37	LEU	C-O	-6.47	1.11	1.23
3	F	180	TRP	CD2-CE2	-6.47	1.33	1.41
3	F	268	PHE	CD1-CE1	-6.47	1.26	1.39
3	O	45	TYR	CD2-CE2	-6.47	1.29	1.39
3	4	469	SER	CB-OG	-6.47	1.33	1.42
2	9	113	VAL	CB-CG2	-6.47	1.39	1.52
2	E	67	PRO	CB-CG	-6.47	1.17	1.50
3	I	305	PRO	C-O	-6.47	1.10	1.23
1	J	1	MET	CB-CG	-6.47	1.30	1.51
2	3	113	VAL	CB-CG2	-6.47	1.39	1.52
2	6	37	LEU	C-O	-6.47	1.11	1.23
2	9	67	PRO	CB-CG	-6.47	1.17	1.50
2	Q	78	GLU	CD-OE2	-6.47	1.18	1.25
2	3	37	LEU	C-O	-6.47	1.11	1.23
1	5	59	GLU	C-O	-6.47	1.11	1.23
1	D	59	GLU	C-O	-6.47	1.11	1.23
3	R	305	PRO	C-O	-6.47	1.10	1.23
3	C	45	TYR	CD2-CE2	-6.46	1.29	1.39
2	X	37	LEU	C-O	-6.46	1.11	1.23
3	C	180	TRP	CD2-CE2	-6.46	1.33	1.41
1	G	59	GLU	C-O	-6.46	1.11	1.23
2	E	113	VAL	CB-CG2	-6.46	1.39	1.52
3	1	345	GLU	CB-CG	-6.46	1.39	1.52
3	7	180	TRP	CD2-CE2	-6.46	1.33	1.41
3	O	416	PRO	CG-CD	-6.46	1.29	1.50
2	T	81	ARG	C-O	-6.46	1.11	1.23
3	Y	416	PRO	CG-CD	-6.46	1.29	1.50
1	Z	21	PHE	CE2-CZ	-6.46	1.25	1.37
3	U	416	PRO	CG-CD	-6.46	1.29	1.50
2	B	37	LEU	C-O	-6.45	1.11	1.23
3	I	416	PRO	CG-CD	-6.45	1.29	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	305	PRO	C-O	-6.45	1.10	1.23
2	K	81	ARG	C-O	-6.45	1.11	1.23
2	Q	37	LEU	C-O	-6.45	1.11	1.23
3	1	416	PRO	CG-CD	-6.45	1.29	1.50
3	C	305	PRO	C-O	-6.45	1.10	1.23
3	O	180	TRP	CD2-CE2	-6.45	1.33	1.41
3	O	508	GLU	CG-CD	6.45	1.61	1.51
3	R	45	TYR	CD2-CE2	-6.45	1.29	1.39
3	4	180	TRP	CD2-CE2	-6.45	1.33	1.41
3	7	305	PRO	C-O	-6.45	1.10	1.23
3	7	416	PRO	CG-CD	-6.45	1.29	1.50
3	1	45	TYR	CD2-CE2	-6.45	1.29	1.39
3	1	305	PRO	C-O	-6.45	1.10	1.23
3	V	416	PRO	CG-CD	-6.45	1.29	1.50
3	C	416	PRO	CG-CD	-6.45	1.29	1.50
3	F	416	PRO	CG-CD	-6.45	1.29	1.50
2	9	37	LEU	C-O	-6.45	1.11	1.23
3	O	440	TRP	CE3-CZ3	-6.44	1.27	1.38
1	2	59	GLU	C-O	-6.44	1.11	1.23
2	6	81	ARG	C-O	-6.44	1.11	1.23
3	I	180	TRP	CD2-CE2	-6.44	1.33	1.41
3	L	305	PRO	C-O	-6.44	1.10	1.23
1	P	59	GLU	C-O	-6.44	1.11	1.23
1	S	59	GLU	C-O	-6.44	1.11	1.23
2	T	37	LEU	C-O	-6.44	1.11	1.23
1	A	59	GLU	C-O	-6.44	1.11	1.23
3	V	345	GLU	CB-CG	-6.44	1.40	1.52
2	X	81	ARG	C-O	-6.44	1.11	1.23
3	7	268	PHE	CD1-CE1	-6.44	1.26	1.39
3	V	305	PRO	C-O	-6.44	1.10	1.23
3	I	268	PHE	CD1-CE1	-6.44	1.26	1.39
3	L	416	PRO	CG-CD	-6.44	1.29	1.50
2	Q	81	ARG	C-O	-6.44	1.11	1.23
2	9	81	ARG	C-O	-6.44	1.11	1.23
3	U	180	TRP	CD2-CE2	-6.44	1.33	1.41
2	H	81	ARG	C-O	-6.44	1.11	1.23
2	N	81	ARG	C-O	-6.44	1.11	1.23
1	2	32	TYR	CE2-CZ	-6.44	1.30	1.38
3	F	440	TRP	CE3-CZ3	-6.43	1.27	1.38
2	K	37	LEU	C-O	-6.43	1.11	1.23
3	O	305	PRO	C-O	-6.43	1.10	1.23
3	R	496	PHE	CG-CD2	-6.43	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7	508	GLU	CG-CD	6.43	1.61	1.51
3	O	496	PHE	CG-CD2	-6.43	1.29	1.38
3	R	569	TYR	CE2-CZ	-6.43	1.30	1.38
3	4	508	GLU	CG-CD	6.43	1.61	1.51
3	U	496	PHE	CG-CD2	-6.43	1.29	1.38
3	Y	305	PRO	C-O	-6.43	1.10	1.23
3	F	477	PHE	CE1-CZ	-6.43	1.25	1.37
1	W	21	PHE	CE2-CZ	-6.43	1.25	1.37
1	2	21	PHE	CE2-CZ	-6.43	1.25	1.37
2	3	81	ARG	C-O	-6.43	1.11	1.23
3	4	416	PRO	CG-CD	-6.43	1.29	1.50
3	L	440	TRP	CE3-CZ3	-6.43	1.27	1.38
2	N	37	LEU	C-O	-6.43	1.11	1.23
3	R	416	PRO	CG-CD	-6.43	1.29	1.50
2	E	81	ARG	C-O	-6.43	1.11	1.23
1	G	21	PHE	CE2-CZ	-6.43	1.25	1.37
3	L	345	GLU	CB-CG	-6.43	1.40	1.52
3	R	508	GLU	CG-CD	6.43	1.61	1.51
3	V	496	PHE	CG-CD2	-6.43	1.29	1.38
2	0	37	LEU	C-O	-6.43	1.11	1.23
3	1	440	TRP	CE3-CZ3	-6.43	1.27	1.38
3	4	305	PRO	C-O	-6.43	1.10	1.23
3	I	45	TYR	CD2-CE2	-6.42	1.29	1.39
1	J	21	PHE	CE2-CZ	-6.42	1.25	1.37
2	K	78	GLU	CD-OE2	-6.42	1.18	1.25
3	Y	440	TRP	CE3-CZ3	-6.42	1.27	1.38
3	1	496	PHE	CG-CD2	-6.42	1.29	1.38
3	7	45	TYR	CD2-CE2	-6.42	1.29	1.39
2	B	81	ARG	C-O	-6.42	1.11	1.23
3	I	345	GLU	CB-CG	-6.42	1.40	1.52
1	W	59	GLU	C-O	-6.42	1.11	1.23
2	0	81	ARG	C-O	-6.42	1.11	1.23
1	M	59	GLU	C-O	-6.42	1.11	1.23
3	R	440	TRP	CE3-CZ3	-6.42	1.27	1.38
1	J	59	GLU	C-O	-6.42	1.11	1.23
3	V	440	TRP	CE3-CZ3	-6.42	1.27	1.38
1	8	21	PHE	CE2-CZ	-6.42	1.25	1.37
3	C	440	TRP	CE3-CZ3	-6.42	1.27	1.38
3	F	345	GLU	CB-CG	-6.42	1.40	1.52
2	H	78	GLU	CD-OE2	-6.42	1.18	1.25
2	0	49	PHE	CE2-CZ	-6.42	1.25	1.37
2	0	78	GLU	CD-OE2	-6.42	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	78	GLU	CD-OE2	-6.42	1.18	1.25
3	R	477	PHE	CE1-CZ	-6.41	1.25	1.37
1	S	21	PHE	CE2-CZ	-6.41	1.25	1.37
3	1	180	TRP	CD2-CE2	-6.41	1.33	1.41
3	I	477	PHE	CE1-CZ	-6.41	1.25	1.37
1	5	32	TYR	CE2-CZ	-6.41	1.30	1.38
1	A	21	PHE	CE2-CZ	-6.41	1.25	1.37
3	I	440	TRP	CE3-CZ3	-6.41	1.27	1.38
3	7	381	GLN	CD-NE2	-6.41	1.16	1.32
2	B	78	GLU	CD-OE2	-6.41	1.18	1.25
2	T	49	PHE	CE2-CZ	-6.41	1.25	1.37
3	V	477	PHE	CE1-CZ	-6.41	1.25	1.37
2	6	78	GLU	CD-OE2	-6.41	1.18	1.25
3	7	440	TRP	CE3-CZ3	-6.41	1.27	1.38
3	7	477	PHE	CE1-CZ	-6.41	1.25	1.37
2	9	49	PHE	CE2-CZ	-6.41	1.25	1.37
3	C	508	GLU	CG-CD	6.41	1.61	1.51
3	C	345	GLU	CB-CG	-6.41	1.40	1.52
1	D	21	PHE	CE2-CZ	-6.41	1.25	1.37
3	I	134	ALA	C-N	-6.41	1.21	1.33
3	O	345	GLU	CB-CG	-6.41	1.40	1.52
3	U	440	TRP	CE3-CZ3	-6.41	1.27	1.38
2	3	49	PHE	CE2-CZ	-6.40	1.25	1.37
3	C	496	PHE	CG-CD2	-6.40	1.29	1.38
1	5	21	PHE	CE2-CZ	-6.40	1.25	1.37
3	C	477	PHE	CE1-CZ	-6.40	1.25	1.37
3	O	134	ALA	C-N	-6.40	1.21	1.33
1	P	21	PHE	CE2-CZ	-6.40	1.25	1.37
1	Z	59	GLU	C-O	-6.40	1.11	1.23
3	7	496	PHE	CG-CD2	-6.40	1.29	1.38
2	E	78	GLU	CD-OE2	-6.40	1.18	1.25
1	M	21	PHE	CE2-CZ	-6.40	1.25	1.37
3	F	496	PHE	CG-CD2	-6.40	1.29	1.38
3	O	228	GLY	C-O	-6.40	1.13	1.23
3	V	381	GLN	CD-NE2	-6.40	1.16	1.32
3	1	477	PHE	CE1-CZ	-6.40	1.25	1.37
1	8	32	TYR	CE2-CZ	-6.40	1.30	1.38
1	8	59	GLU	C-O	-6.40	1.11	1.23
3	4	440	TRP	CE3-CZ3	-6.39	1.27	1.38
3	7	345	GLU	CB-CG	-6.39	1.40	1.52
3	R	345	GLU	CB-CG	-6.39	1.40	1.52
3	Y	508	GLU	CG-CD	6.39	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	477	PHE	CE1-CZ	-6.39	1.25	1.37
3	V	569	TYR	CE2-CZ	-6.39	1.30	1.38
2	B	49	PHE	CE2-CZ	-6.39	1.25	1.37
3	L	381	GLN	CD-NE2	-6.39	1.16	1.32
2	N	49	PHE	CE2-CZ	-6.39	1.25	1.37
1	S	32	TYR	CE2-CZ	-6.39	1.30	1.38
3	V	508	GLU	CG-CD	6.39	1.61	1.51
3	Y	477	PHE	CE1-CZ	-6.39	1.25	1.37
3	U	345	GLU	CB-CG	-6.39	1.40	1.52
1	J	32	TYR	CE2-CZ	-6.38	1.30	1.38
3	4	496	PHE	CG-CD2	-6.38	1.29	1.38
3	U	228	GLY	C-O	-6.38	1.13	1.23
3	4	477	PHE	CE1-CZ	-6.38	1.25	1.37
3	C	381	GLN	CD-NE2	-6.38	1.16	1.32
3	F	508	GLU	CG-CD	6.38	1.61	1.51
2	H	49	PHE	CE2-CZ	-6.38	1.25	1.37
2	K	49	PHE	CE2-CZ	-6.38	1.25	1.37
3	L	508	GLU	CG-CD	6.38	1.61	1.51
2	6	49	PHE	CE2-CZ	-6.38	1.25	1.37
3	7	569	TYR	CE2-CZ	-6.38	1.30	1.38
2	9	78	GLU	CD-OE2	-6.38	1.18	1.25
3	U	134	ALA	C-N	-6.38	1.21	1.33
3	Y	381	GLN	CD-NE2	-6.38	1.17	1.32
3	4	345	GLU	CB-CG	-6.38	1.40	1.52
3	R	381	GLN	CD-NE2	-6.38	1.17	1.32
2	X	78	GLU	CD-OE2	-6.38	1.18	1.25
3	Y	569	TYR	CE2-CZ	-6.38	1.30	1.38
3	U	381	GLN	CD-NE2	-6.38	1.17	1.32
2	N	150	GLU	CG-CD	6.38	1.61	1.51
2	X	49	PHE	CE2-CZ	-6.38	1.25	1.37
3	4	381	GLN	CD-NE2	-6.38	1.17	1.32
3	L	477	PHE	CE1-CZ	-6.38	1.25	1.37
2	Q	49	PHE	CE2-CZ	-6.38	1.25	1.37
3	F	134	ALA	C-N	-6.37	1.21	1.33
1	M	86	PHE	CE2-CZ	-6.37	1.25	1.37
3	O	477	PHE	CE1-CZ	-6.37	1.25	1.37
3	R	134	ALA	C-N	-6.37	1.21	1.33
3	R	228	GLY	C-O	-6.37	1.13	1.23
3	1	381	GLN	CD-NE2	-6.37	1.17	1.32
3	4	569	TYR	CE2-CZ	-6.37	1.30	1.38
3	L	496	PHE	CG-CD2	-6.37	1.29	1.38
3	1	134	ALA	C-N	-6.37	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8	86	PHE	CE2-CZ	-6.37	1.25	1.37
1	A	32	TYR	CE2-CZ	-6.37	1.30	1.38
3	C	134	ALA	C-N	-6.37	1.21	1.33
3	I	381	GLN	CD-NE2	-6.37	1.17	1.32
3	L	134	ALA	C-N	-6.37	1.21	1.33
3	Y	228	GLY	C-O	-6.37	1.13	1.23
3	1	508	GLU	CG-CD	6.37	1.61	1.51
3	U	569	TYR	CE2-CZ	-6.37	1.30	1.38
1	P	86	PHE	CE2-CZ	-6.37	1.25	1.37
1	Z	66[A]	LYS	CB-CG	-6.37	1.35	1.52
1	Z	66[B]	LYS	CB-CG	-6.37	1.35	1.52
2	N	78	GLU	CD-OE2	-6.37	1.18	1.25
3	V	134	ALA	C-N	-6.37	1.21	1.33
2	T	78	GLU	CD-OE2	-6.36	1.18	1.25
2	E	150	GLU	CG-CD	6.36	1.61	1.51
1	D	86	PHE	CE2-CZ	-6.36	1.25	1.37
1	W	32	TYR	CE2-CZ	-6.36	1.30	1.38
3	1	63	ARG	CZ-NH1	-6.36	1.24	1.33
3	1	569	TYR	CE2-CZ	-6.36	1.30	1.38
3	C	569	TYR	CE2-CZ	-6.36	1.30	1.38
1	D	32	TYR	CE2-CZ	-6.36	1.30	1.38
1	G	32	TYR	CE2-CZ	-6.36	1.30	1.38
1	M	32	TYR	CE2-CZ	-6.36	1.30	1.38
3	R	433	LYS	CD-CE	-6.36	1.35	1.51
3	7	134	ALA	C-N	-6.36	1.21	1.33
2	E	49	PHE	CE2-CZ	-6.36	1.25	1.37
1	G	66[A]	LYS	CB-CG	-6.36	1.35	1.52
1	G	66[B]	LYS	CB-CG	-6.36	1.35	1.52
3	I	496	PHE	CG-CD2	-6.36	1.29	1.38
1	W	66[A]	LYS	CB-CG	-6.36	1.35	1.52
1	W	66[B]	LYS	CB-CG	-6.36	1.35	1.52
3	1	228	GLY	C-O	-6.36	1.13	1.23
3	4	228	GLY	C-O	-6.36	1.13	1.23
3	F	381	GLN	CD-NE2	-6.35	1.17	1.32
3	I	228	GLY	C-O	-6.35	1.13	1.23
3	I	508	GLU	CG-CD	6.35	1.61	1.51
1	J	66[A]	LYS	CB-CG	-6.35	1.35	1.52
1	J	66[B]	LYS	CB-CG	-6.35	1.35	1.52
3	L	228	GLY	C-O	-6.35	1.13	1.23
3	V	430	GLU	CB-CG	6.35	1.64	1.52
3	Y	345	GLU	CB-CG	-6.35	1.40	1.52
3	F	569	TYR	CE2-CZ	-6.35	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	66[A]	LYS	CB-CG	-6.35	1.35	1.52
1	P	66[B]	LYS	CB-CG	-6.35	1.35	1.52
1	5	86	PHE	CE2-CZ	-6.35	1.25	1.37
1	A	86	PHE	CE2-CZ	-6.35	1.25	1.37
3	O	381	GLN	CD-NE2	-6.35	1.17	1.32
3	V	228	GLY	C-O	-6.35	1.13	1.23
2	0	69	GLN	CB-CG	-6.35	1.35	1.52
3	Y	134	ALA	C-N	-6.35	1.21	1.33
2	K	69	GLN	CB-CG	-6.35	1.35	1.52
3	L	376	TRP	CE2-CZ2	-6.35	1.28	1.39
1	P	32	TYR	CE2-CZ	-6.35	1.30	1.38
3	V	121	THR	CB-CG2	-6.35	1.31	1.52
3	4	433	LYS	CD-CE	-6.35	1.35	1.51
1	5	66[A]	LYS	CB-CG	-6.35	1.35	1.52
1	5	66[B]	LYS	CB-CG	-6.35	1.35	1.52
1	G	86	PHE	CE2-CZ	-6.34	1.25	1.37
2	T	150	GLU	CG-CD	6.34	1.61	1.51
3	L	121	THR	CB-CG2	-6.34	1.31	1.52
1	M	66[A]	LYS	CB-CG	-6.34	1.35	1.52
1	M	66[B]	LYS	CB-CG	-6.34	1.35	1.52
3	Y	496	PHE	CG-CD2	-6.34	1.29	1.38
1	A	66[A]	LYS	CB-CG	-6.34	1.35	1.52
1	A	66[B]	LYS	CB-CG	-6.34	1.35	1.52
3	C	228	GLY	C-O	-6.34	1.13	1.23
2	H	74	PHE	CG-CD2	-6.34	1.29	1.38
1	Z	32	TYR	CE2-CZ	-6.34	1.30	1.38
1	2	66[A]	LYS	CB-CG	-6.34	1.35	1.52
1	2	66[B]	LYS	CB-CG	-6.34	1.35	1.52
3	4	121	THR	CB-CG2	-6.34	1.31	1.52
3	Y	121	THR	CB-CG2	-6.34	1.31	1.52
3	C	433	LYS	CD-CE	-6.34	1.35	1.51
3	O	569	TYR	CE2-CZ	-6.34	1.30	1.38
1	S	66[A]	LYS	CB-CG	-6.33	1.35	1.52
1	S	66[B]	LYS	CB-CG	-6.33	1.35	1.52
1	W	86	PHE	CE2-CZ	-6.33	1.25	1.37
2	9	74	PHE	CG-CD2	-6.33	1.29	1.38
1	D	66[A]	LYS	CB-CG	-6.33	1.35	1.52
1	D	66[B]	LYS	CB-CG	-6.33	1.35	1.52
2	Q	150	GLU	CG-CD	6.33	1.61	1.51
3	7	433	LYS	CD-CE	-6.33	1.35	1.51
3	U	508	GLU	CG-CD	6.33	1.61	1.51
3	L	433	LYS	CD-CE	-6.33	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	430	GLU	CB-CG	6.33	1.64	1.52
3	U	121	THR	CB-CG2	-6.33	1.31	1.52
3	C	121	THR	CB-CG2	-6.33	1.31	1.52
2	T	69	GLN	CB-CG	-6.33	1.35	1.52
3	I	569	TYR	CE2-CZ	-6.33	1.30	1.38
3	Y	376	TRP	CE2-CZ2	-6.33	1.28	1.39
3	Y	433	LYS	CD-CE	-6.33	1.35	1.51
2	3	69	GLN	CB-CG	-6.33	1.35	1.52
3	4	376	TRP	CE2-CZ2	-6.33	1.28	1.39
2	B	150	GLU	CG-CD	6.33	1.61	1.51
2	N	74	PHE	CG-CD2	-6.33	1.29	1.38
3	7	121	THR	CB-CG2	-6.33	1.31	1.52
3	I	121	THR	CB-CG2	-6.33	1.31	1.52
2	N	69	GLN	CB-CG	-6.33	1.35	1.52
3	1	121	THR	CB-CG2	-6.33	1.31	1.52
3	1	433	LYS	CD-CE	-6.33	1.35	1.51
2	3	74	PHE	CG-CD2	-6.33	1.29	1.38
1	8	66[A]	LYS	CB-CG	-6.33	1.35	1.52
1	8	66[B]	LYS	CB-CG	-6.33	1.35	1.52
2	B	69	GLN	CB-CG	-6.32	1.35	1.52
3	F	433	LYS	CD-CE	-6.32	1.35	1.51
3	L	569	TYR	CE2-CZ	-6.32	1.30	1.38
3	V	433	LYS	CD-CE	-6.32	1.35	1.51
2	X	69	GLN	CB-CG	-6.32	1.35	1.52
2	X	74	PHE	CG-CD2	-6.32	1.29	1.38
2	H	150	GLU	CG-CD	6.32	1.61	1.51
3	I	376	TRP	CE2-CZ2	-6.32	1.29	1.39
2	K	74	PHE	CG-CD2	-6.32	1.29	1.38
3	O	121	THR	CB-CG2	-6.32	1.31	1.52
3	O	433	LYS	CD-CE	-6.32	1.35	1.51
3	L	430	GLU	CB-CG	6.32	1.64	1.52
3	Y	430	GLU	CB-CG	6.32	1.64	1.52
3	4	430	GLU	CB-CG	6.32	1.64	1.52
3	7	387	LYS	CE-NZ	-6.32	1.33	1.49
3	F	228	GLY	C-O	-6.32	1.13	1.23
3	F	121	THR	CB-CG2	-6.32	1.31	1.52
1	S	86	PHE	CE2-CZ	-6.32	1.25	1.37
2	X	150	GLU	CG-CD	6.32	1.61	1.51
3	1	180	TRP	CZ2-CH2	-6.32	1.25	1.37
3	4	134	ALA	C-N	-6.32	1.21	1.33
2	9	69	GLN	CB-CG	-6.32	1.35	1.52
2	H	69	GLN	CB-CG	-6.32	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	150	GLU	CG-CD	6.32	1.61	1.51
2	Q	69	GLN	CB-CG	-6.32	1.35	1.52
3	R	121	THR	CB-CG2	-6.32	1.31	1.52
3	V	387	LYS	CE-NZ	-6.32	1.33	1.49
3	7	430	GLU	CB-CG	6.32	1.64	1.52
3	U	180	TRP	CZ2-CH2	-6.32	1.25	1.37
1	Z	86	PHE	CE2-CZ	-6.31	1.25	1.37
3	I	433	LYS	CD-CE	-6.31	1.35	1.51
3	I	514	ARG	CZ-NH2	-6.31	1.24	1.33
3	O	430	GLU	CB-CG	6.31	1.64	1.52
3	V	376	TRP	CE2-CZ2	-6.31	1.29	1.39
3	Y	221	TYR	CZ-OH	-6.31	1.27	1.37
3	Y	387	LYS	CE-NZ	-6.31	1.33	1.49
3	U	376	TRP	CE2-CZ2	-6.31	1.29	1.39
3	C	376	TRP	CE2-CZ2	-6.31	1.29	1.39
2	E	69	GLN	CB-CG	-6.31	1.35	1.52
2	Q	74	PHE	CG-CD2	-6.31	1.29	1.38
3	U	430	GLU	CB-CG	6.31	1.64	1.52
2	B	74	PHE	CG-CD2	-6.31	1.29	1.38
3	F	430	GLU	CB-CG	6.31	1.64	1.52
1	J	86	PHE	CE2-CZ	-6.31	1.25	1.37
3	L	221	TYR	CZ-OH	-6.31	1.27	1.37
3	O	268	PHE	CG-CD2	-6.31	1.29	1.38
3	O	514	ARG	CZ-NH2	-6.31	1.24	1.33
3	R	430	GLU	CB-CG	6.31	1.64	1.52
3	V	221	TYR	CZ-OH	-6.31	1.27	1.37
3	Y	268	PHE	CG-CD1	-6.31	1.29	1.38
1	2	86	PHE	CE2-CZ	-6.31	1.25	1.37
3	C	430	GLU	CB-CG	6.31	1.64	1.52
3	1	268	PHE	CG-CD2	-6.31	1.29	1.38
3	O	63	ARG	CZ-NH1	-6.30	1.24	1.33
2	6	69	GLN	CB-CG	-6.30	1.35	1.52
3	7	228	GLY	C-O	-6.30	1.13	1.23
3	U	268	PHE	CG-CD2	-6.30	1.29	1.38
3	R	376	TRP	CE2-CZ2	-6.30	1.29	1.39
3	V	268	PHE	CG-CD2	-6.30	1.29	1.38
2	6	150	GLU	CG-CD	6.30	1.61	1.51
3	C	221	TYR	CZ-OH	-6.30	1.27	1.37
3	I	430	GLU	CB-CG	6.30	1.64	1.52
2	3	150	GLU	CG-CD	6.30	1.61	1.51
3	4	180	TRP	CZ2-CH2	-6.30	1.25	1.37
3	U	221	TYR	CZ-OH	-6.30	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	180	TRP	CZ2-CH2	-6.30	1.25	1.37
3	1	376	TRP	CE2-CZ2	-6.30	1.29	1.39
2	9	150	GLU	CG-CD	6.30	1.61	1.51
3	O	569	TYR	CG-CD2	-6.30	1.30	1.39
2	0	150	GLU	CG-CD	6.30	1.61	1.51
3	1	268	PHE	CG-CD1	-6.30	1.29	1.38
3	7	180	TRP	CZ2-CH2	-6.30	1.25	1.37
3	F	221	TYR	CZ-OH	-6.29	1.27	1.37
3	F	268	PHE	CG-CD2	-6.29	1.29	1.38
3	I	221	TYR	CZ-OH	-6.29	1.27	1.37
3	1	387	LYS	CE-NZ	-6.29	1.33	1.49
3	C	387	LYS	CE-NZ	-6.29	1.33	1.49
3	I	569	TYR	CG-CD2	-6.29	1.30	1.39
3	R	387	LYS	CE-NZ	-6.29	1.33	1.49
2	0	74	PHE	CG-CD2	-6.29	1.29	1.38
3	1	477	PHE	CD1-CE1	-6.29	1.26	1.39
3	4	221	TYR	CZ-OH	-6.29	1.27	1.37
3	F	514	ARG	CZ-NH2	-6.29	1.24	1.33
3	R	514	ARG	CZ-NH2	-6.29	1.24	1.33
3	V	514	ARG	CZ-NH2	-6.29	1.24	1.33
3	4	387	LYS	CE-NZ	-6.29	1.33	1.49
3	U	387	LYS	CE-NZ	-6.29	1.33	1.49
3	F	376	TRP	CE2-CZ2	-6.29	1.29	1.39
3	C	180	TRP	CZ2-CH2	-6.29	1.25	1.37
3	C	268	PHE	CG-CD2	-6.29	1.29	1.38
3	F	81	ARG	CG-CD	-6.29	1.36	1.51
3	I	477	PHE	CD1-CE1	-6.29	1.26	1.39
3	O	376	TRP	CE2-CZ2	-6.29	1.29	1.39
3	R	268	PHE	CG-CD2	-6.29	1.29	1.38
3	U	433	LYS	CD-CE	-6.29	1.35	1.51
3	L	268	PHE	CG-CD1	-6.28	1.29	1.38
3	L	514	ARG	CZ-NH2	-6.28	1.24	1.33
3	7	221	TYR	CZ-OH	-6.28	1.27	1.37
3	7	376	TRP	CE2-CZ2	-6.28	1.29	1.39
3	U	475	PRO	CB-CG	-6.28	1.18	1.50
3	C	63	ARG	CZ-NH1	-6.28	1.24	1.33
3	I	180	TRP	CZ2-CH2	-6.28	1.25	1.37
3	L	63	ARG	CZ-NH1	-6.28	1.24	1.33
3	L	477	PHE	CD1-CE1	-6.28	1.26	1.39
3	O	387	LYS	CE-NZ	-6.28	1.33	1.49
3	1	221	TYR	CZ-OH	-6.28	1.27	1.37
3	U	63	ARG	CZ-NH1	-6.28	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	81	ARG	CG-CD	-6.28	1.36	1.51
3	4	268	PHE	CG-CD2	-6.28	1.29	1.38
3	O	475	PRO	CB-CG	-6.28	1.18	1.50
3	V	79	ASP	C-O	-6.28	1.11	1.23
3	V	180	TRP	CZ2-CH2	-6.27	1.25	1.37
3	4	475	PRO	CB-CG	-6.27	1.18	1.50
3	7	268	PHE	CG-CD2	-6.27	1.29	1.38
3	F	475	PRO	CB-CG	-6.27	1.18	1.50
3	I	387	LYS	CE-NZ	-6.27	1.33	1.49
3	L	387	LYS	CE-NZ	-6.27	1.33	1.49
3	L	475	PRO	CB-CG	-6.27	1.18	1.50
3	4	79	ASP	C-O	-6.27	1.11	1.23
3	4	477	PHE	CD1-CE1	-6.27	1.26	1.39
3	U	268	PHE	CG-CD1	-6.27	1.29	1.38
3	I	79	ASP	C-O	-6.27	1.11	1.23
3	Y	569	TYR	CG-CD2	-6.27	1.30	1.39
3	F	79	ASP	C-O	-6.27	1.11	1.23
3	L	268	PHE	CG-CD2	-6.27	1.29	1.38
3	R	180	TRP	CZ2-CH2	-6.27	1.25	1.37
3	V	268	PHE	CG-CD1	-6.27	1.29	1.38
2	E	74	PHE	CG-CD2	-6.27	1.29	1.38
3	F	387	LYS	CE-NZ	-6.27	1.33	1.49
3	I	268	PHE	CG-CD2	-6.27	1.29	1.38
3	1	514	ARG	CZ-NH2	-6.27	1.25	1.33
2	6	74	PHE	CG-CD2	-6.27	1.29	1.38
3	7	268	PHE	CG-CD1	-6.27	1.29	1.38
3	C	477	PHE	CD1-CE1	-6.27	1.26	1.39
3	O	477	PHE	CD1-CE1	-6.27	1.26	1.39
3	7	63	ARG	CZ-NH1	-6.27	1.25	1.33
3	O	79	ASP	C-O	-6.26	1.11	1.23
3	V	475	PRO	CB-CG	-6.26	1.18	1.50
3	Y	477	PHE	CD1-CE1	-6.26	1.26	1.39
2	T	74	PHE	CG-CD2	-6.26	1.29	1.38
3	1	81	ARG	CG-CD	-6.26	1.36	1.51
3	4	63	ARG	CZ-NH1	-6.26	1.25	1.33
3	C	475	PRO	CB-CG	-6.26	1.18	1.50
3	I	268	PHE	CG-CD1	-6.26	1.29	1.38
3	O	527	LYS	CG-CD	-6.26	1.31	1.52
3	R	475	PRO	CB-CG	-6.26	1.18	1.50
3	V	63	ARG	CZ-NH1	-6.26	1.25	1.33
3	Y	514	ARG	CZ-NH2	-6.26	1.25	1.33
3	1	79	ASP	C-O	-6.26	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	79	ASP	C-O	-6.26	1.11	1.23
3	C	268	PHE	CG-CD1	-6.26	1.29	1.38
3	F	477	PHE	CD1-CE1	-6.26	1.26	1.39
3	R	63	ARG	CZ-NH1	-6.26	1.25	1.33
3	R	477	PHE	CD1-CE1	-6.26	1.26	1.39
3	F	268	PHE	CG-CD1	-6.26	1.29	1.38
3	R	79	ASP	C-O	-6.26	1.11	1.23
3	R	221	TYR	CZ-OH	-6.26	1.27	1.37
3	L	180	TRP	CZ2-CH2	-6.25	1.25	1.37
3	1	475	PRO	CB-CG	-6.25	1.18	1.50
3	C	514	ARG	CZ-NH2	-6.25	1.25	1.33
3	F	63	ARG	CZ-NH1	-6.25	1.25	1.33
3	F	527	LYS	CG-CD	-6.25	1.31	1.52
3	V	477	PHE	CD1-CE1	-6.25	1.26	1.39
3	7	475	PRO	CB-CG	-6.25	1.18	1.50
3	7	514	ARG	CZ-NH2	-6.25	1.25	1.33
3	U	79	ASP	C-O	-6.25	1.11	1.23
3	U	477	PHE	CD1-CE1	-6.25	1.26	1.39
3	I	63	ARG	CZ-NH1	-6.25	1.25	1.33
3	I	81	ARG	CG-CD	-6.25	1.36	1.51
3	Y	180	TRP	CZ2-CH2	-6.25	1.25	1.37
3	Y	475	PRO	CB-CG	-6.25	1.18	1.50
3	7	477	PHE	CD1-CE1	-6.25	1.26	1.39
3	C	81	ARG	CG-CD	-6.25	1.36	1.51
3	R	268	PHE	CG-CD1	-6.25	1.29	1.38
3	V	81	ARG	CG-CD	-6.25	1.36	1.51
1	W	86	PHE	CD1-CE1	-6.25	1.26	1.39
3	Y	268	PHE	CG-CD2	-6.25	1.29	1.38
3	I	475	PRO	CB-CG	-6.25	1.18	1.50
3	Y	79	ASP	C-O	-6.25	1.11	1.23
3	1	569	TYR	CG-CD2	-6.25	1.31	1.39
3	7	79	ASP	C-O	-6.25	1.11	1.23
3	7	81	ARG	CG-CD	-6.25	1.36	1.51
3	7	527	LYS	CG-CD	-6.25	1.31	1.52
3	7	569	TYR	CG-CD2	-6.25	1.31	1.39
3	O	180	TRP	CZ2-CH2	-6.25	1.25	1.37
3	O	221	TYR	CZ-OH	-6.25	1.27	1.37
3	Y	63	ARG	CZ-NH1	-6.24	1.25	1.33
3	V	527	LYS	CG-CD	-6.24	1.31	1.52
3	U	21[A]	ILE	CG1-CD1	-6.24	1.07	1.50
3	U	21[B]	ILE	CG1-CD1	-6.24	1.07	1.50
3	U	81	ARG	CG-CD	-6.24	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	527	LYS	CG-CD	-6.24	1.31	1.52
3	F	21[A]	ILE	CG1-CD1	-6.24	1.07	1.50
3	F	21[B]	ILE	CG1-CD1	-6.24	1.07	1.50
3	I	527	LYS	CG-CD	-6.24	1.31	1.52
3	L	527	LYS	CG-CD	-6.24	1.31	1.52
3	Y	527	LYS	CG-CD	-6.24	1.31	1.52
3	4	514	ARG	CZ-NH2	-6.24	1.25	1.33
3	U	514	ARG	CZ-NH2	-6.24	1.25	1.33
3	U	527	LYS	CG-CD	-6.24	1.31	1.52
3	U	569	TYR	CG-CD2	-6.24	1.31	1.39
3	L	79	ASP	C-O	-6.24	1.11	1.23
3	1	527	LYS	CG-CD	-6.24	1.31	1.52
3	4	21[A]	ILE	CG1-CD1	-6.24	1.07	1.50
3	4	21[B]	ILE	CG1-CD1	-6.24	1.07	1.50
3	7	21[A]	ILE	CG1-CD1	-6.24	1.07	1.50
3	7	21[B]	ILE	CG1-CD1	-6.24	1.07	1.50
3	F	569	TYR	CG-CD2	-6.23	1.31	1.39
1	J	86	PHE	CD1-CE1	-6.23	1.26	1.39
3	O	21[A]	ILE	CG1-CD1	-6.23	1.07	1.50
3	O	21[B]	ILE	CG1-CD1	-6.23	1.07	1.50
3	R	527	LYS	CG-CD	-6.23	1.31	1.52
3	Y	81	ARG	CG-CD	-6.23	1.36	1.51
3	C	21[A]	ILE	CG1-CD1	-6.23	1.07	1.50
3	C	21[B]	ILE	CG1-CD1	-6.23	1.07	1.50
3	L	81	ARG	CG-CD	-6.23	1.36	1.51
3	O	81	ARG	CG-CD	-6.23	1.36	1.51
3	Y	21[A]	ILE	CG1-CD1	-6.23	1.07	1.50
3	Y	21[B]	ILE	CG1-CD1	-6.23	1.07	1.50
3	L	569	TYR	CG-CD2	-6.23	1.31	1.39
3	Y	166	PRO	C-O	-6.23	1.10	1.23
3	4	527	LYS	CG-CD	-6.23	1.31	1.52
3	L	21[A]	ILE	CG1-CD1	-6.23	1.07	1.50
3	L	21[B]	ILE	CG1-CD1	-6.23	1.07	1.50
3	I	21[A]	ILE	CG1-CD1	-6.22	1.07	1.50
3	I	21[B]	ILE	CG1-CD1	-6.22	1.07	1.50
3	V	21[A]	ILE	CG1-CD1	-6.22	1.07	1.50
3	V	21[B]	ILE	CG1-CD1	-6.22	1.07	1.50
3	4	569	TYR	CG-CD2	-6.22	1.31	1.39
3	R	21[A]	ILE	CG1-CD1	-6.22	1.07	1.50
3	R	21[B]	ILE	CG1-CD1	-6.22	1.07	1.50
1	S	86	PHE	CD1-CE1	-6.22	1.26	1.39
1	Z	86	PHE	CD1-CE1	-6.22	1.26	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	21[A]	ILE	CG1-CD1	-6.22	1.07	1.50
3	1	21[B]	ILE	CG1-CD1	-6.22	1.07	1.50
3	C	569	TYR	CG-CD2	-6.22	1.31	1.39
1	2	86	PHE	CD1-CE1	-6.22	1.26	1.39
3	4	81	ARG	CG-CD	-6.22	1.36	1.51
1	A	86	PHE	CD1-CE1	-6.22	1.26	1.39
3	V	569	TYR	CG-CD2	-6.22	1.31	1.39
3	4	268	PHE	CG-CD1	-6.22	1.29	1.38
3	O	268	PHE	CG-CD1	-6.21	1.29	1.38
1	P	86	PHE	CD1-CE1	-6.21	1.26	1.39
1	5	86	PHE	CD1-CE1	-6.21	1.26	1.39
3	I	75	VAL	CB-CG2	-6.21	1.39	1.52
3	O	75	VAL	CB-CG2	-6.21	1.39	1.52
1	D	86	PHE	CD1-CE1	-6.21	1.26	1.39
3	1	75	VAL	CB-CG2	-6.21	1.39	1.52
3	7	166	PRO	C-O	-6.21	1.10	1.23
3	L	166	PRO	C-O	-6.20	1.10	1.23
3	L	478	TYR	CZ-OH	-6.20	1.27	1.37
1	M	86	PHE	CD1-CE1	-6.20	1.26	1.39
3	V	407[A]	ARG	CG-CD	-6.20	1.36	1.51
3	V	407[B]	ARG	CG-CD	-6.20	1.36	1.51
3	4	75	VAL	CB-CG2	-6.20	1.39	1.52
3	R	166	PRO	C-O	-6.20	1.10	1.23
3	F	407[A]	ARG	CG-CD	-6.20	1.36	1.51
3	F	407[B]	ARG	CG-CD	-6.20	1.36	1.51
1	G	86	PHE	CD1-CE1	-6.20	1.26	1.39
3	Y	127	GLU	CD-OE2	-6.20	1.18	1.25
3	U	166	PRO	C-O	-6.20	1.10	1.23
3	C	407[A]	ARG	CG-CD	-6.19	1.36	1.51
3	C	407[B]	ARG	CG-CD	-6.19	1.36	1.51
3	F	75	VAL	CB-CG2	-6.19	1.39	1.52
3	F	570	PHE	CD1-CE1	-6.19	1.26	1.39
3	I	166	PRO	C-O	-6.19	1.10	1.23
3	L	407[A]	ARG	CG-CD	-6.19	1.36	1.51
3	L	407[B]	ARG	CG-CD	-6.19	1.36	1.51
3	7	437	LEU	CG-CD2	-6.19	1.28	1.51
3	U	75	VAL	CB-CG2	-6.19	1.39	1.52
3	U	478	TYR	CZ-OH	-6.19	1.27	1.37
3	C	166	PRO	C-O	-6.19	1.10	1.23
3	I	407[A]	ARG	CG-CD	-6.19	1.36	1.51
3	I	407[B]	ARG	CG-CD	-6.19	1.36	1.51
3	I	570	PHE	CD1-CE1	-6.19	1.26	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	478	TYR	CZ-OH	-6.19	1.27	1.37
3	1	407[A]	ARG	CG-CD	-6.19	1.36	1.51
3	1	407[B]	ARG	CG-CD	-6.19	1.36	1.51
3	7	407[A]	ARG	CG-CD	-6.19	1.36	1.51
3	7	407[B]	ARG	CG-CD	-6.19	1.36	1.51
3	R	569	TYR	CG-CD2	-6.19	1.31	1.39
3	C	75	VAL	CB-CG2	-6.19	1.39	1.52
3	1	570	PHE	CD1-CE1	-6.19	1.26	1.39
3	7	127	GLU	CD-OE2	-6.19	1.18	1.25
3	V	570	PHE	CD1-CE1	-6.19	1.26	1.39
3	L	75	VAL	CB-CG2	-6.18	1.39	1.52
3	1	166	PRO	C-O	-6.18	1.10	1.23
3	1	437	LEU	CG-CD2	-6.18	1.28	1.51
3	4	166	PRO	C-O	-6.18	1.10	1.23
3	L	437	LEU	CG-CD2	-6.18	1.28	1.51
3	R	407[A]	ARG	CG-CD	-6.18	1.36	1.51
3	R	407[B]	ARG	CG-CD	-6.18	1.36	1.51
3	V	437	LEU	CG-CD2	-6.18	1.28	1.51
3	U	127	GLU	CD-OE2	-6.18	1.18	1.25
3	U	407[A]	ARG	CG-CD	-6.18	1.36	1.51
3	U	407[B]	ARG	CG-CD	-6.18	1.36	1.51
3	Y	437	LEU	CG-CD2	-6.18	1.28	1.51
3	4	437	LEU	CG-CD2	-6.18	1.28	1.51
3	R	127	GLU	CD-OE2	-6.18	1.18	1.25
3	4	407[A]	ARG	CG-CD	-6.18	1.36	1.51
3	4	407[B]	ARG	CG-CD	-6.18	1.36	1.51
3	7	75	VAL	CB-CG2	-6.18	1.39	1.52
3	F	437	LEU	CG-CD2	-6.18	1.28	1.51
3	R	75	VAL	CB-CG2	-6.18	1.39	1.52
3	I	437	LEU	CG-CD2	-6.17	1.29	1.51
3	L	570	PHE	CD1-CE1	-6.17	1.26	1.39
3	O	166	PRO	C-O	-6.17	1.10	1.23
3	U	570	PHE	CD1-CE1	-6.17	1.26	1.39
3	C	437	LEU	CG-CD2	-6.17	1.29	1.51
3	Y	407[A]	ARG	CG-CD	-6.17	1.36	1.51
3	Y	407[B]	ARG	CG-CD	-6.17	1.36	1.51
3	O	437	LEU	CG-CD2	-6.17	1.29	1.51
3	Y	149	TYR	CZ-OH	-6.17	1.27	1.37
3	L	29	PHE	CG-CD1	-6.17	1.29	1.38
3	Y	75	VAL	CB-CG2	-6.17	1.39	1.52
3	1	149	TYR	CZ-OH	-6.17	1.27	1.37
1	8	86	PHE	CD1-CE1	-6.17	1.26	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	437	LEU	CG-CD2	-6.17	1.29	1.51
3	C	478	TYR	CZ-OH	-6.17	1.27	1.37
3	R	437	LEU	CG-CD2	-6.17	1.29	1.51
3	I	478	TYR	CZ-OH	-6.17	1.27	1.37
3	O	407[A]	ARG	CG-CD	-6.17	1.36	1.51
3	O	407[B]	ARG	CG-CD	-6.17	1.36	1.51
3	R	478	TYR	CZ-OH	-6.17	1.27	1.37
3	C	570	PHE	CD1-CE1	-6.16	1.26	1.39
3	V	75	VAL	CB-CG2	-6.16	1.40	1.52
3	V	149	TYR	CZ-OH	-6.16	1.27	1.37
3	V	166	PRO	C-O	-6.16	1.10	1.23
3	Y	570	PHE	CD1-CE1	-6.16	1.26	1.39
3	O	478	TYR	CZ-OH	-6.16	1.27	1.37
3	Y	29	PHE	CG-CD1	-6.16	1.29	1.38
3	7	478	TYR	CZ-OH	-6.16	1.27	1.37
3	U	29	PHE	CG-CD1	-6.15	1.29	1.38
3	O	570	PHE	CD1-CE1	-6.15	1.26	1.39
3	V	127	GLU	CD-OE2	-6.15	1.18	1.25
3	Y	478	TYR	CZ-OH	-6.15	1.27	1.37
3	4	478	TYR	CZ-OH	-6.15	1.27	1.37
3	F	166	PRO	C-O	-6.15	1.10	1.23
3	1	29	PHE	CG-CD1	-6.15	1.29	1.38
3	R	570	PHE	CD1-CE1	-6.15	1.26	1.39
3	C	149	TYR	CZ-OH	-6.15	1.27	1.37
3	1	127	GLU	CD-OE2	-6.15	1.18	1.25
3	4	149	TYR	CZ-OH	-6.15	1.27	1.37
3	7	257	GLU	C-O	-6.15	1.11	1.23
3	C	127	GLU	CD-OE2	-6.15	1.18	1.25
2	N	160	PHE	CD1-CE1	-6.14	1.26	1.39
3	O	13	PHE	CG-CD2	-6.14	1.29	1.38
3	7	149	TYR	CZ-OH	-6.14	1.27	1.37
3	R	29	PHE	CG-CD1	-6.14	1.29	1.38
3	F	478	TYR	CZ-OH	-6.14	1.27	1.37
3	L	149	TYR	CZ-OH	-6.14	1.27	1.37
3	1	478	TYR	CZ-OH	-6.14	1.27	1.37
3	4	570	PHE	CD1-CE1	-6.14	1.26	1.39
3	C	29	PHE	CG-CD1	-6.13	1.29	1.38
3	7	570	PHE	CD1-CE1	-6.13	1.26	1.39
3	U	149	TYR	CZ-OH	-6.13	1.27	1.37
3	I	29	PHE	CG-CD1	-6.13	1.29	1.38
3	7	29	PHE	CG-CD1	-6.13	1.29	1.38
3	L	257	GLU	C-O	-6.13	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	160	PHE	CD1-CE1	-6.13	1.26	1.39
3	F	29	PHE	CG-CD1	-6.13	1.29	1.38
3	F	257	GLU	C-O	-6.13	1.11	1.23
3	Y	257	GLU	C-O	-6.13	1.11	1.23
3	4	257	GLU	C-O	-6.13	1.11	1.23
3	4	127	GLU	CD-OE2	-6.12	1.19	1.25
3	C	257	GLU	C-O	-6.12	1.11	1.23
3	R	149	TYR	CZ-OH	-6.12	1.27	1.37
3	F	127	GLU	CD-OE2	-6.12	1.19	1.25
3	F	149	TYR	CZ-OH	-6.12	1.27	1.37
3	I	127	GLU	CD-OE2	-6.12	1.19	1.25
3	O	29	PHE	CG-CD1	-6.12	1.29	1.38
3	1	257	GLU	C-O	-6.12	1.11	1.23
3	U	13	PHE	CG-CD2	-6.12	1.29	1.38
3	U	257	GLU	C-O	-6.12	1.11	1.23
2	K	160	PHE	CD1-CE1	-6.12	1.27	1.39
3	O	127	GLU	CD-OE2	-6.12	1.19	1.25
3	O	149	TYR	CZ-OH	-6.11	1.27	1.37
2	Q	160	PHE	CD1-CE1	-6.11	1.27	1.39
3	R	257	GLU	C-O	-6.11	1.11	1.23
3	V	257	GLU	C-O	-6.11	1.11	1.23
3	O	257	GLU	C-O	-6.11	1.11	1.23
1	P	58[A]	LYS	CB-CG	-6.11	1.36	1.52
1	P	58[B]	LYS	CB-CG	-6.11	1.36	1.52
3	F	13	PHE	CG-CD2	-6.11	1.29	1.38
3	I	149	TYR	CZ-OH	-6.11	1.27	1.37
3	I	257	GLU	C-O	-6.11	1.11	1.23
2	0	160	PHE	CD1-CE1	-6.11	1.27	1.39
1	5	58[A]	LYS	CB-CG	-6.11	1.36	1.52
1	5	58[B]	LYS	CB-CG	-6.11	1.36	1.52
1	S	58[A]	LYS	CB-CG	-6.11	1.36	1.52
1	S	58[B]	LYS	CB-CG	-6.11	1.36	1.52
3	4	13	PHE	CG-CD2	-6.11	1.29	1.38
2	6	160	PHE	CD1-CE1	-6.11	1.27	1.39
2	6	49	PHE	CD2-CE2	-6.10	1.27	1.39
3	V	29	PHE	CG-CD1	-6.10	1.29	1.38
3	L	13	PHE	CG-CD2	-6.10	1.29	1.38
3	4	63	ARG	CZ-NH2	-6.10	1.25	1.33
2	E	160	PHE	CD1-CE1	-6.10	1.27	1.39
2	N	49	PHE	CD2-CE2	-6.10	1.27	1.39
3	R	223	VAL	CB-CG1	-6.10	1.40	1.52
3	7	63	ARG	CZ-NH2	-6.10	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	223	VAL	CB-CG1	-6.10	1.40	1.52
3	C	13	PHE	CG-CD2	-6.09	1.29	1.38
1	W	58[A]	LYS	CB-CG	-6.09	1.36	1.52
1	W	58[B]	LYS	CB-CG	-6.09	1.36	1.52
3	4	29	PHE	CG-CD1	-6.09	1.29	1.38
2	B	160	PHE	CD1-CE1	-6.09	1.27	1.39
3	O	63	ARG	CZ-NH2	-6.09	1.25	1.33
2	E	49	PHE	CD2-CE2	-6.09	1.27	1.39
1	J	58[A]	LYS	CB-CG	-6.09	1.36	1.52
1	J	58[B]	LYS	CB-CG	-6.09	1.36	1.52
2	H	160	PHE	CD1-CE1	-6.09	1.27	1.39
2	X	144	GLU	CD-OE2	-6.09	1.19	1.25
3	7	223	VAL	CB-CG1	-6.09	1.40	1.52
3	R	159	PHE	CE1-CZ	-6.09	1.25	1.37
2	X	160	PHE	CD1-CE1	-6.09	1.27	1.39
3	1	159	PHE	CE1-CZ	-6.08	1.25	1.37
3	I	63	ARG	CZ-NH2	-6.08	1.25	1.33
3	L	159	PHE	CE1-CZ	-6.08	1.25	1.37
2	9	49	PHE	CD2-CE2	-6.08	1.27	1.39
1	A	58[A]	LYS	CB-CG	-6.08	1.36	1.52
1	A	58[B]	LYS	CB-CG	-6.08	1.36	1.52
3	R	63	ARG	CZ-NH2	-6.08	1.25	1.33
3	7	13	PHE	CG-CD2	-6.08	1.29	1.38
2	9	160	PHE	CD1-CE1	-6.08	1.27	1.39
2	T	49	PHE	CD2-CE2	-6.08	1.27	1.39
1	Z	58[A]	LYS	CB-CG	-6.08	1.36	1.52
1	Z	58[B]	LYS	CB-CG	-6.08	1.36	1.52
2	Q	49	PHE	CD2-CE2	-6.08	1.27	1.39
3	V	159	PHE	CE1-CZ	-6.08	1.25	1.37
3	1	13	PHE	CG-CD2	-6.08	1.29	1.38
1	2	58[A]	LYS	CB-CG	-6.08	1.36	1.52
1	2	58[B]	LYS	CB-CG	-6.08	1.36	1.52
3	7	289	ILE	CB-CG2	-6.08	1.34	1.52
3	U	189	VAL	CB-CG2	-6.08	1.40	1.52
1	D	58[A]	LYS	CB-CG	-6.08	1.36	1.52
1	D	58[B]	LYS	CB-CG	-6.08	1.36	1.52
1	M	58[A]	LYS	CB-CG	-6.08	1.36	1.52
1	M	58[B]	LYS	CB-CG	-6.08	1.36	1.52
2	3	49	PHE	CD2-CE2	-6.08	1.27	1.39
1	8	58[A]	LYS	CB-CG	-6.08	1.36	1.52
1	8	58[B]	LYS	CB-CG	-6.08	1.36	1.52
3	I	455	GLY	N-CA	-6.07	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	63	ARG	CZ-NH2	-6.07	1.25	1.33
3	L	127	GLU	CD-OE2	-6.07	1.19	1.25
2	B	49	PHE	CD2-CE2	-6.07	1.27	1.39
1	G	58[A]	LYS	CB-CG	-6.07	1.36	1.52
1	G	58[B]	LYS	CB-CG	-6.07	1.36	1.52
3	I	189	VAL	CB-CG2	-6.07	1.40	1.52
3	R	289	ILE	CB-CG2	-6.07	1.34	1.52
3	V	189	VAL	CB-CG2	-6.07	1.40	1.52
3	Y	13	PHE	CG-CD2	-6.07	1.29	1.38
3	4	289	ILE	CB-CG2	-6.07	1.34	1.52
3	F	63	ARG	CZ-NH2	-6.07	1.25	1.33
2	H	49	PHE	CD2-CE2	-6.07	1.27	1.39
3	Y	343	ARG	CZ-NH2	-6.07	1.25	1.33
3	1	343	ARG	CZ-NH2	-6.07	1.25	1.33
3	4	159	PHE	CE1-CZ	-6.07	1.25	1.37
3	I	159	PHE	CE1-CZ	-6.07	1.25	1.37
3	L	440	TRP	CE2-CZ2	-6.07	1.29	1.39
3	O	440	TRP	CE2-CZ2	-6.07	1.29	1.39
3	R	13	PHE	CG-CD2	-6.07	1.29	1.38
3	R	455	GLY	N-CA	-6.07	1.36	1.46
3	Y	289	ILE	CB-CG2	-6.07	1.34	1.52
3	R	343	ARG	CZ-NH2	-6.06	1.25	1.33
3	V	440	TRP	CE2-CZ2	-6.06	1.29	1.39
2	X	49	PHE	CD2-CE2	-6.06	1.27	1.39
2	3	160	PHE	CD1-CE1	-6.06	1.27	1.39
3	U	343	ARG	CZ-NH2	-6.06	1.25	1.33
3	F	289	ILE	CB-CG2	-6.06	1.34	1.52
2	0	49	PHE	CD2-CE2	-6.06	1.27	1.39
3	C	159	PHE	CE1-CZ	-6.06	1.25	1.37
3	F	223	VAL	CB-CG1	-6.06	1.40	1.52
3	1	522	CYS	CB-SG	-6.06	1.72	1.82
3	I	289	ILE	CB-CG2	-6.06	1.34	1.52
2	K	49	PHE	CD2-CE2	-6.06	1.27	1.39
3	O	223	VAL	CB-CG1	-6.06	1.40	1.52
3	V	223	VAL	CB-CG1	-6.06	1.40	1.52
2	0	144	GLU	CD-OE2	-6.06	1.19	1.25
3	7	159	PHE	CE1-CZ	-6.06	1.25	1.37
3	U	159	PHE	CE1-CZ	-6.06	1.25	1.37
3	C	223	VAL	CB-CG1	-6.06	1.40	1.52
3	C	289	ILE	CB-CG2	-6.06	1.34	1.52
3	R	189	VAL	CB-CG2	-6.05	1.40	1.52
3	7	343	ARG	CZ-NH2	-6.05	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	189	VAL	CB-CG2	-6.05	1.40	1.52
3	L	223	VAL	CB-CG1	-6.05	1.40	1.52
3	C	343	ARG	CZ-NH2	-6.05	1.25	1.33
3	F	522	CYS	CB-SG	-6.05	1.72	1.82
3	L	189	VAL	CB-CG2	-6.05	1.40	1.52
3	Y	63	ARG	CZ-NH2	-6.05	1.25	1.33
3	7	145	PRO	CB-CG	-6.05	1.19	1.50
3	I	13	PHE	CG-CD2	-6.05	1.29	1.38
3	Y	455	GLY	N-CA	-6.05	1.36	1.46
3	U	223	VAL	CB-CG1	-6.05	1.40	1.52
3	I	440	TRP	CE2-CZ2	-6.04	1.29	1.39
3	L	343	ARG	CZ-NH2	-6.04	1.25	1.33
3	Y	223	VAL	CB-CG1	-6.04	1.40	1.52
3	L	63	ARG	CZ-NH2	-6.04	1.25	1.33
3	O	289	ILE	CB-CG2	-6.04	1.34	1.52
3	O	343	ARG	CZ-NH2	-6.04	1.25	1.33
3	F	145	PRO	CB-CG	-6.04	1.19	1.50
3	L	145	PRO	CB-CG	-6.04	1.19	1.50
3	1	289	ILE	CB-CG2	-6.04	1.34	1.52
3	4	145	PRO	CB-CG	-6.04	1.19	1.50
3	O	145	PRO	CB-CG	-6.04	1.19	1.50
3	V	289	ILE	CB-CG2	-6.04	1.34	1.52
3	V	455	GLY	N-CA	-6.04	1.36	1.46
3	R	145	PRO	CB-CG	-6.04	1.19	1.50
3	V	13	PHE	CG-CD2	-6.04	1.29	1.38
3	1	145	PRO	CB-CG	-6.04	1.19	1.50
3	C	145	PRO	CB-CG	-6.04	1.19	1.50
3	C	189	VAL	CB-CG2	-6.04	1.40	1.52
3	I	343	ARG	CZ-NH2	-6.04	1.25	1.33
3	O	159	PHE	CE1-CZ	-6.04	1.25	1.37
3	4	223	VAL	CB-CG1	-6.04	1.40	1.52
3	U	145	PRO	CB-CG	-6.04	1.19	1.50
3	U	289	ILE	CB-CG2	-6.04	1.34	1.52
3	7	522	CYS	CB-SG	-6.04	1.72	1.82
3	L	289	ILE	CB-CG2	-6.03	1.34	1.52
2	Q	144	GLU	CD-OE2	-6.03	1.19	1.25
3	V	145	PRO	CB-CG	-6.03	1.19	1.50
3	Y	189	VAL	CB-CG2	-6.03	1.40	1.52
3	R	440	TRP	CE2-CZ2	-6.03	1.29	1.39
3	1	189	VAL	CB-CG2	-6.03	1.40	1.52
3	Y	522	CYS	CB-SG	-6.03	1.72	1.82
3	1	63	ARG	CZ-NH2	-6.03	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6	144	GLU	CD-OE2	-6.03	1.19	1.25
3	Y	145	PRO	CB-CG	-6.03	1.19	1.50
3	1	223	VAL	CB-CG1	-6.03	1.40	1.52
3	1	440	TRP	CE2-CZ2	-6.03	1.29	1.39
3	U	514	ARG	NE-CZ	-6.03	1.25	1.33
3	L	522	CYS	CB-SG	-6.03	1.72	1.82
3	O	189	VAL	CB-CG2	-6.03	1.40	1.52
3	F	440	TRP	CE2-CZ2	-6.02	1.29	1.39
3	C	440	TRP	CE2-CZ2	-6.02	1.29	1.39
3	C	455	GLY	N-CA	-6.02	1.37	1.46
3	7	455	GLY	N-CA	-6.02	1.37	1.46
3	U	522	CYS	CB-SG	-6.02	1.72	1.82
3	F	343	ARG	CZ-NH2	-6.02	1.25	1.33
3	I	145	PRO	CB-CG	-6.02	1.19	1.50
3	I	443	ARG	CZ-NH2	-6.02	1.25	1.33
3	O	522	CYS	CB-SG	-6.02	1.72	1.82
3	U	63	ARG	CZ-NH2	-6.02	1.25	1.33
2	N	144	GLU	CD-OE2	-6.02	1.19	1.25
3	C	522	CYS	CB-SG	-6.01	1.72	1.82
3	F	455	GLY	N-CA	-6.01	1.37	1.46
3	L	443	ARG	CZ-NH2	-6.01	1.25	1.33
3	Y	482	PHE	CD1-CE1	-6.01	1.27	1.39
3	4	343	ARG	CZ-NH2	-6.01	1.25	1.33
3	Y	159	PHE	CE1-CZ	-6.01	1.25	1.37
3	4	440	TRP	CE2-CZ2	-6.01	1.29	1.39
3	1	455	GLY	N-CA	-6.01	1.37	1.46
3	F	159	PHE	CE1-CZ	-6.01	1.25	1.37
3	F	189	VAL	CB-CG2	-6.01	1.40	1.52
3	O	455	GLY	N-CA	-6.01	1.37	1.46
3	V	522	CYS	CB-SG	-6.01	1.72	1.82
3	V	63	ARG	CZ-NH2	-6.00	1.25	1.33
3	V	343	ARG	CZ-NH2	-6.00	1.25	1.33
3	Y	440	TRP	CE2-CZ2	-6.00	1.29	1.39
3	R	443	ARG	CZ-NH2	-6.00	1.25	1.33
3	Y	514	ARG	NE-CZ	-6.00	1.25	1.33
3	4	522	CYS	CB-SG	-6.00	1.72	1.82
3	U	440	TRP	CE2-CZ2	-6.00	1.29	1.39
3	I	522	CYS	CB-SG	-6.00	1.72	1.82
3	R	522	CYS	CB-SG	-6.00	1.72	1.82
3	R	514	ARG	NE-CZ	-6.00	1.25	1.33
3	7	189	VAL	CB-CG2	-5.99	1.40	1.52
3	7	482	PHE	CD1-CE1	-5.99	1.27	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	482	PHE	CD1-CE1	-5.99	1.27	1.39
2	B	144	GLU	CD-OE2	-5.99	1.19	1.25
3	L	455	GLY	N-CA	-5.99	1.37	1.46
3	4	455	GLY	N-CA	-5.99	1.37	1.46
3	I	482	PHE	CD1-CE1	-5.99	1.27	1.39
3	4	482	PHE	CD1-CE1	-5.99	1.27	1.39
3	7	440	TRP	CE2-CZ2	-5.99	1.29	1.39
2	9	144	GLU	CD-OE2	-5.99	1.19	1.25
3	U	455	GLY	N-CA	-5.98	1.37	1.46
3	L	514	ARG	NE-CZ	-5.98	1.25	1.33
3	R	482	PHE	CD1-CE1	-5.98	1.27	1.39
3	1	514	ARG	NE-CZ	-5.98	1.25	1.33
2	K	144	GLU	CD-OE2	-5.98	1.19	1.25
3	V	443	ARG	CZ-NH2	-5.98	1.25	1.33
3	1	482	PHE	CD1-CE1	-5.98	1.27	1.39
3	7	160	PHE	CG-CD1	-5.98	1.29	1.38
3	C	514	ARG	NE-CZ	-5.97	1.25	1.33
3	F	514	ARG	NE-CZ	-5.97	1.25	1.33
3	R	376	TRP	CZ3-CH2	-5.97	1.30	1.40
3	4	443	ARG	CZ-NH2	-5.97	1.25	1.33
3	C	482	PHE	CD1-CE1	-5.97	1.27	1.39
3	L	568	ARG	CZ-NH1	-5.97	1.25	1.33
3	F	482	PHE	CD1-CE1	-5.97	1.27	1.39
2	N	160	PHE	CD2-CE2	-5.97	1.27	1.39
3	U	160	PHE	CG-CD1	-5.97	1.29	1.38
3	O	482	PHE	CD1-CE1	-5.97	1.27	1.39
3	1	376	TRP	CZ3-CH2	-5.97	1.30	1.40
3	7	568	ARG	CZ-NH1	-5.97	1.25	1.33
2	Q	160	PHE	CE1-CZ	-5.96	1.26	1.37
2	X	160	PHE	CE1-CZ	-5.96	1.26	1.37
3	7	376	TRP	CZ3-CH2	-5.96	1.30	1.40
3	C	443	ARG	CZ-NH2	-5.96	1.25	1.33
3	O	175	VAL	C-O	-5.96	1.12	1.23
3	1	568	ARG	CZ-NH1	-5.96	1.25	1.33
3	7	175	VAL	C-O	-5.96	1.12	1.23
2	H	160	PHE	CE1-CZ	-5.96	1.26	1.37
3	U	175	VAL	C-O	-5.96	1.12	1.23
3	U	443	ARG	CZ-NH2	-5.96	1.25	1.33
3	7	514	ARG	NE-CZ	-5.96	1.25	1.33
3	4	175	VAL	C-O	-5.96	1.12	1.23
3	U	482	PHE	CD1-CE1	-5.96	1.27	1.39
3	I	376	TRP	CZ3-CH2	-5.96	1.30	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	376	TRP	CZ3-CH2	-5.95	1.30	1.40
3	I	448	LYS	CG-CD	-5.95	1.32	1.52
3	L	175	VAL	C-O	-5.95	1.12	1.23
3	C	376	TRP	CZ3-CH2	-5.95	1.30	1.40
3	O	443	ARG	CZ-NH2	-5.95	1.25	1.33
3	Y	443	ARG	CZ-NH2	-5.95	1.25	1.33
3	1	443	ARG	CZ-NH2	-5.95	1.25	1.33
2	3	160	PHE	CE1-CZ	-5.95	1.26	1.37
2	6	160	PHE	CD2-CE2	-5.95	1.27	1.39
2	9	160	PHE	CD2-CE2	-5.95	1.27	1.39
2	B	160	PHE	CE1-CZ	-5.95	1.26	1.37
3	I	568	ARG	CZ-NH1	-5.95	1.25	1.33
3	R	448	LYS	CG-CD	-5.95	1.32	1.52
3	L	160	PHE	CG-CD1	-5.95	1.29	1.38
3	1	175	VAL	C-O	-5.95	1.12	1.23
3	R	568	ARG	CZ-NH1	-5.95	1.25	1.33
3	V	160	PHE	CG-CD1	-5.95	1.29	1.38
2	3	139	VAL	CB-CG2	-5.95	1.40	1.52
3	7	448	LYS	CG-CD	-5.95	1.32	1.52
3	F	448	LYS	CG-CD	-5.94	1.32	1.52
2	K	160	PHE	CE1-CZ	-5.94	1.26	1.37
3	L	482	PHE	CD1-CE1	-5.94	1.27	1.39
2	0	139	VAL	CB-CG2	-5.94	1.40	1.52
3	4	514	ARG	NE-CZ	-5.94	1.25	1.33
3	U	376	TRP	CZ3-CH2	-5.94	1.30	1.40
3	C	175	VAL	C-O	-5.94	1.12	1.23
3	F	175	VAL	C-O	-5.94	1.12	1.23
2	N	139	VAL	CB-CG2	-5.94	1.40	1.52
3	R	175	VAL	C-O	-5.94	1.12	1.23
2	T	160	PHE	CE1-CZ	-5.94	1.26	1.37
2	H	144	GLU	CD-OE2	-5.94	1.19	1.25
3	L	376	TRP	CZ3-CH2	-5.94	1.30	1.40
3	Y	568	ARG	CZ-NH1	-5.94	1.25	1.33
1	Z	37	SER	CB-OG	-5.94	1.34	1.42
3	L	449	PRO	CB-CG	-5.94	1.20	1.50
2	3	144	GLU	CD-OE2	-5.94	1.19	1.25
3	4	448	LYS	CG-CD	-5.94	1.32	1.52
3	V	376	TRP	CZ3-CH2	-5.94	1.30	1.40
2	E	160	PHE	CE1-CZ	-5.93	1.26	1.37
3	I	156	VAL	C-N	-5.93	1.20	1.34
3	I	514	ARG	NE-CZ	-5.93	1.25	1.33
3	Y	448	LYS	CG-CD	-5.93	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	160	PHE	CG-CD1	-5.93	1.29	1.38
2	3	160	PHE	CD2-CE2	-5.93	1.27	1.39
2	6	160	PHE	CE1-CZ	-5.93	1.26	1.37
3	U	156	VAL	C-N	-5.93	1.20	1.34
3	U	449	PRO	CB-CG	-5.93	1.20	1.50
3	C	160	PHE	CG-CD1	-5.93	1.29	1.38
3	C	568	ARG	CZ-NH1	-5.93	1.25	1.33
3	V	514	ARG	NE-CZ	-5.93	1.25	1.33
2	X	160	PHE	CD2-CE2	-5.93	1.27	1.39
3	4	160	PHE	CG-CD1	-5.93	1.29	1.38
3	C	448	LYS	CG-CD	-5.93	1.32	1.52
3	I	160	PHE	CG-CD1	-5.93	1.29	1.38
2	E	144	GLU	CD-OE2	-5.93	1.19	1.25
3	L	448	LYS	CG-CD	-5.93	1.32	1.52
3	1	449	PRO	CB-CG	-5.93	1.20	1.50
2	H	160	PHE	CD2-CE2	-5.93	1.27	1.39
3	O	376	TRP	CZ3-CH2	-5.93	1.30	1.40
3	O	514	ARG	NE-CZ	-5.93	1.25	1.33
2	B	139	VAL	CB-CG2	-5.93	1.40	1.52
2	H	139	VAL	CB-CG2	-5.93	1.40	1.52
3	O	448	LYS	CG-CD	-5.93	1.32	1.52
3	V	156	VAL	C-N	-5.93	1.20	1.34
3	Y	175	VAL	C-O	-5.93	1.12	1.23
3	4	440	TRP	CB-CG	-5.93	1.39	1.50
1	8	37	SER	CB-OG	-5.93	1.34	1.42
3	U	568	ARG	CZ-NH1	-5.93	1.25	1.33
2	K	139	VAL	CB-CG2	-5.92	1.40	1.52
2	N	160	PHE	CE1-CZ	-5.92	1.26	1.37
3	V	175	VAL	C-O	-5.92	1.12	1.23
3	V	448	LYS	CG-CD	-5.92	1.32	1.52
2	9	160	PHE	CE1-CZ	-5.92	1.26	1.37
3	R	449	PRO	CB-CG	-5.92	1.20	1.50
3	C	449	PRO	CB-CG	-5.92	1.20	1.50
1	D	37	SER	CB-OG	-5.92	1.34	1.42
2	E	160	PHE	CD2-CE2	-5.92	1.27	1.39
3	F	160	PHE	CG-CD1	-5.92	1.29	1.38
3	O	160	PHE	CG-CD1	-5.92	1.29	1.38
3	1	156	VAL	C-N	-5.92	1.20	1.34
3	U	31	GLU	CB-CG	-5.92	1.40	1.52
2	B	160	PHE	CD2-CE2	-5.92	1.27	1.39
3	F	568	ARG	CZ-NH1	-5.92	1.25	1.33
2	0	160	PHE	CE1-CZ	-5.92	1.26	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	448	LYS	CG-CD	-5.92	1.32	1.52
2	E	139	VAL	CB-CG2	-5.92	1.40	1.52
3	F	449	PRO	CB-CG	-5.92	1.20	1.50
1	2	37	SER	CB-OG	-5.92	1.34	1.42
2	9	139	VAL	CB-CG2	-5.92	1.40	1.52
3	U	448	LYS	CG-CD	-5.92	1.32	1.52
3	O	156	VAL	C-N	-5.92	1.20	1.34
3	R	31	GLU	CB-CG	-5.92	1.41	1.52
3	Y	449	PRO	CB-CG	-5.92	1.20	1.50
3	7	443	ARG	CZ-NH2	-5.92	1.25	1.33
3	O	449	PRO	CB-CG	-5.91	1.20	1.50
3	4	144	SER	CA-CB	-5.91	1.44	1.52
3	4	568	ARG	CZ-NH1	-5.91	1.25	1.33
3	V	449	PRO	CB-CG	-5.91	1.20	1.50
3	7	144	SER	CA-CB	-5.91	1.44	1.52
3	7	449	PRO	CB-CG	-5.91	1.20	1.50
3	F	144	SER	CA-CB	-5.91	1.44	1.52
3	L	156	VAL	C-N	-5.91	1.20	1.34
2	T	139	VAL	CB-CG2	-5.91	1.40	1.52
1	A	37	SER	CB-OG	-5.91	1.34	1.42
3	F	443	ARG	CZ-NH2	-5.91	1.25	1.33
2	K	160	PHE	CD2-CE2	-5.91	1.27	1.39
3	1	144	SER	CA-CB	-5.91	1.44	1.52
3	4	449	PRO	CB-CG	-5.91	1.20	1.50
1	5	37	SER	CB-OG	-5.91	1.34	1.42
3	7	156	VAL	C-N	-5.91	1.20	1.34
3	I	449	PRO	CB-CG	-5.91	1.20	1.50
3	R	160	PHE	CG-CD1	-5.91	1.29	1.38
3	O	568	ARG	CZ-NH1	-5.91	1.25	1.33
3	C	156	VAL	C-N	-5.90	1.20	1.34
3	I	175	VAL	C-O	-5.90	1.12	1.23
2	Q	160	PHE	CD2-CE2	-5.90	1.27	1.39
3	R	156	VAL	C-N	-5.90	1.20	1.34
2	6	139	VAL	CB-CG2	-5.90	1.40	1.52
3	4	376	TRP	CZ3-CH2	-5.90	1.30	1.40
1	G	37	SER	CB-OG	-5.90	1.34	1.42
3	L	440	TRP	CB-CG	-5.90	1.39	1.50
3	V	568	ARG	CZ-NH1	-5.90	1.25	1.33
2	X	139	VAL	CB-CG2	-5.90	1.40	1.52
3	7	560	ILE	CB-CG2	-5.90	1.34	1.52
3	Y	376	TRP	CZ3-CH2	-5.90	1.30	1.40
3	I	144	SER	CA-CB	-5.90	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	37	SER	CB-OG	-5.90	1.34	1.42
2	T	160	PHE	CD2-CE2	-5.90	1.27	1.39
3	U	440	TRP	CB-CG	-5.90	1.39	1.50
3	F	440	TRP	CB-CG	-5.90	1.39	1.50
2	T	144	GLU	CD-OE2	-5.90	1.19	1.25
3	F	31	GLU	CB-CG	-5.89	1.41	1.52
3	O	440	TRP	CB-CG	-5.89	1.39	1.50
2	0	160	PHE	CD2-CE2	-5.89	1.27	1.39
1	J	37	SER	CB-OG	-5.89	1.34	1.42
3	Y	440	TRP	CB-CG	-5.89	1.39	1.50
3	7	31	GLU	CB-CG	-5.89	1.41	1.52
3	I	560	ILE	CB-CG2	-5.89	1.34	1.52
3	7	440	TRP	CB-CG	-5.89	1.39	1.50
3	C	31	GLU	CB-CG	-5.89	1.41	1.52
3	C	440	TRP	CB-CG	-5.89	1.39	1.50
2	Q	139	VAL	CB-CG2	-5.89	1.40	1.52
3	4	156	VAL	C-N	-5.89	1.20	1.34
3	I	31	GLU	CB-CG	-5.89	1.41	1.52
3	R	440	TRP	CB-CG	-5.89	1.39	1.50
3	F	156	VAL	C-N	-5.88	1.20	1.34
3	L	560	ILE	CB-CG2	-5.88	1.34	1.52
3	Y	31	GLU	CB-CG	-5.88	1.41	1.52
3	Y	156	VAL	C-N	-5.88	1.20	1.34
3	Y	160	PHE	CG-CD1	-5.88	1.29	1.38
3	U	560	ILE	CB-CG2	-5.88	1.34	1.52
3	C	560	ILE	CB-CG2	-5.88	1.34	1.52
3	V	31	GLU	CB-CG	-5.88	1.41	1.52
3	R	560	ILE	CB-CG2	-5.88	1.34	1.52
3	L	31	GLU	CB-CG	-5.88	1.41	1.52
1	S	37	SER	CB-OG	-5.88	1.34	1.42
1	W	37	SER	CB-OG	-5.88	1.34	1.42
3	4	560	ILE	CB-CG2	-5.88	1.34	1.52
3	O	560	ILE	CB-CG2	-5.88	1.34	1.52
3	1	300	PRO	CB-CG	-5.88	1.20	1.50
3	L	144	SER	CA-CB	-5.88	1.44	1.52
3	O	31	GLU	CB-CG	-5.88	1.41	1.52
3	I	300	PRO	CB-CG	-5.87	1.20	1.50
3	1	31	GLU	CB-CG	-5.87	1.41	1.52
3	F	300	PRO	CB-CG	-5.87	1.20	1.50
3	I	459	ASN	CG-ND2	-5.87	1.18	1.32
3	O	300	PRO	CB-CG	-5.87	1.20	1.50
1	P	31	ASN	CG-ND2	-5.87	1.18	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	144	SER	CA-CB	-5.87	1.44	1.52
3	Y	560	ILE	CB-CG2	-5.87	1.34	1.52
3	1	440	TRP	CB-CG	-5.87	1.39	1.50
3	U	300	PRO	CB-CG	-5.87	1.20	1.50
3	C	144	SER	CA-CB	-5.87	1.44	1.52
3	V	300	PRO	CB-CG	-5.87	1.20	1.50
3	Y	144	SER	CA-CB	-5.87	1.44	1.52
3	F	560	ILE	CB-CG2	-5.87	1.34	1.52
3	I	440	TRP	CB-CG	-5.87	1.39	1.50
3	4	300	PRO	CB-CG	-5.87	1.20	1.50
1	5	82	VAL	CB-CG1	-5.87	1.40	1.52
3	L	300	PRO	CB-CG	-5.87	1.20	1.50
3	4	31	GLU	CB-CG	-5.87	1.41	1.52
3	U	75	VAL	CB-CG1	-5.87	1.40	1.52
3	C	300	PRO	CB-CG	-5.87	1.20	1.50
3	V	440	TRP	CB-CG	-5.87	1.39	1.50
3	V	560	ILE	CB-CG2	-5.87	1.34	1.52
1	Z	82	VAL	CB-CG1	-5.87	1.40	1.52
3	7	300	PRO	CB-CG	-5.87	1.20	1.50
1	M	37	SER	CB-OG	-5.86	1.34	1.42
1	S	82	VAL	CB-CG1	-5.86	1.40	1.52
3	I	75	VAL	CB-CG1	-5.86	1.40	1.52
3	R	144	SER	CA-CB	-5.86	1.44	1.52
3	R	300	PRO	CB-CG	-5.86	1.20	1.50
3	Y	75	VAL	CB-CG1	-5.86	1.40	1.52
3	U	144	SER	CA-CB	-5.86	1.44	1.52
3	Y	300	PRO	CB-CG	-5.86	1.20	1.50
3	1	560	ILE	CB-CG2	-5.86	1.34	1.52
1	2	31	ASN	CG-ND2	-5.86	1.18	1.32
1	J	31	ASN	CG-ND2	-5.86	1.18	1.32
3	C	75	VAL	CB-CG1	-5.85	1.40	1.52
3	1	75	VAL	CB-CG1	-5.85	1.40	1.52
3	F	75	VAL	CB-CG1	-5.85	1.40	1.52
3	O	75	VAL	CB-CG1	-5.85	1.40	1.52
3	O	144	SER	CA-CB	-5.85	1.44	1.52
1	S	31	ASN	CG-ND2	-5.85	1.18	1.32
1	G	31	ASN	CG-ND2	-5.85	1.18	1.32
1	M	82	VAL	CB-CG1	-5.84	1.40	1.52
3	R	75	VAL	CB-CG1	-5.84	1.40	1.52
2	6	74	PHE	CE1-CZ	-5.84	1.26	1.37
1	G	82	VAL	CB-CG1	-5.84	1.40	1.52
1	P	82	VAL	CB-CG1	-5.84	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	75	VAL	CB-CG1	-5.84	1.40	1.52
1	A	31	ASN	CG-ND2	-5.84	1.18	1.32
1	A	82	VAL	CB-CG1	-5.84	1.40	1.52
1	5	31	ASN	CG-ND2	-5.84	1.18	1.32
3	L	75	VAL	CB-CG1	-5.84	1.40	1.52
3	7	75	VAL	CB-CG1	-5.84	1.40	1.52
1	2	82	VAL	CB-CG1	-5.84	1.40	1.52
1	D	82	VAL	CB-CG1	-5.84	1.40	1.52
1	D	31	ASN	CG-ND2	-5.83	1.18	1.32
2	H	74	PHE	CE1-CZ	-5.83	1.26	1.37
3	V	459	ASN	CG-ND2	-5.83	1.18	1.32
1	W	31	ASN	CG-ND2	-5.83	1.18	1.32
3	Y	459	ASN	CG-ND2	-5.83	1.18	1.32
3	7	193	PRO	CG-CD	-5.83	1.31	1.50
1	J	82	VAL	CB-CG1	-5.83	1.40	1.52
1	W	82	VAL	CB-CG1	-5.83	1.40	1.52
1	8	31	ASN	CG-ND2	-5.83	1.18	1.32
3	O	459	ASN	CG-ND2	-5.83	1.18	1.32
2	0	74	PHE	CE1-CZ	-5.83	1.26	1.37
3	7	459	ASN	CG-ND2	-5.83	1.18	1.32
3	V	147	GLN	CB-CG	-5.82	1.36	1.52
3	1	193	PRO	CG-CD	-5.82	1.31	1.50
3	4	75	VAL	CB-CG1	-5.82	1.40	1.52
3	Y	147	GLN	CB-CG	-5.82	1.36	1.52
3	4	193	PRO	CG-CD	-5.82	1.31	1.50
3	7	519	VAL	CB-CG2	-5.82	1.40	1.52
3	C	459	ASN	CG-ND2	-5.82	1.18	1.32
3	L	459	ASN	CG-ND2	-5.82	1.18	1.32
1	M	31	ASN	CG-ND2	-5.82	1.18	1.32
3	V	193	PRO	CG-CD	-5.82	1.31	1.50
3	I	147	GLN	CB-CG	-5.82	1.36	1.52
3	O	147	GLN	CB-CG	-5.82	1.36	1.52
2	T	74	PHE	CE1-CZ	-5.82	1.26	1.37
1	Z	31	ASN	CG-ND2	-5.82	1.18	1.32
2	9	74	PHE	CE1-CZ	-5.82	1.26	1.37
3	F	459	ASN	CG-ND2	-5.82	1.18	1.32
3	L	193	PRO	CG-CD	-5.82	1.31	1.50
3	O	519	VAL	CB-CG2	-5.82	1.40	1.52
3	F	147	GLN	CB-CG	-5.81	1.36	1.52
3	C	193	PRO	CG-CD	-5.81	1.31	1.50
3	F	193	PRO	CG-CD	-5.81	1.31	1.50
3	Y	193	PRO	CG-CD	-5.81	1.31	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	445	PHE	CE1-CZ	-5.81	1.26	1.37
3	U	445	PHE	CE1-CZ	-5.81	1.26	1.37
1	G	52	SER	CB-OG	-5.81	1.34	1.42
1	M	52	SER	CB-OG	-5.81	1.34	1.42
3	R	193	PRO	CG-CD	-5.81	1.31	1.50
1	S	52	SER	CB-OG	-5.81	1.34	1.42
3	O	193	PRO	CG-CD	-5.81	1.31	1.50
3	I	519	VAL	CB-CG2	-5.80	1.40	1.52
3	R	459	ASN	CG-ND2	-5.80	1.18	1.32
3	1	459	ASN	CG-ND2	-5.80	1.18	1.32
3	1	519	VAL	CB-CG2	-5.80	1.40	1.52
3	4	519	VAL	CB-CG2	-5.80	1.40	1.52
1	8	82	VAL	CB-CG1	-5.80	1.40	1.52
3	U	459	ASN	CG-ND2	-5.80	1.18	1.32
2	E	74	PHE	CE1-CZ	-5.80	1.26	1.37
2	B	74	PHE	CE1-CZ	-5.80	1.26	1.37
3	C	147	GLN	CB-CG	-5.80	1.36	1.52
3	V	519	VAL	CB-CG2	-5.80	1.40	1.52
3	1	147	GLN	CB-CG	-5.80	1.36	1.52
3	4	147	GLN	CB-CG	-5.80	1.36	1.52
3	U	193	PRO	CG-CD	-5.80	1.31	1.50
2	K	74	PHE	CE1-CZ	-5.80	1.26	1.37
3	R	519	VAL	CB-CG2	-5.80	1.40	1.52
2	X	74	PHE	CE1-CZ	-5.80	1.26	1.37
3	4	459	ASN	CG-ND2	-5.80	1.18	1.32
3	V	376	TRP	NE1-CE2	-5.80	1.30	1.37
3	7	147	GLN	CB-CG	-5.80	1.36	1.52
3	I	193	PRO	CG-CD	-5.80	1.31	1.50
3	U	376	TRP	NE1-CE2	-5.80	1.30	1.37
2	Q	74	PHE	CE1-CZ	-5.79	1.26	1.37
3	7	376	TRP	NE1-CE2	-5.79	1.30	1.37
3	L	445	PHE	CE1-CZ	-5.79	1.26	1.37
3	R	147	GLN	CB-CG	-5.79	1.36	1.52
1	5	52	SER	CB-OG	-5.79	1.34	1.42
3	U	147	GLN	CB-CG	-5.79	1.36	1.52
1	5	31	ASN	C-N	-5.79	1.20	1.34
3	F	211	LEU	CG-CD2	-5.79	1.30	1.51
3	L	147	GLN	CB-CG	-5.79	1.36	1.52
3	V	524	THR	C-N	-5.79	1.20	1.34
3	4	445	PHE	CE1-CZ	-5.79	1.26	1.37
3	C	519	VAL	CB-CG2	-5.79	1.40	1.52
3	F	445	PHE	CE1-CZ	-5.79	1.26	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	376	TRP	NE1-CE2	-5.79	1.30	1.37
3	I	524	THR	C-N	-5.78	1.20	1.34
3	V	445	PHE	CE1-CZ	-5.78	1.26	1.37
3	1	211	LEU	CG-CD2	-5.78	1.30	1.51
3	R	256	ASN	CG-ND2	-5.78	1.18	1.32
1	Z	31	ASN	C-N	-5.78	1.20	1.34
1	Z	52	SER	CB-OG	-5.78	1.34	1.42
3	V	256	ASN	CG-ND2	-5.78	1.18	1.32
3	C	445	PHE	CE1-CZ	-5.78	1.26	1.37
3	F	519	VAL	CB-CG2	-5.78	1.40	1.52
3	L	211	LEU	CG-CD2	-5.78	1.30	1.51
3	R	524	THR	C-N	-5.78	1.20	1.34
3	Y	211	LEU	CG-CD2	-5.78	1.30	1.51
3	4	440	TRP	CD2-CE2	-5.78	1.34	1.41
3	7	524	THR	C-N	-5.78	1.20	1.34
3	F	376	TRP	NE1-CE2	-5.77	1.30	1.37
3	L	519	VAL	CB-CG2	-5.77	1.40	1.52
3	C	524	THR	C-N	-5.77	1.20	1.34
3	I	376	TRP	NE1-CE2	-5.77	1.30	1.37
3	I	445	PHE	CE1-CZ	-5.77	1.26	1.37
3	O	211	LEU	CG-CD2	-5.77	1.30	1.51
3	U	524	THR	C-N	-5.77	1.20	1.34
3	R	445	PHE	CE1-CZ	-5.77	1.26	1.37
3	Y	256	ASN	CG-ND2	-5.77	1.18	1.32
3	Y	519	VAL	CB-CG2	-5.77	1.40	1.52
3	U	519	VAL	CB-CG2	-5.77	1.40	1.52
3	L	524	THR	C-N	-5.77	1.20	1.34
2	N	74	PHE	CE1-CZ	-5.77	1.26	1.37
3	R	376	TRP	NE1-CE2	-5.77	1.30	1.37
3	V	211	LEU	CG-CD2	-5.77	1.30	1.51
3	C	211	LEU	CG-CD2	-5.77	1.30	1.51
3	C	376	TRP	NE1-CE2	-5.77	1.30	1.37
3	Y	249	SER	CB-OG	-5.77	1.34	1.42
3	C	256	ASN	CG-ND2	-5.77	1.18	1.32
3	1	524	THR	C-N	-5.77	1.20	1.34
3	4	524	THR	C-N	-5.77	1.20	1.34
3	1	376	TRP	NE1-CE2	-5.76	1.30	1.37
3	4	376	TRP	NE1-CE2	-5.76	1.30	1.37
3	R	211	LEU	CG-CD2	-5.76	1.30	1.51
3	Y	376	TRP	NE1-CE2	-5.76	1.30	1.37
3	Y	524	THR	C-N	-5.76	1.20	1.34
2	3	74	PHE	CE1-CZ	-5.76	1.26	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	SER	CB-OG	-5.76	1.34	1.42
3	L	256	ASN	CG-ND2	-5.76	1.18	1.32
3	O	249	SER	CB-OG	-5.76	1.34	1.42
3	1	256	ASN	CG-ND2	-5.76	1.18	1.32
1	2	31	ASN	C-N	-5.76	1.20	1.34
3	4	211	LEU	CG-CD2	-5.76	1.30	1.51
3	O	524	THR	C-N	-5.76	1.20	1.34
3	4	256	ASN	CG-ND2	-5.76	1.18	1.32
1	W	31	ASN	C-N	-5.76	1.20	1.34
3	1	445	PHE	CE1-CZ	-5.76	1.26	1.37
3	7	211	LEU	CG-CD2	-5.76	1.30	1.51
3	O	440	TRP	CD2-CE2	-5.75	1.34	1.41
1	A	31	ASN	C-N	-5.75	1.20	1.34
1	J	52	SER	CB-OG	-5.75	1.34	1.42
3	U	256	ASN	CG-ND2	-5.75	1.18	1.32
1	D	31	ASN	C-N	-5.75	1.20	1.34
3	I	211	LEU	CG-CD2	-5.75	1.30	1.51
3	7	445	PHE	CE1-CZ	-5.75	1.26	1.37
3	7	256	ASN	CG-ND2	-5.75	1.18	1.32
1	M	31	ASN	C-N	-5.75	1.20	1.34
3	O	445	PHE	CE1-CZ	-5.75	1.26	1.37
3	F	256	ASN	CG-ND2	-5.75	1.18	1.32
3	F	440	TRP	CD2-CE2	-5.75	1.34	1.41
3	F	524	THR	C-N	-5.75	1.20	1.34
1	G	31	ASN	C-N	-5.75	1.20	1.34
3	Y	440	TRP	CD2-CE2	-5.75	1.34	1.41
3	U	211	LEU	CG-CD2	-5.75	1.30	1.51
1	8	31	ASN	C-N	-5.75	1.20	1.34
3	I	256	ASN	CG-ND2	-5.74	1.18	1.32
1	S	31	ASN	C-N	-5.74	1.20	1.34
3	C	440	TRP	CD2-CE2	-5.74	1.34	1.41
1	J	31	ASN	C-N	-5.74	1.20	1.34
3	O	256	ASN	CG-ND2	-5.74	1.18	1.32
1	P	31	ASN	C-N	-5.74	1.20	1.34
3	V	274	HIS	C-N	-5.74	1.20	1.34
3	Y	247	GLN	CD-NE2	-5.74	1.18	1.32
3	V	403	PHE	CB-CG	-5.74	1.41	1.51
3	R	153	SER	CA-CB	-5.74	1.44	1.52
3	4	22	ARG	CZ-NH1	-5.74	1.25	1.33
1	8	52	SER	CB-OG	-5.74	1.34	1.42
3	R	249	SER	CB-OG	-5.73	1.34	1.42
1	W	52	SER	CB-OG	-5.73	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	403	PHE	CB-CG	-5.73	1.41	1.51
3	7	440	TRP	CD2-CE2	-5.73	1.34	1.41
1	D	52	SER	CB-OG	-5.73	1.34	1.42
3	4	153	SER	CA-CB	-5.73	1.44	1.52
3	Y	22	ARG	CZ-NH1	-5.73	1.25	1.33
3	R	274	HIS	C-N	-5.72	1.20	1.34
3	L	376	TRP	NE1-CE2	-5.72	1.30	1.37
3	7	404	ARG	CB-CG	-5.72	1.37	1.52
3	F	127	GLU	CD-OE1	-5.72	1.19	1.25
1	P	52	SER	CB-OG	-5.72	1.34	1.42
3	V	247	GLN	CD-NE2	-5.72	1.18	1.32
3	I	274	HIS	C-N	-5.72	1.21	1.34
3	I	440	TRP	CD2-CE2	-5.72	1.34	1.41
3	R	440	TRP	CD2-CE2	-5.72	1.34	1.41
3	V	404	ARG	CB-CG	-5.72	1.37	1.52
1	2	52	SER	CB-OG	-5.72	1.34	1.42
3	U	440	TRP	CD2-CE2	-5.72	1.34	1.41
3	1	153	SER	CA-CB	-5.71	1.44	1.52
3	C	249	SER	CB-OG	-5.71	1.34	1.42
3	F	247	GLN	CD-NE2	-5.71	1.18	1.32
3	F	403	PHE	CB-CG	-5.71	1.41	1.51
3	4	127	GLU	CD-OE1	-5.71	1.19	1.25
3	7	149	TYR	CD2-CE2	-5.71	1.30	1.39
3	Y	404	ARG	CB-CG	-5.71	1.37	1.52
3	7	396	ASP	CB-CG	5.71	1.63	1.51
3	C	404	ARG	CB-CG	-5.71	1.37	1.52
3	V	153	SER	CA-CB	-5.71	1.44	1.52
3	7	274	HIS	C-N	-5.71	1.21	1.34
3	F	404	ARG	CB-CG	-5.71	1.37	1.52
3	I	127	GLU	CD-OE1	-5.71	1.19	1.25
3	O	153	SER	CA-CB	-5.71	1.44	1.52
3	O	274	HIS	C-N	-5.71	1.21	1.34
3	O	396	ASP	CB-CG	5.71	1.63	1.51
3	R	403	PHE	CB-CG	-5.71	1.41	1.51
3	1	149	TYR	CD2-CE2	-5.71	1.30	1.39
3	1	249	SER	CB-OG	-5.71	1.34	1.42
3	1	440	TRP	CD2-CE2	-5.71	1.34	1.41
3	4	396	ASP	CB-CG	5.71	1.63	1.51
3	R	404	ARG	CB-CG	-5.71	1.37	1.52
3	U	274	HIS	C-N	-5.71	1.21	1.34
3	C	274	HIS	C-N	-5.70	1.21	1.34
3	L	247	GLN	CD-NE2	-5.70	1.18	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	404	ARG	CB-CG	-5.70	1.37	1.52
3	O	22	ARG	CZ-NH1	-5.70	1.25	1.33
3	4	404	ARG	CB-CG	-5.70	1.37	1.52
3	L	249	SER	CB-OG	-5.70	1.34	1.42
3	L	274	HIS	C-N	-5.70	1.21	1.34
3	F	153	SER	CA-CB	-5.70	1.44	1.52
3	I	403	PHE	CB-CG	-5.70	1.41	1.51
3	L	440	TRP	CD2-CE2	-5.70	1.34	1.41
3	R	247	GLN	CD-NE2	-5.70	1.18	1.32
3	1	247	GLN	CD-NE2	-5.70	1.18	1.32
3	U	404	ARG	CB-CG	-5.70	1.37	1.52
3	I	404	ARG	CB-CG	-5.70	1.37	1.52
3	I	247	GLN	CD-NE2	-5.70	1.18	1.32
3	I	249	SER	CB-OG	-5.70	1.34	1.42
2	K	48	THR	CB-CG2	-5.70	1.33	1.52
2	Q	48	THR	CB-CG2	-5.70	1.33	1.52
3	V	440	TRP	CD2-CE2	-5.70	1.34	1.41
3	7	403	PHE	CB-CG	-5.70	1.41	1.51
3	I	290	ILE	CB-CG2	-5.69	1.35	1.52
3	C	247	GLN	CD-NE2	-5.69	1.18	1.32
3	C	403	PHE	CB-CG	-5.69	1.41	1.51
3	F	396	ASP	CB-CG	5.69	1.63	1.51
3	L	22	ARG	CZ-NH1	-5.69	1.25	1.33
3	L	127	GLU	CD-OE1	-5.69	1.19	1.25
3	4	403	PHE	CB-CG	-5.69	1.41	1.51
3	U	153	SER	CA-CB	-5.69	1.44	1.52
3	C	153	SER	CA-CB	-5.69	1.44	1.52
3	C	396	ASP	CB-CG	5.69	1.63	1.51
3	F	22	ARG	CZ-NH1	-5.69	1.25	1.33
3	F	290	ILE	CB-CG2	-5.69	1.35	1.52
3	V	396	ASP	CB-CG	5.69	1.63	1.51
2	X	48	THR	CB-CG2	-5.69	1.33	1.52
3	U	149	TYR	CD2-CE2	-5.69	1.30	1.39
3	U	249	SER	CB-OG	-5.69	1.34	1.42
3	U	396	ASP	CB-CG	5.69	1.63	1.51
3	1	396	ASP	CB-CG	5.69	1.63	1.51
3	I	149	TYR	CD2-CE2	-5.69	1.30	1.39
3	L	403	PHE	CB-CG	-5.69	1.41	1.51
3	V	249	SER	CB-OG	-5.69	1.34	1.42
3	Y	274	HIS	C-N	-5.69	1.21	1.34
3	1	274	HIS	C-N	-5.69	1.21	1.34
3	7	22	ARG	CZ-NH1	-5.69	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	403	PHE	CB-CG	-5.69	1.41	1.51
3	F	249	SER	CB-OG	-5.69	1.34	1.42
3	L	396	ASP	CB-CG	5.69	1.63	1.51
3	O	247	GLN	CD-NE2	-5.69	1.18	1.32
3	O	404	ARG	CB-CG	-5.69	1.37	1.52
3	R	22	ARG	CZ-NH1	-5.69	1.25	1.33
3	V	290	ILE	CB-CG2	-5.69	1.35	1.52
2	0	48	THR	CB-CG2	-5.69	1.33	1.52
3	4	274	HIS	C-N	-5.69	1.21	1.34
3	U	247	GLN	CD-NE2	-5.69	1.18	1.32
3	C	290	ILE	CB-CG2	-5.68	1.35	1.52
2	H	48	THR	CB-CG2	-5.68	1.33	1.52
3	O	290	ILE	CB-CG2	-5.68	1.35	1.52
3	4	149	TYR	CD2-CE2	-5.68	1.30	1.39
2	6	48	THR	CB-CG2	-5.68	1.33	1.52
2	B	48	THR	CB-CG2	-5.68	1.33	1.52
3	L	404	ARG	CB-CG	-5.68	1.37	1.52
3	4	247	GLN	CD-NE2	-5.68	1.18	1.32
3	7	247	GLN	CD-NE2	-5.68	1.18	1.32
3	7	249	SER	CB-OG	-5.68	1.34	1.42
3	C	22	ARG	CZ-NH1	-5.68	1.25	1.33
3	Y	396	ASP	CB-CG	5.68	1.63	1.51
3	4	249	SER	CB-OG	-5.68	1.34	1.42
3	U	22	ARG	CZ-NH1	-5.68	1.25	1.33
3	L	153	SER	CA-CB	-5.68	1.44	1.52
2	N	48	THR	CB-CG2	-5.68	1.33	1.52
3	4	290	ILE	CB-CG2	-5.68	1.35	1.52
3	C	149	TYR	CD2-CE2	-5.67	1.30	1.39
3	F	274	HIS	C-N	-5.67	1.21	1.34
3	V	22	ARG	CZ-NH1	-5.67	1.25	1.33
3	Y	290	ILE	CB-CG2	-5.67	1.35	1.52
3	1	290	ILE	CB-CG2	-5.67	1.35	1.52
3	L	290	ILE	CB-CG2	-5.67	1.35	1.52
3	I	396	ASP	CB-CG	5.67	1.63	1.51
3	R	290	ILE	CB-CG2	-5.67	1.35	1.52
2	T	48	THR	CB-CG2	-5.67	1.33	1.52
3	Y	153	SER	CA-CB	-5.67	1.44	1.52
1	W	95	VAL	CB-CG1	-5.67	1.41	1.52
3	Y	403	PHE	CB-CG	-5.67	1.41	1.51
3	R	396	ASP	CB-CG	5.67	1.63	1.51
3	V	127	GLU	CD-OE1	-5.67	1.19	1.25
3	L	149	TYR	CD2-CE2	-5.67	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	149	TYR	CD2-CE2	-5.67	1.30	1.39
1	P	21	PHE	CD1-CE1	-5.67	1.27	1.39
3	Y	149	TYR	CD2-CE2	-5.66	1.30	1.39
3	1	403	PHE	CB-CG	-5.66	1.41	1.51
2	3	40	CYS	CB-SG	-5.66	1.72	1.81
2	3	48	THR	CB-CG2	-5.66	1.33	1.52
2	9	48	THR	CB-CG2	-5.66	1.33	1.52
3	I	153	SER	CA-CB	-5.66	1.44	1.52
1	P	95	VAL	CB-CG1	-5.66	1.41	1.52
3	R	127	GLU	CD-OE1	-5.66	1.19	1.25
3	V	149	TYR	CD2-CE2	-5.66	1.30	1.39
3	U	290	ILE	CB-CG2	-5.66	1.35	1.52
2	E	48	THR	CB-CG2	-5.66	1.33	1.52
3	7	153	SER	CA-CB	-5.66	1.44	1.52
3	7	290	ILE	CB-CG2	-5.66	1.35	1.52
2	9	40	CYS	CB-SG	-5.65	1.72	1.81
3	R	149	TYR	CD2-CE2	-5.65	1.30	1.39
3	R	191	GLY	N-CA	-5.65	1.37	1.46
1	J	21	PHE	CD1-CE1	-5.65	1.27	1.39
1	8	95	VAL	CB-CG1	-5.65	1.41	1.52
3	C	127	GLU	CD-OE1	-5.65	1.19	1.25
1	A	95	VAL	CB-CG1	-5.64	1.41	1.52
2	H	40	CYS	CB-SG	-5.64	1.72	1.81
1	S	95	VAL	CB-CG1	-5.64	1.41	1.52
3	F	149	TYR	CD2-CE2	-5.64	1.30	1.39
2	0	40	CYS	CB-SG	-5.64	1.72	1.81
3	O	127	GLU	CD-OE1	-5.63	1.19	1.25
3	1	127	GLU	CD-OE1	-5.63	1.19	1.25
1	A	21	PHE	CD1-CE1	-5.63	1.27	1.39
1	J	95	VAL	CB-CG1	-5.63	1.41	1.52
1	G	95	VAL	CB-CG1	-5.63	1.41	1.52
3	Y	127	GLU	CD-OE1	-5.63	1.19	1.25
3	F	155	GLY	N-CA	-5.62	1.37	1.46
1	M	21	PHE	CD1-CE1	-5.62	1.27	1.39
3	O	191	GLY	N-CA	-5.62	1.37	1.46
2	Q	40	CYS	CB-SG	-5.62	1.72	1.81
1	S	21	PHE	CD1-CE1	-5.62	1.28	1.39
1	2	21	PHE	CD1-CE1	-5.62	1.27	1.39
1	D	95	VAL	CB-CG1	-5.62	1.41	1.52
2	T	40	CYS	CB-SG	-5.62	1.72	1.81
1	5	95	VAL	CB-CG1	-5.62	1.41	1.52
2	B	40	CYS	CB-SG	-5.62	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	63	ARG	NE-CZ	-5.62	1.25	1.33
2	3	118	PHE	CD2-CE2	-5.62	1.28	1.39
3	L	155	GLY	N-CA	-5.62	1.37	1.46
1	Z	95	VAL	CB-CG1	-5.62	1.41	1.52
1	2	95	VAL	CB-CG1	-5.62	1.41	1.52
2	E	40	CYS	CB-SG	-5.62	1.72	1.81
3	I	22	ARG	CZ-NH1	-5.62	1.25	1.33
3	U	127	GLU	CD-OE1	-5.62	1.19	1.25
3	I	155	GLY	N-CA	-5.61	1.37	1.46
3	R	472	THR	CB-CG2	-5.61	1.33	1.52
1	W	21	PHE	CD1-CE1	-5.61	1.28	1.39
1	D	21	PHE	CD1-CE1	-5.61	1.28	1.39
3	C	191	GLY	N-CA	-5.61	1.37	1.46
1	M	95	VAL	CB-CG1	-5.61	1.41	1.52
3	Y	191	GLY	N-CA	-5.61	1.37	1.46
2	6	40	CYS	CB-SG	-5.61	1.72	1.81
2	0	118	PHE	CD2-CE2	-5.61	1.28	1.39
3	U	155	GLY	N-CA	-5.61	1.37	1.46
3	O	122	ASP	CB-CG	5.61	1.63	1.51
3	F	191	GLY	N-CA	-5.61	1.37	1.46
3	L	191	GLY	N-CA	-5.61	1.37	1.46
3	R	122	ASP	CB-CG	5.61	1.63	1.51
1	Z	21	PHE	CD1-CE1	-5.61	1.28	1.39
3	1	18	GLY	C-O	-5.61	1.14	1.23
3	4	155	GLY	N-CA	-5.61	1.37	1.46
3	1	22	ARG	CZ-NH1	-5.60	1.25	1.33
3	L	472	THR	CB-CG2	-5.60	1.33	1.52
3	V	122	ASP	CB-CG	5.60	1.63	1.51
3	V	191	GLY	N-CA	-5.60	1.37	1.46
1	5	21	PHE	CD1-CE1	-5.60	1.28	1.39
3	I	472	THR	CB-CG2	-5.60	1.33	1.52
2	X	118	PHE	CD2-CE2	-5.60	1.28	1.39
3	U	472	THR	CB-CG2	-5.60	1.33	1.52
2	X	40	CYS	CB-SG	-5.60	1.72	1.81
3	4	472	THR	CB-CG2	-5.60	1.33	1.52
3	7	127	GLU	CD-OE1	-5.60	1.19	1.25
3	7	191	GLY	N-CA	-5.60	1.37	1.46
3	F	472	THR	CB-CG2	-5.60	1.33	1.52
3	I	191	GLY	N-CA	-5.59	1.37	1.46
2	K	40	CYS	CB-SG	-5.59	1.72	1.81
3	1	472	THR	CB-CG2	-5.59	1.33	1.52
3	U	191	GLY	N-CA	-5.59	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	472	THR	CB-CG2	-5.59	1.33	1.52
3	U	122	ASP	CB-CG	5.59	1.63	1.51
1	8	21	PHE	CD1-CE1	-5.59	1.28	1.39
3	O	472	THR	CB-CG2	-5.59	1.33	1.52
3	Y	122	ASP	CB-CG	5.59	1.63	1.51
3	Y	155	GLY	N-CA	-5.59	1.37	1.46
3	7	472	THR	CB-CG2	-5.59	1.33	1.52
3	V	472	THR	CB-CG2	-5.59	1.33	1.52
3	1	155	GLY	N-CA	-5.59	1.37	1.46
3	4	191	GLY	N-CA	-5.59	1.37	1.46
1	G	21	PHE	CD1-CE1	-5.58	1.28	1.39
3	V	63	ARG	NE-CZ	-5.58	1.25	1.33
1	5	81	GLN	CB-CG	-5.58	1.37	1.52
3	U	63	ARG	NE-CZ	-5.58	1.25	1.33
1	M	81	GLN	CB-CG	-5.58	1.37	1.52
3	C	122	ASP	CB-CG	5.58	1.63	1.51
2	E	118	PHE	CD2-CE2	-5.58	1.28	1.39
3	1	122	ASP	CB-CG	5.58	1.63	1.51
2	B	118	PHE	CD2-CE2	-5.58	1.28	1.39
3	L	122	ASP	CB-CG	5.58	1.63	1.51
1	P	81	GLN	CB-CG	-5.58	1.37	1.52
3	Y	472	THR	CB-CG2	-5.58	1.33	1.52
2	9	118	PHE	CD2-CE2	-5.58	1.28	1.39
1	8	81	GLN	CB-CG	-5.57	1.37	1.52
3	C	155	GLY	N-CA	-5.57	1.37	1.46
3	O	18	GLY	C-O	-5.57	1.14	1.23
2	T	118	PHE	CD2-CE2	-5.57	1.28	1.39
3	1	63	ARG	NE-CZ	-5.57	1.25	1.33
3	Y	63	ARG	NE-CZ	-5.57	1.25	1.33
3	Y	160	PHE	CG-CD2	-5.57	1.30	1.38
3	7	122	ASP	CB-CG	5.57	1.63	1.51
3	F	122	ASP	CB-CG	5.57	1.63	1.51
2	N	40	CYS	CB-SG	-5.57	1.72	1.81
3	R	113	PRO	CG-CD	-5.57	1.32	1.50
3	R	160	PHE	CG-CD2	-5.57	1.30	1.38
3	U	113	PRO	CG-CD	-5.57	1.32	1.50
3	L	201	LYS	CE-NZ	-5.56	1.35	1.49
3	L	343	ARG	CZ-NH1	-5.56	1.25	1.33
3	F	18	GLY	C-O	-5.56	1.14	1.23
3	F	63	ARG	NE-CZ	-5.56	1.25	1.33
2	H	72	SER	CB-OG	-5.56	1.35	1.42
3	O	113	PRO	CG-CD	-5.56	1.32	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	18	GLY	C-O	-5.56	1.14	1.23
3	C	18	GLY	C-O	-5.56	1.14	1.23
3	4	122	ASP	CB-CG	5.56	1.63	1.51
3	C	113	PRO	CG-CD	-5.56	1.32	1.50
1	G	81	GLN	CB-CG	-5.56	1.37	1.52
3	L	113	PRO	CG-CD	-5.56	1.32	1.50
3	Y	113	PRO	CG-CD	-5.56	1.32	1.50
3	U	160	PHE	CG-CD2	-5.56	1.30	1.38
3	F	381	GLN	CB-CG	-5.56	1.37	1.52
3	I	18	GLY	C-O	-5.56	1.14	1.23
3	L	63	ARG	NE-CZ	-5.56	1.25	1.33
3	R	18	GLY	C-O	-5.56	1.14	1.23
3	V	113	PRO	CG-CD	-5.56	1.32	1.50
1	W	81	GLN	CB-CG	-5.56	1.37	1.52
3	7	113	PRO	CG-CD	-5.56	1.32	1.50
3	7	160	PHE	CG-CD2	-5.56	1.30	1.38
3	U	343	ARG	CZ-NH1	-5.56	1.25	1.33
3	O	381	GLN	CB-CG	-5.56	1.37	1.52
1	D	81	GLN	CB-CG	-5.55	1.37	1.52
2	Q	118	PHE	CD2-CE2	-5.55	1.28	1.39
3	R	201	LYS	CE-NZ	-5.55	1.35	1.49
2	X	54	PRO	CG-CD	-5.55	1.32	1.50
3	4	113	PRO	CG-CD	-5.55	1.32	1.50
3	C	160	PHE	CG-CD2	-5.55	1.30	1.38
3	F	160	PHE	CG-CD2	-5.55	1.30	1.38
2	K	54	PRO	CG-CD	-5.55	1.32	1.50
3	L	160	PHE	CG-CD2	-5.55	1.30	1.38
2	6	118	PHE	CD2-CE2	-5.55	1.28	1.39
1	A	81	GLN	CB-CG	-5.55	1.37	1.52
3	C	63	ARG	NE-CZ	-5.55	1.25	1.33
2	K	118	PHE	CD2-CE2	-5.55	1.28	1.39
3	V	381	GLN	CB-CG	-5.55	1.37	1.52
3	1	113	PRO	CG-CD	-5.55	1.32	1.50
3	1	191	GLY	N-CA	-5.55	1.37	1.46
3	4	343	ARG	CZ-NH1	-5.55	1.25	1.33
3	I	122	ASP	CB-CG	5.55	1.63	1.51
3	7	343	ARG	CZ-NH1	-5.55	1.25	1.33
2	H	118	PHE	CD2-CE2	-5.55	1.28	1.39
3	I	343	ARG	CZ-NH1	-5.55	1.25	1.33
3	V	201	LYS	CE-NZ	-5.55	1.35	1.49
3	1	201	LYS	CE-NZ	-5.55	1.35	1.49
3	O	343	ARG	CZ-NH1	-5.55	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	113	PRO	CG-CD	-5.54	1.32	1.50
1	S	81	GLN	CB-CG	-5.54	1.37	1.52
3	F	113	PRO	CG-CD	-5.54	1.32	1.50
3	F	201	LYS	CE-NZ	-5.54	1.35	1.49
3	I	63	ARG	NE-CZ	-5.54	1.25	1.33
1	J	81	GLN	CB-CG	-5.54	1.37	1.52
3	O	155	GLY	N-CA	-5.54	1.37	1.46
2	3	72	SER	CB-OG	-5.54	1.35	1.42
3	4	381	GLN	CB-CG	-5.54	1.37	1.52
3	7	201	LYS	CE-NZ	-5.54	1.35	1.49
3	U	18	GLY	C-O	-5.54	1.14	1.23
2	N	118	PHE	CD2-CE2	-5.54	1.28	1.39
3	R	271	ARG	CZ-NH1	-5.54	1.25	1.33
3	Y	18	GLY	C-O	-5.54	1.14	1.23
3	7	18	GLY	C-O	-5.54	1.14	1.23
2	9	54	PRO	CG-CD	-5.54	1.32	1.50
2	E	54	PRO	CG-CD	-5.54	1.32	1.50
2	T	54	PRO	CG-CD	-5.54	1.32	1.50
1	Z	81	GLN	CB-CG	-5.54	1.37	1.52
3	7	381	GLN	CB-CG	-5.54	1.37	1.52
3	C	381	GLN	CB-CG	-5.54	1.37	1.52
2	6	54	PRO	CG-CD	-5.54	1.32	1.50
2	B	54	PRO	CG-CD	-5.53	1.32	1.50
3	C	201	LYS	CE-NZ	-5.53	1.35	1.49
3	L	18	GLY	C-O	-5.53	1.14	1.23
3	V	160	PHE	CG-CD2	-5.53	1.30	1.38
3	Y	271	ARG	CZ-NH1	-5.53	1.25	1.33
2	0	54	PRO	CG-CD	-5.53	1.32	1.50
3	1	381	GLN	CB-CG	-5.53	1.37	1.52
3	U	454	LYS	C-O	-5.53	1.12	1.23
3	I	381	GLN	CB-CG	-5.53	1.37	1.52
3	O	160	PHE	CG-CD2	-5.53	1.30	1.38
3	1	160	PHE	CG-CD2	-5.53	1.30	1.38
3	4	454	LYS	C-O	-5.53	1.12	1.23
3	C	271	ARG	CZ-NH1	-5.53	1.25	1.33
2	H	54	PRO	CG-CD	-5.53	1.32	1.50
3	I	201	LYS	CE-NZ	-5.53	1.35	1.49
3	L	454	LYS	C-O	-5.53	1.12	1.23
2	N	72	SER	CB-OG	-5.53	1.35	1.42
2	6	72	SER	CB-OG	-5.53	1.35	1.42
3	7	155	GLY	N-CA	-5.53	1.37	1.46
3	U	271	ARG	CZ-NH1	-5.53	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	72	SER	CB-OG	-5.53	1.35	1.42
3	I	271	ARG	CZ-NH1	-5.53	1.25	1.33
2	Q	54	PRO	CG-CD	-5.53	1.32	1.50
3	R	454	LYS	C-O	-5.53	1.12	1.23
3	7	63	ARG	NE-CZ	-5.53	1.25	1.33
2	0	118	PHE	CB-CG	-5.52	1.42	1.51
1	G	12	MET	C-O	-5.52	1.12	1.23
1	S	32	TYR	CG-CD2	-5.52	1.31	1.39
1	W	32	TYR	CG-CD2	-5.52	1.31	1.39
3	4	201	LYS	CE-NZ	-5.52	1.35	1.49
1	5	51	LYS	CG-CD	-5.52	1.33	1.52
3	I	487	LYS	C-O	-5.52	1.12	1.23
3	U	201	LYS	CE-NZ	-5.52	1.35	1.49
3	C	343	ARG	CZ-NH1	-5.52	1.25	1.33
3	F	454	LYS	C-O	-5.52	1.12	1.23
2	H	118	PHE	CB-CG	-5.52	1.42	1.51
2	N	76	PHE	C-O	-5.52	1.12	1.23
3	O	201	LYS	CE-NZ	-5.52	1.35	1.49
3	R	155	GLY	N-CA	-5.52	1.37	1.46
2	T	76	PHE	C-O	-5.52	1.12	1.23
2	T	118	PHE	CB-CG	-5.52	1.42	1.51
3	V	155	GLY	N-CA	-5.52	1.37	1.46
2	9	72	SER	CB-OG	-5.52	1.35	1.42
3	I	160	PHE	CG-CD2	-5.52	1.30	1.38
3	V	18	GLY	C-O	-5.52	1.14	1.23
2	0	72	SER	CB-OG	-5.52	1.35	1.42
1	2	81	GLN	CB-CG	-5.52	1.37	1.52
2	3	54	PRO	CG-CD	-5.52	1.32	1.50
3	7	487	LYS	C-O	-5.52	1.12	1.23
3	Y	201	LYS	CE-NZ	-5.52	1.35	1.49
3	C	454	LYS	C-O	-5.51	1.12	1.23
3	F	487	LYS	C-O	-5.51	1.12	1.23
1	J	51	LYS	CG-CD	-5.51	1.33	1.52
2	Q	72	SER	CB-OG	-5.51	1.35	1.42
1	2	51	LYS	CG-CD	-5.51	1.33	1.52
2	3	76	PHE	C-O	-5.51	1.12	1.23
3	7	271	ARG	CZ-NH1	-5.51	1.25	1.33
3	F	271	ARG	CZ-NH1	-5.51	1.25	1.33
3	Y	381	GLN	CB-CG	-5.51	1.37	1.52
2	3	118	PHE	CB-CG	-5.51	1.42	1.51
1	8	51	LYS	CG-CD	-5.51	1.33	1.52
3	L	381	GLN	CB-CG	-5.51	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	51	LYS	CG-CD	-5.51	1.33	1.52
2	Q	76	PHE	C-O	-5.51	1.12	1.23
3	R	381	GLN	CB-CG	-5.51	1.37	1.52
3	L	487	LYS	C-O	-5.51	1.12	1.23
1	M	51	LYS	CG-CD	-5.51	1.33	1.52
2	T	72	SER	CB-OG	-5.51	1.35	1.42
3	V	487	LYS	C-O	-5.51	1.12	1.23
2	X	72	SER	CB-OG	-5.51	1.35	1.42
2	6	118	PHE	CB-CG	-5.51	1.42	1.51
3	7	454	LYS	C-O	-5.51	1.12	1.23
2	E	72	SER	CB-OG	-5.51	1.35	1.42
3	F	343	ARG	CZ-NH1	-5.51	1.25	1.33
3	V	271	ARG	CZ-NH1	-5.51	1.25	1.33
3	U	381	GLN	CB-CG	-5.51	1.37	1.52
1	A	51	LYS	CG-CD	-5.51	1.33	1.52
1	D	51	LYS	CG-CD	-5.51	1.33	1.52
2	E	118	PHE	CB-CG	-5.51	1.42	1.51
1	J	32	TYR	CG-CD2	-5.51	1.31	1.39
2	N	54	PRO	CG-CD	-5.51	1.32	1.50
3	1	343	ARG	CZ-NH1	-5.51	1.25	1.33
3	1	454	LYS	C-O	-5.51	1.12	1.23
3	C	487	LYS	C-O	-5.50	1.12	1.23
3	R	343	ARG	CZ-NH1	-5.50	1.25	1.33
3	Y	343	ARG	CZ-NH1	-5.50	1.25	1.33
1	Z	51	LYS	CG-CD	-5.50	1.33	1.52
3	4	63	ARG	NE-CZ	-5.50	1.25	1.33
2	K	72	SER	CB-OG	-5.50	1.35	1.42
2	H	76	PHE	C-O	-5.50	1.12	1.23
2	N	118	PHE	CB-CG	-5.50	1.42	1.51
3	4	160	PHE	CG-CD2	-5.50	1.30	1.38
1	8	32	TYR	CG-CD2	-5.50	1.31	1.39
1	W	51	LYS	CG-CD	-5.50	1.33	1.52
1	W	86	PHE	CG-CD2	-5.50	1.30	1.38
2	B	118	PHE	CB-CG	-5.50	1.42	1.51
2	E	76	PHE	C-O	-5.50	1.12	1.23
3	O	487	LYS	C-O	-5.50	1.12	1.23
1	S	51	LYS	CG-CD	-5.50	1.33	1.52
3	V	343	ARG	CZ-NH1	-5.50	1.25	1.33
3	Y	454	LYS	C-O	-5.50	1.12	1.23
3	4	147	GLN	CD-OE1	-5.50	1.11	1.24
1	D	86	PHE	CG-CD2	-5.50	1.30	1.38
1	G	51	LYS	CG-CD	-5.50	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	86	PHE	CG-CD2	-5.50	1.30	1.38
3	V	454	LYS	C-O	-5.50	1.12	1.23
3	Y	487	LYS	C-O	-5.50	1.12	1.23
2	B	76	PHE	C-O	-5.49	1.12	1.23
2	N	66	ARG	CZ-NH2	-5.49	1.25	1.33
2	Q	118	PHE	CB-CG	-5.49	1.42	1.51
2	X	118	PHE	CB-CG	-5.49	1.42	1.51
3	1	271	ARG	CZ-NH1	-5.49	1.25	1.33
3	4	271	ARG	CZ-NH1	-5.49	1.25	1.33
3	U	487	LYS	C-O	-5.49	1.12	1.23
2	9	118	PHE	CB-CG	-5.49	1.42	1.51
3	F	309	TYR	CE1-CZ	-5.49	1.31	1.38
2	3	66	ARG	CZ-NH2	-5.49	1.25	1.33
1	D	32	TYR	CG-CD2	-5.49	1.32	1.39
3	O	63	ARG	NE-CZ	-5.49	1.25	1.33
3	O	454	LYS	C-O	-5.49	1.12	1.23
2	6	66	ARG	CZ-NH2	-5.49	1.25	1.33
3	4	487	LYS	C-O	-5.49	1.12	1.23
3	L	271	ARG	CZ-NH1	-5.49	1.25	1.33
3	R	269	GLU	CB-CG	5.48	1.62	1.52
3	R	532	ARG	NE-CZ	-5.48	1.25	1.33
1	2	32	TYR	CG-CD2	-5.48	1.32	1.39
3	F	164	ILE	CB-CG2	-5.48	1.35	1.52
2	X	76	PHE	C-O	-5.48	1.12	1.23
3	7	147	GLN	CD-OE1	-5.48	1.11	1.24
1	P	86	PHE	CG-CD2	-5.48	1.30	1.38
3	R	487	LYS	C-O	-5.48	1.12	1.23
3	1	487	LYS	C-O	-5.48	1.12	1.23
3	I	147	GLN	CD-OE1	-5.48	1.11	1.24
3	I	454	LYS	C-O	-5.48	1.12	1.23
2	K	76	PHE	C-O	-5.48	1.12	1.23
1	W	12	MET	C-O	-5.48	1.12	1.23
2	0	76	PHE	C-O	-5.48	1.12	1.23
1	2	86	PHE	CG-CD2	-5.48	1.30	1.38
3	4	269	GLU	CB-CG	5.48	1.62	1.52
1	8	86	PHE	CG-CD2	-5.48	1.30	1.38
3	U	147	GLN	CD-OE1	-5.48	1.11	1.24
3	F	147	GLN	CD-OE1	-5.47	1.11	1.24
1	M	32	TYR	CG-CD2	-5.47	1.32	1.39
1	M	86	PHE	CG-CD2	-5.47	1.30	1.38
3	O	271	ARG	CZ-NH1	-5.47	1.25	1.33
1	A	86	PHE	CG-CD2	-5.47	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	376	TRP	CG-CD2	-5.47	1.34	1.43
1	8	12	MET	C-O	-5.47	1.12	1.23
3	F	532	ARG	NE-CZ	-5.47	1.25	1.33
2	Q	66	ARG	CZ-NH2	-5.47	1.25	1.33
3	Y	164	ILE	CB-CG2	-5.47	1.35	1.52
3	U	376	TRP	CG-CD2	-5.47	1.34	1.43
1	A	12	MET	C-O	-5.47	1.12	1.23
2	H	66	ARG	CZ-NH2	-5.47	1.25	1.33
1	D	14	TYR	CE2-CZ	-5.47	1.31	1.38
3	I	376	TRP	CG-CD2	-5.47	1.34	1.43
1	Z	12	MET	C-O	-5.47	1.12	1.23
1	2	12	MET	C-O	-5.47	1.12	1.23
1	5	86	PHE	CG-CD2	-5.47	1.30	1.38
2	6	76	PHE	C-O	-5.47	1.12	1.23
3	7	269	GLU	CB-CG	5.47	1.62	1.52
2	9	76	PHE	C-O	-5.47	1.12	1.23
3	C	147	GLN	CD-OE1	-5.46	1.11	1.24
2	0	66	ARG	CZ-NH2	-5.46	1.25	1.33
3	7	42	GLU	CD-OE2	-5.46	1.19	1.25
3	L	532	ARG	NE-CZ	-5.46	1.25	1.33
1	A	32	TYR	CG-CD2	-5.46	1.32	1.39
2	K	118	PHE	CB-CG	-5.46	1.42	1.51
3	1	164	ILE	CB-CG2	-5.46	1.35	1.52
3	F	291	ARG	CD-NE	-5.46	1.37	1.46
1	P	12	MET	C-O	-5.46	1.12	1.23
1	5	12	MET	C-O	-5.46	1.12	1.23
3	7	164	ILE	CB-CG2	-5.46	1.35	1.52
2	9	66	ARG	CZ-NH2	-5.46	1.25	1.33
2	B	66	ARG	CZ-NH2	-5.46	1.25	1.33
3	R	147	GLN	CD-OE1	-5.46	1.11	1.24
3	V	478	TYR	CD1-CE1	-5.46	1.31	1.39
3	Y	360	SER	CA-CB	-5.46	1.44	1.52
3	Y	376	TRP	CG-CD2	-5.46	1.34	1.43
3	C	164	ILE	CB-CG2	-5.46	1.35	1.52
1	J	86	PHE	CG-CD2	-5.46	1.30	1.38
1	M	12	MET	C-O	-5.46	1.12	1.23
3	V	291	ARG	CD-NE	-5.46	1.37	1.46
3	1	387	LYS	CB-CG	-5.46	1.37	1.52
3	Y	269	GLU	CB-CG	5.45	1.62	1.52
1	D	12	MET	C-O	-5.45	1.12	1.23
3	F	269	GLU	CB-CG	5.45	1.62	1.52
1	G	86	PHE	CG-CD2	-5.45	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	387	LYS	CB-CG	-5.45	1.37	1.52
3	C	269	GLU	CB-CG	5.45	1.62	1.52
3	I	164	ILE	CB-CG2	-5.45	1.35	1.52
3	L	147	GLN	CD-OE1	-5.45	1.11	1.24
3	L	269	GLU	CB-CG	5.45	1.62	1.52
3	O	147	GLN	CD-OE1	-5.45	1.11	1.24
3	R	164	ILE	CB-CG2	-5.45	1.35	1.52
3	V	147	GLN	CD-OE1	-5.45	1.11	1.24
3	V	164	ILE	CB-CG2	-5.45	1.35	1.52
2	X	66	ARG	CZ-NH2	-5.45	1.25	1.33
3	Y	42	GLU	CD-OE2	-5.45	1.19	1.25
3	Y	291	ARG	CD-NE	-5.45	1.37	1.46
3	1	147	GLN	CD-OE1	-5.45	1.11	1.24
3	1	269	GLU	CB-CG	5.45	1.62	1.52
3	U	478	TYR	CD1-CE1	-5.45	1.31	1.39
3	U	532	ARG	NE-CZ	-5.45	1.25	1.33
1	J	12	MET	C-O	-5.45	1.12	1.23
1	S	12	MET	C-O	-5.45	1.12	1.23
1	Z	86	PHE	CG-CD2	-5.45	1.30	1.38
3	Y	147	GLN	CD-OE1	-5.45	1.11	1.24
3	O	269	GLU	CB-CG	5.45	1.62	1.52
3	R	118	GLY	N-CA	-5.45	1.37	1.46
3	Y	478	TYR	CD1-CE1	-5.45	1.31	1.39
3	4	130	ILE	C-N	-5.45	1.21	1.34
3	U	164	ILE	CB-CG2	-5.45	1.35	1.52
3	F	387	LYS	CB-CG	-5.44	1.37	1.52
3	O	164	ILE	CB-CG2	-5.44	1.35	1.52
3	4	164	ILE	CB-CG2	-5.44	1.35	1.52
3	O	42	GLU	CD-OE2	-5.44	1.19	1.25
3	R	360	SER	CA-CB	-5.44	1.44	1.52
3	1	360	SER	CA-CB	-5.44	1.44	1.52
3	V	269	GLU	CB-CG	5.44	1.62	1.52
3	U	387	LYS	CB-CG	-5.44	1.37	1.52
3	C	532	ARG	NE-CZ	-5.44	1.25	1.33
3	L	42	GLU	CD-OE2	-5.44	1.19	1.25
3	L	443	ARG	CD-NE	-5.44	1.37	1.46
3	V	309	TYR	CE1-CZ	-5.44	1.31	1.38
1	Z	32	TYR	CG-CD2	-5.44	1.32	1.39
3	1	478	TYR	CD1-CE1	-5.44	1.31	1.39
3	4	360	SER	CA-CB	-5.44	1.44	1.52
3	L	376	TRP	CG-CD2	-5.44	1.34	1.43
1	G	32	TYR	CG-CD2	-5.43	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	269	GLU	CB-CG	5.43	1.62	1.52
3	V	443	ARG	CD-NE	-5.43	1.37	1.46
3	4	376	TRP	CG-CD2	-5.43	1.34	1.43
3	U	291	ARG	CD-NE	-5.43	1.37	1.46
3	C	376	TRP	CG-CD2	-5.43	1.34	1.43
3	L	164	ILE	CB-CG2	-5.43	1.36	1.52
2	N	128	ASN	CG-ND2	-5.43	1.19	1.32
3	R	443	ARG	CD-NE	-5.43	1.37	1.46
3	Y	387	LYS	CB-CG	-5.43	1.37	1.52
3	1	200	GLY	C-O	-5.43	1.15	1.23
1	8	14	TYR	CE2-CZ	-5.43	1.31	1.38
3	F	360	SER	CA-CB	-5.43	1.44	1.52
2	H	128	ASN	CG-ND2	-5.43	1.19	1.32
3	I	42	GLU	CD-OE2	-5.43	1.19	1.25
3	V	42	GLU	CD-OE2	-5.43	1.19	1.25
3	4	136	ILE	CG1-CD1	-5.43	1.12	1.50
3	U	269	GLU	CB-CG	5.43	1.62	1.52
3	C	291	ARG	CD-NE	-5.43	1.37	1.46
3	F	130	ILE	C-N	-5.43	1.21	1.34
1	S	14	TYR	CE2-CZ	-5.43	1.31	1.38
3	7	532	ARG	NE-CZ	-5.43	1.25	1.33
3	U	136	ILE	CG1-CD1	-5.43	1.12	1.50
3	I	136	ILE	CG1-CD1	-5.43	1.13	1.50
2	K	66	ARG	CZ-NH2	-5.43	1.25	1.33
3	L	387	LYS	CB-CG	-5.43	1.38	1.52
3	O	136	ILE	CG1-CD1	-5.43	1.13	1.50
3	O	360	SER	CA-CB	-5.43	1.44	1.52
3	1	136	ILE	CG1-CD1	-5.43	1.13	1.50
3	7	291	ARG	CD-NE	-5.43	1.37	1.46
3	C	42	GLU	CD-OE2	-5.42	1.19	1.25
3	C	387	LYS	CB-CG	-5.42	1.38	1.52
3	F	136	ILE	CG1-CD1	-5.42	1.13	1.50
3	Y	136	ILE	CG1-CD1	-5.42	1.13	1.50
3	4	532	ARG	NE-CZ	-5.42	1.25	1.33
3	7	136	ILE	CG1-CD1	-5.42	1.13	1.50
3	L	478	TYR	CD1-CE1	-5.42	1.31	1.39
3	R	387	LYS	CB-CG	-5.42	1.38	1.52
3	1	443	ARG	CD-NE	-5.42	1.37	1.46
3	C	136	ILE	CG1-CD1	-5.42	1.13	1.50
3	O	387	LYS	CB-CG	-5.42	1.38	1.52
1	P	32	TYR	CG-CD2	-5.42	1.32	1.39
3	R	136	ILE	CG1-CD1	-5.42	1.13	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	376	TRP	CG-CD2	-5.42	1.34	1.43
3	V	532	ARG	NE-CZ	-5.42	1.26	1.33
1	Z	14	TYR	CE2-CZ	-5.42	1.31	1.38
3	1	291	ARG	CD-NE	-5.42	1.37	1.46
3	4	291	ARG	CD-NE	-5.42	1.37	1.46
1	5	32	TYR	CG-CD2	-5.42	1.32	1.39
3	I	532	ARG	NE-CZ	-5.42	1.26	1.33
3	O	200	GLY	C-O	-5.42	1.15	1.23
2	T	128	ASN	CG-ND2	-5.42	1.19	1.32
3	1	376	TRP	CG-CD2	-5.42	1.34	1.43
3	F	478	TYR	CD1-CE1	-5.42	1.31	1.39
3	I	130	ILE	C-N	-5.42	1.21	1.34
3	O	118	GLY	N-CA	-5.42	1.38	1.46
3	O	130	ILE	C-N	-5.42	1.21	1.34
3	O	532	ARG	NE-CZ	-5.42	1.26	1.33
3	V	136	ILE	CG1-CD1	-5.42	1.13	1.50
2	X	128	ASN	CG-ND2	-5.42	1.19	1.32
3	U	42	GLU	CD-OE2	-5.42	1.19	1.25
3	C	309	TYR	CE1-CZ	-5.42	1.31	1.38
3	L	136	ILE	CG1-CD1	-5.42	1.13	1.50
2	T	66	ARG	CZ-NH2	-5.42	1.26	1.33
3	V	360	SER	CA-CB	-5.42	1.44	1.52
3	1	309	TYR	CE1-CZ	-5.42	1.31	1.38
3	4	309	TYR	CE1-CZ	-5.42	1.31	1.38
3	C	478	TYR	CD1-CE1	-5.42	1.31	1.39
3	I	309	TYR	CE1-CZ	-5.42	1.31	1.38
3	R	291	ARG	CD-NE	-5.42	1.37	1.46
3	V	130	ILE	C-N	-5.42	1.21	1.34
2	0	128	ASN	CG-ND2	-5.42	1.19	1.32
3	O	291	ARG	CD-NE	-5.41	1.37	1.46
3	O	443	ARG	CD-NE	-5.41	1.37	1.46
3	R	130	ILE	C-N	-5.41	1.21	1.34
3	Y	130	ILE	C-N	-5.41	1.21	1.34
2	0	59	LYS	CB-CG	-5.41	1.38	1.52
2	K	128	ASN	CG-ND2	-5.41	1.19	1.32
3	4	443	ARG	CD-NE	-5.41	1.37	1.46
1	8	66[A]	LYS	CG-CD	-5.41	1.34	1.52
1	8	66[B]	LYS	CG-CD	-5.41	1.34	1.52
3	C	130	ILE	C-N	-5.41	1.21	1.34
3	C	360	SER	CA-CB	-5.41	1.44	1.52
3	I	387	LYS	CB-CG	-5.41	1.38	1.52
3	O	478	TYR	CD1-CE1	-5.41	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	478	TYR	CD1-CE1	-5.41	1.31	1.39
1	S	66[A]	LYS	CG-CD	-5.41	1.34	1.52
1	S	66[B]	LYS	CG-CD	-5.41	1.34	1.52
2	6	59	LYS	CB-CG	-5.41	1.38	1.52
2	B	128	ASN	CG-ND2	-5.41	1.19	1.32
3	C	118	GLY	N-CA	-5.41	1.38	1.46
3	I	291	ARG	CD-NE	-5.41	1.37	1.46
3	L	81	ARG	CZ-NH2	-5.41	1.26	1.33
3	V	118	GLY	N-CA	-5.41	1.38	1.46
3	V	200	GLY	C-O	-5.41	1.15	1.23
3	4	118	GLY	N-CA	-5.41	1.38	1.46
3	7	130	ILE	C-N	-5.41	1.21	1.34
3	U	360	SER	CA-CB	-5.41	1.44	1.52
1	G	66[A]	LYS	CG-CD	-5.40	1.34	1.52
1	G	66[B]	LYS	CG-CD	-5.40	1.34	1.52
3	R	309	TYR	CE1-CZ	-5.40	1.31	1.38
3	7	376	TRP	CG-CD2	-5.40	1.34	1.43
3	C	443	ARG	CD-NE	-5.40	1.37	1.46
3	F	443	ARG	CD-NE	-5.40	1.37	1.46
1	G	14	TYR	CE2-CZ	-5.40	1.31	1.38
3	I	118	GLY	N-CA	-5.40	1.38	1.46
3	O	309	TYR	CE1-CZ	-5.40	1.31	1.38
3	V	81	ARG	CZ-NH2	-5.40	1.26	1.33
3	Y	309	TYR	CE1-CZ	-5.40	1.31	1.38
3	4	387	LYS	CB-CG	-5.40	1.38	1.52
3	U	118	GLY	N-CA	-5.40	1.38	1.46
3	U	200	GLY	C-O	-5.40	1.15	1.23
3	U	309	TYR	CE1-CZ	-5.40	1.31	1.38
3	O	440	TRP	CG-CD2	-5.40	1.34	1.43
3	V	376	TRP	CG-CD2	-5.40	1.34	1.43
3	Y	532	ARG	NE-CZ	-5.40	1.26	1.33
3	1	42	GLU	CD-OE2	-5.40	1.19	1.25
3	1	494	VAL	C-N	-5.40	1.21	1.34
3	7	200	GLY	C-O	-5.40	1.15	1.23
3	7	387	LYS	CB-CG	-5.40	1.38	1.52
3	7	478	TYR	CD1-CE1	-5.40	1.31	1.39
3	4	478	TYR	CD1-CE1	-5.40	1.31	1.39
3	7	494	VAL	C-N	-5.40	1.21	1.34
3	U	81	ARG	CZ-NH2	-5.40	1.26	1.33
1	A	66[A]	LYS	CG-CD	-5.40	1.34	1.52
1	A	66[B]	LYS	CG-CD	-5.40	1.34	1.52
2	E	59	LYS	CB-CG	-5.40	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	59	LYS	CB-CG	-5.40	1.38	1.52
2	3	128	ASN	CG-ND2	-5.40	1.19	1.32
3	U	443	ARG	CD-NE	-5.40	1.37	1.46
2	E	128	ASN	CG-ND2	-5.40	1.19	1.32
2	H	59	LYS	CB-CG	-5.40	1.38	1.52
3	V	494	VAL	C-N	-5.40	1.21	1.34
3	7	118	GLY	N-CA	-5.40	1.38	1.46
2	9	128	ASN	CG-ND2	-5.40	1.19	1.32
3	U	130	ILE	C-N	-5.40	1.21	1.34
2	B	59	LYS	CB-CG	-5.39	1.38	1.52
3	L	291	ARG	CD-NE	-5.39	1.37	1.46
1	M	66[A]	LYS	CG-CD	-5.39	1.34	1.52
1	M	66[B]	LYS	CG-CD	-5.39	1.34	1.52
3	1	118	GLY	N-CA	-5.39	1.38	1.46
2	3	59	LYS	CB-CG	-5.39	1.38	1.52
1	A	14	TYR	CE2-CZ	-5.39	1.31	1.38
1	D	66[A]	LYS	CG-CD	-5.39	1.34	1.52
1	D	66[B]	LYS	CG-CD	-5.39	1.34	1.52
3	I	81	ARG	CZ-NH2	-5.39	1.26	1.33
3	I	360	SER	CA-CB	-5.39	1.44	1.52
1	M	14	TYR	CE2-CZ	-5.39	1.31	1.38
2	Q	128	ASN	CG-ND2	-5.39	1.19	1.32
3	1	81	ARG	CZ-NH2	-5.39	1.26	1.33
3	4	42	GLU	CD-OE2	-5.39	1.19	1.25
3	L	200	GLY	C-O	-5.39	1.15	1.23
1	P	66[A]	LYS	CG-CD	-5.39	1.34	1.52
1	P	66[B]	LYS	CG-CD	-5.39	1.34	1.52
1	Z	66[A]	LYS	CG-CD	-5.39	1.34	1.52
1	Z	66[B]	LYS	CG-CD	-5.39	1.34	1.52
3	1	130	ILE	C-N	-5.39	1.21	1.34
3	7	443	ARG	CD-NE	-5.39	1.37	1.46
2	E	66	ARG	CZ-NH2	-5.39	1.26	1.33
2	K	59	LYS	CB-CG	-5.39	1.38	1.52
3	R	42	GLU	CD-OE2	-5.39	1.19	1.25
2	6	128	ASN	CG-ND2	-5.39	1.19	1.32
3	Y	443	ARG	CD-NE	-5.39	1.37	1.46
3	Y	494	VAL	C-N	-5.39	1.21	1.34
1	2	14	TYR	CE2-CZ	-5.39	1.31	1.38
2	9	59	LYS	CB-CG	-5.39	1.38	1.52
3	C	81	ARG	CZ-NH2	-5.38	1.26	1.33
3	R	81	ARG	CZ-NH2	-5.38	1.26	1.33
3	R	200	GLY	C-O	-5.38	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	532	ARG	NE-CZ	-5.38	1.26	1.33
3	4	81	ARG	CZ-NH2	-5.38	1.26	1.33
3	C	200	GLY	C-O	-5.38	1.15	1.23
3	C	494	VAL	C-N	-5.38	1.21	1.34
3	F	118	GLY	N-CA	-5.38	1.38	1.46
3	F	376	TRP	CG-CD2	-5.38	1.34	1.43
3	F	494	VAL	C-N	-5.38	1.21	1.34
1	J	66[A]	LYS	CG-CD	-5.38	1.34	1.52
1	J	66[B]	LYS	CG-CD	-5.38	1.34	1.52
3	O	81	ARG	CZ-NH2	-5.38	1.26	1.33
3	O	494	VAL	C-N	-5.38	1.21	1.34
2	Q	59	LYS	CB-CG	-5.38	1.38	1.52
1	W	66[A]	LYS	CG-CD	-5.38	1.34	1.52
1	W	66[B]	LYS	CG-CD	-5.38	1.34	1.52
3	L	130	ILE	C-N	-5.38	1.21	1.34
3	R	494	VAL	C-N	-5.38	1.21	1.34
1	2	66[A]	LYS	CG-CD	-5.38	1.34	1.52
1	2	66[B]	LYS	CG-CD	-5.38	1.34	1.52
1	5	14	TYR	CE2-CZ	-5.38	1.31	1.38
3	7	81	ARG	CZ-NH2	-5.38	1.26	1.33
3	7	360	SER	CA-CB	-5.38	1.44	1.52
1	J	14	TYR	CE2-CZ	-5.38	1.31	1.38
2	T	59	LYS	CB-CG	-5.38	1.38	1.52
3	7	309	TYR	CE1-CZ	-5.38	1.31	1.38
3	L	360	SER	CA-CB	-5.38	1.44	1.52
1	5	66[A]	LYS	CG-CD	-5.38	1.34	1.52
1	5	66[B]	LYS	CG-CD	-5.38	1.34	1.52
1	P	14	TYR	CE2-CZ	-5.38	1.31	1.38
3	V	440	TRP	CG-CD2	-5.38	1.34	1.43
3	F	200	GLY	C-O	-5.37	1.15	1.23
3	I	494	VAL	C-N	-5.37	1.21	1.34
2	X	59	LYS	CB-CG	-5.37	1.38	1.52
3	1	440	TRP	CG-CD2	-5.37	1.34	1.43
3	4	200	GLY	C-O	-5.37	1.15	1.23
3	4	494	VAL	C-N	-5.37	1.21	1.34
3	F	440	TRP	CG-CD2	-5.37	1.34	1.43
3	U	494	VAL	C-N	-5.37	1.21	1.34
3	F	81	ARG	CZ-NH2	-5.37	1.26	1.33
1	W	14	TYR	CE2-CZ	-5.37	1.31	1.38
1	W	24	LYS	CE-NZ	-5.36	1.35	1.49
3	L	118	GLY	N-CA	-5.36	1.38	1.46
2	6	134	TRP	CD1-NE1	-5.36	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	440	TRP	CG-CD2	-5.36	1.34	1.43
2	K	134	TRP	CD1-NE1	-5.36	1.28	1.38
3	L	494	VAL	C-N	-5.36	1.21	1.34
3	C	440	TRP	CG-CD2	-5.36	1.34	1.43
1	D	99	ILE	CG1-CD1	-5.36	1.13	1.50
3	I	478	TYR	CD1-CE1	-5.36	1.31	1.39
1	Z	99	ILE	CG1-CD1	-5.36	1.13	1.50
3	I	443	ARG	CD-NE	-5.35	1.37	1.46
2	O	134	TRP	CD1-NE1	-5.35	1.28	1.38
1	M	99	ILE	CG1-CD1	-5.35	1.13	1.50
1	G	99	ILE	CG1-CD1	-5.35	1.13	1.50
1	J	24	LYS	CE-NZ	-5.35	1.35	1.49
3	Y	118	GLY	N-CA	-5.35	1.38	1.46
1	5	99	ILE	CG1-CD1	-5.35	1.13	1.50
1	8	99	ILE	CG1-CD1	-5.35	1.13	1.50
3	U	440	TRP	CG-CD2	-5.35	1.34	1.43
1	A	99	ILE	CG1-CD1	-5.35	1.13	1.50
3	I	200	GLY	C-O	-5.35	1.15	1.23
1	J	99	ILE	CG1-CD1	-5.35	1.13	1.50
1	S	99	ILE	CG1-CD1	-5.35	1.13	1.50
1	W	99	ILE	CG1-CD1	-5.35	1.13	1.50
1	2	99	ILE	CG1-CD1	-5.35	1.13	1.50
2	3	134	TRP	CD1-NE1	-5.35	1.28	1.38
3	7	216	ALA	C-O	-5.35	1.13	1.23
3	R	440	TRP	CG-CD2	-5.35	1.34	1.43
1	2	24	LYS	CE-NZ	-5.35	1.35	1.49
3	L	309	TYR	CE1-CZ	-5.34	1.31	1.38
1	P	99	ILE	CG1-CD1	-5.34	1.13	1.50
3	Y	81	ARG	CZ-NH2	-5.34	1.26	1.33
2	K	140	VAL	C-N	5.34	1.44	1.34
1	G	24	LYS	CE-NZ	-5.34	1.35	1.49
1	W	2	GLN	CG-CD	-5.34	1.38	1.51
1	J	2	GLN	CG-CD	-5.34	1.38	1.51
1	8	24	LYS	CE-NZ	-5.34	1.35	1.49
2	B	134	TRP	CD1-NE1	-5.34	1.28	1.38
1	P	24	LYS	CE-NZ	-5.34	1.35	1.49
3	Y	200	GLY	C-O	-5.34	1.15	1.23
3	7	440	TRP	CG-CD2	-5.33	1.34	1.43
1	A	24	LYS	CE-NZ	-5.33	1.35	1.49
1	D	24	LYS	CE-NZ	-5.33	1.35	1.49
2	N	134	TRP	CD1-NE1	-5.33	1.28	1.38
1	5	24	LYS	CE-NZ	-5.33	1.35	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8	2	GLN	CG-CD	-5.33	1.38	1.51
1	Z	24	LYS	CE-NZ	-5.33	1.35	1.49
3	L	101	LYS	C-O	-5.33	1.13	1.23
3	4	440	TRP	CG-CD2	-5.33	1.34	1.43
2	Q	134	TRP	CD1-NE1	-5.32	1.28	1.38
1	S	24	LYS	CE-NZ	-5.32	1.35	1.49
3	F	42	GLU	CD-OE2	-5.32	1.19	1.25
3	4	216	ALA	C-O	-5.32	1.13	1.23
3	V	216	ALA	C-O	-5.32	1.13	1.23
3	7	101	LYS	C-O	-5.32	1.13	1.23
2	E	140	VAL	C-N	5.32	1.44	1.34
1	A	2	GLN	CG-CD	-5.32	1.38	1.51
1	M	24	LYS	CE-NZ	-5.32	1.35	1.49
3	L	440	TRP	CG-CD2	-5.31	1.34	1.43
3	V	350	GLU	CD-OE2	-5.31	1.19	1.25
3	Y	440	TRP	CG-CD2	-5.31	1.34	1.43
2	E	134	TRP	CD1-NE1	-5.31	1.28	1.38
1	G	2	GLN	CG-CD	-5.31	1.38	1.51
2	H	134	TRP	CD1-NE1	-5.31	1.28	1.38
1	M	2	GLN	CG-CD	-5.31	1.38	1.51
3	C	216	ALA	C-O	-5.31	1.13	1.23
3	F	482	PHE	CG-CD2	-5.31	1.30	1.38
3	O	101	LYS	C-O	-5.31	1.13	1.23
2	T	140	VAL	C-N	5.31	1.44	1.34
2	9	134	TRP	CD1-NE1	-5.31	1.28	1.38
2	9	140	VAL	C-N	5.31	1.44	1.34
2	B	140	VAL	C-N	5.31	1.44	1.34
3	I	216	ALA	C-O	-5.30	1.13	1.23
1	P	2	GLN	CG-CD	-5.30	1.38	1.51
3	F	216	ALA	C-O	-5.30	1.13	1.23
2	H	140	VAL	C-N	5.30	1.44	1.34
3	L	177	PRO	C-N	-5.30	1.23	1.33
2	N	140	VAL	C-N	5.30	1.44	1.34
1	Z	2	GLN	CG-CD	-5.30	1.38	1.51
3	1	101	LYS	C-O	-5.30	1.13	1.23
3	U	101	LYS	C-O	-5.30	1.13	1.23
3	I	101	LYS	C-O	-5.30	1.13	1.23
2	0	140	VAL	C-N	5.30	1.44	1.34
3	1	482	PHE	CG-CD2	-5.30	1.30	1.38
3	F	350	GLU	CD-OE2	-5.30	1.19	1.25
3	R	92	ARG	CB-CG	-5.30	1.38	1.52
2	T	134	TRP	CD1-NE1	-5.30	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	140	VAL	C-N	5.30	1.44	1.34
3	U	216	ALA	C-O	-5.30	1.13	1.23
3	L	482	PHE	CG-CD2	-5.29	1.30	1.38
3	L	350	GLU	CD-OE2	-5.29	1.19	1.25
3	R	216	ALA	C-O	-5.29	1.13	1.23
1	S	2	GLN	CG-CD	-5.29	1.38	1.51
3	V	92	ARG	CB-CG	-5.29	1.38	1.52
1	D	2	GLN	CG-CD	-5.29	1.38	1.51
3	F	177	PRO	C-N	-5.29	1.23	1.33
3	Y	216	ALA	C-O	-5.29	1.13	1.23
3	Y	490[A]	GLN	CB-CG	-5.29	1.38	1.52
3	Y	490[B]	GLN	CB-CG	-5.29	1.38	1.52
3	C	101	LYS	C-O	-5.29	1.13	1.23
3	L	216	ALA	C-O	-5.29	1.13	1.23
3	1	92	ARG	CD-NE	-5.29	1.37	1.46
3	I	490[A]	GLN	CB-CG	-5.29	1.38	1.52
3	I	490[B]	GLN	CB-CG	-5.29	1.38	1.52
1	2	2	GLN	CG-CD	-5.29	1.38	1.51
3	7	92	ARG	CB-CG	-5.29	1.38	1.52
3	I	482	PHE	CG-CD2	-5.29	1.30	1.38
2	X	134	TRP	CD1-NE1	-5.29	1.28	1.38
3	U	482	PHE	CG-CD2	-5.29	1.30	1.38
2	Q	105	PHE	CD1-CE1	-5.29	1.28	1.39
3	V	490[A]	GLN	CB-CG	-5.29	1.38	1.52
3	V	490[B]	GLN	CB-CG	-5.29	1.38	1.52
1	2	86	PHE	CG-CD1	-5.29	1.30	1.38
3	4	101	LYS	C-O	-5.29	1.13	1.23
2	6	140	VAL	C-N	5.29	1.44	1.34
3	Y	101	LYS	C-O	-5.28	1.13	1.23
3	4	350	GLU	CD-OE2	-5.28	1.19	1.25
1	5	2	GLN	CG-CD	-5.28	1.39	1.51
2	6	105	PHE	CD1-CE1	-5.28	1.28	1.39
3	1	92	ARG	CB-CG	-5.28	1.38	1.52
2	3	140	VAL	C-N	5.28	1.44	1.34
3	7	177	PRO	C-N	-5.28	1.23	1.33
3	U	92	ARG	CD-NE	-5.28	1.37	1.46
3	O	482	PHE	CG-CD2	-5.28	1.30	1.38
3	1	490[A]	GLN	CB-CG	-5.28	1.38	1.52
3	1	490[B]	GLN	CB-CG	-5.28	1.38	1.52
3	7	350	GLU	CD-OE2	-5.28	1.19	1.25
3	L	473	PRO	CG-CD	-5.27	1.33	1.50
3	R	490[A]	GLN	CB-CG	-5.27	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	490[B]	GLN	CB-CG	-5.27	1.38	1.52
3	F	101	LYS	C-O	-5.27	1.13	1.23
3	I	92	ARG	CB-CG	-5.27	1.38	1.52
1	J	86	PHE	CG-CD1	-5.27	1.30	1.38
3	R	459	ASN	CB-CG	-5.27	1.39	1.51
3	V	101	LYS	C-O	-5.27	1.13	1.23
3	Y	177	PRO	C-N	-5.27	1.23	1.33
3	1	216	ALA	C-O	-5.27	1.13	1.23
3	1	350	GLU	CD-OE2	-5.27	1.19	1.25
3	4	92	ARG	CB-CG	-5.27	1.38	1.52
3	C	482	PHE	CG-CD2	-5.27	1.30	1.38
3	C	490[A]	GLN	CB-CG	-5.27	1.38	1.52
3	C	490[B]	GLN	CB-CG	-5.27	1.38	1.52
3	I	177	PRO	C-N	-5.27	1.23	1.33
3	R	101	LYS	C-O	-5.27	1.13	1.23
3	V	482	PHE	CG-CD2	-5.27	1.30	1.38
3	1	177	PRO	C-N	-5.27	1.23	1.33
3	U	490[A]	GLN	CB-CG	-5.27	1.38	1.52
3	U	490[B]	GLN	CB-CG	-5.27	1.38	1.52
3	C	92	ARG	CB-CG	-5.27	1.38	1.52
3	F	569	TYR	CD1-CE1	-5.27	1.31	1.39
3	O	216	ALA	C-O	-5.27	1.13	1.23
3	O	490[A]	GLN	CB-CG	-5.27	1.38	1.52
3	O	490[B]	GLN	CB-CG	-5.27	1.38	1.52
3	7	460	TRP	CZ2-CH2	-5.27	1.27	1.37
1	S	86	PHE	CG-CD1	-5.27	1.30	1.38
3	U	459	ASN	CB-CG	-5.27	1.39	1.51
3	F	490[A]	GLN	CB-CG	-5.26	1.38	1.52
3	F	490[B]	GLN	CB-CG	-5.26	1.38	1.52
3	I	92	ARG	CD-NE	-5.26	1.37	1.46
3	L	490[A]	GLN	CB-CG	-5.26	1.38	1.52
3	L	490[B]	GLN	CB-CG	-5.26	1.38	1.52
3	O	460	TRP	CZ2-CH2	-5.26	1.27	1.37
2	Q	140	VAL	C-N	5.26	1.44	1.34
1	W	86	PHE	CG-CD1	-5.26	1.30	1.38
3	4	490[A]	GLN	CB-CG	-5.26	1.38	1.52
3	4	490[B]	GLN	CB-CG	-5.26	1.38	1.52
1	M	69	VAL	CB-CG2	-5.26	1.41	1.52
3	R	482	PHE	CG-CD2	-5.26	1.30	1.38
3	4	473	PRO	CG-CD	-5.26	1.33	1.50
3	C	92	ARG	CD-NE	-5.26	1.37	1.46
3	I	473	PRO	CG-CD	-5.26	1.33	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	92	ARG	CB-CG	-5.26	1.38	1.52
1	5	69	VAL	CB-CG2	-5.26	1.41	1.52
1	A	86	PHE	CG-CD1	-5.26	1.30	1.38
3	C	177	PRO	C-N	-5.26	1.23	1.33
3	L	92	ARG	CD-NE	-5.26	1.37	1.46
3	V	459	ASN	CB-CG	-5.26	1.39	1.51
3	Y	92	ARG	CB-CG	-5.26	1.38	1.52
3	4	92	ARG	CD-NE	-5.26	1.37	1.46
3	I	350	GLU	CD-OE2	-5.26	1.19	1.25
2	T	105	PHE	CD1-CE1	-5.26	1.28	1.39
3	Y	350	GLU	CD-OE2	-5.26	1.19	1.25
2	3	105	PHE	CD1-CE1	-5.26	1.28	1.39
2	H	105	PHE	CD1-CE1	-5.25	1.28	1.39
3	V	473	PRO	CG-CD	-5.25	1.33	1.50
3	F	473	PRO	CG-CD	-5.25	1.33	1.50
2	0	105	PHE	CD1-CE1	-5.25	1.28	1.39
3	4	482	PHE	CG-CD2	-5.25	1.30	1.38
1	5	86	PHE	CG-CD1	-5.25	1.30	1.38
3	7	490[A]	GLN	CB-CG	-5.25	1.38	1.52
3	7	490[B]	GLN	CB-CG	-5.25	1.38	1.52
3	C	350	GLU	CD-OE2	-5.25	1.19	1.25
1	G	69	VAL	CB-CG2	-5.25	1.41	1.52
3	L	92	ARG	CB-CG	-5.25	1.38	1.52
3	U	92	ARG	CB-CG	-5.25	1.38	1.52
3	R	350	GLU	CD-OE2	-5.25	1.19	1.25
3	R	473	PRO	CG-CD	-5.25	1.33	1.50
3	U	473	PRO	CG-CD	-5.25	1.33	1.50
3	C	473	PRO	CG-CD	-5.25	1.33	1.50
1	G	86	PHE	CG-CD1	-5.25	1.30	1.38
3	O	569	TYR	CD1-CE1	-5.25	1.31	1.39
1	P	86	PHE	CG-CD1	-5.25	1.30	1.38
3	4	177	PRO	C-N	-5.25	1.23	1.33
3	C	459	ASN	CB-CG	-5.25	1.39	1.51
2	K	74	PHE	CD1-CE1	-5.25	1.28	1.39
3	L	459	ASN	CB-CG	-5.25	1.39	1.51
3	1	473	PRO	CG-CD	-5.25	1.33	1.50
1	S	70	MET	CG-SD	-5.25	1.67	1.81
1	Z	69	VAL	CB-CG2	-5.25	1.41	1.52
3	4	459	ASN	CB-CG	-5.25	1.39	1.51
1	8	86	PHE	CG-CD1	-5.25	1.30	1.38
2	N	74	PHE	CD1-CE1	-5.24	1.28	1.39
3	O	459	ASN	CB-CG	-5.24	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	74	PHE	CD1-CE1	-5.24	1.28	1.39
3	7	92	ARG	CD-NE	-5.24	1.37	1.46
3	7	473	PRO	CG-CD	-5.24	1.33	1.50
2	9	105	PHE	CD1-CE1	-5.24	1.28	1.39
3	O	92	ARG	CD-NE	-5.24	1.37	1.46
1	D	69	VAL	CB-CG2	-5.24	1.41	1.52
3	R	177	PRO	C-N	-5.24	1.23	1.33
2	X	74	PHE	CD1-CE1	-5.24	1.28	1.39
2	B	105	PHE	CD1-CE1	-5.24	1.28	1.39
3	O	473	PRO	CG-CD	-5.24	1.33	1.50
1	W	69	VAL	CB-CG2	-5.24	1.41	1.52
3	Y	482	PHE	CG-CD2	-5.24	1.30	1.38
3	U	350	GLU	CD-OE2	-5.24	1.19	1.25
1	Z	70	MET	CG-SD	-5.24	1.67	1.81
1	2	69	VAL	CB-CG2	-5.24	1.41	1.52
3	7	569	TYR	CD1-CE1	-5.24	1.31	1.39
3	F	92	ARG	CB-CG	-5.24	1.38	1.52
3	F	459	ASN	CB-CG	-5.24	1.39	1.51
3	I	459	ASN	CB-CG	-5.24	1.39	1.51
3	V	177	PRO	C-N	-5.24	1.23	1.33
3	Y	473	PRO	CG-CD	-5.24	1.33	1.50
3	7	459	ASN	CB-CG	-5.24	1.39	1.51
2	T	74	PHE	CD1-CE1	-5.23	1.28	1.39
1	8	70	MET	CG-SD	-5.23	1.67	1.81
1	P	70	MET	CG-SD	-5.23	1.67	1.81
3	1	459	ASN	CB-CG	-5.23	1.39	1.51
1	A	69	VAL	CB-CG2	-5.23	1.41	1.52
1	D	70	MET	CG-SD	-5.23	1.67	1.81
3	V	92	ARG	CD-NE	-5.23	1.37	1.46
1	2	70	MET	CG-SD	-5.23	1.67	1.81
1	5	70	MET	CG-SD	-5.23	1.67	1.81
1	A	70	MET	CG-SD	-5.23	1.67	1.81
2	B	74	PHE	CD1-CE1	-5.23	1.28	1.39
3	O	350	GLU	CD-OE2	-5.23	1.20	1.25
3	V	460	TRP	CZ2-CH2	-5.23	1.27	1.37
1	J	69	VAL	CB-CG2	-5.22	1.41	1.52
3	L	569	TYR	CD1-CE1	-5.22	1.31	1.39
1	M	70	MET	CG-SD	-5.22	1.67	1.81
3	7	482	PHE	CG-CD2	-5.22	1.30	1.38
2	E	105	PHE	CD1-CE1	-5.22	1.28	1.39
3	Y	459	ASN	CB-CG	-5.22	1.39	1.51
2	N	105	PHE	CD1-CE1	-5.22	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	70	MET	CG-SD	-5.22	1.67	1.81
3	O	177	PRO	C-N	-5.22	1.23	1.33
3	F	92	ARG	CD-NE	-5.22	1.37	1.46
3	F	173	THR	C-O	-5.22	1.13	1.23
3	F	460	TRP	CZ2-CH2	-5.22	1.27	1.37
3	I	460	TRP	CZ2-CH2	-5.22	1.27	1.37
1	J	70	MET	CG-SD	-5.22	1.67	1.81
3	C	460	TRP	CZ2-CH2	-5.22	1.27	1.37
3	F	254	SER	C-O	-5.22	1.13	1.23
1	Z	86	PHE	CG-CD1	-5.22	1.30	1.38
3	7	173	THR	C-O	-5.22	1.13	1.23
3	U	569	TYR	CD1-CE1	-5.22	1.31	1.39
3	C	569	TYR	CD1-CE1	-5.21	1.31	1.39
3	R	460	TRP	CZ2-CH2	-5.21	1.27	1.37
3	Y	460	TRP	CZ2-CH2	-5.21	1.27	1.37
3	U	177	PRO	C-N	-5.21	1.23	1.33
1	G	70	MET	CG-SD	-5.21	1.67	1.81
3	R	92	ARG	CD-NE	-5.21	1.37	1.46
3	R	173	THR	C-O	-5.21	1.13	1.23
3	Y	173	THR	C-O	-5.21	1.13	1.23
2	0	74	PHE	CD1-CE1	-5.21	1.28	1.39
2	9	74	PHE	CD1-CE1	-5.21	1.28	1.39
2	E	74	PHE	CD1-CE1	-5.21	1.28	1.39
3	L	460	TRP	CZ2-CH2	-5.21	1.27	1.37
3	O	61	LEU	CG-CD2	-5.21	1.32	1.51
1	P	69	VAL	CB-CG2	-5.21	1.42	1.52
3	R	509	LYS	CD-CE	-5.21	1.38	1.51
3	V	173	THR	C-O	-5.21	1.13	1.23
3	U	460	TRP	CZ2-CH2	-5.21	1.27	1.37
1	D	86	PHE	CG-CD1	-5.21	1.30	1.38
2	K	105	PHE	CD1-CE1	-5.21	1.28	1.39
1	M	86	PHE	CG-CD1	-5.21	1.30	1.38
3	V	254	SER	C-O	-5.21	1.13	1.23
3	1	173	THR	C-O	-5.21	1.13	1.23
3	1	569	TYR	CD1-CE1	-5.21	1.31	1.39
3	7	509	LYS	CD-CE	-5.21	1.38	1.51
3	U	254	SER	C-O	-5.21	1.13	1.23
3	7	61	LEU	CG-CD2	-5.21	1.32	1.51
3	C	173	THR	C-O	-5.20	1.13	1.23
1	S	69	VAL	CB-CG2	-5.20	1.42	1.52
2	X	105	PHE	CD1-CE1	-5.20	1.28	1.39
3	4	173	THR	C-O	-5.20	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	28	LEU	CG-CD1	-5.20	1.32	1.51
3	Y	92	ARG	CD-NE	-5.20	1.37	1.46
3	F	509	LYS	CD-CE	-5.20	1.38	1.51
3	I	509	LYS	CD-CE	-5.20	1.38	1.51
3	O	28	LEU	CG-CD1	-5.20	1.32	1.51
3	O	173	THR	C-O	-5.20	1.13	1.23
3	V	509	LYS	CD-CE	-5.20	1.38	1.51
3	Y	28	LEU	CG-CD1	-5.20	1.32	1.51
3	4	28	LEU	CG-CD1	-5.20	1.32	1.51
3	R	569	TYR	CD1-CE1	-5.20	1.31	1.39
3	1	460	TRP	CZ2-CH2	-5.20	1.27	1.37
3	4	61	LEU	CG-CD2	-5.20	1.32	1.51
2	6	74	PHE	CD1-CE1	-5.20	1.28	1.39
3	7	443	ARG	CZ-NH1	-5.20	1.26	1.33
3	R	28	LEU	CG-CD1	-5.20	1.32	1.51
3	4	460	TRP	CZ2-CH2	-5.20	1.27	1.37
3	C	509	LYS	CD-CE	-5.20	1.38	1.51
3	F	61	LEU	CG-CD2	-5.20	1.32	1.51
3	L	28	LEU	CG-CD1	-5.20	1.32	1.51
3	L	173	THR	C-O	-5.20	1.13	1.23
2	Q	74	PHE	CD1-CE1	-5.20	1.28	1.39
3	R	254	SER	C-O	-5.20	1.13	1.23
3	Y	509	LYS	CD-CE	-5.20	1.38	1.51
3	4	207	ARG	CZ-NH2	-5.20	1.26	1.33
2	9	140	VAL	CB-CG2	-5.20	1.42	1.52
3	U	28	LEU	CG-CD1	-5.20	1.32	1.51
3	L	61	LEU	CG-CD2	-5.19	1.32	1.51
3	C	28	LEU	CG-CD1	-5.19	1.32	1.51
3	V	61	LEU	CG-CD2	-5.19	1.32	1.51
3	Y	61	LEU	CG-CD2	-5.19	1.32	1.51
1	8	69	VAL	CB-CG2	-5.19	1.42	1.52
3	I	61	LEU	CG-CD2	-5.19	1.32	1.51
3	L	254	SER	C-O	-5.19	1.13	1.23
3	L	509	LYS	CD-CE	-5.19	1.38	1.51
3	U	207	ARG	CZ-NH2	-5.19	1.26	1.33
3	C	61	LEU	CG-CD2	-5.19	1.32	1.51
2	H	130	LEU	CG-CD1	-5.19	1.32	1.51
3	1	61	LEU	CG-CD2	-5.19	1.32	1.51
3	1	509	LYS	CD-CE	-5.19	1.38	1.51
3	4	509	LYS	CD-CE	-5.19	1.38	1.51
3	4	569	TYR	CD1-CE1	-5.19	1.31	1.39
2	X	130	LEU	CG-CD1	-5.19	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7	28	LEU	CG-CD1	-5.19	1.32	1.51
3	U	61	LEU	CG-CD2	-5.19	1.32	1.51
3	I	28	LEU	CG-CD1	-5.18	1.32	1.51
3	F	443	ARG	CZ-NH1	-5.18	1.26	1.33
2	H	74	PHE	CD1-CE1	-5.18	1.28	1.39
3	1	28	LEU	CG-CD1	-5.18	1.32	1.51
3	1	443	ARG	CZ-NH1	-5.18	1.26	1.33
3	C	254	SER	C-O	-5.18	1.13	1.23
3	F	28	LEU	CG-CD1	-5.18	1.32	1.51
3	I	569	TYR	CD1-CE1	-5.18	1.31	1.39
3	4	254	SER	C-O	-5.18	1.13	1.23
3	I	514	ARG	CG-CD	-5.18	1.39	1.51
2	K	130	LEU	CG-CD1	-5.18	1.32	1.51
2	T	140	VAL	CB-CG2	-5.18	1.42	1.52
3	1	254	SER	C-O	-5.18	1.13	1.23
2	6	130	LEU	CG-CD1	-5.18	1.32	1.51
3	Y	514	ARG	CG-CD	-5.18	1.39	1.51
2	Q	130	LEU	CG-CD1	-5.18	1.32	1.51
2	B	130	LEU	CG-CD1	-5.17	1.32	1.51
3	I	173	THR	C-O	-5.17	1.13	1.23
3	R	61	LEU	CG-CD2	-5.17	1.32	1.51
3	O	571	PHE	CE2-CZ	-5.17	1.27	1.37
2	K	140	VAL	CB-CG2	-5.17	1.42	1.52
3	R	248	VAL	CB-CG1	-5.17	1.42	1.52
3	Y	207	ARG	CZ-NH2	-5.17	1.26	1.33
2	0	140	VAL	CB-CG2	-5.17	1.42	1.52
3	U	509	LYS	CD-CE	-5.17	1.38	1.51
2	B	140	VAL	CB-CG2	-5.17	1.42	1.52
3	F	207	ARG	CZ-NH2	-5.17	1.26	1.33
2	E	140	VAL	CB-CG2	-5.17	1.42	1.52
3	V	514	ARG	CG-CD	-5.17	1.39	1.51
3	1	248	VAL	CB-CG1	-5.17	1.42	1.52
2	E	130	LEU	CG-CD1	-5.17	1.32	1.51
3	I	207	ARG	CZ-NH2	-5.17	1.26	1.33
3	I	353	LEU	CG-CD2	-5.17	1.32	1.51
2	N	130	LEU	CG-CD1	-5.17	1.32	1.51
2	T	130	LEU	CG-CD1	-5.17	1.32	1.51
2	3	130	LEU	CG-CD1	-5.17	1.32	1.51
3	7	571	PHE	CE2-CZ	-5.17	1.27	1.37
2	9	130	LEU	CG-CD1	-5.17	1.32	1.51
2	N	140	VAL	CB-CG2	-5.16	1.42	1.52
3	O	248	VAL	CB-CG1	-5.16	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	140	VAL	CB-CG2	-5.16	1.42	1.52
3	V	443	ARG	CZ-NH1	-5.16	1.26	1.33
3	1	353	LEU	CG-CD2	-5.16	1.32	1.51
3	7	254	SER	C-O	-5.16	1.13	1.23
3	7	353	LEU	CG-CD2	-5.16	1.32	1.51
3	V	353	LEU	CG-CD2	-5.16	1.32	1.51
3	V	569	TYR	CD1-CE1	-5.16	1.31	1.39
3	L	353	LEU	CG-CD2	-5.16	1.32	1.51
2	0	130	LEU	CG-CD1	-5.16	1.32	1.51
3	U	514	ARG	CG-CD	-5.16	1.39	1.51
3	L	514	ARG	CG-CD	-5.16	1.39	1.51
3	R	353	LEU	CG-CD2	-5.16	1.32	1.51
3	U	173	THR	C-O	-5.16	1.13	1.23
2	6	140	VAL	CB-CG2	-5.16	1.42	1.52
2	H	140	VAL	CB-CG2	-5.16	1.42	1.52
3	4	443	ARG	CZ-NH1	-5.16	1.26	1.33
3	C	248	VAL	CB-CG1	-5.15	1.42	1.52
3	C	353	LEU	CG-CD2	-5.15	1.32	1.51
3	C	514	ARG	CG-CD	-5.15	1.39	1.51
3	O	509	LYS	CD-CE	-5.15	1.38	1.51
3	V	248	VAL	CB-CG1	-5.15	1.42	1.52
3	U	248	VAL	CB-CG1	-5.15	1.42	1.52
3	R	514	ARG	CG-CD	-5.15	1.39	1.51
3	Y	443	ARG	CZ-NH1	-5.15	1.26	1.33
3	1	514	ARG	CG-CD	-5.15	1.39	1.51
3	4	248	VAL	CB-CG1	-5.15	1.42	1.52
3	O	480	PRO	C-N	-5.15	1.22	1.34
3	Y	480	PRO	C-N	-5.15	1.22	1.34
3	4	353	LEU	CG-CD2	-5.15	1.32	1.51
3	F	353	LEU	CG-CD2	-5.15	1.32	1.51
3	L	207	ARG	CZ-NH2	-5.15	1.26	1.33
3	4	514	ARG	CG-CD	-5.15	1.39	1.51
2	X	140	VAL	CB-CG2	-5.14	1.42	1.52
3	U	353	LEU	CG-CD2	-5.14	1.32	1.51
3	C	207	ARG	CZ-NH2	-5.14	1.26	1.33
3	C	443	ARG	CZ-NH1	-5.14	1.26	1.33
3	I	571	PHE	CE2-CZ	-5.14	1.27	1.37
3	L	571	PHE	CE2-CZ	-5.14	1.27	1.37
3	O	443	ARG	CZ-NH1	-5.14	1.26	1.33
3	Y	569	TYR	CD1-CE1	-5.14	1.31	1.39
3	F	105	PRO	CB-CG	-5.14	1.24	1.50
3	F	248	VAL	CB-CG1	-5.14	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	105	PRO	CB-CG	-5.14	1.24	1.50
1	5	10	LYS	CE-NZ	-5.14	1.36	1.49
3	7	105	PRO	CB-CG	-5.14	1.24	1.50
3	F	571	PHE	CE2-CZ	-5.14	1.27	1.37
3	O	105	PRO	CB-CG	-5.14	1.24	1.50
1	P	10	LYS	CE-NZ	-5.14	1.36	1.49
3	1	571	PHE	CE2-CZ	-5.14	1.27	1.37
3	I	254	SER	C-O	-5.14	1.13	1.23
3	L	105	PRO	CB-CG	-5.14	1.24	1.50
3	R	480	PRO	C-N	-5.14	1.22	1.34
3	V	105	PRO	CB-CG	-5.14	1.24	1.50
3	Y	353	LEU	CG-CD2	-5.14	1.32	1.51
3	4	105	PRO	CB-CG	-5.14	1.24	1.50
3	4	571	PHE	CE2-CZ	-5.14	1.27	1.37
3	F	514	ARG	CG-CD	-5.14	1.39	1.51
3	V	370	GLY	C-O	-5.14	1.15	1.23
3	Y	105	PRO	CB-CG	-5.14	1.24	1.50
3	Y	248	VAL	CB-CG1	-5.14	1.42	1.52
3	4	370	GLY	C-O	-5.14	1.15	1.23
3	7	514	ARG	CG-CD	-5.14	1.39	1.51
3	U	105	PRO	CB-CG	-5.14	1.24	1.50
3	U	443	ARG	CZ-NH1	-5.14	1.26	1.33
3	C	105	PRO	CB-CG	-5.13	1.24	1.50
3	I	248	VAL	CB-CG1	-5.13	1.42	1.52
3	O	514	ARG	CG-CD	-5.13	1.39	1.51
1	S	10	LYS	CE-NZ	-5.13	1.36	1.49
3	Y	254	SER	C-O	-5.13	1.13	1.23
3	4	480	PRO	C-N	-5.13	1.22	1.34
1	M	10	LYS	CE-NZ	-5.13	1.36	1.49
3	O	254	SER	C-O	-5.13	1.13	1.23
2	T	91	TYR	CD2-CE2	-5.13	1.31	1.39
3	1	105	PRO	CB-CG	-5.13	1.24	1.50
3	C	571	PHE	CE2-CZ	-5.13	1.27	1.37
3	I	105	PRO	CB-CG	-5.13	1.24	1.50
3	Y	571	PHE	CE2-CZ	-5.13	1.27	1.37
2	3	91	TYR	CD2-CE2	-5.13	1.31	1.39
1	J	10	LYS	CE-NZ	-5.13	1.36	1.49
1	Z	10	LYS	CE-NZ	-5.13	1.36	1.49
3	C	480	PRO	C-N	-5.13	1.22	1.34
3	L	480	PRO	C-N	-5.13	1.22	1.34
3	R	207	ARG	CZ-NH2	-5.13	1.26	1.33
3	V	571	PHE	CE2-CZ	-5.13	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	480	PRO	C-N	-5.13	1.22	1.34
3	7	248	VAL	CB-CG1	-5.13	1.42	1.52
3	O	353	LEU	CG-CD2	-5.13	1.32	1.51
2	3	140	VAL	CB-CG2	-5.13	1.42	1.52
3	I	480	PRO	C-N	-5.12	1.22	1.34
2	K	91	TYR	CD2-CE2	-5.12	1.31	1.39
3	L	248	VAL	CB-CG1	-5.12	1.42	1.52
3	1	207	ARG	CZ-NH2	-5.12	1.26	1.33
3	R	571	PHE	CE2-CZ	-5.12	1.27	1.37
3	4	65	ASN	CG-ND2	-5.12	1.20	1.32
3	U	480	PRO	C-N	-5.12	1.22	1.34
3	R	65	ASN	CG-ND2	-5.12	1.20	1.32
3	7	65	ASN	CG-ND2	-5.12	1.20	1.32
1	A	10	LYS	CE-NZ	-5.12	1.36	1.49
1	8	10	LYS	CE-NZ	-5.12	1.36	1.49
3	Y	65	ASN	CG-ND2	-5.12	1.20	1.32
3	L	443	ARG	CZ-NH1	-5.12	1.26	1.33
3	O	207	ARG	CZ-NH2	-5.12	1.26	1.33
3	1	65	ASN	CG-ND2	-5.12	1.20	1.32
1	2	10	LYS	CE-NZ	-5.12	1.36	1.49
3	O	65	ASN	CG-ND2	-5.11	1.20	1.32
3	R	443	ARG	CZ-NH1	-5.11	1.26	1.33
1	2	64	LEU	CG-CD1	-5.11	1.32	1.51
3	C	65	ASN	CG-ND2	-5.11	1.20	1.32
3	7	480	PRO	C-N	-5.11	1.22	1.34
2	6	91	TYR	CD2-CE2	-5.11	1.31	1.39
3	U	571	PHE	CE2-CZ	-5.11	1.27	1.37
2	B	91	TYR	CD2-CE2	-5.11	1.31	1.39
3	L	65	ASN	CG-ND2	-5.11	1.20	1.32
3	V	207	ARG	CZ-NH2	-5.11	1.26	1.33
1	D	64	LEU	CG-CD1	-5.11	1.32	1.51
3	F	65	ASN	CG-ND2	-5.11	1.20	1.32
3	I	443	ARG	CZ-NH1	-5.11	1.26	1.33
3	V	480	PRO	C-N	-5.11	1.22	1.34
1	W	64	LEU	CG-CD1	-5.11	1.32	1.51
2	X	91	TYR	CD2-CE2	-5.11	1.31	1.39
3	F	480	PRO	C-N	-5.10	1.22	1.34
1	5	64	LEU	CG-CD1	-5.10	1.32	1.51
1	J	64	LEU	CG-CD1	-5.10	1.32	1.51
3	R	482	PHE	CG-CD1	-5.10	1.31	1.38
1	P	64	LEU	CG-CD1	-5.10	1.32	1.51
3	7	207	ARG	CZ-NH2	-5.10	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	LEU	CG-CD1	-5.10	1.32	1.51
1	8	64	LEU	CG-CD1	-5.10	1.32	1.51
3	F	389	SER	CB-OG	-5.10	1.35	1.42
1	S	32	TYR	CG-CD1	-5.10	1.32	1.39
3	U	65	ASN	CG-ND2	-5.10	1.20	1.32
1	S	64	LEU	CG-CD1	-5.10	1.32	1.51
3	4	33	GLU	CG-CD	5.10	1.59	1.51
1	D	10	LYS	CE-NZ	-5.09	1.36	1.49
1	P	32	TYR	CG-CD1	-5.09	1.32	1.39
1	W	10	LYS	CE-NZ	-5.09	1.36	1.49
3	I	389	SER	CB-OG	-5.09	1.35	1.42
3	R	45	TYR	CZ-OH	-5.09	1.29	1.37
3	7	370	GLY	C-O	-5.09	1.15	1.23
1	G	32	TYR	CG-CD1	-5.09	1.32	1.39
1	G	64	LEU	CG-CD1	-5.09	1.33	1.51
3	V	65	ASN	CG-ND2	-5.09	1.20	1.32
2	9	91	TYR	CD2-CE2	-5.09	1.31	1.39
3	I	65	ASN	CG-ND2	-5.09	1.20	1.32
2	0	91	TYR	CD2-CE2	-5.09	1.31	1.39
3	F	33	GLU	CG-CD	5.09	1.59	1.51
1	M	64	LEU	CG-CD1	-5.09	1.33	1.51
3	Y	45	TYR	CZ-OH	-5.09	1.29	1.37
3	1	33	GLU	CG-CD	5.09	1.59	1.51
1	G	10	LYS	CE-NZ	-5.08	1.36	1.49
1	Z	64	LEU	CG-CD1	-5.08	1.33	1.51
3	O	45	TYR	CZ-OH	-5.08	1.29	1.37
3	O	482	PHE	CG-CD1	-5.08	1.31	1.38
2	Q	91	TYR	CD2-CE2	-5.08	1.31	1.39
3	O	389	SER	CB-OG	-5.08	1.35	1.42
2	E	91	TYR	CD2-CE2	-5.08	1.31	1.39
3	I	370	GLY	C-O	-5.08	1.15	1.23
3	C	370	GLY	C-O	-5.08	1.15	1.23
2	N	91	TYR	CD2-CE2	-5.08	1.31	1.39
3	Y	370	GLY	C-O	-5.07	1.15	1.23
3	Y	482	PHE	CG-CD1	-5.07	1.31	1.38
1	D	7	GLU	CG-CD	5.07	1.59	1.51
2	H	91	TYR	CD2-CE2	-5.07	1.31	1.39
3	U	45	TYR	CZ-OH	-5.07	1.29	1.37
1	Z	32	TYR	CG-CD1	-5.07	1.32	1.39
3	V	45	TYR	CZ-OH	-5.07	1.29	1.37
3	U	370	GLY	C-O	-5.07	1.15	1.23
3	V	33	GLU	CG-CD	5.06	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	19	ASP	CB-CG	5.06	1.62	1.51
3	U	460	TRP	CZ3-CH2	-5.06	1.31	1.40
3	O	19	ASP	CB-CG	5.06	1.62	1.51
3	C	45	TYR	CZ-OH	-5.06	1.29	1.37
3	F	460	TRP	CZ3-CH2	-5.06	1.31	1.40
3	R	370	GLY	C-O	-5.06	1.15	1.23
3	4	389	SER	CB-OG	-5.06	1.35	1.42
3	I	45	TYR	CZ-OH	-5.05	1.29	1.37
1	J	32	TYR	CG-CD1	-5.05	1.32	1.39
3	Y	19	ASP	CB-CG	5.05	1.62	1.51
3	4	45	TYR	CZ-OH	-5.05	1.29	1.37
3	U	19	ASP	CB-CG	5.05	1.62	1.51
3	7	33	GLU	CG-CD	5.05	1.59	1.51
1	D	32	TYR	CG-CD1	-5.05	1.32	1.39
3	L	370	GLY	C-O	-5.05	1.15	1.23
3	O	370	GLY	C-O	-5.05	1.15	1.23
3	4	179	PRO	N-CD	-5.05	1.40	1.47
3	L	460	TRP	CZ3-CH2	-5.04	1.31	1.40
1	A	32	TYR	CG-CD1	-5.04	1.32	1.39
3	I	460	TRP	CZ3-CH2	-5.04	1.31	1.40
3	R	19	ASP	CB-CG	5.04	1.62	1.51
3	V	19	ASP	CB-CG	5.04	1.62	1.51
3	C	389	SER	CB-OG	-5.04	1.35	1.42
3	I	482	PHE	CG-CD1	-5.04	1.31	1.38
3	L	33	GLU	CG-CD	5.04	1.59	1.51
1	8	32	TYR	CG-CD1	-5.04	1.32	1.39
3	C	33	GLU	CG-CD	5.04	1.59	1.51
3	F	482	PHE	CG-CD1	-5.04	1.31	1.38
3	Y	33	GLU	CG-CD	5.04	1.59	1.51
3	4	460	TRP	CZ3-CH2	-5.04	1.31	1.40
3	U	33	GLU	CG-CD	5.04	1.59	1.51
3	C	482	PHE	CG-CD1	-5.04	1.31	1.38
3	O	33	GLU	CG-CD	5.04	1.59	1.51
2	0	117	PRO	CB-CG	-5.04	1.24	1.50
3	U	179	PRO	N-CD	-5.04	1.40	1.47
2	Q	117	PRO	CB-CG	-5.03	1.24	1.50
2	9	117	PRO	CB-CG	-5.03	1.24	1.50
3	L	45	TYR	CZ-OH	-5.03	1.29	1.37
3	R	389	SER	CB-OG	-5.03	1.35	1.42
3	1	45	TYR	CZ-OH	-5.03	1.29	1.37
3	C	19	ASP	CB-CG	5.03	1.62	1.51
3	F	19	ASP	CB-CG	5.03	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	389	SER	CB-OG	-5.03	1.35	1.42
3	Y	460	TRP	CZ3-CH2	-5.03	1.32	1.40
3	1	203	ASN	C-O	-5.03	1.13	1.23
2	3	117	PRO	CB-CG	-5.03	1.24	1.50
3	R	460	TRP	CZ3-CH2	-5.03	1.32	1.40
3	V	389	SER	CB-OG	-5.03	1.35	1.42
1	5	32	TYR	CG-CD1	-5.03	1.32	1.39
3	U	389	SER	CB-OG	-5.03	1.35	1.42
2	E	117	PRO	CB-CG	-5.03	1.24	1.50
2	K	117	PRO	CB-CG	-5.03	1.24	1.50
3	1	460	TRP	CZ3-CH2	-5.03	1.32	1.40
2	6	117	PRO	CB-CG	-5.03	1.24	1.50
3	R	203	ASN	C-O	-5.02	1.13	1.23
3	O	203	ASN	C-O	-5.02	1.13	1.23
3	R	179	PRO	N-CD	-5.02	1.40	1.47
2	B	117	PRO	CB-CG	-5.02	1.24	1.50
3	C	460	TRP	CZ3-CH2	-5.02	1.32	1.40
3	L	217	GLY	C-O	-5.02	1.15	1.23
3	F	217	GLY	C-O	-5.02	1.15	1.23
3	I	179	PRO	N-CD	-5.02	1.40	1.47
3	I	409	VAL	CB-CG2	-5.02	1.42	1.52
2	T	117	PRO	CB-CG	-5.02	1.24	1.50
2	X	121	LYS	CE-NZ	-5.02	1.36	1.49
3	4	217	GLY	C-O	-5.02	1.15	1.23
1	8	7	GLU	CG-CD	5.02	1.59	1.51
3	U	217	GLY	C-O	-5.02	1.15	1.23
3	U	482	PHE	CG-CD1	-5.02	1.31	1.38
1	G	7	GLU	CG-CD	5.02	1.59	1.51
2	N	117	PRO	CB-CG	-5.02	1.24	1.50
2	X	117	PRO	CB-CG	-5.02	1.24	1.50
3	Y	389	SER	CB-OG	-5.02	1.35	1.42
3	1	370	GLY	C-O	-5.02	1.15	1.23
3	7	45	TYR	CZ-OH	-5.02	1.29	1.37
3	L	482	PHE	CG-CD1	-5.02	1.31	1.38
3	V	482	PHE	CG-CD1	-5.02	1.31	1.38
1	2	7	GLU	CG-CD	5.02	1.59	1.51
3	F	420	GLN	C-N	-5.01	1.24	1.33
3	O	460	TRP	CZ3-CH2	-5.01	1.32	1.40
3	4	409	VAL	CB-CG2	-5.01	1.42	1.52
3	4	482	PHE	CG-CD1	-5.01	1.31	1.38
2	H	117	PRO	CB-CG	-5.01	1.24	1.50
3	1	482	PHE	CG-CD1	-5.01	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	19	ASP	CB-CG	5.01	1.62	1.51
3	F	45	TYR	CZ-OH	-5.01	1.29	1.37
3	O	179	PRO	N-CD	-5.01	1.40	1.47
3	R	217	GLY	C-O	-5.01	1.15	1.23
3	V	420	GLN	C-N	-5.01	1.24	1.33
1	W	32	TYR	CG-CD1	-5.01	1.32	1.39
2	0	121	LYS	CE-NZ	-5.01	1.36	1.49
2	E	121	LYS	CE-NZ	-5.01	1.36	1.49
3	L	19	ASP	CB-CG	5.01	1.62	1.51
3	R	420	GLN	C-N	-5.01	1.24	1.33
3	V	409	VAL	CB-CG2	-5.01	1.42	1.52
3	V	460	TRP	CZ3-CH2	-5.01	1.32	1.40
3	Y	217	GLY	C-O	-5.01	1.15	1.23
3	F	409	VAL	CB-CG2	-5.01	1.42	1.52
2	H	87	ARG	CZ-NH2	-5.01	1.26	1.33
3	R	409	VAL	CB-CG2	-5.01	1.42	1.52
2	3	87	ARG	CZ-NH2	-5.01	1.26	1.33
3	I	420	GLN	C-N	-5.00	1.24	1.33
3	C	409	VAL	CB-CG2	-5.00	1.42	1.52
3	F	370	GLY	C-O	-5.00	1.15	1.23
3	V	203	ASN	C-O	-5.00	1.13	1.23
3	Y	203	ASN	C-O	-5.00	1.13	1.23
3	1	420	GLN	C-N	-5.00	1.24	1.33
3	7	19	ASP	CB-CG	5.00	1.62	1.51
3	7	389	SER	CB-OG	-5.00	1.35	1.42
1	A	7	GLU	CG-CD	5.00	1.59	1.51
2	H	121	LYS	CE-NZ	-5.00	1.36	1.49
1	J	7	GLU	CG-CD	5.00	1.59	1.51
3	V	217	GLY	C-O	-5.00	1.15	1.23

All (2219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	207	ARG	NE-CZ-NH1	15.14	127.87	120.30
3	L	207	ARG	NE-CZ-NH1	15.13	127.87	120.30
3	R	407[A]	ARG	NE-CZ-NH1	15.12	127.86	120.30
3	R	407[B]	ARG	NE-CZ-NH1	15.12	127.86	120.30
3	7	207	ARG	NE-CZ-NH1	15.12	127.86	120.30
3	L	407[A]	ARG	NE-CZ-NH1	15.11	127.86	120.30
3	L	407[B]	ARG	NE-CZ-NH1	15.11	127.86	120.30
3	V	207	ARG	NE-CZ-NH1	15.11	127.86	120.30
3	Y	407[A]	ARG	NE-CZ-NH1	15.11	127.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	407[B]	ARG	NE-CZ-NH1	15.11	127.85	120.30
3	1	407[A]	ARG	NE-CZ-NH1	15.11	127.85	120.30
3	1	407[B]	ARG	NE-CZ-NH1	15.11	127.85	120.30
3	U	407[A]	ARG	NE-CZ-NH1	15.10	127.85	120.30
3	U	407[B]	ARG	NE-CZ-NH1	15.10	127.85	120.30
3	4	407[A]	ARG	NE-CZ-NH1	15.09	127.84	120.30
3	4	407[B]	ARG	NE-CZ-NH1	15.09	127.84	120.30
3	C	407[A]	ARG	NE-CZ-NH1	15.08	127.84	120.30
3	C	407[B]	ARG	NE-CZ-NH1	15.08	127.84	120.30
3	C	207	ARG	NE-CZ-NH1	15.06	127.83	120.30
3	F	407[A]	ARG	NE-CZ-NH1	15.06	127.83	120.30
3	F	407[B]	ARG	NE-CZ-NH1	15.06	127.83	120.30
3	R	207	ARG	NE-CZ-NH1	15.06	127.83	120.30
3	O	407[A]	ARG	NE-CZ-NH1	15.06	127.83	120.30
3	O	407[B]	ARG	NE-CZ-NH1	15.06	127.83	120.30
3	I	407[A]	ARG	NE-CZ-NH1	15.05	127.83	120.30
3	I	407[B]	ARG	NE-CZ-NH1	15.05	127.83	120.30
3	O	207	ARG	NE-CZ-NH1	15.04	127.82	120.30
3	I	207	ARG	NE-CZ-NH1	15.03	127.82	120.30
3	7	407[A]	ARG	NE-CZ-NH1	15.03	127.82	120.30
3	7	407[B]	ARG	NE-CZ-NH1	15.03	127.82	120.30
3	Y	207	ARG	NE-CZ-NH1	15.01	127.80	120.30
3	U	207	ARG	NE-CZ-NH1	15.01	127.80	120.30
3	4	207	ARG	NE-CZ-NH1	14.99	127.80	120.30
3	F	207	ARG	NE-CZ-NH1	14.99	127.80	120.30
3	V	407[A]	ARG	NE-CZ-NH1	14.95	127.78	120.30
3	V	407[B]	ARG	NE-CZ-NH1	14.95	127.78	120.30
2	Q	104	ARG	NE-CZ-NH1	-14.67	112.96	120.30
2	X	104	ARG	NE-CZ-NH1	-14.66	112.97	120.30
2	3	104	ARG	NE-CZ-NH1	-14.65	112.97	120.30
2	H	104	ARG	NE-CZ-NH1	-14.63	112.98	120.30
2	T	104	ARG	NE-CZ-NH1	-14.63	112.98	120.30
2	9	104	ARG	NE-CZ-NH1	-14.63	112.98	120.30
2	B	104	ARG	NE-CZ-NH1	-14.63	112.99	120.30
2	6	104	ARG	NE-CZ-NH1	-14.58	113.01	120.30
2	K	104	ARG	NE-CZ-NH1	-14.57	113.01	120.30
2	N	104	ARG	NE-CZ-NH1	-14.57	113.02	120.30
2	0	104	ARG	NE-CZ-NH1	-14.57	113.02	120.30
2	E	104	ARG	NE-CZ-NH1	-14.56	113.02	120.30
2	K	104	ARG	NE-CZ-NH2	13.90	127.25	120.30
2	T	104	ARG	NE-CZ-NH2	13.85	127.22	120.30
3	F	341	ARG	NE-CZ-NH2	-13.82	113.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	104	ARG	NE-CZ-NH2	13.82	127.21	120.30
2	3	104	ARG	NE-CZ-NH2	13.82	127.21	120.30
2	Q	104	ARG	NE-CZ-NH2	13.81	127.20	120.30
3	L	341	ARG	NE-CZ-NH2	-13.78	113.41	120.30
2	B	104	ARG	NE-CZ-NH2	13.78	127.19	120.30
3	O	341	ARG	NE-CZ-NH2	-13.76	113.42	120.30
3	1	341	ARG	NE-CZ-NH2	-13.76	113.42	120.30
2	6	104	ARG	NE-CZ-NH2	13.76	127.18	120.30
2	E	104	ARG	NE-CZ-NH2	13.75	127.18	120.30
2	H	104	ARG	NE-CZ-NH2	13.73	127.16	120.30
3	V	341	ARG	NE-CZ-NH2	-13.71	113.45	120.30
3	C	341	ARG	NE-CZ-NH2	-13.70	113.45	120.30
3	R	341	ARG	NE-CZ-NH2	-13.70	113.45	120.30
2	0	104	ARG	NE-CZ-NH2	13.70	127.15	120.30
3	U	341	ARG	NE-CZ-NH2	-13.70	113.45	120.30
3	7	341	ARG	NE-CZ-NH2	-13.69	113.45	120.30
3	I	341	ARG	NE-CZ-NH2	-13.69	113.45	120.30
2	9	104	ARG	NE-CZ-NH2	13.68	127.14	120.30
2	N	104	ARG	NE-CZ-NH2	13.68	127.14	120.30
3	4	341	ARG	NE-CZ-NH2	-13.68	113.46	120.30
3	Y	341	ARG	NE-CZ-NH2	-13.67	113.47	120.30
3	1	268	PHE	CB-CG-CD1	12.77	129.74	120.80
3	L	268	PHE	CB-CG-CD1	12.76	129.73	120.80
3	V	268	PHE	CB-CG-CD1	12.76	129.73	120.80
3	U	268	PHE	CB-CG-CD1	12.75	129.72	120.80
3	Y	268	PHE	CB-CG-CD1	12.73	129.71	120.80
3	4	268	PHE	CB-CG-CD1	12.72	129.71	120.80
3	7	268	PHE	CB-CG-CD1	12.71	129.70	120.80
3	C	268	PHE	CB-CG-CD1	12.70	129.69	120.80
3	I	268	PHE	CB-CG-CD1	12.70	129.69	120.80
3	R	268	PHE	CB-CG-CD1	12.69	129.68	120.80
3	L	341	ARG	NE-CZ-NH1	12.68	126.64	120.30
3	O	268	PHE	CB-CG-CD1	12.68	129.68	120.80
3	R	341	ARG	NE-CZ-NH1	12.67	126.63	120.30
3	I	341	ARG	NE-CZ-NH1	12.65	126.63	120.30
3	F	268	PHE	CB-CG-CD1	12.65	129.66	120.80
3	V	341	ARG	NE-CZ-NH1	12.65	126.62	120.30
3	7	341	ARG	NE-CZ-NH1	12.65	126.62	120.30
3	Y	341	ARG	NE-CZ-NH1	12.64	126.62	120.30
3	C	341	ARG	NE-CZ-NH1	12.63	126.61	120.30
3	O	341	ARG	NE-CZ-NH1	12.62	126.61	120.30
3	F	341	ARG	NE-CZ-NH1	12.61	126.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	341	ARG	NE-CZ-NH1	12.58	126.59	120.30
3	1	341	ARG	NE-CZ-NH1	12.57	126.58	120.30
3	U	341	ARG	NE-CZ-NH1	12.56	126.58	120.30
2	6	158	ARG	NE-CZ-NH1	-12.46	114.07	120.30
2	N	158	ARG	NE-CZ-NH1	-12.43	114.08	120.30
2	T	158	ARG	NE-CZ-NH1	-12.43	114.08	120.30
2	E	158	ARG	NE-CZ-NH1	-12.39	114.11	120.30
2	X	158	ARG	NE-CZ-NH1	-12.37	114.11	120.30
2	H	158	ARG	NE-CZ-NH1	-12.37	114.11	120.30
2	3	158	ARG	NE-CZ-NH1	-12.37	114.12	120.30
2	B	158	ARG	NE-CZ-NH1	-12.36	114.12	120.30
2	Q	158	ARG	NE-CZ-NH1	-12.35	114.12	120.30
2	0	158	ARG	NE-CZ-NH1	-12.32	114.14	120.30
2	K	158	ARG	NE-CZ-NH1	-12.30	114.15	120.30
2	9	158	ARG	NE-CZ-NH1	-12.29	114.15	120.30
3	O	291	ARG	NE-CZ-NH1	12.04	126.32	120.30
3	I	291	ARG	NE-CZ-NH1	12.03	126.31	120.30
3	V	291	ARG	NE-CZ-NH1	12.02	126.31	120.30
3	U	523	ARG	NE-CZ-NH2	11.99	126.30	120.30
3	4	291	ARG	NE-CZ-NH1	11.97	126.29	120.30
3	C	291	ARG	NE-CZ-NH1	11.96	126.28	120.30
3	7	291	ARG	NE-CZ-NH1	11.96	126.28	120.30
3	L	291	ARG	NE-CZ-NH1	11.96	126.28	120.30
3	R	291	ARG	NE-CZ-NH1	11.95	126.28	120.30
3	F	291	ARG	NE-CZ-NH1	11.95	126.28	120.30
3	7	343	ARG	NE-CZ-NH2	-11.95	114.33	120.30
3	Y	291	ARG	NE-CZ-NH1	11.95	126.27	120.30
3	1	523	ARG	NE-CZ-NH2	11.94	126.27	120.30
3	1	291	ARG	NE-CZ-NH1	11.94	126.27	120.30
3	V	523	ARG	NE-CZ-NH2	11.93	126.27	120.30
3	L	523	ARG	NE-CZ-NH2	11.93	126.27	120.30
3	U	291	ARG	NE-CZ-NH1	11.92	126.26	120.30
3	L	343	ARG	NE-CZ-NH2	-11.90	114.35	120.30
3	R	523	ARG	NE-CZ-NH2	11.89	126.25	120.30
3	Y	523	ARG	NE-CZ-NH2	11.88	126.24	120.30
3	F	523	ARG	NE-CZ-NH2	11.87	126.24	120.30
3	1	343	ARG	NE-CZ-NH2	-11.88	114.36	120.30
3	I	523	ARG	NE-CZ-NH2	11.87	126.23	120.30
3	C	523	ARG	NE-CZ-NH2	11.87	126.23	120.30
3	U	343	ARG	NE-CZ-NH2	-11.87	114.37	120.30
3	V	343	ARG	NE-CZ-NH2	-11.86	114.37	120.30
3	C	343	ARG	NE-CZ-NH2	-11.86	114.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7	523	ARG	NE-CZ-NH2	11.84	126.22	120.30
3	Y	343	ARG	NE-CZ-NH2	-11.83	114.39	120.30
3	F	343	ARG	NE-CZ-NH2	-11.82	114.39	120.30
3	O	343	ARG	NE-CZ-NH2	-11.81	114.39	120.30
3	4	343	ARG	NE-CZ-NH2	-11.81	114.39	120.30
3	O	523	ARG	NE-CZ-NH2	11.81	126.20	120.30
3	I	343	ARG	NE-CZ-NH2	-11.78	114.41	120.30
3	R	343	ARG	NE-CZ-NH2	-11.78	114.41	120.30
3	4	523	ARG	NE-CZ-NH2	11.77	126.19	120.30
3	7	343	ARG	NE-CZ-NH1	11.46	126.03	120.30
3	4	343	ARG	NE-CZ-NH1	11.45	126.03	120.30
3	V	343	ARG	NE-CZ-NH1	11.43	126.01	120.30
3	I	343	ARG	NE-CZ-NH1	11.41	126.00	120.30
3	L	343	ARG	NE-CZ-NH1	11.40	126.00	120.30
3	F	343	ARG	NE-CZ-NH1	11.38	125.99	120.30
3	R	343	ARG	NE-CZ-NH1	11.38	125.99	120.30
3	Y	343	ARG	NE-CZ-NH1	11.38	125.99	120.30
3	U	343	ARG	NE-CZ-NH1	11.38	125.99	120.30
3	C	343	ARG	NE-CZ-NH1	11.37	125.99	120.30
3	O	343	ARG	NE-CZ-NH1	11.35	125.97	120.30
3	1	343	ARG	NE-CZ-NH1	11.28	125.94	120.30
2	N	158	ARG	NE-CZ-NH2	10.90	125.75	120.30
2	0	158	ARG	NE-CZ-NH2	10.87	125.73	120.30
2	T	158	ARG	NE-CZ-NH2	10.87	125.73	120.30
2	X	158	ARG	NE-CZ-NH2	10.86	125.73	120.30
2	6	158	ARG	NE-CZ-NH2	10.86	125.73	120.30
2	9	158	ARG	NE-CZ-NH2	10.86	125.73	120.30
2	Q	158	ARG	NE-CZ-NH2	10.85	125.73	120.30
2	H	158	ARG	NE-CZ-NH2	10.85	125.72	120.30
2	B	158	ARG	NE-CZ-NH2	10.84	125.72	120.30
2	K	158	ARG	NE-CZ-NH2	10.84	125.72	120.30
2	3	158	ARG	NE-CZ-NH2	10.80	125.70	120.30
2	E	158	ARG	NE-CZ-NH2	10.80	125.70	120.30
2	K	87	ARG	NE-CZ-NH2	-10.42	115.09	120.30
2	Q	87	ARG	NE-CZ-NH2	-10.38	115.11	120.30
2	3	87	ARG	NE-CZ-NH2	-10.38	115.11	120.30
2	T	87	ARG	NE-CZ-NH2	-10.36	115.12	120.30
2	H	87	ARG	NE-CZ-NH2	-10.35	115.13	120.30
2	B	87	ARG	NE-CZ-NH2	-10.34	115.13	120.30
2	E	87	ARG	NE-CZ-NH2	-10.34	115.13	120.30
2	9	87	ARG	NE-CZ-NH2	-10.33	115.14	120.30
2	X	87	ARG	NE-CZ-NH2	-10.32	115.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	87	ARG	NE-CZ-NH2	-10.30	115.15	120.30
2	0	87	ARG	NE-CZ-NH2	-10.30	115.15	120.30
2	6	87	ARG	NE-CZ-NH2	-10.29	115.16	120.30
3	O	207	ARG	NE-CZ-NH2	-10.07	115.27	120.30
3	7	371	ARG	NE-CZ-NH2	-10.05	115.27	120.30
3	I	371	ARG	NE-CZ-NH2	-10.05	115.27	120.30
3	U	371	ARG	NE-CZ-NH2	-10.04	115.28	120.30
3	O	371	ARG	NE-CZ-NH2	-10.03	115.28	120.30
3	L	207	ARG	NE-CZ-NH2	-10.03	115.29	120.30
3	Y	371	ARG	NE-CZ-NH2	-10.02	115.29	120.30
3	R	371	ARG	NE-CZ-NH2	-9.99	115.30	120.30
3	L	371	ARG	NE-CZ-NH2	-9.99	115.30	120.30
3	1	371	ARG	NE-CZ-NH2	-9.99	115.30	120.30
3	C	207	ARG	NE-CZ-NH2	-9.98	115.31	120.30
3	I	207	ARG	NE-CZ-NH2	-9.98	115.31	120.30
3	Y	207	ARG	NE-CZ-NH2	-9.98	115.31	120.30
3	7	207	ARG	NE-CZ-NH2	-9.98	115.31	120.30
3	C	371	ARG	NE-CZ-NH2	-9.97	115.31	120.30
3	7	441	ASP	CB-CG-OD1	9.97	127.27	118.30
3	U	207	ARG	NE-CZ-NH2	-9.97	115.32	120.30
2	0	85	PHE	CB-CG-CD1	9.96	127.78	120.80
3	1	207	ARG	NE-CZ-NH2	-9.96	115.32	120.30
3	4	207	ARG	NE-CZ-NH2	-9.96	115.32	120.30
3	L	441	ASP	CB-CG-OD1	9.95	127.26	118.30
3	F	441	ASP	CB-CG-OD1	9.95	127.25	118.30
3	V	207	ARG	NE-CZ-NH2	-9.94	115.33	120.30
3	R	207	ARG	NE-CZ-NH2	-9.94	115.33	120.30
2	T	85	PHE	CB-CG-CD1	9.94	127.75	120.80
3	F	371	ARG	NE-CZ-NH2	-9.93	115.34	120.30
2	B	85	PHE	CB-CG-CD1	9.92	127.75	120.80
2	H	85	PHE	CB-CG-CD1	9.92	127.75	120.80
3	F	207	ARG	NE-CZ-NH2	-9.92	115.34	120.30
3	C	441	ASP	CB-CG-OD1	9.91	127.22	118.30
2	Q	85	PHE	CB-CG-CD1	9.91	127.74	120.80
2	6	85	PHE	CB-CG-CD1	9.91	127.74	120.80
2	N	85	PHE	CB-CG-CD1	9.91	127.74	120.80
3	V	371	ARG	NE-CZ-NH2	-9.91	115.35	120.30
3	4	371	ARG	NE-CZ-NH2	-9.91	115.35	120.30
3	O	441	ASP	CB-CG-OD1	9.90	127.21	118.30
2	3	85	PHE	CB-CG-CD1	9.90	127.73	120.80
3	I	441	ASP	CB-CG-OD1	9.90	127.21	118.30
2	X	85	PHE	CB-CG-CD1	9.90	127.73	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	441	ASP	CB-CG-OD1	9.90	127.21	118.30
3	Y	441	ASP	CB-CG-OD1	9.90	127.21	118.30
2	9	85	PHE	CB-CG-CD1	9.90	127.73	120.80
3	4	443	ARG	NE-CZ-NH2	-9.90	115.35	120.30
2	K	85	PHE	CB-CG-CD1	9.89	127.72	120.80
3	O	443	ARG	NE-CZ-NH2	-9.89	115.36	120.30
3	V	441	ASP	CB-CG-OD1	9.88	127.20	118.30
3	U	443	ARG	NE-CZ-NH2	-9.88	115.36	120.30
3	4	441	ASP	CB-CG-OD1	9.88	127.19	118.30
3	R	441	ASP	CB-CG-OD1	9.88	127.19	118.30
3	1	443	ARG	NE-CZ-NH2	-9.87	115.36	120.30
2	E	85	PHE	CB-CG-CD1	9.87	127.71	120.80
3	V	443	ARG	NE-CZ-NH2	-9.86	115.37	120.30
3	Y	443	ARG	NE-CZ-NH2	-9.86	115.37	120.30
3	1	441	ASP	CB-CG-OD1	9.85	127.17	118.30
3	C	443	ARG	NE-CZ-NH2	-9.83	115.38	120.30
3	F	443	ARG	NE-CZ-NH2	-9.82	115.39	120.30
3	7	443	ARG	NE-CZ-NH2	-9.81	115.39	120.30
3	R	443	ARG	NE-CZ-NH2	-9.79	115.40	120.30
3	I	443	ARG	NE-CZ-NH2	-9.77	115.42	120.30
3	L	443	ARG	NE-CZ-NH2	-9.74	115.43	120.30
3	V	378	ARG	NE-CZ-NH1	9.53	125.06	120.30
3	I	108	MET	CG-SD-CE	-9.48	85.03	100.20
3	1	108	MET	CG-SD-CE	-9.48	85.03	100.20
3	I	243	GLU	CA-CB-CG	9.48	134.25	113.40
3	O	243	GLU	CA-CB-CG	9.48	134.25	113.40
3	V	108	MET	CG-SD-CE	-9.47	85.04	100.20
3	V	243	GLU	CA-CB-CG	9.47	134.24	113.40
3	F	243	GLU	CA-CB-CG	9.47	134.24	113.40
3	Y	243	GLU	CA-CB-CG	9.47	134.23	113.40
3	7	243	GLU	CA-CB-CG	9.47	134.23	113.40
3	C	243	GLU	CA-CB-CG	9.47	134.22	113.40
3	R	378	ARG	NE-CZ-NH1	9.46	125.03	120.30
3	U	243	GLU	CA-CB-CG	9.46	134.22	113.40
3	L	378	ARG	NE-CZ-NH1	9.46	125.03	120.30
3	L	108	MET	CG-SD-CE	-9.46	85.07	100.20
3	7	108	MET	CG-SD-CE	-9.46	85.07	100.20
3	O	108	MET	CG-SD-CE	-9.46	85.07	100.20
3	Y	108	MET	CG-SD-CE	-9.45	85.07	100.20
3	1	243	GLU	CA-CB-CG	9.45	134.20	113.40
3	C	108	MET	CG-SD-CE	-9.45	85.08	100.20
3	4	243	GLU	CA-CB-CG	9.45	134.19	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	108	MET	CG-SD-CE	-9.45	85.08	100.20
3	L	243	GLU	CA-CB-CG	9.45	134.19	113.40
3	R	243	GLU	CA-CB-CG	9.45	134.19	113.40
3	4	108	MET	CG-SD-CE	-9.45	85.08	100.20
3	7	378	ARG	NE-CZ-NH1	9.44	125.02	120.30
3	4	378	ARG	NE-CZ-NH1	9.44	125.02	120.30
3	F	108	MET	CG-SD-CE	-9.44	85.10	100.20
3	R	108	MET	CG-SD-CE	-9.43	85.11	100.20
3	I	378	ARG	NE-CZ-NH1	9.43	125.01	120.30
3	C	378	ARG	NE-CZ-NH1	9.42	125.01	120.30
3	1	378	ARG	NE-CZ-NH1	9.42	125.01	120.30
3	Y	378	ARG	NE-CZ-NH1	9.41	125.01	120.30
3	O	378	ARG	NE-CZ-NH1	9.39	125.00	120.30
3	F	378	ARG	NE-CZ-NH1	9.38	124.99	120.30
3	U	378	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	P	23	ARG	NE-CZ-NH1	-9.35	115.63	120.30
1	5	23	ARG	NE-CZ-NH1	-9.34	115.63	120.30
1	W	23	ARG	NE-CZ-NH1	-9.34	115.63	120.30
2	H	66	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	S	23	ARG	NE-CZ-NH1	-9.33	115.64	120.30
1	8	23	ARG	NE-CZ-NH1	-9.32	115.64	120.30
2	E	66	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	D	23	ARG	NE-CZ-NH1	-9.31	115.64	120.30
2	6	66	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	J	23	ARG	NE-CZ-NH1	-9.30	115.65	120.30
1	2	23	ARG	NE-CZ-NH1	-9.30	115.65	120.30
1	M	23	ARG	NE-CZ-NH1	-9.28	115.66	120.30
2	0	66	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	A	23	ARG	NE-CZ-NH1	-9.27	115.67	120.30
1	G	23	ARG	NE-CZ-NH1	-9.25	115.67	120.30
2	3	66	ARG	NE-CZ-NH2	-9.23	115.68	120.30
2	Q	66	ARG	NE-CZ-NH2	-9.22	115.69	120.30
2	B	66	ARG	NE-CZ-NH2	-9.21	115.69	120.30
2	X	66	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	Z	23	ARG	NE-CZ-NH1	-9.20	115.70	120.30
2	N	66	ARG	NE-CZ-NH2	-9.18	115.71	120.30
2	K	66	ARG	NE-CZ-NH2	-9.18	115.71	120.30
2	T	66	ARG	NE-CZ-NH2	-9.17	115.71	120.30
2	9	66	ARG	NE-CZ-NH2	-9.09	115.75	120.30
2	T	74	PHE	CB-CG-CD1	8.98	127.08	120.80
2	X	74	PHE	CB-CG-CD1	8.97	127.08	120.80
2	0	74	PHE	CB-CG-CD1	8.95	127.06	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	74	PHE	CB-CG-CD1	8.94	127.06	120.80
2	H	74	PHE	CB-CG-CD1	8.94	127.06	120.80
2	B	74	PHE	CB-CG-CD1	8.93	127.05	120.80
2	N	74	PHE	CB-CG-CD1	8.93	127.05	120.80
2	6	74	PHE	CB-CG-CD1	8.93	127.05	120.80
2	K	74	PHE	CB-CG-CD1	8.92	127.04	120.80
2	Q	74	PHE	CB-CG-CD1	8.91	127.04	120.80
2	3	74	PHE	CB-CG-CD1	8.91	127.03	120.80
2	9	74	PHE	CB-CG-CD1	8.90	127.03	120.80
3	7	159	PHE	CB-CG-CD1	8.50	126.75	120.80
3	F	159	PHE	CB-CG-CD1	8.50	126.75	120.80
3	O	159	PHE	CB-CG-CD1	8.49	126.74	120.80
3	V	159	PHE	CB-CG-CD1	8.48	126.74	120.80
3	C	159	PHE	CB-CG-CD1	8.47	126.73	120.80
3	I	159	PHE	CB-CG-CD1	8.47	126.73	120.80
3	4	159	PHE	CB-CG-CD1	8.47	126.73	120.80
3	Y	159	PHE	CB-CG-CD1	8.46	126.72	120.80
3	1	159	PHE	CB-CG-CD1	8.46	126.72	120.80
3	R	159	PHE	CB-CG-CD1	8.45	126.71	120.80
3	U	159	PHE	CB-CG-CD1	8.42	126.69	120.80
3	L	159	PHE	CB-CG-CD1	8.36	126.65	120.80
3	7	131	LEU	CB-CG-CD2	8.32	125.15	111.00
3	F	131	LEU	CB-CG-CD2	8.32	125.14	111.00
3	Y	131	LEU	CB-CG-CD2	8.32	125.15	111.00
3	I	131	LEU	CB-CG-CD2	8.32	125.14	111.00
3	V	131	LEU	CB-CG-CD2	8.32	125.14	111.00
3	4	131	LEU	CB-CG-CD2	8.32	125.14	111.00
3	C	131	LEU	CB-CG-CD2	8.31	125.13	111.00
3	L	131	LEU	CB-CG-CD2	8.31	125.13	111.00
3	R	131	LEU	CB-CG-CD2	8.31	125.13	111.00
3	O	131	LEU	CB-CG-CD2	8.30	125.12	111.00
3	1	131	LEU	CB-CG-CD2	8.30	125.12	111.00
3	U	131	LEU	CB-CG-CD2	8.30	125.11	111.00
1	8	23	ARG	NE-CZ-NH2	8.27	124.44	120.30
2	0	66	ARG	NE-CZ-NH1	8.22	124.41	120.30
2	H	66	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	M	23	ARG	NE-CZ-NH2	8.19	124.40	120.30
1	P	23	ARG	NE-CZ-NH2	8.19	124.40	120.30
2	E	66	ARG	NE-CZ-NH1	8.19	124.39	120.30
2	K	66	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	W	23	ARG	NE-CZ-NH2	8.18	124.39	120.30
1	2	23	ARG	NE-CZ-NH2	8.18	124.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	66	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	Z	23	ARG	NE-CZ-NH2	8.13	124.36	120.30
2	N	66	ARG	NE-CZ-NH1	8.12	124.36	120.30
2	3	66	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	A	23	ARG	NE-CZ-NH2	8.11	124.36	120.30
2	X	66	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	D	23	ARG	NE-CZ-NH2	8.11	124.35	120.30
2	Q	66	ARG	NE-CZ-NH1	8.11	124.35	120.30
2	6	66	ARG	NE-CZ-NH1	8.10	124.35	120.30
2	T	66	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	G	23	ARG	NE-CZ-NH2	8.09	124.35	120.30
3	R	192	LEU	CA-CB-CG	8.07	133.86	115.30
3	I	192	LEU	CA-CB-CG	8.07	133.86	115.30
3	O	192	LEU	CA-CB-CG	8.06	133.84	115.30
3	Y	192	LEU	CA-CB-CG	8.06	133.83	115.30
3	C	192	LEU	CA-CB-CG	8.06	133.83	115.30
3	V	192	LEU	CA-CB-CG	8.05	133.83	115.30
1	5	23	ARG	NE-CZ-NH2	8.06	124.33	120.30
3	7	192	LEU	CA-CB-CG	8.05	133.82	115.30
2	9	66	ARG	NE-CZ-NH1	8.05	124.33	120.30
3	U	192	LEU	CA-CB-CG	8.05	133.81	115.30
3	F	192	LEU	CA-CB-CG	8.05	133.81	115.30
3	L	192	LEU	CA-CB-CG	8.05	133.81	115.30
3	4	192	LEU	CA-CB-CG	8.05	133.81	115.30
3	1	192	LEU	CA-CB-CG	8.05	133.81	115.30
1	J	23	ARG	NE-CZ-NH2	8.04	124.32	120.30
1	S	23	ARG	NE-CZ-NH2	8.02	124.31	120.30
3	Y	445	PHE	CB-CG-CD2	8.01	126.40	120.80
3	O	445	PHE	CB-CG-CD2	7.99	126.39	120.80
3	F	63	ARG	NE-CZ-NH1	-7.97	116.32	120.30
3	1	445	PHE	CB-CG-CD2	7.96	126.37	120.80
3	L	445	PHE	CB-CG-CD2	7.95	126.36	120.80
3	R	445	PHE	CB-CG-CD2	7.95	126.36	120.80
3	4	445	PHE	CB-CG-CD2	7.94	126.36	120.80
3	7	445	PHE	CB-CG-CD2	7.94	126.36	120.80
3	F	445	PHE	CB-CG-CD2	7.94	126.36	120.80
3	C	445	PHE	CB-CG-CD2	7.93	126.35	120.80
3	Y	63	ARG	NE-CZ-NH1	-7.93	116.33	120.30
3	U	445	PHE	CB-CG-CD2	7.93	126.35	120.80
3	I	63	ARG	NE-CZ-NH1	-7.91	116.34	120.30
3	V	445	PHE	CB-CG-CD2	7.91	126.34	120.80
3	I	445	PHE	CB-CG-CD2	7.90	126.33	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	378	ARG	NE-CZ-NH2	-7.89	116.36	120.30
3	V	378	ARG	NE-CZ-NH2	-7.89	116.36	120.30
3	O	63	ARG	NE-CZ-NH1	-7.88	116.36	120.30
3	4	378	ARG	NE-CZ-NH2	-7.88	116.36	120.30
3	R	378	ARG	NE-CZ-NH2	-7.86	116.37	120.30
3	Y	378	ARG	NE-CZ-NH2	-7.84	116.38	120.30
3	C	63	ARG	NE-CZ-NH1	-7.84	116.38	120.30
3	7	63	ARG	NE-CZ-NH1	-7.83	116.39	120.30
3	L	378	ARG	NE-CZ-NH2	-7.82	116.39	120.30
3	4	63	ARG	NE-CZ-NH1	-7.82	116.39	120.30
3	C	378	ARG	NE-CZ-NH2	-7.80	116.40	120.30
3	I	378	ARG	NE-CZ-NH2	-7.80	116.40	120.30
3	7	378	ARG	NE-CZ-NH2	-7.80	116.40	120.30
3	V	63	ARG	NE-CZ-NH1	-7.77	116.42	120.30
3	L	63	ARG	NE-CZ-NH1	-7.77	116.42	120.30
3	F	378	ARG	NE-CZ-NH2	-7.76	116.42	120.30
3	U	63	ARG	NE-CZ-NH1	-7.76	116.42	120.30
3	1	268	PHE	CB-CG-CD2	-7.73	115.39	120.80
3	L	268	PHE	CB-CG-CD2	-7.71	115.40	120.80
3	R	63	ARG	NE-CZ-NH1	-7.71	116.44	120.30
3	V	268	PHE	CB-CG-CD2	-7.71	115.40	120.80
3	U	268	PHE	CB-CG-CD2	-7.70	115.41	120.80
1	5	11	LEU	CB-CG-CD1	7.70	124.08	111.00
1	G	11	LEU	CB-CG-CD1	7.70	124.08	111.00
3	O	378	ARG	NE-CZ-NH2	-7.70	116.45	120.30
3	F	268	PHE	CB-CG-CD2	-7.69	115.42	120.80
1	Z	11	LEU	CB-CG-CD1	7.69	124.07	111.00
3	1	63	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	8	11	LEU	CB-CG-CD1	7.68	124.06	111.00
1	2	11	LEU	CB-CG-CD1	7.68	124.05	111.00
1	A	11	LEU	CB-CG-CD1	7.68	124.05	111.00
1	J	11	LEU	CB-CG-CD1	7.68	124.05	111.00
1	D	11	LEU	CB-CG-CD1	7.67	124.05	111.00
3	I	268	PHE	CB-CG-CD2	-7.67	115.43	120.80
3	Y	268	PHE	CB-CG-CD2	-7.67	115.43	120.80
1	M	11	LEU	CB-CG-CD1	7.67	124.05	111.00
3	4	268	PHE	CB-CG-CD2	-7.67	115.43	120.80
3	C	268	PHE	CB-CG-CD2	-7.67	115.43	120.80
1	W	11	LEU	CB-CG-CD1	7.66	124.03	111.00
1	S	11	LEU	CB-CG-CD1	7.65	124.01	111.00
1	P	11	LEU	CB-CG-CD1	7.65	124.00	111.00
3	U	378	ARG	NE-CZ-NH2	-7.65	116.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	268	PHE	CB-CG-CD2	-7.65	115.45	120.80
3	7	268	PHE	CB-CG-CD2	-7.64	115.45	120.80
3	O	268	PHE	CB-CG-CD2	-7.59	115.48	120.80
2	Q	141	PRO	CA-N-CD	-7.57	100.91	111.50
2	9	141	PRO	CA-N-CD	-7.56	100.92	111.50
2	6	141	PRO	CA-N-CD	-7.55	100.93	111.50
2	E	141	PRO	CA-N-CD	-7.55	100.93	111.50
2	T	141	PRO	CA-N-CD	-7.55	100.93	111.50
2	0	141	PRO	CA-N-CD	-7.55	100.93	111.50
2	B	141	PRO	CA-N-CD	-7.55	100.93	111.50
2	3	141	PRO	CA-N-CD	-7.55	100.94	111.50
3	7	530	LEU	CB-CG-CD1	7.55	123.83	111.00
2	Q	154[A]	ARG	NE-CZ-NH2	-7.54	116.53	120.30
2	Q	154[B]	ARG	NE-CZ-NH2	-7.54	116.53	120.30
2	H	141	PRO	CA-N-CD	-7.54	100.94	111.50
2	N	154[A]	ARG	NE-CZ-NH2	-7.54	116.53	120.30
2	N	154[B]	ARG	NE-CZ-NH2	-7.54	116.53	120.30
3	U	530	LEU	CB-CG-CD1	7.54	123.81	111.00
3	L	530	LEU	CB-CG-CD1	7.54	123.81	111.00
2	X	141	PRO	CA-N-CD	-7.54	100.95	111.50
3	1	530	LEU	CB-CG-CD1	7.54	123.81	111.00
3	V	530	LEU	CB-CG-CD1	7.53	123.81	111.00
3	Y	530	LEU	CB-CG-CD1	7.53	123.81	111.00
3	I	530	LEU	CB-CG-CD1	7.53	123.80	111.00
2	N	141	PRO	CA-N-CD	-7.53	100.97	111.50
3	C	530	LEU	CB-CG-CD1	7.52	123.79	111.00
3	F	530	LEU	CB-CG-CD1	7.52	123.79	111.00
3	O	530	LEU	CB-CG-CD1	7.52	123.79	111.00
2	K	141	PRO	CA-N-CD	-7.52	100.97	111.50
3	4	530	LEU	CB-CG-CD1	7.52	123.79	111.00
3	R	530	LEU	CB-CG-CD1	7.51	123.76	111.00
2	X	154[A]	ARG	NE-CZ-NH2	-7.48	116.56	120.30
2	X	154[B]	ARG	NE-CZ-NH2	-7.48	116.56	120.30
2	H	154[A]	ARG	NE-CZ-NH2	-7.47	116.56	120.30
2	H	154[B]	ARG	NE-CZ-NH2	-7.47	116.56	120.30
2	B	154[A]	ARG	NE-CZ-NH2	-7.47	116.57	120.30
2	B	154[B]	ARG	NE-CZ-NH2	-7.47	116.57	120.30
2	3	154[A]	ARG	NE-CZ-NH2	-7.47	116.57	120.30
2	3	154[B]	ARG	NE-CZ-NH2	-7.47	116.57	120.30
2	E	154[A]	ARG	NE-CZ-NH2	-7.46	116.57	120.30
2	E	154[B]	ARG	NE-CZ-NH2	-7.46	116.57	120.30
3	L	458	ILE	CA-CB-CG1	7.45	125.15	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	458	ILE	CA-CB-CG1	7.44	125.13	111.00
2	0	154[A]	ARG	NE-CZ-NH2	-7.43	116.58	120.30
2	0	154[B]	ARG	NE-CZ-NH2	-7.43	116.58	120.30
3	7	458	ILE	CA-CB-CG1	7.42	125.11	111.00
3	O	458	ILE	CA-CB-CG1	7.42	125.10	111.00
2	T	154[A]	ARG	NE-CZ-NH2	-7.42	116.59	120.30
2	T	154[B]	ARG	NE-CZ-NH2	-7.42	116.59	120.30
3	1	458	ILE	CA-CB-CG1	7.42	125.10	111.00
3	C	458	ILE	CA-CB-CG1	7.42	125.09	111.00
3	U	458	ILE	CA-CB-CG1	7.42	125.09	111.00
3	V	458	ILE	CA-CB-CG1	7.41	125.08	111.00
2	6	154[A]	ARG	NE-CZ-NH2	-7.41	116.59	120.30
2	6	154[B]	ARG	NE-CZ-NH2	-7.41	116.59	120.30
2	K	154[A]	ARG	NE-CZ-NH2	-7.41	116.60	120.30
2	K	154[B]	ARG	NE-CZ-NH2	-7.41	116.60	120.30
3	F	458	ILE	CA-CB-CG1	7.41	125.07	111.00
3	Y	458	ILE	CA-CB-CG1	7.40	125.05	111.00
3	4	458	ILE	CA-CB-CG1	7.40	125.05	111.00
2	9	154[A]	ARG	NE-CZ-NH2	-7.40	116.60	120.30
2	9	154[B]	ARG	NE-CZ-NH2	-7.40	116.60	120.30
3	R	458	ILE	CA-CB-CG1	7.39	125.04	111.00
3	L	441	ASP	CB-CG-OD2	-7.38	111.65	118.30
3	I	122	ASP	CB-CG-OD2	7.38	124.94	118.30
3	1	304	ASN	CA-C-N	7.38	137.76	117.10
3	4	122	ASP	CB-CG-OD2	7.38	124.94	118.30
3	L	304	ASN	CA-C-N	7.38	137.75	117.10
3	O	304	ASN	CA-C-N	7.38	137.75	117.10
3	Y	122	ASP	CB-CG-OD2	7.38	124.94	118.30
3	C	122	ASP	CB-CG-OD2	7.37	124.93	118.30
3	V	441	ASP	CB-CG-OD2	-7.37	111.67	118.30
3	R	304	ASN	CA-C-N	7.37	137.72	117.10
3	1	122	ASP	CB-CG-OD2	7.36	124.93	118.30
3	U	304	ASN	CA-C-N	7.36	137.71	117.10
3	C	304	ASN	CA-C-N	7.36	137.71	117.10
3	F	304	ASN	CA-C-N	7.36	137.71	117.10
3	4	304	ASN	CA-C-N	7.36	137.71	117.10
3	F	122	ASP	CB-CG-OD2	7.36	124.92	118.30
3	F	441	ASP	CB-CG-OD2	-7.36	111.68	118.30
3	R	122	ASP	CB-CG-OD2	7.36	124.92	118.30
3	U	441	ASP	CB-CG-OD2	-7.36	111.68	118.30
3	I	304	ASN	CA-C-N	7.35	137.69	117.10
3	7	304	ASN	CA-C-N	7.35	137.69	117.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7	441	ASP	CB-CG-OD2	-7.35	111.68	118.30
3	Y	304	ASN	CA-C-N	7.35	137.68	117.10
3	O	122	ASP	CB-CG-OD2	7.34	124.91	118.30
3	O	441	ASP	CB-CG-OD2	-7.34	111.69	118.30
3	U	122	ASP	CB-CG-OD2	7.34	124.91	118.30
3	V	122	ASP	CB-CG-OD2	7.34	124.91	118.30
3	V	304	ASN	CA-C-N	7.34	137.66	117.10
3	L	122	ASP	CB-CG-OD2	7.34	124.91	118.30
3	4	441	ASP	CB-CG-OD2	-7.34	111.69	118.30
3	C	441	ASP	CB-CG-OD2	-7.34	111.69	118.30
3	F	479	ARG	NE-CZ-NH1	-7.33	116.64	120.30
3	I	441	ASP	CB-CG-OD2	-7.33	111.71	118.30
3	7	122	ASP	CB-CG-OD2	7.32	124.89	118.30
3	R	441	ASP	CB-CG-OD2	-7.32	111.72	118.30
3	Y	441	ASP	CB-CG-OD2	-7.30	111.73	118.30
3	7	479	ARG	NE-CZ-NH1	-7.28	116.66	120.30
3	R	407[A]	ARG	NE-CZ-NH2	-7.27	116.66	120.30
3	R	407[B]	ARG	NE-CZ-NH2	-7.27	116.66	120.30
3	L	479	ARG	NE-CZ-NH1	-7.27	116.67	120.30
3	1	441	ASP	CB-CG-OD2	-7.25	111.77	118.30
3	O	407[A]	ARG	NE-CZ-NH2	-7.23	116.69	120.30
3	O	407[B]	ARG	NE-CZ-NH2	-7.23	116.69	120.30
3	I	479	ARG	NE-CZ-NH1	-7.23	116.69	120.30
3	V	479	ARG	NE-CZ-NH1	-7.21	116.70	120.30
3	Y	479	ARG	NE-CZ-NH1	-7.20	116.70	120.30
3	C	479	ARG	NE-CZ-NH1	-7.20	116.70	120.30
3	4	479	ARG	NE-CZ-NH1	-7.20	116.70	120.30
3	I	407[A]	ARG	NE-CZ-NH2	-7.19	116.70	120.30
3	I	407[B]	ARG	NE-CZ-NH2	-7.19	116.70	120.30
3	F	407[A]	ARG	NE-CZ-NH2	-7.19	116.71	120.30
3	F	407[B]	ARG	NE-CZ-NH2	-7.19	116.71	120.30
3	U	407[A]	ARG	NE-CZ-NH2	-7.19	116.71	120.30
3	U	407[B]	ARG	NE-CZ-NH2	-7.19	116.71	120.30
3	L	407[A]	ARG	NE-CZ-NH2	-7.18	116.71	120.30
3	L	407[B]	ARG	NE-CZ-NH2	-7.18	116.71	120.30
3	C	407[A]	ARG	NE-CZ-NH2	-7.18	116.71	120.30
3	C	407[B]	ARG	NE-CZ-NH2	-7.18	116.71	120.30
3	Y	407[A]	ARG	NE-CZ-NH2	-7.18	116.71	120.30
3	Y	407[B]	ARG	NE-CZ-NH2	-7.18	116.71	120.30
3	7	407[A]	ARG	NE-CZ-NH2	-7.17	116.71	120.30
3	7	407[B]	ARG	NE-CZ-NH2	-7.17	116.71	120.30
3	1	407[A]	ARG	NE-CZ-NH2	-7.17	116.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	407[B]	ARG	NE-CZ-NH2	-7.17	116.71	120.30
3	O	479	ARG	NE-CZ-NH1	-7.17	116.72	120.30
3	R	479	ARG	NE-CZ-NH1	-7.16	116.72	120.30
3	U	479	ARG	NE-CZ-NH1	-7.16	116.72	120.30
3	1	479	ARG	NE-CZ-NH1	-7.15	116.72	120.30
3	4	407[A]	ARG	NE-CZ-NH2	-7.13	116.73	120.30
3	4	407[B]	ARG	NE-CZ-NH2	-7.13	116.73	120.30
3	V	407[A]	ARG	NE-CZ-NH2	-7.12	116.74	120.30
3	V	407[B]	ARG	NE-CZ-NH2	-7.12	116.74	120.30
2	0	93	LYS	CD-CE-NZ	7.09	128.02	111.70
2	H	93	LYS	CD-CE-NZ	7.09	128.01	111.70
2	N	93	LYS	CD-CE-NZ	7.09	128.01	111.70
2	T	93	LYS	CD-CE-NZ	7.09	128.00	111.70
2	Q	93	LYS	CD-CE-NZ	7.09	128.00	111.70
2	B	93	LYS	CD-CE-NZ	7.08	127.98	111.70
3	U	440	TRP	CA-CB-CG	7.07	127.13	113.70
2	E	93	LYS	CD-CE-NZ	7.07	127.95	111.70
2	X	93	LYS	CD-CE-NZ	7.07	127.96	111.70
2	6	93	LYS	CD-CE-NZ	7.07	127.95	111.70
2	K	93	LYS	CD-CE-NZ	7.06	127.94	111.70
2	9	93	LYS	CD-CE-NZ	7.06	127.94	111.70
2	3	93	LYS	CD-CE-NZ	7.06	127.94	111.70
3	1	440	TRP	CA-CB-CG	7.04	127.08	113.70
3	C	440	TRP	CA-CB-CG	7.04	127.08	113.70
3	R	440	TRP	CA-CB-CG	7.04	127.08	113.70
3	O	440	TRP	CA-CB-CG	7.04	127.08	113.70
3	7	440	TRP	CA-CB-CG	7.04	127.07	113.70
3	V	440	TRP	CA-CB-CG	7.04	127.07	113.70
3	L	440	TRP	CA-CB-CG	7.03	127.06	113.70
3	4	440	TRP	CA-CB-CG	7.03	127.06	113.70
3	F	440	TRP	CA-CB-CG	7.03	127.06	113.70
3	Y	440	TRP	CA-CB-CG	7.03	127.05	113.70
3	I	440	TRP	CA-CB-CG	7.02	127.04	113.70
2	N	83	LEU	CA-CB-CG	7.00	131.40	115.30
3	7	437	LEU	CA-CB-CG	6.99	131.38	115.30
2	H	83	LEU	CA-CB-CG	6.99	131.37	115.30
3	I	437	LEU	CA-CB-CG	6.99	131.37	115.30
2	3	83	LEU	CA-CB-CG	6.99	131.38	115.30
2	X	83	LEU	CA-CB-CG	6.99	131.37	115.30
3	U	437	LEU	CA-CB-CG	6.99	131.37	115.30
3	R	437	LEU	CA-CB-CG	6.98	131.36	115.30
3	O	437	LEU	CA-CB-CG	6.98	131.36	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	83	LEU	CA-CB-CG	6.98	131.36	115.30
2	B	83	LEU	CA-CB-CG	6.98	131.36	115.30
2	Q	83	LEU	CA-CB-CG	6.98	131.35	115.30
2	9	83	LEU	CA-CB-CG	6.98	131.36	115.30
2	E	83	LEU	CA-CB-CG	6.98	131.35	115.30
2	K	83	LEU	CA-CB-CG	6.98	131.35	115.30
2	Q	87	ARG	NE-CZ-NH1	6.98	123.79	120.30
2	X	87	ARG	NE-CZ-NH1	6.98	123.79	120.30
2	T	83	LEU	CA-CB-CG	6.97	131.34	115.30
3	C	437	LEU	CA-CB-CG	6.97	131.33	115.30
2	0	83	LEU	CA-CB-CG	6.97	131.33	115.30
3	V	437	LEU	CA-CB-CG	6.97	131.32	115.30
2	9	87	ARG	NE-CZ-NH1	6.96	123.78	120.30
3	1	437	LEU	CA-CB-CG	6.96	131.31	115.30
3	4	437	LEU	CA-CB-CG	6.96	131.31	115.30
3	L	437	LEU	CA-CB-CG	6.96	131.30	115.30
2	K	87	ARG	NE-CZ-NH1	6.95	123.78	120.30
3	F	437	LEU	CA-CB-CG	6.95	131.28	115.30
3	Y	437	LEU	CA-CB-CG	6.94	131.26	115.30
3	1	304	ASN	O-C-N	-6.94	107.92	121.10
3	L	304	ASN	O-C-N	-6.94	107.92	121.10
3	R	304	ASN	O-C-N	-6.93	107.93	121.10
3	F	304	ASN	O-C-N	-6.93	107.94	121.10
3	I	527	LYS	CD-CE-NZ	6.93	127.64	111.70
3	I	304	ASN	O-C-N	-6.93	107.94	121.10
3	O	527	LYS	CD-CE-NZ	6.93	127.63	111.70
3	L	527	LYS	CD-CE-NZ	6.92	127.63	111.70
3	O	304	ASN	O-C-N	-6.92	107.95	121.10
3	C	304	ASN	O-C-N	-6.92	107.96	121.10
3	R	527	LYS	CD-CE-NZ	6.92	127.61	111.70
3	Y	304	ASN	O-C-N	-6.92	107.95	121.10
3	Y	527	LYS	CD-CE-NZ	6.92	127.61	111.70
2	0	87	ARG	NE-CZ-NH1	6.92	123.76	120.30
2	B	87	ARG	NE-CZ-NH1	6.91	123.76	120.30
3	4	304	ASN	O-C-N	-6.91	107.96	121.10
3	U	304	ASN	O-C-N	-6.91	107.97	121.10
3	U	527	LYS	CD-CE-NZ	6.91	127.59	111.70
3	C	527	LYS	CD-CE-NZ	6.91	127.59	111.70
2	T	87	ARG	NE-CZ-NH1	6.91	123.75	120.30
3	7	304	ASN	O-C-N	-6.91	107.98	121.10
3	1	527	LYS	CD-CE-NZ	6.90	127.58	111.70
3	V	527	LYS	CD-CE-NZ	6.90	127.58	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	527	LYS	CD-CE-NZ	6.90	127.58	111.70
3	7	527	LYS	CD-CE-NZ	6.90	127.58	111.70
3	V	304	ASN	O-C-N	-6.90	107.99	121.10
3	O	364	SER	CA-C-O	-6.90	105.61	120.10
2	E	87	ARG	NE-CZ-NH1	6.89	123.74	120.30
3	F	527	LYS	CD-CE-NZ	6.88	127.53	111.70
3	I	364	SER	CA-C-O	-6.88	105.64	120.10
3	4	364	SER	CA-C-O	-6.88	105.64	120.10
3	R	364	SER	CA-C-O	-6.88	105.65	120.10
3	Y	95	LYS	CA-CB-CG	6.88	128.54	113.40
3	7	364	SER	CA-C-O	-6.88	105.65	120.10
3	Y	364	SER	CA-C-O	-6.88	105.65	120.10
3	1	364	SER	CA-C-O	-6.88	105.65	120.10
3	F	364	SER	CA-C-O	-6.88	105.66	120.10
2	H	87	ARG	NE-CZ-NH1	6.87	123.74	120.30
3	C	364	SER	CA-C-O	-6.87	105.67	120.10
3	7	95	LYS	CA-CB-CG	6.87	128.51	113.40
3	U	364	SER	CA-C-O	-6.87	105.67	120.10
3	L	364	SER	CA-C-O	-6.87	105.68	120.10
3	I	95	LYS	CA-CB-CG	6.86	128.50	113.40
3	V	364	SER	CA-C-O	-6.86	105.69	120.10
2	3	87	ARG	NE-CZ-NH1	6.86	123.73	120.30
3	4	95	LYS	CA-CB-CG	6.86	128.50	113.40
3	1	95	LYS	CA-CB-CG	6.86	128.50	113.40
3	U	95	LYS	CA-CB-CG	6.86	128.49	113.40
3	C	95	LYS	CA-CB-CG	6.86	128.49	113.40
3	O	95	LYS	CA-CB-CG	6.86	128.49	113.40
3	F	95	LYS	CA-CB-CG	6.86	128.48	113.40
3	R	95	LYS	CA-CB-CG	6.86	128.48	113.40
3	Y	571	PHE	CB-CG-CD2	6.85	125.60	120.80
3	V	95	LYS	CA-CB-CG	6.85	128.47	113.40
3	L	95	LYS	CA-CB-CG	6.85	128.46	113.40
2	N	87	ARG	NE-CZ-NH1	6.84	123.72	120.30
2	6	87	ARG	NE-CZ-NH1	6.83	123.71	120.30
3	7	571	PHE	CB-CG-CD2	6.82	125.57	120.80
3	R	571	PHE	CB-CG-CD2	6.80	125.56	120.80
3	F	571	PHE	CB-CG-CD2	6.79	125.56	120.80
3	V	571	PHE	CB-CG-CD2	6.79	125.55	120.80
3	1	571	PHE	CB-CG-CD2	6.77	125.54	120.80
3	C	571	PHE	CB-CG-CD2	6.77	125.54	120.80
3	I	571	PHE	CB-CG-CD2	6.76	125.53	120.80
3	L	22	ARG	NE-CZ-NH1	6.75	123.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	571	PHE	CB-CG-CD2	6.75	125.52	120.80
3	R	269	GLU	C-N-CA	6.75	136.47	122.30
3	U	269	GLU	C-N-CA	6.74	136.46	122.30
3	U	571	PHE	CB-CG-CD2	6.74	125.52	120.80
2	N	86	ASP	CB-CG-OD2	6.74	124.37	118.30
3	L	571	PHE	CB-CG-CD2	6.74	125.52	120.80
3	1	269	GLU	C-N-CA	6.74	136.44	122.30
3	7	269	GLU	C-N-CA	6.73	136.44	122.30
3	F	269	GLU	C-N-CA	6.73	136.43	122.30
2	H	86	ASP	CB-CG-OD2	6.73	124.35	118.30
3	L	269	GLU	C-N-CA	6.73	136.43	122.30
3	V	190	GLU	CA-CB-CG	6.73	128.20	113.40
2	X	95	LEU	CA-CB-CG	6.73	130.77	115.30
3	4	571	PHE	CB-CG-CD2	6.73	125.51	120.80
3	R	22	ARG	NE-CZ-NH1	6.72	123.66	120.30
3	4	269	GLU	C-N-CA	6.72	136.42	122.30
2	9	86	ASP	CB-CG-OD2	6.72	124.35	118.30
2	N	95	LEU	CA-CB-CG	6.72	130.76	115.30
3	C	269	GLU	C-N-CA	6.72	136.41	122.30
3	V	269	GLU	C-N-CA	6.72	136.41	122.30
2	Q	95	LEU	CA-CB-CG	6.72	130.75	115.30
3	I	269	GLU	C-N-CA	6.71	136.40	122.30
3	O	269	GLU	C-N-CA	6.71	136.40	122.30
3	4	190	GLU	CA-CB-CG	6.71	128.17	113.40
3	O	190	GLU	CA-CB-CG	6.71	128.17	113.40
3	R	190	GLU	CA-CB-CG	6.71	128.17	113.40
3	L	190	GLU	CA-CB-CG	6.71	128.16	113.40
2	K	86	ASP	CB-CG-OD2	6.71	124.34	118.30
2	6	95	LEU	CA-CB-CG	6.71	130.73	115.30
2	B	95	LEU	CA-CB-CG	6.71	130.72	115.30
3	C	190	GLU	CA-CB-CG	6.71	128.15	113.40
2	E	95	LEU	CA-CB-CG	6.70	130.72	115.30
2	0	95	LEU	CA-CB-CG	6.70	130.72	115.30
2	9	95	LEU	CA-CB-CG	6.70	130.72	115.30
2	3	95	LEU	CA-CB-CG	6.70	130.71	115.30
2	T	95	LEU	CA-CB-CG	6.70	130.71	115.30
3	1	190	GLU	CA-CB-CG	6.70	128.14	113.40
2	6	86	ASP	CB-CG-OD2	6.70	124.33	118.30
3	I	190	GLU	CA-CB-CG	6.70	128.13	113.40
2	3	86	ASP	CB-CG-OD2	6.70	124.33	118.30
3	7	190	GLU	CA-CB-CG	6.70	128.14	113.40
3	Y	190	GLU	CA-CB-CG	6.70	128.13	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	269	GLU	C-N-CA	6.70	136.36	122.30
3	F	190	GLU	CA-CB-CG	6.69	128.13	113.40
2	B	86	ASP	CB-CG-OD2	6.69	124.32	118.30
2	H	95	LEU	CA-CB-CG	6.69	130.69	115.30
2	K	95	LEU	CA-CB-CG	6.69	130.69	115.30
3	7	22	ARG	NE-CZ-NH1	6.68	123.64	120.30
3	U	190	GLU	CA-CB-CG	6.68	128.10	113.40
2	0	86	ASP	CB-CG-OD2	6.68	124.31	118.30
2	E	86	ASP	CB-CG-OD2	6.67	124.31	118.30
3	Y	22	ARG	NE-CZ-NH1	6.67	123.63	120.30
3	O	22	ARG	NE-CZ-NH1	6.66	123.63	120.30
2	X	86	ASP	CB-CG-OD2	6.66	124.30	118.30
2	Q	86	ASP	CB-CG-OD2	6.66	124.29	118.30
3	U	22	ARG	NE-CZ-NH1	6.65	123.63	120.30
3	C	22	ARG	NE-CZ-NH1	6.65	123.63	120.30
3	V	22	ARG	NE-CZ-NH1	6.65	123.63	120.30
2	T	86	ASP	CB-CG-OD2	6.65	124.28	118.30
3	I	22	ARG	NE-CZ-NH1	6.64	123.62	120.30
3	U	368	ALA	C-N-CA	6.63	138.28	121.70
3	Y	368	ALA	C-N-CA	6.63	138.28	121.70
3	I	368	ALA	C-N-CA	6.63	138.26	121.70
3	7	368	ALA	C-N-CA	6.62	138.26	121.70
3	I	45	TYR	N-CA-CB	6.62	122.52	110.60
3	4	22	ARG	NE-CZ-NH1	6.62	123.61	120.30
3	C	368	ALA	C-N-CA	6.62	138.25	121.70
3	F	368	ALA	C-N-CA	6.62	138.25	121.70
3	1	368	ALA	C-N-CA	6.62	138.25	121.70
3	4	368	ALA	C-N-CA	6.62	138.24	121.70
3	L	368	ALA	C-N-CA	6.61	138.23	121.70
3	O	368	ALA	C-N-CA	6.61	138.24	121.70
3	R	368	ALA	C-N-CA	6.61	138.22	121.70
3	V	368	ALA	C-N-CA	6.60	138.21	121.70
3	U	45	TYR	N-CA-CB	6.60	122.48	110.60
3	C	45	TYR	N-CA-CB	6.58	122.45	110.60
3	L	45	TYR	N-CA-CB	6.58	122.45	110.60
3	7	45	TYR	N-CA-CB	6.58	122.44	110.60
3	O	45	TYR	N-CA-CB	6.58	122.44	110.60
3	4	45	TYR	N-CA-CB	6.58	122.44	110.60
3	R	45	TYR	N-CA-CB	6.57	122.43	110.60
3	U	89	VAL	C-N-CA	6.57	136.10	122.30
3	1	45	TYR	N-CA-CB	6.57	122.42	110.60
3	F	45	TYR	N-CA-CB	6.57	122.42	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	89	VAL	C-N-CA	6.56	136.08	122.30
3	Y	45	TYR	N-CA-CB	6.56	122.41	110.60
3	1	22	ARG	NE-CZ-NH1	6.56	123.58	120.30
3	V	45	TYR	N-CA-CB	6.55	122.40	110.60
3	1	89	VAL	C-N-CA	6.55	136.07	122.30
3	4	89	VAL	C-N-CA	6.55	136.06	122.30
3	U	480	PRO	CA-N-CD	-6.55	102.33	111.50
3	F	22	ARG	NE-CZ-NH1	6.55	123.58	120.30
3	C	89	VAL	C-N-CA	6.54	136.04	122.30
3	F	480	PRO	CA-N-CD	-6.54	102.35	111.50
3	F	89	VAL	C-N-CA	6.54	136.03	122.30
3	7	480	PRO	CA-N-CD	-6.54	102.35	111.50
3	O	89	VAL	C-N-CA	6.54	136.03	122.30
3	Y	89	VAL	C-N-CA	6.54	136.02	122.30
3	I	480	PRO	CA-N-CD	-6.53	102.35	111.50
3	I	89	VAL	C-N-CA	6.53	136.02	122.30
3	O	480	PRO	CA-N-CD	-6.53	102.36	111.50
3	V	480	PRO	CA-N-CD	-6.53	102.36	111.50
3	V	89	VAL	C-N-CA	6.53	136.01	122.30
3	R	480	PRO	CA-N-CD	-6.52	102.37	111.50
3	1	480	PRO	CA-N-CD	-6.52	102.37	111.50
3	C	480	PRO	CA-N-CD	-6.52	102.37	111.50
3	L	480	PRO	CA-N-CD	-6.52	102.37	111.50
3	7	89	VAL	C-N-CA	6.52	135.99	122.30
3	4	480	PRO	CA-N-CD	-6.51	102.38	111.50
3	Y	480	PRO	CA-N-CD	-6.51	102.39	111.50
3	R	89	VAL	C-N-CA	6.51	135.97	122.30
1	8	6	ARG	CA-CB-CG	6.49	127.67	113.40
1	P	6	ARG	CA-CB-CG	6.48	127.67	113.40
1	D	6	ARG	CA-CB-CG	6.48	127.66	113.40
1	Z	6	ARG	CA-CB-CG	6.48	127.66	113.40
1	J	6	ARG	CA-CB-CG	6.48	127.65	113.40
1	G	6	ARG	CA-CB-CG	6.47	127.64	113.40
1	S	6	ARG	CA-CB-CG	6.47	127.64	113.40
1	2	6	ARG	CA-CB-CG	6.47	127.64	113.40
1	A	6	ARG	CA-CB-CG	6.47	127.64	113.40
1	W	6	ARG	CA-CB-CG	6.46	127.62	113.40
1	5	6	ARG	CA-CB-CG	6.46	127.62	113.40
1	M	6	ARG	CA-CB-CG	6.46	127.61	113.40
3	O	514	ARG	NE-CZ-NH2	-6.45	117.08	120.30
2	9	85	PHE	CB-CG-CD2	-6.42	116.30	120.80
3	1	70	LEU	CB-CG-CD1	6.41	121.91	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6	85	PHE	CB-CG-CD2	-6.41	116.31	120.80
2	T	85	PHE	CB-CG-CD2	-6.41	116.31	120.80
3	7	70	LEU	CB-CG-CD1	6.41	121.90	111.00
3	R	70	LEU	CB-CG-CD1	6.41	121.89	111.00
3	Y	70	LEU	CB-CG-CD1	6.41	121.89	111.00
2	X	85	PHE	CB-CG-CD2	-6.40	116.32	120.80
2	H	85	PHE	CB-CG-CD2	-6.40	116.32	120.80
3	U	70	LEU	CB-CG-CD1	6.40	121.88	111.00
3	C	70	LEU	CB-CG-CD1	6.40	121.88	111.00
2	E	85	PHE	CB-CG-CD2	-6.39	116.32	120.80
3	O	70	LEU	CB-CG-CD1	6.39	121.87	111.00
3	I	70	LEU	CB-CG-CD1	6.39	121.87	111.00
3	L	70	LEU	CB-CG-CD1	6.39	121.86	111.00
2	B	85	PHE	CB-CG-CD2	-6.39	116.33	120.80
3	V	70	LEU	CB-CG-CD1	6.38	121.85	111.00
3	F	70	LEU	CB-CG-CD1	6.38	121.85	111.00
3	4	70	LEU	CB-CG-CD1	6.38	121.85	111.00
2	N	85	PHE	CB-CG-CD2	-6.38	116.34	120.80
3	Y	514	ARG	NE-CZ-NH2	-6.38	117.11	120.30
2	0	85	PHE	CB-CG-CD2	-6.37	116.34	120.80
3	L	210	LEU	CB-CG-CD1	6.37	121.83	111.00
2	Q	85	PHE	CB-CG-CD2	-6.37	116.34	120.80
3	F	210	LEU	CB-CG-CD1	6.36	121.81	111.00
3	Y	210	LEU	CB-CG-CD1	6.36	121.81	111.00
3	L	460	TRP	CA-CB-CG	6.36	125.78	113.70
3	V	210	LEU	CB-CG-CD1	6.36	121.81	111.00
3	U	514	ARG	NE-CZ-NH2	-6.36	117.12	120.30
3	1	210	LEU	CB-CG-CD1	6.36	121.81	111.00
3	7	210	LEU	CB-CG-CD1	6.36	121.81	111.00
3	4	210	LEU	CB-CG-CD1	6.36	121.80	111.00
3	C	210	LEU	CB-CG-CD1	6.35	121.80	111.00
3	1	514	ARG	NE-CZ-NH2	-6.35	117.13	120.30
3	R	210	LEU	CB-CG-CD1	6.35	121.79	111.00
3	I	460	TRP	CA-CB-CG	6.35	125.76	113.70
2	K	85	PHE	CB-CG-CD2	-6.35	116.36	120.80
3	O	460	TRP	CA-CB-CG	6.35	125.76	113.70
2	3	85	PHE	CB-CG-CD2	-6.34	116.36	120.80
3	7	460	TRP	CA-CB-CG	6.34	125.75	113.70
3	O	210	LEU	CB-CG-CD1	6.34	121.78	111.00
3	U	210	LEU	CB-CG-CD1	6.34	121.78	111.00
3	4	451	MET	CA-CB-CG	6.34	124.08	113.30
3	U	173	THR	C-N-CA	6.34	137.55	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	451	MET	CA-CB-CG	6.34	124.08	113.30
3	V	460	TRP	CA-CB-CG	6.34	125.74	113.70
3	U	460	TRP	CA-CB-CG	6.34	125.74	113.70
3	F	460	TRP	CA-CB-CG	6.34	125.74	113.70
3	I	210	LEU	CB-CG-CD1	6.33	121.77	111.00
3	C	460	TRP	CA-CB-CG	6.33	125.73	113.70
3	C	514	ARG	NE-CZ-NH2	-6.33	117.14	120.30
3	I	514	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	2	22	LYS	CD-CE-NZ	6.33	126.26	111.70
3	4	514	ARG	NE-CZ-NH2	-6.33	117.14	120.30
2	K	53	LYS	CA-CB-CG	6.33	127.32	113.40
3	Y	173	THR	C-N-CA	6.33	137.51	121.70
3	I	173	THR	C-N-CA	6.32	137.51	121.70
3	I	225	GLU	CA-CB-CG	6.32	127.31	113.40
2	Q	53	LYS	CA-CB-CG	6.32	127.31	113.40
3	Y	451	MET	CA-CB-CG	6.32	124.05	113.30
3	4	173	THR	C-N-CA	6.32	137.51	121.70
3	7	225	GLU	CA-CB-CG	6.32	127.31	113.40
1	8	22	LYS	CD-CE-NZ	6.32	126.25	111.70
3	F	514	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	D	22	LYS	CD-CE-NZ	6.32	126.23	111.70
3	F	451	MET	CA-CB-CG	6.32	124.04	113.30
2	H	53	LYS	CA-CB-CG	6.32	127.31	113.40
3	I	451	MET	CA-CB-CG	6.32	124.04	113.30
3	L	451	MET	CA-CB-CG	6.32	124.05	113.30
3	R	225	GLU	CA-CB-CG	6.32	127.30	113.40
3	7	514	ARG	NE-CZ-NH2	-6.32	117.14	120.30
2	E	53	LYS	CA-CB-CG	6.32	127.30	113.40
3	F	225	GLU	CA-CB-CG	6.32	127.30	113.40
2	T	53	LYS	CA-CB-CG	6.32	127.30	113.40
3	Y	460	TRP	CA-CB-CG	6.32	125.70	113.70
3	1	451	MET	CA-CB-CG	6.32	124.04	113.30
3	1	460	TRP	CA-CB-CG	6.32	125.70	113.70
3	O	173	THR	C-N-CA	6.32	137.49	121.70
3	Y	225	GLU	CA-CB-CG	6.32	127.30	113.40
3	C	225	GLU	CA-CB-CG	6.31	127.29	113.40
3	C	451	MET	CA-CB-CG	6.31	124.03	113.30
2	B	53	LYS	CA-CB-CG	6.31	127.29	113.40
3	C	173	THR	C-N-CA	6.31	137.48	121.70
3	L	173	THR	C-N-CA	6.31	137.48	121.70
1	5	22	LYS	CD-CE-NZ	6.31	126.22	111.70
2	6	53	LYS	CA-CB-CG	6.31	127.29	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	225	GLU	CA-CB-CG	6.31	127.29	113.40
1	A	22	LYS	CD-CE-NZ	6.31	126.21	111.70
1	M	22	LYS	CD-CE-NZ	6.31	126.21	111.70
3	R	460	TRP	CA-CB-CG	6.31	125.69	113.70
3	V	225	GLU	CA-CB-CG	6.31	127.28	113.40
1	P	22	LYS	CD-CE-NZ	6.31	126.21	111.70
1	S	22	LYS	CD-CE-NZ	6.31	126.20	111.70
3	4	460	TRP	CA-CB-CG	6.31	125.68	113.70
3	7	173	THR	C-N-CA	6.31	137.47	121.70
3	7	451	MET	CA-CB-CG	6.31	124.02	113.30
3	F	173	THR	C-N-CA	6.30	137.46	121.70
3	R	451	MET	CA-CB-CG	6.30	124.02	113.30
3	V	451	MET	CA-CB-CG	6.30	124.02	113.30
3	1	225	GLU	CA-CB-CG	6.30	127.27	113.40
2	9	53	LYS	CA-CB-CG	6.30	127.27	113.40
3	O	225	GLU	CA-CB-CG	6.30	127.27	113.40
2	X	53	LYS	CA-CB-CG	6.30	127.27	113.40
1	Z	22	LYS	CD-CE-NZ	6.30	126.19	111.70
2	3	53	LYS	CA-CB-CG	6.30	127.26	113.40
1	J	22	LYS	CD-CE-NZ	6.30	126.19	111.70
2	0	53	LYS	CA-CB-CG	6.30	127.26	113.40
3	1	173	THR	C-N-CA	6.30	137.44	121.70
1	G	22	LYS	CD-CE-NZ	6.30	126.18	111.70
3	L	514	ARG	NE-CZ-NH2	-6.30	117.15	120.30
2	N	53	LYS	CA-CB-CG	6.30	127.25	113.40
1	W	22	LYS	CD-CE-NZ	6.30	126.18	111.70
3	O	451	MET	CA-CB-CG	6.29	124.00	113.30
3	V	173	THR	C-N-CA	6.29	137.44	121.70
3	L	225	GLU	CA-CB-CG	6.29	127.25	113.40
3	R	173	THR	C-N-CA	6.29	137.43	121.70
3	4	225	GLU	CA-CB-CG	6.29	127.24	113.40
3	U	81	ARG	CG-CD-NE	6.29	125.00	111.80
3	F	443	ARG	NE-CZ-NH1	6.28	123.44	120.30
3	7	81	ARG	CG-CD-NE	6.28	124.99	111.80
3	F	81	ARG	CG-CD-NE	6.28	124.99	111.80
3	C	81	ARG	CG-CD-NE	6.28	124.98	111.80
3	I	396	ASP	CB-CG-OD1	6.28	123.95	118.30
3	Y	81	ARG	CG-CD-NE	6.28	124.98	111.80
3	4	81	ARG	CG-CD-NE	6.28	124.98	111.80
3	V	81	ARG	CG-CD-NE	6.27	124.97	111.80
3	R	81	ARG	CG-CD-NE	6.27	124.97	111.80
3	U	443	ARG	NE-CZ-NH1	6.27	123.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	81	ARG	CG-CD-NE	6.27	124.96	111.80
3	I	81	ARG	CG-CD-NE	6.26	124.95	111.80
3	O	81	ARG	CG-CD-NE	6.26	124.95	111.80
3	I	269	GLU	CA-CB-CG	6.26	127.17	113.40
3	L	81	ARG	CG-CD-NE	6.26	124.95	111.80
3	V	514	ARG	NE-CZ-NH2	-6.26	117.17	120.30
3	C	179	PRO	CA-N-CD	-6.26	102.74	111.50
3	U	269	GLU	CA-CB-CG	6.26	127.17	113.40
3	Y	269	GLU	CA-CB-CG	6.25	127.16	113.40
3	L	269	GLU	CA-CB-CG	6.25	127.16	113.40
3	C	269	GLU	CA-CB-CG	6.25	127.14	113.40
3	Y	396	ASP	CB-CG-OD1	6.25	123.92	118.30
3	L	117	VAL	CA-CB-CG2	6.25	120.27	110.90
3	O	269	GLU	CA-CB-CG	6.24	127.14	113.40
3	1	269	GLU	CA-CB-CG	6.24	127.14	113.40
3	4	269	GLU	CA-CB-CG	6.24	127.13	113.40
3	7	269	GLU	CA-CB-CG	6.24	127.14	113.40
3	V	269	GLU	CA-CB-CG	6.24	127.13	113.40
3	Y	443	ARG	NE-CZ-NH1	6.24	123.42	120.30
3	F	269	GLU	CA-CB-CG	6.24	127.12	113.40
3	R	117	VAL	CA-CB-CG2	6.24	120.25	110.90
3	R	269	GLU	CA-CB-CG	6.23	127.11	113.40
3	V	443	ARG	NE-CZ-NH1	6.23	123.41	120.30
3	C	396	ASP	CB-CG-OD1	6.22	123.90	118.30
3	O	396	ASP	CB-CG-OD1	6.22	123.90	118.30
3	R	396	ASP	CB-CG-OD1	6.22	123.90	118.30
3	Y	117	VAL	CA-CB-CG2	6.22	120.23	110.90
3	7	443	ARG	NE-CZ-NH1	6.22	123.41	120.30
3	1	117	VAL	CA-CB-CG2	6.21	120.22	110.90
3	R	514	ARG	NE-CZ-NH2	-6.21	117.19	120.30
3	U	117	VAL	CA-CB-CG2	6.21	120.22	110.90
3	C	117	VAL	CA-CB-CG2	6.21	120.22	110.90
3	7	396	ASP	CB-CG-OD1	6.21	123.89	118.30
3	V	396	ASP	CB-CG-OD1	6.21	123.89	118.30
3	4	443	ARG	NE-CZ-NH1	6.20	123.40	120.30
3	F	117	VAL	CA-CB-CG2	6.20	120.20	110.90
3	I	117	VAL	CA-CB-CG2	6.20	120.20	110.90
3	1	396	ASP	CB-CG-OD1	6.20	123.88	118.30
3	7	117	VAL	CA-CB-CG2	6.20	120.20	110.90
3	4	396	ASP	CB-CG-OD1	6.20	123.88	118.30
3	O	117	VAL	CA-CB-CG2	6.20	120.19	110.90
3	I	189	VAL	CG1-CB-CG2	6.19	120.81	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	443	ARG	NE-CZ-NH1	6.19	123.40	120.30
3	L	396	ASP	CB-CG-OD1	6.19	123.87	118.30
3	L	443	ARG	NE-CZ-NH1	6.19	123.40	120.30
3	F	189	VAL	CG1-CB-CG2	6.19	120.80	110.90
3	V	117	VAL	CA-CB-CG2	6.19	120.18	110.90
3	F	396	ASP	CB-CG-OD1	6.18	123.86	118.30
3	O	443	ARG	NE-CZ-NH1	6.18	123.39	120.30
3	R	189	VAL	CG1-CB-CG2	6.18	120.79	110.90
3	V	189	VAL	CG1-CB-CG2	6.18	120.79	110.90
3	7	404	ARG	CB-CG-CD	6.18	127.67	111.60
3	U	189	VAL	CG1-CB-CG2	6.18	120.79	110.90
3	Y	53	ASP	C-N-CA	6.18	135.28	122.30
3	4	117	VAL	CA-CB-CG2	6.18	120.17	110.90
3	F	53	ASP	C-N-CA	6.18	135.28	122.30
3	L	53	ASP	C-N-CA	6.18	135.28	122.30
3	U	404	ARG	CB-CG-CD	6.18	127.67	111.60
3	1	404	ARG	CB-CG-CD	6.18	127.66	111.60
3	Y	189	VAL	CG1-CB-CG2	6.18	120.78	110.90
3	Y	404	ARG	CB-CG-CD	6.18	127.66	111.60
3	4	189	VAL	CG1-CB-CG2	6.17	120.78	110.90
3	C	189	VAL	CG1-CB-CG2	6.17	120.78	110.90
3	R	131	LEU	CA-CB-CG	6.17	129.50	115.30
3	1	189	VAL	CG1-CB-CG2	6.17	120.78	110.90
3	V	404	ARG	CB-CG-CD	6.17	127.64	111.60
3	7	131	LEU	CA-CB-CG	6.17	129.49	115.30
3	7	193	PRO	CA-N-CD	-6.17	102.86	111.50
3	C	404	ARG	CB-CG-CD	6.17	127.64	111.60
3	I	404	ARG	CB-CG-CD	6.17	127.64	111.60
3	I	443	ARG	NE-CZ-NH1	6.17	123.38	120.30
3	I	131	LEU	CA-CB-CG	6.17	129.48	115.30
3	L	404	ARG	CB-CG-CD	6.17	127.63	111.60
3	1	193	PRO	CA-N-CD	-6.16	102.87	111.50
3	F	131	LEU	CA-CB-CG	6.16	129.47	115.30
3	O	131	LEU	CA-CB-CG	6.16	129.47	115.30
3	F	404	ARG	CB-CG-CD	6.16	127.61	111.60
3	R	404	ARG	CB-CG-CD	6.16	127.62	111.60
3	Y	131	LEU	CA-CB-CG	6.16	129.47	115.30
3	1	443	ARG	NE-CZ-NH1	6.16	123.38	120.30
3	7	189	VAL	CG1-CB-CG2	6.16	120.76	110.90
3	R	193	PRO	CA-N-CD	-6.16	102.88	111.50
3	V	131	LEU	CA-CB-CG	6.16	129.47	115.30
3	1	53	ASP	C-N-CA	6.16	135.24	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7	53	ASP	C-N-CA	6.16	135.24	122.30
3	U	396	ASP	CB-CG-OD1	6.16	123.84	118.30
3	4	404	ARG	CB-CG-CD	6.16	127.61	111.60
3	C	53	ASP	C-N-CA	6.16	135.23	122.30
3	O	189	VAL	CG1-CB-CG2	6.16	120.75	110.90
3	C	131	LEU	CA-CB-CG	6.15	129.46	115.30
3	L	131	LEU	CA-CB-CG	6.15	129.46	115.30
3	U	131	LEU	CA-CB-CG	6.15	129.45	115.30
3	F	193	PRO	CA-N-CD	-6.15	102.89	111.50
3	L	189	VAL	CG1-CB-CG2	6.15	120.74	110.90
3	R	53	ASP	C-N-CA	6.15	135.22	122.30
3	O	53	ASP	C-N-CA	6.15	135.21	122.30
3	O	404	ARG	CB-CG-CD	6.15	127.58	111.60
3	4	131	LEU	CA-CB-CG	6.15	129.44	115.30
3	L	68	LEU	CB-CG-CD1	6.15	121.45	111.00
3	F	68	LEU	CB-CG-CD1	6.14	121.44	111.00
3	O	571	PHE	C-N-CA	6.14	135.20	122.30
3	V	68	LEU	CB-CG-CD1	6.14	121.44	111.00
3	V	53	ASP	C-N-CA	6.14	135.20	122.30
3	1	68	LEU	CB-CG-CD1	6.14	121.44	111.00
3	1	131	LEU	CA-CB-CG	6.14	129.43	115.30
3	4	193	PRO	CA-N-CD	-6.14	102.90	111.50
3	U	53	ASP	C-N-CA	6.14	135.19	122.30
3	Y	68	LEU	CB-CG-CD1	6.14	121.43	111.00
3	C	193	PRO	CA-N-CD	-6.14	102.91	111.50
3	U	571	PHE	C-N-CA	6.14	135.19	122.30
3	I	53	ASP	C-N-CA	6.13	135.18	122.30
3	C	68	LEU	CB-CG-CD1	6.13	121.43	111.00
3	4	53	ASP	C-N-CA	6.13	135.18	122.30
3	4	571	PHE	C-N-CA	6.13	135.18	122.30
3	L	193	PRO	CA-N-CD	-6.13	102.92	111.50
3	O	68	LEU	CB-CG-CD1	6.13	121.42	111.00
3	1	571	PHE	C-N-CA	6.13	135.18	122.30
3	R	68	LEU	CB-CG-CD1	6.13	121.42	111.00
3	Y	193	PRO	CA-N-CD	-6.13	102.92	111.50
3	4	68	LEU	CB-CG-CD1	6.13	121.42	111.00
3	C	571	PHE	C-N-CA	6.13	135.17	122.30
3	I	571	PHE	C-N-CA	6.13	135.16	122.30
3	O	193	PRO	CA-N-CD	-6.13	102.92	111.50
3	V	193	PRO	CA-N-CD	-6.13	102.92	111.50
3	7	68	LEU	CB-CG-CD1	6.13	121.41	111.00
3	U	68	LEU	CB-CG-CD1	6.12	121.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	571	PHE	C-N-CA	6.12	135.15	122.30
3	L	571	PHE	C-N-CA	6.12	135.15	122.30
3	I	68	LEU	CB-CG-CD1	6.12	121.40	111.00
3	R	443	ARG	NE-CZ-NH1	6.12	123.36	120.30
3	R	571	PHE	C-N-CA	6.12	135.14	122.30
3	7	571	PHE	C-N-CA	6.11	135.13	122.30
3	Y	571	PHE	C-N-CA	6.11	135.12	122.30
3	U	193	PRO	CA-N-CD	-6.10	102.96	111.50
3	V	571	PHE	C-N-CA	6.10	135.10	122.30
3	I	193	PRO	CA-N-CD	-6.09	102.97	111.50
1	M	30[A]	LEU	CB-CG-CD2	6.08	121.33	111.00
1	M	30[B]	LEU	CB-CG-CD2	6.08	121.33	111.00
1	S	30[A]	LEU	CB-CG-CD2	6.08	121.33	111.00
1	S	30[B]	LEU	CB-CG-CD2	6.08	121.33	111.00
1	5	30[A]	LEU	CB-CG-CD2	6.07	121.32	111.00
1	5	30[B]	LEU	CB-CG-CD2	6.07	121.32	111.00
1	A	30[A]	LEU	CB-CG-CD2	6.06	121.31	111.00
1	A	30[B]	LEU	CB-CG-CD2	6.06	121.31	111.00
1	D	30[A]	LEU	CB-CG-CD2	6.06	121.30	111.00
1	D	30[B]	LEU	CB-CG-CD2	6.06	121.30	111.00
1	G	30[A]	LEU	CB-CG-CD2	6.06	121.30	111.00
1	G	30[B]	LEU	CB-CG-CD2	6.06	121.30	111.00
1	Z	30[A]	LEU	CB-CG-CD2	6.06	121.30	111.00
1	Z	30[B]	LEU	CB-CG-CD2	6.06	121.30	111.00
1	8	30[A]	LEU	CB-CG-CD2	6.06	121.30	111.00
1	8	30[B]	LEU	CB-CG-CD2	6.06	121.30	111.00
1	J	30[A]	LEU	CB-CG-CD2	6.06	121.30	111.00
1	J	30[B]	LEU	CB-CG-CD2	6.06	121.30	111.00
3	L	187	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	P	30[A]	LEU	CB-CG-CD2	6.06	121.30	111.00
1	P	30[B]	LEU	CB-CG-CD2	6.06	121.30	111.00
3	V	449	PRO	CA-N-CD	-6.05	103.02	111.50
1	W	30[A]	LEU	CB-CG-CD2	6.05	121.29	111.00
1	W	30[B]	LEU	CB-CG-CD2	6.05	121.29	111.00
1	2	30[A]	LEU	CB-CG-CD2	6.05	121.28	111.00
1	2	30[B]	LEU	CB-CG-CD2	6.05	121.28	111.00
3	O	449	PRO	CA-N-CD	-6.04	103.04	111.50
3	F	449	PRO	CA-N-CD	-6.04	103.04	111.50
3	Y	187	ARG	NE-CZ-NH1	6.04	123.32	120.30
3	7	449	PRO	CA-N-CD	-6.03	103.06	111.50
3	U	221	TYR	CA-CB-CG	6.03	124.85	113.40
3	L	449	PRO	CA-N-CD	-6.02	103.07	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	221	TYR	CA-CB-CG	6.02	124.83	113.40
3	4	449	PRO	CA-N-CD	-6.02	103.08	111.50
3	C	449	PRO	CA-N-CD	-6.01	103.08	111.50
3	F	221	TYR	CA-CB-CG	6.01	124.83	113.40
3	U	449	PRO	CA-N-CD	-6.01	103.08	111.50
3	Y	142	LEU	CA-CB-CG	6.01	129.12	115.30
3	1	221	TYR	CA-CB-CG	6.01	124.82	113.40
3	1	449	PRO	CA-N-CD	-6.01	103.09	111.50
3	4	221	TYR	CA-CB-CG	6.01	124.81	113.40
3	L	142	LEU	CA-CB-CG	6.01	129.11	115.30
3	O	221	TYR	CA-CB-CG	6.01	124.81	113.40
1	M	44	MET	CA-CB-CG	6.00	123.51	113.30
3	1	142	LEU	CA-CB-CG	6.00	129.11	115.30
3	U	187	ARG	NE-CZ-NH1	6.00	123.30	120.30
3	7	142	LEU	CA-CB-CG	6.00	129.10	115.30
3	C	221	TYR	CA-CB-CG	6.00	124.80	113.40
3	I	187	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	2	44	MET	CA-CB-CG	6.00	123.50	113.30
3	1	187	ARG	NE-CZ-NH1	6.00	123.30	120.30
3	I	449	PRO	CA-N-CD	-6.00	103.11	111.50
3	7	187	ARG	NE-CZ-NH1	6.00	123.30	120.30
3	O	142	LEU	CA-CB-CG	5.99	129.09	115.30
1	W	44	MET	CA-CB-CG	5.99	123.49	113.30
3	R	449	PRO	CA-N-CD	-5.99	103.11	111.50
3	C	142	LEU	CA-CB-CG	5.99	129.08	115.30
3	V	142	LEU	CA-CB-CG	5.99	129.08	115.30
3	Y	449	PRO	CA-N-CD	-5.99	103.11	111.50
1	5	44	MET	CA-CB-CG	5.99	123.49	113.30
3	F	142	LEU	CA-CB-CG	5.99	129.07	115.30
3	I	221	TYR	CA-CB-CG	5.99	124.77	113.40
3	L	221	TYR	CA-CB-CG	5.99	124.77	113.40
3	R	142	LEU	CA-CB-CG	5.99	129.07	115.30
1	Z	44	MET	CA-CB-CG	5.99	123.48	113.30
3	U	142	LEU	CA-CB-CG	5.99	129.07	115.30
3	I	142	LEU	CA-CB-CG	5.98	129.06	115.30
3	V	221	TYR	CA-CB-CG	5.98	124.77	113.40
3	4	142	LEU	CA-CB-CG	5.98	129.06	115.30
3	7	221	TYR	CA-CB-CG	5.98	124.77	113.40
1	G	44	MET	CA-CB-CG	5.98	123.47	113.30
1	P	44	MET	CA-CB-CG	5.98	123.47	113.30
1	A	44	MET	CA-CB-CG	5.98	123.46	113.30
3	F	308	PRO	CA-N-CD	-5.98	103.13	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	308	PRO	CA-N-CD	-5.98	103.13	111.50
3	Y	221	TYR	CA-CB-CG	5.98	124.76	113.40
3	V	308	PRO	CA-N-CD	-5.97	103.14	111.50
1	S	44	MET	CA-CB-CG	5.97	123.45	113.30
1	5	88	ASP	CB-CG-OD1	5.97	123.67	118.30
1	W	88	ASP	CB-CG-OD1	5.97	123.67	118.30
1	J	44	MET	CA-CB-CG	5.97	123.45	113.30
1	D	44	MET	CA-CB-CG	5.97	123.44	113.30
1	D	88	ASP	CB-CG-OD1	5.97	123.67	118.30
1	8	88	ASP	CB-CG-OD1	5.96	123.66	118.30
3	C	308	PRO	CA-N-CD	-5.95	103.17	111.50
1	8	44	MET	CA-CB-CG	5.95	123.42	113.30
3	F	187	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	M	88	ASP	CB-CG-OD1	5.95	123.65	118.30
1	P	88	ASP	CB-CG-OD1	5.95	123.65	118.30
3	R	187	ARG	NE-CZ-NH1	5.95	123.27	120.30
3	Y	514	ARG	CB-CG-CD	5.95	127.06	111.60
1	A	88	ASP	CB-CG-OD1	5.95	123.65	118.30
3	4	308	PRO	CA-N-CD	-5.95	103.17	111.50
3	R	514	ARG	CB-CG-CD	5.95	127.06	111.60
1	2	88	ASP	CB-CG-OD1	5.94	123.65	118.30
1	G	88	ASP	CB-CG-OD1	5.94	123.65	118.30
3	F	514	ARG	CB-CG-CD	5.94	127.05	111.60
3	I	514	ARG	CB-CG-CD	5.94	127.04	111.60
3	U	514	ARG	CB-CG-CD	5.94	127.04	111.60
3	C	187	ARG	NE-CZ-NH1	5.94	123.27	120.30
3	L	514	ARG	CB-CG-CD	5.94	127.03	111.60
3	Y	308	PRO	CA-N-CD	-5.94	103.19	111.50
3	V	187	ARG	NE-CZ-NH1	5.94	123.27	120.30
3	C	514	ARG	CB-CG-CD	5.93	127.03	111.60
3	7	514	ARG	CB-CG-CD	5.93	127.03	111.60
3	U	308	PRO	CA-N-CD	-5.93	103.19	111.50
3	7	308	PRO	CA-N-CD	-5.93	103.19	111.50
3	1	308	PRO	CA-N-CD	-5.93	103.20	111.50
3	L	308	PRO	CA-N-CD	-5.93	103.20	111.50
1	Z	88	ASP	CB-CG-OD1	5.93	123.64	118.30
3	O	308	PRO	CA-N-CD	-5.93	103.20	111.50
3	R	308	PRO	CA-N-CD	-5.93	103.20	111.50
3	V	514	ARG	CB-CG-CD	5.93	127.01	111.60
3	4	514	ARG	CB-CG-CD	5.93	127.01	111.60
3	O	187	ARG	NE-CZ-NH1	5.92	123.26	120.30
3	1	514	ARG	CB-CG-CD	5.92	127.00	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	514	ARG	CB-CG-CD	5.92	126.98	111.60
1	S	88	ASP	CB-CG-OD1	5.91	123.62	118.30
3	I	439	LEU	CA-CB-CG	5.91	128.89	115.30
3	O	439	LEU	CA-CB-CG	5.91	128.89	115.30
3	1	439	LEU	CA-CB-CG	5.91	128.89	115.30
1	J	88	ASP	CB-CG-OD1	5.90	123.61	118.30
3	C	439	LEU	CA-CB-CG	5.90	128.87	115.30
3	F	439	LEU	CA-CB-CG	5.90	128.88	115.30
3	U	439	LEU	CA-CB-CG	5.90	128.88	115.30
3	4	439	LEU	CA-CB-CG	5.90	128.87	115.30
3	R	439	LEU	CA-CB-CG	5.90	128.87	115.30
3	7	439	LEU	CA-CB-CG	5.90	128.87	115.30
3	V	439	LEU	CA-CB-CG	5.90	128.86	115.30
3	Y	439	LEU	CA-CB-CG	5.89	128.84	115.30
3	4	187	ARG	NE-CZ-NH1	5.88	123.24	120.30
3	L	439	LEU	CA-CB-CG	5.87	128.81	115.30
3	7	376	TRP	CG-CD1-NE1	5.85	115.95	110.10
3	L	376	TRP	CG-CD1-NE1	5.84	115.94	110.10
1	2	26	ARG	NE-CZ-NH2	5.83	123.22	120.30
3	Y	404	ARG	CG-CD-NE	5.82	124.03	111.80
3	L	404	ARG	CG-CD-NE	5.82	124.02	111.80
3	4	201	LYS	CG-CD-CE	5.82	129.36	111.90
3	I	404	ARG	CG-CD-NE	5.82	124.02	111.80
3	V	404	ARG	CG-CD-NE	5.82	124.01	111.80
3	7	404	ARG	CG-CD-NE	5.82	124.01	111.80
3	U	404	ARG	CG-CD-NE	5.81	124.01	111.80
3	I	201	LYS	CG-CD-CE	5.81	129.34	111.90
3	O	404	ARG	CG-CD-NE	5.81	124.01	111.80
3	1	201	LYS	CG-CD-CE	5.81	129.33	111.90
3	C	201	LYS	CG-CD-CE	5.81	129.32	111.90
3	C	404	ARG	CG-CD-NE	5.81	124.00	111.80
3	L	390	ARG	NE-CZ-NH1	5.81	123.20	120.30
3	R	201	LYS	CG-CD-CE	5.81	129.32	111.90
3	V	201	LYS	CG-CD-CE	5.81	129.32	111.90
3	L	201	LYS	CG-CD-CE	5.80	129.32	111.90
3	O	201	LYS	CG-CD-CE	5.80	129.31	111.90
3	Y	201	LYS	CG-CD-CE	5.80	129.32	111.90
3	4	404	ARG	CG-CD-NE	5.80	123.99	111.80
3	F	376	TRP	CG-CD1-NE1	5.80	115.90	110.10
1	M	26	ARG	NE-CZ-NH2	5.80	123.20	120.30
2	E	94	ARG	CD-NE-CZ	5.80	131.72	123.60
3	7	201	LYS	CG-CD-CE	5.80	129.30	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	201	LYS	CG-CD-CE	5.80	129.30	111.90
2	N	94	ARG	CD-NE-CZ	5.80	131.72	123.60
3	R	404	ARG	CG-CD-NE	5.80	123.98	111.80
3	C	376	TRP	CG-CD1-NE1	5.80	115.90	110.10
3	O	376	TRP	CG-CD1-NE1	5.80	115.90	110.10
3	1	404	ARG	CG-CD-NE	5.80	123.97	111.80
3	V	376	TRP	CG-CD1-NE1	5.79	115.89	110.10
3	Y	376	TRP	CG-CD1-NE1	5.79	115.89	110.10
3	F	201	LYS	CG-CD-CE	5.79	129.28	111.90
3	R	376	TRP	CG-CD1-NE1	5.79	115.89	110.10
1	S	26	ARG	NE-CZ-NH2	5.79	123.20	120.30
3	I	376	TRP	CG-CD1-NE1	5.79	115.89	110.10
3	1	376	TRP	CG-CD1-NE1	5.79	115.89	110.10
3	U	36	LEU	CA-CB-CG	5.79	128.61	115.30
3	F	404	ARG	CG-CD-NE	5.79	123.95	111.80
3	V	36	LEU	CA-CB-CG	5.79	128.60	115.30
1	W	26	ARG	NE-CZ-NH2	5.79	123.19	120.30
3	Y	36	LEU	CA-CB-CG	5.78	128.60	115.30
3	C	36	LEU	CA-CB-CG	5.78	128.59	115.30
3	R	36	LEU	CA-CB-CG	5.78	128.60	115.30
3	V	390	ARG	NE-CZ-NH1	5.78	123.19	120.30
3	1	36	LEU	CA-CB-CG	5.78	128.59	115.30
3	7	36	LEU	CA-CB-CG	5.78	128.59	115.30
2	9	94	ARG	CD-NE-CZ	5.78	131.69	123.60
3	L	36	LEU	CA-CB-CG	5.78	128.59	115.30
2	6	94	ARG	CD-NE-CZ	5.78	131.69	123.60
3	F	36	LEU	CA-CB-CG	5.78	128.58	115.30
1	J	26	ARG	NE-CZ-NH2	5.78	123.19	120.30
3	V	201	LYS	CB-CG-CD	5.77	126.61	111.60
3	4	376	TRP	CG-CD1-NE1	5.77	115.87	110.10
1	P	26	ARG	NE-CZ-NH2	5.77	123.19	120.30
3	R	201	LYS	CB-CG-CD	5.77	126.60	111.60
3	Y	390	ARG	NE-CZ-NH1	5.77	123.19	120.30
2	K	94	ARG	CD-NE-CZ	5.77	131.67	123.60
3	O	201	LYS	CB-CG-CD	5.76	126.59	111.60
2	6	94	ARG	CA-CB-CG	5.76	126.08	113.40
1	A	26	ARG	NE-CZ-NH2	5.76	123.18	120.30
3	I	36	LEU	CA-CB-CG	5.76	128.54	115.30
3	O	36	LEU	CA-CB-CG	5.76	128.55	115.30
3	Y	201	LYS	CB-CG-CD	5.76	126.58	111.60
3	1	201	LYS	CB-CG-CD	5.76	126.57	111.60
3	U	70	LEU	CA-CB-CG	5.76	128.55	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	201	LYS	CB-CG-CD	5.76	126.58	111.60
3	F	201	LYS	CB-CG-CD	5.76	126.57	111.60
3	4	36	LEU	CA-CB-CG	5.76	128.54	115.30
2	K	94	ARG	CA-CB-CG	5.75	126.06	113.40
2	N	94	ARG	CA-CB-CG	5.75	126.06	113.40
3	4	70	LEU	CA-CB-CG	5.75	128.54	115.30
2	B	94	ARG	CD-NE-CZ	5.75	131.65	123.60
3	C	201	LYS	CB-CG-CD	5.75	126.56	111.60
3	I	201	LYS	CB-CG-CD	5.75	126.56	111.60
2	Q	94	ARG	CD-NE-CZ	5.75	131.65	123.60
3	F	70	LEU	CA-CB-CG	5.75	128.52	115.30
3	L	127	GLU	OE1-CD-OE2	-5.75	116.40	123.30
2	X	94	ARG	CA-CB-CG	5.75	126.04	113.40
3	L	201	LYS	CB-CG-CD	5.75	126.54	111.60
3	Y	70	LEU	CA-CB-CG	5.75	128.51	115.30
3	4	201	LYS	CB-CG-CD	5.75	126.54	111.60
3	7	70	LEU	CA-CB-CG	5.75	128.51	115.30
1	8	26	ARG	NE-CZ-NH2	5.75	123.17	120.30
3	L	70	LEU	CA-CB-CG	5.74	128.51	115.30
3	O	454	LYS	C-N-CA	5.74	134.36	122.30
3	U	454	LYS	C-N-CA	5.74	134.36	122.30
2	0	94	ARG	CD-NE-CZ	5.74	131.64	123.60
3	7	201	LYS	CB-CG-CD	5.74	126.53	111.60
2	B	94	ARG	CA-CB-CG	5.74	126.03	113.40
2	E	94	ARG	CA-CB-CG	5.74	126.03	113.40
3	V	70	LEU	CA-CB-CG	5.74	128.50	115.30
2	3	94	ARG	CA-CB-CG	5.74	126.03	113.40
3	U	376	TRP	CG-CD1-NE1	5.74	115.84	110.10
3	C	70	LEU	CA-CB-CG	5.74	128.49	115.30
2	T	94	ARG	CD-NE-CZ	5.74	131.63	123.60
2	0	94	ARG	CA-CB-CG	5.74	126.02	113.40
3	7	454	LYS	C-N-CA	5.74	134.34	122.30
3	O	70	LEU	CA-CB-CG	5.73	128.48	115.30
3	R	454	LYS	C-N-CA	5.73	134.34	122.30
2	9	94	ARG	CA-CB-CG	5.73	126.01	113.40
3	C	454	LYS	C-N-CA	5.73	134.34	122.30
2	X	94	ARG	CD-NE-CZ	5.73	131.62	123.60
3	F	454	LYS	C-N-CA	5.73	134.33	122.30
2	H	94	ARG	CD-NE-CZ	5.73	131.62	123.60
3	I	70	LEU	CA-CB-CG	5.73	128.47	115.30
3	R	70	LEU	CA-CB-CG	5.73	128.47	115.30
1	Z	26	ARG	NE-CZ-NH2	5.73	123.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	127	GLU	OE1-CD-OE2	-5.73	116.43	123.30
3	O	127	GLU	OE1-CD-OE2	-5.73	116.43	123.30
2	T	94	ARG	CA-CB-CG	5.73	126.00	113.40
2	H	94	ARG	CA-CB-CG	5.72	125.99	113.40
3	L	102	SER	C-N-CA	5.72	134.32	122.30
3	O	102	SER	C-N-CA	5.72	134.32	122.30
3	V	454	LYS	C-N-CA	5.72	134.32	122.30
3	Y	454	LYS	C-N-CA	5.72	134.32	122.30
2	3	94	ARG	CD-NE-CZ	5.72	131.62	123.60
3	I	102	SER	C-N-CA	5.72	134.32	122.30
3	R	390	ARG	NE-CZ-NH1	5.72	123.16	120.30
3	7	431	VAL	C-N-CA	5.72	134.32	122.30
3	I	454	LYS	C-N-CA	5.72	134.31	122.30
3	1	70	LEU	CA-CB-CG	5.72	128.45	115.30
3	1	102	SER	C-N-CA	5.72	134.31	122.30
3	Y	427	GLY	N-CA-C	5.72	127.39	113.10
3	1	454	LYS	C-N-CA	5.72	134.31	122.30
3	4	454	LYS	C-N-CA	5.72	134.30	122.30
3	C	390	ARG	NE-CZ-NH1	5.71	123.16	120.30
3	L	454	LYS	C-N-CA	5.71	134.30	122.30
2	Q	94	ARG	CA-CB-CG	5.71	125.97	113.40
3	F	102	SER	C-N-CA	5.71	134.30	122.30
3	U	102	SER	C-N-CA	5.71	134.29	122.30
3	F	390	ARG	NE-CZ-NH1	5.71	123.15	120.30
3	1	127	GLU	OE1-CD-OE2	-5.71	116.45	123.30
3	4	102	SER	C-N-CA	5.71	134.28	122.30
3	C	127	GLU	OE1-CD-OE2	-5.71	116.45	123.30
3	C	431	VAL	C-N-CA	5.71	134.28	122.30
3	I	431	VAL	C-N-CA	5.71	134.28	122.30
3	O	390	ARG	NE-CZ-NH1	5.71	123.15	120.30
3	R	127	GLU	OE1-CD-OE2	-5.71	116.45	123.30
3	F	427	GLY	N-CA-C	5.70	127.36	113.10
3	R	102	SER	C-N-CA	5.70	134.28	122.30
3	1	431	VAL	C-N-CA	5.70	134.28	122.30
3	7	127	GLU	OE1-CD-OE2	-5.70	116.46	123.30
3	C	102	SER	C-N-CA	5.70	134.28	122.30
3	U	431	VAL	C-N-CA	5.70	134.27	122.30
3	R	431	VAL	C-N-CA	5.70	134.27	122.30
3	Y	431	VAL	C-N-CA	5.70	134.27	122.30
1	5	26	ARG	NE-CZ-NH2	5.70	123.15	120.30
3	7	390	ARG	NE-CZ-NH1	5.70	123.15	120.30
3	U	427	GLY	N-CA-C	5.70	127.35	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	127	GLU	OE1-CD-OE2	-5.70	116.46	123.30
3	L	427	GLY	N-CA-C	5.70	127.34	113.10
3	V	102	SER	C-N-CA	5.70	134.27	122.30
3	V	431	VAL	C-N-CA	5.70	134.27	122.30
1	G	26	ARG	NE-CZ-NH2	5.70	123.15	120.30
3	R	427	GLY	N-CA-C	5.70	127.34	113.10
3	4	431	VAL	C-N-CA	5.70	134.26	122.30
3	Y	102	SER	C-N-CA	5.69	134.26	122.30
3	7	102	SER	C-N-CA	5.69	134.26	122.30
3	C	427	GLY	N-CA-C	5.69	127.33	113.10
3	V	427	GLY	N-CA-C	5.69	127.33	113.10
3	1	427	GLY	N-CA-C	5.69	127.33	113.10
3	F	431	VAL	C-N-CA	5.69	134.25	122.30
3	I	427	GLY	N-CA-C	5.69	127.32	113.10
3	Y	127	GLU	OE1-CD-OE2	-5.69	116.48	123.30
3	4	427	GLY	N-CA-C	5.69	127.32	113.10
3	I	390	ARG	NE-CZ-NH1	5.68	123.14	120.30
3	O	431	VAL	C-N-CA	5.68	134.24	122.30
3	7	427	GLY	N-CA-C	5.68	127.31	113.10
1	D	26	ARG	NE-CZ-NH2	5.68	123.14	120.30
3	L	431	VAL	C-N-CA	5.68	134.23	122.30
3	4	127	GLU	OE1-CD-OE2	-5.68	116.48	123.30
3	V	127	GLU	OE1-CD-OE2	-5.68	116.49	123.30
3	O	152	LEU	CA-CB-CG	5.68	128.35	115.30
3	U	478	TYR	C-N-CA	5.68	135.89	121.70
3	O	427	GLY	N-CA-C	5.67	127.29	113.10
3	U	390	ARG	NE-CZ-NH1	5.67	123.14	120.30
3	L	152	LEU	CA-CB-CG	5.67	128.34	115.30
3	V	478	TYR	C-N-CA	5.67	135.88	121.70
3	U	152	LEU	CA-CB-CG	5.67	128.34	115.30
3	I	127	GLU	OE1-CD-OE2	-5.67	116.50	123.30
3	R	152	LEU	CA-CB-CG	5.67	128.34	115.30
3	Y	478	TYR	C-N-CA	5.67	135.87	121.70
3	1	478	TYR	C-N-CA	5.67	135.86	121.70
3	4	478	TYR	C-N-CA	5.67	135.87	121.70
3	7	478	TYR	C-N-CA	5.67	135.86	121.70
3	C	152	LEU	CA-CB-CG	5.67	128.33	115.30
3	C	478	TYR	C-N-CA	5.66	135.86	121.70
3	I	478	TYR	C-N-CA	5.66	135.86	121.70
3	L	478	TYR	C-N-CA	5.66	135.86	121.70
3	1	152	LEU	CA-CB-CG	5.66	128.33	115.30
3	R	478	TYR	C-N-CA	5.66	135.85	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	390	ARG	NE-CZ-NH1	5.66	123.13	120.30
3	V	152	LEU	CA-CB-CG	5.66	128.32	115.30
3	O	478	TYR	C-N-CA	5.66	135.85	121.70
3	7	152	LEU	CA-CB-CG	5.66	128.31	115.30
3	F	152	LEU	CA-CB-CG	5.65	128.30	115.30
3	4	152	LEU	CA-CB-CG	5.65	128.30	115.30
3	I	152	LEU	CA-CB-CG	5.65	128.30	115.30
3	F	478	TYR	C-N-CA	5.65	135.82	121.70
3	Y	152	LEU	CA-CB-CG	5.65	128.29	115.30
3	1	390	ARG	NE-CZ-NH1	5.65	123.12	120.30
2	X	133	GLY	N-CA-C	5.64	127.21	113.10
3	L	129	LEU	CB-CG-CD2	5.64	120.59	111.00
3	7	129	LEU	CB-CG-CD2	5.64	120.58	111.00
2	K	133	GLY	N-CA-C	5.63	127.18	113.10
3	I	129	LEU	CB-CG-CD2	5.63	120.57	111.00
2	N	133	GLY	N-CA-C	5.63	127.16	113.10
3	I	90	GLY	N-CA-C	5.62	127.16	113.10
2	9	133	GLY	N-CA-C	5.62	127.16	113.10
3	C	129	LEU	CB-CG-CD2	5.62	120.56	111.00
2	Q	133	GLY	N-CA-C	5.62	127.16	113.10
3	R	129	LEU	CB-CG-CD2	5.62	120.56	111.00
3	F	90	GLY	N-CA-C	5.62	127.15	113.10
3	7	448	LYS	CB-CG-CD	5.62	126.22	111.60
3	I	448	LYS	CB-CG-CD	5.62	126.21	111.60
2	B	133	GLY	N-CA-C	5.62	127.15	113.10
3	L	90	GLY	N-CA-C	5.62	127.14	113.10
2	T	133	GLY	N-CA-C	5.62	127.15	113.10
3	V	129	LEU	CB-CG-CD2	5.62	120.55	111.00
3	Y	485	MET	CA-CB-CG	5.62	122.85	113.30
2	E	133	GLY	N-CA-C	5.62	127.14	113.10
3	V	90	GLY	N-CA-C	5.61	127.14	113.10
3	U	129	LEU	CB-CG-CD2	5.61	120.54	111.00
3	C	90	GLY	N-CA-C	5.61	127.12	113.10
2	H	133	GLY	N-CA-C	5.61	127.12	113.10
2	3	133	GLY	N-CA-C	5.61	127.13	113.10
3	U	90	GLY	N-CA-C	5.61	127.13	113.10
3	L	485	MET	CA-CB-CG	5.61	122.83	113.30
3	1	129	LEU	CB-CG-CD2	5.61	120.53	111.00
3	O	129	LEU	CB-CG-CD2	5.61	120.53	111.00
3	R	485	MET	CA-CB-CG	5.61	122.83	113.30
3	Y	90	GLY	N-CA-C	5.61	127.12	113.10
3	Y	129	LEU	CB-CG-CD2	5.61	120.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	448	LYS	CB-CG-CD	5.61	126.17	111.60
3	1	90	GLY	N-CA-C	5.61	127.12	113.10
2	6	133	GLY	N-CA-C	5.61	127.11	113.10
3	7	90	GLY	N-CA-C	5.61	127.11	113.10
3	C	485	MET	CA-CB-CG	5.60	122.83	113.30
3	F	129	LEU	CB-CG-CD2	5.60	120.53	111.00
3	R	90	GLY	N-CA-C	5.60	127.11	113.10
2	0	133	GLY	N-CA-C	5.60	127.11	113.10
3	4	90	GLY	N-CA-C	5.60	127.11	113.10
3	L	448	LYS	CB-CG-CD	5.60	126.16	111.60
3	R	448	LYS	CB-CG-CD	5.60	126.16	111.60
3	4	129	LEU	CB-CG-CD2	5.60	120.52	111.00
3	C	448	LYS	CB-CG-CD	5.60	126.15	111.60
3	1	485	MET	CA-CB-CG	5.60	122.82	113.30
1	2	23	ARG	CB-CG-CD	5.60	126.16	111.60
3	U	448	LYS	CB-CG-CD	5.60	126.15	111.60
3	O	448	LYS	CB-CG-CD	5.60	126.15	111.60
1	J	23	ARG	CB-CG-CD	5.59	126.14	111.60
3	O	485	MET	CA-CB-CG	5.59	122.81	113.30
3	4	448	LYS	CB-CG-CD	5.59	126.14	111.60
3	F	448	LYS	CB-CG-CD	5.59	126.14	111.60
3	F	485	MET	CA-CB-CG	5.59	122.81	113.30
3	O	90	GLY	N-CA-C	5.59	127.07	113.10
1	S	23	ARG	CB-CG-CD	5.59	126.13	111.60
3	V	448	LYS	CB-CG-CD	5.59	126.13	111.60
1	Z	23	ARG	CB-CG-CD	5.59	126.13	111.60
3	1	448	LYS	CB-CG-CD	5.59	126.13	111.60
3	I	485	MET	CA-CB-CG	5.59	122.80	113.30
3	V	485	MET	CA-CB-CG	5.59	122.80	113.30
3	4	485	MET	CA-CB-CG	5.59	122.80	113.30
2	Q	149	LEU	CB-CG-CD2	5.58	120.49	111.00
1	A	23	ARG	CB-CG-CD	5.58	126.12	111.60
1	G	23	ARG	CB-CG-CD	5.58	126.12	111.60
3	V	183	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	8	23	ARG	CB-CG-CD	5.58	126.12	111.60
2	6	149	LEU	CB-CG-CD2	5.58	120.49	111.00
2	T	149	LEU	CB-CG-CD2	5.58	120.48	111.00
2	B	149	LEU	CB-CG-CD2	5.58	120.48	111.00
3	7	485	MET	CA-CB-CG	5.58	122.78	113.30
1	W	23	ARG	CB-CG-CD	5.58	126.10	111.60
2	0	149	LEU	CB-CG-CD2	5.58	120.48	111.00
2	3	149	LEU	CB-CG-CD2	5.58	120.48	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	23	ARG	CB-CG-CD	5.58	126.09	111.60
1	M	23	ARG	CB-CG-CD	5.57	126.09	111.60
1	P	23	ARG	CB-CG-CD	5.57	126.09	111.60
2	N	149	LEU	CB-CG-CD2	5.57	120.47	111.00
2	X	149	LEU	CB-CG-CD2	5.57	120.47	111.00
3	U	485	MET	CA-CB-CG	5.57	122.77	113.30
2	E	149	LEU	CB-CG-CD2	5.57	120.47	111.00
3	4	291	ARG	NE-CZ-NH2	-5.57	117.52	120.30
2	H	149	LEU	CB-CG-CD2	5.57	120.46	111.00
1	D	23	ARG	CB-CG-CD	5.56	126.07	111.60
3	F	183	ARG	NE-CZ-NH2	5.56	123.08	120.30
3	F	227	TRP	CA-CB-CG	5.56	124.27	113.70
3	O	227	TRP	CA-CB-CG	5.56	124.27	113.70
2	K	149	LEU	CB-CG-CD2	5.56	120.46	111.00
3	1	291	ARG	NE-CZ-NH2	-5.56	117.52	120.30
3	4	227	TRP	CA-CB-CG	5.56	124.27	113.70
3	7	227	TRP	CA-CB-CG	5.56	124.27	113.70
1	G	56	VAL	CA-CB-CG2	5.56	119.23	110.90
3	R	227	TRP	CA-CB-CG	5.55	124.25	113.70
2	9	149	LEU	CB-CG-CD2	5.55	120.44	111.00
1	M	56	VAL	CA-CB-CG2	5.55	119.23	110.90
3	C	227	TRP	CA-CB-CG	5.55	124.25	113.70
3	R	183	ARG	NE-CZ-NH2	5.55	123.08	120.30
3	Y	227	TRP	CA-CB-CG	5.55	124.25	113.70
3	I	227	TRP	CA-CB-CG	5.55	124.24	113.70
1	8	56	VAL	CA-CB-CG2	5.55	119.22	110.90
3	1	185	MET	CB-CG-SD	5.54	129.03	112.40
3	4	185	MET	CB-CG-SD	5.54	129.03	112.40
3	Y	291	ARG	NE-CZ-NH2	-5.54	117.53	120.30
3	V	227	TRP	CA-CB-CG	5.54	124.23	113.70
3	Y	185	MET	CB-CG-SD	5.54	129.03	112.40
3	1	183	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	2	56	VAL	CA-CB-CG2	5.54	119.21	110.90
3	7	183	ARG	NE-CZ-NH2	5.54	123.07	120.30
3	L	183	ARG	NE-CZ-NH2	5.54	123.07	120.30
3	L	227	TRP	CA-CB-CG	5.54	124.22	113.70
3	R	185	MET	CB-CG-SD	5.54	129.02	112.40
3	U	227	TRP	CA-CB-CG	5.54	124.22	113.70
3	C	185	MET	CB-CG-SD	5.54	129.01	112.40
1	S	56	VAL	CA-CB-CG2	5.54	119.20	110.90
1	P	56	VAL	CA-CB-CG2	5.53	119.20	110.90
3	1	227	TRP	CA-CB-CG	5.53	124.21	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7	185	MET	CB-CG-SD	5.53	129.00	112.40
3	U	185	MET	CB-CG-SD	5.53	129.00	112.40
3	F	185	MET	CB-CG-SD	5.53	128.99	112.40
3	F	291	ARG	NE-CZ-NH2	-5.53	117.53	120.30
3	I	185	MET	CB-CG-SD	5.53	128.99	112.40
3	F	88	ASP	CB-CG-OD1	5.53	123.28	118.30
1	5	56	VAL	CA-CB-CG2	5.53	119.19	110.90
3	L	185	MET	CB-CG-SD	5.53	128.97	112.40
3	O	185	MET	CB-CG-SD	5.53	128.98	112.40
3	V	185	MET	CB-CG-SD	5.52	128.97	112.40
3	O	88	ASP	CB-CG-OD1	5.52	123.27	118.30
3	1	91	ILE	C-N-CA	5.52	135.50	121.70
1	A	56	VAL	CA-CB-CG2	5.52	119.17	110.90
1	Z	56	VAL	CA-CB-CG2	5.52	119.18	110.90
1	W	56	VAL	CA-CB-CG2	5.51	119.17	110.90
3	C	183	ARG	NE-CZ-NH2	5.51	123.06	120.30
2	H	104	ARG	CD-NE-CZ	5.51	131.32	123.60
1	J	56	VAL	CA-CB-CG2	5.51	119.17	110.90
2	9	104	ARG	CD-NE-CZ	5.51	131.31	123.60
3	Y	91	ILE	C-N-CA	5.51	135.47	121.70
3	1	88	ASP	CB-CG-OD1	5.51	123.25	118.30
2	N	104	ARG	CD-NE-CZ	5.50	131.31	123.60
3	I	91	ILE	C-N-CA	5.50	135.46	121.70
2	E	104	ARG	CD-NE-CZ	5.50	131.30	123.60
2	0	104	ARG	CD-NE-CZ	5.50	131.30	123.60
3	7	91	ILE	C-N-CA	5.50	135.46	121.70
3	L	291	ARG	NE-CZ-NH2	-5.50	117.55	120.30
3	R	91	ILE	C-N-CA	5.50	135.45	121.70
3	4	91	ILE	C-N-CA	5.50	135.44	121.70
3	C	91	ILE	C-N-CA	5.50	135.44	121.70
2	9	78	GLU	CA-CB-CG	5.50	125.49	113.40
3	L	88	ASP	CB-CG-OD1	5.49	123.24	118.30
3	R	88	ASP	CB-CG-OD1	5.49	123.24	118.30
3	V	88	ASP	CB-CG-OD1	5.49	123.24	118.30
3	O	91	ILE	C-N-CA	5.49	135.43	121.70
3	4	183	ARG	NE-CZ-NH2	5.49	123.05	120.30
2	6	104	ARG	CD-NE-CZ	5.49	131.29	123.60
3	Y	88	ASP	CB-CG-OD1	5.49	123.24	118.30
2	T	104	ARG	CD-NE-CZ	5.49	131.28	123.60
2	X	78	GLU	CA-CB-CG	5.49	125.47	113.40
3	7	88	ASP	CB-CG-OD1	5.49	123.24	118.30
3	F	91	ILE	C-N-CA	5.48	135.41	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	104	ARG	CD-NE-CZ	5.48	131.28	123.60
2	3	104	ARG	CD-NE-CZ	5.48	131.28	123.60
2	B	104	ARG	CD-NE-CZ	5.48	131.27	123.60
3	L	91	ILE	C-N-CA	5.48	135.40	121.70
2	K	78	GLU	CA-CB-CG	5.48	125.45	113.40
3	U	91	ILE	C-N-CA	5.48	135.40	121.70
2	B	78	GLU	CA-CB-CG	5.48	125.45	113.40
3	C	88	ASP	CB-CG-OD1	5.48	123.23	118.30
1	D	56	VAL	CA-CB-CG2	5.48	119.12	110.90
2	E	78	GLU	CA-CB-CG	5.48	125.45	113.40
2	0	78	GLU	CA-CB-CG	5.48	125.45	113.40
3	U	183	ARG	NE-CZ-NH2	5.48	123.04	120.30
2	6	37	LEU	C-N-CA	5.48	133.80	122.30
2	H	78	GLU	CA-CB-CG	5.47	125.44	113.40
3	I	160	PHE	C-N-CA	5.47	133.80	122.30
3	V	91	ILE	C-N-CA	5.47	135.39	121.70
2	0	37	LEU	C-N-CA	5.47	133.79	122.30
2	B	37	LEU	C-N-CA	5.47	133.79	122.30
3	C	291	ARG	NE-CZ-NH2	-5.47	117.56	120.30
2	K	104	ARG	CD-NE-CZ	5.47	131.26	123.60
2	Q	37	LEU	C-N-CA	5.47	133.79	122.30
2	Q	78	GLU	CA-CB-CG	5.47	125.44	113.40
2	Q	104	ARG	CD-NE-CZ	5.47	131.26	123.60
3	7	160	PHE	C-N-CA	5.47	133.79	122.30
3	R	291	ARG	NE-CZ-NH2	-5.47	117.56	120.30
2	X	37	LEU	C-N-CA	5.47	133.79	122.30
3	Y	183	ARG	NE-CZ-NH2	5.47	123.03	120.30
3	7	291	ARG	NE-CZ-NH2	-5.47	117.56	120.30
2	T	37	LEU	C-N-CA	5.47	133.78	122.30
3	Y	160	PHE	C-N-CA	5.47	133.79	122.30
3	4	88	ASP	CB-CG-OD1	5.47	123.22	118.30
2	N	78	GLU	CA-CB-CG	5.47	125.43	113.40
3	R	160	PHE	C-N-CA	5.47	133.78	122.30
2	3	78	GLU	CA-CB-CG	5.47	125.43	113.40
2	9	37	LEU	C-N-CA	5.47	133.78	122.30
3	I	291	ARG	NE-CZ-NH2	-5.47	117.57	120.30
3	L	160	PHE	C-N-CA	5.47	133.78	122.30
3	O	291	ARG	NE-CZ-NH2	-5.47	117.57	120.30
2	3	37	LEU	C-N-CA	5.47	133.78	122.30
3	I	496	PHE	CB-CG-CD1	5.46	124.62	120.80
2	K	37	LEU	C-N-CA	5.46	133.78	122.30
3	4	160	PHE	C-N-CA	5.46	133.78	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	88	ASP	CB-CG-OD1	5.46	123.22	118.30
3	1	145	PRO	CA-N-CD	-5.46	103.85	111.50
3	C	160	PHE	C-N-CA	5.46	133.77	122.30
3	O	183	ARG	NE-CZ-NH2	5.46	123.03	120.30
2	T	78	GLU	CA-CB-CG	5.46	125.42	113.40
3	V	160	PHE	C-N-CA	5.46	133.77	122.30
3	1	160	PHE	C-N-CA	5.46	133.77	122.30
2	H	37	LEU	C-N-CA	5.46	133.76	122.30
2	N	37	LEU	C-N-CA	5.46	133.76	122.30
3	F	160	PHE	C-N-CA	5.46	133.76	122.30
3	U	88	ASP	CB-CG-OD1	5.46	123.21	118.30
3	U	160	PHE	C-N-CA	5.46	133.76	122.30
2	E	37	LEU	C-N-CA	5.45	133.75	122.30
2	6	78	GLU	CA-CB-CG	5.45	125.40	113.40
3	7	145	PRO	CA-N-CD	-5.45	103.87	111.50
3	O	160	PHE	C-N-CA	5.45	133.74	122.30
3	V	496	PHE	CB-CG-CD1	5.45	124.61	120.80
3	F	145	PRO	CA-N-CD	-5.45	103.88	111.50
3	L	496	PHE	CB-CG-CD1	5.45	124.61	120.80
3	I	145	PRO	CA-N-CD	-5.44	103.88	111.50
3	I	183	ARG	NE-CZ-NH2	5.44	123.02	120.30
3	C	145	PRO	CA-N-CD	-5.44	103.88	111.50
3	L	145	PRO	CA-N-CD	-5.44	103.89	111.50
3	Y	187	ARG	CB-CG-CD	5.43	125.73	111.60
3	4	187	ARG	CB-CG-CD	5.43	125.72	111.60
3	V	291	ARG	NE-CZ-NH2	-5.43	117.58	120.30
3	O	145	PRO	CA-N-CD	-5.43	103.90	111.50
3	4	496	PHE	CB-CG-CD1	5.43	124.60	120.80
3	F	187	ARG	CB-CG-CD	5.43	125.71	111.60
3	O	187	ARG	CB-CG-CD	5.43	125.71	111.60
3	I	187	ARG	CB-CG-CD	5.43	125.71	111.60
3	R	187	ARG	CB-CG-CD	5.43	125.71	111.60
3	V	187	ARG	CB-CG-CD	5.42	125.70	111.60
3	V	381	GLN	CA-CB-CG	5.42	125.33	113.40
3	C	187	ARG	CB-CG-CD	5.42	125.70	111.60
1	W	1	MET	CB-CG-SD	5.42	128.66	112.40
3	Y	145	PRO	CA-N-CD	-5.42	103.91	111.50
2	H	145	ARG	O-C-N	-5.42	110.80	121.10
3	V	145	PRO	CA-N-CD	-5.42	103.91	111.50
3	1	211	LEU	C-N-CA	5.42	135.25	121.70
3	U	211	LEU	C-N-CA	5.42	135.25	121.70
3	U	291	ARG	NE-CZ-NH2	-5.42	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	381	GLN	CA-CB-CG	5.42	125.32	113.40
3	V	211	LEU	C-N-CA	5.42	135.24	121.70
3	U	187	ARG	CB-CG-CD	5.42	125.68	111.60
3	I	381	GLN	CA-CB-CG	5.42	125.31	113.40
3	O	323	VAL	CA-CB-CG2	5.42	119.02	110.90
3	R	323	VAL	CA-CB-CG2	5.42	119.02	110.90
1	S	1	MET	CB-CG-SD	5.42	128.65	112.40
3	Y	211	LEU	C-N-CA	5.42	135.24	121.70
3	1	187	ARG	CB-CG-CD	5.42	125.68	111.60
2	E	145	ARG	O-C-N	-5.41	110.81	121.10
3	F	496	PHE	CB-CG-CD1	5.41	124.59	120.80
3	O	381	GLN	CA-CB-CG	5.41	125.31	113.40
3	Y	323	VAL	CA-CB-CG2	5.41	119.02	110.90
1	2	1	MET	CB-CG-SD	5.41	128.64	112.40
3	4	211	LEU	C-N-CA	5.41	135.23	121.70
1	M	1	MET	CB-CG-SD	5.41	128.63	112.40
1	P	1	MET	CB-CG-SD	5.41	128.64	112.40
3	R	145	PRO	CA-N-CD	-5.41	103.92	111.50
3	F	381	GLN	CA-CB-CG	5.41	125.30	113.40
3	L	187	ARG	CB-CG-CD	5.41	125.67	111.60
2	0	145	ARG	O-C-N	-5.41	110.82	121.10
2	Q	145	ARG	O-C-N	-5.41	110.83	121.10
3	R	211	LEU	C-N-CA	5.41	135.22	121.70
3	7	226	ASP	CB-CG-OD1	5.41	123.17	118.30
3	C	381	GLN	CA-CB-CG	5.41	125.30	113.40
3	Y	226	ASP	CB-CG-OD1	5.41	123.17	118.30
3	Y	496	PHE	CB-CG-CD1	5.41	124.58	120.80
3	4	145	PRO	CA-N-CD	-5.41	103.93	111.50
3	7	187	ARG	CB-CG-CD	5.41	125.66	111.60
3	4	381	GLN	CA-CB-CG	5.41	125.29	113.40
1	D	1	MET	CB-CG-SD	5.40	128.61	112.40
1	A	1	MET	CB-CG-SD	5.40	128.60	112.40
3	F	211	LEU	C-N-CA	5.40	135.20	121.70
3	R	381	GLN	CA-CB-CG	5.40	125.28	113.40
3	7	211	LEU	C-N-CA	5.40	135.20	121.70
3	U	145	PRO	CA-N-CD	-5.40	103.94	111.50
3	L	211	LEU	C-N-CA	5.40	135.20	121.70
1	8	1	MET	CB-CG-SD	5.40	128.60	112.40
1	G	1	MET	CB-CG-SD	5.40	128.59	112.40
1	2	32	TYR	CA-CB-CG	5.40	123.66	113.40
1	J	1	MET	CB-CG-SD	5.40	128.59	112.40
3	O	496	PHE	CB-CG-CD1	5.40	124.58	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1	MET	CB-CG-SD	5.40	128.59	112.40
3	C	496	PHE	CB-CG-CD1	5.39	124.58	120.80
3	I	211	LEU	C-N-CA	5.39	135.18	121.70
3	O	211	LEU	C-N-CA	5.39	135.19	121.70
3	L	381	GLN	CA-CB-CG	5.39	125.26	113.40
3	1	323	VAL	CA-CB-CG2	5.39	118.99	110.90
3	7	381	GLN	CA-CB-CG	5.39	125.26	113.40
3	7	496	PHE	CB-CG-CD1	5.39	124.57	120.80
2	9	145	ARG	O-C-N	-5.39	110.86	121.10
3	F	323	VAL	CA-CB-CG2	5.39	118.98	110.90
2	K	145	ARG	O-C-N	-5.39	110.86	121.10
2	T	145	ARG	O-C-N	-5.39	110.86	121.10
1	Z	1	MET	CB-CG-SD	5.39	128.57	112.40
2	B	145	ARG	O-C-N	-5.39	110.86	121.10
3	L	323	VAL	CA-CB-CG2	5.39	118.98	110.90
3	Y	381	GLN	CA-CB-CG	5.39	125.25	113.40
2	6	145	ARG	O-C-N	-5.39	110.86	121.10
3	C	323	VAL	CA-CB-CG2	5.39	118.98	110.90
3	F	83	GLY	C-N-CA	5.38	135.16	121.70
3	4	323	VAL	CA-CB-CG2	5.38	118.98	110.90
3	U	496	PHE	CB-CG-CD1	5.38	124.57	120.80
1	A	32	TYR	CA-CB-CG	5.38	123.62	113.40
1	M	32	TYR	CA-CB-CG	5.38	123.63	113.40
3	I	323	VAL	CA-CB-CG2	5.38	118.97	110.90
1	W	32	TYR	CA-CB-CG	5.38	123.62	113.40
3	Y	238	LEU	CB-CG-CD1	5.38	120.14	111.00
3	1	83	GLY	C-N-CA	5.38	135.15	121.70
3	V	323	VAL	CA-CB-CG2	5.38	118.97	110.90
3	7	83	GLY	C-N-CA	5.38	135.15	121.70
3	V	83	GLY	C-N-CA	5.38	135.14	121.70
3	1	226	ASP	CB-CG-OD1	5.38	123.14	118.30
1	8	32	TYR	CA-CB-CG	5.38	123.61	113.40
3	U	323	VAL	CA-CB-CG2	5.38	118.97	110.90
3	O	83	GLY	C-N-CA	5.38	135.14	121.70
3	7	323	VAL	CA-CB-CG2	5.38	118.96	110.90
3	L	83	GLY	C-N-CA	5.37	135.13	121.70
3	1	381	GLN	CA-CB-CG	5.37	125.22	113.40
2	3	145	ARG	O-C-N	-5.37	110.89	121.10
1	5	32	TYR	CA-CB-CG	5.37	123.61	113.40
2	X	145	ARG	O-C-N	-5.37	110.90	121.10
1	J	32	TYR	CA-CB-CG	5.37	123.60	113.40
1	P	32	TYR	CA-CB-CG	5.37	123.60	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	83	GLY	C-N-CA	5.37	135.12	121.70
2	N	145	ARG	O-C-N	-5.37	110.90	121.10
3	C	83	GLY	C-N-CA	5.37	135.11	121.70
3	R	496	PHE	CB-CG-CD1	5.37	124.56	120.80
3	I	226	ASP	CB-CG-OD1	5.36	123.13	118.30
3	Y	83	GLY	C-N-CA	5.36	135.11	121.70
3	U	83	GLY	C-N-CA	5.36	135.11	121.70
1	D	32	TYR	CA-CB-CG	5.36	123.58	113.40
3	C	226	ASP	CB-CG-OD1	5.36	123.12	118.30
3	R	226	ASP	CB-CG-OD1	5.36	123.12	118.30
3	I	83	GLY	C-N-CA	5.36	135.10	121.70
1	S	32	TYR	CA-CB-CG	5.36	123.58	113.40
3	U	238	LEU	CB-CG-CD1	5.36	120.11	111.00
1	G	32	TYR	CA-CB-CG	5.36	123.58	113.40
3	R	238	LEU	CB-CG-CD1	5.36	120.11	111.00
1	Z	32	TYR	CA-CB-CG	5.36	123.58	113.40
3	L	238	LEU	CB-CG-CD1	5.35	120.10	111.00
3	O	238	LEU	CB-CG-CD1	5.35	120.10	111.00
3	1	238	LEU	CB-CG-CD1	5.35	120.09	111.00
3	4	83	GLY	C-N-CA	5.35	135.07	121.70
3	4	238	LEU	CB-CG-CD1	5.35	120.09	111.00
3	F	226	ASP	CB-CG-OD1	5.35	123.11	118.30
3	V	226	ASP	CB-CG-OD1	5.35	123.11	118.30
3	C	238	LEU	CB-CG-CD1	5.35	120.09	111.00
1	G	78	PRO	CA-N-CD	-5.34	104.02	111.50
3	7	238	LEU	CB-CG-CD1	5.34	120.09	111.00
3	L	226	ASP	CB-CG-OD1	5.34	123.11	118.30
3	I	238	LEU	CB-CG-CD1	5.34	120.08	111.00
3	7	412	ILE	CG1-CB-CG2	5.34	123.15	111.40
3	I	412	ILE	CG1-CB-CG2	5.34	123.15	111.40
3	V	238	LEU	CB-CG-CD1	5.34	120.08	111.00
3	7	144	SER	CA-CB-OG	5.34	125.62	111.20
1	D	78	PRO	CA-N-CD	-5.34	104.03	111.50
3	F	412	ILE	CG1-CB-CG2	5.34	123.14	111.40
3	O	205	TYR	CA-C-N	5.34	126.87	116.20
3	O	412	ILE	CG1-CB-CG2	5.33	123.14	111.40
3	F	144	SER	CA-CB-OG	5.33	125.59	111.20
3	L	412	ILE	CG1-CB-CG2	5.33	123.13	111.40
3	R	361	MET	CA-CB-CG	5.33	122.36	113.30
3	U	361	MET	CA-CB-CG	5.33	122.36	113.30
3	F	361	MET	CA-CB-CG	5.33	122.36	113.30
3	R	144	SER	CA-CB-OG	5.33	125.59	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	144	SER	CA-CB-OG	5.33	125.59	111.20
1	M	78	PRO	CA-N-CD	-5.33	104.04	111.50
3	U	144	SER	CA-CB-OG	5.33	125.59	111.20
3	U	205	TYR	CA-C-N	5.33	126.86	116.20
3	O	226	ASP	CB-CG-OD1	5.33	123.09	118.30
3	V	144	SER	CA-CB-OG	5.33	125.58	111.20
3	Y	144	SER	CA-CB-OG	5.33	125.58	111.20
3	1	144	SER	CA-CB-OG	5.33	125.58	111.20
1	5	78	PRO	CA-N-CD	-5.33	104.04	111.50
1	A	78	PRO	CA-N-CD	-5.33	104.05	111.50
3	C	412	ILE	CG1-CB-CG2	5.33	123.11	111.40
3	I	144	SER	CA-CB-OG	5.33	125.58	111.20
3	V	412	ILE	CG1-CB-CG2	5.33	123.11	111.40
1	Z	78	PRO	CA-N-CD	-5.33	104.04	111.50
3	U	412	ILE	CG1-CB-CG2	5.33	123.12	111.40
3	O	144	SER	CA-CB-OG	5.32	125.57	111.20
3	1	412	ILE	CG1-CB-CG2	5.32	123.11	111.40
1	2	78	PRO	CA-N-CD	-5.32	104.05	111.50
3	4	412	ILE	CG1-CB-CG2	5.32	123.11	111.40
3	F	238	LEU	CB-CG-CD1	5.32	120.05	111.00
3	4	361	MET	CA-CB-CG	5.32	122.35	113.30
3	C	144	SER	CA-CB-OG	5.32	125.56	111.20
3	V	205	TYR	CA-C-N	5.32	126.84	116.20
3	Y	412	ILE	CG1-CB-CG2	5.32	123.11	111.40
1	8	78	PRO	CA-N-CD	-5.32	104.05	111.50
3	L	462	ALA	N-CA-CB	5.32	117.55	110.10
3	R	205	TYR	CA-C-N	5.32	126.84	116.20
3	Y	205	TYR	CA-C-N	5.32	126.84	116.20
3	U	226	ASP	CB-CG-OD1	5.32	123.09	118.30
3	U	478	TYR	CE1-CZ-OH	5.32	134.46	120.10
3	C	205	TYR	CA-C-N	5.32	126.83	116.20
3	L	144	SER	CA-CB-OG	5.31	125.55	111.20
3	L	205	TYR	CA-C-N	5.31	126.83	116.20
1	J	78	PRO	CA-N-CD	-5.31	104.06	111.50
3	V	361	MET	CA-CB-CG	5.31	122.33	113.30
3	1	496	PHE	CB-CG-CD1	5.31	124.52	120.80
3	L	443	ARG	CA-CB-CG	5.31	125.08	113.40
3	4	226	ASP	CB-CG-OD1	5.31	123.08	118.30
1	P	78	PRO	CA-N-CD	-5.30	104.07	111.50
1	W	78	PRO	CA-N-CD	-5.30	104.07	111.50
3	Y	443	ARG	CA-CB-CG	5.30	125.07	113.40
3	1	443	ARG	CA-CB-CG	5.30	125.07	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	443	ARG	CA-CB-CG	5.30	125.07	113.40
3	C	478	TYR	CE1-CZ-OH	5.30	134.42	120.10
3	I	443	ARG	CA-CB-CG	5.30	125.07	113.40
3	O	443	ARG	CA-CB-CG	5.30	125.07	113.40
3	7	205	TYR	CA-C-N	5.30	126.81	116.20
3	C	361	MET	CA-CB-CG	5.30	122.31	113.30
3	R	443	ARG	CA-CB-CG	5.30	125.06	113.40
3	1	462	ALA	N-CA-CB	5.30	117.52	110.10
3	1	478	TYR	CE1-CZ-OH	5.30	134.41	120.10
3	4	443	ARG	CA-CB-CG	5.30	125.06	113.40
3	7	443	ARG	CA-CB-CG	5.30	125.06	113.40
3	V	478	TYR	CE1-CZ-OH	5.30	134.41	120.10
3	Y	478	TYR	CE1-CZ-OH	5.30	134.41	120.10
3	U	443	ARG	CA-CB-CG	5.30	125.06	113.40
3	I	361	MET	CA-CB-CG	5.30	122.31	113.30
3	L	478	TYR	CE1-CZ-OH	5.30	134.40	120.10
1	S	78	PRO	CA-N-CD	-5.30	104.08	111.50
3	V	443	ARG	CA-CB-CG	5.30	125.06	113.40
3	7	462	ALA	N-CA-CB	5.30	117.52	110.10
3	F	478	TYR	CE1-CZ-OH	5.30	134.40	120.10
3	I	205	TYR	CA-C-N	5.30	126.80	116.20
3	R	412	ILE	CG1-CB-CG2	5.30	123.05	111.40
3	4	462	ALA	N-CA-CB	5.30	117.52	110.10
3	O	478	TYR	CE1-CZ-OH	5.29	134.40	120.10
3	O	361	MET	CA-CB-CG	5.29	122.30	113.30
3	4	205	TYR	CA-C-N	5.29	126.79	116.20
3	F	205	TYR	CA-C-N	5.29	126.78	116.20
3	F	443	ARG	CA-CB-CG	5.29	125.04	113.40
3	4	478	TYR	CE1-CZ-OH	5.29	134.39	120.10
3	Y	361	MET	CA-CB-CG	5.29	122.29	113.30
3	7	361	MET	CA-CB-CG	5.29	122.29	113.30
3	7	478	TYR	CE1-CZ-OH	5.29	134.38	120.10
3	L	361	MET	CA-CB-CG	5.29	122.29	113.30
3	R	478	TYR	CE1-CZ-OH	5.29	134.38	120.10
3	R	462	ALA	N-CA-CB	5.29	117.50	110.10
3	U	462	ALA	N-CA-CB	5.29	117.50	110.10
3	F	462	ALA	N-CA-CB	5.29	117.50	110.10
3	I	462	ALA	N-CA-CB	5.29	117.50	110.10
3	1	205	TYR	CA-C-N	5.29	126.77	116.20
3	C	462	ALA	N-CA-CB	5.28	117.50	110.10
3	I	478	TYR	CE1-CZ-OH	5.28	134.37	120.10
3	Y	462	ALA	N-CA-CB	5.28	117.49	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	361	MET	CA-CB-CG	5.27	122.26	113.30
1	8	48	ARG	CG-CD-NE	5.27	122.87	111.80
1	G	48	ARG	CG-CD-NE	5.27	122.86	111.80
3	F	68	LEU	CA-CB-CG	5.26	127.41	115.30
3	O	462	ALA	N-CA-CB	5.26	117.47	110.10
1	2	48	ARG	CG-CD-NE	5.26	122.86	111.80
1	P	48	ARG	CG-CD-NE	5.26	122.85	111.80
1	5	48	ARG	CG-CD-NE	5.26	122.85	111.80
1	D	48	ARG	CG-CD-NE	5.26	122.84	111.80
1	J	48	ARG	CG-CD-NE	5.26	122.84	111.80
1	M	48	ARG	CG-CD-NE	5.26	122.84	111.80
3	1	68	LEU	CA-CB-CG	5.26	127.39	115.30
3	O	68	LEU	CA-CB-CG	5.25	127.39	115.30
3	V	462	ALA	N-CA-CB	5.25	117.46	110.10
1	A	48	ARG	CG-CD-NE	5.25	122.83	111.80
3	V	68	LEU	CA-CB-CG	5.25	127.38	115.30
1	S	48	ARG	CG-CD-NE	5.25	122.83	111.80
1	Z	48	ARG	CG-CD-NE	5.25	122.83	111.80
1	W	48	ARG	CG-CD-NE	5.25	122.83	111.80
3	L	68	LEU	CA-CB-CG	5.25	127.37	115.30
3	U	42	GLU	CA-CB-CG	5.25	124.94	113.40
3	C	68	LEU	CA-CB-CG	5.24	127.36	115.30
3	7	68	LEU	CA-CB-CG	5.24	127.36	115.30
3	I	108	MET	CB-CG-SD	-5.24	96.67	112.40
3	7	108	MET	CB-CG-SD	-5.24	96.67	112.40
3	R	68	LEU	CA-CB-CG	5.24	127.35	115.30
3	4	68	LEU	CA-CB-CG	5.24	127.35	115.30
3	L	108	MET	CB-CG-SD	-5.24	96.69	112.40
3	U	108	MET	CB-CG-SD	-5.24	96.69	112.40
3	I	68	LEU	CA-CB-CG	5.24	127.34	115.30
3	Y	68	LEU	CA-CB-CG	5.24	127.34	115.30
3	1	108	MET	CB-CG-SD	-5.23	96.70	112.40
3	4	108	MET	CB-CG-SD	-5.23	96.70	112.40
3	I	42	GLU	CA-CB-CG	5.23	124.91	113.40
3	C	108	MET	CB-CG-SD	-5.23	96.72	112.40
3	V	108	MET	CB-CG-SD	-5.23	96.72	112.40
3	U	68	LEU	CA-CB-CG	5.23	127.32	115.30
3	4	42	GLU	CA-CB-CG	5.23	124.90	113.40
3	O	108	MET	CB-CG-SD	-5.22	96.73	112.40
3	V	42	GLU	CA-CB-CG	5.22	124.90	113.40
3	Y	42	GLU	CA-CB-CG	5.22	124.89	113.40
3	F	108	MET	CB-CG-SD	-5.22	96.74	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	429	VAL	CA-CB-CG2	5.22	118.73	110.90
3	I	244	MET	CA-CB-CG	5.22	122.17	113.30
3	Y	108	MET	CB-CG-SD	-5.22	96.74	112.40
3	C	42	GLU	CA-CB-CG	5.22	124.88	113.40
3	F	42	GLU	CA-CB-CG	5.22	124.88	113.40
3	R	108	MET	CB-CG-SD	-5.22	96.75	112.40
1	D	57[A]	MET	CB-CG-SD	5.21	128.04	112.40
1	D	57[B]	MET	CB-CG-SD	5.21	128.04	112.40
3	R	244	MET	CA-CB-CG	5.21	122.17	113.30
3	R	42	GLU	CA-CB-CG	5.21	124.87	113.40
1	S	57[A]	MET	CB-CG-SD	5.21	128.03	112.40
1	S	57[B]	MET	CB-CG-SD	5.21	128.03	112.40
3	1	244	MET	CA-CB-CG	5.21	122.16	113.30
3	7	244	MET	CA-CB-CG	5.21	122.16	113.30
3	1	42	GLU	CA-CB-CG	5.21	124.86	113.40
3	L	443	ARG	CG-CD-NE	5.21	122.74	111.80
3	O	42	GLU	CA-CB-CG	5.21	124.86	113.40
3	I	429	VAL	CA-CB-CG2	5.21	118.71	110.90
3	L	42	GLU	CA-CB-CG	5.21	124.85	113.40
3	U	429	VAL	CA-CB-CG2	5.21	118.71	110.90
3	C	244	MET	CA-CB-CG	5.21	122.15	113.30
1	G	57[A]	MET	CB-CG-SD	5.21	128.01	112.40
1	G	57[B]	MET	CB-CG-SD	5.21	128.01	112.40
3	7	42	GLU	CA-CB-CG	5.20	124.85	113.40
3	7	429	VAL	CA-CB-CG2	5.20	118.71	110.90
3	L	429	VAL	CA-CB-CG2	5.20	118.70	110.90
3	R	443	ARG	CG-CD-NE	5.20	122.72	111.80
3	V	244	MET	CA-CB-CG	5.20	122.14	113.30
1	A	57[A]	MET	CB-CG-SD	5.20	128.00	112.40
1	A	57[B]	MET	CB-CG-SD	5.20	128.00	112.40
3	F	443	ARG	CG-CD-NE	5.20	122.72	111.80
3	4	429	VAL	CA-CB-CG2	5.20	118.70	110.90
3	U	244	MET	CA-CB-CG	5.20	122.14	113.30
3	F	429	VAL	CA-CB-CG2	5.20	118.70	110.90
1	J	57[A]	MET	CB-CG-SD	5.20	127.99	112.40
1	J	57[B]	MET	CB-CG-SD	5.20	127.99	112.40
3	L	244	MET	CA-CB-CG	5.20	122.14	113.30
3	O	443	ARG	CG-CD-NE	5.20	122.72	111.80
1	P	57[A]	MET	CB-CG-SD	5.20	127.99	112.40
1	P	57[B]	MET	CB-CG-SD	5.20	127.99	112.40
3	C	429	VAL	CA-CB-CG2	5.20	118.69	110.90
3	L	186	LEU	CA-CB-CG	5.20	127.25	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	57[A]	MET	CB-CG-SD	5.20	127.99	112.40
1	2	57[B]	MET	CB-CG-SD	5.20	127.99	112.40
3	4	244	MET	CA-CB-CG	5.20	122.13	113.30
3	4	250	VAL	C-N-CA	5.19	134.69	121.70
1	5	57[A]	MET	CB-CG-SD	5.19	127.98	112.40
1	5	57[B]	MET	CB-CG-SD	5.19	127.98	112.40
3	F	244	MET	CA-CB-CG	5.19	122.13	113.30
3	O	429	VAL	CA-CB-CG2	5.19	118.69	110.90
3	R	250	VAL	C-N-CA	5.19	134.68	121.70
1	W	57[A]	MET	CB-CG-SD	5.19	127.98	112.40
1	W	57[B]	MET	CB-CG-SD	5.19	127.98	112.40
3	1	186	LEU	CA-CB-CG	5.19	127.24	115.30
3	4	443	ARG	CG-CD-NE	5.19	122.70	111.80
1	M	57[A]	MET	CB-CG-SD	5.19	127.97	112.40
1	M	57[B]	MET	CB-CG-SD	5.19	127.97	112.40
3	V	443	ARG	CG-CD-NE	5.19	122.70	111.80
1	Z	57[A]	MET	CB-CG-SD	5.19	127.97	112.40
1	Z	57[B]	MET	CB-CG-SD	5.19	127.97	112.40
3	1	429	VAL	CA-CB-CG2	5.19	118.69	110.90
2	9	121	LYS	CD-CE-NZ	-5.19	99.76	111.70
3	C	443	ARG	CG-CD-NE	5.19	122.70	111.80
3	O	186	LEU	CA-CB-CG	5.19	127.23	115.30
3	R	429	VAL	CA-CB-CG2	5.19	118.68	110.90
3	L	149	TYR	CG-CD1-CE1	5.19	125.45	121.30
3	V	149	TYR	CG-CD1-CE1	5.19	125.45	121.30
3	V	429	VAL	CA-CB-CG2	5.19	118.68	110.90
3	7	443	ARG	CG-CD-NE	5.19	122.69	111.80
1	8	57[A]	MET	CB-CG-SD	5.19	127.96	112.40
1	8	57[B]	MET	CB-CG-SD	5.19	127.96	112.40
3	Y	443	ARG	CG-CD-NE	5.18	122.69	111.80
3	L	250	VAL	C-N-CA	5.18	134.66	121.70
3	O	244	MET	CA-CB-CG	5.18	122.11	113.30
3	Y	250	VAL	C-N-CA	5.18	134.65	121.70
3	U	443	ARG	CG-CD-NE	5.18	122.68	111.80
3	C	250	VAL	C-N-CA	5.18	134.65	121.70
3	F	250	VAL	C-N-CA	5.18	134.65	121.70
3	I	152	LEU	CB-CG-CD2	5.18	119.81	111.00
3	O	250	VAL	C-N-CA	5.18	134.65	121.70
3	7	250	VAL	C-N-CA	5.18	134.65	121.70
3	V	250	VAL	C-N-CA	5.18	134.64	121.70
3	Y	244	MET	CA-CB-CG	5.18	122.10	113.30
3	R	186	LEU	CA-CB-CG	5.17	127.20	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	121	LYS	CD-CE-NZ	-5.17	99.80	111.70
3	V	152	LEU	CB-CG-CD2	5.17	119.79	111.00
3	1	250	VAL	C-N-CA	5.17	134.63	121.70
3	1	443	ARG	CG-CD-NE	5.17	122.66	111.80
3	4	152	LEU	CB-CG-CD2	5.17	119.79	111.00
3	U	250	VAL	C-N-CA	5.17	134.63	121.70
3	C	186	LEU	CA-CB-CG	5.17	127.19	115.30
3	I	186	LEU	CA-CB-CG	5.17	127.19	115.30
3	7	186	LEU	CA-CB-CG	5.17	127.19	115.30
3	I	443	ARG	CG-CD-NE	5.17	122.65	111.80
3	V	25	ASP	CB-CG-OD2	-5.17	113.65	118.30
3	Y	152	LEU	CB-CG-CD2	5.17	119.79	111.00
2	B	121	LYS	CD-CE-NZ	-5.17	99.82	111.70
2	K	121	LYS	CD-CE-NZ	-5.17	99.81	111.70
3	L	503	ASP	CB-CG-OD2	5.17	122.95	118.30
2	0	121	LYS	CD-CE-NZ	-5.17	99.82	111.70
3	4	186	LEU	CA-CB-CG	5.17	127.18	115.30
2	Q	121	LYS	CD-CE-NZ	-5.17	99.82	111.70
3	I	250	VAL	C-N-CA	5.16	134.61	121.70
3	I	503	ASP	CB-CG-OD2	5.16	122.95	118.30
3	V	186	LEU	CA-CB-CG	5.16	127.17	115.30
3	Y	186	LEU	CA-CB-CG	5.16	127.17	115.30
3	F	186	LEU	CA-CB-CG	5.16	127.17	115.30
3	1	503	ASP	CB-CG-OD2	5.16	122.94	118.30
2	N	121	LYS	CD-CE-NZ	-5.16	99.83	111.70
2	6	121	LYS	CD-CE-NZ	-5.16	99.84	111.70
3	U	186	LEU	CA-CB-CG	5.16	127.16	115.30
3	O	503	ASP	CB-CG-OD2	5.16	122.94	118.30
2	H	121	LYS	CD-CE-NZ	-5.15	99.85	111.70
3	F	152	LEU	CB-CG-CD2	5.15	119.76	111.00
3	F	503	ASP	CB-CG-OD2	5.15	122.94	118.30
2	X	121	LYS	CD-CE-NZ	-5.15	99.85	111.70
2	3	121	LYS	CD-CE-NZ	-5.15	99.85	111.70
2	E	121	LYS	CD-CE-NZ	-5.15	99.85	111.70
3	R	152	LEU	CB-CG-CD2	5.15	119.76	111.00
3	R	503	ASP	CB-CG-OD2	5.15	122.94	118.30
3	C	152	LEU	CB-CG-CD2	5.15	119.75	111.00
3	1	152	LEU	CB-CG-CD2	5.15	119.75	111.00
3	O	152	LEU	CB-CG-CD2	5.15	119.75	111.00
3	L	152	LEU	CB-CG-CD2	5.14	119.74	111.00
3	V	376	TRP	CA-CB-CG	5.14	123.46	113.70
3	1	25	ASP	CB-CG-OD2	-5.14	113.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	149	TYR	CG-CD1-CE1	5.14	125.41	121.30
3	U	503	ASP	CB-CG-OD2	5.14	122.92	118.30
3	L	376	TRP	CA-CB-CG	5.13	123.45	113.70
3	7	376	TRP	CA-CB-CG	5.13	123.46	113.70
3	U	25	ASP	CB-CG-OD2	-5.13	113.68	118.30
3	4	25	ASP	CB-CG-OD2	-5.13	113.69	118.30
3	U	152	LEU	CB-CG-CD2	5.13	119.72	111.00
3	C	503	ASP	CB-CG-OD2	5.12	122.91	118.30
3	F	25	ASP	CB-CG-OD2	-5.12	113.69	118.30
3	R	376	TRP	CA-CB-CG	5.12	123.44	113.70
3	1	376	TRP	CA-CB-CG	5.12	123.44	113.70
3	C	376	TRP	CA-CB-CG	5.12	123.43	113.70
3	I	364	SER	N-CA-CB	5.12	118.18	110.50
3	I	376	TRP	CA-CB-CG	5.12	123.43	113.70
3	7	152	LEU	CB-CG-CD2	5.12	119.71	111.00
3	F	376	TRP	CA-CB-CG	5.12	123.43	113.70
3	Y	376	TRP	CA-CB-CG	5.12	123.43	113.70
3	L	25	ASP	CB-CG-OD2	-5.12	113.69	118.30
3	O	376	TRP	CA-CB-CG	5.12	123.42	113.70
3	R	149	TYR	CG-CD1-CE1	5.12	125.39	121.30
3	Y	571	PHE	CB-CG-CD1	-5.11	117.22	120.80
3	L	364	SER	N-CA-CB	5.11	118.17	110.50
3	7	364	SER	N-CA-CB	5.11	118.17	110.50
3	F	149	TYR	CG-CD1-CE1	5.11	125.39	121.30
3	C	25	ASP	CB-CG-OD2	-5.11	113.71	118.30
3	4	376	TRP	CA-CB-CG	5.11	123.40	113.70
3	C	364	SER	N-CA-CB	5.10	118.16	110.50
3	O	25	ASP	CB-CG-OD2	-5.10	113.71	118.30
3	Y	364	SER	N-CA-CB	5.10	118.16	110.50
3	U	364	SER	N-CA-CB	5.10	118.15	110.50
3	V	364	SER	N-CA-CB	5.10	118.15	110.50
3	F	364	SER	N-CA-CB	5.10	118.15	110.50
3	V	503	ASP	CB-CG-OD2	5.10	122.89	118.30
3	U	149	TYR	CG-CD1-CE1	5.10	125.38	121.30
3	U	376	TRP	CA-CB-CG	5.10	123.38	113.70
3	C	149	TYR	CG-CD1-CE1	5.10	125.38	121.30
3	R	25	ASP	CB-CG-OD2	-5.10	113.71	118.30
3	R	364	SER	N-CA-CB	5.10	118.14	110.50
3	O	364	SER	N-CA-CB	5.09	118.14	110.50
3	F	571	PHE	CB-CG-CD1	-5.09	117.24	120.80
3	Y	25	ASP	CB-CG-OD2	-5.09	113.72	118.30
3	Y	503	ASP	CB-CG-OD2	5.09	122.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7	503	ASP	CB-CG-OD2	5.09	122.88	118.30
3	4	364	SER	N-CA-CB	5.09	118.13	110.50
3	4	199	LEU	C-N-CA	5.09	132.98	122.30
3	1	364	SER	N-CA-CB	5.08	118.13	110.50
3	7	25	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	J	10	LYS	CD-CE-NZ	5.08	123.39	111.70
3	7	199	LEU	C-N-CA	5.08	132.97	122.30
1	Z	10	LYS	CD-CE-NZ	5.08	123.39	111.70
3	1	199	LEU	C-N-CA	5.08	132.97	122.30
1	S	10	LYS	CD-CE-NZ	5.08	123.39	111.70
1	2	10	LYS	CD-CE-NZ	5.08	123.38	111.70
3	I	25	ASP	CB-CG-OD2	-5.08	113.73	118.30
3	I	509	LYS	CB-CG-CD	5.07	124.79	111.60
3	R	199	LEU	C-N-CA	5.07	132.96	122.30
1	5	10	LYS	CD-CE-NZ	5.07	123.37	111.70
1	A	10	LYS	CD-CE-NZ	5.07	123.36	111.70
1	P	10	LYS	CD-CE-NZ	5.07	123.36	111.70
3	V	509	LYS	CB-CG-CD	5.07	124.78	111.60
3	F	509	LYS	CB-CG-CD	5.07	124.78	111.60
3	I	149	TYR	CG-CD1-CE1	5.07	125.36	121.30
1	M	10	LYS	CD-CE-NZ	5.07	123.35	111.70
3	V	199	LEU	C-N-CA	5.07	132.94	122.30
3	4	509	LYS	CB-CG-CD	5.06	124.77	111.60
1	D	10	LYS	CD-CE-NZ	5.06	123.34	111.70
3	L	199	LEU	C-N-CA	5.06	132.93	122.30
3	V	571	PHE	CB-CG-CD1	-5.06	117.26	120.80
3	1	509	LYS	CB-CG-CD	5.06	124.76	111.60
3	7	509	LYS	CB-CG-CD	5.06	124.76	111.60
2	Q	141	PRO	N-CA-C	-5.06	98.94	112.10
1	W	10	LYS	CD-CE-NZ	5.06	123.34	111.70
3	C	199	LEU	C-N-CA	5.06	132.92	122.30
3	C	509	LYS	CB-CG-CD	5.06	124.75	111.60
2	K	141	PRO	N-CA-C	-5.06	98.95	112.10
2	T	141	PRO	N-CA-C	-5.06	98.95	112.10
3	O	509	LYS	CB-CG-CD	5.06	124.75	111.60
2	N	61	ARG	NE-CZ-NH1	5.05	122.83	120.30
3	O	149	TYR	CG-CD1-CE1	5.05	125.34	121.30
3	Y	509	LYS	CB-CG-CD	5.05	124.74	111.60
3	4	503	ASP	CB-CG-OD2	5.05	122.85	118.30
3	Y	149	TYR	CG-CD1-CE1	5.05	125.34	121.30
3	O	199	LEU	C-N-CA	5.05	132.91	122.30
3	R	509	LYS	CB-CG-CD	5.05	124.73	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	199	LEU	C-N-CA	5.05	132.91	122.30
2	6	141	PRO	N-CA-C	-5.05	98.97	112.10
2	E	141	PRO	N-CA-C	-5.05	98.97	112.10
3	L	509	LYS	CB-CG-CD	5.05	124.73	111.60
3	U	509	LYS	CB-CG-CD	5.05	124.73	111.60
3	U	199	LEU	C-N-CA	5.05	132.90	122.30
3	7	571	PHE	CB-CG-CD1	-5.05	117.27	120.80
1	8	10	LYS	CD-CE-NZ	5.05	123.31	111.70
3	F	199	LEU	C-N-CA	5.04	132.89	122.30
3	7	149	TYR	CG-CD1-CE1	5.04	125.34	121.30
2	B	141	PRO	N-CA-C	-5.04	98.98	112.10
2	0	141	PRO	N-CA-C	-5.04	98.98	112.10
2	H	141	PRO	N-CA-C	-5.04	98.99	112.10
3	L	571	PHE	CB-CG-CD1	-5.04	117.27	120.80
2	N	141	PRO	N-CA-C	-5.04	98.99	112.10
3	O	571	PHE	CB-CG-CD1	-5.04	117.27	120.80
3	1	571	PHE	CB-CG-CD1	-5.04	117.27	120.80
2	3	141	PRO	N-CA-C	-5.04	98.99	112.10
3	F	434[A]	MET	C-N-CA	-5.04	109.10	121.70
3	F	434[B]	MET	C-N-CA	-5.04	109.10	121.70
3	R	434[A]	MET	C-N-CA	-5.04	109.10	121.70
3	R	434[B]	MET	C-N-CA	-5.04	109.10	121.70
3	1	434[A]	MET	C-N-CA	-5.04	109.10	121.70
3	1	434[B]	MET	C-N-CA	-5.04	109.10	121.70
3	I	199	LEU	C-N-CA	5.04	132.88	122.30
2	X	141	PRO	N-CA-C	-5.04	99.00	112.10
3	U	420	GLN	CA-CB-CG	5.04	124.48	113.40
2	9	141	PRO	N-CA-C	-5.04	99.01	112.10
1	G	10	LYS	CD-CE-NZ	5.03	123.28	111.70
3	O	530	LEU	CB-CG-CD2	5.03	119.56	111.00
3	7	420	GLN	CA-CB-CG	5.03	124.47	113.40
3	L	434[A]	MET	C-N-CA	-5.03	109.12	121.70
3	L	434[B]	MET	C-N-CA	-5.03	109.12	121.70
3	C	571	PHE	CB-CG-CD1	-5.03	117.28	120.80
3	1	420	GLN	CA-CB-CG	5.03	124.46	113.40
3	4	434[A]	MET	C-N-CA	-5.03	109.14	121.70
3	4	434[B]	MET	C-N-CA	-5.03	109.14	121.70
3	I	434[A]	MET	C-N-CA	-5.02	109.14	121.70
3	I	434[B]	MET	C-N-CA	-5.02	109.14	121.70
3	1	149	TYR	CG-CD1-CE1	5.02	125.32	121.30
3	R	420	GLN	CA-CB-CG	5.02	124.45	113.40
2	3	61	ARG	NE-CZ-NH1	5.02	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7	156	VAL	C-N-CA	5.02	134.26	121.70
3	7	434[A]	MET	C-N-CA	-5.02	109.14	121.70
3	7	434[B]	MET	C-N-CA	-5.02	109.14	121.70
3	U	434[A]	MET	C-N-CA	-5.02	109.15	121.70
3	U	434[B]	MET	C-N-CA	-5.02	109.15	121.70
3	C	434[A]	MET	C-N-CA	-5.02	109.15	121.70
3	C	434[B]	MET	C-N-CA	-5.02	109.15	121.70
3	V	434[A]	MET	C-N-CA	-5.02	109.15	121.70
3	V	434[B]	MET	C-N-CA	-5.02	109.15	121.70
3	Y	156	VAL	C-N-CA	5.02	134.25	121.70
3	C	420	GLN	CA-CB-CG	5.02	124.44	113.40
3	F	156	VAL	C-N-CA	5.02	134.25	121.70
3	O	420	GLN	CA-CB-CG	5.02	124.44	113.40
3	R	571	PHE	CB-CG-CD1	-5.02	117.29	120.80
3	Y	420	GLN	CA-CB-CG	5.02	124.44	113.40
3	F	530	LEU	CB-CG-CD2	5.02	119.53	111.00
3	R	530	LEU	CB-CG-CD2	5.02	119.53	111.00
3	U	299	LEU	CB-CG-CD1	5.02	119.53	111.00
3	L	420	GLN	CA-CB-CG	5.02	124.44	113.40
3	O	156	VAL	C-N-CA	5.02	134.24	121.70
3	V	420	GLN	CA-CB-CG	5.02	124.44	113.40
3	U	571	PHE	CB-CG-CD1	-5.02	117.29	120.80
3	O	434[A]	MET	C-N-CA	-5.01	109.17	121.70
3	O	434[B]	MET	C-N-CA	-5.01	109.17	121.70
3	V	156	VAL	C-N-CA	5.01	134.24	121.70
3	Y	530	LEU	CB-CG-CD2	5.01	119.52	111.00
3	4	420	GLN	CA-CB-CG	5.01	124.43	113.40
3	U	156	VAL	C-N-CA	5.01	134.24	121.70
3	F	299	LEU	CB-CG-CD1	5.01	119.52	111.00
2	H	61	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	K	61	ARG	NE-CZ-NH1	5.01	122.81	120.30
3	4	530	LEU	CB-CG-CD2	5.01	119.52	111.00
3	L	299	LEU	CB-CG-CD1	5.01	119.52	111.00
1	Z	91	ARG	CA-CB-CG	5.01	124.42	113.40
1	5	91	ARG	CA-CB-CG	5.01	124.42	113.40
3	C	156	VAL	C-N-CA	5.01	134.22	121.70
3	C	530	LEU	CB-CG-CD2	5.01	119.52	111.00
3	F	406[A]	LEU	CA-CB-CG	5.01	126.82	115.30
3	F	406[B]	LEU	CA-CB-CG	5.01	126.82	115.30
3	L	530	LEU	CB-CG-CD2	5.01	119.52	111.00
1	M	91	ARG	CA-CB-CG	5.01	124.42	113.40
3	V	530	LEU	CB-CG-CD2	5.01	119.52	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	91	ARG	CA-CB-CG	5.01	124.42	113.40
3	R	299	LEU	CB-CG-CD1	5.01	119.51	111.00
3	Y	299	LEU	CB-CG-CD1	5.01	119.51	111.00
3	Y	420	GLN	C-N-CA	5.01	132.82	122.30
3	Y	434[A]	MET	C-N-CA	-5.01	109.18	121.70
3	Y	434[B]	MET	C-N-CA	-5.01	109.18	121.70
1	D	91	ARG	CA-CB-CG	5.01	124.41	113.40
3	F	420	GLN	CA-CB-CG	5.01	124.42	113.40
3	I	571	PHE	CB-CG-CD1	-5.01	117.30	120.80
3	1	299	LEU	CB-CG-CD1	5.01	119.51	111.00
3	7	530	LEU	CB-CG-CD2	5.01	119.51	111.00
1	S	91	ARG	CA-CB-CG	5.00	124.41	113.40
3	Y	406[A]	LEU	CA-CB-CG	5.00	126.81	115.30
3	Y	406[B]	LEU	CA-CB-CG	5.00	126.81	115.30
3	O	406[A]	LEU	CA-CB-CG	5.00	126.81	115.30
3	O	406[B]	LEU	CA-CB-CG	5.00	126.81	115.30
3	V	299	LEU	CB-CG-CD1	5.00	119.50	111.00
3	1	156	VAL	C-N-CA	5.00	134.21	121.70
1	2	91	ARG	CA-CB-CG	5.00	124.41	113.40
3	4	406[A]	LEU	CA-CB-CG	5.00	126.81	115.30
3	4	406[B]	LEU	CA-CB-CG	5.00	126.81	115.30
1	A	91	ARG	CA-CB-CG	5.00	124.40	113.40
3	C	299	LEU	CB-CG-CD1	5.00	119.50	111.00
3	V	478	TYR	CG-CD2-CE2	5.00	125.30	121.30
3	4	299	LEU	CB-CG-CD1	5.00	119.50	111.00
3	U	530	LEU	CB-CG-CD2	5.00	119.50	111.00

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	1	287	PRO	Peptide
1	2	15	THR	Mainchain
3	4	287	PRO	Peptide
1	5	15	THR	Mainchain
3	7	287	PRO	Peptide
1	8	15	THR	Mainchain
1	A	15	THR	Mainchain
3	C	287	PRO	Peptide
1	D	15	THR	Mainchain
3	F	287	PRO	Peptide
1	G	15	THR	Mainchain

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Mol	Chain	Res	Type	Group
3	I	287	PRO	Peptide
1	J	15	THR	Mainchain
3	L	287	PRO	Peptide
1	M	15	THR	Mainchain
3	O	287	PRO	Peptide
1	P	15	THR	Mainchain
3	R	287	PRO	Peptide
1	S	15	THR	Mainchain
3	U	287	PRO	Peptide
3	V	287	PRO	Peptide
1	W	15	THR	Mainchain
3	Y	287	PRO	Peptide
1	Z	15	THR	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	805	856	818	8	0
1	5	805	856	818	4	0
1	8	805	856	818	6	0
1	A	805	856	818	3	0
1	D	805	856	818	5	0
1	G	805	856	818	6	0
1	J	805	856	818	3	0
1	M	805	856	818	3	0
1	P	805	856	818	3	0
1	S	805	856	818	10	0
1	W	805	856	818	4	0
1	Z	805	856	818	3	0
2	0	1042	1019	1008	9	0
2	3	1042	1019	1008	10	0
2	6	1042	1019	1008	8	0
2	9	1042	1019	1008	7	0
2	B	1042	1019	1008	7	0
2	E	1042	1019	1008	6	0
2	H	1042	1019	1008	6	0
2	K	1042	1019	1008	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	1042	1019	1008	7	0
2	Q	1042	1019	1008	11	0
2	T	1042	1019	1008	7	0
2	X	1042	1019	1008	6	0
3	1	4271	4222	4151	43	0
3	4	4271	4222	4151	40	0
3	7	4271	4222	4151	43	0
3	C	4271	4222	4151	41	0
3	F	4271	4222	4151	37	0
3	I	4271	4222	4151	40	0
3	L	4271	4222	4151	54	0
3	O	4271	4222	4152	43	0
3	R	4271	4222	4151	52	0
3	U	4271	4222	4152	41	0
3	V	4271	4222	4152	40	0
3	Y	4271	4222	4151	43	0
4	1	2	0	0	0	0
4	4	2	0	0	0	0
4	7	2	0	0	0	0
4	C	2	0	0	0	0
4	F	2	0	0	0	0
4	I	2	0	0	0	0
4	L	2	0	0	0	0
4	O	2	0	0	0	0
4	R	2	0	0	0	0
4	U	2	0	0	0	0
4	V	2	0	0	0	0
4	Y	2	0	0	0	0
5	0	57	0	0	2	0
5	1	224	0	0	6	0
5	2	25	0	0	0	0
5	3	57	0	0	2	0
5	4	216	0	0	5	0
5	5	25	0	0	0	0
5	6	57	0	0	3	0
5	7	220	0	0	6	0
5	8	25	0	0	0	0
5	9	56	0	0	2	0
5	A	25	0	0	0	0
5	B	59	0	0	2	0
5	C	224	0	0	6	0
5	D	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	59	0	0	2	0
5	F	225	0	0	5	0
5	G	27	0	0	0	0
5	H	58	0	0	3	0
5	I	227	0	0	7	0
5	J	25	0	0	0	0
5	K	59	0	0	2	0
5	L	227	0	0	9	0
5	M	25	0	0	0	0
5	N	57	0	0	6	0
5	O	222	0	0	7	0
5	P	25	0	0	0	0
5	Q	57	0	0	2	0
5	R	216	0	0	7	0
5	S	25	0	0	0	0
5	T	58	0	0	2	0
5	U	223	0	0	9	0
5	V	227	0	0	7	0
5	W	25	0	0	0	0
5	X	58	0	0	2	0
5	Y	226	0	0	7	0
5	Z	26	0	0	0	0
All	All	77112	73164	71727	565	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 4.

All (565) 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)
2:9:141:PRO:N	2:9:141:PRO:CA	1.70	1.48
2:E:141:PRO:N	2:E:141:PRO:CA	1.70	1.47
2:6:141:PRO:N	2:6:141:PRO:CA	1.70	1.46
2:N:141:PRO:N	2:N:141:PRO:CA	1.70	1.45
2:X:141:PRO:N	2:X:141:PRO:CA	1.70	1.44
2:B:141:PRO:N	2:B:141:PRO:CA	1.70	1.43
2:H:141:PRO:N	2:H:141:PRO:CA	1.70	1.42
2:3:141:PRO:CA	2:3:141:PRO:N	1.70	1.39
2:T:141:PRO:N	2:T:141:PRO:CA	1.70	1.38
2:Q:141:PRO:N	2:Q:141:PRO:CA	1.70	1.37
2:K:141:PRO:N	2:K:141:PRO:CA	1.70	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:PRO:N	3:C:179:PRO:CA	1.68	1.33
2:0:141:PRO:N	2:0:141:PRO:CA	1.70	1.33
3:L:487:LYS:HE3	3:R:511:GLY:O	1.57	1.03
3:L:167:THR:OG1	3:V:122:ASP:OD2	1.89	0.89
3:C:511:GLY:O	3:Y:487:LYS:HE3	1.78	0.83
3:L:491:ASP:OD2	3:R:187:ARG:NE	2.14	0.81
3:F:122:ASP:OD2	3:Y:167:THR:OG1	2.00	0.78
2:Q:79:VAL:HG21	2:Q:83:LEU:HD12	1.72	0.72
2:0:79:VAL:HG21	2:0:83:LEU:HD12	1.72	0.72
3:L:123:ALA:HB3	5:L:853:HOH:O	1.89	0.72
2:9:79:VAL:HG21	2:9:83:LEU:HD12	1.72	0.72
3:O:511:GLY:O	3:7:487:LYS:HE3	1.89	0.71
2:T:79:VAL:HG21	2:T:83:LEU:HD12	1.72	0.71
2:B:79:VAL:HG21	2:B:83:LEU:HD12	1.72	0.71
3:1:123:ALA:HB3	5:1:862:HOH:O	1.90	0.71
3:I:487:LYS:HE3	3:4:511:GLY:O	1.90	0.71
2:N:79:VAL:HG21	2:N:83:LEU:HD12	1.72	0.71
2:X:79:VAL:HG21	2:X:83:LEU:HD12	1.72	0.71
2:H:79:VAL:HG21	2:H:83:LEU:HD12	1.72	0.71
2:6:79:VAL:HG21	2:6:83:LEU:HD12	1.72	0.70
3:C:487:LYS:HE3	3:F:511:GLY:O	1.92	0.70
3:I:123:ALA:HB3	5:I:856:HOH:O	1.91	0.70
2:3:79:VAL:HG21	2:3:83:LEU:HD12	1.72	0.70
3:R:53:ASP:OD2	3:V:203:ASN:HB3	1.92	0.70
2:K:79:VAL:HG21	2:K:83:LEU:HD12	1.72	0.69
2:E:79:VAL:HG21	2:E:83:LEU:HD12	1.72	0.69
2:6:141:PRO:N	2:6:141:PRO:C	2.46	0.69
2:X:141:PRO:N	2:X:141:PRO:C	2.46	0.69
3:O:203:ASN:HB3	3:7:53:ASP:OD2	1.93	0.69
3:R:181:ASN:OD1	5:R:701:HOH:O	2.11	0.69
5:O:865:HOH:O	3:7:123:ALA:HB3	1.92	0.69
2:3:141:PRO:N	2:3:141:PRO:C	2.46	0.69
2:H:141:PRO:N	2:H:141:PRO:C	2.46	0.68
2:N:141:PRO:N	2:N:141:PRO:C	2.46	0.68
3:O:53:ASP:OD2	3:1:203:ASN:HB3	1.93	0.68
2:T:141:PRO:N	2:T:141:PRO:C	2.46	0.68
3:I:167:THR:OG1	3:U:122:ASP:OD2	2.08	0.68
2:Q:141:PRO:N	2:Q:141:PRO:C	2.46	0.68
3:U:408:TYR:O	3:U:411:LYS:HB2	1.94	0.68
3:C:408:TYR:O	3:C:411:LYS:HB2	1.94	0.68
3:F:408:TYR:O	3:F:411:LYS:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:408:TYR:O	3:4:411:LYS:HB2	1.94	0.68
2:E:141:PRO:N	2:E:141:PRO:C	2.46	0.68
2:9:141:PRO:N	2:9:141:PRO:C	2.46	0.68
3:V:408:TYR:O	3:V:411:LYS:HB2	1.94	0.68
3:7:408:TYR:O	3:7:411:LYS:HB2	1.94	0.67
2:B:141:PRO:N	2:B:141:PRO:C	2.46	0.67
3:I:408:TYR:O	3:I:411:LYS:HB2	1.94	0.67
3:R:408:TYR:O	3:R:411:LYS:HB2	1.94	0.67
3:Y:123:ALA:HB3	5:Y:853:HOH:O	1.95	0.67
3:Y:408:TYR:O	3:Y:411:LYS:HB2	1.94	0.67
3:1:408:TYR:O	3:1:411:LYS:HB2	1.94	0.67
3:L:408:TYR:O	3:L:411:LYS:HB2	1.94	0.67
3:Y:266:ASP:O	5:Y:701:HOH:O	2.12	0.67
3:O:408:TYR:O	3:O:411:LYS:HB2	1.94	0.66
2:K:141:PRO:N	2:K:141:PRO:C	2.46	0.66
1:D:45:GLU:OE1	1:W:26:ARG:NH2	2.26	0.66
2:K:146:PRO:HB3	5:N:252:HOH:O	1.96	0.66
2:0:141:PRO:N	2:0:141:PRO:C	2.46	0.65
5:L:868:HOH:O	3:V:119:VAL:HG22	1.96	0.65
3:4:53:ASP:OD2	3:U:203:ASN:HB3	1.96	0.65
1:J:26:ARG:NH2	1:S:45:GLU:OE1	2.24	0.64
3:4:123:ALA:HB3	5:U:865:HOH:O	1.97	0.64
3:L:266:ASP:OD1	2:0:134:TRP:HZ3	1.79	0.64
3:4:487:LYS:HE3	3:U:511:GLY:O	1.98	0.64
3:C:123:ALA:HB3	5:C:851:HOH:O	1.98	0.64
3:1:53:ASP:OD2	3:7:203:ASN:HB3	1.97	0.63
2:9:79:VAL:CG2	2:9:83:LEU:HD12	2.30	0.62
2:B:79:VAL:CG2	2:B:83:LEU:HD12	2.30	0.62
2:X:79:VAL:CG2	2:X:83:LEU:HD12	2.30	0.62
2:6:79:VAL:CG2	2:6:83:LEU:HD12	2.30	0.62
3:V:292:VAL:HG23	5:V:864:HOH:O	2.00	0.62
2:H:79:VAL:CG2	2:H:83:LEU:HD12	2.30	0.62
2:N:79:VAL:CG2	2:N:83:LEU:HD12	2.30	0.62
3:L:312:ASN:ND2	1:S:88:ASP:OD1	2.27	0.62
2:3:79:VAL:CG2	2:3:83:LEU:HD12	2.30	0.62
2:T:79:VAL:CG2	2:T:83:LEU:HD12	2.29	0.62
3:O:122:ASP:OD2	3:1:167:THR:OG1	2.15	0.61
2:E:79:VAL:CG2	2:E:83:LEU:HD12	2.30	0.61
3:L:292:VAL:HG23	5:L:867:HOH:O	2.00	0.61
3:O:487:LYS:HE3	3:1:511:GLY:O	2.00	0.61
2:Q:66:ARG:HB2	3:V:260:TYR:CE1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:292:VAL:HG23	5:R:867:HOH:O	2.00	0.61
3:1:292:VAL:HG23	5:1:868:HOH:O	2.00	0.61
3:U:292:VAL:HG23	5:U:864:HOH:O	2.00	0.61
3:I:292:VAL:HG23	5:I:869:HOH:O	2.00	0.61
2:O:79:VAL:CG2	2:O:83:LEU:HD12	2.30	0.61
2:K:79:VAL:CG2	2:K:83:LEU:HD12	2.30	0.61
3:O:292:VAL:HG23	5:O:863:HOH:O	2.00	0.61
3:4:292:VAL:HG23	5:4:862:HOH:O	2.00	0.61
3:C:292:VAL:HG23	5:C:868:HOH:O	2.00	0.61
3:Y:292:VAL:HG23	5:Y:867:HOH:O	2.00	0.60
1:Z:45:GLU:OE1	1:5:26:ARG:NH2	2.32	0.60
3:F:292:VAL:HG23	5:F:867:HOH:O	2.00	0.60
2:Q:79:VAL:CG2	2:Q:83:LEU:HD12	2.30	0.60
1:G:26:ARG:NH2	1:8:45:GLU:OE1	2.33	0.60
3:7:292:VAL:HG23	5:7:864:HOH:O	2.00	0.60
3:1:487:LYS:HE3	3:7:511:GLY:O	2.02	0.59
3:R:173:THR:HG22	3:R:224:HIS:CG	2.37	0.59
3:4:173:THR:HG22	3:4:224:HIS:CG	2.37	0.59
3:7:173:THR:HG22	3:7:224:HIS:CG	2.37	0.59
3:1:173:THR:HG22	3:1:224:HIS:CG	2.37	0.59
3:I:173:THR:HG22	3:I:224:HIS:CG	2.37	0.59
3:C:173:THR:HG22	3:C:224:HIS:CG	2.37	0.59
3:U:173:THR:HG22	3:U:224:HIS:CG	2.37	0.59
3:F:487:LYS:HE3	3:Y:511:GLY:O	2.02	0.59
3:L:173:THR:HG22	3:L:224:HIS:CG	2.37	0.59
3:V:173:THR:HG22	3:V:224:HIS:CG	2.37	0.59
3:F:173:THR:HG22	3:F:224:HIS:CG	2.37	0.59
3:L:491:ASP:CG	3:R:187:ARG:HH21	2.06	0.59
3:I:53:ASP:OD2	3:4:203:ASN:HB3	2.03	0.59
3:V:377:LEU:HD11	3:V:565:MET:O	2.03	0.59
3:U:377:LEU:HD11	3:U:565:MET:O	2.03	0.59
2:B:96:ASN:O	5:B:201:HOH:O	2.17	0.58
3:L:45:TYR:OH	3:R:173:THR:HG23	2.03	0.58
3:1:377:LEU:HD11	3:1:565:MET:O	2.03	0.58
2:K:134:TRP:HZ3	3:1:266:ASP:OD1	1.86	0.58
3:O:173:THR:HG22	3:O:224:HIS:CG	2.37	0.58
3:7:377:LEU:HD11	3:7:565:MET:O	2.03	0.58
2:H:96:ASN:O	5:H:201:HOH:O	2.17	0.58
3:I:377:LEU:HD11	3:I:565:MET:O	2.03	0.58
3:L:377:LEU:HD11	3:L:565:MET:O	2.03	0.58
3:R:377:LEU:HD11	3:R:565:MET:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:96:ASN:O	5:3:201:HOH:O	2.17	0.58
3:Y:173:THR:HG22	3:Y:224:HIS:CG	2.37	0.58
2:K:96:ASN:O	5:K:201:HOH:O	2.17	0.58
2:X:96:ASN:O	5:X:201:HOH:O	2.17	0.58
2:N:96:ASN:O	5:N:201:HOH:O	2.17	0.58
2:T:96:ASN:O	5:T:201:HOH:O	2.17	0.58
2:O:96:ASN:O	5:O:201:HOH:O	2.17	0.58
3:4:377:LEU:HD11	3:4:565:MET:O	2.03	0.58
3:F:377:LEU:HD11	3:F:565:MET:O	2.03	0.57
2:Q:96:ASN:O	5:Q:201:HOH:O	2.17	0.57
3:F:123:ALA:HB3	5:F:809:HOH:O	2.04	0.57
3:I:511:GLY:O	3:U:487:LYS:HE3	2.04	0.57
3:O:377:LEU:HD11	3:O:565:MET:O	2.03	0.57
2:E:96:ASN:O	5:E:201:HOH:O	2.17	0.57
2:6:96:ASN:O	5:6:201:HOH:O	2.17	0.57
3:Y:377:LEU:HD11	3:Y:565:MET:O	2.03	0.57
3:C:377:LEU:HD11	3:C:565:MET:O	2.03	0.57
3:L:150:HIS:CE1	1:S:5:PRO:HB2	2.39	0.56
3:C:53:ASP:OD2	3:F:203:ASN:HB3	2.05	0.56
3:O:123:ALA:HB3	5:1:869:HOH:O	2.05	0.56
3:7:145:PRO:HD3	5:7:882:HOH:O	2.06	0.56
2:9:96:ASN:O	5:9:201:HOH:O	2.17	0.56
2:K:146:PRO:HB3	5:N:216:HOH:O	2.05	0.56
3:C:179:PRO:N	3:C:179:PRO:C	2.55	0.56
2:3:66:ARG:HB2	3:U:260:TYR:CE1	2.40	0.56
3:I:122:ASP:OD2	3:4:167:THR:OG1	2.18	0.55
3:O:145:PRO:HD3	5:7:893:HOH:O	2.06	0.55
3:L:481:MET:SD	3:R:166:PRO:HD3	2.48	0.54
5:O:894:HOH:O	3:1:145:PRO:HD3	2.07	0.54
3:L:169:GLY:HA3	3:V:122:ASP:OD1	2.07	0.53
3:4:145:PRO:HD3	5:4:880:HOH:O	2.09	0.53
5:L:899:HOH:O	3:R:146:GLN:HG2	2.09	0.53
3:L:53:ASP:OD2	3:R:203:ASN:HB3	2.08	0.52
3:I:173:THR:HG22	3:I:224:HIS:CD2	2.45	0.52
2:N:66:ARG:HB2	3:1:260:TYR:CE1	2.44	0.52
3:4:173:THR:HG22	3:4:224:HIS:CD2	2.45	0.52
3:1:249:SER:HA	3:1:274:HIS:O	2.10	0.52
3:U:173:THR:HG22	3:U:224:HIS:CD2	2.45	0.52
3:V:173:THR:HG22	3:V:224:HIS:CD2	2.45	0.52
3:7:249:SER:HA	3:7:274:HIS:O	2.10	0.52
3:C:203:ASN:HB3	3:Y:53:ASP:OD2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:168:ASP:OD2	5:R:702:HOH:O	2.19	0.52
3:R:249:SER:HA	3:R:274:HIS:O	2.10	0.52
3:7:173:THR:HG22	3:7:224:HIS:CD2	2.45	0.52
3:C:249:SER:HA	3:C:274:HIS:O	2.10	0.52
3:I:249:SER:HA	3:I:274:HIS:O	2.10	0.52
3:L:491:ASP:OD2	3:R:187:ARG:NH2	2.43	0.52
3:O:173:THR:HG22	3:O:224:HIS:CD2	2.45	0.52
3:C:173:THR:HG22	3:C:224:HIS:CD2	2.45	0.51
3:F:173:THR:HG22	3:F:224:HIS:CD2	2.45	0.51
3:O:249:SER:HA	3:O:274:HIS:O	2.10	0.51
3:V:249:SER:HA	3:V:274:HIS:O	2.10	0.51
3:Y:173:THR:HG22	3:Y:224:HIS:CD2	2.45	0.51
3:1:173:THR:HG22	3:1:224:HIS:CD2	2.45	0.51
3:4:300:PRO:HB3	5:4:862:HOH:O	2.10	0.51
3:U:123:ALA:HB3	5:U:829:HOH:O	2.10	0.51
3:C:290:ILE:HD11	3:C:353:LEU:HD12	1.93	0.51
3:F:249:SER:HA	3:F:274:HIS:O	2.10	0.51
3:O:260:TYR:CE1	2:6:66:ARG:HB2	2.44	0.51
3:O:290:ILE:HD11	3:O:353:LEU:HD12	1.93	0.51
3:R:173:THR:HG22	3:R:224:HIS:CD2	2.45	0.51
3:I:502:LEU:HD22	3:I:518:ALA:HB2	1.93	0.51
3:R:502:LEU:HD22	3:R:518:ALA:HB2	1.93	0.51
3:U:300:PRO:HB3	5:U:864:HOH:O	2.10	0.51
3:L:300:PRO:HB3	5:L:867:HOH:O	2.10	0.51
3:R:290:ILE:HD11	3:R:353:LEU:HD12	1.93	0.51
3:R:300:PRO:HB3	5:R:867:HOH:O	2.10	0.51
3:C:138:THR:HA	3:C:160:PHE:HB2	1.93	0.51
3:F:502:LEU:HD22	3:F:518:ALA:HB2	1.93	0.51
3:I:290:ILE:HD11	3:I:353:LEU:HD12	1.93	0.51
3:L:173:THR:HG22	3:L:224:HIS:CD2	2.45	0.51
3:L:290:ILE:HD11	3:L:353:LEU:HD12	1.93	0.51
1:Z:71:ASP:O	3:1:568:ARG:NH1	2.44	0.51
1:A:71:ASP:O	3:C:568:ARG:NH1	2.44	0.51
1:D:71:ASP:O	3:F:568:ARG:NH1	2.44	0.51
1:W:71:ASP:O	3:Y:568:ARG:NH1	2.44	0.51
3:Y:249:SER:HA	3:Y:274:HIS:O	2.10	0.51
3:1:290:ILE:HD11	3:1:353:LEU:HD12	1.93	0.51
1:G:71:ASP:O	3:I:568:ARG:NH1	2.44	0.51
3:L:138:THR:HA	3:L:160:PHE:HB2	1.93	0.51
2:6:159:GLY:HA3	5:6:236:HOH:O	2.11	0.51
3:7:138:THR:HA	3:7:160:PHE:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:71:ASP:O	3:V:568:ARG:NH1	2.44	0.51
3:V:290:ILE:HD11	3:V:353:LEU:HD12	1.93	0.51
3:V:300:PRO:HB3	5:V:864:HOH:O	2.10	0.51
3:Y:502:LEU:HD22	3:Y:518:ALA:HB2	1.93	0.51
3:4:502:LEU:HD22	3:4:518:ALA:HB2	1.93	0.51
3:7:290:ILE:HD11	3:7:353:LEU:HD12	1.93	0.51
3:7:300:PRO:HB3	5:7:864:HOH:O	2.10	0.51
2:9:159:GLY:HA3	5:9:236:HOH:O	2.11	0.51
3:L:249:SER:HA	3:L:274:HIS:O	2.10	0.51
1:5:71:ASP:O	3:7:568:ARG:NH1	2.44	0.51
1:8:71:ASP:O	3:U:568:ARG:NH1	2.44	0.51
3:U:249:SER:HA	3:U:274:HIS:O	2.10	0.51
3:I:203:ASN:HB3	3:U:53:ASP:OD2	2.10	0.50
3:Y:290:ILE:HD11	3:Y:353:LEU:HD12	1.93	0.50
3:4:138:THR:HA	3:4:160:PHE:HB2	1.93	0.50
3:4:290:ILE:HD11	3:4:353:LEU:HD12	1.93	0.50
1:J:71:ASP:O	3:L:568:ARG:NH1	2.44	0.50
2:T:159:GLY:HA3	5:T:237:HOH:O	2.11	0.50
3:Y:300:PRO:HB3	5:Y:867:HOH:O	2.10	0.50
1:2:71:ASP:O	3:4:568:ARG:NH1	2.44	0.50
3:U:502:LEU:HD22	3:U:518:ALA:HB2	1.93	0.50
3:I:260:TYR:CE1	2:9:66:ARG:HB2	2.47	0.50
3:L:502:LEU:HD22	3:L:518:ALA:HB2	1.93	0.50
2:N:159:GLY:HA3	5:N:237:HOH:O	2.11	0.50
3:R:138:THR:HA	3:R:160:PHE:HB2	1.93	0.50
3:1:300:PRO:HB3	5:1:868:HOH:O	2.10	0.50
3:4:249:SER:HA	3:4:274:HIS:O	2.10	0.50
2:B:159:GLY:HA3	5:B:237:HOH:O	2.11	0.50
3:C:502:LEU:HD22	3:C:518:ALA:HB2	1.93	0.50
3:O:138:THR:HA	3:O:160:PHE:HB2	1.93	0.50
3:O:300:PRO:HB3	5:O:863:HOH:O	2.10	0.50
3:O:502:LEU:HD22	3:O:518:ALA:HB2	1.93	0.50
3:V:138:THR:HA	3:V:160:PHE:HB2	1.93	0.50
3:I:138:THR:HA	3:I:160:PHE:HB2	1.93	0.50
3:L:266:ASP:O	5:L:701:HOH:O	2.19	0.50
3:L:511:GLY:O	3:V:487:LYS:HE3	2.11	0.50
1:P:71:ASP:O	3:R:568:ARG:NH1	2.44	0.50
2:K:159:GLY:HA3	5:K:237:HOH:O	2.11	0.50
3:1:502:LEU:HD22	3:1:518:ALA:HB2	1.93	0.50
3:F:300:PRO:HB3	5:F:867:HOH:O	2.10	0.50
3:C:300:PRO:HB3	5:C:868:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:290:ILE:HD11	3:F:353:LEU:HD12	1.93	0.50
2:H:159:GLY:HA3	5:H:236:HOH:O	2.11	0.50
3:I:300:PRO:HB3	5:I:869:HOH:O	2.10	0.49
2:Q:159:GLY:HA3	5:Q:237:HOH:O	2.11	0.49
3:1:138:THR:HA	3:1:160:PHE:HB2	1.93	0.49
3:7:502:LEU:HD22	3:7:518:ALA:HB2	1.93	0.49
2:E:159:GLY:HA3	5:E:237:HOH:O	2.11	0.49
3:U:145:PRO:HD3	5:U:893:HOH:O	2.11	0.49
3:U:290:ILE:HD11	3:U:353:LEU:HD12	1.93	0.49
3:C:484:ALA:HA	3:C:489[B]:MET:HG2	1.95	0.49
3:Y:138:THR:HA	3:Y:160:PHE:HB2	1.93	0.49
3:U:138:THR:HA	3:U:160:PHE:HB2	1.93	0.49
3:F:138:THR:HA	3:F:160:PHE:HB2	1.93	0.49
1:G:45:GLU:OE1	1:2:26:ARG:NH2	2.40	0.49
1:M:71:ASP:O	3:O:568:ARG:NH1	2.44	0.49
3:Y:484:ALA:HA	3:Y:489[B]:MET:HG2	1.95	0.49
3:4:484:ALA:HA	3:4:489[B]:MET:HG2	1.95	0.49
3:O:173:THR:HG23	3:7:45:TYR:OH	2.13	0.49
3:V:502:LEU:HD22	3:V:518:ALA:HB2	1.93	0.49
3:U:484:ALA:HA	3:U:489[B]:MET:HG2	1.95	0.49
3:F:484:ALA:HA	3:F:489[B]:MET:HG2	1.95	0.49
3:R:484:ALA:HA	3:R:489[B]:MET:HG2	1.94	0.49
3:F:145:PRO:HD3	5:F:887:HOH:O	2.12	0.49
2:0:159:GLY:HA3	5:0:235:HOH:O	2.11	0.49
3:1:122:ASP:OD2	3:7:167:THR:OG1	2.13	0.49
2:3:159:GLY:HA3	5:3:236:HOH:O	2.11	0.49
1:G:49:ASP:OD1	1:2:28:LEU:HD11	2.13	0.49
3:R:123:ALA:HB3	5:R:866:HOH:O	2.13	0.49
2:X:159:GLY:HA3	5:X:236:HOH:O	2.11	0.49
3:1:484:ALA:HA	3:1:489[B]:MET:HG2	1.94	0.48
2:K:126:GLY:HA2	3:R:232:ASN:CG	2.34	0.48
2:Q:157:GLU:HG3	2:3:153[A]:ARG:NH2	2.29	0.48
3:V:484:ALA:HA	3:V:489[B]:MET:HG2	1.95	0.48
2:K:146:PRO:HG3	5:N:237:HOH:O	2.12	0.48
3:7:484:ALA:HA	3:7:489[B]:MET:HG2	1.94	0.48
3:C:145:PRO:HD3	5:C:888:HOH:O	2.13	0.48
3:L:484:ALA:HA	3:L:489[B]:MET:HG2	1.94	0.48
3:I:484:ALA:HA	3:I:489[B]:MET:HG2	1.94	0.48
3:1:139:HIS:CE1	3:1:276:PHE:CD2	3.02	0.48
3:C:139:HIS:CE1	3:C:276:PHE:CD2	3.02	0.48
3:I:139:HIS:CE1	3:I:276:PHE:CD2	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:484:ALA:HA	3:O:489[B]:MET:HG2	1.94	0.48
3:Y:139:HIS:CE1	3:Y:276:PHE:CD2	3.02	0.48
3:1:318:PHE:O	3:1:322:MET:HG3	2.14	0.48
3:4:139:HIS:CE1	3:4:276:PHE:CD2	3.02	0.48
3:F:139:HIS:CE1	3:F:276:PHE:CD2	3.02	0.48
3:I:318:PHE:O	3:I:322:MET:HG3	2.14	0.48
3:R:139:HIS:CE1	3:R:276:PHE:CD2	3.02	0.48
3:R:225:GLU:HG2	3:R:251:HIS:CD2	2.49	0.47
3:Y:225:GLU:HG2	3:Y:251:HIS:CD2	2.49	0.47
3:C:225:GLU:HG2	3:C:251:HIS:CD2	2.49	0.47
3:O:187:ARG:NE	3:7:491:ASP:OD2	2.43	0.47
3:V:225:GLU:HG2	3:V:251:HIS:CD2	2.49	0.47
3:C:318:PHE:O	3:C:322:MET:HG3	2.14	0.47
3:F:225:GLU:HG2	3:F:251:HIS:CD2	2.49	0.47
3:O:263:ASP:OD2	5:O:701:HOH:O	2.20	0.47
3:O:318:PHE:O	3:O:322:MET:HG3	2.14	0.47
3:1:225:GLU:HG2	3:1:251:HIS:CD2	2.50	0.47
3:U:225:GLU:HG2	3:U:251:HIS:CD2	2.49	0.47
3:L:225:GLU:HG2	3:L:251:HIS:CD2	2.49	0.47
3:O:225:GLU:HG2	3:O:251:HIS:CD2	2.50	0.47
3:V:193:PRO:HB3	3:V:489[B]:MET:HE2	1.97	0.47
3:7:139:HIS:CE1	3:7:276:PHE:CD2	3.02	0.47
3:U:139:HIS:CE1	3:U:276:PHE:CD2	3.02	0.47
3:L:572:GLY:N	1:S:7:GLU:HG2	2.29	0.47
3:V:139:HIS:CE1	3:V:276:PHE:CD2	3.02	0.47
3:I:225:GLU:HG2	3:I:251:HIS:CD2	2.50	0.47
3:O:139:HIS:CE1	3:O:276:PHE:CD2	3.02	0.47
3:F:318:PHE:O	3:F:322:MET:HG3	2.14	0.47
3:L:139:HIS:CE1	3:L:276:PHE:CD2	3.02	0.47
3:R:318:PHE:O	3:R:322:MET:HG3	2.14	0.47
3:V:145:PRO:HD3	5:V:895:HOH:O	2.14	0.47
3:V:318:PHE:O	3:V:322:MET:HG3	2.14	0.47
3:Y:318:PHE:O	3:Y:322:MET:HG3	2.14	0.47
3:4:225:GLU:HG2	3:4:251:HIS:CD2	2.49	0.47
3:7:318:PHE:O	3:7:322:MET:HG3	2.14	0.47
3:U:263:ASP:OD2	5:U:701:HOH:O	2.21	0.47
2:Q:145:ARG:NE	3:Y:266:ASP:OD1	2.47	0.47
1:P:45:GLU:OE1	1:S:26:ARG:NH2	2.37	0.46
3:4:318:PHE:O	3:4:322:MET:HG3	2.14	0.46
3:L:318:PHE:O	3:L:322:MET:HG3	2.14	0.46
3:L:572:GLY:O	1:S:85:ILE:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:225:GLU:HG2	3:7:251:HIS:CD2	2.49	0.46
2:K:125:TYR:HB3	3:R:205:TYR:CG	2.51	0.46
1:M:28:LEU:HD11	1:5:49:ASP:OD1	2.16	0.46
3:Y:145:PRO:HD3	5:Y:870:HOH:O	2.15	0.46
2:0:126:GLY:HA2	3:7:232:ASN:CG	2.36	0.46
3:O:203:ASN:HB2	3:7:53:ASP:HB3	1.98	0.46
3:L:251:HIS:CE1	3:L:283:GLY:HA3	2.51	0.46
3:1:251:HIS:CE1	3:1:283:GLY:HA3	2.51	0.46
3:U:318:PHE:O	3:U:322:MET:HG3	2.14	0.46
3:F:122:ASP:OD1	3:Y:169:GLY:HA3	2.15	0.46
3:I:483:GLY:O	3:I:489[A]:MET:HA	2.16	0.46
3:Y:251:HIS:CE1	3:Y:283:GLY:HA3	2.51	0.46
3:7:483:GLY:O	3:7:489[A]:MET:HA	2.16	0.46
3:O:193:PRO:HB3	3:O:489[B]:MET:HE2	1.98	0.46
3:Y:483:GLY:O	3:Y:489[A]:MET:HA	2.16	0.46
3:1:483:GLY:O	3:1:489[A]:MET:HA	2.16	0.46
3:I:428:SER:OG	3:I:433:LYS:NZ	2.41	0.46
3:O:483:GLY:O	3:O:489[A]:MET:HA	2.16	0.46
3:4:483:GLY:O	3:4:489[A]:MET:HA	2.16	0.46
3:U:251:HIS:CE1	3:U:283:GLY:HA3	2.51	0.46
2:Q:157:GLU:HG3	2:3:153[B]:ARG:HH22	1.81	0.45
3:R:483:GLY:O	3:R:489[A]:MET:HA	2.16	0.45
3:R:251:HIS:CE1	3:R:283:GLY:HA3	2.51	0.45
3:O:251:HIS:CE1	3:O:283:GLY:HA3	2.51	0.45
3:4:251:HIS:CE1	3:4:283:GLY:HA3	2.51	0.45
3:I:145:PRO:HD3	5:I:888:HOH:O	2.15	0.45
3:L:53:ASP:HB3	3:R:203:ASN:CB	2.46	0.45
3:L:469:SER:O	3:R:369:MET:N	2.49	0.45
3:C:186:LEU:O	3:C:189:VAL:HG22	2.17	0.45
3:C:187:ARG:NE	3:Y:491:ASP:OD2	2.39	0.45
3:C:251:HIS:CE1	3:C:283:GLY:HA3	2.51	0.45
3:I:251:HIS:CE1	3:I:283:GLY:HA3	2.51	0.45
3:L:53:ASP:HB3	3:R:203:ASN:HB2	1.99	0.45
3:7:251:HIS:CE1	3:7:283:GLY:HA3	2.51	0.45
3:U:483:GLY:O	3:U:489[A]:MET:HA	2.16	0.45
3:F:53:ASP:OD1	3:Y:228:GLY:HA3	2.16	0.45
5:H:254:HOH:O	2:T:146:PRO:HB3	2.17	0.45
2:K:70:VAL:HA	3:R:257:GLU:HG3	1.99	0.45
3:R:186:LEU:O	3:R:189:VAL:HG22	2.17	0.45
3:V:428:SER:OG	3:V:433:LYS:NZ	2.41	0.45
3:V:483:GLY:O	3:V:489[A]:MET:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:483:GLY:O	3:C:489[A]:MET:HA	2.16	0.45
3:F:251:HIS:CE1	3:F:283:GLY:HA3	2.51	0.45
3:O:186:LEU:O	3:O:189:VAL:HG22	2.17	0.45
3:V:251:HIS:CE1	3:V:283:GLY:HA3	2.51	0.45
3:4:360:SER:CB	3:4:530:LEU:HD13	2.47	0.45
3:7:186:LEU:O	3:7:189:VAL:HG22	2.17	0.45
3:F:186:LEU:O	3:F:189:VAL:HG22	2.17	0.45
3:F:483:GLY:O	3:F:489[A]:MET:HA	2.16	0.45
3:O:360:SER:CB	3:O:530:LEU:HD13	2.47	0.45
3:L:266:ASP:OD1	2:0:134:TRP:CZ3	2.66	0.44
3:V:360:SER:CB	3:V:530:LEU:HD13	2.47	0.44
1:A:28:LEU:HD11	1:W:49:ASP:OD1	2.18	0.44
3:I:186:LEU:O	3:I:189:VAL:HG22	2.17	0.44
2:K:146:PRO:CB	5:N:216:HOH:O	2.64	0.44
3:L:483:GLY:O	3:L:489[A]:MET:HA	2.16	0.44
5:L:898:HOH:O	3:R:145:PRO:HD3	2.17	0.44
3:7:360:SER:CB	3:7:530:LEU:HD13	2.47	0.44
3:R:360:SER:CB	3:R:530:LEU:HD13	2.47	0.44
3:C:360:SER:CB	3:C:530:LEU:HD13	2.47	0.44
3:C:428:SER:OG	3:C:433:LYS:NZ	2.41	0.44
3:F:360:SER:CB	3:F:530:LEU:HD13	2.47	0.44
3:L:186:LEU:O	3:L:189:VAL:HG22	2.17	0.44
3:F:53:ASP:OD2	3:Y:203:ASN:HB3	2.17	0.44
3:F:428:SER:OG	3:F:433:LYS:NZ	2.41	0.44
3:I:360:SER:CB	3:I:530:LEU:HD13	2.47	0.44
3:L:360:SER:CB	3:L:530:LEU:HD13	2.47	0.44
3:L:491:ASP:OD2	3:R:187:ARG:CZ	2.65	0.44
3:R:193:PRO:HB3	3:R:489[B]:MET:HE2	1.99	0.44
3:1:186:LEU:O	3:1:189:VAL:HG22	2.17	0.44
1:8:18:ASP:O	1:8:22:LYS:HG3	2.18	0.44
3:U:186:LEU:O	3:U:189:VAL:HG22	2.17	0.44
1:D:5:PRO:HB2	3:Y:150:HIS:CE1	2.52	0.44
1:2:18:ASP:O	1:2:22:LYS:HG3	2.18	0.44
3:4:45:TYR:OH	3:U:173:THR:HG23	2.18	0.44
1:5:18:ASP:O	1:5:22:LYS:HG3	2.18	0.44
3:U:360:SER:CB	3:U:530:LEU:HD13	2.47	0.44
3:R:428:SER:OG	3:R:433:LYS:NZ	2.41	0.44
3:Y:186:LEU:O	3:Y:189:VAL:HG22	2.17	0.44
3:1:360:SER:CB	3:1:530:LEU:HD13	2.47	0.44
1:W:18:ASP:O	1:W:22:LYS:HG3	2.18	0.44
1:Z:18:ASP:O	1:Z:22:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:186:LEU:O	3:4:189:VAL:HG22	2.17	0.43
1:D:18:ASP:O	1:D:22:LYS:HG3	2.18	0.43
3:F:193:PRO:HB3	3:F:489[B]:MET:HE2	1.99	0.43
3:V:186:LEU:O	3:V:189:VAL:HG22	2.17	0.43
3:L:487:LYS:NZ	3:R:513:ASP:OD2	2.44	0.43
3:Y:193:PRO:HB3	3:Y:489[B]:MET:HE2	2.00	0.43
3:Y:360:SER:CB	3:Y:530:LEU:HD13	2.47	0.43
3:U:193:PRO:HB3	3:U:489[B]:MET:HE2	2.00	0.43
1:A:18:ASP:O	1:A:22:LYS:HG3	2.18	0.43
3:L:193:PRO:HB3	3:L:489[B]:MET:HE2	1.99	0.43
1:P:18:ASP:O	1:P:22:LYS:HG3	2.18	0.43
1:J:18:ASP:O	1:J:22:LYS:HG3	2.18	0.43
2:Q:157:GLU:HG3	2:3:153[B]:ARG:NH2	2.33	0.43
3:1:306:THR:HA	5:1:712:HOH:O	2.19	0.43
1:G:18:ASP:O	1:G:22:LYS:HG3	2.18	0.43
3:O:306:THR:HA	5:O:716:HOH:O	2.19	0.43
3:C:166:PRO:HD3	3:Y:481:MET:SD	2.58	0.43
1:S:18:ASP:O	1:S:22:LYS:HG3	2.18	0.43
1:2:96:HIS:HE2	3:U:319:ASP:CG	2.22	0.43
2:B:146:PRO:HB3	5:6:253:HOH:O	2.19	0.42
1:D:7:GLU:HG2	3:Y:572:GLY:N	2.34	0.42
3:F:306:THR:HA	5:F:715:HOH:O	2.19	0.42
3:O:187:ARG:HH21	3:7:491:ASP:CG	2.22	0.42
3:V:266:ASP:O	5:V:701:HOH:O	2.20	0.42
3:7:193:PRO:HB3	3:7:489[B]:MET:HE2	2.01	0.42
3:O:182:ILE:HD13	3:O:218:VAL:HG13	2.02	0.42
3:O:232:ASN:CG	2:6:126:GLY:HA2	2.39	0.42
3:R:306:THR:HA	5:R:717:HOH:O	2.19	0.42
1:M:18:ASP:O	1:M:22:LYS:HG3	2.18	0.42
3:V:182:ILE:HD13	3:V:218:VAL:HG13	2.02	0.42
3:7:182:ILE:HD13	3:7:218:VAL:HG13	2.01	0.42
3:Y:182:ILE:HD13	3:Y:218:VAL:HG13	2.02	0.42
3:I:193:PRO:HB3	3:I:489[B]:MET:HE2	2.00	0.42
1:2:45:GLU:OE1	1:8:26:ARG:NH2	2.42	0.42
3:F:82:LEU:HD21	3:F:99:ILE:HD13	2.02	0.42
3:F:464:GLY:HA2	3:F:475:PRO:O	2.20	0.42
3:I:182:ILE:HD13	3:I:218:VAL:HG13	2.02	0.42
3:O:296:PRO:O	3:O:526:SER:HB2	2.20	0.42
3:1:53:ASP:OD1	3:7:228:GLY:HA3	2.20	0.42
3:4:82:LEU:HD21	3:4:99:ILE:HD13	2.02	0.42
3:4:306:THR:HA	5:4:715:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:296:PRO:O	3:L:526:SER:HB2	2.20	0.42
3:Y:464:GLY:HA2	3:Y:475:PRO:O	2.20	0.42
3:4:296:PRO:O	3:4:526:SER:HB2	2.20	0.42
3:I:45:TYR:OH	3:4:173:THR:HG23	2.19	0.42
3:R:82:LEU:HD21	3:R:99:ILE:HD13	2.02	0.42
3:R:296:PRO:O	3:R:526:SER:HB2	2.20	0.42
3:1:428:SER:OG	3:1:433:LYS:NZ	2.41	0.42
3:7:306:THR:HA	5:7:714:HOH:O	2.19	0.42
3:U:296:PRO:O	3:U:526:SER:HB2	2.20	0.42
3:C:82:LEU:HD21	3:C:99:ILE:HD13	2.02	0.42
3:R:182:ILE:HD13	3:R:218:VAL:HG13	2.02	0.42
3:1:182:ILE:HD13	3:1:218:VAL:HG13	2.02	0.42
3:U:182:ILE:HD13	3:U:218:VAL:HG13	2.01	0.42
3:C:296:PRO:O	3:C:526:SER:HB2	2.20	0.41
3:I:306:THR:HA	5:I:715:HOH:O	2.19	0.41
3:O:45:TYR:CZ	3:1:169:GLY:HA2	2.55	0.41
3:1:41:GLU:OE2	5:1:701:HOH:O	2.22	0.41
3:1:464:GLY:HA2	3:1:475:PRO:O	2.20	0.41
3:7:296:PRO:O	3:7:526:SER:HB2	2.20	0.41
3:U:306:THR:HA	5:U:718:HOH:O	2.19	0.41
3:C:464:GLY:HA2	3:C:475:PRO:O	2.20	0.41
3:I:296:PRO:O	3:I:526:SER:HB2	2.20	0.41
3:L:182:ILE:HD13	3:L:218:VAL:HG13	2.02	0.41
3:L:228:GLY:HA3	3:V:53:ASP:OD1	2.19	0.41
3:R:464:GLY:HA2	3:R:475:PRO:O	2.20	0.41
3:R:487:LYS:HE3	3:V:511:GLY:O	2.20	0.41
3:V:41:GLU:OE2	5:V:702:HOH:O	2.22	0.41
3:Y:82:LEU:HD21	3:Y:99:ILE:HD13	2.02	0.41
3:1:45:TYR:OH	3:7:173:THR:HG23	2.20	0.41
3:4:193:PRO:HB3	3:4:489[B]:MET:HE2	2.00	0.41
3:7:82:LEU:HD21	3:7:99:ILE:HD13	2.02	0.41
3:V:278:THR:HB	5:V:800:HOH:O	2.20	0.41
3:V:306:THR:HA	5:V:715:HOH:O	2.19	0.41
3:4:464:GLY:HA2	3:4:475:PRO:O	2.20	0.41
3:U:41:GLU:OE2	5:U:702:HOH:O	2.22	0.41
3:I:82:LEU:HD21	3:I:99:ILE:HD13	2.02	0.41
3:V:464:GLY:HA2	3:V:475:PRO:O	2.20	0.41
3:Y:306:THR:HA	5:Y:713:HOH:O	2.19	0.41
3:C:182:ILE:HD13	3:C:218:VAL:HG13	2.02	0.41
3:C:306:THR:HA	5:C:715:HOH:O	2.19	0.41
1:S:18:ASP:OD1	1:S:22:LYS:NZ	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:428:SER:OG	3:Y:433:LYS:NZ	2.41	0.41
3:1:82:LEU:HD21	3:1:99:ILE:HD13	2.02	0.41
3:7:464:GLY:HA2	3:7:475:PRO:O	2.20	0.41
3:F:224:HIS:ND1	3:F:226:ASP:HB2	2.36	0.41
3:I:464:GLY:HA2	3:I:475:PRO:O	2.20	0.41
3:L:278:THR:HB	5:L:799:HOH:O	2.21	0.41
3:L:306:THR:HA	5:L:716:HOH:O	2.19	0.41
3:O:224:HIS:ND1	3:O:226:ASP:HB2	2.36	0.41
3:V:296:PRO:O	3:V:526:SER:HB2	2.20	0.41
3:Y:278:THR:HB	5:Y:797:HOH:O	2.21	0.41
3:7:224:HIS:ND1	3:7:226:ASP:HB2	2.36	0.41
3:U:464:GLY:HA2	3:U:475:PRO:O	2.20	0.41
3:L:82:LEU:HD21	3:L:99:ILE:HD13	2.02	0.41
3:L:464:GLY:HA2	3:L:475:PRO:O	2.20	0.41
3:O:278:THR:HB	5:O:798:HOH:O	2.21	0.41
3:V:224:HIS:ND1	3:V:226:ASP:HB2	2.36	0.41
3:U:278:THR:HB	5:U:801:HOH:O	2.21	0.41
3:C:17:THR:HA	3:C:32:ILE:HG22	2.03	0.41
1:G:28:LEU:HD11	1:8:49:ASP:OD1	2.20	0.41
3:I:224:HIS:ND1	3:I:226:ASP:HB2	2.36	0.41
3:O:82:LEU:HD21	3:O:99:ILE:HD13	2.02	0.41
3:O:464:GLY:HA2	3:O:475:PRO:O	2.20	0.41
3:4:182:ILE:HD13	3:4:218:VAL:HG13	2.02	0.41
3:C:224:HIS:ND1	3:C:226:ASP:HB2	2.36	0.41
3:C:278:THR:HB	5:C:798:HOH:O	2.21	0.41
3:F:17:THR:HA	3:F:32:ILE:HG22	2.03	0.41
3:I:278:THR:HB	5:I:798:HOH:O	2.20	0.41
3:L:228:GLY:HA3	3:V:53:ASP:CG	2.41	0.41
3:L:572:GLY:H	1:S:7:GLU:HG2	1.86	0.41
3:R:17:THR:HA	3:R:32:ILE:HG22	2.03	0.41
3:R:224:HIS:ND1	3:R:226:ASP:HB2	2.36	0.41
3:1:193:PRO:HB3	3:1:489[B]:MET:HE2	2.02	0.41
3:1:224:HIS:ND1	3:1:226:ASP:HB2	2.36	0.41
1:2:53:VAL:HG23	3:U:312:ASN:HB3	2.03	0.41
3:4:17:THR:HA	3:4:32:ILE:HG22	2.03	0.41
3:4:41:GLU:OE2	5:4:701:HOH:O	2.22	0.41
3:I:41:GLU:OE2	5:I:701:HOH:O	2.22	0.41
3:L:17:THR:HA	3:L:32:ILE:HG22	2.03	0.41
3:I:17:THR:HA	3:I:32:ILE:HG22	2.03	0.40
3:R:278:THR:HB	5:R:799:HOH:O	2.21	0.40
3:V:82:LEU:HD21	3:V:99:ILE:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:296:PRO:O	3:1:526:SER:HB2	2.20	0.40
3:4:224:HIS:ND1	3:4:226:ASP:HB2	2.36	0.40
3:C:193:PRO:HB3	3:C:489[B]:MET:HE2	2.02	0.40
3:F:182:ILE:HD13	3:F:218:VAL:HG13	2.02	0.40
3:Y:360:SER:HB3	3:Y:530:LEU:HD13	2.03	0.40
3:1:17:THR:HA	3:1:32:ILE:HG22	2.03	0.40
3:7:278:THR:HB	5:7:800:HOH:O	2.21	0.40
3:U:82:LEU:HD21	3:U:99:ILE:HD13	2.02	0.40
3:C:360:SER:HB3	3:C:530:LEU:HD13	2.03	0.40
3:F:296:PRO:O	3:F:526:SER:HB2	2.20	0.40
3:Y:296:PRO:O	3:Y:526:SER:HB2	2.20	0.40
3:4:289:ILE:O	3:4:292:VAL:HG22	2.22	0.40
3:U:289:ILE:O	3:U:292:VAL:HG22	2.22	0.40
3:C:289:ILE:O	3:C:292:VAL:HG22	2.22	0.40
3:L:307:LEU:HA	3:L:308:PRO:HA	1.99	0.40
3:O:187:ARG:NH2	3:7:491:ASP:OD2	2.53	0.40
3:R:307:LEU:HA	3:R:308:PRO:HA	1.99	0.40
3:1:53:ASP:HB3	3:7:203:ASN:HB2	2.03	0.40
1:2:49:ASP:OD1	1:8:28:LEU:HD11	2.22	0.40
3:4:428:SER:OG	3:4:433:LYS:NZ	2.41	0.40
3:4:481:MET:SD	3:U:166:PRO:HD3	2.62	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	2	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	5	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	8	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	A	106/100 (106%)	103 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	G	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	J	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	M	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	P	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	S	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	W	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
1	Z	106/100 (106%)	103 (97%)	3 (3%)	0	100	100
2	0	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	3	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	6	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	9	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	B	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	E	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	H	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	K	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	N	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	Q	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	T	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
2	X	132/132 (100%)	120 (91%)	9 (7%)	3 (2%)	5	1
3	1	569/571 (100%)	536 (94%)	33 (6%)	0	100	100
3	4	569/571 (100%)	537 (94%)	32 (6%)	0	100	100
3	7	569/571 (100%)	537 (94%)	32 (6%)	0	100	100
3	C	569/571 (100%)	538 (95%)	31 (5%)	0	100	100
3	F	569/571 (100%)	537 (94%)	32 (6%)	0	100	100
3	I	569/571 (100%)	536 (94%)	33 (6%)	0	100	100
3	L	569/571 (100%)	537 (94%)	32 (6%)	0	100	100
3	O	569/571 (100%)	536 (94%)	33 (6%)	0	100	100
3	R	569/571 (100%)	537 (94%)	32 (6%)	0	100	100
3	U	569/571 (100%)	536 (94%)	33 (6%)	0	100	100
3	V	569/571 (100%)	537 (94%)	32 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Y	569/571 (100%)	537 (94%)	32 (6%)	0	100	100
All	All	9684/9636 (100%)	9117 (94%)	531 (6%)	36 (0%)	32	20

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	32	GLU
2	E	32	GLU
2	H	32	GLU
2	K	32	GLU
2	N	32	GLU
2	Q	32	GLU
2	T	32	GLU
2	X	32	GLU
2	0	32	GLU
2	3	32	GLU
2	6	32	GLU
2	9	32	GLU
2	B	81	ARG
2	E	81	ARG
2	H	81	ARG
2	K	81	ARG
2	N	81	ARG
2	Q	81	ARG
2	T	81	ARG
2	X	81	ARG
2	0	81	ARG
2	3	81	ARG
2	6	81	ARG
2	9	81	ARG
2	B	80	ASN
2	E	80	ASN
2	H	80	ASN
2	K	80	ASN
2	N	80	ASN
2	Q	80	ASN
2	T	80	ASN
2	X	80	ASN
2	0	80	ASN
2	3	80	ASN
2	6	80	ASN
2	9	80	ASN

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	2	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	5	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	8	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	A	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	D	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	G	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	J	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	M	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	P	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	S	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	W	95/87 (109%)	92 (97%)	3 (3%)	34	24
1	Z	95/87 (109%)	92 (97%)	3 (3%)	34	24
2	0	112/110 (102%)	109 (97%)	3 (3%)	40	30
2	3	112/110 (102%)	109 (97%)	3 (3%)	40	30
2	6	112/110 (102%)	109 (97%)	3 (3%)	40	30
2	9	112/110 (102%)	109 (97%)	3 (3%)	40	30
2	B	112/110 (102%)	109 (97%)	3 (3%)	40	30
2	E	112/110 (102%)	109 (97%)	3 (3%)	40	30
2	H	112/110 (102%)	109 (97%)	3 (3%)	40	30
2	K	112/110 (102%)	109 (97%)	3 (3%)	40	30
2	N	112/110 (102%)	109 (97%)	3 (3%)	40	30
2	Q	112/110 (102%)	109 (97%)	3 (3%)	40	30
2	T	112/110 (102%)	109 (97%)	3 (3%)	40	30
2	X	112/110 (102%)	109 (97%)	3 (3%)	40	30
3	1	458/456 (100%)	452 (99%)	6 (1%)	65	62
3	4	458/456 (100%)	452 (99%)	6 (1%)	65	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	7	458/456 (100%)	452 (99%)	6 (1%)	65	62
3	C	458/456 (100%)	452 (99%)	6 (1%)	65	62
3	F	458/456 (100%)	452 (99%)	6 (1%)	65	62
3	I	458/456 (100%)	452 (99%)	6 (1%)	65	62
3	L	458/456 (100%)	452 (99%)	6 (1%)	65	62
3	O	458/456 (100%)	452 (99%)	6 (1%)	65	62
3	R	458/456 (100%)	452 (99%)	6 (1%)	65	62
3	U	458/456 (100%)	452 (99%)	6 (1%)	65	62
3	V	458/456 (100%)	452 (99%)	6 (1%)	65	62
3	Y	458/456 (100%)	452 (99%)	6 (1%)	65	62
All	All	7980/7836 (102%)	7836 (98%)	144 (2%)	60	47

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16[A]	LEU
1	A	16[B]	LEU
1	A	75	ASP
2	B	46	PRO
2	B	51	GLU
2	B	110	GLU
3	C	3	GLN
3	C	37	ARG
3	C	203	ASN
3	C	434[A]	MET
3	C	434[B]	MET
3	C	454	LYS
1	D	16[A]	LEU
1	D	16[B]	LEU
1	D	75	ASP
2	E	46	PRO
2	E	51	GLU
2	E	110	GLU
3	F	3	GLN
3	F	37	ARG
3	F	203	ASN
3	F	434[A]	MET
3	F	434[B]	MET

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Mol	Chain	Res	Type
3	F	454	LYS
1	G	16[A]	LEU
1	G	16[B]	LEU
1	G	75	ASP
2	H	46	PRO
2	H	51	GLU
2	H	110	GLU
3	I	3	GLN
3	I	37	ARG
3	I	203	ASN
3	I	434[A]	MET
3	I	434[B]	MET
3	I	454	LYS
1	J	16[A]	LEU
1	J	16[B]	LEU
1	J	75	ASP
2	K	46	PRO
2	K	51	GLU
2	K	110	GLU
3	L	3	GLN
3	L	37	ARG
3	L	203	ASN
3	L	434[A]	MET
3	L	434[B]	MET
3	L	454	LYS
1	M	16[A]	LEU
1	M	16[B]	LEU
1	M	75	ASP
2	N	46	PRO
2	N	51	GLU
2	N	110	GLU
3	O	3	GLN
3	O	37	ARG
3	O	203	ASN
3	O	434[A]	MET
3	O	434[B]	MET
3	O	454	LYS
1	P	16[A]	LEU
1	P	16[B]	LEU
1	P	75	ASP
2	Q	46	PRO
2	Q	51	GLU

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Mol	Chain	Res	Type
2	Q	110	GLU
3	R	3	GLN
3	R	37	ARG
3	R	203	ASN
3	R	434[A]	MET
3	R	434[B]	MET
3	R	454	LYS
1	S	16[A]	LEU
1	S	16[B]	LEU
1	S	75	ASP
2	T	46	PRO
2	T	51	GLU
2	T	110	GLU
3	V	3	GLN
3	V	37	ARG
3	V	203	ASN
3	V	434[A]	MET
3	V	434[B]	MET
3	V	454	LYS
1	W	16[A]	LEU
1	W	16[B]	LEU
1	W	75	ASP
2	X	46	PRO
2	X	51	GLU
2	X	110	GLU
3	Y	3	GLN
3	Y	37	ARG
3	Y	203	ASN
3	Y	434[A]	MET
3	Y	434[B]	MET
3	Y	454	LYS
1	Z	16[A]	LEU
1	Z	16[B]	LEU
1	Z	75	ASP
2	0	46	PRO
2	0	51	GLU
2	0	110	GLU
3	1	3	GLN
3	1	37	ARG
3	1	203	ASN
3	1	434[A]	MET
3	1	434[B]	MET

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Mol	Chain	Res	Type
3	1	454	LYS
1	2	16[A]	LEU
1	2	16[B]	LEU
1	2	75	ASP
2	3	46	PRO
2	3	51	GLU
2	3	110	GLU
3	4	3	GLN
3	4	37	ARG
3	4	203	ASN
3	4	434[A]	MET
3	4	434[B]	MET
3	4	454	LYS
1	5	16[A]	LEU
1	5	16[B]	LEU
1	5	75	ASP
2	6	46	PRO
2	6	51	GLU
2	6	110	GLU
3	7	3	GLN
3	7	37	ARG
3	7	203	ASN
3	7	434[A]	MET
3	7	434[B]	MET
3	7	454	LYS
1	8	16[A]	LEU
1	8	16[B]	LEU
1	8	75	ASP
2	9	46	PRO
2	9	51	GLU
2	9	110	GLU
3	U	3	GLN
3	U	37	ARG
3	U	203	ASN
3	U	434[A]	MET
3	U	434[B]	MET
3	U	454	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	52	ASN

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Mol	Chain	Res	Type
3	C	60	HIS
3	C	528	HIS
2	E	52	ASN
3	F	60	HIS
3	F	420	GLN
3	F	528	HIS
2	H	52	ASN
3	I	60	HIS
3	I	528	HIS
2	K	52	ASN
3	L	60	HIS
3	L	528	HIS
2	N	52	ASN
3	O	60	HIS
3	O	528	HIS
2	Q	52	ASN
3	R	60	HIS
3	R	181	ASN
3	R	528	HIS
2	T	52	ASN
3	V	60	HIS
3	V	420	GLN
3	V	528	HIS
2	X	52	ASN
3	Y	60	HIS
3	Y	528	HIS
2	0	52	ASN
3	1	60	HIS
3	1	528	HIS
2	3	52	ASN
3	4	60	HIS
3	4	528	HIS
2	6	52	ASN
3	7	60	HIS
3	7	528	HIS
2	9	52	ASN
3	U	60	HIS
3	U	528	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	KCX	R	222	3,4	9,11,12	1.66	3 (33%)	5,12,14	2.65	1 (20%)
3	KCX	U	222	3,4	9,11,12	1.67	3 (33%)	5,12,14	2.64	1 (20%)
3	KCX	Y	222	3,4	9,11,12	1.66	3 (33%)	5,12,14	2.65	1 (20%)
3	KCX	L	222	3,4	9,11,12	1.65	3 (33%)	5,12,14	2.66	1 (20%)
3	KCX	4	222	3,4	9,11,12	1.66	3 (33%)	5,12,14	2.66	1 (20%)
3	KCX	1	222	3,4	9,11,12	1.67	3 (33%)	5,12,14	2.66	1 (20%)
3	KCX	7	222	3,4	9,11,12	1.46	2 (22%)	5,12,14	1.13	0
3	KCX	C	222	3,4	9,11,12	1.67	3 (33%)	5,12,14	2.65	1 (20%)
3	KCX	F	222	3,4	9,11,12	1.46	2 (22%)	5,12,14	1.12	0
3	KCX	O	222	3,4	9,11,12	1.66	3 (33%)	5,12,14	2.66	1 (20%)
3	KCX	V	222	3,4	9,11,12	1.46	2 (22%)	5,12,14	1.13	0
3	KCX	I	222	3,4	9,11,12	1.66	3 (33%)	5,12,14	2.65	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KCX	R	222	3,4	-	0/9/10/12	-
3	KCX	U	222	3,4	-	0/9/10/12	-
3	KCX	Y	222	3,4	-	0/9/10/12	-
3	KCX	L	222	3,4	-	0/9/10/12	-
3	KCX	4	222	3,4	-	0/9/10/12	-
3	KCX	1	222	3,4	-	0/9/10/12	-
3	KCX	7	222	3,4	-	0/9/10/12	-
3	KCX	C	222	3,4	-	0/9/10/12	-
3	KCX	F	222	3,4	-	0/9/10/12	-
3	KCX	O	222	3,4	-	0/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KCX	V	222	3,4	-	0/9/10/12	-
3	KCX	I	222	3,4	-	0/9/10/12	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	222	KCX	OQ1-CX	2.97	1.27	1.21
3	C	222	KCX	OQ1-CX	2.94	1.27	1.21
3	I	222	KCX	OQ1-CX	2.93	1.27	1.21
3	4	222	KCX	OQ1-CX	2.93	1.27	1.21
3	L	222	KCX	OQ1-CX	2.92	1.27	1.21
3	Y	222	KCX	OQ1-CX	2.92	1.27	1.21
3	U	222	KCX	OQ1-CX	2.91	1.27	1.21
3	O	222	KCX	OQ1-CX	2.91	1.27	1.21
3	R	222	KCX	OQ1-CX	2.90	1.27	1.21
3	7	222	KCX	CB-CA	-2.33	1.50	1.53
3	V	222	KCX	CB-CA	-2.32	1.50	1.53
3	4	222	KCX	CB-CA	-2.31	1.50	1.53
3	O	222	KCX	CB-CA	-2.30	1.50	1.53
3	C	222	KCX	CB-CA	-2.29	1.50	1.53
3	1	222	KCX	CB-CA	-2.29	1.50	1.53
3	I	222	KCX	CB-CA	-2.29	1.50	1.53
3	U	222	KCX	CB-CA	-2.28	1.50	1.53
3	R	222	KCX	CB-CA	-2.28	1.50	1.53
3	F	222	KCX	CB-CA	-2.27	1.50	1.53
3	U	222	KCX	CX-NZ	-2.27	1.31	1.35
3	R	222	KCX	CX-NZ	-2.27	1.31	1.35
3	F	222	KCX	CX-NZ	-2.27	1.31	1.35
3	I	222	KCX	CX-NZ	-2.26	1.31	1.35
3	Y	222	KCX	CB-CA	-2.26	1.50	1.53
3	C	222	KCX	CX-NZ	-2.26	1.31	1.35
3	7	222	KCX	CX-NZ	-2.25	1.31	1.35
3	Y	222	KCX	CX-NZ	-2.25	1.31	1.35
3	L	222	KCX	CB-CA	-2.25	1.50	1.53
3	1	222	KCX	CX-NZ	-2.25	1.31	1.35
3	V	222	KCX	CX-NZ	-2.25	1.31	1.35
3	O	222	KCX	CX-NZ	-2.24	1.31	1.35
3	4	222	KCX	CX-NZ	-2.23	1.31	1.35
3	L	222	KCX	CX-NZ	-2.19	1.31	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	222	KCX	OQ1-CX-NZ	-5.53	116.39	124.96
3	4	222	KCX	OQ1-CX-NZ	-5.53	116.39	124.96
3	O	222	KCX	OQ1-CX-NZ	-5.53	116.39	124.96
3	1	222	KCX	OQ1-CX-NZ	-5.52	116.40	124.96
3	Y	222	KCX	OQ1-CX-NZ	-5.51	116.41	124.96
3	C	222	KCX	OQ1-CX-NZ	-5.51	116.42	124.96
3	I	222	KCX	OQ1-CX-NZ	-5.51	116.42	124.96
3	R	222	KCX	OQ1-CX-NZ	-5.50	116.43	124.96
3	U	222	KCX	OQ1-CX-NZ	-5.48	116.46	124.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	I	7
3	O	7
3	V	7
3	1	7
3	U	7
3	7	6
3	C	6
3	F	6
3	L	6
3	R	6
3	Y	6
3	4	6
2	B	3
2	E	3
2	H	3
2	K	3
2	N	3
2	Q	3
2	T	3
2	X	3
2	0	3
2	3	3
2	6	3
2	9	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	156:VAL	C	157:ALA	N	1.20
1	O	156:VAL	C	157:ALA	N	1.20
1	V	156:VAL	C	157:ALA	N	1.20
1	1	156:VAL	C	157:ALA	N	1.20
1	U	156:VAL	C	157:ALA	N	1.20
1	7	201:LYS	C	202:GLY	N	1.19
1	C	201:LYS	C	202:GLY	N	1.18
1	C	396:ASP	C	397:ALA	N	1.18
1	F	201:LYS	C	202:GLY	N	1.18
1	F	396:ASP	C	397:ALA	N	1.18
1	I	201:LYS	C	202:GLY	N	1.18
1	I	396:ASP	C	397:ALA	N	1.18
1	L	201:LYS	C	202:GLY	N	1.18
1	L	396:ASP	C	397:ALA	N	1.18
1	O	201:LYS	C	202:GLY	N	1.18
1	O	396:ASP	C	397:ALA	N	1.18

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	201:LYS	C	202:GLY	N	1.18
1	R	396:ASP	C	397:ALA	N	1.18
1	V	201:LYS	C	202:GLY	N	1.18
1	V	396:ASP	C	397:ALA	N	1.18
1	Y	201:LYS	C	202:GLY	N	1.18
1	Y	396:ASP	C	397:ALA	N	1.18
1	1	201:LYS	C	202:GLY	N	1.18
1	1	396:ASP	C	397:ALA	N	1.18
1	4	201:LYS	C	202:GLY	N	1.18
1	4	396:ASP	C	397:ALA	N	1.18
1	7	396:ASP	C	397:ALA	N	1.18
1	U	201:LYS	C	202:GLY	N	1.18
1	U	396:ASP	C	397:ALA	N	1.18
1	B	52:ASN	C	53:LYS	N	1.16
1	C	294:SER	C	295:GLN	N	1.16
1	E	52:ASN	C	53:LYS	N	1.16
1	F	294:SER	C	295:GLN	N	1.16
1	H	52:ASN	C	53:LYS	N	1.16
1	I	294:SER	C	295:GLN	N	1.16
1	K	52:ASN	C	53:LYS	N	1.16
1	L	294:SER	C	295:GLN	N	1.16
1	N	52:ASN	C	53:LYS	N	1.16
1	O	294:SER	C	295:GLN	N	1.16
1	Q	52:ASN	C	53:LYS	N	1.16
1	R	294:SER	C	295:GLN	N	1.16
1	T	52:ASN	C	53:LYS	N	1.16
1	V	294:SER	C	295:GLN	N	1.16
1	X	52:ASN	C	53:LYS	N	1.16
1	Y	294:SER	C	295:GLN	N	1.16
1	0	52:ASN	C	53:LYS	N	1.16
1	1	294:SER	C	295:GLN	N	1.16
1	3	52:ASN	C	53:LYS	N	1.16
1	4	294:SER	C	295:GLN	N	1.16
1	6	52:ASN	C	53:LYS	N	1.16
1	7	294:SER	C	295:GLN	N	1.16
1	9	52:ASN	C	53:LYS	N	1.16
1	U	294:SER	C	295:GLN	N	1.16
1	B	153[A]:ARG	C	154:ARG	N	1.15
1	E	153[A]:ARG	C	154:ARG	N	1.15
1	H	153[A]:ARG	C	154:ARG	N	1.15
1	K	153[A]:ARG	C	154:ARG	N	1.15
1	N	153[A]:ARG	C	154:ARG	N	1.15

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Q	153[A]:ARG	C	154:ARG	N	1.15
1	T	153[A]:ARG	C	154:ARG	N	1.15
1	X	153[A]:ARG	C	154:ARG	N	1.15
1	0	153[A]:ARG	C	154:ARG	N	1.15
1	3	153[A]:ARG	C	154:ARG	N	1.15
1	6	153[A]:ARG	C	154:ARG	N	1.15
1	9	153[A]:ARG	C	154:ARG	N	1.15
1	C	199:LEU	C	200:GLY	N	1.14
1	F	199:LEU	C	200:GLY	N	1.14
1	I	199:LEU	C	200:GLY	N	1.14
1	L	199:LEU	C	200:GLY	N	1.14
1	O	199:LEU	C	200:GLY	N	1.14
1	R	199:LEU	C	200:GLY	N	1.14
1	V	199:LEU	C	200:GLY	N	1.14
1	Y	199:LEU	C	200:GLY	N	1.14
1	1	199:LEU	C	200:GLY	N	1.14
1	4	199:LEU	C	200:GLY	N	1.14
1	7	199:LEU	C	200:GLY	N	1.14
1	U	199:LEU	C	200:GLY	N	1.14
1	B	153[B]:ARG	C	154:ARG	N	1.13
1	E	153[B]:ARG	C	154:ARG	N	1.13
1	H	153[B]:ARG	C	154:ARG	N	1.13
1	K	153[B]:ARG	C	154:ARG	N	1.13
1	N	153[B]:ARG	C	154:ARG	N	1.13
1	Q	153[B]:ARG	C	154:ARG	N	1.13
1	T	153[B]:ARG	C	154:ARG	N	1.13
1	X	153[B]:ARG	C	154:ARG	N	1.13
1	0	153[B]:ARG	C	154:ARG	N	1.13
1	3	153[B]:ARG	C	154:ARG	N	1.13
1	6	153[B]:ARG	C	154:ARG	N	1.13
1	9	153[B]:ARG	C	154:ARG	N	1.13
1	C	364:SER	C	365:ASP	N	1.12
1	F	364:SER	C	365:ASP	N	1.12
1	I	364:SER	C	365:ASP	N	1.12
1	L	364:SER	C	365:ASP	N	1.12
1	O	364:SER	C	365:ASP	N	1.12
1	R	364:SER	C	365:ASP	N	1.12
1	V	364:SER	C	365:ASP	N	1.12
1	Y	364:SER	C	365:ASP	N	1.12
1	1	364:SER	C	365:ASP	N	1.12
1	4	364:SER	C	365:ASP	N	1.12
1	7	364:SER	C	365:ASP	N	1.12

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	364:SER	C	365:ASP	N	1.12
1	C	29:PHE	C	30:ILE	N	1.11
1	F	29:PHE	C	30:ILE	N	1.11
1	I	29:PHE	C	30:ILE	N	1.11
1	L	29:PHE	C	30:ILE	N	1.11
1	O	29:PHE	C	30:ILE	N	1.11
1	R	29:PHE	C	30:ILE	N	1.11
1	V	29:PHE	C	30:ILE	N	1.11
1	Y	29:PHE	C	30:ILE	N	1.11
1	1	29:PHE	C	30:ILE	N	1.11
1	4	29:PHE	C	30:ILE	N	1.11
1	7	29:PHE	C	30:ILE	N	1.11
1	U	29:PHE	C	30:ILE	N	1.11

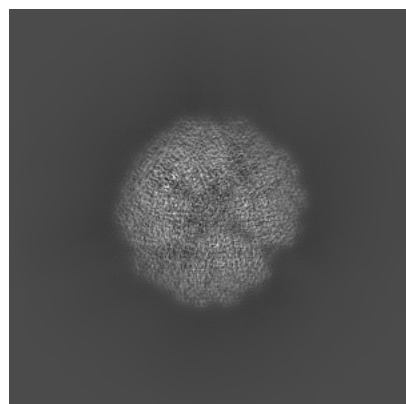
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10835. These allow visual inspection of the internal detail of the map and identification of artifacts.

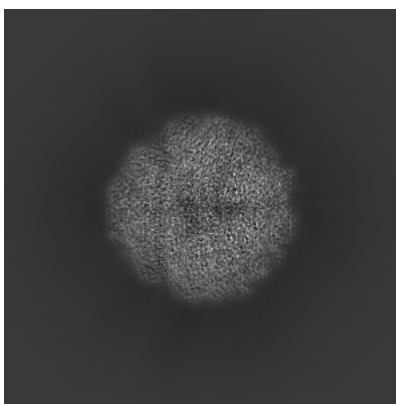
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

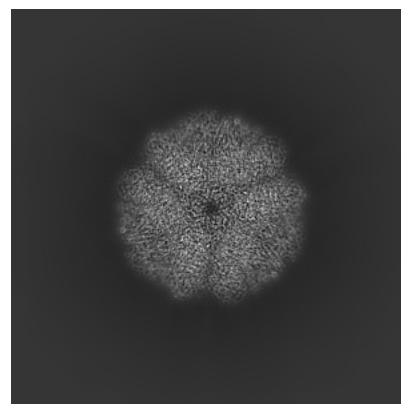
6.1.1 Primary map



X

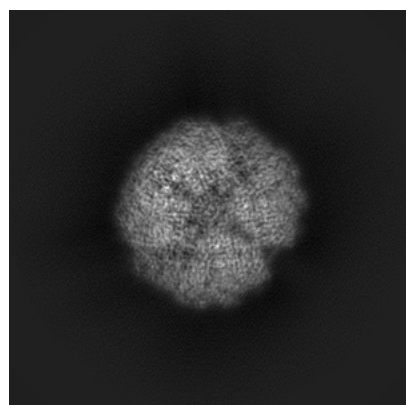


Y

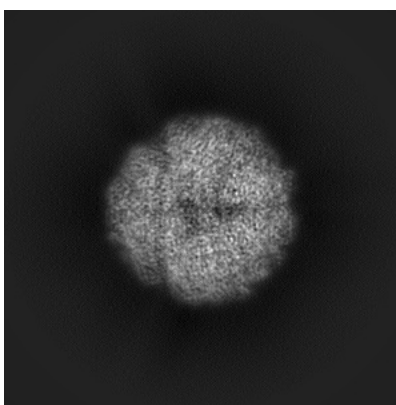


Z

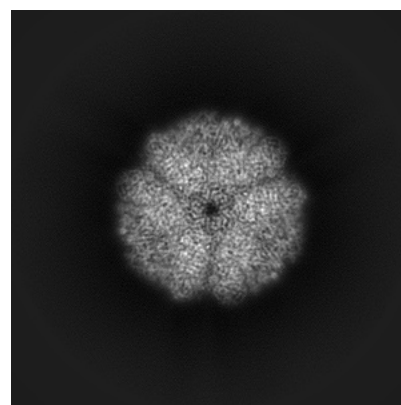
6.1.2 Raw map



X



Y

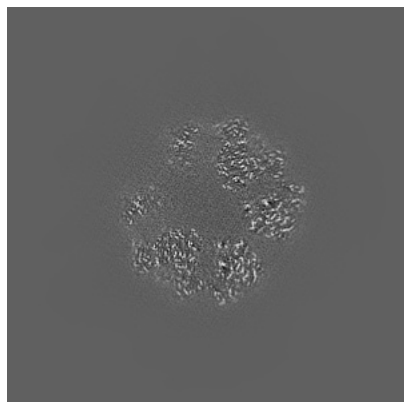


Z

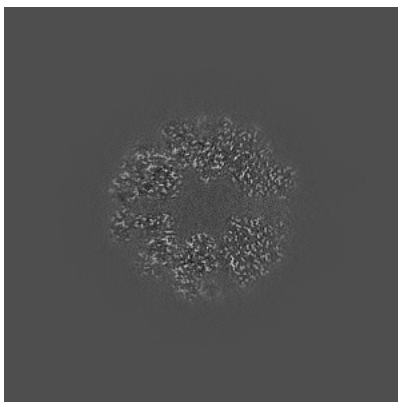
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

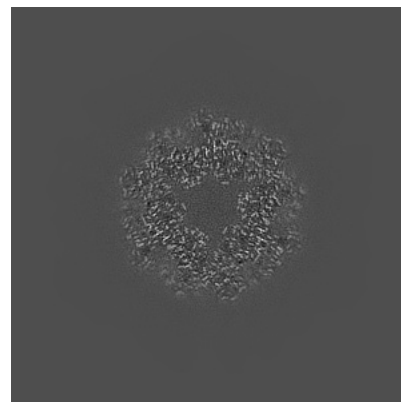
6.2.1 Primary map



X Index: 256

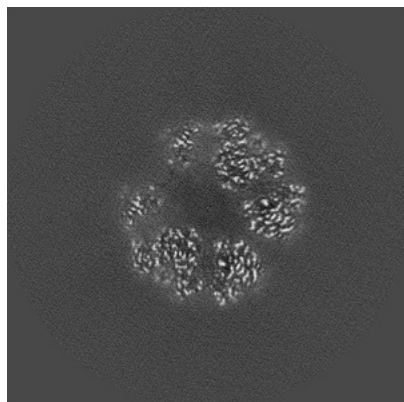


Y Index: 256

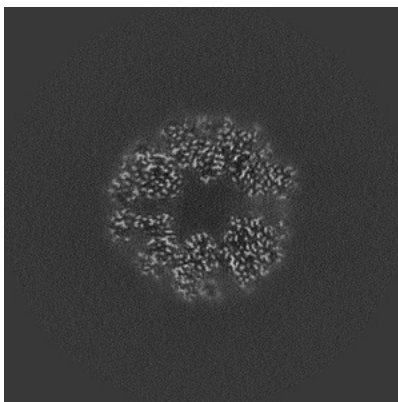


Z Index: 256

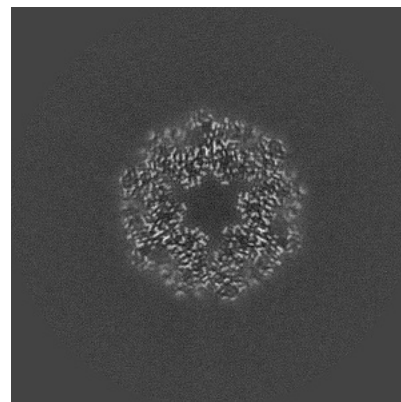
6.2.2 Raw map



X Index: 256



Y Index: 256

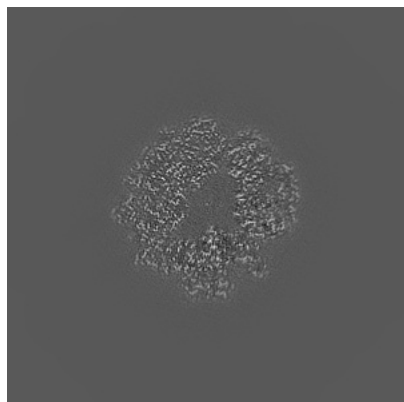


Z Index: 256

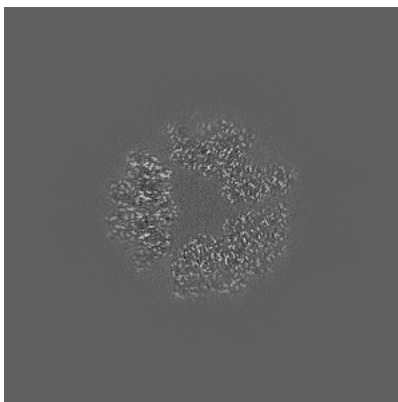
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

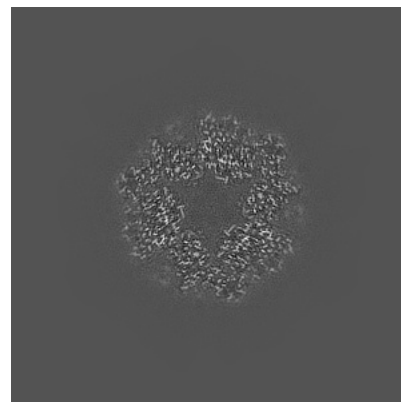
6.3.1 Primary map



X Index: 288

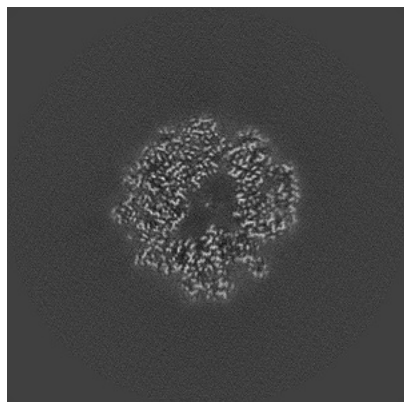


Y Index: 243

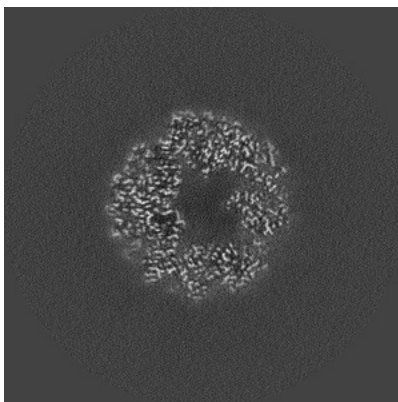


Z Index: 250

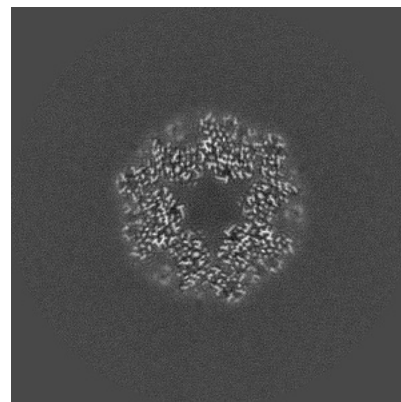
6.3.2 Raw map



X Index: 288



Y Index: 273

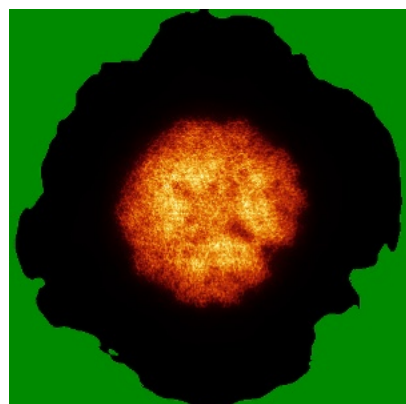


Z Index: 250

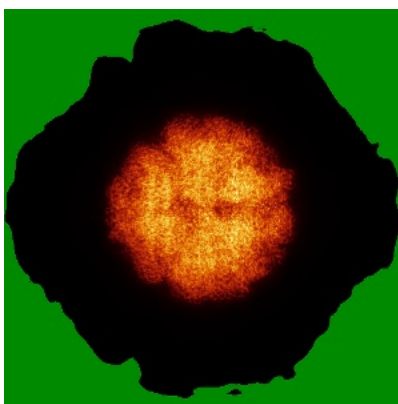
The images above show the largest variance slices of the map in three orthogonal directions.

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

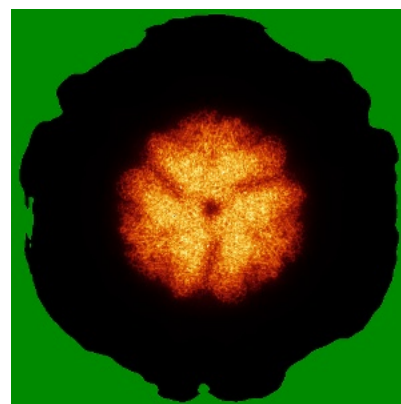
6.4.1 Primary map



X

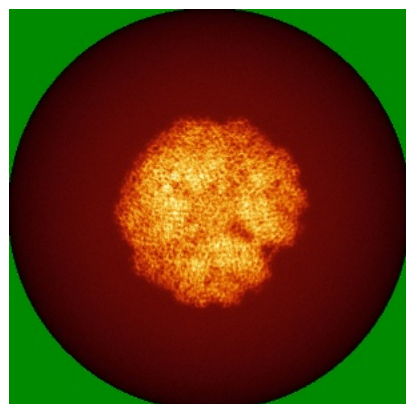


Y

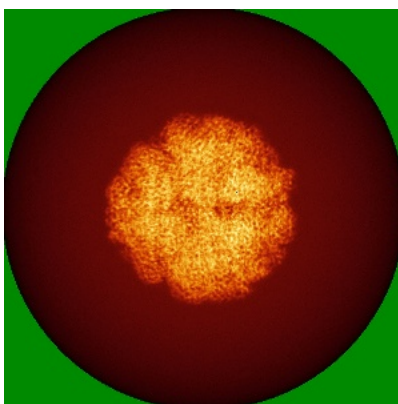


Z

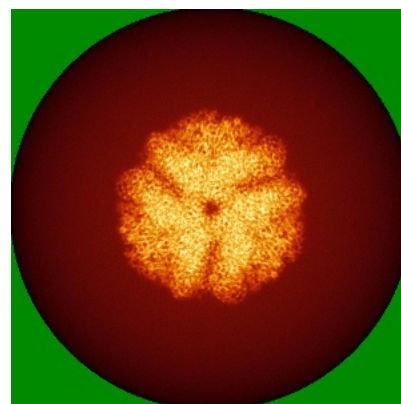
6.4.2 Raw map



X



Y

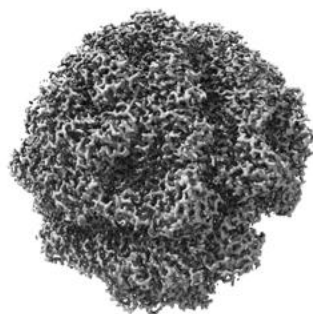


Z

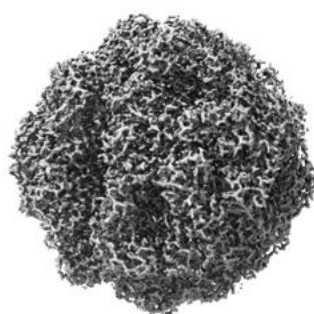
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

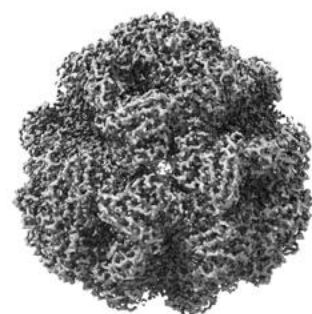
6.5.1 Primary map



X



Y



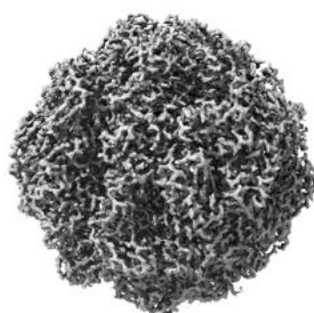
Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

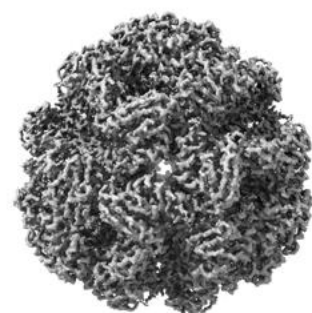
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

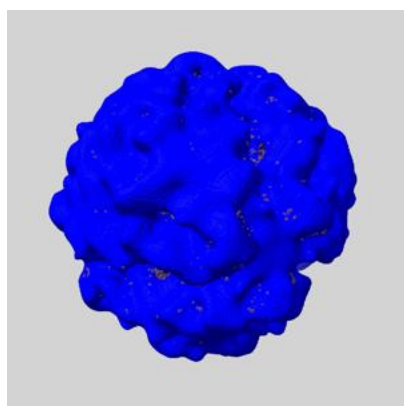
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

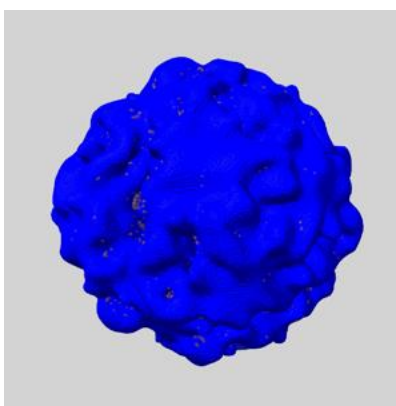
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

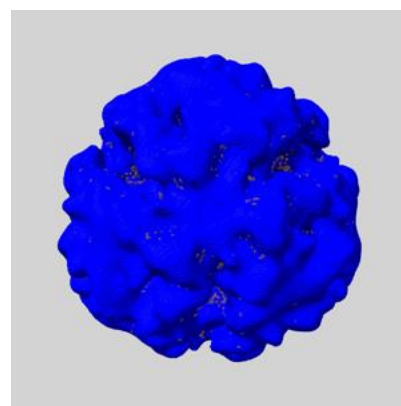
6.6.1 emd_10835_msk_1.map [i](#)



X



Y

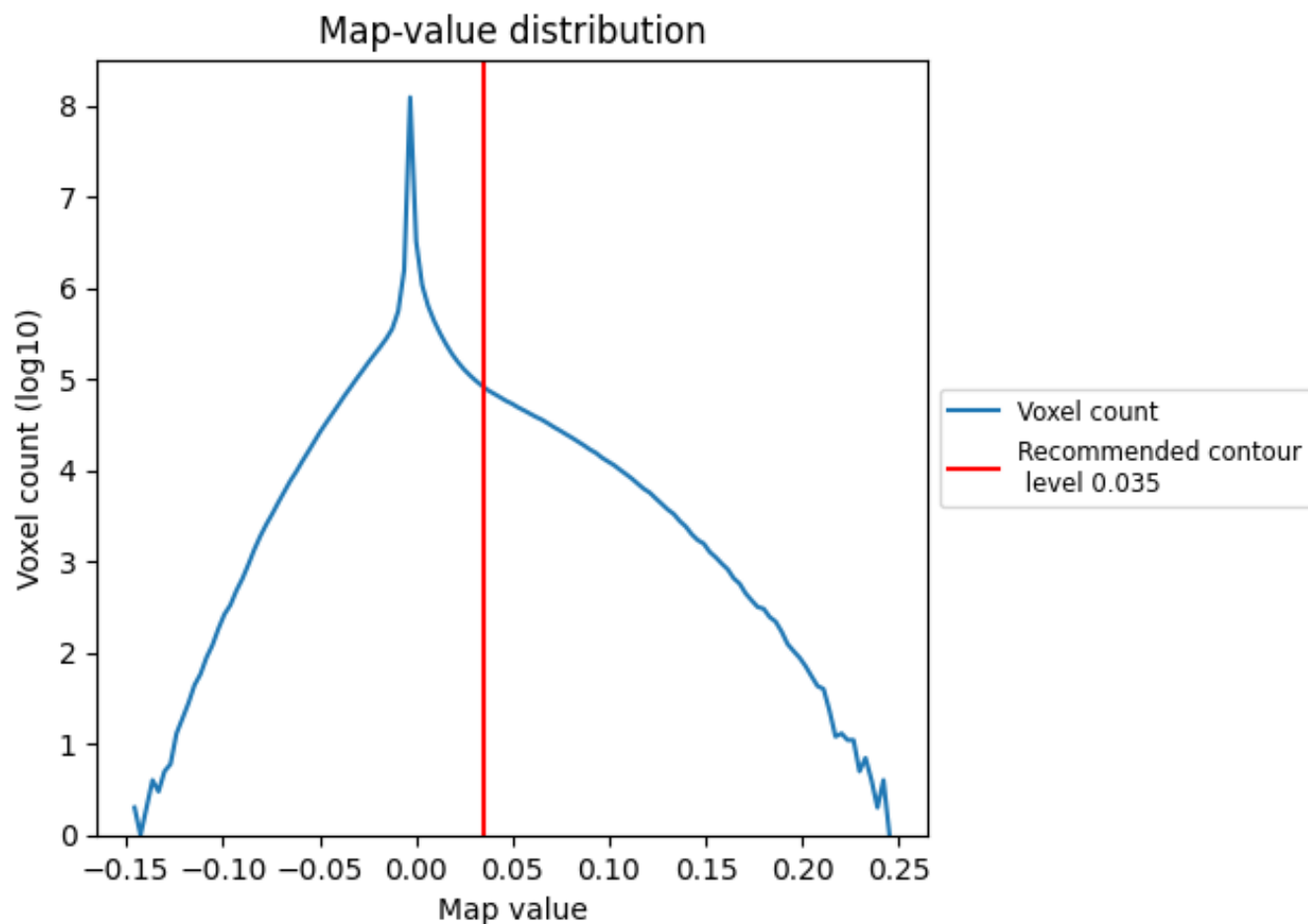


Z

7 Map analysis [i](#)

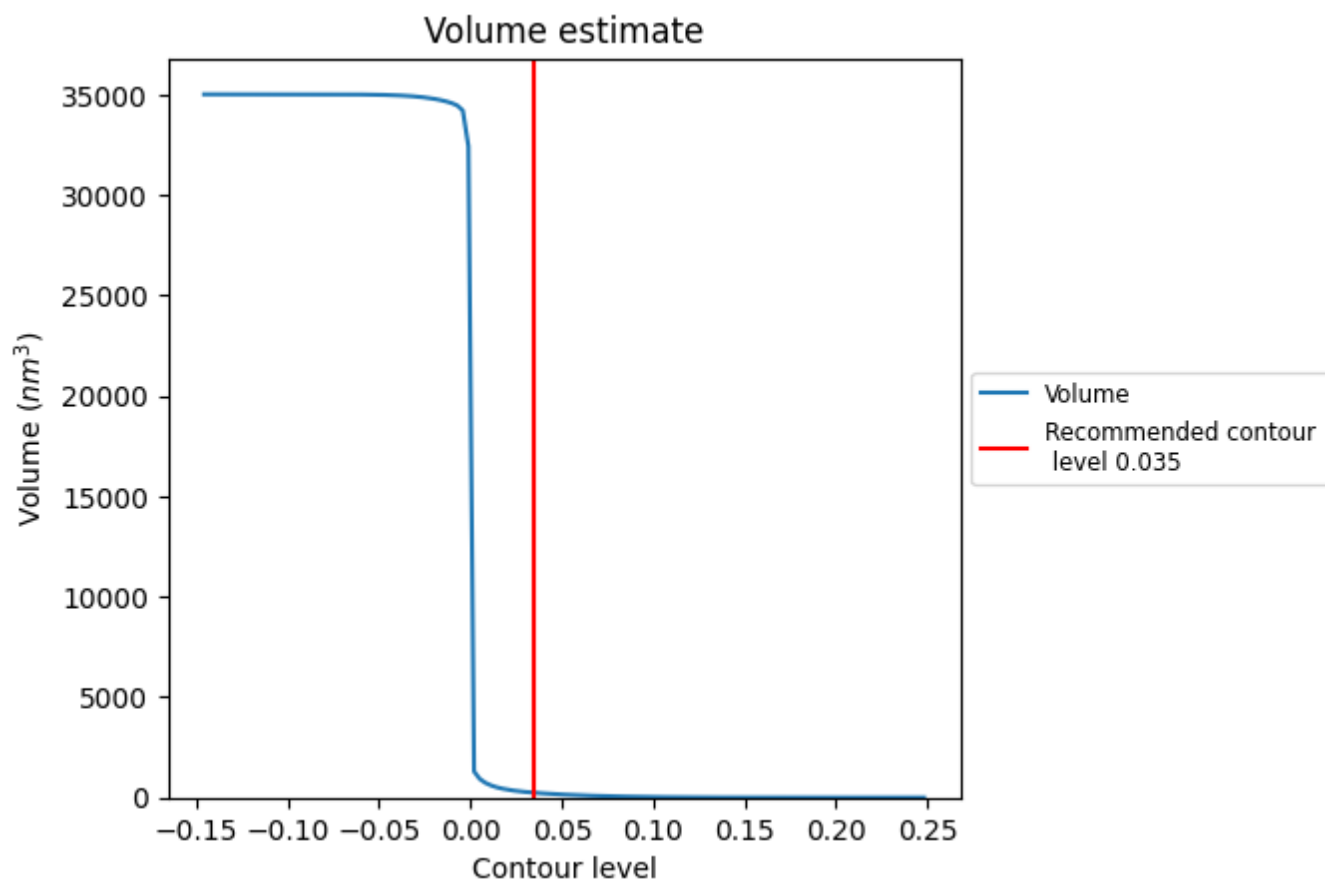
This section contains the results of statistical analysis of the map.

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.

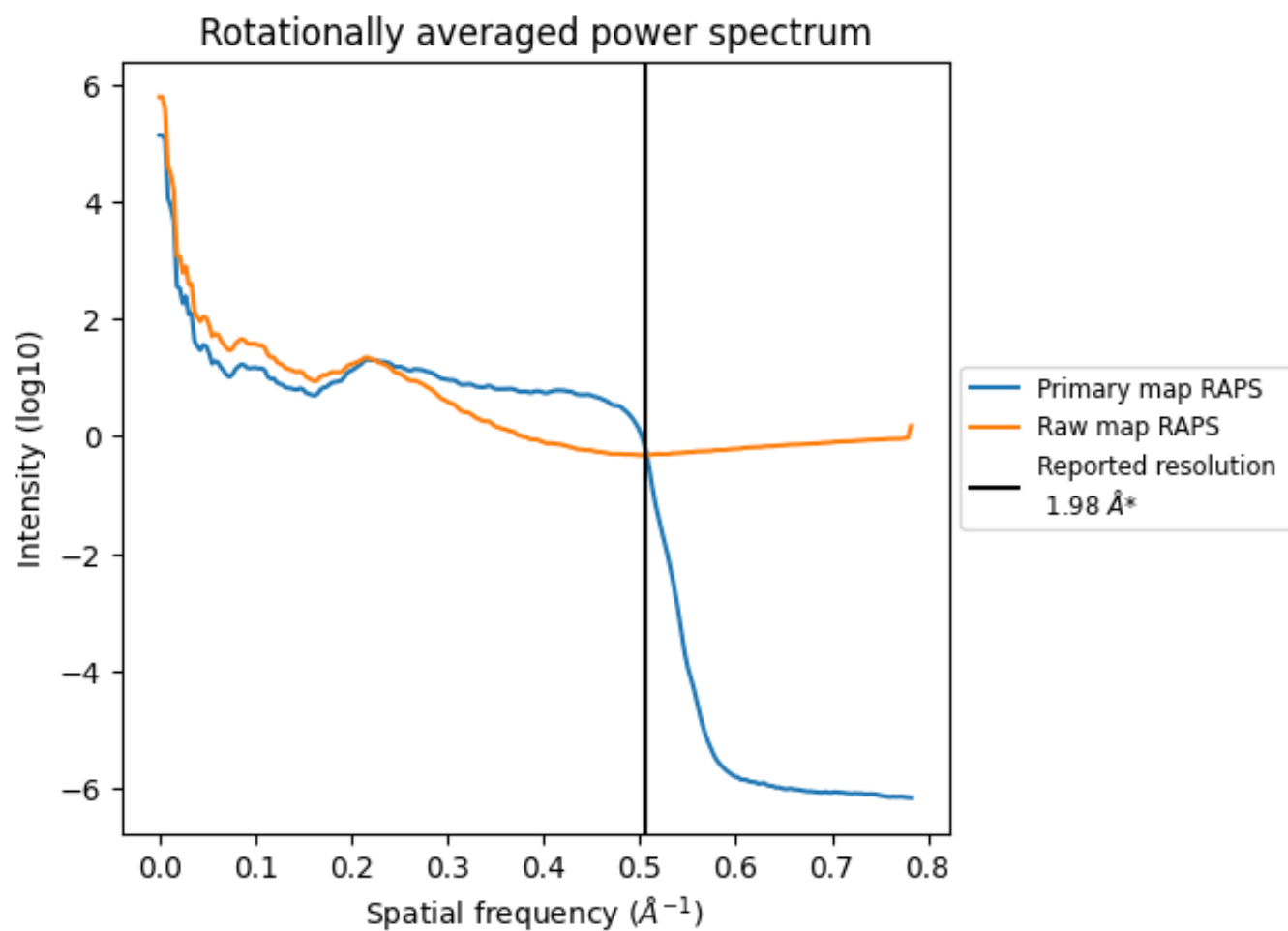
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 240 nm^3 ; this corresponds to an approximate mass of 217 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 ⓘ

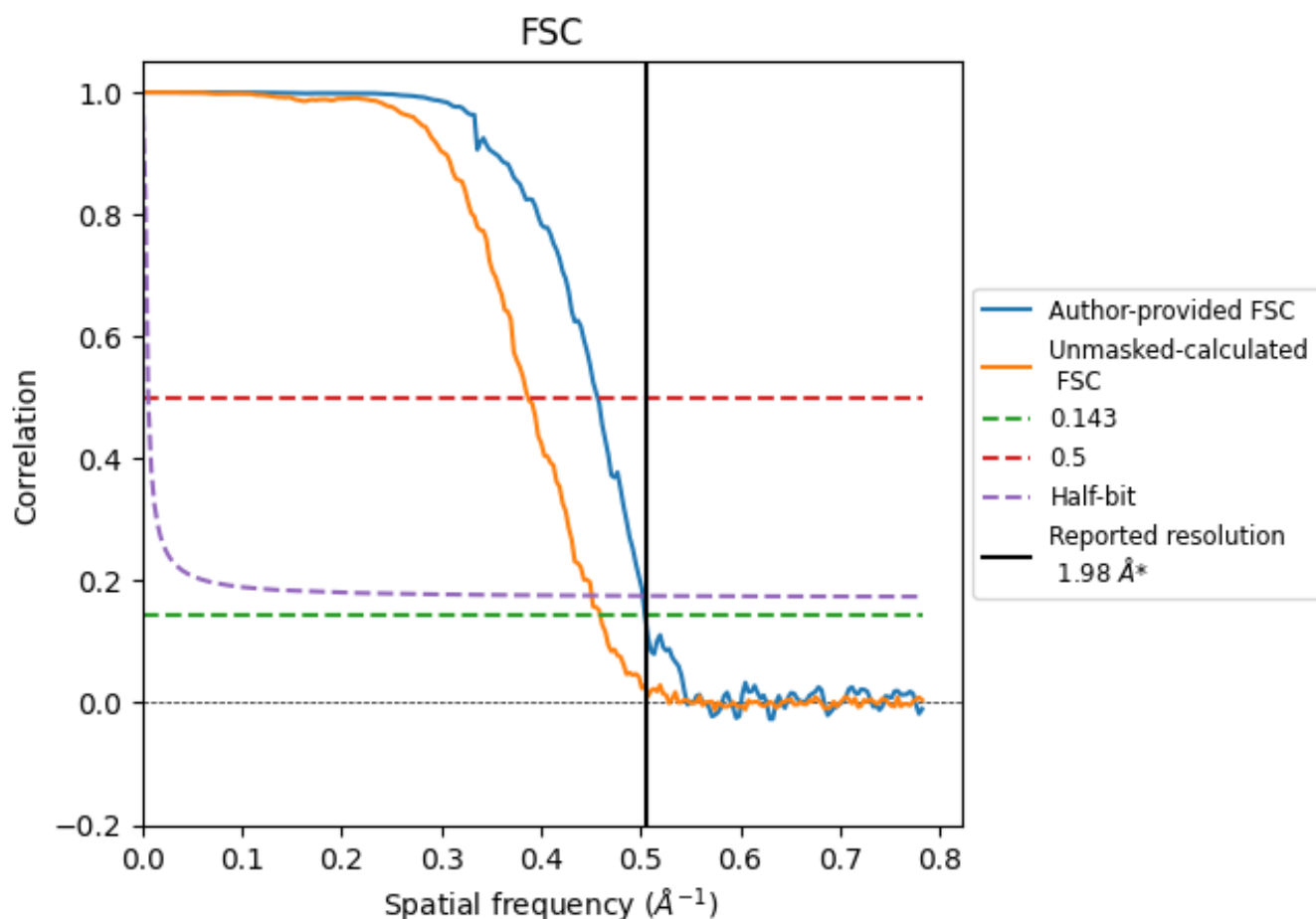


*Reported resolution corresponds to spatial frequency of 0.505 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.505 \AA^{-1}

8.2 Resolution estimates [i](#)

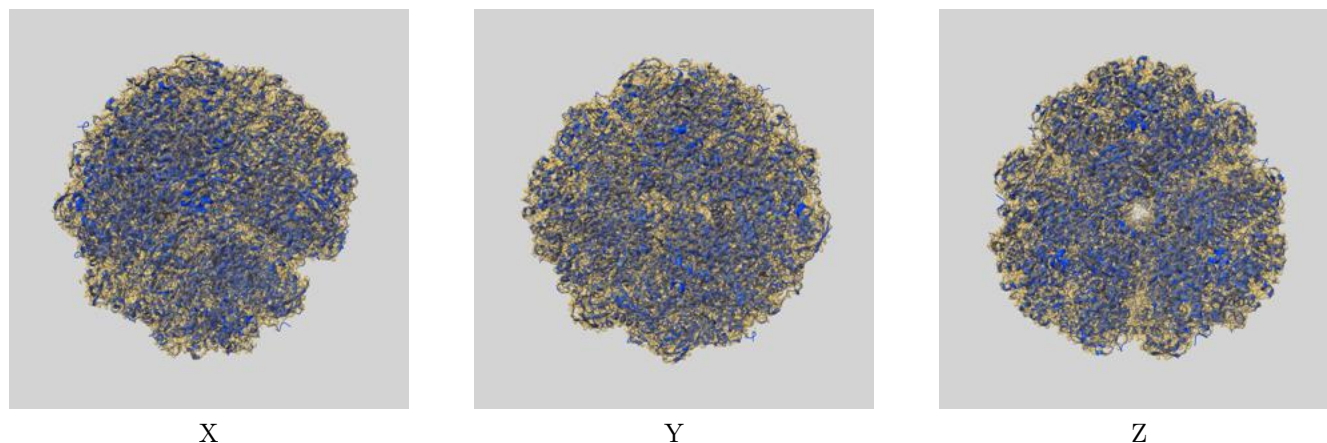
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.98	-	-
Author-provided FSC curve	1.98	2.19	1.99
Unmasked-calculated*	2.18	2.58	2.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.18 differs from the reported value 1.98 by more than 10 %

9 Map-model fit [i](#)

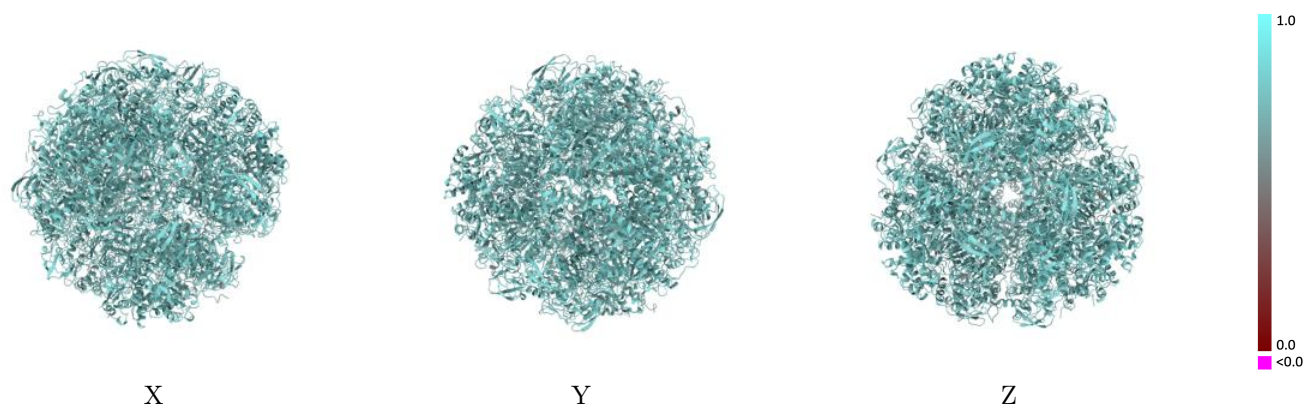
This section contains information regarding the fit between EMDB map EMD-10835 and PDB model 6YL3. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



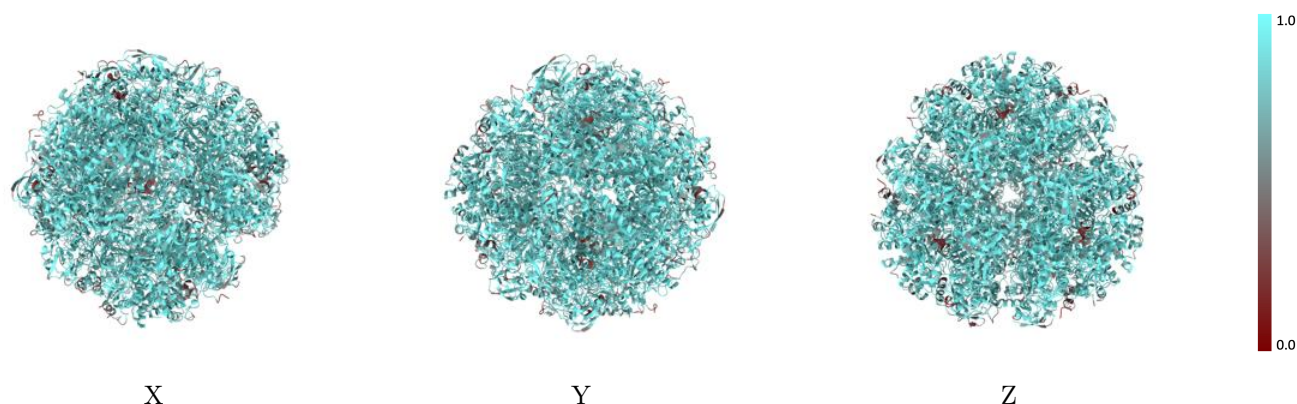
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



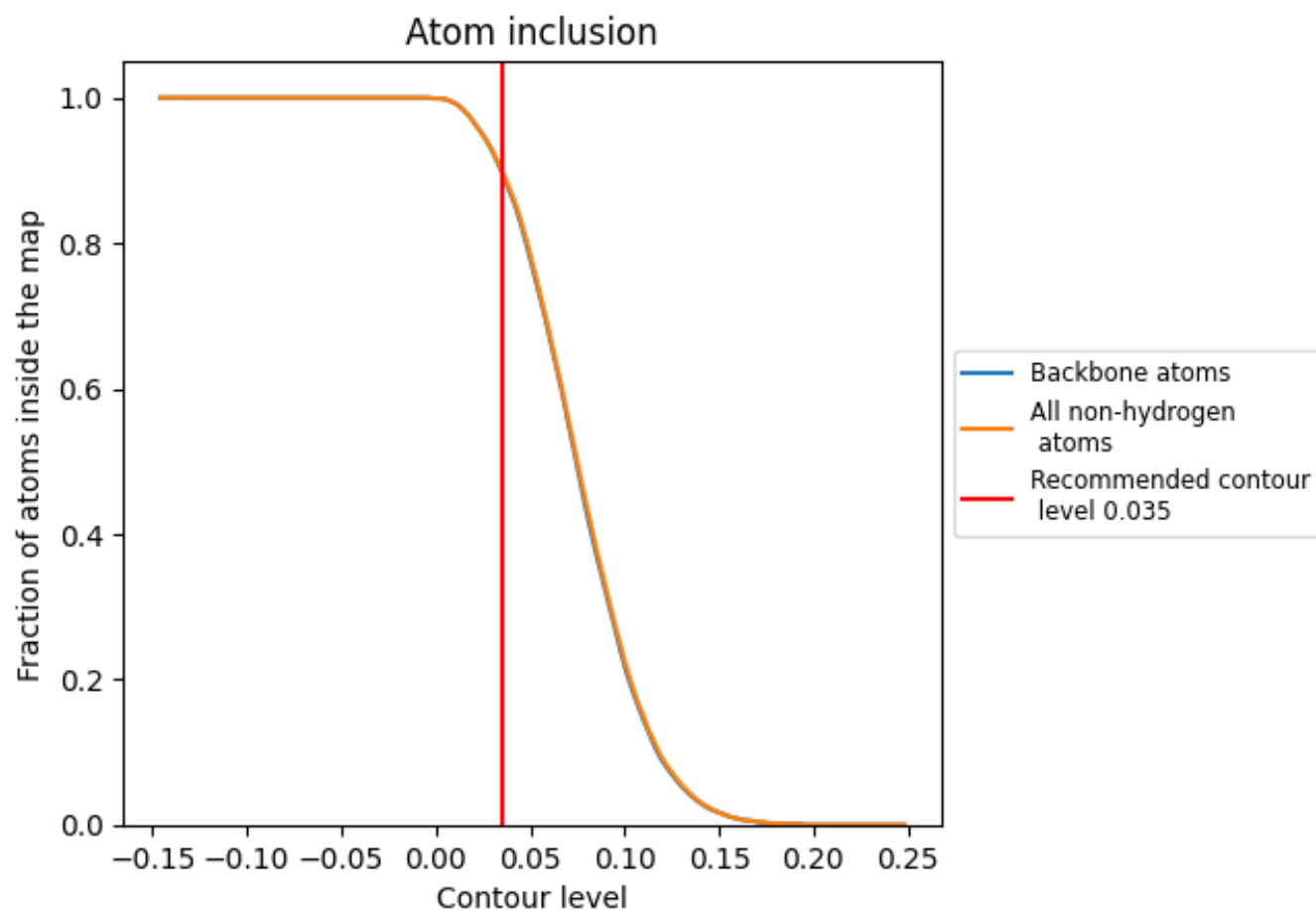
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9000	 0.7670
0	 0.8400	 0.7590
1	 0.9230	 0.7790
2	 0.8770	 0.7620
3	 0.8310	 0.7530
4	 0.9210	 0.7720
5	 0.8810	 0.7610
6	 0.8330	 0.7460
7	 0.9220	 0.7760
8	 0.8770	 0.7570
9	 0.8260	 0.7350
A	 0.8790	 0.7670
B	 0.8420	 0.7630
C	 0.9260	 0.7840
D	 0.8800	 0.7660
E	 0.8340	 0.7590
F	 0.9250	 0.7800
G	 0.8750	 0.7600
H	 0.8390	 0.7560
I	 0.9200	 0.7740
J	 0.8770	 0.7660
K	 0.8250	 0.7360
L	 0.9120	 0.7490
M	 0.8750	 0.7660
N	 0.8340	 0.7560
O	 0.9210	 0.7730
P	 0.8800	 0.7650
Q	 0.8340	 0.7410
R	 0.9200	 0.7700
S	 0.8790	 0.7670
T	 0.8240	 0.7380
U	 0.9140	 0.7600
V	 0.9190	 0.7660
W	 0.8770	 0.7620
X	 0.8380	 0.7580



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Chain	Atom inclusion	Q-score
Y	 0.9230	 0.7760
Z	 0.8830	 0.7640