



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:01 PM UTC

PDB ID : 5MPD / pdb\_00005mpd  
EMDB ID : EMD-3534  
Title : 26S proteasome in presence of ATP (s1)  
Authors : Wehmer, M.; Rudack, T.; Beck, F.; Aufderheide, A.; Pfeifer, G.; Plitzko, J.M.;  
Foerster, F.; Schulten, K.; Baumeister, W.; Sakata, E.  
Deposited on : 2016-12-16  
Resolution : 4.10 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](mailto: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>.

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

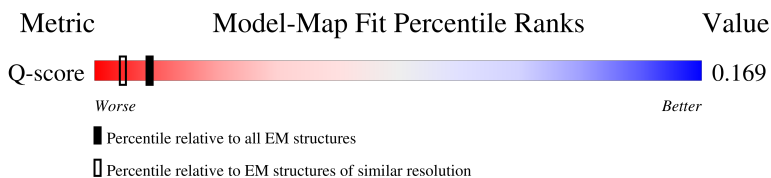
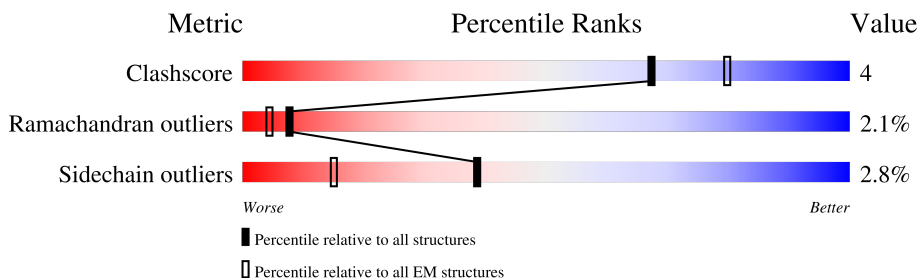
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 ( 3.60 - 4.60 )

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  $\geq 3$ , 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	W	268	
2	V	306	
3	T	274	
4	X	156	

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Mol	Chain	Length	Quality of chain
5	Y	89	
6	Z	993	
7	N	945	
8	S	523	
9	P	445	
10	Q	434	
11	R	429	
12	U	338	
13	O	393	

## 2 Entry composition i

There are 13 unique types of molecules in this entry. The entry contains 40974 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	W	197	1534	962	269	300	3	0	0

- Molecule 2 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	V	289	2274	1425	389	446	14	0	0

- Molecule 3 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	T	266	2192	1405	349	432	6	0	0

- Molecule 4 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	X	127	1032	664	169	195	4	0	0

- Molecule 5 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	Y	51	435	264	69	102	0	0

- Molecule 6 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Z	906	7005	4416	1150	1409	30	0	0

- Molecule 7 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	N	890	6882	4373	1156	1325	28	0	0

- Molecule 8 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	S	475	3894	2488	653	738	15	0	0

- Molecule 9 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	P	440	3608	2297	604	697	10	0	0

- Molecule 10 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Q	434	3499	2225	577	681	16	0	0

- Molecule 11 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	R	381	3060	1955	502	593	10	0	0

- Molecule 12 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	U	298	2373	1496	404	466	7	0	0

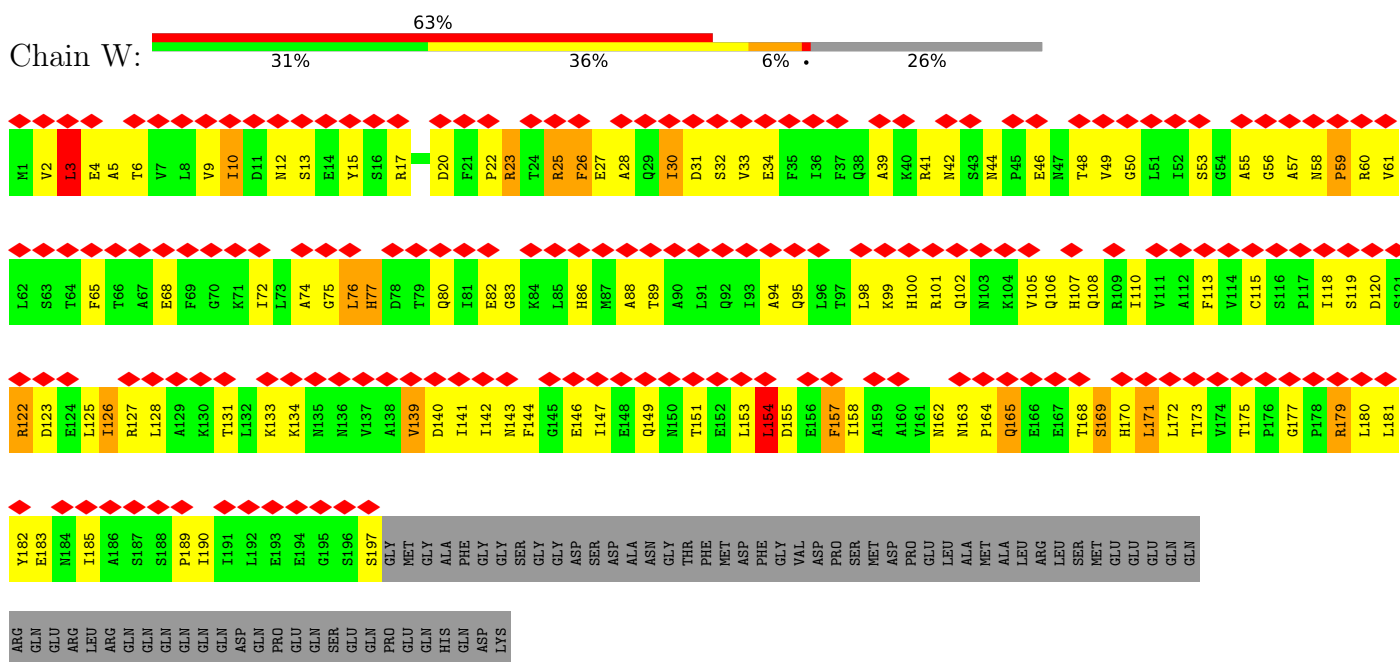
- Molecule 13 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O	388	3186	2051	519	608	8	0	0

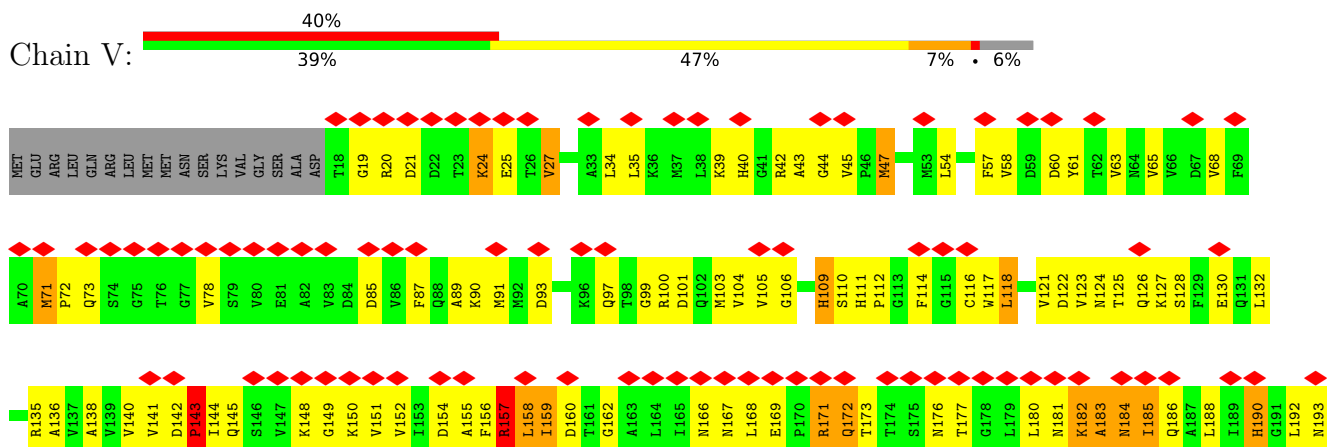
### 3 Residue-property plots

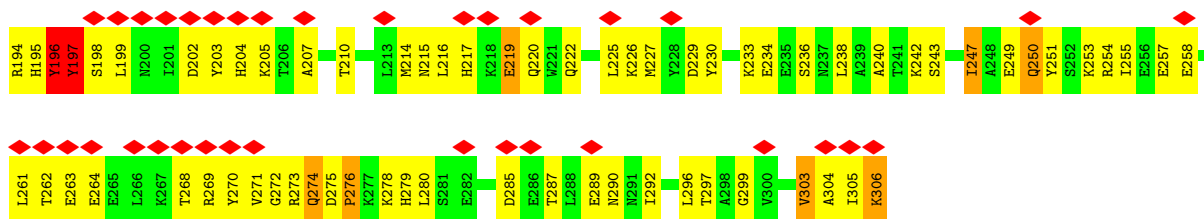
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 26S proteasome regulatory subunit RPN10

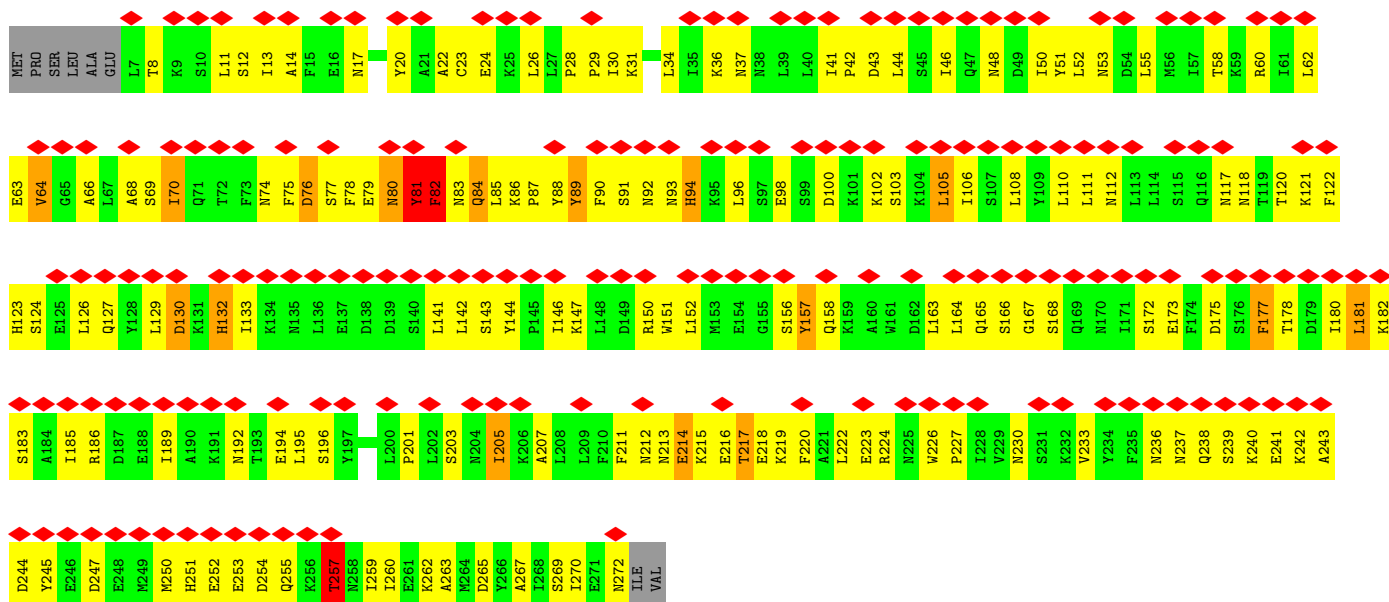


- Molecule 2: Ubiquitin carboxyl-terminal hydrolase RPN11

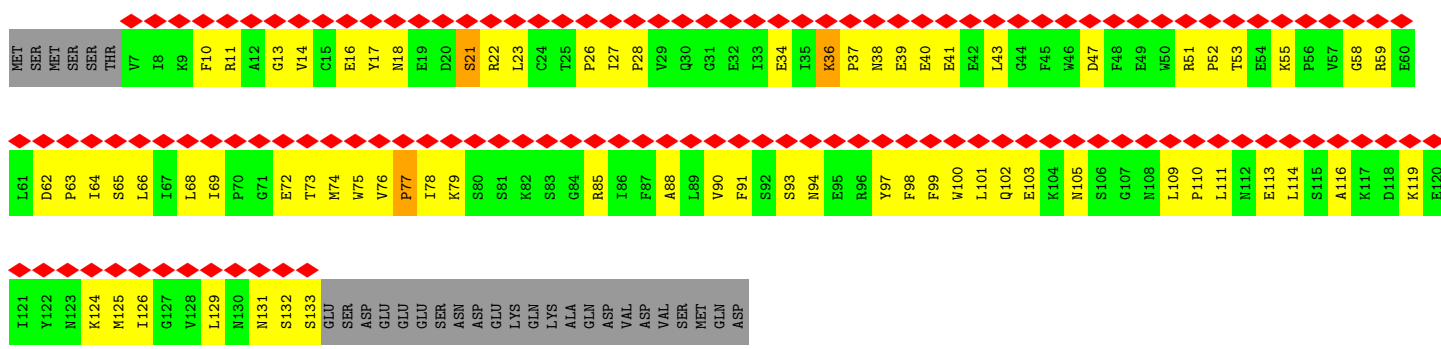
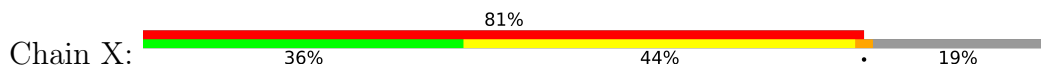




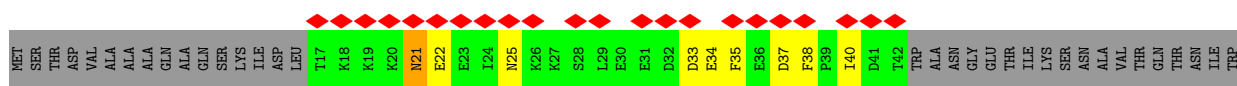
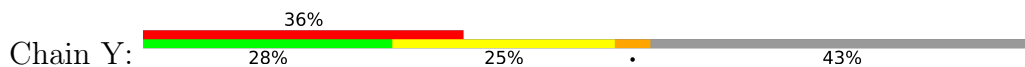
• Molecule 3: 26S proteasome regulatory subunit RPN12



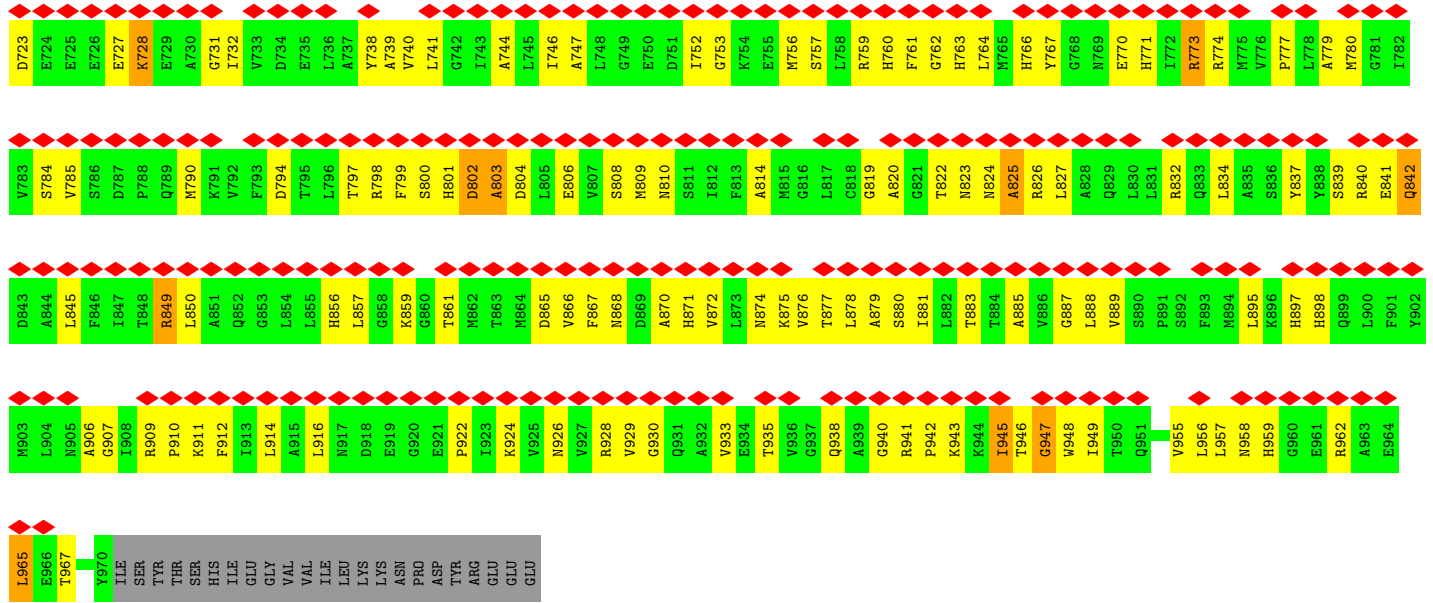
• Molecule 4: 26S proteasome regulatory subunit RPN13



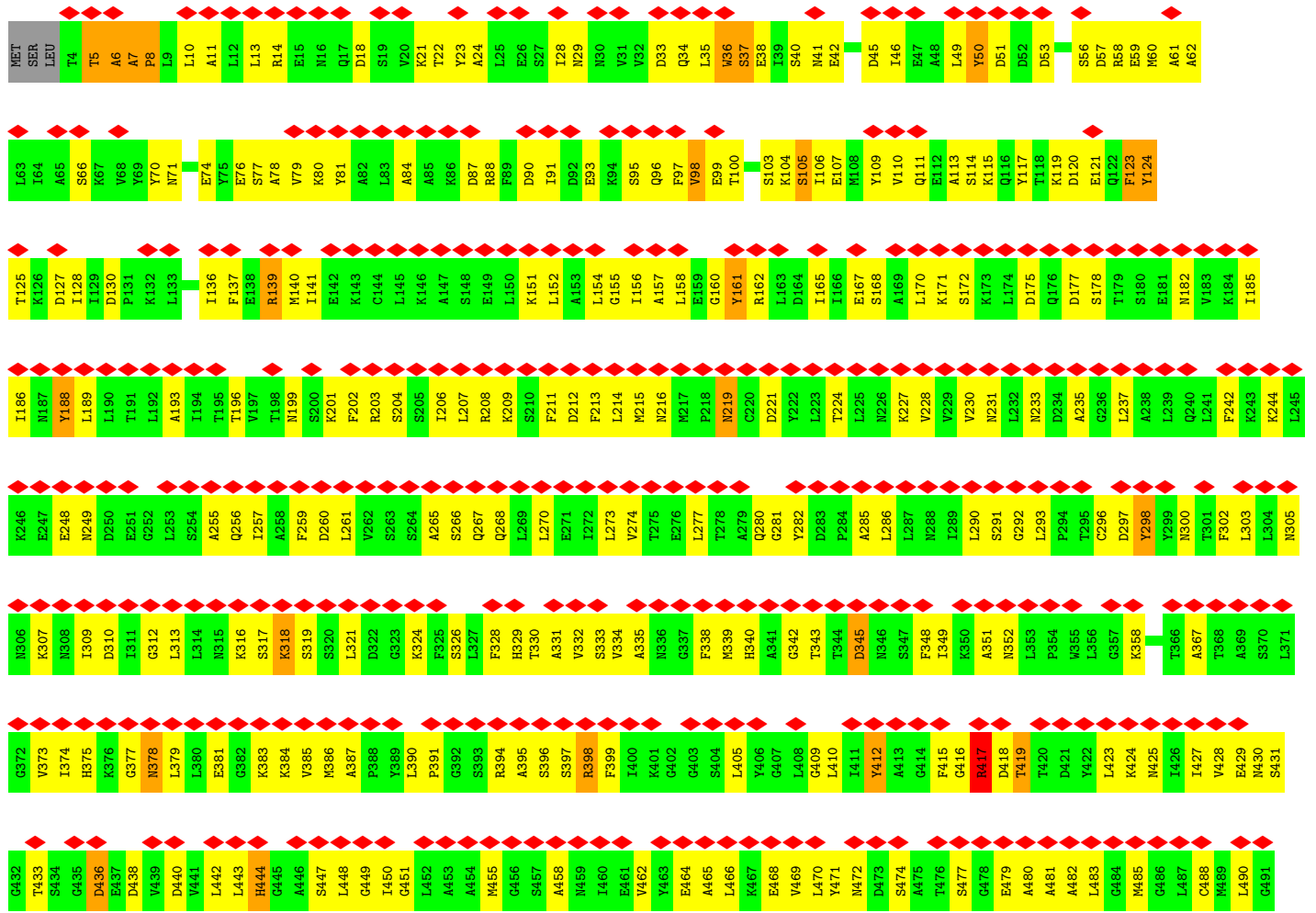
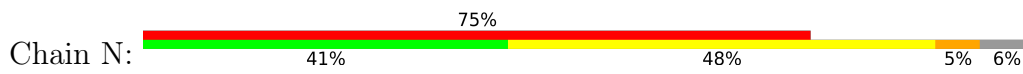
• Molecule 5: 26S proteasome complex subunit SEM1

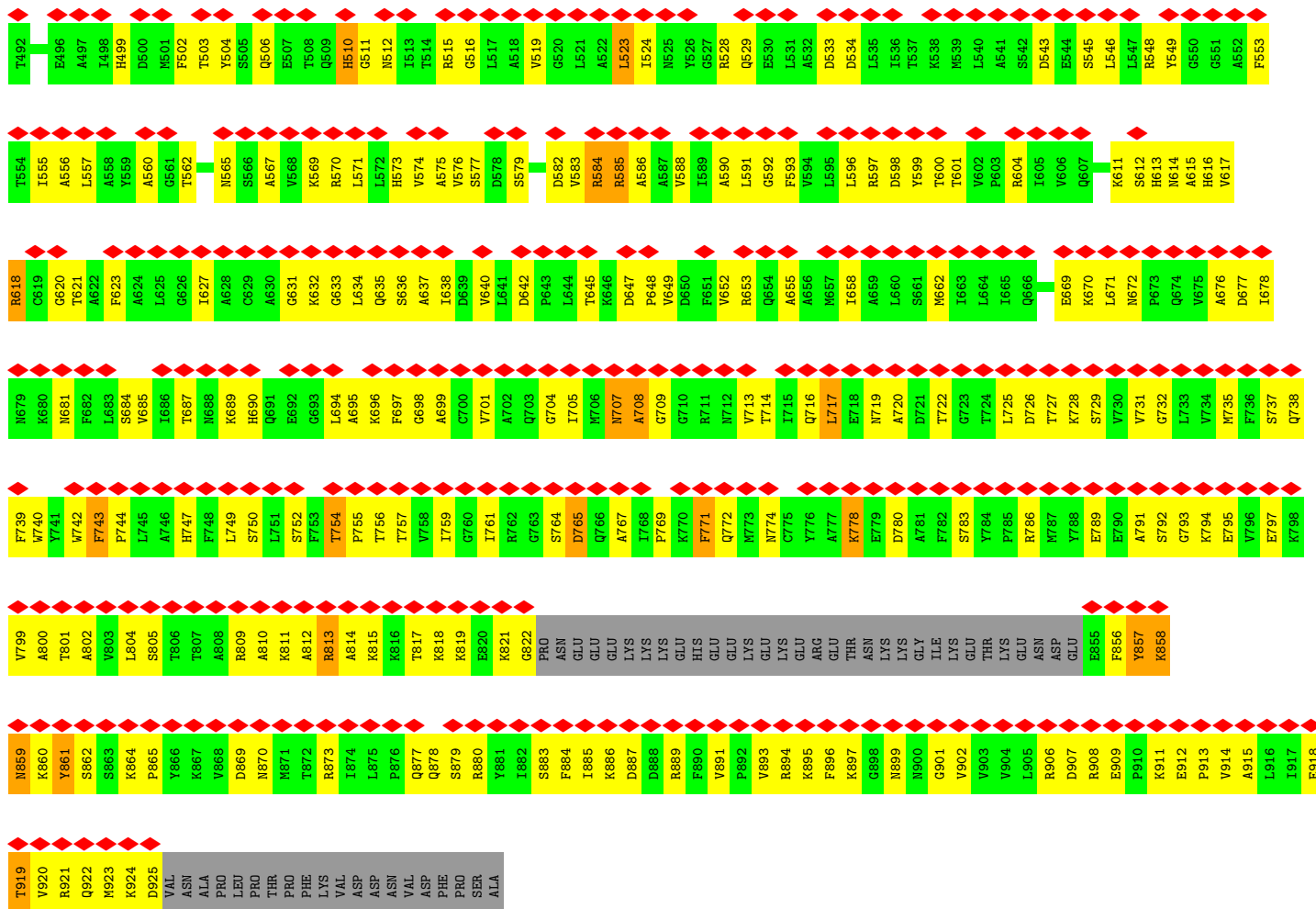




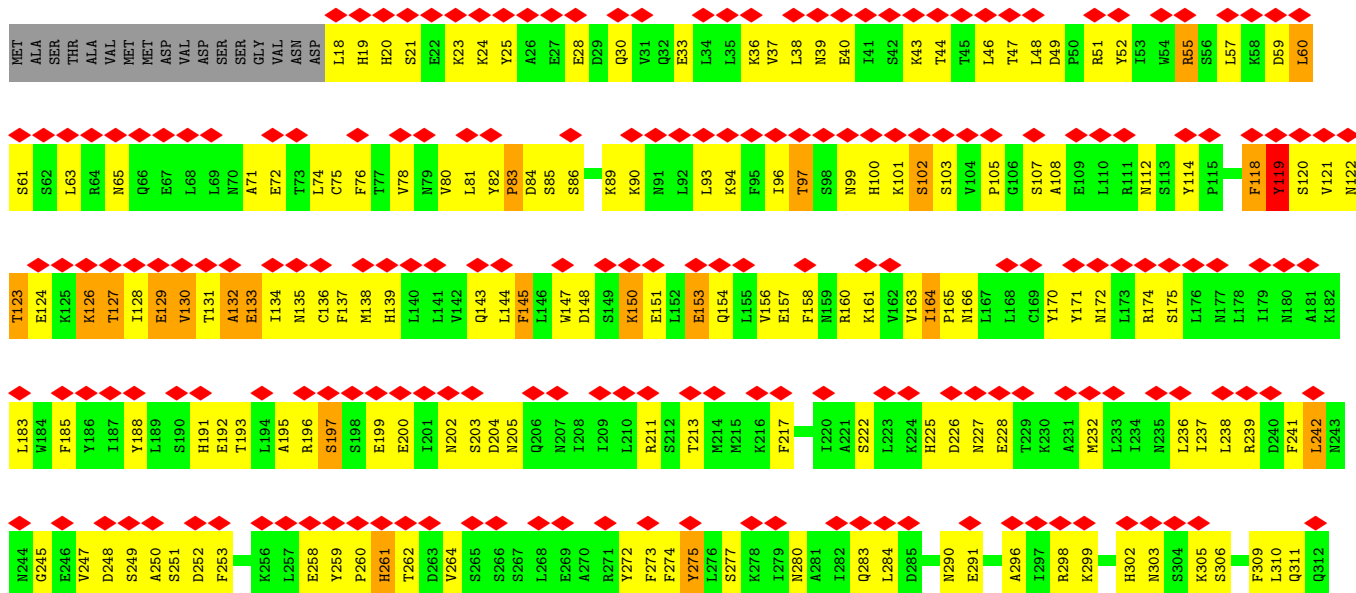
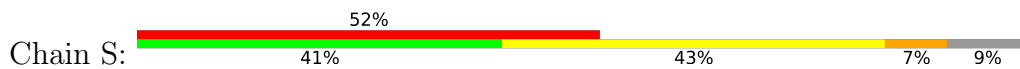


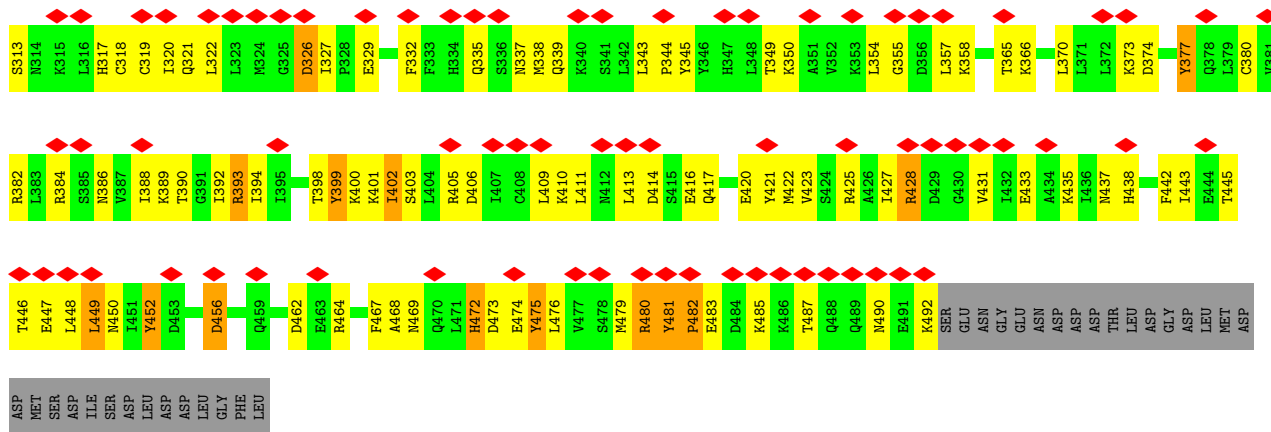
• Molecule 7: 26S proteasome regulatory subunit RPN2



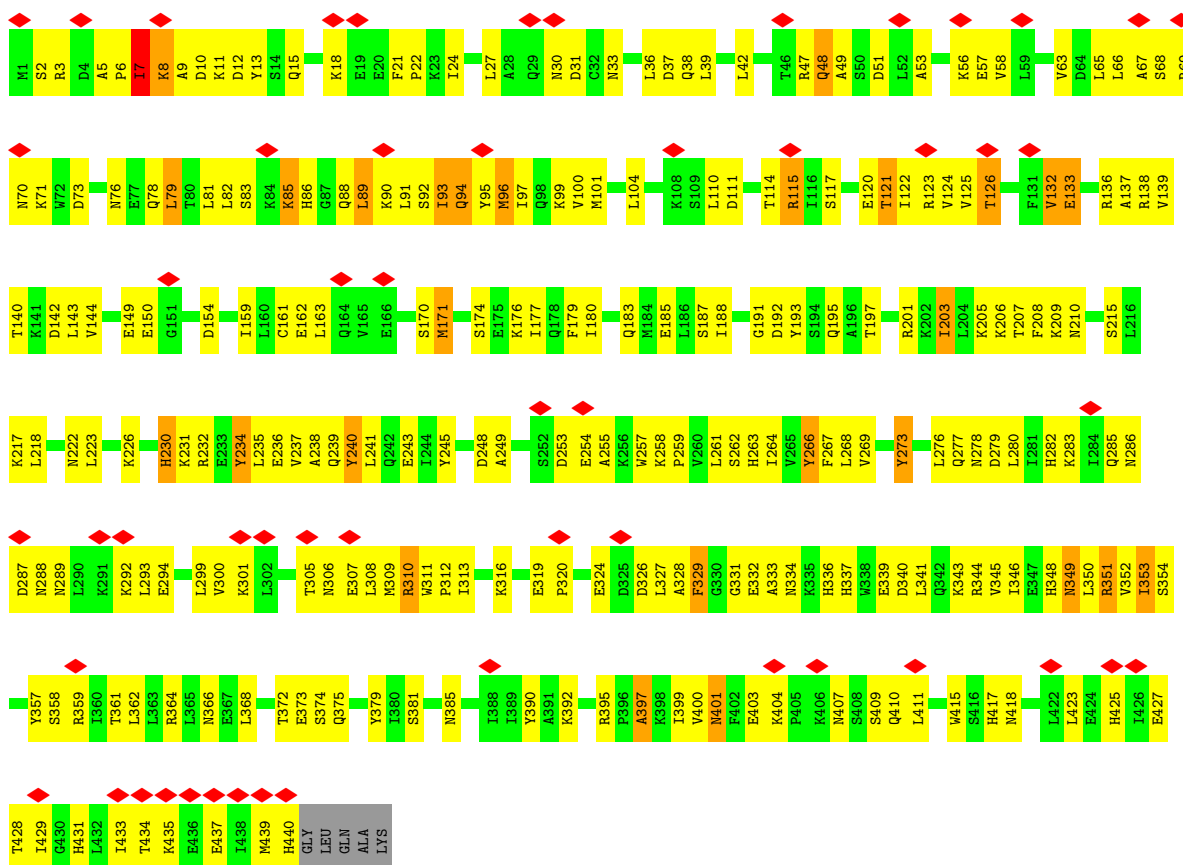
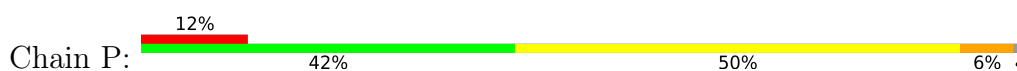


• Molecule 8: 26S proteasome regulatory subunit RPN3

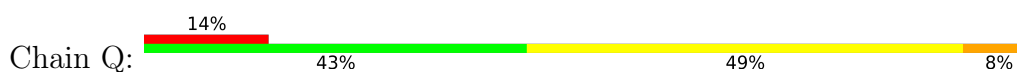


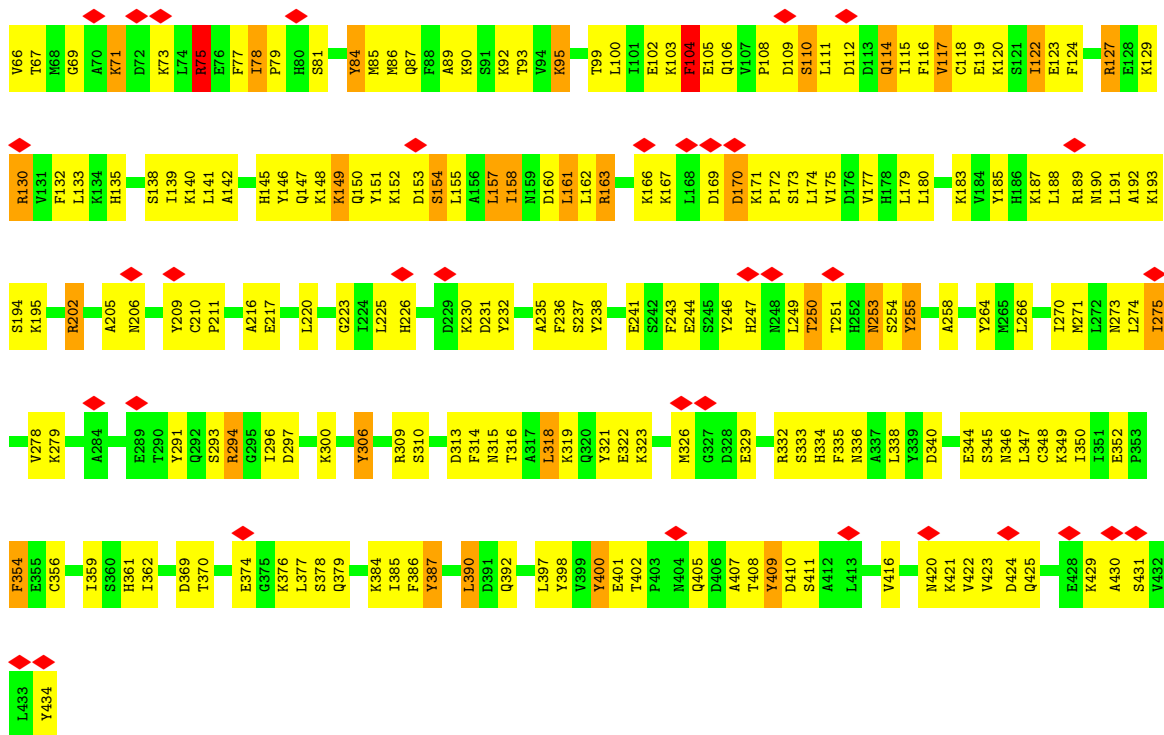


• Molecule 9: 26S proteasome regulatory subunit RPN5

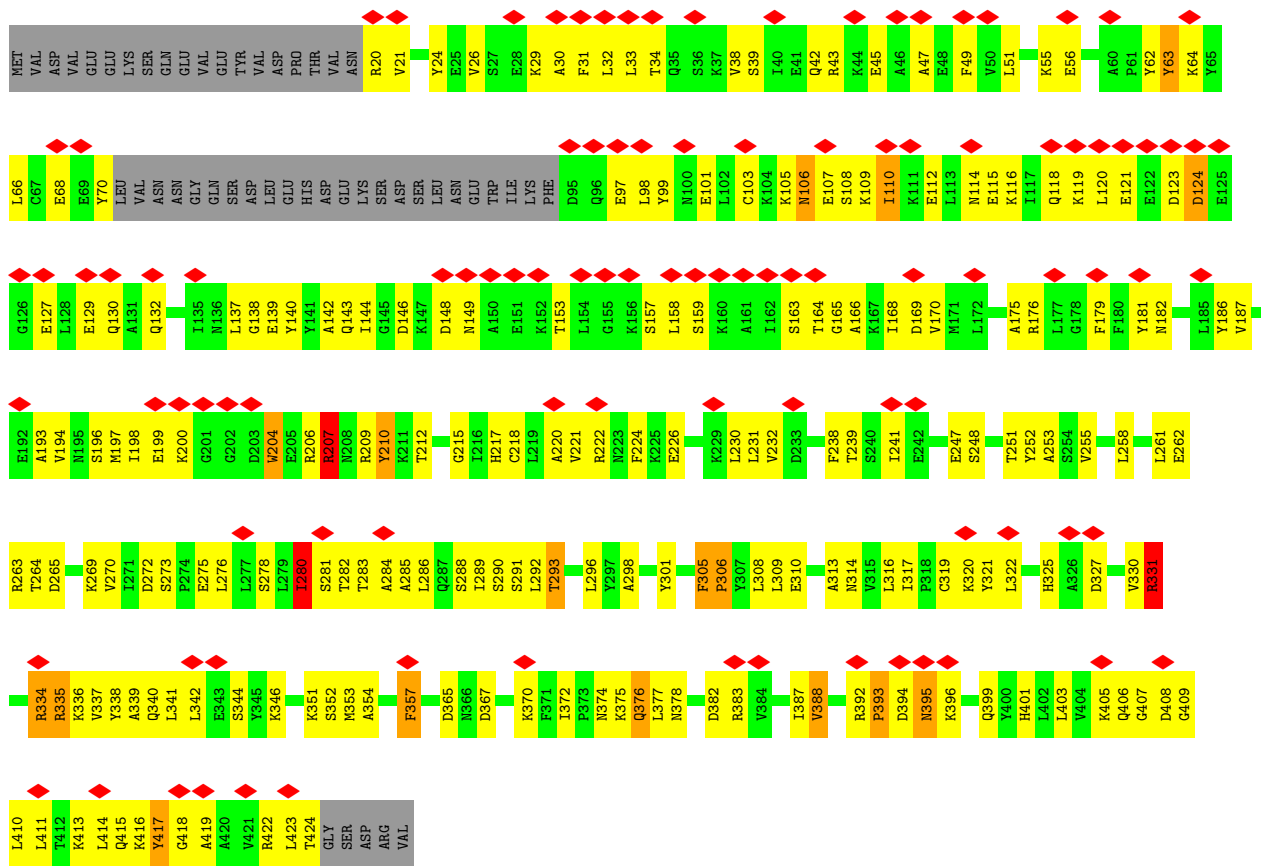


• Molecule 10: 26S proteasome regulatory subunit RPN6

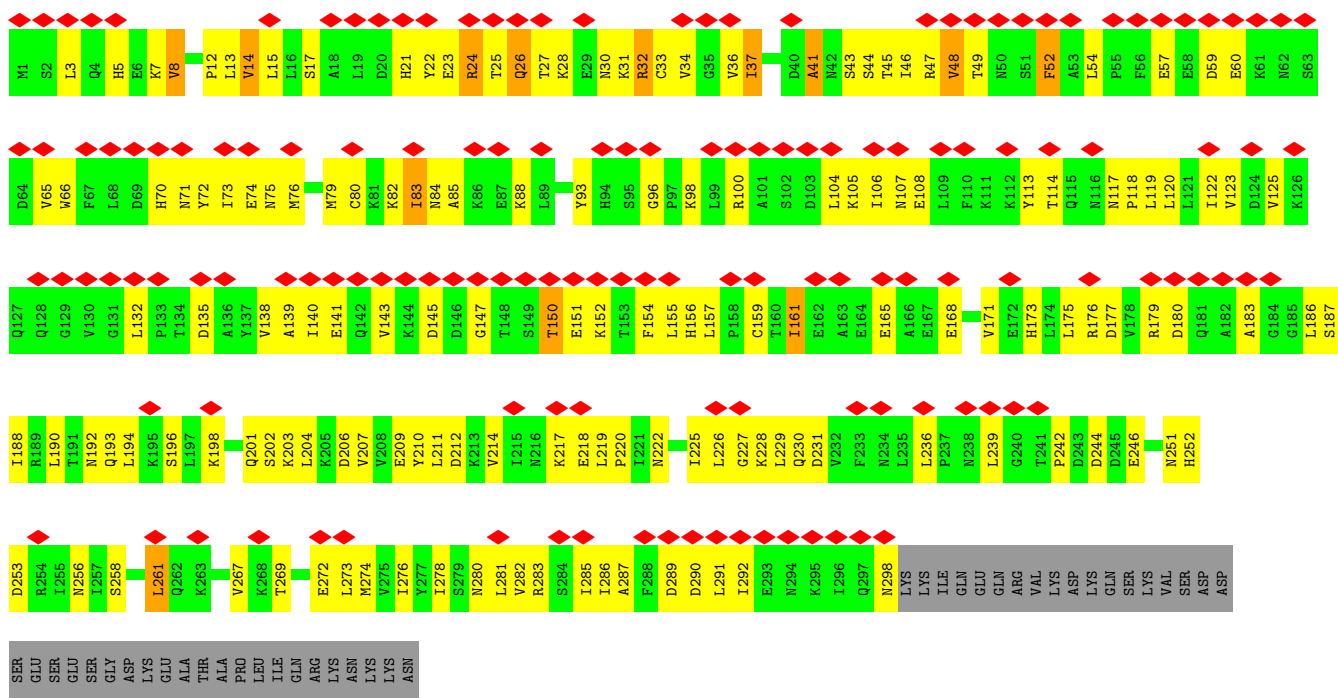




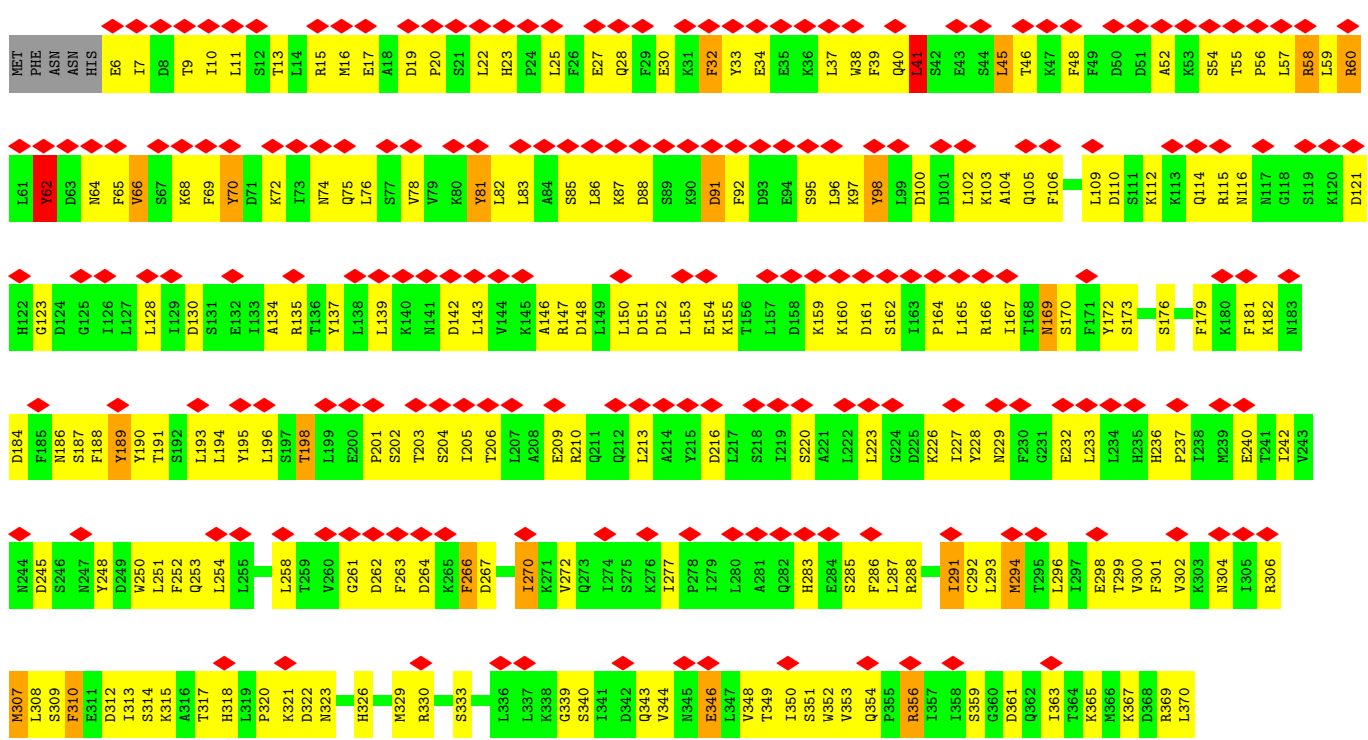
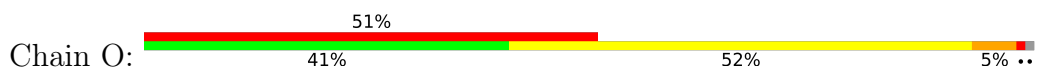
• Molecule 11: 26S proteasome regulatory subunit RPN7

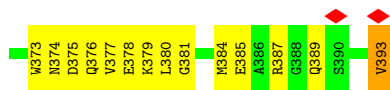


• Molecule 12: 26S proteasome regulatory subunit RPN8



• Molecule 13: 26S proteasome regulatory subunit RPN9





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	286500	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 ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.211	Depositor
Minimum map value	-0.133	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.38, 1.38, 1.38	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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	W	2.23	61/1557 (3.9%)	2.34	97/2111 (4.6%)
2	V	2.31	92/2309 (4.0%)	2.39	128/3115 (4.1%)
3	T	2.26	83/2235 (3.7%)	2.45	151/3017 (5.0%)
4	X	2.23	31/1058 (2.9%)	2.32	51/1432 (3.6%)
5	Y	2.24	18/438 (4.1%)	2.28	22/583 (3.8%)
6	Z	2.22	254/7122 (3.6%)	2.43	499/9645 (5.2%)
7	N	2.33	293/6994 (4.2%)	2.40	440/9455 (4.7%)
8	S	2.24	150/3966 (3.8%)	2.49	295/5355 (5.5%)
9	P	2.24	138/3663 (3.8%)	2.38	238/4940 (4.8%)
10	Q	2.24	119/3556 (3.3%)	2.42	252/4787 (5.3%)
11	R	2.24	128/3110 (4.1%)	2.41	193/4193 (4.6%)
12	U	2.17	77/2407 (3.2%)	2.38	156/3258 (4.8%)
13	O	2.20	112/3247 (3.4%)	2.43	222/4380 (5.1%)
All	All	2.25	1556/41662 (3.7%)	2.41	2744/56271 (4.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	W	0	6
2	V	0	5
3	T	0	6
4	X	0	2
5	Y	0	1
6	Z	0	12
7	N	0	23
8	S	0	14
9	P	0	8
10	Q	0	19
11	R	0	12
12	U	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	O	0	11
All	All	0	123

All (1556) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	8	PRO	CA-CB	42.98	2.17	1.53
8	S	127	THR	CA-CB	16.44	1.80	1.53
7	N	738	GLN	CA-C	-13.02	1.37	1.52
2	V	196	TYR	CA-CB	12.27	1.74	1.53
5	Y	89	GLN	C-OXT	-11.57	1.00	1.23
9	P	440	HIS	C-O	-11.57	1.00	1.23
3	T	272	ASN	C-O	-11.57	1.00	1.23
13	O	393	VAL	C-O	-11.57	1.00	1.23
10	Q	434	TYR	C-O	-11.56	1.00	1.23
2	V	306	LYS	C-O	-11.55	1.00	1.23
4	X	133	SER	C-O	-11.55	1.00	1.23
7	N	925	ASP	C-O	-11.55	1.00	1.23
1	W	197	SER	C-O	-11.54	1.00	1.23
10	Q	434	TYR	C-OXT	-11.54	1.00	1.23
11	R	424	THR	C-O	-11.54	1.00	1.23
13	O	393	VAL	C-OXT	-11.54	1.00	1.23
2	V	306	LYS	C-OXT	-11.54	1.00	1.23
8	S	492	LYS	C-O	-11.53	1.00	1.23
5	Y	89	GLN	C-O	-11.51	1.00	1.23
7	N	909	GLU	C-N	11.40	1.42	1.33
1	W	25	ARG	NE-CZ	11.21	1.45	1.33
2	V	216	LEU	N-CA	-10.74	1.37	1.47
6	Z	753	GLY	CA-C	-10.69	1.39	1.52
9	P	261	LEU	C-N	10.58	1.47	1.33
6	Z	806	GLU	CA-C	10.49	1.61	1.52
10	Q	162	LEU	CA-C	-10.21	1.44	1.52
7	N	155	GLY	N-CA	-10.15	1.33	1.45
7	N	88	ARG	NE-CZ	10.14	1.44	1.33
7	N	604	ARG	CZ-NH2	10.09	1.46	1.33
13	O	162	SER	C-N	10.07	1.44	1.33
2	V	140	VAL	CA-C	-10.00	1.40	1.52
9	P	423	LEU	CA-C	-9.97	1.39	1.52
3	T	265	ASP	N-CA	-9.90	1.34	1.46
10	Q	254	SER	CA-C	-9.74	1.39	1.52
7	N	485	MET	CA-C	-9.69	1.40	1.52
3	T	186	ARG	NE-CZ	9.59	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Q	226	HIS	ND1-CE1	9.57	1.42	1.32
7	N	889	ARG	NE-CZ	9.45	1.43	1.33
7	N	417	ARG	NE-CZ	9.38	1.43	1.33
8	S	103	SER	C-N	9.35	1.44	1.33
12	U	34	VAL	N-CA	-9.34	1.35	1.46
9	P	2	SER	CA-C	-9.28	1.42	1.52
10	Q	50	ARG	CD-NE	9.28	1.59	1.46
7	N	516	GLY	CA-C	-9.22	1.41	1.52
8	S	476	LEU	CA-C	-9.14	1.41	1.52
2	V	171	ARG	NE-CZ	9.06	1.43	1.33
3	T	224	ARG	CD-NE	8.98	1.58	1.46
6	Z	856	HIS	ND1-CE1	8.96	1.41	1.32
9	P	47	ARG	NE-CZ	8.92	1.42	1.33
3	T	118	ASN	CA-C	-8.87	1.42	1.53
9	P	263	HIS	ND1-CE1	8.87	1.41	1.32
3	T	17	ASN	CA-C	8.85	1.64	1.52
9	P	310	ARG	CD-NE	8.84	1.58	1.46
7	N	893	VAL	N-CA	-8.78	1.36	1.46
7	N	802	ALA	C-N	8.78	1.44	1.33
12	U	253	ASP	CA-CB	8.76	1.67	1.53
5	Y	65	ASP	CA-CB	-8.76	1.35	1.53
3	T	260	ILE	N-CA	-8.75	1.35	1.46
6	Z	924	LYS	CA-C	-8.75	1.41	1.52
9	P	425	HIS	CA-C	-8.68	1.41	1.52
12	U	32	ARG	CD-NE	8.67	1.58	1.46
12	U	132	LEU	CA-C	-8.65	1.43	1.53
13	O	41	LEU	N-CA	-8.62	1.35	1.46
9	P	266	TYR	CA-C	-8.60	1.41	1.52
7	N	66	SER	CA-C	-8.59	1.42	1.52
7	N	786	ARG	NE-CZ	8.59	1.42	1.33
10	Q	349	LYS	CA-CB	8.59	1.66	1.53
9	P	136	ARG	CA-C	-8.58	1.41	1.52
9	P	332	GLU	N-CA	-8.56	1.36	1.46
10	Q	390	LEU	CA-CB	8.53	1.64	1.53
9	P	114	THR	CA-C	-8.51	1.42	1.52
10	Q	416	VAL	CA-C	-8.47	1.42	1.52
13	O	375	ASP	CA-C	-8.46	1.41	1.52
8	S	311	GLN	CA-C	-8.45	1.41	1.52
11	R	207	ARG	NE-CZ	8.39	1.42	1.33
2	V	261	LEU	CA-CB	8.38	1.65	1.53
6	Z	558	LEU	N-CA	-8.32	1.36	1.46
10	Q	3	LEU	N-CA	-8.30	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O	60	ARG	N-CA	-8.24	1.36	1.46
8	S	480	ARG	CD-NE	8.24	1.57	1.46
3	T	11	LEU	CA-CB	8.23	1.66	1.53
10	Q	17	GLU	N-CA	8.20	1.56	1.46
7	N	906	ARG	NE-CZ	8.19	1.42	1.33
6	Z	819	GLY	CA-C	-8.18	1.43	1.52
7	N	488	CYS	C-N	8.18	1.44	1.33
13	O	173	SER	N-CA	-8.17	1.36	1.46
3	T	66	ALA	CA-C	-8.17	1.42	1.52
1	W	180	LEU	CA-C	-8.15	1.41	1.52
3	T	69	SER	CA-C	-8.14	1.41	1.52
7	N	902	VAL	CA-CB	-8.13	1.44	1.54
12	U	120	LEU	N-CA	-8.11	1.35	1.46
6	Z	876	VAL	C-N	8.11	1.44	1.33
9	P	161	CYS	N-CA	-8.09	1.35	1.46
13	O	135	ARG	NE-CZ	8.09	1.42	1.33
3	T	252	GLU	N-CA	-8.09	1.36	1.46
7	N	571	LEU	CA-C	-8.08	1.42	1.52
1	W	101	ARG	CD-NE	8.08	1.57	1.46
13	O	201	PRO	C-N	8.08	1.44	1.33
7	N	139	ARG	NE-CZ	8.05	1.42	1.33
8	S	392	ILE	CA-C	-8.03	1.42	1.53
8	S	119	TYR	C-N	8.03	1.44	1.33
10	Q	210	CYS	CA-C	8.03	1.62	1.53
7	N	869	ASP	C-N	8.02	1.44	1.33
9	P	188	ILE	N-CA	8.02	1.56	1.46
13	O	106	PHE	CA-CB	8.01	1.66	1.53
7	N	440	ASP	CA-C	-7.99	1.42	1.52
7	N	759	ILE	CA-C	-7.99	1.42	1.52
6	Z	773	ARG	CA-C	-7.98	1.42	1.52
3	T	37	ASN	N-CA	-7.98	1.36	1.46
6	Z	759	ARG	CZ-NH2	7.94	1.43	1.33
7	N	885	ILE	CA-C	-7.92	1.44	1.53
6	Z	498	ALA	C-O	-7.92	1.17	1.24
7	N	772	GLN	CA-C	-7.91	1.43	1.52
7	N	37	SER	C-N	7.90	1.44	1.33
6	Z	400	ILE	C-N	7.89	1.43	1.33
7	N	209	LYS	CA-C	-7.89	1.42	1.52
6	Z	361	HIS	ND1-CE1	7.88	1.40	1.32
3	T	23	CYS	C-N	7.87	1.43	1.33
2	V	180	LEU	CA-CB	7.87	1.63	1.53
2	V	159	ILE	N-CA	-7.84	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	101	ARG	CZ-NH2	7.82	1.43	1.33
11	R	56	GLU	N-CA	-7.82	1.36	1.46
11	R	334	ARG	NE-CZ	7.79	1.41	1.33
11	R	112	GLU	CA-C	-7.78	1.42	1.52
13	O	41	LEU	CA-CB	-7.78	1.41	1.53
4	X	129	LEU	N-CA	-7.77	1.36	1.46
8	S	211	ARG	NE-CZ	7.77	1.41	1.33
6	Z	849	ARG	NE-CZ	7.76	1.41	1.33
3	T	60	ARG	NE-CZ	7.73	1.41	1.33
8	S	171	TYR	CA-CB	-7.73	1.39	1.53
4	X	132	SER	C-N	7.71	1.44	1.33
13	O	32	PHE	CA-CB	7.70	1.65	1.53
3	T	251	HIS	ND1-CE1	7.70	1.40	1.32
12	U	202	SER	C-N	7.68	1.43	1.33
2	V	101	ASP	C-N	7.67	1.42	1.33
7	N	649	VAL	CA-C	-7.67	1.44	1.52
8	S	490	ASN	CA-C	-7.66	1.43	1.52
4	X	22	ARG	CZ-NH1	7.63	1.43	1.32
6	Z	439	TYR	N-CA	-7.61	1.37	1.46
11	R	221	VAL	CA-CB	-7.61	1.44	1.54
2	V	236	SER	CA-CB	7.61	1.65	1.53
6	Z	420	ALA	C-N	7.60	1.44	1.34
8	S	298	ARG	N-CA	-7.60	1.37	1.46
2	V	230	TYR	N-CA	-7.60	1.35	1.46
9	P	240	TYR	CA-C	7.60	1.62	1.52
11	R	106	ASN	C-N	7.60	1.43	1.33
4	X	22	ARG	CD-NE	7.59	1.56	1.46
7	N	699	ALA	N-CA	-7.59	1.37	1.46
9	P	234	TYR	CA-C	-7.59	1.42	1.52
7	N	499	HIS	C-N	7.59	1.44	1.33
3	T	41	ILE	C-N	7.58	1.39	1.33
13	O	306	ARG	NE-CZ	7.58	1.41	1.33
7	N	374	ILE	N-CA	-7.57	1.37	1.46
9	P	203	ILE	CA-C	-7.56	1.43	1.52
9	P	249	ALA	N-CA	-7.56	1.37	1.46
3	T	92	ASN	CA-C	-7.55	1.46	1.53
13	O	115	ARG	C-N	7.55	1.44	1.33
7	N	162	ARG	C-N	7.55	1.45	1.33
11	R	276	LEU	N-CA	-7.54	1.37	1.46
5	Y	25	ASN	CA-CB	7.54	1.65	1.53
12	U	5	HIS	ND1-CE1	7.54	1.40	1.32
3	T	233	VAL	N-CA	-7.53	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Q	13	ARG	CZ-NH1	7.51	1.43	1.32
13	O	236	HIS	ND1-CE1	7.51	1.40	1.32
2	V	20	ARG	N-CA	-7.50	1.36	1.46
7	N	165	ILE	N-CA	-7.50	1.37	1.46
7	N	352	ASN	N-CA	-7.50	1.36	1.46
10	Q	171	LYS	C-N	7.50	1.42	1.33
7	N	640	VAL	CA-C	-7.49	1.43	1.52
5	Y	69	VAL	CA-CB	-7.48	1.44	1.54
7	N	897	LYS	CA-C	-7.47	1.43	1.52
7	N	394	ARG	NE-CZ	7.47	1.41	1.33
8	S	76	PHE	CA-CB	7.44	1.65	1.53
2	V	35	LEU	CA-C	-7.43	1.43	1.52
6	Z	286	VAL	N-CA	-7.42	1.37	1.46
12	U	231	ASP	CA-C	-7.42	1.42	1.52
8	S	384	ARG	NE-CZ	7.42	1.41	1.33
7	N	633	GLY	C-N	7.41	1.43	1.33
8	S	51	ARG	CA-C	7.41	1.62	1.52
11	R	222	ARG	CA-C	-7.40	1.43	1.52
7	N	618	ARG	CA-C	-7.38	1.43	1.52
12	U	36	VAL	C-N	7.37	1.42	1.33
7	N	616	HIS	CA-C	-7.37	1.43	1.52
8	S	485	LYS	C-N	7.36	1.44	1.33
9	P	136	ARG	NE-CZ	7.34	1.41	1.33
12	U	152	LYS	CA-C	-7.34	1.43	1.52
7	N	29	ASN	C-N	7.33	1.43	1.33
11	R	278	SER	CA-C	-7.32	1.42	1.52
2	V	269	ARG	NE-CZ	7.32	1.41	1.33
9	P	94	GLN	N-CA	-7.30	1.36	1.46
1	W	179	ARG	CZ-NH1	7.30	1.43	1.32
1	W	2	VAL	CA-C	-7.29	1.44	1.52
6	Z	8	LYS	CA-CB	7.29	1.66	1.53
7	N	670	LYS	CA-C	-7.29	1.42	1.52
3	T	42	PRO	N-CA	-7.28	1.40	1.47
6	Z	203	LEU	CA-C	-7.28	1.43	1.52
12	U	118	PRO	CA-C	-7.28	1.44	1.52
13	O	16	MET	N-CA	-7.28	1.37	1.46
3	T	42	PRO	CA-C	-7.27	1.45	1.52
9	P	126	THR	CA-C	-7.26	1.43	1.52
9	P	65	LEU	CA-CB	7.25	1.64	1.53
12	U	283	ARG	NE-CZ	7.25	1.41	1.33
1	W	110	ILE	CA-C	-7.25	1.43	1.52
11	R	310	GLU	CA-C	-7.24	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	275	TYR	N-CA	-7.24	1.37	1.46
9	P	348	HIS	ND1-CE1	7.23	1.39	1.32
7	N	395	ALA	CA-C	-7.23	1.43	1.52
7	N	891	VAL	CA-C	-7.23	1.45	1.52
10	Q	34	ASP	C-N	7.22	1.43	1.33
8	S	38	LEU	C-N	7.21	1.43	1.33
3	T	186	ARG	CD-NE	7.20	1.56	1.46
11	R	331	ARG	NE-CZ	7.20	1.41	1.33
7	N	584	ARG	CZ-NH2	7.19	1.42	1.33
6	Z	124	MET	CA-C	-7.18	1.43	1.52
6	Z	801	HIS	ND1-CE1	7.17	1.39	1.32
11	R	365	ASP	C-N	7.17	1.43	1.33
13	O	152	ASP	CA-C	-7.17	1.43	1.52
3	T	147	LYS	N-CA	-7.17	1.37	1.46
9	P	237	VAL	CA-CB	-7.17	1.45	1.54
10	Q	135	HIS	C-N	7.16	1.43	1.33
2	V	20	ARG	CZ-NH1	7.15	1.42	1.32
3	T	100	ASP	N-CA	-7.15	1.37	1.46
7	N	203	ARG	NE-CZ	7.15	1.41	1.33
9	P	324	GLU	N-CA	-7.15	1.37	1.46
6	Z	949	ILE	N-CA	-7.14	1.37	1.46
7	N	545	SER	N-CA	-7.13	1.37	1.46
7	N	14	ARG	NE-CZ	7.13	1.40	1.33
8	S	382	ARG	CZ-NH2	7.13	1.42	1.33
6	Z	434	GLN	CA-C	-7.13	1.43	1.52
12	U	59	ASP	CA-C	-7.12	1.43	1.52
7	N	418	ASP	CA-C	-7.12	1.43	1.52
11	R	314	ASN	CA-C	-7.12	1.43	1.52
13	O	356	ARG	CZ-NH2	7.12	1.42	1.33
9	P	243	GLU	C-N	7.11	1.42	1.33
6	Z	883	THR	CA-C	-7.11	1.43	1.52
7	N	417	ARG	CD-NE	7.10	1.56	1.46
10	Q	49	LYS	N-CA	-7.09	1.37	1.46
2	V	54	LEU	C-N	7.09	1.40	1.33
9	P	99	LYS	C-N	7.08	1.42	1.33
11	R	291	SER	C-N	7.08	1.43	1.33
7	N	894	ARG	NE-CZ	7.08	1.40	1.33
3	T	82	PHE	C-N	7.07	1.42	1.33
13	O	58	ARG	NE-CZ	7.06	1.40	1.33
6	Z	824	ASN	CA-C	7.06	1.60	1.52
8	S	228	GLU	CA-C	-7.05	1.43	1.52
6	Z	752	ILE	C-N	7.04	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	71	LEU	N-CA	-7.04	1.37	1.46
6	Z	103	TYR	CA-C	-7.03	1.43	1.52
10	Q	192	ALA	CA-C	-7.03	1.43	1.52
8	S	302	HIS	ND1-CE1	7.02	1.39	1.32
7	N	819	LYS	N-CA	-7.02	1.37	1.46
4	X	39	GLU	CA-C	-7.02	1.43	1.52
7	N	127	ASP	N-CA	-7.01	1.37	1.46
8	S	249	SER	C-N	7.01	1.43	1.34
8	S	405	ARG	NE-CZ	7.00	1.40	1.33
4	X	72	GLU	C-N	7.00	1.42	1.33
7	N	814	ALA	C-N	6.98	1.42	1.33
13	O	291	ILE	CA-CB	-6.97	1.45	1.54
7	N	196	THR	CA-C	-6.97	1.47	1.52
13	O	23	HIS	ND1-CE1	6.97	1.39	1.32
4	X	17	TYR	CA-CB	6.97	1.64	1.53
12	U	168	GLU	C-N	6.97	1.42	1.33
9	P	404	LYS	CA-C	-6.96	1.45	1.53
9	P	3	ARG	NE-CZ	6.96	1.40	1.33
6	Z	343	ALA	C-N	6.96	1.43	1.33
7	N	684	SER	C-N	6.95	1.42	1.33
8	S	131	THR	C-N	6.94	1.43	1.33
9	P	326	ASP	C-N	6.93	1.43	1.33
7	N	338	PHE	C-O	-6.93	1.16	1.24
10	Q	202	ARG	C-N	6.93	1.43	1.33
11	R	255	VAL	N-CA	-6.93	1.38	1.46
7	N	653	ARG	NE-CZ	6.92	1.40	1.33
7	N	114	SER	N-CA	-6.91	1.38	1.46
2	V	135	ARG	NE-CZ	6.91	1.40	1.33
6	Z	210	TYR	CA-C	-6.91	1.43	1.52
2	V	254	ARG	NE-CZ	6.91	1.40	1.33
6	Z	965	LEU	CA-C	-6.91	1.44	1.52
2	V	65	VAL	CA-CB	-6.90	1.45	1.53
3	T	52	LEU	C-N	6.90	1.43	1.33
12	U	60	GLU	C-N	6.90	1.42	1.33
4	X	11	ARG	CD-NE	6.89	1.55	1.46
7	N	373	VAL	N-CA	-6.89	1.37	1.46
6	Z	295	ARG	CD-NE	6.89	1.55	1.46
11	R	370	LYS	CA-C	-6.89	1.44	1.52
11	R	405	LYS	CA-CB	6.89	1.64	1.53
5	Y	68	GLU	N-CA	-6.88	1.37	1.46
6	Z	87	LYS	N-CA	-6.88	1.40	1.46
11	R	393	PRO	CA-CB	6.88	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	114	TYR	CA-CB	6.87	1.64	1.53
2	V	104	VAL	N-CA	-6.87	1.38	1.46
11	R	383	ARG	CZ-NH1	6.87	1.42	1.32
13	O	182	LYS	N-CA	-6.87	1.37	1.46
7	N	305	ASN	N-CA	-6.86	1.38	1.46
7	N	865	PRO	C-N	6.86	1.42	1.33
7	N	266	SER	CA-C	-6.86	1.44	1.52
10	Q	115	ILE	CA-C	6.86	1.61	1.52
2	V	128	SER	N-CA	-6.85	1.38	1.46
7	N	285	ALA	C-O	-6.85	1.16	1.24
11	R	33	LEU	CA-C	-6.85	1.43	1.52
11	R	115	GLU	N-CA	-6.85	1.37	1.46
13	O	184	ASP	CA-C	-6.85	1.44	1.53
12	U	161	ILE	N-CA	-6.84	1.37	1.46
6	Z	706	LYS	C-N	6.83	1.42	1.33
2	V	40	HIS	CG-ND1	6.82	1.45	1.38
6	Z	136	ARG	N-CA	-6.82	1.38	1.46
7	N	24	ALA	C-N	6.82	1.42	1.33
6	Z	572	ILE	N-CA	-6.81	1.37	1.46
6	Z	12	ILE	C-O	-6.81	1.16	1.24
9	P	66	LEU	CA-C	-6.80	1.43	1.52
7	N	614	ASN	N-CA	-6.80	1.37	1.46
10	Q	202	ARG	NE-CZ	6.80	1.40	1.33
12	U	236	LEU	CA-C	-6.79	1.45	1.52
7	N	397	SER	CA-CB	6.79	1.66	1.53
9	P	268	LEU	C-N	6.79	1.42	1.33
6	Z	424	SER	C-N	6.78	1.42	1.33
11	R	392	ARG	CZ-NH1	6.78	1.42	1.32
7	N	921	ARG	CD-NE	6.78	1.55	1.46
11	R	207	ARG	CZ-NH1	6.77	1.42	1.32
11	R	217	HIS	CE1-NE2	-6.76	1.25	1.32
13	O	242	ILE	CA-CB	-6.76	1.45	1.54
6	Z	247	GLN	C-N	6.75	1.42	1.33
6	Z	555	ALA	N-CA	-6.75	1.38	1.46
9	P	63	VAL	CA-CB	6.75	1.62	1.54
6	Z	371	SER	CA-CB	6.75	1.64	1.53
8	S	89	LYS	CA-C	-6.75	1.44	1.52
6	Z	329	ILE	CA-C	-6.74	1.44	1.52
11	R	344	SER	CA-C	-6.74	1.43	1.52
6	Z	962	ARG	NE-CZ	6.74	1.40	1.33
10	Q	85	MET	N-CA	-6.74	1.38	1.46
9	P	364	ARG	NE-CZ	6.73	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Q	370	THR	CA-C	-6.73	1.44	1.52
8	S	196	ARG	CD-NE	6.72	1.55	1.46
10	Q	294	ARG	CD-NE	6.72	1.55	1.46
6	Z	155	ARG	CZ-NH2	6.72	1.42	1.33
6	Z	962	ARG	CD-NE	6.72	1.55	1.46
3	T	103	SER	CA-CB	6.72	1.63	1.53
10	Q	95	LYS	N-CA	6.72	1.54	1.46
9	P	174	SER	CA-C	-6.72	1.44	1.52
9	P	439	MET	CA-C	-6.71	1.44	1.52
2	V	254	ARG	C-N	6.71	1.41	1.33
9	P	359	ARG	CA-C	-6.71	1.44	1.52
8	S	447	GLU	CA-C	-6.71	1.44	1.52
12	U	45	THR	CA-C	-6.71	1.44	1.52
7	N	515	ARG	CD-NE	6.70	1.55	1.46
7	N	615	ALA	CA-C	-6.70	1.43	1.52
8	S	160	ARG	C-N	6.70	1.42	1.33
12	U	173	HIS	ND1-CE1	6.70	1.39	1.32
8	S	319	CYS	N-CA	-6.69	1.38	1.46
9	P	358	SER	N-CA	-6.69	1.37	1.46
12	U	207	VAL	N-CA	-6.69	1.38	1.46
7	N	212	ASP	CA-C	-6.69	1.43	1.52
7	N	570	ARG	NE-CZ	6.69	1.40	1.33
12	U	201	GLN	N-CA	-6.68	1.38	1.46
8	S	93	LEU	C-N	6.68	1.42	1.33
2	V	118	LEU	CA-C	-6.68	1.44	1.52
11	R	284	ALA	CA-C	-6.68	1.44	1.52
6	Z	75	ILE	N-CA	-6.67	1.39	1.46
13	O	210	ARG	NE-CZ	6.67	1.40	1.33
10	Q	319	LYS	CA-C	-6.67	1.43	1.52
6	Z	37	GLN	CA-C	-6.66	1.43	1.52
6	Z	152	GLU	N-CA	-6.65	1.38	1.46
13	O	69	PHE	CA-CB	6.65	1.62	1.53
9	P	429	ILE	N-CA	-6.65	1.38	1.46
10	Q	294	ARG	NE-CZ	6.64	1.40	1.33
6	Z	861	THR	CA-C	-6.64	1.43	1.52
13	O	263	PHE	CA-C	-6.64	1.43	1.52
8	S	273	PHE	N-CA	-6.64	1.37	1.46
9	P	100	VAL	CA-CB	-6.64	1.46	1.54
8	S	309	PHE	CA-CB	6.63	1.63	1.53
8	S	129	GLU	N-CA	-6.63	1.38	1.46
13	O	227	ILE	CA-C	-6.63	1.45	1.52
8	S	382	ARG	CD-NE	6.62	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Q	332	ARG	CZ-NH2	6.62	1.42	1.33
7	N	729	SER	CA-C	-6.62	1.44	1.52
9	P	22	PRO	CA-CB	-6.62	1.44	1.53
2	V	278	LYS	CA-CB	6.61	1.63	1.53
2	V	279	HIS	CG-ND1	6.61	1.45	1.38
3	T	163	LEU	CA-CB	6.61	1.63	1.53
9	P	180	ILE	N-CA	-6.61	1.38	1.46
9	P	427	GLU	N-CA	-6.61	1.38	1.46
8	S	46	LEU	CA-C	-6.61	1.43	1.52
13	O	134	ALA	N-CA	-6.61	1.38	1.46
8	S	71	ALA	N-CA	-6.61	1.39	1.46
7	N	560	ALA	CA-C	-6.60	1.44	1.52
11	R	194	VAL	CA-C	-6.60	1.43	1.52
12	U	226	LEU	CA-C	-6.60	1.44	1.52
7	N	887	ASP	CA-C	-6.60	1.44	1.52
6	Z	221	VAL	CA-C	6.60	1.61	1.52
7	N	697	PHE	N-CA	-6.60	1.38	1.46
11	R	209	ARG	CZ-NH2	6.59	1.42	1.33
8	S	199	GLU	CA-C	-6.59	1.44	1.52
11	R	159	SER	N-CA	-6.59	1.38	1.46
3	T	87	PRO	C-N	6.59	1.42	1.33
11	R	222	ARG	CZ-NH2	6.58	1.42	1.33
6	Z	959	HIS	CD2-NE2	-6.58	1.30	1.37
8	S	154	GLN	CA-C	-6.58	1.44	1.52
7	N	921	ARG	CZ-NH2	6.58	1.42	1.33
6	Z	471	LEU	C-N	6.57	1.41	1.33
13	O	30	GLU	CA-C	6.57	1.61	1.52
8	S	157	GLU	CA-C	-6.57	1.44	1.52
10	Q	270	ILE	N-CA	-6.57	1.38	1.46
13	O	147	ARG	NE-CZ	6.57	1.40	1.33
8	S	144	LEU	C-N	6.56	1.42	1.33
10	Q	350	ILE	CA-C	-6.56	1.44	1.52
6	Z	516	THR	CA-C	-6.56	1.44	1.52
12	U	24	ARG	CZ-NH2	6.55	1.42	1.33
3	T	83	ASN	CA-CB	6.55	1.63	1.53
5	Y	83	ARG	NE-CZ	6.55	1.40	1.33
6	Z	826	ARG	CZ-NH2	6.54	1.42	1.33
10	Q	19	GLN	CA-C	-6.54	1.44	1.52
10	Q	33	LYS	CA-CB	6.54	1.63	1.53
7	N	813	ARG	NE-CZ	6.54	1.40	1.33
10	Q	217	GLU	CA-C	-6.54	1.44	1.52
2	V	54	LEU	CA-C	-6.53	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	430	LEU	N-CA	-6.53	1.38	1.46
13	O	261	GLY	CA-C	6.53	1.60	1.51
2	V	207	ALA	CA-C	-6.52	1.43	1.52
7	N	482	ALA	N-CA	-6.52	1.38	1.46
11	R	97	GLU	N-CA	6.51	1.54	1.46
12	U	186	LEU	C-N	6.51	1.42	1.33
7	N	394	ARG	CA-C	-6.51	1.44	1.52
12	U	209	GLU	C-N	6.51	1.42	1.33
13	O	15	ARG	N-CA	-6.51	1.38	1.46
7	N	809	ARG	NE-CZ	6.51	1.40	1.33
11	R	423	LEU	N-CA	-6.50	1.38	1.46
11	R	55	LYS	CA-C	-6.49	1.44	1.52
9	P	434	THR	C-N	6.49	1.42	1.33
6	Z	276	ASN	CA-CB	6.49	1.63	1.53
7	N	757	THR	N-CA	-6.49	1.37	1.46
8	S	414	ASP	C-N	6.49	1.41	1.33
6	Z	957	LEU	CA-C	-6.48	1.44	1.52
6	Z	246	CYS	N-CA	-6.48	1.37	1.46
6	Z	391	ASN	CA-CB	6.48	1.61	1.53
6	Z	623	ARG	NE-CZ	6.48	1.40	1.33
7	N	22	THR	N-CA	-6.48	1.38	1.46
6	Z	945	ILE	N-CA	-6.47	1.38	1.46
6	Z	214	HIS	ND1-CE1	6.47	1.39	1.32
8	S	310	LEU	C-N	6.47	1.42	1.33
6	Z	331	GLY	N-CA	-6.47	1.37	1.45
11	R	38	VAL	N-CA	-6.46	1.38	1.46
10	Q	369	ASP	C-N	6.46	1.42	1.33
2	V	167	ASN	N-CA	-6.46	1.36	1.46
12	U	100	ARG	CZ-NH1	6.45	1.41	1.32
7	N	412	TYR	N-CA	-6.45	1.37	1.46
8	S	49	ASP	C-N	6.45	1.43	1.33
4	X	27	ILE	CA-C	-6.44	1.47	1.53
7	N	113	ALA	CA-C	-6.44	1.44	1.52
6	Z	867	PHE	CA-C	6.44	1.61	1.52
7	N	309	ILE	CA-C	6.44	1.60	1.52
7	N	7	ALA	N-CA	-6.44	1.39	1.46
6	Z	897	HIS	CG-ND1	6.44	1.45	1.38
13	O	98	TYR	CA-C	-6.43	1.44	1.52
6	Z	914	LEU	CA-C	-6.43	1.44	1.52
7	N	465	ALA	CA-C	-6.43	1.44	1.52
10	Q	209	TYR	CA-C	-6.43	1.44	1.52
10	Q	211	PRO	CA-C	-6.43	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	164	THR	N-CA	-6.43	1.38	1.46
11	R	320	LYS	N-CA	-6.42	1.38	1.46
7	N	221	ASP	CA-CB	6.41	1.64	1.53
6	Z	151	HIS	ND1-CE1	6.41	1.39	1.32
8	S	365	THR	C-O	-6.40	1.16	1.24
2	V	268	THR	C-N	6.40	1.42	1.33
13	O	52	ALA	CA-CB	-6.40	1.44	1.53
7	N	307	LYS	C-N	6.39	1.42	1.33
12	U	117	ASN	CA-C	-6.39	1.45	1.52
7	N	211	PHE	C-N	6.39	1.42	1.34
10	Q	314	PHE	CA-CB	6.37	1.63	1.53
4	X	69	ILE	CA-C	-6.37	1.48	1.53
9	P	58	VAL	C-O	-6.37	1.16	1.24
8	S	251	SER	CA-CB	6.37	1.63	1.53
12	U	206	ASP	N-CA	-6.36	1.38	1.46
8	S	100	HIS	ND1-CE1	6.36	1.39	1.32
3	T	263	ALA	N-CA	-6.35	1.38	1.46
6	Z	928	ARG	CZ-NH2	6.35	1.41	1.33
9	P	10	ASP	N-CA	-6.35	1.38	1.46
12	U	179	ARG	CZ-NH2	6.35	1.41	1.33
9	P	162	GLU	N-CA	-6.35	1.38	1.46
7	N	431	SER	C-N	6.34	1.42	1.33
8	S	260	PRO	C-N	6.34	1.43	1.33
9	P	283	LYS	CA-CB	6.34	1.63	1.53
2	V	151	VAL	CA-CB	-6.34	1.45	1.54
7	N	791	ALA	N-CA	-6.34	1.38	1.46
10	Q	31	LEU	C-N	6.33	1.41	1.33
10	Q	329	GLU	CA-C	-6.33	1.44	1.52
9	P	310	ARG	NE-CZ	6.33	1.40	1.33
6	Z	249	MET	C-N	6.33	1.41	1.33
7	N	598	ASP	CA-CB	6.33	1.64	1.53
13	O	54	SER	C-N	6.33	1.42	1.33
3	T	11	LEU	C-N	6.33	1.42	1.33
7	N	908	ARG	CA-CB	6.32	1.63	1.53
7	N	398	ARG	CZ-NH2	6.32	1.41	1.33
13	O	270	ILE	CA-CB	-6.31	1.46	1.54
10	Q	278	VAL	CA-CB	-6.31	1.46	1.54
6	Z	747	ALA	CA-C	-6.31	1.44	1.52
13	O	287	LEU	N-CA	-6.31	1.38	1.46
8	S	393	ARG	CD-NE	6.30	1.55	1.46
3	T	244	ASP	CA-C	-6.30	1.44	1.52
6	Z	138	ARG	CZ-NH1	6.30	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	600	THR	CA-CB	6.30	1.65	1.53
13	O	301	PHE	CA-C	-6.29	1.44	1.52
2	V	305	ILE	N-CA	-6.29	1.38	1.46
7	N	128	ILE	N-CA	-6.29	1.39	1.46
10	Q	100	LEU	CA-C	-6.29	1.44	1.52
7	N	767	ALA	C-N	6.29	1.38	1.33
8	S	370	LEU	N-CA	-6.29	1.38	1.46
11	R	164	THR	C-N	6.28	1.41	1.33
4	X	23	LEU	CA-C	-6.28	1.44	1.52
3	T	165	GLN	CA-C	-6.28	1.44	1.52
1	W	128	LEU	CA-C	-6.28	1.44	1.52
1	W	108	GLN	C-O	6.26	1.31	1.24
6	Z	214	HIS	CE1-NE2	-6.26	1.26	1.32
9	P	3	ARG	CZ-NH2	6.26	1.41	1.33
11	R	142	ALA	N-CA	-6.26	1.38	1.46
4	X	59	ARG	CZ-NH1	6.26	1.41	1.32
1	W	89	THR	C-O	-6.26	1.16	1.24
7	N	800	ALA	CA-CB	6.26	1.63	1.53
8	S	472	HIS	ND1-CE1	6.25	1.38	1.32
5	Y	86	ARG	NE-CZ	6.25	1.40	1.33
13	O	254	LEU	CA-C	-6.25	1.44	1.52
8	S	24	LYS	N-CA	-6.25	1.39	1.46
10	Q	361	HIS	N-CA	-6.25	1.38	1.46
6	Z	475	GLN	N-CA	-6.24	1.38	1.46
8	S	108	ALA	CA-C	-6.24	1.45	1.52
7	N	14	ARG	CZ-NH2	6.24	1.41	1.33
9	P	351	ARG	CZ-NH1	6.24	1.41	1.32
6	Z	34	GLU	C-N	6.24	1.42	1.33
6	Z	573	LEU	CA-CB	6.24	1.63	1.53
7	N	618	ARG	NE-CZ	6.24	1.40	1.33
4	X	66	LEU	CA-C	-6.24	1.45	1.52
4	X	73	THR	C-N	6.24	1.42	1.33
8	S	160	ARG	CD-NE	6.24	1.54	1.46
2	V	152	VAL	CA-C	-6.23	1.46	1.52
6	Z	943	LYS	CA-C	-6.23	1.45	1.52
6	Z	344	LYS	CA-C	-6.23	1.44	1.52
9	P	218	LEU	C-N	6.23	1.42	1.33
6	Z	586	GLU	C-O	-6.22	1.16	1.24
1	W	118	ILE	CA-C	-6.22	1.45	1.52
11	R	220	ALA	C-N	6.22	1.42	1.33
11	R	247	GLU	N-CA	-6.22	1.38	1.46
7	N	235	ALA	C-N	6.22	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	74	MET	N-CA	-6.21	1.38	1.45
10	Q	425	GLN	N-CA	6.21	1.53	1.46
7	N	597	ARG	CZ-NH2	6.21	1.41	1.33
2	V	180	LEU	CA-C	-6.20	1.45	1.52
6	Z	832	ARG	CD-NE	6.20	1.54	1.46
7	N	286	LEU	CA-C	-6.20	1.44	1.52
6	Z	494	GLY	N-CA	-6.20	1.37	1.45
12	U	82	LYS	CA-C	-6.20	1.44	1.52
7	N	128	ILE	C-N	6.19	1.40	1.33
4	X	52	PRO	CA-C	-6.19	1.43	1.52
13	O	167	ILE	N-CA	-6.19	1.39	1.46
2	V	304	ALA	CA-CB	6.18	1.63	1.53
9	P	9	ALA	C-N	6.18	1.42	1.34
8	S	296	ALA	N-CA	-6.18	1.38	1.46
12	U	57	GLU	N-CA	6.18	1.53	1.46
2	V	87	PHE	CA-C	-6.17	1.44	1.52
6	Z	756	MET	N-CA	-6.17	1.38	1.46
8	S	322	LEU	CA-CB	6.17	1.62	1.53
7	N	300	ASN	N-CA	-6.17	1.39	1.46
9	P	230	HIS	ND1-CE1	6.17	1.38	1.32
7	N	5	THR	N-CA	-6.17	1.38	1.45
9	P	232	ARG	CA-CB	6.17	1.62	1.53
6	Z	13	ASP	N-CA	6.16	1.53	1.46
6	Z	600	GLU	C-N	-6.16	1.26	1.33
8	S	172	ASN	C-N	6.16	1.42	1.33
1	W	134	LYS	CA-C	-6.15	1.44	1.52
9	P	379	TYR	N-CA	-6.15	1.38	1.46
2	V	39	LYS	N-CA	-6.15	1.39	1.46
7	N	533	ASP	N-CA	-6.14	1.39	1.46
9	P	209	LYS	N-CA	6.14	1.53	1.46
6	Z	216	GLY	CA-C	-6.13	1.43	1.51
7	N	719	ASN	N-CA	-6.13	1.38	1.46
6	Z	40	GLU	N-CA	-6.13	1.38	1.46
7	N	909	GLU	CA-CB	6.13	1.61	1.52
10	Q	401	GLU	CA-CB	6.13	1.62	1.53
6	Z	432	GLY	C-N	6.13	1.42	1.33
13	O	262	ASP	CA-CB	6.12	1.62	1.53
5	Y	77	LEU	N-CA	-6.12	1.38	1.46
6	Z	779	ALA	CA-C	-6.12	1.45	1.52
13	O	121	ASP	N-CA	-6.12	1.38	1.46
7	N	430	ASN	CA-CB	6.12	1.64	1.53
8	S	232	MET	CA-C	-6.12	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Q	127	ARG	C-N	6.11	1.39	1.33
13	O	300	VAL	N-CA	-6.11	1.39	1.46
6	Z	608	TYR	CA-C	-6.10	1.44	1.52
12	U	7	LYS	CA-C	-6.10	1.44	1.52
6	Z	55	ARG	NE-CZ	6.10	1.39	1.33
6	Z	198	GLU	CA-CB	6.10	1.62	1.53
11	R	296	LEU	N-CA	-6.09	1.39	1.46
1	W	58	ASN	CA-CB	6.09	1.61	1.53
7	N	391	PRO	CA-C	-6.09	1.44	1.52
6	Z	160	GLU	C-O	-6.09	1.16	1.24
12	U	72	TYR	CA-CB	6.09	1.63	1.53
13	O	69	PHE	CA-C	-6.09	1.45	1.53
9	P	397	ALA	CA-C	-6.09	1.44	1.52
8	S	399	TYR	CA-C	-6.09	1.45	1.52
10	Q	421	LYS	N-CA	-6.09	1.39	1.46
12	U	113	TYR	CA-CB	6.09	1.62	1.53
13	O	288	ARG	CZ-NH2	6.08	1.41	1.33
8	S	90	LYS	N-CA	-6.08	1.39	1.46
3	T	94	HIS	ND1-CE1	6.08	1.38	1.32
10	Q	241	GLU	CA-CB	6.08	1.62	1.53
6	Z	868	ASN	N-CA	-6.08	1.39	1.46
6	Z	481	PRO	N-CA	-6.08	1.40	1.47
7	N	912	GLU	N-CA	-6.07	1.37	1.45
6	Z	68	LEU	CA-CB	6.07	1.61	1.53
7	N	331	ALA	C-N	6.07	1.41	1.33
3	T	132	HIS	CA-CB	6.07	1.63	1.53
11	R	414	LEU	CA-C	-6.07	1.44	1.52
8	S	200	GLU	N-CA	-6.07	1.38	1.45
8	S	170	TYR	N-CA	-6.07	1.38	1.45
3	T	91	SER	CA-C	-6.06	1.44	1.52
7	N	230	VAL	CA-C	-6.06	1.45	1.52
6	Z	621	LEU	CA-C	-6.06	1.45	1.52
10	Q	51	ARG	CZ-NH1	6.06	1.41	1.32
13	O	202	SER	C-N	6.06	1.41	1.33
7	N	902	VAL	C-N	6.06	1.41	1.33
8	S	302	HIS	CA-C	-6.05	1.45	1.52
6	Z	875	LYS	CA-C	-6.05	1.45	1.52
6	Z	400	ILE	N-CA	-6.04	1.39	1.46
7	N	728	LYS	CA-CB	6.04	1.62	1.53
6	Z	380	ASN	CA-C	-6.04	1.45	1.52
6	Z	801	HIS	CD2-NE2	6.04	1.44	1.37
11	R	261	LEU	C-N	6.04	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	488	CYS	CA-C	-6.04	1.45	1.52
7	N	383	LYS	C-N	6.04	1.41	1.33
7	N	817	THR	N-CA	-6.04	1.39	1.46
8	S	99	ASN	CA-C	-6.04	1.45	1.52
2	V	297	THR	N-CA	-6.04	1.39	1.46
9	P	392	LYS	N-CA	-6.04	1.39	1.46
10	Q	356	CYS	CA-C	-6.03	1.45	1.53
11	R	272	ASP	N-CA	-6.03	1.38	1.46
11	R	337	VAL	C-N	6.03	1.41	1.33
13	O	28	GLN	C-N	6.03	1.41	1.33
7	N	8	PRO	CA-C	-6.03	1.43	1.52
6	Z	486	SER	N-CA	-6.03	1.39	1.46
7	N	604	ARG	NE-CZ	6.03	1.39	1.33
11	R	206	ARG	NE-CZ	6.03	1.39	1.33
10	Q	223	GLY	N-CA	-6.02	1.38	1.45
6	Z	536	GLY	C-N	6.02	1.41	1.33
9	P	319	GLU	C-N	6.02	1.38	1.33
10	Q	174	LEU	N-CA	-6.02	1.38	1.46
1	W	142	ILE	CA-C	-6.01	1.45	1.52
3	T	254	ASP	CA-C	-6.01	1.44	1.52
7	N	778	LYS	C-N	6.01	1.41	1.33
12	U	141	GLU	CA-C	-6.01	1.45	1.52
11	R	403	LEU	N-CA	-6.01	1.39	1.46
8	S	112	ASN	CA-CB	6.01	1.62	1.53
3	T	75	PHE	CA-CB	6.01	1.62	1.53
11	R	409	GLY	CA-C	6.01	1.58	1.52
6	Z	762	GLY	CA-C	-6.01	1.45	1.52
6	Z	553	ARG	CD-NE	6.00	1.54	1.46
9	P	132	VAL	C-O	-6.00	1.17	1.24
6	Z	197	LYS	CA-C	-6.00	1.45	1.52
8	S	164	ILE	CA-C	-6.00	1.46	1.52
12	U	227	GLY	CA-C	-6.00	1.45	1.51
10	Q	11	ALA	N-CA	-6.00	1.39	1.46
10	Q	154	SER	N-CA	-6.00	1.39	1.46
11	R	317	ILE	CA-C	6.00	1.59	1.52
11	R	418	GLY	N-CA	6.00	1.53	1.45
1	W	115	CYS	C-N	6.00	1.40	1.33
7	N	332	VAL	CA-C	-6.00	1.44	1.52
1	W	181	LEU	N-CA	-5.99	1.39	1.46
11	R	248	SER	CA-C	-5.99	1.45	1.52
6	Z	551	LEU	CA-C	-5.99	1.45	1.52
6	Z	566	LEU	N-CA	-5.98	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	267	ALA	CA-C	-5.98	1.45	1.52
11	R	392	ARG	CA-CB	5.98	1.58	1.53
13	O	92	PHE	C-N	5.98	1.42	1.34
8	S	138	MET	C-N	5.98	1.41	1.33
6	Z	55	ARG	CZ-NH2	5.98	1.41	1.33
7	N	612	SER	CA-C	5.98	1.60	1.52
8	S	86	SER	CA-CB	5.98	1.62	1.53
11	R	306	PRO	CA-CB	-5.97	1.44	1.53
7	N	670	LYS	C-N	5.97	1.41	1.33
8	S	237	ILE	CA-C	5.97	1.60	1.52
8	S	468	ALA	N-CA	-5.97	1.39	1.46
12	U	27	THR	CA-C	-5.97	1.45	1.52
7	N	597	ARG	NE-CZ	5.96	1.39	1.33
10	Q	139	ILE	CA-C	-5.96	1.45	1.52
8	S	317	HIS	ND1-CE1	5.96	1.38	1.32
11	R	200	LYS	CA-CB	5.96	1.62	1.53
4	X	59	ARG	CZ-NH2	5.95	1.41	1.33
12	U	15	LEU	CA-C	5.95	1.60	1.52
4	X	63	PRO	C-N	5.95	1.36	1.33
7	N	80	LYS	CA-C	-5.95	1.44	1.52
13	O	242	ILE	N-CA	-5.95	1.39	1.46
6	Z	471	LEU	CA-C	-5.94	1.45	1.52
9	P	357	TYR	CB-CG	-5.94	1.38	1.51
11	R	108	SER	C-N	5.94	1.41	1.33
3	T	217	THR	CA-C	5.94	1.60	1.52
6	Z	543	THR	C-N	5.94	1.42	1.33
11	R	413	LYS	CA-CB	5.94	1.62	1.53
2	V	287	THR	N-CA	-5.94	1.38	1.46
6	Z	351	PRO	N-CA	-5.93	1.41	1.47
7	N	117	TYR	N-CA	-5.93	1.39	1.46
7	N	794	LYS	C-N	5.93	1.41	1.33
12	U	177	ASP	N-CA	-5.93	1.38	1.45
9	P	354	SER	CA-C	-5.93	1.45	1.52
6	Z	244	ARG	CZ-NH2	5.93	1.41	1.33
13	O	323	ASN	C-N	5.93	1.41	1.33
6	Z	790	MET	C-N	5.93	1.42	1.33
7	N	310	ASP	N-CA	5.93	1.53	1.46
6	Z	814	ALA	CA-C	5.92	1.60	1.52
8	S	128	ILE	CA-C	-5.92	1.45	1.52
13	O	62	TYR	C-N	5.92	1.41	1.33
6	Z	383	SER	CA-C	-5.91	1.45	1.52
7	N	185	ILE	CA-C	-5.91	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	U	48	VAL	CA-CB	-5.91	1.47	1.54
11	R	148	ASP	CA-C	-5.91	1.45	1.52
1	W	41	ARG	CZ-NH2	5.91	1.41	1.33
10	Q	332	ARG	CZ-NH1	5.91	1.41	1.32
6	Z	4	GLU	C-N	5.90	1.39	1.32
7	N	351	ALA	CA-C	5.90	1.60	1.52
13	O	6	GLU	C-N	5.90	1.40	1.34
5	Y	74	THR	N-CA	-5.90	1.39	1.46
6	Z	199	ASP	CA-CB	5.90	1.62	1.53
11	R	209	ARG	CZ-NH1	5.90	1.41	1.32
2	V	100	ARG	NE-CZ	5.90	1.39	1.33
7	N	429	GLU	CA-C	-5.90	1.45	1.52
8	S	217	PHE	N-CA	-5.90	1.39	1.46
9	P	159	ILE	CA-C	-5.90	1.45	1.52
6	Z	128	GLU	N-CA	-5.89	1.39	1.46
7	N	77	SER	CA-C	-5.89	1.44	1.52
1	W	77	HIS	CD2-NE2	5.89	1.44	1.37
10	Q	130	ARG	CA-C	-5.89	1.45	1.52
12	U	83	ILE	C-N	5.89	1.41	1.33
13	O	62	TYR	CA-CB	5.89	1.62	1.53
4	X	131	ASN	CA-C	-5.89	1.45	1.53
7	N	277	LEU	CA-C	-5.89	1.44	1.52
9	P	11	LYS	C-O	-5.89	1.17	1.24
6	Z	872	VAL	CA-C	-5.88	1.45	1.52
9	P	431	HIS	CE1-NE2	5.88	1.38	1.32
7	N	653	ARG	CD-NE	5.88	1.54	1.46
12	U	156	HIS	ND1-CE1	5.88	1.38	1.32
6	Z	767	TYR	N-CA	5.87	1.53	1.46
6	Z	145	ASP	N-CA	-5.87	1.39	1.46
11	R	309	LEU	N-CA	-5.87	1.39	1.46
10	Q	251	THR	CA-C	-5.87	1.45	1.52
11	R	269	LYS	C-N	5.87	1.41	1.33
2	V	34	LEU	CA-CB	5.86	1.62	1.53
10	Q	188	LEU	CB-CG	5.86	1.65	1.53
13	O	387	ARG	CD-NE	5.86	1.54	1.46
10	Q	172	PRO	N-CD	-5.86	1.39	1.47
7	N	106	ILE	CA-C	-5.86	1.45	1.52
12	U	135	ASP	N-CA	5.86	1.52	1.45
7	N	53	ASP	C-N	5.85	1.41	1.33
13	O	353	VAL	N-CA	-5.85	1.39	1.46
11	R	417	TYR	CA-C	-5.85	1.45	1.52
6	Z	58	GLU	CA-C	-5.85	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	293	LEU	CA-CB	5.85	1.60	1.53
8	S	36	LYS	C-N	5.85	1.41	1.33
10	Q	244	GLU	N-CA	-5.85	1.39	1.46
8	S	51	ARG	CZ-NH2	5.84	1.41	1.33
3	T	105	LEU	CA-CB	5.84	1.62	1.53
7	N	818	LYS	N-CA	-5.84	1.38	1.46
10	Q	274	LEU	CA-C	-5.84	1.45	1.53
6	Z	877	THR	CA-C	-5.84	1.45	1.52
6	Z	429	ASN	C-N	5.84	1.41	1.33
7	N	141	ILE	CA-C	-5.84	1.45	1.52
3	T	146	ILE	CA-C	-5.83	1.45	1.52
3	T	151	TRP	NE1-CE2	-5.83	1.31	1.37
10	Q	247	HIS	N-CA	-5.83	1.39	1.46
12	U	190	LEU	CA-C	-5.83	1.45	1.52
9	P	121	THR	CA-C	-5.83	1.45	1.52
6	Z	156	HIS	C-N	5.83	1.41	1.34
6	Z	128	GLU	C-N	5.83	1.41	1.33
6	Z	236	PHE	N-CA	-5.82	1.38	1.46
7	N	737	SER	CA-C	-5.82	1.44	1.52
7	N	752	SER	CA-CB	5.82	1.64	1.53
6	Z	296	SER	CA-CB	5.82	1.62	1.53
11	R	62	TYR	CA-C	-5.82	1.44	1.52
2	V	109	HIS	N-CA	-5.82	1.38	1.45
9	P	301	LYS	C-N	5.82	1.41	1.33
9	P	392	LYS	CA-C	-5.82	1.45	1.52
13	O	193	LEU	CA-C	-5.81	1.45	1.52
3	T	60	ARG	CZ-NH1	5.81	1.40	1.32
7	N	386	MET	C-N	5.81	1.41	1.33
7	N	662	MET	CA-C	-5.81	1.44	1.52
9	P	139	VAL	CA-CB	-5.81	1.46	1.54
11	R	422	ARG	CZ-NH2	5.81	1.41	1.33
2	V	303	VAL	C-N	5.81	1.41	1.33
6	Z	856	HIS	CD2-NE2	5.80	1.44	1.37
7	N	611	LYS	N-CA	-5.80	1.39	1.46
11	R	280	ILE	C-N	5.80	1.41	1.33
1	W	58	ASN	CA-C	-5.80	1.46	1.52
1	W	48	THR	C-N	5.79	1.41	1.33
7	N	555	ILE	C-N	5.79	1.41	1.33
11	R	406	GLN	CA-CB	5.79	1.63	1.53
6	Z	622	HIS	CA-C	-5.79	1.45	1.52
7	N	303	LEU	CA-C	-5.79	1.45	1.52
9	P	351	ARG	CA-CB	5.79	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	53	SER	CA-CB	-5.78	1.44	1.53
6	Z	620	LEU	CA-C	-5.78	1.45	1.52
1	W	169	SER	C-N	5.78	1.40	1.33
12	U	84	ASN	C-N	5.78	1.42	1.33
8	S	322	LEU	C-N	5.78	1.41	1.33
4	X	111	LEU	CA-CB	5.77	1.62	1.53
8	S	423	VAL	N-CA	-5.77	1.39	1.46
9	P	12	ASP	C-O	-5.77	1.17	1.24
9	P	38	GLN	CA-CB	-5.77	1.44	1.53
10	Q	397	LEU	CA-C	-5.77	1.45	1.52
7	N	633	GLY	CA-C	-5.77	1.47	1.52
2	V	272	GLY	N-CA	-5.76	1.37	1.45
9	P	8	LYS	C-N	5.76	1.41	1.33
10	Q	152	LYS	N-CA	-5.76	1.39	1.46
2	V	104	VAL	C-O	-5.75	1.18	1.24
7	N	729	SER	N-CA	-5.75	1.39	1.46
2	V	276	PRO	C-N	5.75	1.41	1.33
7	N	424	LYS	N-CA	-5.75	1.39	1.46
11	R	43	ARG	CD-NE	5.75	1.54	1.46
11	R	419	ALA	CA-C	-5.75	1.45	1.52
1	W	5	ALA	CA-C	-5.75	1.45	1.52
8	S	410	LYS	C-N	5.75	1.41	1.33
7	N	678	ILE	N-CA	-5.75	1.39	1.46
7	N	696	LYS	C-O	-5.74	1.17	1.24
7	N	822	GLY	N-CA	5.74	1.54	1.45
9	P	401	ASN	CA-C	-5.74	1.45	1.52
1	W	175	THR	CA-C	-5.74	1.45	1.52
11	R	383	ARG	CD-NE	5.74	1.54	1.46
6	Z	138	ARG	NE-CZ	5.73	1.39	1.33
9	P	115	ARG	C-N	5.73	1.41	1.33
6	Z	519	PRO	CA-C	5.72	1.60	1.52
7	N	387	ALA	N-CA	-5.72	1.40	1.46
13	O	189	TYR	C-N	5.72	1.41	1.33
7	N	562	THR	CA-C	-5.72	1.45	1.52
11	R	341	LEU	CA-C	5.72	1.60	1.52
2	V	93	ASP	CA-CB	5.72	1.62	1.53
5	Y	86	ARG	CZ-NH2	5.72	1.40	1.33
7	N	771	PHE	C-N	5.71	1.41	1.33
2	V	104	VAL	C-N	5.71	1.40	1.33
6	Z	56	LEU	C-N	5.71	1.41	1.33
11	R	197	MET	N-CA	-5.71	1.38	1.46
6	Z	152	GLU	CA-C	-5.71	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	553	PHE	N-CA	-5.71	1.38	1.46
7	N	216	ASN	CA-C	-5.70	1.45	1.52
11	R	209	ARG	CA-C	5.70	1.60	1.52
6	Z	808	SER	C-N	-5.70	1.26	1.33
9	P	351	ARG	CD-NE	5.70	1.54	1.46
13	O	365	LYS	CA-C	-5.70	1.45	1.52
1	W	39	ALA	N-CA	5.70	1.53	1.46
8	S	406	ASP	CA-C	-5.69	1.45	1.52
2	V	126	GLN	CA-C	-5.69	1.45	1.52
2	V	234	GLU	CA-C	-5.69	1.45	1.52
6	Z	397	ASP	N-CA	-5.69	1.39	1.46
3	T	181	LEU	CA-C	-5.69	1.45	1.52
10	Q	326	MET	C-N	5.69	1.40	1.33
13	O	97	LYS	N-CA	5.68	1.52	1.46
7	N	216	ASN	N-CA	-5.68	1.39	1.46
8	S	327	ILE	CA-C	-5.68	1.47	1.52
9	P	96	MET	C-N	5.68	1.41	1.34
7	N	71	ASN	CA-C	-5.68	1.45	1.52
7	N	300	ASN	CA-CB	5.68	1.62	1.53
11	R	165	GLY	CA-C	-5.68	1.45	1.51
2	V	105	VAL	C-N	5.68	1.39	1.33
11	R	403	LEU	C-N	5.68	1.41	1.33
3	T	196	SER	CA-C	-5.67	1.45	1.52
6	Z	619	ASP	CA-CB	5.67	1.60	1.53
6	Z	369	PHE	N-CA	-5.67	1.39	1.45
8	S	310	LEU	CA-C	-5.67	1.45	1.52
6	Z	367	SER	N-CA	5.67	1.52	1.46
2	V	25	GLU	CA-CB	5.67	1.61	1.53
2	V	158	LEU	N-CA	-5.67	1.39	1.46
7	N	317	SER	CA-C	-5.67	1.45	1.52
12	U	196	SER	CA-C	-5.67	1.45	1.52
11	R	194	VAL	N-CA	-5.66	1.39	1.46
1	W	99	LYS	CA-CB	5.66	1.62	1.53
4	X	58	GLY	C-N	5.66	1.40	1.33
8	S	384	ARG	CD-NE	5.66	1.54	1.46
11	R	121	GLU	CA-C	-5.66	1.45	1.52
2	V	258	GLU	C-N	5.66	1.41	1.33
3	T	30	ILE	C-N	5.66	1.41	1.33
8	S	63	LEU	N-CA	-5.66	1.39	1.46
7	N	870	ASN	N-CA	-5.66	1.38	1.45
9	P	3	ARG	CA-C	-5.66	1.45	1.52
13	O	310	PHE	CA-C	-5.66	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	78	ALA	CA-C	-5.65	1.45	1.52
10	Q	10	GLU	CA-CB	5.65	1.62	1.53
10	Q	61	LEU	C-N	5.65	1.41	1.34
10	Q	321	TYR	CA-CB	5.65	1.61	1.53
9	P	205	LYS	CA-CB	5.65	1.63	1.53
10	Q	15	VAL	CA-C	-5.65	1.45	1.52
7	N	477	SER	N-CA	-5.64	1.38	1.46
3	T	66	ALA	CA-CB	5.64	1.62	1.53
3	T	196	SER	N-CA	-5.64	1.39	1.46
7	N	880	ARG	CZ-NH1	5.64	1.40	1.32
6	Z	528	LEU	N-CA	-5.64	1.39	1.46
11	R	149	ASN	C-N	5.64	1.41	1.33
6	Z	39	SER	CA-CB	5.64	1.62	1.53
6	Z	234	PRO	CA-CB	5.64	1.61	1.53
7	N	87	ASP	C-N	5.64	1.41	1.33
6	Z	57	LYS	N-CA	-5.63	1.39	1.46
12	U	282	VAL	N-CA	-5.63	1.39	1.46
4	X	110	PRO	N-CD	-5.63	1.39	1.47
6	Z	773	ARG	NE-CZ	5.63	1.39	1.33
11	R	39	SER	C-N	5.63	1.40	1.34
8	S	480	ARG	NE-CZ	5.63	1.39	1.33
11	R	20	ARG	CZ-NH1	5.63	1.40	1.32
6	Z	475	GLN	CA-CB	5.63	1.62	1.53
8	S	417	GLN	N-CA	-5.63	1.39	1.46
2	V	20	ARG	NE-CZ	5.62	1.39	1.33
7	N	291	SER	CA-C	-5.62	1.44	1.52
7	N	819	LYS	CA-C	-5.62	1.45	1.52
9	P	176	LYS	CA-C	-5.62	1.45	1.52
6	Z	208	VAL	C-O	-5.62	1.19	1.24
6	Z	431	ASP	C-O	-5.62	1.17	1.23
6	Z	493	LEU	CA-CB	5.62	1.62	1.53
6	Z	469	PRO	CA-C	-5.61	1.45	1.52
13	O	296	LEU	CA-C	-5.61	1.45	1.52
6	Z	2	VAL	C-N	5.61	1.41	1.33
1	W	65	PHE	CA-CB	5.61	1.62	1.53
2	V	275	ASP	CA-CB	5.61	1.62	1.53
7	N	324	LYS	CA-C	-5.61	1.45	1.52
3	T	90	PHE	C-N	5.61	1.41	1.33
3	T	111	LEU	CB-CG	5.61	1.64	1.53
7	N	449	GLY	C-N	5.60	1.40	1.33
8	S	475	TYR	CA-C	-5.60	1.45	1.52
9	P	333	ALA	C-N	5.60	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	39	ASN	CA-CB	5.60	1.62	1.53
9	P	310	ARG	CA-C	-5.59	1.45	1.52
3	T	205	ILE	CA-C	5.59	1.59	1.52
6	Z	287	ARG	CZ-NH2	5.59	1.40	1.33
7	N	91	ILE	C-N	5.59	1.41	1.33
6	Z	623	ARG	CZ-NH2	5.59	1.40	1.33
9	P	138	ARG	CD-NE	5.59	1.54	1.46
13	O	307	MET	CA-C	-5.59	1.45	1.52
9	P	207	THR	CA-C	-5.59	1.45	1.52
2	V	111	HIS	CD2-NE2	5.59	1.44	1.37
6	Z	508	LEU	CA-C	-5.59	1.45	1.52
8	S	174	ARG	CD-NE	5.59	1.54	1.46
2	V	268	THR	CA-C	-5.58	1.46	1.53
2	V	242	LYS	N-CA	-5.58	1.39	1.46
7	N	161	TYR	CA-CB	5.58	1.61	1.53
3	T	226	TRP	CA-C	5.58	1.57	1.52
6	Z	205	LEU	CA-C	-5.58	1.44	1.52
6	Z	840	ARG	CD-NE	5.58	1.54	1.46
8	S	43	LYS	C-N	5.58	1.41	1.33
13	O	216	ASP	C-N	5.57	1.41	1.33
1	W	141	ILE	CA-C	-5.57	1.46	1.52
6	Z	491	LEU	CA-C	-5.57	1.45	1.52
6	Z	89	LEU	N-CA	-5.57	1.39	1.46
6	Z	898	HIS	CA-CB	5.57	1.62	1.53
11	R	232	VAL	CA-CB	5.57	1.61	1.54
1	W	125	LEU	C-O	-5.57	1.17	1.24
7	N	462	VAL	CA-C	-5.57	1.45	1.52
11	R	342	LEU	N-CA	5.57	1.53	1.46
10	Q	293	SER	C-N	5.57	1.41	1.33
8	S	483	GLU	N-CA	-5.56	1.39	1.46
2	V	44	GLY	C-N	5.56	1.39	1.33
8	S	193	THR	CA-C	-5.56	1.45	1.52
13	O	220	SER	CA-CB	5.56	1.61	1.53
10	Q	102	GLU	CA-C	-5.56	1.45	1.52
12	U	202	SER	CA-C	-5.55	1.45	1.52
2	V	261	LEU	C-N	5.55	1.41	1.33
10	Q	36	SER	C-N	5.55	1.41	1.33
10	Q	135	HIS	CA-CB	5.55	1.63	1.53
11	R	43	ARG	CZ-NH2	5.55	1.40	1.33
7	N	249	ASN	N-CA	-5.55	1.39	1.46
9	P	262	SER	CA-CB	5.55	1.61	1.53
6	Z	856	HIS	CG-CD2	5.55	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	106	GLN	N-CA	-5.54	1.39	1.46
6	Z	219	ASP	C-N	5.54	1.41	1.33
7	N	168	SER	CA-C	-5.54	1.45	1.52
8	S	394	ILE	N-CA	-5.54	1.39	1.46
12	U	8	VAL	N-CA	-5.54	1.39	1.46
13	O	333	SER	CA-C	-5.54	1.45	1.52
11	R	416	LYS	C-N	5.54	1.41	1.33
6	Z	202	ARG	CA-C	-5.54	1.45	1.52
7	N	468	GLU	N-CA	-5.54	1.38	1.46
13	O	320	PRO	CA-C	-5.54	1.45	1.52
11	R	210	TYR	N-CA	-5.54	1.39	1.46
8	S	261	HIS	CE1-NE2	-5.54	1.27	1.32
11	R	383	ARG	NE-CZ	5.54	1.39	1.33
13	O	196	LEU	CA-CB	5.54	1.62	1.53
9	P	359	ARG	NE-CZ	5.53	1.39	1.33
11	R	38	VAL	CA-CB	-5.53	1.47	1.54
3	T	55	LEU	CA-CB	5.53	1.62	1.53
7	N	565	ASN	C-N	5.53	1.41	1.33
9	P	30	ASN	C-N	5.53	1.40	1.33
2	V	169	GLU	C-O	-5.53	1.19	1.24
7	N	260	ASP	CA-C	-5.53	1.45	1.52
10	Q	122	ILE	N-CA	5.53	1.53	1.46
10	Q	230	LYS	CA-CB	5.53	1.61	1.53
7	N	543	ASP	C-N	5.53	1.41	1.33
8	S	204	ASP	CA-C	5.53	1.59	1.52
8	S	366	LYS	CA-CB	5.53	1.62	1.53
4	X	88	ALA	C-N	5.52	1.41	1.33
9	P	123	ARG	CZ-NH1	5.52	1.40	1.32
10	Q	247	HIS	CA-C	-5.52	1.45	1.52
3	T	8	THR	C-N	5.52	1.42	1.33
9	P	57	GLU	C-O	-5.52	1.17	1.24
7	N	548	ARG	NE-CZ	5.52	1.39	1.33
13	O	272	VAL	CA-C	-5.52	1.45	1.52
2	V	205	LYS	CA-C	-5.51	1.45	1.52
10	Q	123	GLU	C-N	5.51	1.41	1.33
10	Q	336	ASN	C-N	5.51	1.41	1.33
4	X	85	ARG	CZ-NH2	5.51	1.40	1.33
6	Z	941	ARG	C-O	-5.51	1.19	1.24
6	Z	703	SER	CA-CB	5.51	1.62	1.53
2	V	215	ASN	N-CA	-5.51	1.39	1.46
7	N	694	LEU	N-CA	5.50	1.53	1.46
7	N	786	ARG	CD-NE	5.50	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	197	TYR	C-N	5.50	1.41	1.33
7	N	901	GLY	N-CA	-5.50	1.37	1.45
13	O	103	LYS	C-N	5.50	1.40	1.33
10	Q	189	ARG	NE-CZ	5.50	1.39	1.33
10	Q	232	TYR	N-CA	-5.50	1.39	1.46
8	S	119	TYR	N-CA	-5.50	1.39	1.46
1	W	60	ARG	NE-CZ	5.49	1.39	1.33
7	N	182	ASN	CA-C	-5.49	1.45	1.52
9	P	410	GLN	C-N	5.49	1.41	1.33
13	O	17	GLU	N-CA	-5.49	1.38	1.46
9	P	287	ASP	CA-C	5.49	1.60	1.52
1	W	120	ASP	CA-C	-5.49	1.45	1.52
2	V	68	VAL	C-O	-5.49	1.17	1.23
2	V	226	LYS	N-CA	-5.49	1.39	1.46
3	T	251	HIS	CB-CG	-5.49	1.42	1.50
7	N	170	LEU	CA-CB	5.49	1.62	1.53
1	W	74	ALA	CA-C	-5.49	1.45	1.52
7	N	529	GLN	CA-C	-5.49	1.45	1.52
9	P	267	PHE	C-N	5.49	1.41	1.33
4	X	26	PRO	C-N	5.48	1.38	1.33
2	V	21	ASP	C-O	-5.48	1.17	1.24
7	N	23	TYR	N-CA	-5.48	1.39	1.46
11	R	354	ALA	C-N	5.48	1.41	1.33
3	T	98	GLU	C-N	5.48	1.40	1.33
7	N	448	LEU	N-CA	5.48	1.52	1.46
11	R	341	LEU	N-CA	-5.48	1.39	1.46
13	O	75	GLN	CA-CB	5.48	1.61	1.53
6	Z	193	PHE	C-O	-5.48	1.17	1.24
11	R	331	ARG	CA-C	-5.48	1.45	1.52
8	S	124	GLU	C-N	5.47	1.41	1.34
9	P	192	ASP	C-O	5.47	1.30	1.23
6	Z	237	VAL	N-CA	-5.47	1.39	1.46
12	U	98	LYS	N-CA	-5.47	1.38	1.45
11	R	107	GLU	C-N	5.47	1.41	1.33
1	W	153	LEU	C-N	5.47	1.41	1.33
9	P	120	GLU	C-O	-5.47	1.17	1.24
13	O	137	TYR	C-N	5.47	1.41	1.33
1	W	163	ASN	C-N	5.46	1.40	1.33
8	S	131	THR	CA-C	5.46	1.60	1.52
3	T	12	SER	CA-C	-5.46	1.45	1.52
7	N	375	HIS	N-CA	-5.46	1.38	1.46
7	N	515	ARG	NE-CZ	5.46	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	171	LEU	CA-C	-5.46	1.46	1.52
7	N	423	LEU	C-N	5.46	1.41	1.34
7	N	510	HIS	CA-CB	5.46	1.61	1.53
6	Z	55	ARG	CD-NE	5.46	1.53	1.46
8	S	388	ILE	N-CA	-5.46	1.40	1.46
10	Q	294	ARG	CZ-NH1	5.46	1.40	1.32
12	U	74	GLU	CA-C	5.45	1.59	1.52
7	N	908	ARG	NE-CZ	5.45	1.39	1.33
8	S	61	SER	C-N	5.45	1.41	1.33
11	R	399	GLN	N-CA	-5.45	1.39	1.46
13	O	166	ARG	CZ-NH1	5.45	1.40	1.32
3	T	144	TYR	CA-C	5.45	1.58	1.52
7	N	137	PHE	N-CA	-5.45	1.40	1.46
7	N	887	ASP	C-N	5.45	1.40	1.33
10	Q	15	VAL	N-CA	-5.45	1.40	1.46
10	Q	52	ASN	CA-C	-5.45	1.45	1.52
1	W	172	LEU	C-N	5.44	1.41	1.33
8	S	21	SER	C-N	5.44	1.40	1.33
3	T	102	LYS	CA-CB	5.44	1.62	1.53
7	N	56	SER	CA-CB	5.44	1.62	1.54
13	O	330	ARG	CZ-NH1	5.44	1.40	1.32
6	Z	759	ARG	CD-NE	5.44	1.53	1.46
12	U	256	ASN	CA-C	-5.44	1.46	1.52
9	P	185	GLU	N-CA	-5.43	1.39	1.46
8	S	195	ALA	CA-C	-5.43	1.45	1.52
1	W	133	LYS	CA-CB	5.43	1.62	1.53
6	Z	418	ALA	C-N	5.43	1.40	1.33
8	S	262	THR	CA-CB	-5.43	1.44	1.53
10	Q	99	THR	N-CA	5.43	1.52	1.46
3	T	74	ASN	CA-CB	5.43	1.60	1.52
6	Z	773	ARG	CZ-NH2	5.43	1.40	1.33
7	N	121	GLU	CA-C	-5.43	1.45	1.52
11	R	119	LYS	N-CA	-5.43	1.39	1.46
13	O	264	ASP	N-CA	-5.43	1.39	1.46
12	U	157	LEU	CA-C	-5.42	1.46	1.52
7	N	125	THR	CA-C	-5.42	1.45	1.52
7	N	620	GLY	C-N	5.42	1.41	1.33
6	Z	553	ARG	NE-CZ	5.42	1.39	1.33
7	N	722	THR	C-N	5.42	1.41	1.33
6	Z	452	LEU	CA-C	-5.41	1.45	1.52
9	P	423	LEU	N-CA	-5.41	1.39	1.46
1	W	4	GLU	C-N	5.40	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	190	HIS	CG-CD2	5.40	1.41	1.35
6	Z	256	LEU	C-N	5.40	1.39	1.33
7	N	864	LYS	C-N	5.40	1.40	1.33
9	P	39	LEU	CA-CB	5.40	1.62	1.53
11	R	206	ARG	CA-CB	5.40	1.63	1.53
4	X	125	MET	CA-C	-5.39	1.45	1.52
9	P	337	HIS	C-N	5.39	1.41	1.33
6	Z	709	LYS	N-CA	-5.39	1.40	1.46
8	S	133	GLU	C-N	5.39	1.40	1.33
8	S	151	GLU	CA-CB	5.39	1.59	1.52
9	P	179	PHE	N-CA	-5.39	1.40	1.46
1	W	28	ALA	C-N	5.39	1.41	1.34
8	S	122	ASN	C-N	5.39	1.41	1.33
8	S	202	ASN	CA-C	5.39	1.60	1.52
10	Q	50	ARG	CA-C	-5.39	1.45	1.52
12	U	193	GLN	N-CA	-5.39	1.40	1.46
2	V	222	GLN	N-CA	-5.38	1.40	1.46
7	N	209	LYS	N-CA	-5.38	1.40	1.46
8	S	456	ASP	N-CA	-5.38	1.40	1.46
1	W	23	ARG	CZ-NH2	5.38	1.40	1.33
1	W	30	ILE	CA-C	-5.38	1.46	1.52
3	T	257	THR	C-N	5.38	1.40	1.33
6	Z	8	LYS	N-CA	-5.38	1.39	1.46
6	Z	430	LEU	C-O	-5.38	1.17	1.24
6	Z	906	ALA	C-N	5.38	1.38	1.33
2	V	197	TYR	CA-CB	5.38	1.62	1.53
6	Z	581	VAL	CA-CB	-5.38	1.48	1.54
7	N	921	ARG	NE-CZ	5.38	1.39	1.33
9	P	174	SER	N-CA	-5.38	1.39	1.46
9	P	346	ILE	N-CA	-5.38	1.39	1.46
11	R	20	ARG	NE-CZ	5.37	1.39	1.33
12	U	212	ASP	N-CA	-5.37	1.40	1.46
6	Z	253	VAL	CA-CB	5.37	1.56	1.54
9	P	197	THR	CA-C	-5.37	1.45	1.52
13	O	97	LYS	CA-CB	5.37	1.61	1.53
6	Z	564	ARG	CZ-NH1	5.36	1.40	1.32
12	U	204	LEU	CA-CB	5.36	1.61	1.53
13	O	387	ARG	C-N	5.36	1.41	1.33
7	N	658	ILE	N-CA	-5.36	1.40	1.46
6	Z	777	PRO	CA-C	-5.36	1.44	1.52
8	S	97	THR	C-N	5.36	1.40	1.33
10	Q	3	LEU	C-O	-5.36	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	U	218	GLU	CA-C	-5.36	1.47	1.53
7	N	631	GLY	C-N	5.36	1.40	1.33
12	U	28	LYS	N-CA	-5.36	1.39	1.46
9	P	236	GLU	C-N	5.35	1.40	1.33
10	Q	122	ILE	CA-C	5.35	1.59	1.52
6	Z	349	THR	CA-C	-5.35	1.45	1.52
7	N	265	ALA	C-O	-5.35	1.17	1.23
8	S	225	HIS	CA-C	-5.35	1.46	1.53
2	V	253	LYS	CA-CB	5.35	1.61	1.53
9	P	82	LEU	N-CA	-5.35	1.40	1.46
11	R	143	GLN	CA-C	-5.35	1.45	1.52
8	S	59	ASP	C-N	5.35	1.40	1.33
13	O	369	ARG	CZ-NH1	5.35	1.40	1.32
11	R	422	ARG	NE-CZ	5.34	1.39	1.33
13	O	59	LEU	C-N	5.34	1.40	1.33
10	Q	75	ARG	NE-CZ	5.34	1.39	1.33
7	N	100	THR	CA-C	-5.34	1.46	1.52
13	O	112	LYS	CA-C	-5.34	1.46	1.52
5	Y	68	GLU	C-O	-5.33	1.17	1.23
6	Z	247	GLN	CD-NE2	5.33	1.44	1.33
7	N	93	GLU	C-N	5.33	1.41	1.33
7	N	50	TYR	CA-CB	5.33	1.61	1.53
9	P	57	GLU	N-CA	-5.33	1.39	1.46
11	R	410	LEU	CA-C	-5.33	1.46	1.52
13	O	34	GLU	C-O	-5.33	1.18	1.24
7	N	740	TRP	N-CA	-5.33	1.40	1.46
5	Y	74	THR	CA-C	-5.33	1.46	1.52
7	N	208	ARG	NE-CZ	5.33	1.39	1.33
10	Q	163	ARG	CD-NE	5.33	1.53	1.46
8	S	262	THR	C-N	5.32	1.41	1.33
6	Z	173	ALA	CA-CB	-5.32	1.44	1.53
6	Z	347	ASN	CG-ND2	5.32	1.44	1.33
7	N	596	LEU	N-CA	-5.32	1.39	1.46
8	S	400	LYS	C-N	5.32	1.40	1.33
11	R	193	ALA	C-O	-5.32	1.17	1.24
12	U	43	SER	CA-C	-5.32	1.46	1.52
13	O	293	LEU	CA-C	-5.32	1.45	1.52
3	T	172	SER	N-CA	-5.32	1.39	1.46
7	N	920	VAL	CA-CB	-5.32	1.47	1.54
6	Z	876	VAL	N-CA	-5.31	1.40	1.46
7	N	107	GLU	CA-CB	5.31	1.61	1.53
6	Z	798	ARG	CZ-NH2	5.31	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	443	LEU	CB-CG	5.31	1.64	1.53
9	P	115	ARG	NE-CZ	5.31	1.38	1.33
12	U	14	VAL	CA-CB	-5.31	1.48	1.54
1	W	98	LEU	C-N	5.31	1.41	1.34
6	Z	418	ALA	CA-C	-5.31	1.46	1.52
6	Z	463	HIS	CB-CG	-5.31	1.42	1.50
8	S	253	PHE	N-CA	-5.31	1.40	1.46
10	Q	187	LYS	N-CA	-5.31	1.39	1.46
6	Z	286	VAL	C-O	-5.30	1.18	1.24
6	Z	326	VAL	CA-C	-5.30	1.46	1.52
6	Z	598	ALA	CA-C	-5.30	1.46	1.52
7	N	891	VAL	N-CA	-5.30	1.40	1.46
9	P	343	LYS	N-CA	-5.30	1.39	1.46
10	Q	193	LYS	N-CA	-5.30	1.38	1.46
5	Y	22	GLU	N-CA	-5.30	1.40	1.46
7	N	71	ASN	C-N	5.30	1.40	1.33
9	P	191	GLY	CA-C	5.30	1.59	1.51
11	R	103	CYS	CA-C	5.30	1.59	1.52
1	W	80	GLN	C-N	5.30	1.39	1.34
6	Z	293	MET	N-CA	-5.30	1.39	1.46
8	S	358	LYS	C-N	5.30	1.40	1.33
9	P	425	HIS	ND1-CE1	5.30	1.37	1.32
8	S	37	VAL	C-N	5.30	1.40	1.33
11	R	21	VAL	CA-C	5.30	1.57	1.52
11	R	66	LEU	CA-C	-5.30	1.45	1.52
10	Q	235	ALA	C-O	-5.29	1.18	1.24
1	W	44	ASN	CA-CB	5.29	1.61	1.53
6	Z	583	ASP	C-O	-5.29	1.18	1.24
8	S	428	ARG	CA-C	5.29	1.59	1.52
9	P	344	ARG	NE-CZ	5.29	1.38	1.33
7	N	90	ASP	CA-C	-5.29	1.45	1.52
9	P	217	LYS	C-O	-5.29	1.18	1.24
3	T	168	SER	CA-C	-5.29	1.45	1.52
11	R	290	SER	CA-CB	5.29	1.61	1.53
3	T	270	ILE	C-O	-5.28	1.17	1.24
6	Z	395	CYS	CA-C	-5.28	1.46	1.52
6	Z	909	ARG	NE-CZ	5.28	1.38	1.33
10	Q	226	HIS	CD2-NE2	5.28	1.43	1.37
2	V	143	PRO	N-CA	-5.28	1.40	1.47
6	Z	803	ALA	CA-C	-5.28	1.45	1.52
10	Q	51	ARG	CD-NE	5.27	1.53	1.46
10	Q	379	GLN	C-N	5.27	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	36	LYS	C-N	5.27	1.40	1.33
4	X	11	ARG	NE-CZ	5.27	1.38	1.33
1	W	23	ARG	NE-CZ	5.27	1.38	1.33
6	Z	214	HIS	C-N	5.27	1.41	1.33
7	N	384	LYS	N-CA	-5.27	1.40	1.46
2	V	58	VAL	CA-C	-5.27	1.46	1.52
11	R	68	GLU	CA-C	-5.26	1.46	1.52
13	O	326	HIS	CA-CB	5.26	1.61	1.53
6	Z	81	SER	CA-CB	5.26	1.61	1.53
13	O	233	LEU	CA-CB	5.26	1.61	1.53
6	Z	279	THR	C-O	-5.26	1.17	1.24
13	O	229	ASN	C-N	5.26	1.41	1.34
7	N	685	VAL	CA-CB	-5.26	1.47	1.54
12	U	229	LEU	CA-C	-5.26	1.45	1.52
2	V	160	ASP	CA-CB	5.26	1.61	1.53
6	Z	524	ALA	C-N	5.26	1.41	1.33
12	U	47	ARG	NE-CZ	5.26	1.38	1.33
7	N	696	LYS	CA-C	5.26	1.59	1.52
8	S	428	ARG	NE-CZ	5.26	1.38	1.33
13	O	186	ASN	C-N	5.25	1.41	1.33
6	Z	773	ARG	CD-NE	5.25	1.53	1.46
8	S	107	SER	C-N	5.25	1.40	1.33
8	S	185	PHE	CA-CB	5.25	1.61	1.53
9	P	65	LEU	C-O	-5.25	1.18	1.24
10	Q	338	LEU	CA-C	-5.25	1.46	1.52
11	R	109	LYS	C-N	5.25	1.40	1.33
12	U	151	GLU	N-CA	-5.25	1.39	1.46
12	U	211	LEU	N-CA	-5.25	1.40	1.46
7	N	427	ILE	N-CA	5.25	1.52	1.46
6	Z	784	SER	CA-C	-5.25	1.45	1.52
7	N	342	GLY	C-N	5.25	1.40	1.33
1	W	83	GLY	C-N	5.25	1.40	1.33
7	N	302	PHE	CA-C	-5.25	1.46	1.52
6	Z	138	ARG	CZ-NH2	5.24	1.40	1.33
6	Z	571	GLY	C-N	5.24	1.40	1.33
7	N	14	ARG	CD-NE	5.24	1.53	1.46
7	N	567	ALA	CA-C	-5.24	1.46	1.52
12	U	143	VAL	N-CA	-5.24	1.40	1.46
6	Z	834	LEU	C-N	5.24	1.40	1.33
6	Z	412	GLY	C-O	-5.24	1.17	1.24
6	Z	161	ILE	C-N	5.24	1.41	1.33
7	N	307	LYS	N-CA	-5.24	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	354	LEU	C-N	5.24	1.40	1.33
11	R	291	SER	CA-C	-5.24	1.46	1.52
1	W	139	VAL	C-O	5.24	1.29	1.23
6	Z	946	THR	CA-CB	-5.24	1.46	1.53
8	S	100	HIS	CG-CD2	5.24	1.41	1.35
8	S	473	ASP	CA-C	-5.24	1.46	1.52
13	O	283	HIS	N-CA	-5.24	1.40	1.46
2	V	157	ARG	CZ-NH2	5.23	1.40	1.33
3	T	230	ASN	C-N	5.23	1.41	1.33
6	Z	405	ASN	CA-C	-5.23	1.45	1.52
12	U	123	VAL	C-N	5.23	1.40	1.33
13	O	240	GLU	N-CA	-5.23	1.39	1.46
13	O	339	GLY	CA-C	-5.23	1.45	1.52
4	X	93	SER	CA-C	5.23	1.59	1.52
6	Z	15	GLN	N-CA	-5.23	1.40	1.46
8	S	154	GLN	CD-NE2	5.23	1.44	1.33
7	N	579	SER	CA-CB	5.23	1.61	1.53
9	P	49	ALA	CA-C	-5.23	1.46	1.52
10	Q	114	GLN	N-CA	-5.23	1.40	1.46
11	R	336	LYS	C-O	-5.23	1.17	1.24
11	R	32	LEU	N-CA	-5.23	1.40	1.46
1	W	22	PRO	CA-C	-5.22	1.46	1.52
6	Z	183	LYS	C-N	5.22	1.40	1.33
7	N	585	ARG	CZ-NH2	5.22	1.40	1.33
7	N	588	VAL	CA-C	-5.22	1.45	1.52
8	S	443	ILE	CA-C	-5.22	1.46	1.52
7	N	801	THR	CB-OG1	5.22	1.52	1.43
6	Z	756	MET	CA-CB	5.22	1.61	1.53
8	S	320	ILE	CA-C	-5.22	1.46	1.52
7	N	902	VAL	N-CA	-5.22	1.39	1.46
7	N	914	VAL	C-N	5.22	1.40	1.33
12	U	289	ASP	N-CA	-5.22	1.40	1.46
13	O	91	ASP	N-CA	-5.21	1.39	1.46
7	N	313	LEU	N-CA	-5.21	1.40	1.46
10	Q	237	SER	CA-C	-5.21	1.46	1.52
11	R	289	ILE	N-CA	-5.21	1.39	1.46
6	Z	348	LEU	CA-C	5.21	1.59	1.52
10	Q	150	GLN	CA-CB	5.21	1.59	1.52
11	R	207	ARG	C-O	-5.21	1.17	1.24
11	R	325	HIS	CD2-NE2	5.21	1.43	1.37
13	O	38	TRP	CA-C	-5.20	1.45	1.52
13	O	258	LEU	CA-C	5.20	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	913	PRO	N-CD	-5.20	1.40	1.47
11	R	33	LEU	C-N	5.20	1.40	1.33
13	O	188	PHE	CA-CB	5.20	1.61	1.53
7	N	571	LEU	N-CA	-5.20	1.39	1.46
7	N	597	ARG	CA-C	5.20	1.59	1.52
9	P	294	GLU	CA-C	-5.20	1.45	1.52
7	N	648	PRO	C-O	5.20	1.30	1.24
9	P	70	ASN	C-N	5.20	1.41	1.34
13	O	189	TYR	CA-C	5.20	1.59	1.52
6	Z	820	ALA	N-CA	-5.19	1.40	1.46
7	N	813	ARG	CZ-NH2	5.19	1.40	1.33
9	P	210	ASN	CA-C	-5.19	1.47	1.53
12	U	157	LEU	C-N	5.19	1.39	1.33
12	U	188	ILE	C-N	5.19	1.41	1.34
6	Z	432	GLY	CA-C	-5.19	1.44	1.51
6	Z	857	LEU	CA-CB	5.19	1.61	1.53
7	N	490	LEU	CA-C	-5.19	1.46	1.52
13	O	379	LYS	CA-C	-5.19	1.46	1.52
2	V	148	LYS	CA-C	-5.19	1.46	1.52
10	Q	195	LYS	C-N	5.19	1.40	1.33
6	Z	809	MET	CA-C	-5.19	1.46	1.52
12	U	47	ARG	CA-CB	5.19	1.61	1.53
13	O	60	ARG	CZ-NH2	5.19	1.40	1.33
7	N	604	ARG	C-N	5.18	1.40	1.33
3	T	166	SER	C-N	5.18	1.41	1.33
3	T	252	GLU	CA-CB	5.18	1.59	1.52
6	Z	20	PRO	CA-CB	5.18	1.60	1.53
6	Z	880	SER	N-CA	-5.18	1.40	1.46
10	Q	422	VAL	CA-C	-5.18	1.46	1.52
13	O	210	ARG	CZ-NH2	5.18	1.40	1.33
1	W	142	ILE	C-N	5.18	1.40	1.33
7	N	298	TYR	CA-C	5.18	1.59	1.52
1	W	165	GLN	N-CA	-5.18	1.39	1.46
6	Z	41	GLU	N-CA	-5.18	1.40	1.46
8	S	238	LEU	N-CA	-5.18	1.40	1.46
3	T	110	LEU	C-N	5.18	1.40	1.33
6	Z	948	TRP	C-N	5.18	1.40	1.33
7	N	49	LEU	CA-C	5.18	1.59	1.52
8	S	298	ARG	CZ-NH2	5.18	1.40	1.33
9	P	373	GLU	CA-CB	5.18	1.61	1.53
2	V	116	CYS	CA-C	-5.17	1.45	1.52
6	Z	544	THR	CA-C	-5.17	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	198	SER	CA-CB	5.17	1.61	1.53
4	X	77	PRO	CA-C	-5.17	1.45	1.52
10	Q	306	TYR	CA-CB	5.17	1.61	1.53
8	S	83	PRO	C-N	5.17	1.41	1.33
7	N	160	GLY	CA-C	5.17	1.58	1.51
2	V	285	ASP	N-CA	5.17	1.52	1.46
7	N	199	ASN	CA-C	-5.17	1.46	1.52
2	V	296	LEU	CA-CB	5.17	1.61	1.53
3	T	240	LYS	C-N	5.17	1.40	1.33
7	N	321	LEU	CA-C	5.16	1.59	1.52
7	N	815	LYS	N-CA	-5.16	1.40	1.46
6	Z	405	ASN	C-N	5.16	1.41	1.34
9	P	239	GLN	N-CA	-5.16	1.40	1.46
10	Q	243	PHE	C-N	5.16	1.41	1.33
10	Q	271	MET	CA-CB	5.16	1.61	1.53
6	Z	822	THR	C-N	5.16	1.40	1.33
2	V	289	GLU	CA-CB	5.16	1.61	1.53
9	P	171	MET	CA-CB	5.16	1.62	1.53
11	R	263	ARG	CZ-NH1	5.16	1.40	1.32
11	R	321	TYR	N-CA	-5.16	1.40	1.46
7	N	761	ILE	CA-C	-5.15	1.45	1.52
1	W	113	PHE	N-CA	5.15	1.52	1.46
5	Y	87	GLU	N-CA	-5.15	1.40	1.46
6	Z	454	GLY	C-N	5.15	1.40	1.33
9	P	259	PRO	N-CA	-5.15	1.40	1.47
12	U	82	LYS	C-N	5.15	1.40	1.33
13	O	154	GLU	CA-C	5.15	1.59	1.52
2	V	238	LEU	N-CA	-5.15	1.40	1.46
5	Y	86	ARG	CZ-NH1	5.15	1.40	1.32
7	N	528	ARG	CA-C	5.15	1.59	1.52
2	V	45	VAL	CA-C	-5.15	1.47	1.52
11	R	372	ILE	CA-CB	-5.15	1.47	1.54
1	W	17	ARG	CZ-NH1	5.14	1.40	1.32
3	T	150	ARG	CZ-NH1	5.14	1.40	1.32
7	N	428	VAL	N-CA	-5.14	1.39	1.46
8	S	332	PHE	CA-CB	5.14	1.61	1.53
10	Q	155	LEU	C-N	5.14	1.41	1.33
2	V	169	GLU	N-CA	-5.14	1.41	1.46
7	N	125	THR	C-N	5.14	1.40	1.33
7	N	687	THR	CA-C	5.14	1.59	1.52
9	P	316	LYS	CA-CB	5.14	1.62	1.53
11	R	207	ARG	CA-C	-5.14	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	209	ARG	C-O	5.14	1.30	1.24
7	N	59	GLU	C-N	5.13	1.41	1.33
7	N	385	VAL	CA-C	5.13	1.59	1.52
9	P	397	ALA	C-N	5.13	1.40	1.33
10	Q	105	GLU	N-CA	-5.13	1.40	1.46
6	Z	317	GLN	CA-CB	5.13	1.61	1.53
6	Z	803	ALA	C-N	5.13	1.40	1.33
6	Z	849	ARG	CD-NE	5.13	1.53	1.46
9	P	13	TYR	CA-C	-5.13	1.45	1.52
13	O	267	ASP	N-CA	-5.13	1.40	1.46
3	T	224	ARG	C-N	5.13	1.40	1.33
10	Q	378	SER	CA-CB	5.13	1.61	1.53
6	Z	447	VAL	N-CA	-5.13	1.39	1.46
6	Z	276	ASN	C-N	5.13	1.40	1.33
7	N	189	LEU	N-CA	-5.13	1.39	1.46
8	S	136	CYS	N-CA	5.13	1.52	1.46
2	V	186	GLN	N-CA	-5.12	1.40	1.46
7	N	811	LYS	C-N	5.12	1.40	1.33
3	T	239	SER	C-N	5.12	1.40	1.33
6	Z	956	LEU	CA-C	-5.12	1.46	1.53
9	P	206	LYS	C-O	5.12	1.30	1.24
13	O	11	LEU	CA-C	-5.12	1.46	1.52
13	O	146	ALA	N-CA	-5.12	1.40	1.46
5	Y	21	ASN	N-CA	-5.12	1.40	1.46
9	P	69	ARG	N-CA	5.12	1.52	1.46
6	Z	717	THR	C-N	5.12	1.40	1.33
7	N	801	THR	CA-C	-5.12	1.46	1.52
10	Q	423	VAL	N-CA	-5.12	1.39	1.46
1	W	115	CYS	N-CA	-5.12	1.40	1.46
10	Q	297	ASP	CA-C	-5.12	1.46	1.52
13	O	105	GLN	CA-C	-5.12	1.46	1.52
10	Q	93	THR	N-CA	-5.11	1.40	1.46
9	P	409	SER	CA-C	-5.11	1.46	1.52
4	X	17	TYR	N-CA	-5.11	1.40	1.46
13	O	96	LEU	N-CA	-5.11	1.40	1.46
13	O	285	SER	CA-C	-5.11	1.46	1.52
13	O	314	SER	C-O	-5.11	1.18	1.24
1	W	60	ARG	CD-NE	5.11	1.53	1.46
9	P	68	SER	N-CA	-5.11	1.39	1.46
13	O	292	CYS	C-N	5.11	1.40	1.33
11	R	353	MET	CA-CB	5.10	1.61	1.53
6	Z	300	ALA	CA-CB	5.10	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	448	LEU	C-O	-5.10	1.18	1.24
7	N	511	GLY	CA-C	-5.10	1.46	1.52
8	S	261	HIS	ND1-CE1	5.10	1.37	1.32
12	U	155	LEU	N-CA	-5.10	1.40	1.46
6	Z	495	ILE	N-CA	-5.10	1.40	1.46
8	S	55	ARG	CD-NE	5.10	1.53	1.46
9	P	313	ILE	N-CA	-5.10	1.39	1.46
2	V	124	ASN	CA-CB	5.10	1.61	1.53
7	N	120	ASP	C-O	5.10	1.30	1.23
9	P	85	LYS	CA-CB	5.10	1.62	1.53
13	O	19	ASP	C-N	5.10	1.39	1.34
1	W	118	ILE	N-CA	-5.10	1.40	1.46
2	V	159	ILE	C-N	5.09	1.40	1.33
8	S	161	LYS	N-CA	-5.09	1.40	1.46
2	V	269	ARG	CD-NE	5.09	1.53	1.46
6	Z	293	MET	C-N	5.09	1.40	1.33
7	N	139	ARG	CZ-NH1	5.09	1.39	1.32
8	S	260	PRO	C-O	-5.09	1.17	1.23
9	P	149	GLU	C-N	5.09	1.40	1.33
6	Z	563	VAL	N-CA	-5.09	1.39	1.46
11	R	293	THR	CA-C	-5.09	1.46	1.52
13	O	102	LEU	CA-C	5.09	1.59	1.52
7	N	5	THR	C-N	5.09	1.40	1.33
6	Z	381	LEU	CA-C	-5.09	1.46	1.52
6	Z	311	ALA	C-N	5.08	1.40	1.33
7	N	151	LYS	N-CA	5.08	1.52	1.46
9	P	95	TYR	CA-CB	5.08	1.61	1.53
7	N	481	ALA	CA-C	-5.08	1.46	1.52
8	S	344	PRO	CA-C	-5.08	1.44	1.52
10	Q	86	MET	CG-SD	-5.08	1.68	1.80
6	Z	164	VAL	CA-C	-5.08	1.46	1.52
6	Z	494	GLY	C-N	5.08	1.40	1.33
8	S	19	HIS	CG-CD2	5.08	1.41	1.35
9	P	411	LEU	CA-C	-5.08	1.46	1.52
7	N	270	LEU	N-CA	-5.08	1.40	1.46
8	S	192	GLU	CA-C	-5.08	1.46	1.52
7	N	103	SER	CA-CB	5.08	1.61	1.53
13	O	329	MET	CA-CB	5.08	1.61	1.53
7	N	894	ARG	CZ-NH2	5.07	1.40	1.33
7	N	193	ALA	N-CA	-5.07	1.40	1.46
11	R	175	ALA	N-CA	-5.07	1.40	1.46
2	V	233	LYS	N-CA	-5.07	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	716	GLN	CA-C	-5.07	1.46	1.52
7	N	255	ALA	N-CA	-5.07	1.40	1.46
3	T	77	SER	C-N	5.07	1.40	1.33
6	Z	941	ARG	N-CA	-5.07	1.41	1.46
3	T	88	TYR	CA-CB	5.07	1.61	1.53
5	Y	81	LEU	C-N	5.06	1.40	1.33
6	Z	39	SER	N-CA	-5.06	1.39	1.46
7	N	591	LEU	C-N	5.06	1.41	1.33
8	S	242	LEU	C-N	5.06	1.41	1.34
10	Q	161	LEU	C-N	5.06	1.40	1.33
12	U	83	ILE	CA-C	-5.06	1.46	1.52
9	P	117	SER	CA-CB	5.06	1.61	1.53
3	T	143	SER	N-CA	-5.06	1.40	1.46
7	N	601	THR	N-CA	-5.06	1.39	1.46
3	T	118	ASN	CA-CB	5.06	1.61	1.52
8	S	272	TYR	C-O	-5.06	1.18	1.24
8	S	377	TYR	CA-CB	5.06	1.61	1.53
9	P	33	ASN	CA-CB	5.06	1.61	1.53
3	T	262	LYS	N-CA	-5.06	1.40	1.46
13	O	143	LEU	N-CA	-5.06	1.39	1.46
6	Z	456	GLY	CA-C	5.05	1.57	1.51
8	S	248	ASP	CA-C	-5.05	1.46	1.52
11	R	221	VAL	CA-C	-5.05	1.46	1.52
11	R	408	ASP	N-CA	-5.05	1.40	1.46
2	V	130	GLU	CA-C	-5.05	1.46	1.52
7	N	332	VAL	C-N	-5.05	1.27	1.33
8	S	402	ILE	CA-C	5.05	1.58	1.52
8	S	420	GLU	N-CA	-5.05	1.40	1.46
10	Q	149	LYS	N-CA	-5.05	1.38	1.46
11	R	401	HIS	CA-C	5.05	1.59	1.52
1	W	26	PHE	N-CA	-5.05	1.40	1.46
8	S	305	LYS	C-N	5.05	1.41	1.33
13	O	322	ASP	N-CA	-5.05	1.40	1.46
7	N	883	SER	CA-CB	5.05	1.62	1.53
10	Q	104	PHE	N-CA	-5.05	1.40	1.46
6	Z	832	ARG	CZ-NH2	5.05	1.40	1.33
7	N	6	ALA	C-N	5.05	1.40	1.33
7	N	201	LYS	C-O	5.05	1.30	1.24
10	Q	300	LYS	N-CA	-5.05	1.39	1.46
11	R	34	THR	C-N	5.05	1.40	1.33
6	Z	318	LYS	C-N	5.04	1.41	1.34
8	S	472	HIS	CE1-NE2	-5.04	1.27	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	491	LEU	C-O	-5.04	1.18	1.24
12	U	122	ILE	CA-C	-5.04	1.48	1.53
6	Z	161	ILE	N-CA	-5.04	1.40	1.46
6	Z	357	ILE	N-CA	-5.04	1.39	1.46
6	Z	371	SER	C-N	5.04	1.40	1.33
1	W	59	PRO	C-N	5.04	1.40	1.33
3	T	129	LEU	CA-CB	5.04	1.61	1.53
12	U	23	GLU	CA-CB	5.04	1.62	1.53
10	Q	249	LEU	CB-CG	5.04	1.63	1.53
11	R	285	ALA	C-O	-5.04	1.18	1.24
12	U	183	ALA	CA-C	-5.04	1.47	1.53
3	T	123	HIS	CB-CG	5.04	1.57	1.50
7	N	780	ASP	CA-C	-5.04	1.46	1.52
9	P	91	LEU	CA-CB	5.04	1.61	1.53
7	N	273	LEU	CA-C	-5.03	1.46	1.52
7	N	797	GLU	CA-C	-5.03	1.46	1.52
10	Q	112	ASP	C-N	5.03	1.40	1.33
7	N	242	PHE	CA-CB	5.03	1.62	1.53
6	Z	889	VAL	CA-CB	-5.03	1.48	1.54
7	N	40	SER	CA-CB	-5.03	1.45	1.53
9	P	261	LEU	N-CA	-5.03	1.40	1.46
9	P	307	GLU	C-N	5.03	1.40	1.33
7	N	735	MET	C-N	5.03	1.40	1.33
6	Z	148	GLY	C-N	5.02	1.40	1.33
1	W	168	THR	C-N	5.02	1.40	1.33
6	Z	589	SER	CA-CB	5.02	1.62	1.53
11	R	265	ASP	N-CA	-5.02	1.39	1.46
1	W	3	LEU	C-N	5.02	1.41	1.33
7	N	290	LEU	CB-CG	5.02	1.63	1.53
7	N	398	ARG	NE-CZ	5.02	1.38	1.33
10	Q	79	PRO	C-N	5.02	1.41	1.33
7	N	810	ALA	CA-C	-5.02	1.45	1.52
8	S	60	LEU	CA-C	-5.02	1.46	1.52
11	R	138	GLY	CA-C	-5.02	1.46	1.52
3	T	26	LEU	C-N	5.01	1.40	1.33
3	T	124	SER	N-CA	-5.01	1.40	1.46
8	S	349	THR	N-CA	-5.01	1.40	1.46
7	N	444	HIS	ND1-CE1	5.01	1.37	1.32
11	R	175	ALA	C-N	5.01	1.40	1.33
6	Z	209	PRO	C-N	5.01	1.40	1.33
7	N	889	ARG	CA-CB	5.00	1.60	1.53
11	R	288	SER	CA-C	-5.00	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	458	ALA	CA-CB	5.00	1.61	1.53
8	S	358	LYS	CA-CB	5.00	1.61	1.53
6	Z	75	ILE	C-N	5.00	1.41	1.33
6	Z	145	ASP	C-N	5.00	1.39	1.33
7	N	705	ILE	N-CA	-5.00	1.40	1.46
8	S	238	LEU	C-N	5.00	1.40	1.33
10	Q	329	GLU	CA-CB	5.00	1.61	1.53
12	U	252	HIS	ND1-CE1	5.00	1.37	1.32

All (2744) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	8	PRO	N-CA-CB	-31.93	68.21	103.33
2	V	196	TYR	CB-CA-C	-25.15	60.37	110.42
5	Y	65	ASP	CB-CA-C	-15.49	80.67	110.10
8	S	197	SER	CA-C-O	-14.97	105.28	120.70
8	S	20	HIS	N-CA-C	14.33	126.40	111.07
2	V	196	TYR	N-CA-CB	13.99	134.13	110.49
8	S	127	THR	N-CA-CB	-13.01	90.11	110.28
2	V	197	TYR	N-CA-CB	12.52	131.64	110.49
10	Q	162	LEU	N-CA-C	-12.48	92.75	111.34
3	T	82	PHE	CA-CB-CG	11.91	125.72	113.80
13	O	41	LEU	N-CA-CB	-11.83	92.66	110.16
3	T	236	ASN	N-CA-C	11.81	124.24	111.36
3	T	50	ILE	N-CA-C	-11.55	99.06	110.72
11	R	204	TRP	N-CA-C	-11.37	99.13	113.23
3	T	75	PHE	CA-CB-CG	-11.18	102.62	113.80
12	U	117	ASN	CA-CB-CG	-11.14	101.46	112.60
2	V	183	ALA	CA-C-N	10.79	142.16	121.54
2	V	183	ALA	C-N-CA	10.79	142.16	121.54
6	Z	324	GLU	N-CA-C	-10.73	99.37	111.82
12	U	276	ILE	N-CA-C	-10.60	99.81	110.62
8	S	72	GLU	CA-C-N	10.57	134.60	120.65
8	S	72	GLU	C-N-CA	10.57	134.60	120.65
9	P	30	ASN	CA-CB-CG	-10.55	102.05	112.60
6	Z	612	GLY	O-C-N	10.49	132.00	122.77
3	T	42	PRO	N-CA-C	-10.40	102.55	114.92
5	Y	65	ASP	CA-CB-CG	10.34	122.94	112.60
7	N	483	LEU	CA-C-N	10.32	131.59	120.03
7	N	483	LEU	C-N-CA	10.32	131.59	120.03
6	Z	627	LYS	N-CA-C	10.30	122.51	111.28
6	Z	186	GLY	CA-C-O	-10.20	115.19	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	810	ASN	CA-CB-CG	-10.13	102.47	112.60
1	W	170	HIS	CA-CB-CG	10.13	123.93	113.80
7	N	244	LYS	N-CA-C	-10.12	99.24	111.69
12	U	228	LYS	N-CA-C	10.09	122.35	111.36
13	O	179	PHE	CA-CB-CG	-9.99	103.81	113.80
6	Z	150	GLY	N-CA-C	-9.98	103.69	114.67
8	S	145	PHE	CA-CB-CG	-9.94	103.86	113.80
2	V	220	GLN	N-CA-C	-9.91	99.30	111.40
1	W	10	ILE	N-CA-C	-9.89	94.33	108.17
5	Y	87	GLU	N-CA-C	9.80	121.97	111.28
8	S	302	HIS	CA-CB-CG	-9.75	104.05	113.80
7	N	765	ASP	CA-CB-CG	9.60	122.20	112.60
8	S	126	LYS	N-CA-CB	9.57	129.85	113.10
11	R	215	GLY	CA-C-N	9.57	134.01	120.42
11	R	215	GLY	C-N-CA	9.57	134.01	120.42
2	V	182	LYS	O-C-N	-9.53	110.95	122.20
8	S	317	HIS	CA-CB-CG	9.52	123.32	113.80
6	Z	475	GLN	N-CA-C	9.49	121.63	111.28
7	N	425	ASN	CA-CB-CG	-9.45	103.15	112.60
11	R	394	ASP	CA-CB-CG	-9.43	103.17	112.60
9	P	326	ASP	CA-CB-CG	-9.42	103.18	112.60
1	W	154	LEU	N-CA-C	9.41	124.08	112.23
6	Z	723	ASP	CA-CB-CG	-9.39	103.21	112.60
7	N	671	LEU	O-C-N	-9.39	112.17	122.12
13	O	64	ASN	CA-CB-CG	-9.39	103.21	112.60
5	Y	65	ASP	N-CA-CB	9.38	126.44	110.50
7	N	677	ASP	CA-CB-CG	-9.34	103.26	112.60
13	O	41	LEU	CB-CA-C	9.30	126.67	110.85
10	Q	258	ALA	N-CA-C	-9.26	101.27	111.36
8	S	71	ALA	CA-C-N	9.25	132.68	120.28
8	S	71	ALA	C-N-CA	9.25	132.68	120.28
2	V	91	MET	CA-C-O	-9.24	111.12	120.82
12	U	244	ASP	CA-CB-CG	-9.23	103.37	112.60
6	Z	23	GLN	CB-CG-CD	-9.22	96.92	112.60
12	U	273	LEU	N-CA-C	9.20	122.15	111.11
6	Z	340	LEU	N-CA-C	-9.16	97.09	111.02
1	W	17	ARG	N-CA-C	-9.11	102.34	112.72
7	N	109	TYR	N-CA-C	9.02	121.12	111.28
11	R	217	HIS	N-CA-C	-8.99	101.45	111.07
11	R	377	LEU	N-CA-C	-8.97	102.85	113.88
13	O	155	LYS	N-CA-C	8.93	121.01	111.28
10	Q	52	ASN	N-CA-C	8.91	121.80	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	389	GLN	CA-C-N	8.90	132.57	120.38
13	O	389	GLN	C-N-CA	8.90	132.57	120.38
7	N	769	PRO	CA-C-O	-8.90	110.98	122.19
8	S	467	PHE	CA-C-N	8.88	132.17	120.28
8	S	467	PHE	C-N-CA	8.88	132.17	120.28
2	V	63	VAL	N-CA-CB	8.87	122.64	111.46
11	R	265	ASP	CA-CB-CG	-8.87	103.73	112.60
7	N	681	ASN	OD1-CG-ND2	8.87	131.47	122.60
3	T	132	HIS	CA-C-N	8.86	132.38	120.77
3	T	132	HIS	C-N-CA	8.86	132.38	120.77
6	Z	121	ILE	N-CA-C	-8.85	101.93	110.42
2	V	152	VAL	N-CA-CB	8.82	120.61	110.82
3	T	220	PHE	CA-CB-CG	-8.81	104.99	113.80
8	S	479	MET	N-CA-C	8.81	120.88	111.28
13	O	83	LEU	CA-C-N	8.80	132.07	120.28
13	O	83	LEU	C-N-CA	8.80	132.07	120.28
7	N	621	THR	CA-C-O	8.78	129.99	120.24
3	T	123	HIS	CA-CB-CG	-8.77	105.03	113.80
4	X	47	ASP	CA-CB-CG	-8.73	103.87	112.60
9	P	236	GLU	N-CA-CB	8.73	123.08	110.16
3	T	81	TYR	CA-C-N	8.72	132.31	120.54
3	T	81	TYR	C-N-CA	8.72	132.31	120.54
13	O	116	ASN	OD1-CG-ND2	8.70	131.30	122.60
13	O	92	PHE	CA-CB-CG	-8.69	105.11	113.80
12	U	52	PHE	CA-CB-CG	-8.68	105.12	113.80
9	P	334	ASN	CA-CB-CG	-8.67	103.93	112.60
7	N	884	PHE	CA-CB-CG	-8.65	105.15	113.80
11	R	262	GLU	CA-C-N	8.64	132.21	120.54
11	R	262	GLU	C-N-CA	8.64	132.21	120.54
8	S	338	MET	N-CA-C	-8.63	103.28	113.21
9	P	253	ASP	CA-CB-CG	-8.62	103.98	112.60
6	Z	326	VAL	N-CA-C	-8.62	102.43	110.53
6	Z	806	GLU	CA-C-N	8.54	131.49	120.56
6	Z	806	GLU	C-N-CA	8.54	131.49	120.56
8	S	127	THR	CA-CB-CG2	8.53	125.00	110.50
9	P	76	ASN	O-C-N	8.52	130.85	122.07
7	N	345	ASP	CA-CB-CG	-8.50	104.10	112.60
11	R	282	THR	N-CA-C	-8.49	101.37	112.41
6	Z	959	HIS	CG-CD2-NE2	8.48	115.68	107.20
6	Z	15	GLN	OE1-CD-NE2	8.48	131.08	122.60
3	T	80	ASN	CA-CB-CG	8.45	121.05	112.60
8	S	33	GLU	CA-C-N	8.45	131.42	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	33	GLU	C-N-CA	8.45	131.42	120.44
7	N	99	GLU	N-CA-C	-8.44	102.29	112.59
12	U	179	ARG	N-CA-CB	8.42	124.72	110.49
13	O	150	LEU	N-CA-CB	8.42	122.62	110.16
5	Y	75	ASN	N-CA-C	8.42	120.45	111.28
7	N	613	HIS	CA-CB-CG	-8.41	105.39	113.80
4	X	69	ILE	CA-C-O	-8.39	114.20	119.15
8	S	197	SER	N-CA-C	-8.38	102.09	111.14
4	X	68	LEU	CA-C-N	8.37	128.62	122.59
4	X	68	LEU	C-N-CA	8.37	128.62	122.59
8	S	335	GLN	N-CA-C	-8.36	102.10	113.30
9	P	122	ILE	CA-C-N	8.34	131.45	120.28
9	P	122	ILE	C-N-CA	8.34	131.45	120.28
3	T	88	TYR	CA-C-N	8.32	131.42	120.28
3	T	88	TYR	C-N-CA	8.32	131.42	120.28
6	Z	779	ALA	CA-C-N	8.31	132.09	120.29
6	Z	779	ALA	C-N-CA	8.31	132.09	120.29
9	P	76	ASN	CA-C-O	-8.30	112.10	120.82
13	O	359	SER	CA-C-N	8.30	129.32	120.03
13	O	359	SER	C-N-CA	8.30	129.32	120.03
2	V	121	VAL	N-CA-C	-8.29	102.35	110.72
10	Q	22	GLU	CA-C-N	8.29	132.21	120.28
10	Q	22	GLU	C-N-CA	8.29	132.21	120.28
6	Z	359	LYS	CA-C-O	-8.29	111.77	120.55
11	R	342	LEU	CA-C-O	-8.29	110.74	120.10
6	Z	37	GLN	OE1-CD-NE2	-8.28	114.32	122.60
10	Q	2	SER	CA-C-N	8.26	131.33	120.26
10	Q	2	SER	C-N-CA	8.26	131.33	120.26
7	N	418	ASP	N-CA-C	8.24	119.89	111.07
9	P	418	ASN	N-CA-C	-8.22	102.27	111.07
7	N	615	ALA	N-CA-C	8.21	121.35	111.82
9	P	319	GLU	CA-C-N	8.21	129.20	120.83
9	P	319	GLU	C-N-CA	8.21	129.20	120.83
4	X	79	LYS	N-CA-C	-8.19	103.74	114.31
11	R	132	GLN	OE1-CD-NE2	8.18	130.78	122.60
1	W	126	ILE	N-CA-C	-8.17	102.85	110.53
3	T	76	ASP	CA-C-N	8.17	131.56	120.54
3	T	76	ASP	C-N-CA	8.17	131.56	120.54
11	R	101	GLU	CA-C-O	-8.16	111.78	120.92
13	O	110	ASP	CA-CB-CG	8.15	120.75	112.60
10	Q	32	ASP	CA-CB-CG	-8.14	104.45	112.60
7	N	296	CYS	N-CA-C	-8.14	102.36	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	947	GLY	CA-C-N	8.13	131.83	120.29
6	Z	947	GLY	C-N-CA	8.13	131.83	120.29
8	S	171	TYR	CB-CA-C	8.13	124.58	109.71
10	Q	334	HIS	CA-CB-CG	-8.13	105.67	113.80
7	N	204	SER	N-CA-CB	8.11	122.03	109.94
10	Q	103	LYS	CA-C-O	-8.11	112.22	120.90
7	N	49	LEU	CA-C-O	-8.10	111.97	120.55
12	U	145	ASP	CA-C-O	8.07	128.94	120.30
7	N	512	ASN	CA-CB-CG	8.05	120.65	112.60
6	Z	58	GLU	N-CA-CB	8.05	121.98	109.83
6	Z	207	ILE	CA-C-N	8.04	126.76	120.33
6	Z	207	ILE	C-N-CA	8.04	126.76	120.33
10	Q	78	ILE	O-C-N	-8.03	114.37	120.07
8	S	20	HIS	O-C-N	8.00	130.31	122.07
9	P	407	ASN	CA-CB-CG	-8.00	104.60	112.60
7	N	333	SER	CA-C-O	-7.98	112.44	120.82
13	O	253	GLN	N-CA-CB	7.98	121.85	110.12
9	P	10	ASP	CA-C-N	7.97	130.81	120.44
9	P	10	ASP	C-N-CA	7.97	130.81	120.44
7	N	812	ALA	CA-C-N	7.97	130.80	120.44
7	N	812	ALA	C-N-CA	7.97	130.80	120.44
6	Z	56	LEU	CA-C-N	7.97	130.96	120.28
6	Z	56	LEU	C-N-CA	7.97	130.96	120.28
9	P	286	ASN	CA-C-N	7.97	132.81	121.02
9	P	286	ASN	C-N-CA	7.97	132.81	121.02
9	P	340	ASP	CA-CB-CG	7.96	120.56	112.60
2	V	172	GLN	N-CA-CB	7.96	122.47	110.22
8	S	469	ASN	N-CA-C	-7.95	102.69	111.36
8	S	318	CYS	CB-CA-C	-7.95	98.40	110.88
11	R	286	LEU	CA-C-N	7.94	131.57	120.29
11	R	286	LEU	C-N-CA	7.94	131.57	120.29
12	U	30	ASN	CA-CB-CG	-7.94	104.66	112.60
2	V	47	MET	CA-C-N	7.94	132.01	120.82
2	V	47	MET	C-N-CA	7.94	132.01	120.82
11	R	411	LEU	CA-C-N	7.93	130.75	120.44
11	R	411	LEU	C-N-CA	7.93	130.75	120.44
1	W	170	HIS	CE1-NE2-CD2	-7.93	101.07	109.00
8	S	100	HIS	CA-CB-CG	-7.93	105.87	113.80
10	Q	205	ALA	N-CA-C	-7.93	102.65	112.88
11	R	408	ASP	CA-CB-CG	-7.93	104.67	112.60
13	O	88	ASP	CA-CB-CG	-7.91	104.69	112.60
10	Q	420	ASN	N-CA-C	7.90	119.89	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	258	ALA	CA-C-N	7.89	130.70	120.44
10	Q	258	ALA	C-N-CA	7.89	130.70	120.44
10	Q	423	VAL	CA-CB-CG2	7.87	123.78	110.40
6	Z	353	VAL	N-CA-CB	7.87	115.46	110.50
7	N	582	ASP	CA-CB-CG	-7.84	104.76	112.60
10	Q	171	LYS	CA-C-N	7.83	127.55	119.56
10	Q	171	LYS	C-N-CA	7.83	127.55	119.56
7	N	438	ASP	CA-CB-CG	-7.82	104.78	112.60
8	S	74	LEU	CA-C-N	7.82	131.10	120.54
8	S	74	LEU	C-N-CA	7.82	131.10	120.54
13	O	78	VAL	N-CA-C	7.81	117.92	110.42
1	W	2	VAL	N-CA-CB	7.80	119.91	110.31
6	Z	470	ALA	CA-C-N	7.80	131.07	120.54
6	Z	470	ALA	C-N-CA	7.80	131.07	120.54
12	U	79	MET	CA-C-N	7.80	131.51	120.28
12	U	79	MET	C-N-CA	7.80	131.51	120.28
7	N	418	ASP	CB-CA-C	-7.78	98.66	110.88
13	O	95	SER	O-C-N	7.78	130.36	122.12
6	Z	804	ASP	CA-CB-CG	-7.77	104.83	112.60
9	P	69	ARG	N-CA-C	-7.77	104.23	112.93
6	Z	881	ILE	N-CA-C	-7.76	103.24	110.53
9	P	79	LEU	CA-C-O	-7.75	112.21	120.42
6	Z	334	LYS	CA-C-O	7.74	128.87	119.97
1	W	77	HIS	CE1-NE2-CD2	-7.74	101.26	109.00
4	X	100	TRP	CG-CD2-CE3	-7.74	126.16	133.90
7	N	783	SER	N-CA-CB	7.73	121.32	110.26
6	Z	491	LEU	N-CA-CB	7.73	121.60	110.16
6	Z	257	PRO	CA-C-N	7.72	128.33	120.38
6	Z	257	PRO	C-N-CA	7.72	128.33	120.38
7	N	743	PHE	O-C-N	-7.71	112.46	121.32
10	Q	158	ILE	O-C-N	7.70	129.34	121.87
8	S	160	ARG	CA-C-N	7.69	130.92	120.54
8	S	160	ARG	C-N-CA	7.69	130.92	120.54
7	N	233	ASN	OD1-CG-ND2	7.69	130.29	122.60
7	N	249	ASN	OD1-CG-ND2	7.68	130.28	122.60
6	Z	732	ILE	CA-C-N	7.68	130.24	120.56
6	Z	732	ILE	C-N-CA	7.68	130.24	120.56
9	P	339	GLU	CB-CA-C	-7.68	97.62	110.68
13	O	130	ASP	CA-C-N	7.68	130.57	120.28
13	O	130	ASP	C-N-CA	7.68	130.57	120.28
6	Z	374	LEU	CA-C-O	7.67	129.67	120.92
9	P	352	VAL	CA-C-N	7.67	131.31	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	352	VAL	C-N-CA	7.67	131.31	120.42
3	T	84	GLN	CA-C-N	7.66	130.89	120.54
3	T	84	GLN	C-N-CA	7.66	130.89	120.54
8	S	481	TYR	O-C-N	7.66	127.30	120.48
7	N	546	LEU	N-CA-C	7.65	119.62	111.28
1	W	77	HIS	ND1-CE1-NE2	7.65	116.05	108.40
11	R	327	ASP	CA-CB-CG	-7.64	104.96	112.60
13	O	76	LEU	O-C-N	-7.64	113.44	122.15
11	R	157	SER	CA-C-N	7.64	130.51	120.28
11	R	157	SER	C-N-CA	7.64	130.51	120.28
4	X	69	ILE	CA-C-N	7.63	128.07	119.83
4	X	69	ILE	C-N-CA	7.63	128.07	119.83
13	O	68	LYS	N-CA-C	7.63	119.59	111.28
10	Q	338	LEU	CA-C-O	-7.62	112.82	120.82
6	Z	800	SER	CA-C-N	7.61	130.81	120.38
6	Z	800	SER	C-N-CA	7.61	130.81	120.38
4	X	109	LEU	CA-C-O	-7.61	112.26	120.17
9	P	437	GLU	N-CA-C	-7.60	102.93	111.14
11	R	340	GLN	N-CA-C	-7.59	103.09	111.36
10	Q	14	LEU	N-CA-C	7.59	119.55	111.28
11	R	31	PHE	CA-CB-CG	-7.59	106.21	113.80
2	V	279	HIS	N-CA-C	7.59	120.62	111.82
2	V	168	LEU	CA-C-N	7.58	130.59	120.58
2	V	168	LEU	C-N-CA	7.58	130.59	120.58
9	P	282	HIS	CA-CB-CG	-7.58	106.22	113.80
9	P	79	LEU	N-CA-C	7.57	119.61	111.36
6	Z	455	ILE	CA-C-N	7.56	128.53	119.99
6	Z	455	ILE	C-N-CA	7.56	128.53	119.99
7	N	805	SER	CA-C-O	-7.55	112.42	120.42
6	Z	722	ASP	CA-CB-CG	7.54	120.14	112.60
7	N	84	ALA	N-CA-C	-7.53	104.23	113.41
8	S	83	PRO	CA-C-N	7.53	135.91	121.54
8	S	83	PRO	C-N-CA	7.53	135.91	121.54
10	Q	175	VAL	N-CA-C	-7.53	103.20	110.42
7	N	783	SER	N-CA-C	-7.52	100.58	110.43
2	V	274	GLN	N-CA-C	-7.52	94.78	110.80
10	Q	255	TYR	N-CA-C	-7.52	103.16	111.36
13	O	58	ARG	NE-CZ-NH1	-7.52	113.98	121.50
7	N	177	ASP	N-CA-C	-7.51	103.03	111.07
12	U	192	ASN	CA-C-N	7.51	130.20	120.44
12	U	192	ASN	C-N-CA	7.51	130.20	120.44
7	N	374	ILE	N-CA-C	-7.49	103.23	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	49	PHE	N-CA-CB	7.49	121.13	110.12
13	O	64	ASN	N-CA-C	7.49	119.08	111.07
1	W	12	ASN	CA-CB-CG	-7.49	105.11	112.60
3	T	230	ASN	CA-C-O	7.47	130.17	121.28
6	Z	59	ASP	N-CA-C	-7.47	104.67	114.31
9	P	328	ALA	N-CA-CB	7.46	123.11	110.49
12	U	156	HIS	CB-CG-CD2	-7.46	121.50	131.20
4	X	100	TRP	CE2-CD2-CE3	7.46	126.26	118.80
8	S	102	SER	N-CA-C	-7.46	94.91	110.80
6	Z	930	GLY	CA-C-N	7.46	132.01	120.75
6	Z	930	GLY	C-N-CA	7.46	132.01	120.75
7	N	670	LYS	CA-C-N	7.46	130.28	120.28
7	N	670	LYS	C-N-CA	7.46	130.28	120.28
7	N	743	PHE	CA-C-N	7.46	129.16	119.84
7	N	743	PHE	C-N-CA	7.46	129.16	119.84
13	O	315	LYS	CA-C-O	-7.46	112.51	120.42
7	N	50	TYR	N-CA-C	7.46	119.49	111.36
2	V	71	MET	CA-C-O	-7.46	113.55	119.66
7	N	699	ALA	CA-C-N	7.44	130.11	120.44
7	N	699	ALA	C-N-CA	7.44	130.11	120.44
7	N	732	GLY	CA-C-O	-7.44	113.39	121.05
6	Z	958	ASN	OD1-CG-ND2	7.44	130.04	122.60
3	T	112	ASN	CA-CB-CG	-7.43	105.17	112.60
7	N	600	THR	N-CA-C	-7.43	104.21	113.28
7	N	585	ARG	CA-C-N	7.43	130.23	120.28
7	N	585	ARG	C-N-CA	7.43	130.23	120.28
9	P	349	ASN	CA-CB-CG	7.42	120.02	112.60
1	W	189	PRO	N-CA-CB	7.41	111.03	103.25
6	Z	444	GLU	CA-C-N	7.41	127.12	119.56
6	Z	444	GLU	C-N-CA	7.41	127.12	119.56
7	N	635	GLN	N-CA-C	-7.41	102.90	112.23
13	O	97	LYS	CA-C-N	7.41	130.21	120.28
13	O	97	LYS	C-N-CA	7.41	130.21	120.28
11	R	285	ALA	CB-CA-C	-7.41	99.25	110.88
6	Z	161	ILE	O-C-N	7.40	129.05	121.87
7	N	618	ARG	O-C-N	-7.40	114.27	122.12
1	W	49	VAL	CA-C-N	7.40	128.04	121.82
1	W	49	VAL	C-N-CA	7.40	128.04	121.82
9	P	313	ILE	N-CA-C	-7.40	105.19	111.56
9	P	331	GLY	CA-C-N	7.40	130.50	120.44
9	P	331	GLY	C-N-CA	7.40	130.50	120.44
10	Q	111	LEU	O-C-N	7.40	132.43	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	428	THR	N-CA-CB	7.39	120.98	110.12
8	S	302	HIS	N-CA-C	-7.39	102.25	112.30
6	Z	433	LEU	CA-C-N	7.38	130.76	120.29
6	Z	433	LEU	C-N-CA	7.38	130.76	120.29
10	Q	310	SER	CA-C-O	7.38	128.33	120.36
13	O	266	PHE	CA-C-N	7.37	130.16	120.28
13	O	266	PHE	C-N-CA	7.37	130.16	120.28
5	Y	72	ASP	CA-CB-CG	-7.37	105.23	112.60
1	W	56	GLY	CA-C-N	7.36	130.14	120.28
1	W	56	GLY	C-N-CA	7.36	130.14	120.28
6	Z	128	GLU	CA-C-N	7.35	130.13	120.28
6	Z	128	GLU	C-N-CA	7.35	130.13	120.28
12	U	287	ALA	CA-C-O	-7.35	112.63	120.42
7	N	8	PRO	CA-N-CD	7.34	122.28	112.00
10	Q	153	ASP	CB-CA-C	-7.34	98.37	110.85
7	N	576	VAL	N-CA-C	7.32	118.12	110.72
12	U	5	HIS	CE1-NE2-CD2	-7.32	101.68	109.00
3	T	251	HIS	CG-CD2-NE2	7.32	114.52	107.20
6	Z	387	ASN	CA-CB-CG	-7.32	105.28	112.60
7	N	379	LEU	O-C-N	-7.32	113.62	122.48
7	N	128	ILE	N-CA-C	-7.31	103.16	110.62
7	N	53	ASP	CA-C-N	7.31	130.41	120.54
7	N	53	ASP	C-N-CA	7.31	130.41	120.54
6	Z	629	VAL	O-C-N	7.30	129.07	121.91
11	R	222	ARG	N-CA-C	-7.30	103.32	111.28
6	Z	541	ASP	N-CA-C	-7.30	101.43	111.28
3	T	129	LEU	N-CA-C	7.29	120.28	111.82
8	S	175	SER	N-CA-C	7.29	120.09	111.71
2	V	155	ALA	N-CA-CB	7.29	122.42	110.69
11	R	120	LEU	N-CA-CB	7.28	121.44	110.22
13	O	54	SER	CA-C-N	7.28	131.74	120.60
13	O	54	SER	C-N-CA	7.28	131.74	120.60
6	Z	53	VAL	N-CA-C	-7.28	103.20	110.62
4	X	103	GLU	CB-CG-CD	-7.27	100.23	112.60
3	T	44	LEU	N-CA-CB	7.27	122.78	110.49
6	Z	710	SER	CA-C-N	7.27	130.35	120.54
6	Z	710	SER	C-N-CA	7.27	130.35	120.54
6	Z	175	ASP	CA-CB-CG	7.27	119.87	112.60
11	R	408	ASP	CA-C-N	7.27	128.00	120.00
11	R	408	ASP	C-N-CA	7.27	128.00	120.00
7	N	742	TRP	CB-CG-CD2	-7.26	116.64	126.80
6	Z	790	MET	N-CA-CB	7.26	122.18	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	565	PHE	CB-CA-C	-7.25	98.76	110.79
11	R	388	VAL	N-CA-C	-7.24	95.07	107.24
12	U	71	ASN	CA-CB-CG	-7.24	105.36	112.60
2	V	42	ARG	N-CA-C	-7.24	103.47	111.36
2	V	150	LYS	CA-C-O	-7.24	112.01	120.62
6	Z	214	HIS	CA-C-O	-7.23	111.65	119.97
7	N	797	GLU	N-CA-C	7.23	118.81	111.07
6	Z	429	ASN	OD1-CG-ND2	7.23	129.83	122.60
6	Z	530	LEU	O-C-N	-7.23	113.91	122.15
6	Z	231	ASP	CA-C-N	7.22	130.93	120.38
6	Z	231	ASP	C-N-CA	7.22	130.93	120.38
3	T	75	PHE	N-CA-C	7.22	119.83	111.02
7	N	319	SER	N-CA-C	7.22	119.15	111.28
6	Z	403	ASN	CA-CB-CG	-7.21	105.39	112.60
6	Z	320	SER	CA-C-N	7.20	130.25	120.38
6	Z	320	SER	C-N-CA	7.20	130.25	120.38
8	S	318	CYS	N-CA-CB	7.19	120.44	110.01
11	R	346	LYS	N-CA-C	-7.19	103.38	111.14
9	P	311	TRP	CA-C-O	-7.18	111.37	118.34
13	O	123	GLY	N-CA-C	-7.18	105.91	115.32
4	X	36	LYS	CA-C-O	-7.18	112.34	120.46
6	Z	164	VAL	O-C-N	-7.18	114.43	121.83
6	Z	819	GLY	O-C-N	7.18	129.08	122.19
8	S	100	HIS	CE1-NE2-CD2	-7.18	101.82	109.00
7	N	821	LYS	N-CA-C	-7.17	104.56	113.38
10	Q	169	ASP	CA-C-N	7.17	135.24	121.54
10	Q	169	ASP	C-N-CA	7.17	135.24	121.54
6	Z	129	ASN	CA-C-N	7.17	133.91	121.07
6	Z	129	ASN	C-N-CA	7.17	133.91	121.07
11	R	283	THR	CA-C-N	7.17	130.47	120.29
11	R	283	THR	C-N-CA	7.17	130.47	120.29
7	N	597	ARG	N-CA-C	7.16	118.73	111.07
10	Q	1	MET	CA-C-N	7.16	130.37	120.63
10	Q	1	MET	C-N-CA	7.16	130.37	120.63
8	S	437	ASN	CA-CB-CG	-7.15	105.45	112.60
13	O	160	LYS	N-CA-CB	7.15	120.63	109.83
1	W	123	ASP	CA-CB-CG	-7.15	105.45	112.60
9	P	277	GLN	CA-C-N	7.15	129.73	120.44
9	P	277	GLN	C-N-CA	7.15	129.73	120.44
6	Z	351	PRO	N-CA-C	-7.15	106.42	114.92
6	Z	432	GLY	CA-C-N	7.14	132.13	120.63
6	Z	432	GLY	C-N-CA	7.14	132.13	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	214	LEU	CA-C-N	7.13	131.15	120.31
7	N	214	LEU	C-N-CA	7.13	131.15	120.31
2	V	154	ASP	CA-CB-CG	-7.12	105.48	112.60
2	V	247	ILE	N-CA-C	-7.12	103.32	113.07
6	Z	17	GLN	CA-C-O	-7.12	112.06	120.10
13	O	40	GLN	OE1-CD-NE2	7.12	129.72	122.60
3	T	127	GLN	N-CA-CB	7.12	120.69	110.16
8	S	322	LEU	CA-C-N	7.12	129.82	120.28
8	S	322	LEU	C-N-CA	7.12	129.82	120.28
6	Z	406	TRP	CE2-CD2-CE3	7.11	125.91	118.80
8	S	227	ASN	OD1-CG-ND2	7.11	129.71	122.60
8	S	413	LEU	CA-C-N	7.11	129.69	120.44
8	S	413	LEU	C-N-CA	7.11	129.69	120.44
10	Q	29	SER	CA-C-N	7.11	130.68	120.79
10	Q	29	SER	C-N-CA	7.11	130.68	120.79
11	R	42	GLN	CA-C-O	-7.11	112.89	120.42
6	Z	307	HIS	ND1-CE1-NE2	7.10	115.50	108.40
13	O	361	ASP	CA-CB-CG	-7.10	105.50	112.60
6	Z	790	MET	N-CA-C	-7.10	104.61	113.20
6	Z	437	ASP	CA-C-O	-7.09	113.03	120.55
1	W	170	HIS	ND1-CE1-NE2	7.09	115.49	108.40
13	O	20	PRO	N-CA-C	-7.08	104.71	114.27
6	Z	298	PHE	CA-C-N	7.08	130.35	120.29
6	Z	298	PHE	C-N-CA	7.08	130.35	120.29
6	Z	629	VAL	N-CA-C	-7.08	103.62	110.42
8	S	161	LYS	CA-C-O	-7.08	113.32	120.90
4	X	55	LYS	N-CA-C	7.08	117.74	109.60
3	T	93	ASN	CA-C-N	7.07	135.05	121.54
3	T	93	ASN	C-N-CA	7.07	135.05	121.54
11	R	357	PHE	CA-CB-CG	-7.07	106.73	113.80
11	R	231	LEU	CB-CA-C	-7.06	98.85	110.85
12	U	258	SER	O-C-N	7.05	129.60	122.12
2	V	233	LYS	CB-CA-C	-7.04	99.77	110.90
6	Z	218	GLU	CA-C-N	7.04	130.03	120.38
6	Z	218	GLU	C-N-CA	7.04	130.03	120.38
9	P	10	ASP	N-CA-C	7.04	119.99	111.82
2	V	157	ARG	NE-CZ-NH1	7.04	128.53	121.50
7	N	701	VAL	O-C-N	7.04	128.69	121.87
10	Q	369	ASP	CA-C-N	7.04	129.59	120.44
10	Q	369	ASP	C-N-CA	7.04	129.59	120.44
1	W	170	HIS	CG-CD2-NE2	7.03	114.23	107.20
13	O	330	ARG	NE-CZ-NH1	7.03	128.53	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	177	VAL	N-CA-CB	7.03	119.57	110.57
2	V	204	HIS	ND1-CE1-NE2	7.02	115.42	108.40
6	Z	441	TYR	CA-CB-CG	-7.02	101.26	113.90
9	P	117	SER	CA-C-N	7.02	131.78	120.55
9	P	117	SER	C-N-CA	7.02	131.78	120.55
10	Q	352	GLU	CA-C-O	-7.01	111.54	118.34
10	Q	41	ALA	N-CA-C	-7.01	104.53	113.23
7	N	701	VAL	CA-C-O	-7.01	113.66	120.95
11	R	114	ASN	OD1-CG-ND2	7.01	129.61	122.60
11	R	335	ARG	O-C-N	7.00	130.13	122.15
7	N	529	GLN	OE1-CD-NE2	-7.00	115.60	122.60
10	Q	293	SER	CA-C-O	7.00	129.35	121.51
12	U	5	HIS	ND1-CE1-NE2	7.00	115.39	108.40
9	P	415	TRP	CA-C-N	6.99	129.53	120.44
9	P	415	TRP	C-N-CA	6.99	129.53	120.44
11	R	109	LYS	CA-C-N	6.99	129.93	120.77
11	R	109	LYS	C-N-CA	6.99	129.93	120.77
7	N	175	ASP	CA-CB-CG	-6.99	105.61	112.60
9	P	361	THR	N-CA-CB	6.99	120.91	110.29
6	Z	962	ARG	N-CA-C	-6.98	102.89	111.33
11	R	98	LEU	CA-C-N	6.98	129.93	120.44
11	R	98	LEU	C-N-CA	6.98	129.93	120.44
8	S	262	THR	N-CA-C	-6.98	102.89	111.40
10	Q	294	ARG	CD-NE-CZ	-6.97	114.64	124.40
8	S	274	PHE	O-C-N	6.97	129.62	122.09
6	Z	475	GLN	CA-C-N	6.97	129.62	120.28
6	Z	475	GLN	C-N-CA	6.97	129.62	120.28
8	S	39	ASN	CA-C-N	6.97	129.50	120.44
8	S	39	ASN	C-N-CA	6.97	129.50	120.44
9	P	354	SER	O-C-N	6.97	130.09	122.15
13	O	223	LEU	CA-C-N	6.97	130.12	121.06
13	O	223	LEU	C-N-CA	6.97	130.12	121.06
2	V	177	THR	N-CA-C	-6.96	103.69	111.28
3	T	158	GLN	CA-C-N	6.96	130.17	120.29
3	T	158	GLN	C-N-CA	6.96	130.17	120.29
6	Z	866	VAL	N-CA-C	-6.96	103.99	110.53
11	R	392	ARG	NE-CZ-NH2	6.96	125.46	119.20
13	O	250	TRP	CA-C-N	6.96	129.90	120.44
13	O	250	TRP	C-N-CA	6.96	129.90	120.44
9	P	299	LEU	N-CA-C	6.95	118.51	111.07
1	W	50	GLY	N-CA-C	-6.95	101.00	111.14
10	Q	243	PHE	CA-CB-CG	-6.95	106.85	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	492	LYS	CA-C-O	-6.95	108.99	120.80
10	Q	103	LYS	O-C-N	6.95	129.31	122.09
6	Z	587	THR	CA-C-N	6.94	129.97	120.46
6	Z	587	THR	C-N-CA	6.94	129.97	120.46
7	N	51	ASP	CA-CB-CG	-6.94	105.66	112.60
8	S	191	HIS	CA-CB-CG	6.94	120.74	113.80
11	R	424	THR	CA-C-O	-6.94	109.00	120.80
7	N	754	THR	CA-C-N	6.94	126.70	119.76
7	N	754	THR	C-N-CA	6.94	126.70	119.76
4	X	133	SER	CA-C-O	-6.94	109.01	120.80
10	Q	431	SER	CA-C-N	6.94	129.97	120.46
10	Q	431	SER	C-N-CA	6.94	129.97	120.46
3	T	238	GLN	CA-C-N	6.94	129.90	120.54
3	T	238	GLN	C-N-CA	6.94	129.90	120.54
6	Z	841	GLU	N-CA-C	-6.93	98.10	109.40
6	Z	930	GLY	N-CA-C	6.93	123.95	112.30
7	N	157	ALA	CA-C-N	6.93	129.46	120.44
7	N	157	ALA	C-N-CA	6.93	129.46	120.44
7	N	925	ASP	CA-C-O	-6.93	109.01	120.80
10	Q	429	LYS	O-C-N	-6.93	114.11	122.22
9	P	440	HIS	CA-C-O	-6.93	109.01	120.80
1	W	68	GLU	CA-C-O	6.93	128.53	120.49
9	P	179	PHE	O-C-N	6.93	129.21	122.07
11	R	168	ILE	O-C-N	6.93	128.70	121.91
8	S	59	ASP	CA-C-N	6.93	129.45	120.44
8	S	59	ASP	C-N-CA	6.93	129.45	120.44
9	P	83	SER	N-CA-C	6.93	119.42	111.11
1	W	197	SER	CA-C-O	-6.92	109.03	120.80
8	S	100	HIS	ND1-CE1-NE2	6.92	115.32	108.40
7	N	818	LYS	CA-C-N	6.92	129.55	120.28
7	N	818	LYS	C-N-CA	6.92	129.55	120.28
8	S	71	ALA	N-CA-C	-6.91	104.76	112.57
3	T	272	ASN	CA-C-O	-6.91	109.06	120.80
6	Z	60	ASP	N-CA-CB	6.91	120.26	109.83
2	V	274	GLN	N-CA-CB	6.90	122.16	110.49
7	N	257	ILE	CA-C-N	6.90	130.09	120.29
7	N	257	ILE	C-N-CA	6.90	130.09	120.29
2	V	214	MET	N-CA-C	-6.90	102.11	112.04
6	Z	218	GLU	N-CA-CB	6.90	120.97	110.28
8	S	374	ASP	CA-C-N	6.90	132.67	122.74
8	S	374	ASP	C-N-CA	6.90	132.67	122.74
13	O	109	LEU	O-C-N	6.90	129.43	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	245	TYR	O-C-N	6.90	130.29	122.22
8	S	329	GLU	CA-C-N	6.89	130.08	120.29
8	S	329	GLU	C-N-CA	6.89	130.08	120.29
13	O	143	LEU	N-CA-C	-6.89	103.55	112.23
6	Z	201	LEU	CA-C-N	6.89	129.40	120.44
6	Z	201	LEU	C-N-CA	6.89	129.40	120.44
9	P	282	HIS	CE1-NE2-CD2	-6.89	102.11	109.00
10	Q	345	SER	N-CA-CB	6.89	120.25	110.12
8	S	28	GLU	CA-C-N	6.88	129.84	120.54
8	S	28	GLU	C-N-CA	6.88	129.84	120.54
6	Z	711	SER	O-C-N	6.88	129.24	122.09
7	N	120	ASP	CB-CA-C	-6.87	98.28	109.89
1	W	75	GLY	CA-C-N	6.86	130.03	120.29
1	W	75	GLY	C-N-CA	6.86	130.03	120.29
12	U	285	ILE	CA-C-N	6.86	129.21	120.56
12	U	285	ILE	C-N-CA	6.86	129.21	120.56
6	Z	764	LEU	N-CA-C	-6.86	103.73	111.07
6	Z	17	GLN	CB-CG-CD	-6.85	100.95	112.60
7	N	592	GLY	CA-C-O	6.85	127.51	120.80
11	R	239	THR	N-CA-C	-6.85	98.87	109.76
2	V	196	TYR	CA-CB-CG	-6.85	101.57	113.90
8	S	259	TYR	CA-C-N	6.85	126.81	120.03
8	S	259	TYR	C-N-CA	6.85	126.81	120.03
11	R	110	ILE	CA-C-O	-6.85	114.29	121.41
10	Q	354	PHE	CA-CB-CG	6.84	120.64	113.80
13	O	48	PHE	CA-C-O	-6.84	113.81	121.00
6	Z	112	LYS	N-CA-C	-6.84	103.90	111.36
11	R	308	LEU	CA-C-N	6.84	130.00	120.29
11	R	308	LEU	C-N-CA	6.84	130.00	120.29
7	N	907	ASP	CA-CB-CG	-6.84	105.76	112.60
7	N	429	GLU	N-CA-CB	6.83	119.98	110.07
7	N	583	VAL	CB-CA-C	-6.83	102.79	112.22
4	X	124	LYS	O-C-N	6.83	129.35	122.12
7	N	795	GLU	O-C-N	6.82	129.35	122.12
10	Q	135	HIS	CE1-NE2-CD2	-6.82	102.18	109.00
6	Z	389	PHE	CA-CB-CG	-6.82	106.98	113.80
12	U	75	ASN	CA-CB-CG	6.82	119.42	112.60
3	T	100	ASP	CA-CB-CG	-6.81	105.79	112.60
6	Z	494	GLY	CA-C-N	6.81	129.27	120.56
6	Z	494	GLY	C-N-CA	6.81	129.27	120.56
9	P	288	ASN	CA-C-N	6.81	130.08	120.28
9	P	288	ASN	C-N-CA	6.81	130.08	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	31	LEU	CA-C-N	6.81	129.73	120.54
10	Q	31	LEU	C-N-CA	6.81	129.73	120.54
10	Q	271	MET	N-CA-C	-6.80	103.93	111.82
8	S	136	CYS	CA-C-N	6.80	129.95	120.29
8	S	136	CYS	C-N-CA	6.80	129.95	120.29
9	P	395	ARG	O-C-N	-6.80	114.32	120.71
8	S	438	HIS	O-C-N	6.80	129.37	122.03
6	Z	133	ASP	CA-CB-CG	-6.80	105.80	112.60
6	Z	834	LEU	CA-C-N	6.79	129.38	120.28
6	Z	834	LEU	C-N-CA	6.79	129.38	120.28
9	P	431	HIS	N-CA-C	-6.79	103.95	111.36
11	R	110	ILE	CB-CA-C	6.79	120.39	111.70
7	N	623	PHE	CA-CB-CG	-6.79	107.01	113.80
13	O	236	HIS	CA-C-O	-6.79	113.64	120.63
1	W	95	GLN	OE1-CD-NE2	-6.78	115.82	122.60
2	V	47	MET	N-CA-C	-6.78	100.40	110.23
6	Z	313	ILE	N-CA-C	-6.78	103.88	110.72
11	R	255	VAL	N-CA-C	6.78	116.92	110.42
10	Q	422	VAL	O-C-N	-6.77	115.27	121.91
13	O	187	SER	N-CA-CB	6.77	120.18	110.16
11	R	182	ASN	CA-CB-CG	-6.77	105.83	112.60
7	N	704	GLY	CA-C-O	-6.77	113.09	120.40
11	R	406	GLN	CA-C-N	6.76	128.81	120.22
11	R	406	GLN	C-N-CA	6.76	128.81	120.22
10	Q	407	ALA	CA-C-N	6.76	129.67	120.54
10	Q	407	ALA	C-N-CA	6.76	129.67	120.54
6	Z	291	GLU	CA-C-N	6.76	129.23	120.44
6	Z	291	GLU	C-N-CA	6.76	129.23	120.44
10	Q	177	VAL	N-CA-C	-6.76	104.17	110.53
9	P	235	LEU	CA-C-N	6.76	129.89	120.29
9	P	235	LEU	C-N-CA	6.76	129.89	120.29
7	N	543	ASP	CA-CB-CG	-6.76	105.84	112.60
13	O	83	LEU	N-CA-CB	6.76	120.20	110.06
4	X	53	THR	N-CA-C	-6.75	105.66	114.04
6	Z	472	LEU	CA-C-O	-6.75	113.64	121.07
6	Z	4	GLU	N-CA-CB	6.75	125.75	111.10
12	U	274	MET	N-CA-C	6.75	118.64	111.28
10	Q	56	THR	CA-C-O	-6.75	113.73	120.82
13	O	15	ARG	NE-CZ-NH1	6.74	128.24	121.50
7	N	690	HIS	CA-C-N	6.74	130.93	120.75
7	N	690	HIS	C-N-CA	6.74	130.93	120.75
10	Q	67	THR	N-CA-C	-6.74	102.26	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	39	ASN	OD1-CG-ND2	6.73	129.33	122.60
9	P	73	ASP	CA-C-N	6.72	129.29	120.28
9	P	73	ASP	C-N-CA	6.72	129.29	120.28
9	P	337	HIS	CE1-NE2-CD2	-6.72	102.28	109.00
6	Z	959	HIS	CE1-NE2-CD2	-6.72	102.28	109.00
7	N	425	ASN	N-CA-C	-6.72	103.88	111.07
7	N	470	LEU	N-CA-CB	6.72	120.10	110.16
13	O	203	THR	N-CA-C	-6.72	104.39	112.59
7	N	907	ASP	CA-C-O	6.72	127.52	120.54
8	S	139	HIS	CA-CB-CG	6.71	120.51	113.80
9	P	53	ALA	CA-C-O	-6.71	113.44	120.55
9	P	183	GLN	CB-CA-C	-6.71	99.65	110.79
6	Z	824	ASN	N-CA-C	-6.71	104.23	114.16
8	S	303	ASN	CA-C-N	6.71	129.81	120.29
8	S	303	ASN	C-N-CA	6.71	129.81	120.29
9	P	339	GLU	CA-C-N	6.70	129.93	120.28
9	P	339	GLU	C-N-CA	6.70	129.93	120.28
7	N	60	MET	CA-C-N	6.70	129.26	120.28
7	N	60	MET	C-N-CA	6.70	129.26	120.28
6	Z	349	THR	N-CA-C	-6.69	104.07	111.36
7	N	577	SER	CB-CA-C	-6.69	97.97	110.01
9	P	333	ALA	CA-C-N	6.69	129.91	120.28
9	P	333	ALA	C-N-CA	6.69	129.91	120.28
7	N	270	LEU	CA-C-O	-6.69	113.46	120.55
1	W	55	ALA	CA-C-N	6.69	131.13	121.44
1	W	55	ALA	C-N-CA	6.69	131.13	121.44
4	X	13	GLY	O-C-N	-6.68	117.78	123.59
6	Z	771	HIS	N-CA-C	-6.68	103.47	111.69
7	N	726	ASP	N-CA-CB	6.68	120.83	110.21
13	O	384	MET	CA-C-N	6.68	129.12	120.44
13	O	384	MET	C-N-CA	6.68	129.12	120.44
8	S	472	HIS	N-CA-CB	6.68	119.93	110.12
3	T	250	MET	N-CA-CB	6.67	121.03	110.49
7	N	436	ASP	CA-CB-CG	6.67	119.28	112.60
11	R	144	ILE	N-CA-C	-6.67	106.22	112.83
6	Z	895	LEU	CA-C-N	6.67	133.27	122.53
6	Z	895	LEU	C-N-CA	6.67	133.27	122.53
10	Q	411	SER	N-CA-C	-6.67	103.82	112.23
8	S	75	CYS	CA-C-N	6.67	129.22	120.28
8	S	75	CYS	C-N-CA	6.67	129.22	120.28
13	O	346	GLU	N-CA-CB	6.67	121.76	110.49
6	Z	195	PHE	CA-CB-CG	-6.66	107.14	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	766	HIS	CE1-NE2-CD2	-6.66	102.34	109.00
13	O	286	PHE	N-CA-CB	6.66	119.66	110.01
8	S	226	ASP	CA-C-N	6.66	129.20	120.28
8	S	226	ASP	C-N-CA	6.66	129.20	120.28
4	X	97	TYR	CA-C-O	6.65	128.58	120.60
9	P	37	ASP	N-CA-C	-6.65	103.95	111.07
13	O	181	PHE	CB-CA-C	-6.65	99.55	110.85
7	N	51	ASP	N-CA-CB	6.64	119.88	110.12
9	P	381	SER	CA-C-N	6.64	129.18	120.28
9	P	381	SER	C-N-CA	6.64	129.18	120.28
10	Q	167	LYS	N-CA-C	-6.64	105.09	113.72
6	Z	770	GLU	CA-C-O	-6.64	114.33	121.56
7	N	549	TYR	CA-C-N	6.64	128.44	120.14
7	N	549	TYR	C-N-CA	6.64	128.44	120.14
8	S	425	ARG	CA-C-O	-6.64	113.39	120.42
8	S	236	LEU	O-C-N	6.63	129.15	122.12
10	Q	26	VAL	N-CA-CB	6.63	119.05	110.57
1	W	102	GLN	CB-CA-C	-6.62	100.49	110.88
7	N	57	ASP	CA-C-N	6.62	130.75	120.82
7	N	57	ASP	C-N-CA	6.62	130.75	120.82
6	Z	946	THR	N-CA-C	-6.62	97.73	108.52
6	Z	491	LEU	O-C-N	-6.62	114.61	122.15
8	S	350	LYS	N-CA-CB	6.62	119.80	109.94
12	U	21	HIS	CA-CB-CG	6.62	120.42	113.80
10	Q	374	GLU	N-CA-CB	6.61	119.60	110.01
9	P	122	ILE	N-CA-C	-6.61	102.83	111.09
13	O	191	THR	N-CA-C	6.61	118.48	111.28
9	P	33	ASN	CA-CB-CG	-6.61	105.99	112.60
6	Z	497	PHE	CA-CB-CG	-6.60	107.20	113.80
3	T	42	PRO	CB-CA-C	6.60	117.39	110.00
8	S	438	HIS	CA-CB-CG	6.60	120.40	113.80
12	U	14	VAL	N-CA-CB	6.60	118.27	110.55
6	Z	827	LEU	N-CA-C	-6.59	104.02	111.14
11	R	298	ALA	N-CA-C	-6.59	105.23	113.28
8	S	290	ASN	CB-CA-C	-6.59	100.53	110.88
8	S	19	HIS	ND1-CE1-NE2	6.59	114.99	108.40
11	R	232	VAL	O-C-N	-6.59	115.04	121.83
6	Z	237	VAL	N-CA-CB	6.59	122.10	111.23
10	Q	210	CYS	CA-C-O	-6.58	113.56	119.75
7	N	506	GLN	CB-CG-CD	-6.58	101.41	112.60
3	T	93	ASN	OD1-CG-ND2	6.58	129.18	122.60
5	Y	40	ILE	N-CA-C	-6.58	103.91	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	582	ASP	N-CA-C	-6.58	104.19	111.36
7	N	878	GLN	N-CA-C	-6.58	105.82	114.31
11	R	310	GLU	CB-CA-C	-6.58	100.55	110.88
7	N	907	ASP	CA-C-N	6.58	129.39	120.38
7	N	907	ASP	C-N-CA	6.58	129.39	120.38
6	Z	292	ASP	CA-CB-CG	6.58	119.18	112.60
7	N	358	LYS	CA-C-O	-6.57	111.29	119.38
8	S	145	PHE	CA-C-O	-6.57	113.87	120.90
8	S	389	LYS	N-CA-C	6.57	118.44	111.28
10	Q	338	LEU	O-C-N	6.57	128.84	122.07
3	T	96	LEU	N-CA-C	-6.57	102.40	110.61
6	Z	208	VAL	CA-C-O	-6.57	114.29	118.69
2	V	136	ALA	N-CA-CB	6.56	119.73	109.69
7	N	565	ASN	N-CA-C	-6.56	103.62	111.69
10	Q	63	GLN	N-CA-C	-6.56	105.09	113.23
9	P	301	LYS	CA-C-O	-6.56	111.56	119.49
10	Q	424	ASP	CA-CB-CG	6.56	119.16	112.60
6	Z	868	ASN	CB-CA-C	-6.55	99.91	110.79
8	S	130	VAL	N-CA-C	-6.55	106.28	113.43
6	Z	617	ILE	CA-C-N	6.55	129.06	120.28
6	Z	617	ILE	C-N-CA	6.55	129.06	120.28
7	N	231	ASN	CA-CB-CG	-6.55	106.05	112.60
10	Q	148	LYS	CA-C-N	6.55	134.02	123.93
10	Q	148	LYS	C-N-CA	6.55	134.02	123.93
11	R	252	TYR	CB-CA-C	-6.55	99.91	110.79
6	Z	335	LEU	CA-C-N	6.55	129.59	120.29
6	Z	335	LEU	C-N-CA	6.55	129.59	120.29
9	P	18	LYS	N-CA-CB	6.55	119.96	110.20
6	Z	513	ALA	CB-CA-C	6.55	123.45	110.42
7	N	567	ALA	N-CA-CB	6.55	119.85	110.16
7	N	590	ALA	CA-C-N	6.54	129.05	120.28
7	N	590	ALA	C-N-CA	6.54	129.05	120.28
7	N	285	ALA	CA-C-O	6.54	127.48	120.55
6	Z	922	PRO	CB-CA-C	6.54	119.87	111.56
7	N	731	VAL	CA-C-N	6.54	127.38	119.99
7	N	731	VAL	C-N-CA	6.54	127.38	119.99
7	N	61	ALA	CA-C-N	6.54	129.57	120.29
7	N	61	ALA	C-N-CA	6.54	129.57	120.29
9	P	248	ASP	CA-CB-CG	-6.54	106.06	112.60
6	Z	898	HIS	CA-C-N	6.54	132.71	122.78
6	Z	898	HIS	C-N-CA	6.54	132.71	122.78
8	S	302	HIS	CA-C-N	6.54	130.43	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	302	HIS	C-N-CA	6.54	130.43	120.82
6	Z	467	VAL	N-CA-CB	6.53	120.13	111.90
8	S	239	ARG	N-CA-CB	6.53	119.72	110.12
13	O	147	ARG	O-C-N	-6.53	115.30	122.09
3	T	207	ALA	CA-C-N	6.53	129.32	120.44
3	T	207	ALA	C-N-CA	6.53	129.32	120.44
8	S	30	GLN	N-CA-C	6.53	118.05	111.07
8	S	94	LYS	O-C-N	6.52	129.03	122.12
2	V	225	LEU	N-CA-C	-6.52	105.36	113.38
1	W	142	ILE	N-CA-C	-6.52	97.79	107.51
6	Z	545	SER	CA-C-N	6.52	129.68	120.42
6	Z	545	SER	C-N-CA	6.52	129.68	120.42
7	N	813	ARG	CB-CA-C	-6.52	100.65	110.88
9	P	282	HIS	CG-CD2-NE2	6.52	113.72	107.20
13	O	374	ASN	CA-CB-CG	-6.52	106.08	112.60
9	P	231	LYS	N-CA-C	-6.51	104.91	112.92
11	R	55	LYS	CA-C-N	6.51	129.29	120.44
11	R	55	LYS	C-N-CA	6.51	129.29	120.44
6	Z	959	HIS	N-CA-C	-6.51	103.77	112.94
7	N	110	VAL	N-CA-CB	6.50	118.16	110.55
10	Q	238	TYR	O-C-N	-6.50	115.23	122.12
13	O	176	SER	CA-C-N	6.50	129.00	120.28
13	O	176	SER	C-N-CA	6.50	129.00	120.28
4	X	91	PHE	CA-CB-CG	-6.50	107.30	113.80
6	Z	361	HIS	CA-CB-CG	-6.50	107.30	113.80
12	U	291	LEU	CA-C-O	6.50	127.31	120.42
7	N	348	PHE	CA-CB-CG	6.50	120.30	113.80
1	W	151	THR	CA-CB-OG1	6.50	119.34	109.60
6	Z	924	LYS	O-C-N	-6.50	114.52	122.25
6	Z	206	ASP	N-CA-C	6.50	118.02	111.07
7	N	672	ASN	CA-C-N	6.49	126.42	119.28
7	N	672	ASN	C-N-CA	6.49	126.42	119.28
7	N	556	ALA	N-CA-CB	6.49	119.61	109.94
6	Z	771	HIS	O-C-N	6.49	130.66	122.23
9	P	124	VAL	CA-CB-CG1	6.49	121.43	110.40
8	S	18	LEU	CA-C-N	6.48	128.87	120.44
8	S	18	LEU	C-N-CA	6.48	128.87	120.44
10	Q	253	ASN	CA-CB-CG	-6.48	106.12	112.60
2	V	204	HIS	CE1-NE2-CD2	-6.48	102.52	109.00
7	N	409	GLY	N-CA-C	6.48	121.73	113.24
13	O	245	ASP	CA-C-O	6.48	128.32	121.19
8	S	319	CYS	N-CA-C	6.47	118.00	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	244	ARG	CB-CA-C	-6.47	100.72	110.88
8	S	19	HIS	CE1-NE2-CD2	-6.47	102.53	109.00
9	P	417	HIS	N-CA-C	6.47	118.33	111.28
3	T	164	LEU	CB-CA-C	-6.46	100.06	110.79
9	P	345	VAL	CA-CB-CG1	6.46	121.39	110.40
8	S	30	GLN	OE1-CD-NE2	6.46	129.06	122.60
8	S	326	ASP	N-CA-CB	6.46	120.80	110.46
11	R	292	LEU	N-CA-C	6.46	118.32	111.28
12	U	54	LEU	CA-C-O	-6.46	113.10	119.69
10	Q	190	ASN	N-CA-CB	6.46	120.90	110.77
8	S	158	PHE	CA-C-N	6.45	128.83	120.44
8	S	158	PHE	C-N-CA	6.45	128.83	120.44
6	Z	524	ALA	N-CA-C	-6.45	104.25	111.28
7	N	485	MET	CA-C-O	-6.44	114.06	120.70
13	O	9	THR	N-CA-CB	6.44	120.26	110.28
3	T	121	LYS	CA-C-O	-6.44	112.56	119.97
6	Z	136	ARG	N-CA-CB	6.44	119.58	110.12
7	N	793	GLY	CA-C-O	-6.44	114.05	121.00
12	U	202	SER	O-C-N	6.44	128.94	122.12
6	Z	888	LEU	O-C-N	6.44	130.13	122.79
7	N	891	VAL	CA-C-N	-6.43	113.15	119.78
7	N	891	VAL	C-N-CA	-6.43	113.15	119.78
8	S	24	LYS	CA-C-N	6.43	128.80	120.44
8	S	24	LYS	C-N-CA	6.43	128.80	120.44
3	T	245	TYR	N-CA-C	6.43	118.29	111.28
6	Z	130	GLY	N-CA-C	-6.43	105.18	115.08
1	W	133	LYS	N-CA-C	-6.43	104.36	111.82
9	P	82	LEU	CA-C-O	-6.43	114.07	120.82
7	N	390	LEU	CA-C-N	6.43	126.34	119.85
7	N	390	LEU	C-N-CA	6.43	126.34	119.85
8	S	438	HIS	N-CA-CB	6.43	119.30	109.98
3	T	126	LEU	N-CA-C	6.42	118.28	111.28
6	Z	777	PRO	N-CA-CB	6.42	110.40	103.33
9	P	305	THR	N-CA-CB	6.42	119.41	109.97
6	Z	701	ILE	CA-C-O	-6.42	114.28	120.95
3	T	182	LYS	CB-CA-C	-6.41	100.81	110.88
12	U	292	ILE	CA-C-N	6.41	129.51	120.28
12	U	292	ILE	C-N-CA	6.41	129.51	120.28
13	O	380	LEU	N-CA-C	6.41	118.35	111.36
2	V	230	TYR	CA-C-N	6.41	129.51	120.28
2	V	230	TYR	C-N-CA	6.41	129.51	120.28
8	S	76	PHE	CA-C-N	6.41	129.11	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	76	PHE	C-N-CA	6.41	129.11	120.65
10	Q	110	SER	O-C-N	6.41	131.11	122.59
10	Q	430	ALA	N-CA-C	-6.41	105.22	113.16
8	S	153	GLU	CA-C-N	6.40	128.76	120.44
8	S	153	GLU	C-N-CA	6.40	128.76	120.44
7	N	695	ALA	CA-C-O	-6.40	113.77	120.55
9	P	333	ALA	CB-CA-C	-6.40	99.97	110.85
6	Z	746	ILE	CA-C-O	-6.40	114.07	120.85
9	P	320	PRO	N-CA-C	-6.40	108.03	114.68
6	Z	916	LEU	N-CA-C	-6.39	104.39	111.36
7	N	104	LYS	N-CA-C	-6.39	104.31	111.28
10	Q	116	PHE	CA-C-N	6.39	128.61	120.56
10	Q	116	PHE	C-N-CA	6.39	128.61	120.56
13	O	30	GLU	CA-C-N	6.39	128.75	120.44
13	O	30	GLU	C-N-CA	6.39	128.75	120.44
2	V	122	ASP	CA-CB-CG	-6.39	106.21	112.60
11	R	415	GLN	OE1-CD-NE2	6.39	128.99	122.60
12	U	25	THR	N-CA-CB	6.39	119.92	110.53
6	Z	258	PRO	N-CA-C	6.38	118.49	110.70
11	R	168	ILE	CA-C-N	6.38	129.16	120.54
11	R	168	ILE	C-N-CA	6.38	129.16	120.54
13	O	378	GLU	CA-CB-CG	6.38	126.86	114.10
6	Z	175	ASP	CA-C-O	6.38	127.03	119.56
12	U	281	LEU	CA-C-N	6.38	129.20	120.46
12	U	281	LEU	C-N-CA	6.38	129.20	120.46
2	V	202	ASP	CA-CB-CG	-6.38	106.22	112.60
6	Z	897	HIS	ND1-CE1-NE2	6.38	114.78	108.40
10	Q	105	GLU	O-C-N	6.38	128.72	122.09
8	S	401	LYS	CA-C-O	-6.38	113.48	120.30
5	Y	67	VAL	N-CA-C	-6.37	105.52	111.45
1	W	100	HIS	ND1-CE1-NE2	6.37	114.77	108.40
8	S	170	TYR	CA-C-N	6.37	131.97	122.99
8	S	170	TYR	C-N-CA	6.37	131.97	122.99
13	O	344	VAL	N-CA-C	-6.37	103.37	112.35
6	Z	889	VAL	N-CA-C	-6.37	98.95	108.12
7	N	479	GLU	CB-CG-CD	-6.37	101.78	112.60
10	Q	12	ARG	CA-C-N	6.36	129.13	120.54
10	Q	12	ARG	C-N-CA	6.36	129.13	120.54
7	N	256	GLN	N-CA-C	6.36	117.87	111.07
8	S	374	ASP	CA-CB-CG	-6.36	106.24	112.60
12	U	156	HIS	CB-CG-ND1	6.36	132.23	122.70
13	O	204	SER	CA-C-N	6.36	133.41	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	204	SER	C-N-CA	6.36	133.41	121.97
13	O	187	SER	CB-CA-C	-6.35	100.05	110.85
13	O	285	SER	CB-CA-C	-6.35	100.91	110.88
7	N	472	ASN	CA-C-N	6.35	131.16	122.34
7	N	472	ASN	C-N-CA	6.35	131.16	122.34
13	O	68	LYS	O-C-N	6.35	128.85	122.12
2	V	60	ASP	N-CA-C	-6.35	104.99	114.64
10	Q	43	GLY	N-CA-C	-6.34	98.15	113.18
8	S	118	PHE	N-CA-CB	6.34	121.20	110.49
11	R	42	GLN	O-C-N	6.34	129.38	122.15
13	O	66	VAL	CA-C-O	-6.34	114.45	121.17
2	V	243	SER	N-CA-CB	6.33	119.54	110.16
12	U	253	ASP	N-CA-C	-6.33	104.29	111.07
10	Q	249	LEU	CA-C-N	6.33	131.33	121.26
10	Q	249	LEU	C-N-CA	6.33	131.33	121.26
6	Z	15	GLN	O-C-N	-6.33	114.94	122.15
8	S	193	THR	CA-C-N	6.33	129.28	120.29
8	S	193	THR	C-N-CA	6.33	129.28	120.29
9	P	289	ASN	CA-C-N	6.33	128.76	120.28
9	P	289	ASN	C-N-CA	6.33	128.76	120.28
10	Q	408	THR	CA-C-N	6.33	128.76	120.28
10	Q	408	THR	C-N-CA	6.33	128.76	120.28
2	V	233	LYS	N-CA-CB	6.33	119.24	110.07
6	Z	763	HIS	CE1-NE2-CD2	-6.33	102.67	109.00
8	S	261	HIS	ND1-CE1-NE2	6.32	114.72	108.40
11	R	115	GLU	CB-CG-CD	-6.32	101.85	112.60
12	U	219	LEU	N-CA-C	-6.32	101.61	109.64
3	T	64	VAL	N-CA-C	-6.32	104.33	110.72
6	Z	215	ASN	O-C-N	6.32	129.35	122.15
7	N	98	VAL	N-CA-C	-6.32	97.62	106.53
6	Z	307	HIS	CE1-NE2-CD2	-6.32	102.68	109.00
2	V	290	ASN	OD1-CG-ND2	6.31	128.91	122.60
9	P	431	HIS	CB-CG-CD2	-6.31	122.99	131.20
9	P	435	LYS	CA-C-N	6.31	130.70	120.60
9	P	435	LYS	C-N-CA	6.31	130.70	120.60
6	Z	876	VAL	CA-C-N	6.31	128.74	120.28
6	Z	876	VAL	C-N-CA	6.31	128.74	120.28
9	P	344	ARG	CA-C-N	6.31	129.10	120.46
9	P	344	ARG	C-N-CA	6.31	129.10	120.46
10	Q	90	LYS	CA-C-O	-6.31	114.24	121.68
12	U	154	PHE	N-CA-C	-6.30	98.14	108.41
3	T	62	LEU	CA-C-N	6.30	129.24	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	62	LEU	C-N-CA	6.30	129.24	120.29
6	Z	211	PHE	CA-C-O	-6.30	113.87	120.55
10	Q	71	LYS	CA-C-N	6.30	128.72	120.28
10	Q	71	LYS	C-N-CA	6.30	128.72	120.28
13	O	354	GLN	CA-C-N	6.30	126.31	119.89
13	O	354	GLN	C-N-CA	6.30	126.31	119.89
2	V	181	ASN	CA-CB-CG	-6.30	106.30	112.60
6	Z	634	ASP	CA-CB-CG	6.30	118.90	112.60
12	U	220	PRO	CB-CA-C	6.30	119.59	111.21
2	V	99	GLY	N-CA-C	-6.29	106.55	115.30
7	N	899	ASN	OD1-CG-ND2	-6.29	116.31	122.60
11	R	392	ARG	O-C-N	6.29	125.05	121.27
2	V	73	GLN	CB-CA-C	-6.29	99.82	109.89
8	S	261	HIS	N-CA-C	-6.29	105.26	114.39
8	S	416	GLU	CA-C-N	6.29	128.71	120.28
8	S	416	GLU	C-N-CA	6.29	128.71	120.28
6	Z	287	ARG	O-C-N	6.29	128.63	122.09
10	Q	87	GLN	OE1-CD-NE2	-6.29	116.31	122.60
8	S	469	ASN	N-CA-CB	6.28	119.46	110.16
8	S	313	SER	N-CA-CB	6.28	119.45	110.16
6	Z	912	PHE	N-CA-CB	6.28	119.24	110.26
6	Z	618	GLN	OE1-CD-NE2	-6.27	116.33	122.60
10	Q	110	SER	CA-C-O	-6.27	111.54	120.51
11	R	127	GLU	N-CA-C	-6.27	104.36	111.07
13	O	326	HIS	CA-C-N	6.27	128.68	120.28
13	O	326	HIS	C-N-CA	6.27	128.68	120.28
13	O	13	THR	O-C-N	6.27	128.76	122.12
9	P	163	LEU	N-CA-C	6.27	118.63	111.11
10	Q	409	TYR	CB-CG-CD2	-6.27	111.40	120.80
7	N	79	VAL	CA-C-O	-6.27	114.21	120.85
6	Z	856	HIS	CE1-NE2-CD2	-6.26	102.74	109.00
7	N	720	ALA	CA-C-N	6.26	129.19	120.29
7	N	720	ALA	C-N-CA	6.26	129.19	120.29
6	Z	701	ILE	CA-C-N	6.26	129.00	120.54
6	Z	701	ILE	C-N-CA	6.26	129.00	120.54
6	Z	439	TYR	CB-CG-CD1	6.26	130.19	120.80
10	Q	78	ILE	CB-CA-C	-6.25	107.72	114.35
13	O	58	ARG	CA-C-N	6.25	128.98	120.54
13	O	58	ARG	C-N-CA	6.25	128.98	120.54
4	X	102	GLN	N-CA-C	-6.25	104.55	111.36
7	N	97	PHE	N-CA-C	-6.25	105.43	114.12
6	Z	52	LEU	O-C-N	6.25	128.51	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	586	GLU	O-C-N	6.25	128.74	122.12
7	N	583	VAL	CA-C-O	-6.24	114.23	120.85
13	O	76	LEU	N-CA-C	-6.24	104.56	111.36
10	Q	315	ASN	CB-CA-C	-6.24	100.44	110.79
10	Q	335	PHE	N-CA-C	6.24	119.06	111.82
9	P	362	LEU	N-CA-C	6.24	118.16	111.36
6	Z	58	GLU	CB-CA-C	-6.24	99.37	109.72
9	P	374	SER	N-CA-C	6.24	117.74	111.07
13	O	190	TYR	O-C-N	6.24	128.49	122.07
13	O	277	ILE	N-CA-C	-6.23	100.62	107.73
2	V	168	LEU	N-CA-C	-6.23	105.68	113.28
7	N	913	PRO	CA-C-O	-6.23	114.33	121.56
4	X	101	LEU	N-CA-C	-6.23	99.72	109.25
13	O	385	GLU	N-CA-C	-6.23	104.41	111.07
11	R	26	VAL	CA-C-O	-6.23	114.80	121.27
7	N	28	ILE	O-C-N	6.22	127.91	121.87
9	P	31	ASP	CA-CB-CG	6.22	118.82	112.60
7	N	416	GLY	CA-C-N	6.22	130.15	120.82
7	N	416	GLY	C-N-CA	6.22	130.15	120.82
13	O	159	LYS	N-CA-C	-6.22	104.60	111.82
9	P	7	ILE	CA-C-N	6.22	129.12	120.29
9	P	7	ILE	C-N-CA	6.22	129.12	120.29
10	Q	147	GLN	CB-CG-CD	-6.22	102.03	112.60
13	O	195	TYR	CA-C-N	6.22	129.12	120.29
13	O	195	TYR	C-N-CA	6.22	129.12	120.29
10	Q	108	PRO	CA-C-N	6.21	131.37	121.18
10	Q	108	PRO	C-N-CA	6.21	131.37	121.18
11	R	164	THR	CA-C-N	6.21	127.01	119.99
11	R	164	THR	C-N-CA	6.21	127.01	119.99
2	V	296	LEU	CA-C-O	-6.21	114.30	120.82
9	P	241	LEU	N-CA-C	-6.21	104.51	111.28
6	Z	151	HIS	CB-CA-C	-6.21	99.22	109.65
12	U	198	LYS	N-CA-C	-6.21	104.59	111.36
1	W	162	ASN	N-CA-C	6.20	119.46	110.28
8	S	202	ASN	N-CA-CB	6.20	119.90	110.28
6	Z	731	GLY	CA-C-N	6.20	128.95	120.46
6	Z	731	GLY	C-N-CA	6.20	128.95	120.46
7	N	105	SER	CA-C-N	6.20	128.37	120.56
7	N	105	SER	C-N-CA	6.20	128.37	120.56
7	N	399	PHE	CA-CB-CG	-6.20	107.60	113.80
7	N	479	GLU	O-C-N	6.20	128.78	122.09
10	Q	397	LEU	O-C-N	6.20	130.46	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	46	ILE	CA-C-N	6.20	129.09	120.29
7	N	46	ILE	C-N-CA	6.20	129.09	120.29
7	N	592	GLY	N-CA-C	6.20	120.39	112.83
7	N	750	SER	CA-C-O	6.20	127.10	120.10
12	U	107	ASN	OD1-CG-ND2	6.20	128.80	122.60
10	Q	361	HIS	CE1-NE2-CD2	-6.19	102.81	109.00
2	V	27	VAL	N-CA-CB	6.19	118.45	111.21
6	Z	413	ASP	CA-CB-CG	-6.19	106.41	112.60
8	S	321	GLN	N-CA-C	6.19	118.03	111.28
9	P	58	VAL	N-CA-C	-6.19	104.47	110.72
10	Q	315	ASN	N-CA-CB	6.19	119.22	110.12
1	W	76	LEU	N-CA-C	-6.19	104.61	111.36
7	N	719	ASN	N-CA-CB	6.18	119.06	109.85
3	T	74	ASN	CA-C-N	6.18	129.38	120.79
3	T	74	ASN	C-N-CA	6.18	129.38	120.79
8	S	61	SER	CA-C-O	6.18	127.31	120.82
7	N	638	ILE	CA-C-O	-6.18	114.53	120.95
9	P	88	GLN	CA-C-O	-6.17	111.68	120.51
11	R	140	TYR	N-CA-C	-6.17	104.63	111.36
6	Z	267	THR	N-CA-CB	6.17	119.19	110.12
7	N	466	LEU	N-CA-C	-6.17	104.63	111.36
7	N	171	LYS	O-C-N	-6.17	115.58	122.12
7	N	732	GLY	CA-C-N	6.17	129.69	120.31
7	N	732	GLY	C-N-CA	6.17	129.69	120.31
10	Q	385	ILE	N-CA-C	-6.17	105.13	110.74
8	S	253	PHE	CB-CG-CD1	-6.17	110.22	120.70
7	N	154	LEU	CA-C-N	6.16	126.95	119.99
7	N	154	LEU	C-N-CA	6.16	126.95	119.99
8	S	417	GLN	CA-C-N	6.16	128.82	120.44
8	S	417	GLN	C-N-CA	6.16	128.82	120.44
13	O	209	GLU	CA-C-N	6.16	128.54	120.28
13	O	209	GLU	C-N-CA	6.16	128.54	120.28
6	Z	709	LYS	CA-C-N	6.16	128.82	120.44
6	Z	709	LYS	C-N-CA	6.16	128.82	120.44
8	S	147	TRP	CA-C-N	6.16	128.86	120.54
8	S	147	TRP	C-N-CA	6.16	128.86	120.54
9	P	263	HIS	N-CA-CB	6.16	118.94	110.01
7	N	880	ARG	CB-CG-CD	6.16	125.46	111.30
9	P	349	ASN	N-CA-C	6.16	117.99	111.28
10	Q	348	CYS	N-CA-CB	6.15	119.17	110.12
4	X	76	VAL	N-CA-CB	-6.15	105.85	112.37
8	S	85	SER	O-C-N	6.15	128.63	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	378	ASN	CA-CB-CG	6.15	118.75	112.60
8	S	482	PRO	O-C-N	6.14	129.60	122.23
6	Z	428	TRP	N-CA-C	-6.14	105.09	112.58
6	Z	603	VAL	CA-CB-CG2	-6.14	99.97	110.40
6	Z	799	PHE	CA-CB-CG	-6.14	107.66	113.80
11	R	339	ALA	CA-C-N	6.14	129.01	120.29
11	R	339	ALA	C-N-CA	6.14	129.01	120.29
12	U	76	MET	CA-C-N	6.14	128.82	120.54
12	U	76	MET	C-N-CA	6.14	128.82	120.54
12	U	218	GLU	CA-C-N	6.14	128.92	120.39
12	U	218	GLU	C-N-CA	6.14	128.92	120.39
3	T	14	ALA	N-CA-CB	6.13	119.67	110.22
6	Z	36	GLU	N-CA-C	-6.13	105.83	113.38
7	N	377	GLY	CA-C-N	6.13	133.26	121.54
7	N	377	GLY	C-N-CA	6.13	133.26	121.54
1	W	122	ARG	CA-C-N	6.13	128.78	120.38
1	W	122	ARG	C-N-CA	6.13	128.78	120.38
6	Z	97	PRO	N-CA-CB	6.13	110.01	103.39
10	Q	30	LEU	O-C-N	-6.13	115.52	122.08
11	R	139	GLU	O-C-N	-6.13	115.04	122.22
6	Z	310	LEU	CA-C-N	6.13	128.50	120.28
6	Z	310	LEU	C-N-CA	6.13	128.50	120.28
6	Z	574	TYR	CB-CG-CD2	-6.13	111.61	120.80
11	R	401	HIS	ND1-CE1-NE2	6.13	114.53	108.40
8	S	57	LEU	CA-C-N	6.12	128.40	120.44
8	S	57	LEU	C-N-CA	6.12	128.40	120.44
11	R	374	ASN	CA-CB-CG	-6.12	106.48	112.60
13	O	130	ASP	N-CA-CB	6.12	119.12	110.12
9	P	236	GLU	CA-C-O	-6.12	113.94	120.42
12	U	280	ASN	CB-CA-C	-6.12	100.63	110.79
12	U	281	LEU	O-C-N	-6.12	115.64	122.12
11	R	231	LEU	N-CA-CB	6.11	119.21	110.16
3	T	213	ASN	CA-CB-CG	-6.11	106.49	112.60
3	T	28	PRO	CA-C-O	-6.11	111.70	120.56
6	Z	129	ASN	N-CA-C	-6.11	104.62	111.28
10	Q	145	HIS	CG-CD2-NE2	6.11	113.31	107.20
6	Z	803	ALA	N-CA-C	-6.11	97.80	110.80
10	Q	48	ASP	N-CA-CB	6.11	120.81	110.49
6	Z	727	GLU	CA-C-N	6.10	133.20	121.54
6	Z	727	GLU	C-N-CA	6.10	133.20	121.54
10	Q	89	ALA	N-CA-C	6.10	119.81	111.39
10	Q	124	PHE	CB-CG-CD1	6.10	131.07	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	46	THR	CA-C-N	6.10	128.46	120.28
13	O	46	THR	C-N-CA	6.10	128.46	120.28
6	Z	196	SER	N-CA-C	-6.10	104.63	111.28
7	N	575	ALA	CB-CA-C	-6.10	100.48	110.85
2	V	157	ARG	NE-CZ-NH2	-6.10	113.71	119.20
7	N	469	VAL	N-CA-C	-6.10	104.40	110.62
6	Z	258	PRO	CB-CA-C	6.09	118.36	110.92
8	S	431	VAL	N-CA-C	-6.09	104.56	110.72
10	Q	266	LEU	N-CA-C	-6.09	104.72	111.36
2	V	203	TYR	CA-CB-CG	-6.09	102.93	113.90
11	R	293	THR	CA-C-N	6.09	128.81	120.46
11	R	293	THR	C-N-CA	6.09	128.81	120.46
3	T	122	PHE	CB-CA-C	-6.09	101.32	110.88
12	U	280	ASN	CA-CB-CG	-6.09	106.51	112.60
6	Z	480	ASN	O-C-N	-6.09	115.88	121.30
9	P	417	HIS	CE1-NE2-CD2	-6.09	102.91	109.00
2	V	127	LYS	O-C-N	-6.08	115.21	122.15
7	N	742	TRP	CE2-CD2-CE3	6.08	124.88	118.80
8	S	163	VAL	N-CA-C	6.07	116.81	110.62
6	Z	145	ASP	N-CA-CB	6.07	120.12	110.65
8	S	253	PHE	CD1-CG-CD2	6.07	127.71	118.60
9	P	417	HIS	ND1-CE1-NE2	6.07	114.47	108.40
11	R	193	ALA	CA-C-N	6.07	130.06	120.47
11	R	193	ALA	C-N-CA	6.07	130.06	120.47
11	R	199	GLU	N-CA-C	-6.07	105.91	113.38
1	W	34	GLU	CA-C-N	6.07	128.41	120.28
1	W	34	GLU	C-N-CA	6.07	128.41	120.28
7	N	919	THR	N-CA-CB	6.07	119.04	110.36
2	V	103	MET	CG-SD-CE	-6.07	87.56	100.90
13	O	313	ILE	CA-C-N	6.07	128.73	120.54
13	O	313	ILE	C-N-CA	6.07	128.73	120.54
3	T	255	GLN	N-CA-C	-6.06	105.17	113.30
8	S	311	GLN	CA-C-N	6.06	128.41	120.28
8	S	311	GLN	C-N-CA	6.06	128.41	120.28
8	S	24	LYS	N-CA-C	6.06	117.56	111.07
12	U	37	ILE	N-CA-C	-6.06	99.68	108.17
8	S	191	HIS	CA-C-N	6.06	128.40	120.28
8	S	191	HIS	C-N-CA	6.06	128.40	120.28
6	Z	480	ASN	CA-CB-CG	6.06	118.66	112.60
13	O	308	LEU	N-CA-C	-6.06	98.76	109.06
8	S	25	TYR	CA-C-N	6.06	128.72	120.54
8	S	25	TYR	C-N-CA	6.06	128.72	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	630	LYS	CA-C-N	6.05	126.81	120.03
6	Z	630	LYS	C-N-CA	6.05	126.81	120.03
10	Q	225	LEU	N-CA-C	-6.05	105.56	113.12
13	O	23	HIS	CE1-NE2-CD2	-6.05	102.95	109.00
13	O	116	ASN	O-C-N	6.05	129.05	122.15
6	Z	87	LYS	O-C-N	-6.05	115.60	120.38
3	T	243	ALA	CA-C-N	6.04	128.70	120.54
3	T	243	ALA	C-N-CA	6.04	128.70	120.54
6	Z	24	THR	CA-C-N	6.04	127.39	119.84
6	Z	24	THR	C-N-CA	6.04	127.39	119.84
7	N	645	THR	CA-C-N	6.04	132.51	122.54
7	N	645	THR	C-N-CA	6.04	132.51	122.54
8	S	134	ILE	CA-C-O	-6.04	114.77	121.17
10	Q	114	GLN	N-CA-C	6.04	117.56	110.97
13	O	376	GLN	N-CA-C	6.04	117.86	111.28
7	N	351	ALA	N-CA-C	-6.04	104.61	111.07
12	U	212	ASP	CA-CB-CG	-6.04	106.56	112.60
6	Z	801	HIS	CA-C-N	6.04	133.07	121.54
6	Z	801	HIS	C-N-CA	6.04	133.07	121.54
7	N	178	SER	N-CA-CB	6.04	120.75	111.46
8	S	357	LEU	CA-C-O	-6.04	114.48	120.70
7	N	742	TRP	N-CA-C	-6.03	97.75	108.13
7	N	207	LEU	N-CA-CB	6.03	118.99	110.12
9	P	417	HIS	CA-C-N	6.03	128.28	120.44
9	P	417	HIS	C-N-CA	6.03	128.28	120.44
12	U	207	VAL	CB-CA-C	-6.03	104.25	111.97
10	Q	21	ASN	CA-C-N	6.03	128.85	120.29
10	Q	21	ASN	C-N-CA	6.03	128.85	120.29
7	N	632	LYS	CA-C-N	6.03	125.83	120.10
7	N	632	LYS	C-N-CA	6.03	125.83	120.10
2	V	271	VAL	CA-CB-CG1	6.03	120.64	110.40
6	Z	600	GLU	N-CA-C	6.03	117.85	111.28
6	Z	801	HIS	CE1-NE2-CD2	-6.03	102.97	109.00
11	R	181	TYR	CA-CB-CG	-6.03	103.06	113.90
12	U	154	PHE	CA-C-N	6.03	131.31	123.00
12	U	154	PHE	C-N-CA	6.03	131.31	123.00
13	O	56	PRO	N-CA-C	6.03	121.44	114.03
2	V	142	ASP	CB-CA-C	6.02	116.72	109.85
6	Z	125	THR	N-CA-CB	6.02	118.97	110.12
9	P	300	VAL	CB-CA-C	-6.02	104.13	112.02
9	P	381	SER	O-C-N	-6.02	115.59	122.09
11	R	226	GLU	N-CA-C	-6.02	104.28	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	23	TYR	N-CA-CB	6.02	118.97	110.12
12	U	12	PRO	CA-C-N	6.02	128.35	120.28
12	U	12	PRO	C-N-CA	6.02	128.35	120.28
13	O	291	ILE	N-CA-C	-6.02	104.48	110.62
10	Q	11	ALA	CA-C-N	6.02	128.66	120.54
10	Q	11	ALA	C-N-CA	6.02	128.66	120.54
6	Z	363	ASP	CA-CB-CG	6.02	118.62	112.60
2	V	43	ALA	CA-C-O	-6.01	114.05	120.42
7	N	922	GLN	O-C-N	6.01	128.50	122.12
10	Q	124	PHE	CB-CG-CD2	-6.01	110.47	120.70
10	Q	160	ASP	N-CA-C	-6.01	104.66	112.23
10	Q	296	ILE	CA-C-N	6.01	128.62	120.44
10	Q	296	ILE	C-N-CA	6.01	128.62	120.44
8	S	456	ASP	CA-CB-CG	-6.01	106.59	112.60
6	Z	13	ASP	CA-CB-CG	-6.01	106.59	112.60
7	N	379	LEU	CA-C-O	6.01	125.40	118.97
9	P	215	SER	N-CA-CB	6.01	119.59	110.28
8	S	143	GLN	CA-C-N	6.00	128.25	120.44
8	S	143	GLN	C-N-CA	6.00	128.25	120.44
6	Z	136	ARG	CB-CA-C	-6.00	100.83	110.79
10	Q	141	LEU	CA-C-N	6.00	128.24	120.44
10	Q	141	LEU	C-N-CA	6.00	128.24	120.44
6	Z	280	ASP	CA-C-N	6.00	128.24	120.44
6	Z	280	ASP	C-N-CA	6.00	128.24	120.44
6	Z	611	THR	N-CA-C	-6.00	105.28	114.16
7	N	10	LEU	O-C-N	6.00	128.25	122.07
11	R	105	LYS	N-CA-C	6.00	118.31	111.11
13	O	189	TYR	N-CA-C	-6.00	104.74	111.28
7	N	689	LYS	N-CA-C	-6.00	105.92	113.72
9	P	350	LEU	O-C-N	6.00	128.48	122.12
6	Z	850	LEU	O-C-N	-6.00	115.89	122.07
13	O	33	TYR	CA-C-O	-6.00	114.52	120.82
7	N	601	THR	CA-C-N	6.00	125.13	120.33
7	N	601	THR	C-N-CA	6.00	125.13	120.33
6	Z	859	LYS	CA-C-N	5.99	132.15	121.48
6	Z	859	LYS	C-N-CA	5.99	132.15	121.48
9	P	104	LEU	N-CA-CB	5.99	118.93	110.12
6	Z	497	PHE	N-CA-C	-5.99	105.46	112.89
11	R	291	SER	N-CA-C	-5.99	104.75	111.28
8	S	121	VAL	CA-C-O	-5.99	114.82	121.17
9	P	63	VAL	CA-C-N	5.99	128.80	120.29
9	P	63	VAL	C-N-CA	5.99	128.80	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	269	TYR	N-CA-CB	5.99	118.69	110.01
1	W	32	SER	N-CA-CB	5.98	119.02	110.16
6	Z	593	HIS	CE1-NE2-CD2	-5.98	103.02	109.00
7	N	80	LYS	CA-C-N	5.98	130.85	120.68
7	N	80	LYS	C-N-CA	5.98	130.85	120.68
7	N	911	LYS	N-CA-C	-5.98	106.14	113.50
4	X	119	LYS	CA-C-N	5.98	128.30	120.28
4	X	119	LYS	C-N-CA	5.98	128.30	120.28
8	S	283	GLN	CA-C-N	5.98	132.97	121.54
8	S	283	GLN	C-N-CA	5.98	132.97	121.54
11	R	129	GLU	N-CA-C	5.98	119.05	111.69
13	O	210	ARG	O-C-N	-5.98	115.78	122.12
4	X	75	TRP	CA-C-N	5.98	128.53	123.33
4	X	75	TRP	C-N-CA	5.98	128.53	123.33
3	T	117	ASN	N-CA-C	-5.98	103.21	111.28
8	S	166	ASN	O-C-N	5.98	128.23	122.07
10	Q	250	THR	CA-C-O	5.98	127.25	120.80
7	N	804	LEU	CA-C-O	5.98	126.89	120.55
4	X	98	PHE	CA-CB-CG	-5.97	107.83	113.80
7	N	690	HIS	CA-CB-CG	-5.97	107.83	113.80
13	O	172	TYR	CA-C-N	5.97	128.56	120.44
13	O	172	TYR	C-N-CA	5.97	128.56	120.44
13	O	288	ARG	CB-CA-C	-5.97	100.88	110.79
6	Z	48	ASP	CA-C-N	5.97	128.20	120.44
6	Z	48	ASP	C-N-CA	5.97	128.20	120.44
8	S	338	MET	CA-C-N	5.97	129.09	120.79
8	S	338	MET	C-N-CA	5.97	129.09	120.79
10	Q	135	HIS	ND1-CE1-NE2	5.97	114.37	108.40
1	W	6	THR	CA-C-O	-5.96	113.92	120.36
7	N	902	VAL	N-CA-CB	5.96	117.22	110.72
8	S	148	ASP	CA-C-N	5.96	128.52	120.65
8	S	148	ASP	C-N-CA	5.96	128.52	120.65
8	S	474	GLU	O-C-N	5.96	128.43	122.12
3	T	13	ILE	N-CA-C	-5.95	104.23	112.50
4	X	132	SER	N-CA-C	-5.95	107.83	114.62
11	R	64	LYS	N-CA-CB	5.95	118.87	110.12
11	R	218	CYS	CA-C-N	5.95	128.26	120.28
11	R	218	CYS	C-N-CA	5.95	128.26	120.28
3	T	259	ILE	CA-C-N	5.95	128.87	120.42
3	T	259	ILE	C-N-CA	5.95	128.87	120.42
8	S	284	LEU	N-CA-CB	5.95	120.54	110.49
11	R	166	ALA	N-CA-CB	5.95	118.86	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	238	GLN	CB-CG-CD	-5.95	102.49	112.60
8	S	124	GLU	CA-C-O	-5.95	114.12	120.42
8	S	450	ASN	CA-CB-CG	-5.95	106.65	112.60
6	Z	219	ASP	N-CA-C	5.94	118.52	111.33
11	R	29	LYS	N-CA-C	5.94	117.76	111.28
11	R	99	TYR	CA-CB-CG	-5.94	103.20	113.90
7	N	249	ASN	CB-CG-ND2	-5.94	107.49	116.40
13	O	363	ILE	O-C-N	5.94	127.95	121.83
6	Z	879	ALA	CA-C-N	5.94	128.24	120.28
6	Z	879	ALA	C-N-CA	5.94	128.24	120.28
13	O	28	GLN	CB-CG-CD	-5.94	102.51	112.60
6	Z	712	ASP	CA-C-O	5.93	126.84	120.55
7	N	21	LYS	CB-CA-C	-5.93	100.76	110.85
7	N	334	VAL	CA-C-N	5.93	128.22	120.28
7	N	334	VAL	C-N-CA	5.93	128.22	120.28
9	P	379	TYR	N-CA-CB	5.93	119.43	110.30
7	N	211	PHE	N-CA-CB	5.93	118.61	110.01
7	N	786	ARG	NE-CZ-NH1	-5.93	115.57	121.50
2	V	85	ASP	CA-CB-CG	-5.92	106.68	112.60
11	R	298	ALA	O-C-N	-5.92	114.00	122.41
1	W	100	HIS	CE1-NE2-CD2	-5.92	103.08	109.00
2	V	149	GLY	O-C-N	5.92	127.93	122.19
8	S	138	MET	CA-C-N	5.92	128.14	120.44
8	S	138	MET	C-N-CA	5.92	128.14	120.44
10	Q	160	ASP	CA-CB-CG	-5.92	106.68	112.60
11	R	157	SER	O-C-N	-5.92	115.97	122.07
3	T	53	ASN	O-C-N	5.92	128.90	122.15
6	Z	277	GLU	CA-C-N	5.92	131.49	121.14
6	Z	277	GLU	C-N-CA	5.92	131.49	121.14
6	Z	702	LYS	N-CA-CB	5.92	118.75	109.94
7	N	348	PHE	CB-CA-C	-5.92	100.79	110.85
11	R	116	LYS	CA-C-N	5.92	128.56	120.46
11	R	116	LYS	C-N-CA	5.92	128.56	120.46
8	S	392	ILE	CA-C-N	5.91	128.21	120.28
8	S	392	ILE	C-N-CA	5.91	128.21	120.28
8	S	373	LYS	N-CA-C	-5.91	104.92	111.36
1	W	32	SER	CA-C-O	-5.91	114.15	120.42
1	W	173	THR	CA-C-O	5.91	126.82	120.32
4	X	63	PRO	CA-C-N	5.91	127.88	121.97
4	X	63	PRO	C-N-CA	5.91	127.88	121.97
6	Z	164	VAL	CA-C-N	5.91	128.20	120.28
6	Z	164	VAL	C-N-CA	5.91	128.20	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	77	PHE	CB-CG-CD1	5.91	130.74	120.70
9	P	262	SER	N-CA-C	-5.90	104.75	111.07
13	O	374	ASN	N-CA-C	-5.90	104.92	111.36
3	T	226	TRP	CA-C-O	-5.90	114.19	119.86
11	R	351	LYS	CB-CG-CD	5.90	124.87	111.30
12	U	207	VAL	N-CA-CB	5.90	117.45	110.55
7	N	215	MET	CG-SD-CE	-5.89	87.93	100.90
3	T	203	SER	CA-C-N	5.89	129.27	120.31
3	T	203	SER	C-N-CA	5.89	129.27	120.31
3	T	238	GLN	N-CA-C	5.89	117.37	111.07
9	P	68	SER	N-CA-CB	5.89	118.71	109.69
3	T	86	LYS	CA-C-N	5.89	126.30	119.47
3	T	86	LYS	C-N-CA	5.89	126.30	119.47
9	P	349	ASN	O-C-N	5.89	128.36	122.12
8	S	306	SER	N-CA-CB	5.89	119.44	110.44
6	Z	911	LYS	CA-C-N	5.88	130.81	120.87
6	Z	911	LYS	C-N-CA	5.88	130.81	120.87
2	V	106	GLY	O-C-N	-5.88	117.56	124.15
7	N	725	LEU	CA-C-N	5.88	130.24	122.42
7	N	725	LEU	C-N-CA	5.88	130.24	122.42
9	P	110	LEU	CA-C-N	5.88	128.44	120.38
9	P	110	LEU	C-N-CA	5.88	128.44	120.38
1	W	42	ASN	CA-C-O	5.88	126.73	119.97
7	N	203	ARG	N-CA-C	5.88	117.36	111.07
7	N	755	PRO	N-CA-CB	5.88	108.81	103.34
7	N	923	MET	CA-C-N	5.88	128.08	120.44
7	N	923	MET	C-N-CA	5.88	128.08	120.44
6	Z	825	ALA	CA-C-N	5.88	131.42	121.14
6	Z	825	ALA	C-N-CA	5.88	131.42	121.14
8	S	248	ASP	CA-CB-CG	-5.88	106.72	112.60
6	Z	767	TYR	O-C-N	5.87	128.85	122.15
7	N	228	VAL	O-C-N	5.87	127.57	121.87
7	N	789	GLU	CA-C-O	-5.87	112.86	119.79
10	Q	26	VAL	CB-CA-C	-5.87	104.33	112.02
7	N	756	THR	N-CA-CB	5.87	119.99	110.77
7	N	573	HIS	CE1-NE2-CD2	-5.87	103.13	109.00
10	Q	246	TYR	N-CA-CB	5.87	118.95	110.20
12	U	70	HIS	CA-C-N	5.87	128.63	120.29
12	U	70	HIS	C-N-CA	5.87	128.63	120.29
12	U	267	VAL	CA-C-N	5.87	128.07	120.44
12	U	267	VAL	C-N-CA	5.87	128.07	120.44
3	T	41	ILE	O-C-N	-5.87	114.41	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	741	LEU	CA-C-O	-5.87	113.22	119.97
7	N	621	THR	N-CA-CB	5.87	118.94	110.20
9	P	289	ASN	CA-CB-CG	-5.87	106.73	112.60
5	Y	80	GLU	CA-C-N	5.87	128.14	120.28
5	Y	80	GLU	C-N-CA	5.87	128.14	120.28
11	R	158	LEU	N-CA-CB	5.87	118.74	110.12
3	T	68	ALA	N-CA-CB	5.87	118.86	110.06
9	P	375	GLN	CA-C-N	5.87	128.06	120.44
9	P	375	GLN	C-N-CA	5.87	128.06	120.44
2	V	155	ALA	CB-CA-C	-5.86	98.83	109.38
6	Z	346	LEU	N-CA-CB	5.86	118.51	110.01
7	N	329	HIS	CA-C-O	-5.86	114.21	120.42
7	N	379	LEU	CA-C-N	5.86	128.41	120.44
7	N	379	LEU	C-N-CA	5.86	128.41	120.44
9	P	222	ASN	CA-C-N	5.86	128.13	120.28
9	P	222	ASN	C-N-CA	5.86	128.13	120.28
9	P	329	PHE	N-CA-C	-5.86	101.52	110.14
13	O	318	HIS	CA-C-O	-5.86	114.31	121.28
11	R	108	SER	CA-C-N	5.86	128.45	120.54
11	R	108	SER	C-N-CA	5.86	128.45	120.54
6	Z	52	LEU	CA-C-O	-5.86	114.67	120.82
3	T	180	ILE	N-CA-C	-5.85	104.80	110.42
6	Z	871	HIS	ND1-CE1-NE2	5.85	114.25	108.40
12	U	203	LYS	CB-CA-C	-5.85	101.69	110.88
7	N	305	ASN	CA-CB-CG	-5.85	106.75	112.60
7	N	270	LEU	CA-C-N	5.85	128.12	120.28
7	N	270	LEU	C-N-CA	5.85	128.12	120.28
9	P	306	ASN	CA-CB-CG	-5.85	106.75	112.60
6	Z	275	GLN	CB-CG-CD	-5.85	102.66	112.60
8	S	160	ARG	N-CA-C	5.84	117.32	111.07
9	P	142	ASP	N-CA-CB	5.84	118.91	110.20
11	R	149	ASN	N-CA-C	-5.84	105.98	113.23
13	O	294	MET	N-CA-C	-5.84	105.04	111.82
13	O	302	VAL	CA-CB-CG1	-5.84	100.47	110.40
6	Z	728	LYS	CG-CD-CE	5.84	124.73	111.30
10	Q	92	LYS	CA-C-N	5.84	128.42	120.54
10	Q	92	LYS	C-N-CA	5.84	128.42	120.54
3	T	106	ILE	O-C-N	5.84	127.63	121.91
11	R	218	CYS	O-C-N	-5.83	115.09	122.27
7	N	573	HIS	N-CA-C	-5.83	105.00	111.36
1	W	185	ILE	CA-C-O	-5.83	114.89	120.95
2	V	166	ASN	CA-CB-CG	-5.83	106.77	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	275	ILE	O-C-N	5.83	128.48	122.07
3	T	192	ASN	O-C-N	-5.83	116.07	122.07
8	S	156	VAL	CA-C-O	5.83	127.33	121.27
12	U	138	VAL	CA-C-O	5.83	126.51	120.39
4	X	113	GLU	N-CA-C	-5.82	105.37	112.88
6	Z	839	SER	CB-CA-C	-5.82	101.13	110.79
7	N	111	GLN	N-CA-C	5.82	118.09	111.11
5	Y	22	GLU	N-CA-CB	5.82	118.44	110.01
6	Z	232	LYS	N-CA-C	5.82	119.19	111.75
8	S	343	LEU	N-CA-CB	5.82	118.97	110.30
10	Q	110	SER	N-CA-C	5.82	123.19	110.80
13	O	83	LEU	N-CA-C	5.82	118.37	111.33
7	N	196	THR	CA-C-N	-5.81	115.10	122.37
7	N	196	THR	C-N-CA	-5.81	115.10	122.37
11	R	382	ASP	CB-CA-C	-5.81	99.70	109.53
1	W	179	ARG	O-C-N	5.81	130.32	122.59
2	V	111	HIS	CE1-NE2-CD2	-5.81	103.19	109.00
4	X	40	GLU	O-C-N	-5.81	115.96	122.12
7	N	53	ASP	N-CA-C	-5.81	105.68	112.89
10	Q	140	LYS	CA-C-N	5.81	128.07	120.28
10	Q	140	LYS	C-N-CA	5.81	128.07	120.28
6	Z	208	VAL	CA-C-N	5.81	125.35	119.19
6	Z	208	VAL	C-N-CA	5.81	125.35	119.19
10	Q	33	LYS	CB-CA-C	-5.81	101.51	110.81
12	U	202	SER	CB-CA-C	-5.81	101.15	110.79
6	Z	763	HIS	ND1-CE1-NE2	5.81	114.21	108.40
11	R	119	LYS	CA-C-N	5.81	128.64	120.28
11	R	119	LYS	C-N-CA	5.81	128.64	120.28
11	R	110	ILE	N-CA-C	5.81	116.27	110.23
1	W	164	PRO	CA-C-N	5.80	132.63	121.54
1	W	164	PRO	C-N-CA	5.80	132.63	121.54
10	Q	32	ASP	O-C-N	5.80	128.13	122.09
9	P	372	THR	CA-CB-OG1	5.80	118.31	109.60
10	Q	333	SER	N-CA-CB	5.80	118.58	109.94
2	V	156	PHE	CA-C-O	5.80	128.22	121.44
3	T	89	TYR	N-CA-C	5.80	117.60	111.28
10	Q	405	GLN	N-CA-CB	5.80	118.52	110.17
13	O	194	LEU	CA-C-N	5.80	128.05	120.28
13	O	194	LEU	C-N-CA	5.80	128.05	120.28
6	Z	967	THR	CA-C-O	5.79	127.89	121.11
12	U	59	ASP	CA-CB-CG	-5.79	106.81	112.60
9	P	143	LEU	CB-CA-C	-5.79	101.17	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	336	HIS	CG-CD2-NE2	5.79	112.99	107.20
11	R	337	VAL	CA-CB-CG1	5.79	120.25	110.40
2	V	123	VAL	CA-C-O	-5.79	114.71	120.85
8	S	203	SER	N-CA-C	-5.79	104.97	111.28
10	Q	216	ALA	O-C-N	5.79	128.04	122.07
6	Z	172	ASP	N-CA-C	-5.79	105.05	111.36
1	W	74	ALA	N-CA-C	-5.79	105.05	111.36
10	Q	142	ALA	CA-C-N	5.79	127.97	120.44
10	Q	142	ALA	C-N-CA	5.79	127.97	120.44
7	N	96	GLN	N-CA-C	-5.79	105.41	112.88
2	V	304	ALA	N-CA-C	-5.79	104.89	111.14
3	T	237	ASN	CA-CB-CG	-5.78	106.82	112.60
11	R	124	ASP	CA-C-N	-5.78	113.83	122.74
11	R	124	ASP	C-N-CA	-5.78	113.83	122.74
13	O	152	ASP	CA-CB-CG	-5.78	106.82	112.60
6	Z	308	LYS	CA-C-O	-5.78	114.75	120.82
8	S	398	THR	N-CA-C	5.78	117.58	111.28
7	N	727	THR	CA-C-N	5.78	128.29	120.38
7	N	727	THR	C-N-CA	5.78	128.29	120.38
11	R	319	CYS	CA-C-N	5.78	127.95	120.44
11	R	319	CYS	C-N-CA	5.78	127.95	120.44
1	W	28	ALA	N-CA-C	-5.78	105.12	111.82
8	S	80	VAL	CA-CB-CG1	5.77	120.22	110.40
9	P	428	THR	CA-C-N	5.77	128.37	120.46
9	P	428	THR	C-N-CA	5.77	128.37	120.46
13	O	370	LEU	CB-CA-C	-5.77	101.04	110.85
11	R	408	ASP	N-CA-C	-5.77	105.07	111.36
12	U	269	THR	CA-CB-OG1	5.77	118.25	109.60
13	O	181	PHE	CA-C-N	5.77	130.35	120.72
13	O	181	PHE	C-N-CA	5.77	130.35	120.72
12	U	145	ASP	N-CA-CB	5.77	119.65	110.65
3	T	253	GLU	N-CA-C	-5.76	107.49	114.75
6	Z	399	LEU	N-CA-C	5.76	117.56	111.28
7	N	309	ILE	O-C-N	5.76	129.52	122.72
7	N	783	SER	CA-C-O	5.76	128.21	121.87
8	S	245	GLY	CA-C-N	5.76	131.11	122.23
8	S	245	GLY	C-N-CA	5.76	131.11	122.23
8	S	403	SER	N-CA-CB	5.76	118.53	109.83
9	P	226	LYS	CA-C-O	5.76	126.87	120.82
10	Q	191	LEU	N-CA-C	-5.76	105.58	113.30
6	Z	172	ASP	CA-CB-CG	-5.76	106.84	112.60
7	N	417	ARG	N-CA-CB	5.76	119.17	109.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	U	214	VAL	N-CA-C	-5.76	103.72	111.44
3	T	244	ASP	N-CA-CB	5.76	118.52	109.94
6	Z	528	LEU	O-C-N	-5.75	116.02	122.12
9	P	261	LEU	CA-C-O	5.75	126.60	120.10
3	T	84	GLN	CA-C-O	5.75	127.40	121.07
3	T	130	ASP	CA-CB-CG	-5.75	106.85	112.60
10	Q	112	ASP	CA-CB-CG	5.75	118.35	112.60
11	R	42	GLN	N-CA-C	-5.75	105.09	111.36
8	S	75	CYS	O-C-N	5.75	128.07	122.09
10	Q	100	LEU	O-C-N	5.75	127.99	122.07
12	U	244	ASP	O-C-N	5.75	129.34	122.27
11	R	270	VAL	CA-CB-CG1	5.75	120.17	110.40
8	S	390	THR	CA-C-O	-5.75	114.46	120.55
13	O	76	LEU	CA-C-O	5.75	126.51	120.42
1	W	140	ASP	CB-CA-C	-5.74	99.78	109.72
6	Z	337	GLU	CA-C-N	5.74	127.97	120.28
6	Z	337	GLU	C-N-CA	5.74	127.97	120.28
10	Q	69	GLY	CA-C-O	5.74	130.08	122.39
5	Y	38	PHE	N-CA-CB	5.74	118.85	110.30
2	V	109	HIS	CA-CB-CG	5.74	119.54	113.80
5	Y	37	ASP	CB-CA-C	-5.74	101.87	110.88
10	Q	376	LYS	CA-C-N	5.74	127.97	120.28
10	Q	376	LYS	C-N-CA	5.74	127.97	120.28
11	R	68	GLU	N-CA-C	-5.74	105.11	111.36
12	U	119	LEU	CA-C-N	5.74	131.63	123.14
12	U	119	LEU	C-N-CA	5.74	131.63	123.14
8	S	481	TYR	CA-C-O	-5.73	113.11	118.73
9	P	279	ASP	CA-CB-CG	5.73	118.33	112.60
12	U	230	GLN	CA-C-O	-5.73	114.48	120.55
4	X	124	LYS	CA-C-O	-5.73	114.48	120.55
9	P	195	GLN	CB-CA-C	-5.73	101.89	110.88
6	Z	557	GLU	CA-C-N	5.73	127.89	120.44
6	Z	557	GLU	C-N-CA	5.73	127.89	120.44
7	N	415	PHE	N-CA-C	-5.73	104.03	111.71
9	P	292	LYS	CA-C-O	-5.73	114.35	120.42
9	P	42	LEU	CA-C-O	-5.72	114.78	120.90
4	X	76	VAL	CA-C-O	-5.72	115.96	119.51
6	Z	579	GLU	CB-CG-CD	-5.72	102.87	112.60
7	N	519	VAL	N-CA-C	-5.72	104.78	110.62
8	S	211	ARG	CA-C-N	5.72	127.88	120.44
8	S	211	ARG	C-N-CA	5.72	127.88	120.44
9	P	132	VAL	CA-C-N	5.72	129.40	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	132	VAL	C-N-CA	5.72	129.40	120.82
3	T	28	PRO	CB-CA-C	5.72	117.90	110.92
7	N	924	LYS	N-CA-C	-5.72	104.95	111.07
7	N	429	GLU	O-C-N	-5.72	115.92	122.09
4	X	16	GLU	CB-CG-CD	-5.72	102.88	112.60
11	R	32	LEU	CA-C-O	5.72	126.61	120.55
11	R	258	LEU	N-CA-C	5.72	117.97	111.11
6	Z	574	TYR	CB-CG-CD1	5.71	129.37	120.80
13	O	128	LEU	N-CA-C	5.71	117.51	111.28
4	X	94	ASN	N-CA-C	-5.71	105.21	113.21
6	Z	351	PRO	CA-C-O	5.71	125.19	118.68
6	Z	439	TYR	CA-C-N	5.71	128.50	120.28
6	Z	439	TYR	C-N-CA	5.71	128.50	120.28
6	Z	324	GLU	CA-C-O	-5.71	113.40	119.97
7	N	920	VAL	N-CA-C	-5.71	103.95	111.09
6	Z	375	ASP	CA-CB-CG	-5.71	106.89	112.60
6	Z	433	LEU	CA-C-O	5.71	126.35	119.61
3	T	133	ILE	CA-C-O	-5.71	115.47	121.41
9	P	273	TYR	CB-CA-C	-5.71	100.76	109.89
11	R	310	GLU	N-CA-CB	5.71	118.28	110.01
13	O	220	SER	CB-CA-C	-5.71	101.32	110.79
9	P	440	HIS	CE1-NE2-CD2	-5.71	103.30	109.00
9	P	95	TYR	CA-C-N	5.70	127.85	120.44
9	P	95	TYR	C-N-CA	5.70	127.85	120.44
9	P	9	ALA	N-CA-C	-5.70	104.97	111.07
10	Q	431	SER	N-CA-C	-5.70	105.59	112.54
7	N	204	SER	CB-CA-C	-5.70	101.69	110.81
7	N	316	LYS	N-CA-C	-5.70	104.99	111.14
12	U	41	ALA	CA-C-N	5.70	130.45	122.36
12	U	41	ALA	C-N-CA	5.70	130.45	122.36
2	V	169	GLU	CA-C-O	-5.70	113.09	118.33
9	P	67	ALA	CA-C-N	5.70	128.85	120.82
9	P	67	ALA	C-N-CA	5.70	128.85	120.82
6	Z	897	HIS	CE1-NE2-CD2	-5.69	103.31	109.00
9	P	278	ASN	N-CA-CB	5.69	118.27	110.01
6	Z	54	GLU	CA-C-O	-5.69	114.39	120.42
7	N	744	PRO	O-C-N	-5.69	114.95	122.64
6	Z	272	TYR	N-CA-C	5.69	118.22	111.33
6	Z	385	PHE	CA-C-N	5.69	129.46	120.47
6	Z	385	PHE	C-N-CA	5.69	129.46	120.47
8	S	123	THR	CB-CA-C	-5.69	101.35	110.79
10	Q	226	HIS	CG-CD2-NE2	5.69	112.89	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	81	TYR	CA-C-O	-5.69	114.84	120.70
3	T	28	PRO	N-CA-C	5.69	117.64	110.70
7	N	119	LYS	N-CA-C	-5.68	105.17	111.36
8	S	227	ASN	CA-C-O	5.68	126.58	120.55
8	S	302	HIS	CE1-NE2-CD2	-5.68	103.31	109.00
1	W	177	GLY	CA-C-O	-5.68	113.39	121.52
6	Z	197	LYS	CA-C-N	5.68	127.83	120.44
6	Z	197	LYS	C-N-CA	5.68	127.83	120.44
7	N	786	ARG	N-CA-CB	5.68	118.41	109.83
7	N	878	GLN	CA-C-O	5.68	125.08	118.77
6	Z	168	GLN	OE1-CD-NE2	5.67	128.28	122.60
8	S	384	ARG	NE-CZ-NH2	-5.67	114.10	119.20
10	Q	329	GLU	N-CA-C	-5.67	104.71	111.69
11	R	45	GLU	N-CA-C	-5.67	105.18	111.36
3	T	141	LEU	N-CA-CB	5.67	120.07	110.49
8	S	449	LEU	CB-CA-C	5.67	121.70	110.42
8	S	462	ASP	CA-CB-CG	5.67	118.27	112.60
9	P	187	SER	N-CA-CB	5.67	119.80	110.39
10	Q	146	TYR	CA-C-N	5.67	128.92	120.31
10	Q	146	TYR	C-N-CA	5.67	128.92	120.31
13	O	330	ARG	NH1-CZ-NH2	-5.67	111.93	119.30
6	Z	630	LYS	O-C-N	5.66	128.12	122.12
7	N	219	ASN	CB-CG-ND2	5.66	124.89	116.40
6	Z	524	ALA	CA-C-N	5.66	129.74	120.63
6	Z	524	ALA	C-N-CA	5.66	129.74	120.63
7	N	617	VAL	N-CA-C	-5.66	105.21	110.53
8	S	280	ASN	CA-C-N	5.66	128.18	120.54
8	S	280	ASN	C-N-CA	5.66	128.18	120.54
9	P	125	VAL	CA-C-N	5.66	132.35	121.54
9	P	125	VAL	C-N-CA	5.66	132.35	121.54
13	O	350	ILE	N-CA-C	-5.66	100.27	108.87
7	N	470	LEU	CB-CA-C	-5.66	101.24	110.85
6	Z	761	PHE	CA-C-N	5.65	126.26	119.98
6	Z	761	PHE	C-N-CA	5.65	126.26	119.98
8	S	291	GLU	CA-C-N	5.65	128.32	120.29
8	S	291	GLU	C-N-CA	5.65	128.32	120.29
8	S	261	HIS	CE1-NE2-CD2	-5.65	103.35	109.00
13	O	312	ASP	CB-CA-C	-5.65	101.41	110.79
2	V	106	GLY	CA-C-O	5.65	126.14	121.05
6	Z	300	ALA	N-CA-CB	5.65	118.43	110.12
6	Z	551	LEU	N-CA-C	5.65	117.44	111.28
8	S	401	LYS	N-CA-C	-5.65	99.20	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	U	286	ILE	CA-C-N	5.65	128.31	120.29
12	U	286	ILE	C-N-CA	5.65	128.31	120.29
11	R	407	GLY	CA-C-N	5.65	128.31	120.29
11	R	407	GLY	C-N-CA	5.65	128.31	120.29
7	N	672	ASN	CB-CA-C	-5.64	101.55	110.02
12	U	159	CYS	CA-C-O	5.64	126.69	120.71
6	Z	328	ASP	CB-CA-C	-5.64	102.02	110.88
6	Z	392	LEU	O-C-N	5.64	129.52	122.86
6	Z	898	HIS	N-CA-C	-5.64	105.60	112.88
1	W	57	ALA	N-CA-C	-5.64	105.13	111.28
8	S	133	GLU	CA-C-N	5.64	127.67	120.56
8	S	133	GLU	C-N-CA	5.64	127.67	120.56
13	O	114	GLN	OE1-CD-NE2	5.64	128.24	122.60
1	W	61	VAL	N-CA-C	-5.64	99.46	107.98
2	V	87	PHE	N-CA-CB	5.64	118.41	110.12
13	O	66	VAL	N-CA-CB	5.64	117.15	110.55
3	T	53	ASN	CA-C-O	-5.64	114.44	120.42
7	N	172	SER	N-CA-C	-5.64	105.13	112.23
3	T	251	HIS	N-CA-C	-5.63	98.80	110.80
10	Q	172	PRO	N-CA-CB	5.63	109.11	103.48
8	S	158	PHE	CB-CG-CD2	5.63	130.27	120.70
10	Q	50	ARG	NE-CZ-NH1	5.63	127.13	121.50
12	U	31	LYS	CA-C-O	5.63	126.52	120.32
2	V	222	GLN	CA-C-N	5.63	128.60	120.38
2	V	222	GLN	C-N-CA	5.63	128.60	120.38
12	U	231	ASP	CA-CB-CG	-5.63	106.97	112.60
6	Z	257	PRO	N-CA-C	-5.63	103.84	110.70
7	N	259	PHE	N-CA-CB	5.63	118.49	110.16
11	R	212	THR	CA-C-O	-5.63	114.00	120.24
12	U	192	ASN	N-CA-C	5.63	117.41	111.28
13	O	194	LEU	O-C-N	5.63	128.08	122.12
12	U	108	GLU	CA-C-O	5.62	126.51	120.55
6	Z	488	ALA	N-CA-C	-5.62	105.23	111.36
7	N	115	LYS	CA-C-O	-5.62	114.92	120.82
11	R	401	HIS	CE1-NE2-CD2	-5.62	103.38	109.00
10	Q	163	ARG	CA-C-N	5.62	127.81	120.28
10	Q	163	ARG	C-N-CA	5.62	127.81	120.28
12	U	226	LEU	O-C-N	-5.62	116.17	122.12
6	Z	85	VAL	CA-C-N	5.62	126.86	119.84
6	Z	85	VAL	C-N-CA	5.62	126.86	119.84
2	V	110	SER	CA-C-O	5.61	126.42	120.36
10	Q	344	GLU	N-CA-C	5.61	117.08	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	405	LEU	CA-C-N	5.61	130.08	120.71
7	N	405	LEU	C-N-CA	5.61	130.08	120.71
8	S	150	LYS	N-CA-CB	5.61	119.97	110.49
6	Z	709	LYS	N-CA-C	5.61	117.07	111.07
7	N	188	TYR	CB-CA-C	-5.61	101.47	110.79
6	Z	191	SER	CA-CB-OG	5.61	122.32	111.10
6	Z	210	TYR	N-CA-C	-5.61	105.25	111.36
6	Z	740	VAL	N-CA-C	-5.61	105.06	110.72
8	S	422	MET	O-C-N	5.61	128.15	122.09
2	V	250	GLN	CA-C-O	-5.61	114.61	120.55
8	S	241	PHE	CA-C-N	5.61	127.79	120.28
8	S	241	PHE	C-N-CA	5.61	127.79	120.28
6	Z	766	HIS	ND1-CE1-NE2	5.60	114.00	108.40
9	P	333	ALA	N-CA-CB	5.60	118.45	110.16
10	Q	362	ILE	O-C-N	5.60	127.31	121.87
9	P	269	VAL	CA-C-N	5.60	130.94	121.14
9	P	269	VAL	C-N-CA	5.60	130.94	121.14
1	W	80	GLN	CA-C-N	5.60	129.59	121.52
1	W	80	GLN	C-N-CA	5.60	129.59	121.52
13	O	213	LEU	CA-C-N	5.60	127.78	120.28
13	O	213	LEU	C-N-CA	5.60	127.78	120.28
7	N	343	THR	N-CA-C	5.60	117.03	108.52
8	S	137	PHE	CA-C-N	5.60	127.72	120.44
8	S	137	PHE	C-N-CA	5.60	127.72	120.44
2	V	292	ILE	N-CA-C	-5.60	105.27	110.53
7	N	637	ALA	CA-C-N	5.60	128.13	120.46
7	N	637	ALA	C-N-CA	5.60	128.13	120.46
9	P	255	ALA	CB-CA-C	-5.60	101.50	110.79
6	Z	386	VAL	CA-CB-CG2	-5.59	100.89	110.40
8	S	46	LEU	CA-C-N	5.59	132.22	121.54
8	S	46	LEU	C-N-CA	5.59	132.22	121.54
11	R	301	TYR	CA-C-O	5.59	124.92	118.55
6	Z	551	LEU	CB-CA-C	-5.59	101.51	110.79
13	O	74	ASN	N-CA-CB	5.59	118.86	109.92
2	V	114	PHE	O-C-N	-5.59	115.92	122.96
6	Z	400	ILE	CA-C-O	5.59	126.76	120.95
11	R	273	SER	CA-C-O	-5.59	115.02	119.71
10	Q	51	ARG	N-CA-CB	5.58	119.93	110.49
12	U	80	CYS	O-C-N	5.58	128.75	122.22
2	V	145	GLN	N-CA-C	-5.58	106.47	113.28
7	N	18	ASP	CA-C-N	5.58	127.76	120.28
7	N	18	ASP	C-N-CA	5.58	127.76	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	379	LEU	N-CA-C	-5.58	106.83	113.97
7	N	436	ASP	CA-C-N	5.58	128.79	120.31
7	N	436	ASP	C-N-CA	5.58	128.79	120.31
11	R	415	GLN	CG-CD-NE2	-5.58	108.03	116.40
6	Z	421	SER	N-CA-CB	5.58	118.92	110.28
7	N	586	ALA	CA-C-O	-5.58	114.64	120.55
9	P	223	LEU	N-CA-CB	5.58	118.31	110.12
9	P	425	HIS	CB-CG-ND1	5.58	131.06	122.70
8	S	205	ASN	CA-CB-CG	-5.57	107.03	112.60
3	T	70	ILE	CB-CA-C	-5.57	104.53	112.22
8	S	469	ASN	CA-CB-CG	5.57	118.17	112.60
10	Q	5	GLY	CA-C-N	5.57	127.68	120.44
10	Q	5	GLY	C-N-CA	5.57	127.68	120.44
3	T	20	TYR	N-CA-C	-5.57	106.16	113.17
3	T	219	LYS	N-CA-CB	5.57	118.08	110.01
6	Z	258	PRO	CA-C-O	-5.57	112.49	120.56
6	Z	627	LYS	CA-C-N	5.57	127.68	120.44
6	Z	627	LYS	C-N-CA	5.57	127.68	120.44
7	N	280	GLN	N-CA-C	-5.57	105.22	112.23
7	N	321	LEU	CA-C-N	5.57	130.63	121.39
7	N	321	LEU	C-N-CA	5.57	130.63	121.39
7	N	655	ALA	CA-C-O	-5.57	113.57	119.97
11	R	130	GLN	N-CA-CB	5.57	118.30	110.12
8	S	448	LEU	N-CA-C	-5.57	104.85	111.03
12	U	145	ASP	O-C-N	-5.57	116.81	123.27
13	O	321	LYS	CA-C-O	-5.57	113.81	120.10
3	T	24	GLU	N-CA-C	5.56	117.02	111.07
6	Z	214	HIS	ND1-CE1-NE2	5.56	113.96	108.40
9	P	57	GLU	N-CA-C	5.56	117.42	111.36
7	N	277	LEU	CA-C-N	5.56	127.73	120.28
7	N	277	LEU	C-N-CA	5.56	127.73	120.28
8	S	199	GLU	N-CA-C	-5.56	100.12	109.07
9	P	257	TRP	CB-CG-CD2	-5.56	119.02	126.80
10	Q	75	ARG	O-C-N	5.56	129.98	122.59
12	U	246	GLU	CA-C-N	5.56	128.07	120.46
12	U	246	GLU	C-N-CA	5.56	128.07	120.46
6	Z	382	ALA	CA-C-N	5.55	128.18	120.29
6	Z	382	ALA	C-N-CA	5.55	128.18	120.29
11	R	396	LYS	N-CA-CB	5.55	118.28	110.12
13	O	65	PHE	CB-CG-CD1	5.55	130.14	120.70
13	O	304	ASN	CA-C-N	5.55	128.91	120.13
13	O	304	ASN	C-N-CA	5.55	128.91	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	349	THR	CA-C-O	5.55	126.32	120.54
12	U	139	ALA	CA-C-O	-5.55	112.57	120.51
6	Z	439	TYR	N-CA-C	5.55	117.33	111.28
7	N	186	ILE	N-CA-C	5.55	116.28	110.62
7	N	259	PHE	CA-CB-CG	-5.55	108.25	113.80
1	W	123	ASP	CB-CA-C	-5.54	101.25	110.68
3	T	215	LYS	CA-C-N	5.54	128.74	120.31
3	T	215	LYS	C-N-CA	5.54	128.74	120.31
3	T	245	TYR	O-C-N	5.54	128.00	122.12
7	N	74	GLU	CA-C-N	5.54	128.26	120.28
7	N	74	GLU	C-N-CA	5.54	128.26	120.28
7	N	394	ARG	NE-CZ-NH2	5.54	124.19	119.20
7	N	878	GLN	CB-CG-CD	-5.54	103.18	112.60
10	Q	78	ILE	CA-C-N	5.54	125.64	119.87
10	Q	78	ILE	C-N-CA	5.54	125.64	119.87
2	V	100	ARG	CD-NE-CZ	5.54	132.16	124.40
6	Z	153	TYR	CA-C-N	5.54	128.05	120.46
6	Z	153	TYR	C-N-CA	5.54	128.05	120.46
1	W	56	GLY	O-C-N	5.54	128.03	122.77
9	P	345	VAL	N-CA-CB	5.54	118.07	110.54
12	U	252	HIS	CA-C-N	5.54	127.64	120.44
12	U	252	HIS	C-N-CA	5.54	127.64	120.44
4	X	41	GLU	N-CA-CB	5.54	120.32	111.91
7	N	418	ASP	O-C-N	5.54	127.77	122.07
7	N	419	THR	N-CA-C	-5.53	105.40	111.82
9	P	381	SER	CA-C-O	5.53	126.40	120.70
10	Q	251	THR	N-CA-C	-5.53	100.28	109.46
13	O	87	LYS	N-CA-C	-5.53	104.89	111.69
11	R	410	LEU	O-C-N	-5.53	115.84	122.15
12	U	220	PRO	N-CA-C	-5.53	102.51	111.19
10	Q	241	GLU	N-CA-C	-5.53	105.33	111.36
11	R	181	TYR	CA-C-O	5.53	126.18	119.38
2	V	24	LYS	CB-CA-C	5.53	119.63	109.46
6	Z	766	HIS	CA-CB-CG	5.53	119.33	113.80
13	O	7	ILE	CA-C-N	5.53	127.69	120.28
13	O	7	ILE	C-N-CA	5.53	127.69	120.28
2	V	160	ASP	CA-C-N	5.53	127.68	120.28
2	V	160	ASP	C-N-CA	5.53	127.68	120.28
3	T	46	ILE	N-CA-C	-5.53	101.06	108.35
8	S	154	GLN	O-C-N	5.53	127.76	122.07
10	Q	87	GLN	CB-CA-C	-5.53	101.62	110.79
7	N	326	SER	N-CA-CB	5.52	118.34	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	764	SER	CB-CA-C	-5.52	101.23	110.56
3	T	147	LYS	N-CA-CB	5.52	118.23	110.12
7	N	749	LEU	CA-C-N	5.52	128.23	120.28
7	N	749	LEU	C-N-CA	5.52	128.23	120.28
11	R	413	LYS	CA-C-O	5.52	126.40	120.55
7	N	699	ALA	CB-CA-C	-5.52	102.18	110.90
10	Q	183	LYS	CA-C-N	5.52	127.51	120.56
10	Q	183	LYS	C-N-CA	5.52	127.51	120.56
13	O	153	LEU	CA-C-N	5.52	127.61	120.44
13	O	153	LEU	C-N-CA	5.52	127.61	120.44
6	Z	112	LYS	CA-CB-CG	5.52	125.13	114.10
13	O	348	VAL	N-CA-CB	5.52	118.81	111.64
1	W	101	ARG	CA-C-N	5.51	127.61	120.44
1	W	101	ARG	C-N-CA	5.51	127.61	120.44
2	V	136	ALA	O-C-N	-5.51	116.11	122.95
9	P	236	GLU	N-CA-C	-5.51	105.35	111.36
12	U	290	ASP	N-CA-C	-5.51	105.27	111.28
10	Q	33	LYS	CA-C-N	5.51	127.61	120.44
10	Q	33	LYS	C-N-CA	5.51	127.61	120.44
6	Z	825	ALA	N-CA-CB	5.51	119.80	110.49
13	O	139	LEU	O-C-N	5.51	128.67	122.22
3	T	142	LEU	N-CA-C	5.51	118.04	111.71
10	Q	77	PHE	CB-CA-C	-5.51	101.49	110.85
7	N	636	SER	CA-C-N	5.50	127.66	120.28
7	N	636	SER	C-N-CA	5.50	127.66	120.28
8	S	250	ALA	N-CA-C	5.50	118.04	111.71
10	Q	194	SER	N-CA-C	-5.50	105.36	111.36
6	Z	607	ALA	CB-CA-C	-5.50	101.66	110.79
12	U	17	SER	N-CA-C	5.50	116.96	111.07
7	N	292	GLY	CA-C-O	5.50	125.23	119.07
8	S	311	GLN	CB-CA-C	-5.50	101.66	110.79
10	Q	258	ALA	N-CA-CB	5.50	118.30	110.16
13	O	130	ASP	N-CA-C	-5.50	105.28	111.28
7	N	474	SER	CA-C-N	5.50	128.10	120.29
7	N	474	SER	C-N-CA	5.50	128.10	120.29
12	U	211	LEU	N-CA-CB	5.50	118.20	110.12
7	N	707	ASN	N-CA-C	-5.50	106.42	113.02
11	R	193	ALA	CA-C-O	5.50	126.25	120.42
2	V	141	VAL	N-CA-C	-5.49	99.83	107.80
6	Z	880	SER	CA-C-N	5.49	127.59	120.56
6	Z	880	SER	C-N-CA	5.49	127.59	120.56
11	R	107	GLU	CA-C-O	-5.49	115.02	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	525	MET	CA-C-N	5.49	127.90	120.65
6	Z	525	MET	C-N-CA	5.49	127.90	120.65
7	N	653	ARG	CB-CA-C	-5.49	101.51	110.85
11	R	374	ASN	N-CA-C	-5.49	106.62	113.38
7	N	569	LYS	O-C-N	5.49	127.94	122.12
8	S	467	PHE	O-C-N	-5.49	116.30	122.12
6	Z	924	LYS	N-CA-C	-5.49	105.80	112.88
7	N	13	LEU	CA-C-O	-5.49	113.90	120.10
7	N	81	TYR	CB-CG-CD1	5.49	129.03	120.80
7	N	390	LEU	N-CA-CB	5.49	118.12	110.11
8	S	490	ASN	CA-CB-CG	-5.49	107.11	112.60
9	P	81	LEU	CA-C-N	5.49	127.57	120.44
9	P	81	LEU	C-N-CA	5.49	127.57	120.44
13	O	57	LEU	CA-C-N	5.49	127.58	120.44
13	O	57	LEU	C-N-CA	5.49	127.58	120.44
3	T	219	LYS	CA-C-N	5.49	128.65	120.31
3	T	219	LYS	C-N-CA	5.49	128.65	120.31
10	Q	111	LEU	CA-C-N	5.49	132.02	121.54
10	Q	111	LEU	C-N-CA	5.49	132.02	121.54
1	W	27	GLU	N-CA-C	-5.49	106.09	112.89
5	Y	73	PHE	CA-C-O	-5.49	114.73	120.55
6	Z	929	VAL	CA-C-N	5.49	129.38	121.54
6	Z	929	VAL	C-N-CA	5.49	129.38	121.54
7	N	523	LEU	CA-C-O	-5.49	115.06	120.82
6	Z	439	TYR	CA-C-O	-5.48	114.74	120.55
7	N	281	GLY	CA-C-N	5.48	128.63	120.90
7	N	281	GLY	C-N-CA	5.48	128.63	120.90
10	Q	13	ARG	NE-CZ-NH2	5.48	124.14	119.20
12	U	106	ILE	N-CA-C	-5.48	105.18	110.72
3	T	167	GLY	CA-C-N	5.48	128.17	120.28
3	T	167	GLY	C-N-CA	5.48	128.17	120.28
2	V	210	THR	CA-C-N	5.48	128.17	120.28
2	V	210	THR	C-N-CA	5.48	128.17	120.28
9	P	341	LEU	CA-C-N	5.48	127.88	120.65
9	P	341	LEU	C-N-CA	5.48	127.88	120.65
3	T	94	HIS	CB-CG-CD2	5.48	138.32	131.20
7	N	213	PHE	CA-CB-CG	-5.48	108.32	113.80
8	S	393	ARG	N-CA-CB	5.48	118.17	110.12
9	P	101	MET	CA-C-O	-5.48	114.74	120.55
9	P	278	ASN	CB-CG-ND2	-5.48	108.18	116.40
11	R	176	ARG	CD-NE-CZ	-5.48	116.73	124.40
1	W	86	HIS	CE1-NE2-CD2	-5.48	103.52	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	208	ARG	CA-C-N	5.47	127.56	120.44
7	N	208	ARG	C-N-CA	5.47	127.56	120.44
7	N	719	ASN	OD1-CG-ND2	5.47	128.07	122.60
8	S	275	TYR	CA-C-N	5.47	127.93	120.54
8	S	275	TYR	C-N-CA	5.47	127.93	120.54
2	V	138	ALA	N-CA-C	-5.47	99.37	108.34
6	Z	355	GLU	CB-CA-C	-5.47	102.26	110.90
8	S	317	HIS	CA-C-N	5.47	127.55	120.44
8	S	317	HIS	C-N-CA	5.47	127.55	120.44
11	R	164	THR	O-C-N	-5.47	116.32	122.12
6	Z	620	LEU	N-CA-C	-5.47	99.15	110.80
9	P	124	VAL	N-CA-CB	5.47	118.78	110.58
12	U	104	LEU	O-C-N	-5.47	115.54	122.27
2	V	138	ALA	N-CA-CB	5.47	119.35	110.77
3	T	157	TYR	CA-CB-CG	-5.47	104.06	113.90
4	X	129	LEU	O-C-N	5.47	127.92	122.12
6	Z	220	ALA	CA-C-N	5.46	127.95	120.46
6	Z	220	ALA	C-N-CA	5.46	127.95	120.46
6	Z	371	SER	CA-C-N	5.46	128.63	120.87
6	Z	371	SER	C-N-CA	5.46	128.63	120.87
6	Z	962	ARG	CA-C-O	-5.46	114.73	120.63
7	N	201	LYS	O-C-N	5.46	127.91	122.12
8	S	405	ARG	O-C-N	-5.46	116.33	122.12
12	U	229	LEU	CB-CA-C	-5.46	100.52	110.63
3	T	120	THR	CA-C-N	5.46	128.61	120.31
3	T	120	THR	C-N-CA	5.46	128.61	120.31
13	O	91	ASP	N-CA-CB	5.46	117.99	109.85
9	P	258	LYS	N-CA-C	5.46	121.88	109.81
3	T	20	TYR	CA-CB-CG	-5.46	104.07	113.90
12	U	278	ILE	O-C-N	5.46	127.17	121.87
1	W	46	GLU	N-CA-C	-5.46	106.39	113.16
2	V	24	LYS	CA-C-N	5.46	129.10	121.24
2	V	24	LYS	C-N-CA	5.46	129.10	121.24
10	Q	139	ILE	CA-C-O	-5.46	115.27	120.95
12	U	147	GLY	CA-C-N	5.46	128.99	120.75
12	U	147	GLY	C-N-CA	5.46	128.99	120.75
6	Z	140	LEU	CB-CA-C	-5.46	101.57	110.85
10	Q	361	HIS	CA-CB-CG	5.46	119.26	113.80
12	U	276	ILE	O-C-N	-5.46	116.58	121.87
6	Z	334	LYS	N-CA-CB	5.46	118.73	110.28
9	P	264	ILE	CA-C-O	-5.45	115.60	121.27
9	P	390	TYR	N-CA-C	-5.45	100.51	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	333	SER	O-C-N	5.45	127.69	122.07
7	N	735	MET	CA-C-N	5.45	127.58	120.28
7	N	735	MET	C-N-CA	5.45	127.58	120.28
10	Q	109	ASP	N-CA-C	-5.45	104.58	113.19
13	O	148	ASP	N-CA-CB	5.45	119.28	110.40
6	Z	309	GLN	CA-C-N	5.45	128.59	120.31
6	Z	309	GLN	C-N-CA	5.45	128.59	120.31
9	P	27	LEU	N-CA-CB	5.45	118.61	110.22
9	P	348	HIS	CA-CB-CG	-5.45	108.35	113.80
10	Q	99	THR	O-C-N	-5.45	116.42	122.09
10	Q	158	ILE	CA-C-O	-5.45	115.28	120.95
12	U	125	VAL	N-CA-C	-5.45	106.99	112.17
1	W	101	ARG	CA-CB-CG	5.45	124.99	114.10
7	N	396	SER	N-CA-C	-5.45	104.76	111.40
9	P	397	ALA	N-CA-CB	5.45	119.69	110.49
4	X	37	PRO	N-CA-C	-5.44	101.26	112.47
6	Z	74	SER	CA-C-O	-5.44	112.90	119.49
5	Y	38	PHE	CA-C-N	-5.44	113.42	119.19
5	Y	38	PHE	C-N-CA	-5.44	113.42	119.19
6	Z	89	LEU	N-CA-CB	5.44	117.90	110.01
6	Z	766	HIS	CB-CG-CD2	5.44	138.27	131.20
9	P	276	LEU	CA-C-N	5.44	127.89	120.54
9	P	276	LEU	C-N-CA	5.44	127.89	120.54
10	Q	392	GLN	N-CA-C	-5.44	105.43	111.36
11	R	170	VAL	CA-C-O	-5.44	115.29	120.95
12	U	201	GLN	CB-CG-CD	-5.44	103.35	112.60
3	T	189	ILE	O-C-N	5.44	127.55	121.90
6	Z	433	LEU	N-CA-C	5.44	119.41	112.34
10	Q	231	ASP	CA-CB-CG	5.44	118.04	112.60
11	R	322	LEU	CA-C-O	5.44	125.86	119.28
12	U	198	LYS	CA-C-N	5.44	126.14	119.99
12	U	198	LYS	C-N-CA	5.44	126.14	119.99
6	Z	457	ILE	CA-C-O	-5.44	115.30	120.95
4	X	88	ALA	CA-C-O	5.43	126.30	120.32
6	Z	358	TYR	N-CA-CB	5.43	118.11	110.12
7	N	340	HIS	ND1-CE1-NE2	5.43	113.83	108.40
10	Q	243	PHE	CB-CG-CD1	-5.43	111.46	120.70
6	Z	714	ASP	N-CA-CB	5.43	118.03	109.94
11	R	47	ALA	O-C-N	5.43	127.88	122.12
13	O	356	ARG	CA-C-N	5.43	128.62	120.69
13	O	356	ARG	C-N-CA	5.43	128.62	120.69
8	S	213	THR	CA-C-O	-5.43	114.66	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	147	ARG	CA-CB-CG	5.43	124.96	114.10
4	X	27	ILE	N-CA-C	-5.43	101.79	107.60
6	Z	205	LEU	CA-C-N	5.43	127.50	120.44
6	Z	205	LEU	C-N-CA	5.43	127.50	120.44
6	Z	404	ASP	CA-C-N	5.43	131.91	121.54
6	Z	404	ASP	C-N-CA	5.43	131.91	121.54
7	N	627	ILE	CA-C-N	5.43	128.00	120.29
7	N	627	ILE	C-N-CA	5.43	128.00	120.29
8	S	132	ALA	CA-C-N	5.43	127.56	120.28
8	S	132	ALA	C-N-CA	5.43	127.56	120.28
13	O	343	GLN	N-CA-C	-5.43	106.50	113.23
6	Z	785	VAL	CB-CA-C	-5.43	104.91	112.02
3	T	241	GLU	CA-C-N	5.42	127.55	120.28
3	T	241	GLU	C-N-CA	5.42	127.55	120.28
7	N	227	LYS	CA-C-N	5.42	127.89	120.46
7	N	227	LYS	C-N-CA	5.42	127.89	120.46
7	N	297	ASP	N-CA-CB	5.42	118.09	110.12
7	N	879	SER	CB-CA-C	-5.42	101.79	110.79
9	P	137	ALA	N-CA-C	5.42	117.27	111.36
2	V	57	PHE	CA-C-O	5.42	126.22	120.36
6	Z	889	VAL	CA-CB-CG1	5.42	119.62	110.40
6	Z	935	THR	CB-CA-C	-5.42	102.43	110.67
6	Z	633	GLU	CB-CA-C	-5.42	101.79	110.79
7	N	764	SER	O-C-N	5.42	128.84	122.34
7	N	821	LYS	N-CA-CB	5.42	118.61	110.53
3	T	108	LEU	N-CA-C	5.42	117.19	111.28
7	N	267	GLN	CA-C-N	5.42	127.54	120.28
7	N	267	GLN	C-N-CA	5.42	127.54	120.28
1	W	20	ASP	CA-CB-CG	-5.42	107.19	112.60
7	N	764	SER	CA-C-O	-5.41	113.23	119.56
9	P	93	ILE	O-C-N	5.41	127.12	121.87
1	W	3	LEU	N-CA-CB	5.41	119.64	110.49
6	Z	8	LYS	CA-C-O	-5.41	115.64	121.38
6	Z	474	LEU	N-CA-C	5.41	119.88	113.28
8	S	290	ASN	N-CA-C	5.41	116.86	111.07
12	U	65	VAL	O-C-N	-5.41	117.42	123.26
13	O	25	LEU	N-CA-CB	5.41	118.00	109.94
13	O	213	LEU	O-C-N	-5.41	116.39	122.12
9	P	37	ASP	N-CA-CB	5.41	117.85	110.01
13	O	309	SER	CA-C-N	5.41	128.53	120.31
13	O	309	SER	C-N-CA	5.41	128.53	120.31
9	P	15	GLN	N-CA-C	-5.41	105.47	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	97	GLN	CA-C-O	5.40	126.03	119.38
10	Q	11	ALA	CA-C-O	5.40	126.49	120.82
12	U	218	GLU	N-CA-C	-5.40	103.99	111.28
13	O	85	SER	N-CA-CB	5.40	119.51	110.32
6	Z	215	ASN	N-CA-C	-5.40	105.47	111.36
6	Z	885	ALA	CA-C-O	5.40	124.46	118.52
8	S	195	ALA	CA-C-O	-5.40	114.00	120.10
2	V	114	PHE	CB-CA-C	-5.40	98.63	110.67
2	V	299	GLY	CA-C-N	5.40	127.47	120.56
2	V	299	GLY	C-N-CA	5.40	127.47	120.56
3	T	117	ASN	CA-CB-CG	-5.40	107.20	112.60
6	Z	346	LEU	CB-CA-C	-5.39	102.41	110.88
7	N	62	ALA	N-CA-C	-5.39	105.48	111.36
4	X	105	ASN	N-CA-C	-5.39	104.99	113.02
6	Z	117	ASP	CA-C-N	5.39	127.85	120.46
6	Z	117	ASP	C-N-CA	5.39	127.85	120.46
10	Q	81	SER	N-CA-CB	5.39	118.14	110.16
12	U	202	SER	CA-C-O	-5.39	114.83	120.55
11	R	330	VAL	N-CA-CB	5.39	117.87	110.54
11	R	310	GLU	CA-C-O	-5.39	115.16	120.82
13	O	34	GLU	CA-C-O	-5.39	115.16	120.82
6	Z	151	HIS	CA-C-N	5.39	127.94	120.29
6	Z	151	HIS	C-N-CA	5.39	127.94	120.29
7	N	428	VAL	CA-C-N	5.39	127.77	120.44
7	N	428	VAL	C-N-CA	5.39	127.77	120.44
7	N	696	LYS	CA-C-N	5.39	127.50	120.28
7	N	696	LYS	C-N-CA	5.39	127.50	120.28
7	N	735	MET	CG-SD-CE	-5.39	89.05	100.90
11	R	338	TYR	CB-CG-CD2	-5.39	112.72	120.80
12	U	48	VAL	N-CA-C	-5.39	99.99	108.23
8	S	261	HIS	CG-CD2-NE2	5.38	112.58	107.20
13	O	55	THR	CA-C-N	5.38	125.47	119.87
13	O	55	THR	C-N-CA	5.38	125.47	119.87
6	Z	837	TYR	CA-CB-CG	-5.38	104.22	113.90
7	N	865	PRO	N-CA-CB	5.38	109.03	103.38
6	Z	780	MET	CA-C-N	5.38	125.95	119.98
6	Z	780	MET	C-N-CA	5.38	125.95	119.98
9	P	133	GLU	CA-C-N	5.38	127.34	120.56
9	P	133	GLU	C-N-CA	5.38	127.34	120.56
13	O	86	LEU	N-CA-C	-5.38	106.39	113.17
6	Z	425	ILE	CA-C-N	5.38	131.11	122.83
6	Z	425	ILE	C-N-CA	5.38	131.11	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	52	TYR	O-C-N	5.38	127.82	122.12
13	O	298	GLU	O-C-N	-5.38	116.28	122.09
13	O	377	VAL	N-CA-C	-5.38	105.14	110.62
8	S	442	PHE	CA-C-N	5.38	130.03	123.10
8	S	442	PHE	C-N-CA	5.38	130.03	123.10
7	N	642	ASP	CA-CB-CG	5.37	117.97	112.60
8	S	329	GLU	N-CA-CB	5.37	117.94	109.83
11	R	422	ARG	CB-CA-C	-5.37	101.87	110.79
13	O	351	SER	N-CA-C	-5.37	105.40	113.89
3	T	81	TYR	N-CA-CB	5.37	117.80	110.01
6	Z	319	THR	CA-C-N	5.37	127.74	120.38
6	Z	319	THR	C-N-CA	5.37	127.74	120.38
6	Z	359	LYS	N-CA-C	-5.37	105.42	111.28
11	R	367	ASP	CA-CB-CG	-5.37	107.23	112.60
6	Z	222	ASP	CA-CB-CG	-5.37	107.23	112.60
1	W	94	ALA	N-CA-C	-5.37	105.33	111.07
6	Z	385	PHE	CB-CG-CD2	-5.37	111.58	120.70
11	R	30	ALA	O-C-N	5.37	127.81	122.12
13	O	206	THR	N-CA-CB	5.37	118.61	110.45
13	O	387	ARG	CB-CA-C	-5.37	101.48	110.29
3	T	156	SER	CB-CA-C	-5.37	102.66	111.68
12	U	45	THR	CA-CB-OG1	5.37	117.65	109.60
13	O	373	TRP	CB-CA-C	-5.37	99.27	109.95
6	Z	342	LEU	CB-CA-C	-5.37	101.78	110.79
6	Z	456	GLY	CA-C-N	5.37	127.81	120.46
6	Z	456	GLY	C-N-CA	5.37	127.81	120.46
8	S	445	THR	N-CA-CB	5.36	117.85	109.97
7	N	799	VAL	CA-C-O	-5.36	115.38	120.95
8	S	222	SER	N-CA-C	-5.36	105.52	111.36
10	Q	62	GLY	N-CA-C	-5.36	108.02	114.66
12	U	44	SER	O-C-N	5.36	127.59	122.07
3	T	121	LYS	CA-C-N	5.36	127.41	120.44
3	T	121	LYS	C-N-CA	5.36	127.41	120.44
3	T	223	GLU	N-CA-CB	-5.36	101.97	110.22
6	Z	64	TYR	N-CA-C	-5.36	106.68	113.43
6	Z	122	LEU	N-CA-CB	5.36	119.13	110.40
6	Z	412	GLY	CA-C-N	5.36	128.45	120.31
6	Z	412	GLY	C-N-CA	5.36	128.45	120.31
6	Z	845	LEU	CB-CA-C	-5.36	101.79	110.79
7	N	440	ASP	CA-CB-CG	-5.36	107.24	112.60
8	S	52	TYR	CA-C-N	5.36	127.31	120.56
8	S	52	TYR	C-N-CA	5.36	127.31	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	227	ASN	CB-CA-C	-5.36	101.90	110.79
9	P	282	HIS	ND1-CE1-NE2	5.36	113.76	108.40
10	Q	409	TYR	N-CA-CB	5.36	117.99	110.12
13	O	112	LYS	CA-C-N	5.36	129.78	120.68
13	O	112	LYS	C-N-CA	5.36	129.78	120.68
13	O	354	GLN	N-CA-C	-5.36	100.90	109.04
6	Z	618	GLN	CB-CA-C	-5.35	101.90	110.79
9	P	121	THR	CA-CB-OG1	5.35	117.63	109.60
11	R	252	TYR	N-CA-C	5.35	117.11	111.28
1	W	139	VAL	CA-C-O	5.35	126.36	120.64
7	N	224	THR	CA-C-N	5.35	127.98	120.28
7	N	224	THR	C-N-CA	5.35	127.98	120.28
12	U	73	ILE	N-CA-C	-5.35	105.28	110.42
7	N	647	ASP	CA-C-O	-5.35	114.87	120.70
8	S	355	GLY	CA-C-N	5.35	130.00	121.66
8	S	355	GLY	C-N-CA	5.35	130.00	121.66
3	T	177	PHE	N-CA-C	-5.34	106.82	113.55
9	P	357	TYR	N-CA-CB	5.34	118.58	109.87
12	U	196	SER	O-C-N	-5.34	116.06	122.15
3	T	214	GLU	N-CA-CB	5.34	118.56	110.28
6	Z	744	ALA	CA-C-N	5.34	127.44	120.28
6	Z	744	ALA	C-N-CA	5.34	127.44	120.28
11	R	62	TYR	N-CA-C	-5.34	105.50	112.23
6	Z	151	HIS	CE1-NE2-CD2	-5.34	103.66	109.00
6	Z	374	LEU	O-C-N	-5.34	116.33	122.95
8	S	199	GLU	CA-CB-CG	-5.34	103.42	114.10
7	N	652	VAL	N-CA-CB	5.34	118.58	110.58
12	U	88	LYS	N-CA-C	-5.33	101.25	109.52
6	Z	271	ILE	O-C-N	5.33	127.14	121.91
6	Z	365	SER	CA-C-N	5.33	131.73	121.54
6	Z	365	SER	C-N-CA	5.33	131.73	121.54
6	Z	942	PRO	N-CA-CB	5.33	108.85	103.25
9	P	57	GLU	O-C-N	5.33	128.23	122.15
11	R	313	ALA	N-CA-C	5.33	117.09	111.28
6	Z	59	ASP	CA-CB-CG	5.33	117.93	112.60
6	Z	413	ASP	CA-C-N	5.33	125.90	119.98
6	Z	413	ASP	C-N-CA	5.33	125.90	119.98
6	Z	912	PHE	CA-CB-CG	-5.33	108.47	113.80
7	N	41	ASN	OD1-CG-ND2	5.33	127.93	122.60
8	S	172	ASN	N-CA-CB	5.33	117.85	110.17
8	S	321	GLN	OE1-CD-NE2	-5.33	117.27	122.60
9	P	51	ASP	N-CA-CB	5.33	117.80	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	34	ASP	N-CA-CB	5.33	117.74	110.01
8	S	33	GLU	N-CA-C	5.33	116.77	111.07
10	Q	377	LEU	N-CA-C	-5.33	105.47	111.28
3	T	60	ARG	N-CA-C	-5.32	105.48	111.28
3	T	103	SER	CA-C-O	-5.32	115.20	120.90
6	Z	633	GLU	N-CA-CB	5.32	117.95	110.12
6	Z	849	ARG	N-CA-CB	5.32	120.77	111.13
11	R	120	LEU	N-CA-C	5.32	117.83	111.71
11	R	265	ASP	N-CA-C	-5.32	106.63	113.23
13	O	114	GLN	O-C-N	5.32	127.76	122.12
3	T	183	SER	N-CA-C	-5.32	105.65	111.82
6	Z	580	GLN	N-CA-CB	5.32	119.07	110.40
10	Q	109	ASP	CA-C-N	5.32	131.70	121.54
10	Q	109	ASP	C-N-CA	5.32	131.70	121.54
7	N	282	TYR	CB-CG-CD2	5.32	128.78	120.80
7	N	611	LYS	CA-C-N	5.32	129.23	121.31
7	N	611	LYS	C-N-CA	5.32	129.23	121.31
8	S	20	HIS	CE1-NE2-CD2	-5.32	103.68	109.00
12	U	5	HIS	CG-CD2-NE2	5.32	112.52	107.20
13	O	104	ALA	CA-C-N	5.32	127.72	120.54
13	O	104	ALA	C-N-CA	5.32	127.72	120.54
2	V	183	ALA	CA-C-O	-5.32	116.26	122.37
6	Z	328	ASP	N-CA-CB	5.32	117.72	110.01
7	N	726	ASP	CA-C-N	5.32	127.35	120.44
7	N	726	ASP	C-N-CA	5.32	127.35	120.44
11	R	395	ASN	O-C-N	-5.32	115.52	122.59
7	N	230	VAL	N-CA-CB	5.31	117.37	110.57
9	P	188	ILE	O-C-N	5.31	127.42	121.90
3	T	82	PHE	CB-CA-C	5.31	119.31	110.81
6	Z	938	GLN	N-CA-CB	5.31	117.85	110.04
8	S	23	LYS	CA-C-O	-5.31	115.25	120.82
4	X	34	GLU	CB-CG-CD	-5.31	103.58	112.60
6	Z	169	VAL	O-C-N	-5.31	116.38	121.90
7	N	107	GLU	CB-CA-C	-5.31	102.55	110.88
13	O	22	LEU	N-CA-C	-5.31	106.19	113.30
13	O	233	LEU	N-CA-CB	5.31	117.92	110.12
3	T	22	ALA	N-CA-CB	5.30	117.92	110.12
6	Z	65	GLU	CA-C-N	5.30	127.92	120.28
6	Z	65	GLU	C-N-CA	5.30	127.92	120.28
7	N	130	ASP	CA-C-O	-5.30	112.89	120.16
13	O	310	PHE	CA-C-N	5.30	127.39	120.28
13	O	310	PHE	C-N-CA	5.30	127.39	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	464	GLU	CB-CA-C	-5.30	101.99	110.79
6	Z	592	GLU	CA-C-O	5.30	126.20	120.32
7	N	802	ALA	N-CA-C	5.30	117.06	111.28
9	P	154	ASP	O-C-N	5.30	127.82	122.09
6	Z	823	ASN	CA-CB-CG	-5.30	107.30	112.60
8	S	464	ARG	CB-CA-C	-5.30	102.56	110.88
10	Q	384	LYS	N-CA-C	-5.30	104.10	111.52
3	T	216	GLU	N-CA-CB	5.30	118.49	110.28
10	Q	315	ASN	N-CA-C	5.30	117.06	111.28
7	N	571	LEU	N-CA-C	5.30	118.20	111.69
9	P	254	GLU	N-CA-C	5.30	120.06	111.37
10	Q	345	SER	CA-C-N	5.30	127.81	120.29
10	Q	345	SER	C-N-CA	5.30	127.81	120.29
12	U	225	ILE	CA-C-N	5.30	127.38	120.28
12	U	225	ILE	C-N-CA	5.30	127.38	120.28
1	W	119	SER	N-CA-C	-5.29	104.76	113.50
1	W	131	THR	O-C-N	5.29	128.19	122.15
2	V	90	LYS	CB-CA-C	-5.29	102.53	110.90
12	U	49	THR	N-CA-CB	5.29	118.15	110.26
9	P	21	PHE	N-CA-CB	5.29	119.55	110.34
7	N	387	ALA	CA-C-N	5.29	125.10	119.28
7	N	387	ALA	C-N-CA	5.29	125.10	119.28
7	N	896	PHE	CB-CA-C	-5.29	101.25	109.61
6	Z	483	THR	CA-C-O	-5.29	114.81	120.42
10	Q	57	SER	N-CA-CB	5.29	117.68	110.01
10	Q	273	ASN	CA-CB-CG	5.29	117.89	112.60
12	U	298	ASN	OD1-CG-ND2	-5.29	117.31	122.60
13	O	198	THR	CA-C-O	5.29	125.83	119.43
6	Z	933	VAL	N-CA-CB	5.29	120.99	111.21
7	N	503	THR	N-CA-CB	5.29	117.89	110.12
7	N	348	PHE	N-CA-CB	5.29	117.98	110.16
7	N	649	VAL	N-CA-CB	5.29	116.81	110.31
7	N	923	MET	CA-C-O	-5.29	115.27	120.82
10	Q	157	LEU	CA-C-N	5.29	127.70	120.46
10	Q	157	LEU	C-N-CA	5.29	127.70	120.46
10	Q	322	GLU	CB-CA-C	-5.29	101.70	110.68
9	P	336	HIS	CE1-NE2-CD2	-5.28	103.72	109.00
10	Q	35	SER	N-CA-C	5.28	117.45	111.11
10	Q	84	TYR	CA-C-N	5.28	127.31	120.44
10	Q	84	TYR	C-N-CA	5.28	127.31	120.44
1	W	107	HIS	ND1-CE1-NE2	5.28	113.68	108.40
2	V	264	GLU	CA-C-N	5.28	127.88	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	264	GLU	C-N-CA	5.28	127.88	120.28
7	N	690	HIS	CE1-NE2-CD2	-5.28	103.72	109.00
8	S	469	ASN	CB-CG-ND2	-5.28	108.48	116.40
9	P	71	LYS	N-CA-CB	5.28	118.47	110.28
11	R	34	THR	O-C-N	5.28	127.73	122.08
10	Q	123	GLU	CA-C-N	5.28	127.35	120.28
10	Q	123	GLU	C-N-CA	5.28	127.35	120.28
2	V	122	ASP	CA-C-N	5.28	127.92	120.42
2	V	122	ASP	C-N-CA	5.28	127.92	120.42
6	Z	476	ASP	CA-C-N	5.28	127.78	120.29
6	Z	476	ASP	C-N-CA	5.28	127.78	120.29
13	O	72	LYS	N-CA-CB	5.28	117.94	110.13
4	X	100	TRP	CA-C-O	5.28	127.18	121.06
9	P	289	ASN	N-CA-CB	5.28	118.34	110.22
11	R	163	SER	N-CA-CB	5.28	117.77	110.17
12	U	105	LYS	CA-C-N	5.28	127.91	120.42
12	U	105	LYS	C-N-CA	5.28	127.91	120.42
13	O	237	PRO	CA-C-N	5.28	129.27	120.62
13	O	237	PRO	C-N-CA	5.28	129.27	120.62
6	Z	422	ILE	N-CA-C	-5.27	105.24	110.62
9	P	170	SER	N-CA-C	5.27	117.78	111.71
6	Z	840	ARG	N-CA-CB	5.27	119.18	110.69
8	S	299	LYS	CA-C-O	-5.27	114.96	120.55
10	Q	57	SER	CA-C-N	5.27	127.68	120.46
10	Q	57	SER	C-N-CA	5.27	127.68	120.46
10	Q	171	LYS	N-CA-C	5.27	118.28	110.32
11	R	169	ASP	O-C-N	5.27	127.57	122.09
12	U	194	LEU	CA-C-N	5.27	127.35	120.28
12	U	194	LEU	C-N-CA	5.27	127.35	120.28
8	S	139	HIS	N-CA-CB	5.27	117.65	110.01
11	R	305	PHE	CB-CG-CD2	-5.27	111.74	120.70
6	Z	238	ASP	CA-C-N	5.27	127.65	120.54
6	Z	238	ASP	C-N-CA	5.27	127.65	120.54
6	Z	285	ALA	CA-C-O	5.27	126.03	119.97
7	N	34	GLN	CA-C-O	5.27	125.98	119.81
7	N	42	GLU	N-CA-C	5.27	119.40	112.92
7	N	571	LEU	CA-C-O	-5.27	114.39	120.24
7	N	923	MET	N-CA-C	-5.27	105.43	111.07
11	R	116	LYS	O-C-N	-5.27	116.44	122.08
13	O	367	LYS	N-CA-CB	5.27	117.65	110.01
7	N	553	PHE	N-CA-C	-5.27	106.81	113.18
7	N	698	GLY	CA-C-N	5.27	127.61	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	698	GLY	C-N-CA	5.27	127.61	120.44
13	O	169	ASN	CA-CB-CG	-5.27	107.33	112.60
7	N	156	ILE	O-C-N	-5.27	116.41	121.83
6	Z	57	LYS	N-CA-C	-5.26	105.54	111.28
6	Z	290	GLU	N-CA-CB	5.26	117.71	109.97
7	N	524	ILE	N-CA-C	5.26	117.63	111.05
12	U	261	LEU	O-C-N	-5.26	116.15	122.15
12	U	66	TRP	CB-CG-CD2	-5.26	119.43	126.80
3	T	48	ASN	N-CA-C	-5.26	101.71	109.18
3	T	218	GLU	CA-C-O	5.26	125.83	119.31
7	N	613	HIS	N-CA-C	-5.26	106.91	113.38
8	S	386	ASN	N-CA-C	5.26	117.76	111.71
8	S	472	HIS	O-C-N	5.26	127.69	122.12
1	W	88	ALA	CB-CA-C	-5.26	102.59	110.90
2	V	19	GLY	N-CA-C	-5.26	108.43	115.32
8	S	377	TYR	CA-C-O	-5.26	115.27	120.90
10	Q	170	ASP	CA-CB-CG	5.26	117.86	112.60
6	Z	331	GLY	CA-C-N	5.26	128.31	120.90
6	Z	331	GLY	C-N-CA	5.26	128.31	120.90
12	U	3	LEU	N-CA-C	-5.26	106.55	113.17
11	R	230	LEU	N-CA-CB	5.25	117.94	110.16
7	N	774	ASN	N-CA-CB	5.25	118.74	110.23
9	P	267	PHE	CA-CB-CG	-5.25	108.55	113.80
7	N	747	HIS	CE1-NE2-CD2	-5.25	103.75	109.00
9	P	285	GLN	N-CA-CB	5.25	117.84	110.12
6	Z	89	LEU	CA-C-O	-5.25	115.31	120.82
10	Q	346	ASN	O-C-N	-5.25	116.17	122.15
1	W	139	VAL	O-C-N	-5.25	117.00	123.03
3	T	247	ASP	N-CA-C	5.25	119.16	112.34
5	Y	38	PHE	CA-CB-CG	-5.25	108.55	113.80
7	N	878	GLN	OE1-CD-NE2	-5.25	117.35	122.60
8	S	428	ARG	NE-CZ-NH2	-5.25	114.48	119.20
12	U	227	GLY	CA-C-O	5.25	126.45	121.05
13	O	151	ASP	CA-C-N	5.25	127.31	120.28
13	O	151	ASP	C-N-CA	5.25	127.31	120.28
1	W	86	HIS	ND1-CE1-NE2	5.24	113.64	108.40
6	Z	794	ASP	N-CA-CB	5.24	117.83	110.12
7	N	312	GLY	O-C-N	5.24	128.00	122.28
13	O	263	PHE	CA-CB-CG	-5.24	108.56	113.80
9	P	278	ASN	CA-CB-CG	-5.24	107.36	112.60
1	W	165	GLN	CA-C-N	5.24	127.56	120.44
1	W	165	GLN	C-N-CA	5.24	127.56	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	126	ILE	O-C-N	5.24	127.23	121.83
5	Y	73	PHE	CB-CG-CD2	5.24	129.61	120.70
6	Z	251	ALA	CA-C-O	-5.24	115.00	120.55
8	S	309	PHE	CD1-CG-CD2	-5.24	110.74	118.60
10	Q	173	SER	CA-C-N	5.24	130.88	121.66
10	Q	173	SER	C-N-CA	5.24	130.88	121.66
12	U	26	GLN	CB-CG-CD	-5.24	103.69	112.60
8	S	204	ASP	CA-CB-CG	-5.24	107.36	112.60
6	Z	78	SER	CA-C-N	5.24	127.56	120.44
6	Z	78	SER	C-N-CA	5.24	127.56	120.44
6	Z	600	GLU	CA-C-O	-5.24	115.00	120.55
7	N	335	ALA	CB-CA-C	-5.24	102.10	110.79
13	O	340	SER	N-CA-C	-5.24	101.33	109.24
1	W	9	VAL	N-CA-CB	5.23	118.05	111.46
6	Z	607	ALA	CA-C-O	-5.23	115.00	120.55
7	N	810	ALA	CB-CA-C	-5.23	100.95	110.63
7	N	56	SER	O-C-N	5.23	127.58	122.19
10	Q	15	VAL	CB-CA-C	-5.23	105.08	112.14
11	R	253	ALA	CA-C-O	-5.23	115.00	120.55
13	O	173	SER	CA-C-N	5.23	127.24	120.44
13	O	173	SER	C-N-CA	5.23	127.24	120.44
9	P	94	GLN	O-C-N	5.23	129.68	122.46
2	V	243	SER	CA-C-N	5.23	128.97	120.60
2	V	243	SER	C-N-CA	5.23	128.97	120.60
6	Z	307	HIS	CB-CG-CD2	-5.23	124.40	131.20
10	Q	348	CYS	O-C-N	5.23	127.66	122.12
11	R	378	ASN	CA-CB-CG	-5.23	107.37	112.60
12	U	175	LEU	N-CA-C	-5.23	102.01	110.32
7	N	367	ALA	CA-C-O	-5.22	115.33	120.82
8	S	452	TYR	CB-CA-C	5.22	119.46	110.79
8	S	476	LEU	N-CA-CB	-5.22	102.50	110.07
4	X	109	LEU	CB-CA-C	-5.22	101.27	109.52
9	P	308	LEU	N-CA-C	5.22	117.27	110.43
9	P	354	SER	CA-C-O	-5.22	114.89	120.42
10	Q	313	ASP	CA-C-O	-5.22	114.89	120.42
12	U	239	LEU	N-CA-CB	5.22	118.81	110.46
4	X	40	GLU	CB-CG-CD	-5.22	103.73	112.60
6	Z	450	GLY	CA-C-N	5.22	127.27	120.28
6	Z	450	GLY	C-N-CA	5.22	127.27	120.28
6	Z	264	PHE	CB-CG-CD2	-5.22	111.83	120.70
9	P	79	LEU	N-CA-CB	-5.22	102.44	110.16
9	P	366	ASN	CA-CB-CG	5.22	117.82	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	222	LEU	O-C-N	-5.21	116.21	122.15
7	N	891	VAL	CA-C-O	-5.21	112.96	119.95
12	U	187	SER	O-C-N	5.21	127.44	122.07
7	N	104	LYS	CA-C-N	5.21	127.27	120.28
7	N	104	LYS	C-N-CA	5.21	127.27	120.28
9	P	183	GLN	CA-C-O	-5.21	115.03	120.55
10	Q	279	LYS	CB-CG-CD	5.21	123.29	111.30
2	V	273	ARG	N-CA-CB	5.21	117.81	110.36
3	T	214	GLU	N-CA-C	5.21	117.87	111.82
6	Z	757	SER	N-CA-CB	5.21	118.36	110.28
7	N	410	LEU	O-C-N	5.21	127.72	122.09
12	U	85	ALA	CA-C-N	5.21	127.52	120.38
12	U	85	ALA	C-N-CA	5.21	127.52	120.38
12	U	272	GLU	N-CA-C	5.21	117.04	111.36
7	N	237	LEU	CA-C-O	5.21	125.94	120.42
6	Z	556	ILE	CA-C-N	5.21	131.49	121.54
6	Z	556	ILE	C-N-CA	5.21	131.49	121.54
7	N	167	GLU	N-CA-CB	5.21	117.51	109.91
7	N	618	ARG	N-CA-C	5.21	116.96	111.28
8	S	469	ASN	CA-C-N	5.21	127.26	120.28
8	S	469	ASN	C-N-CA	5.21	127.26	120.28
12	U	31	LYS	O-C-N	-5.21	117.12	123.27
12	U	150	THR	N-CA-CB	5.21	119.29	110.49
6	Z	397	ASP	N-CA-C	-5.21	105.21	112.03
6	Z	465	GLY	N-CA-C	-5.21	107.80	115.30
6	Z	824	ASN	CA-CB-CG	5.21	117.81	112.60
6	Z	118	VAL	CA-CB-CG1	5.20	119.25	110.40
11	R	293	THR	O-C-N	-5.20	116.71	122.07
3	T	227	PRO	CA-N-CD	5.20	119.28	112.00
8	S	228	GLU	CA-C-N	5.20	127.67	120.29
8	S	228	GLU	C-N-CA	5.20	127.67	120.29
1	W	105	VAL	CA-C-N	5.20	128.23	120.90
1	W	105	VAL	C-N-CA	5.20	128.23	120.90
8	S	134	ILE	O-C-N	5.20	127.00	121.91
9	P	56	LYS	O-C-N	-5.20	116.61	122.12
6	Z	106	TRP	N-CA-C	-5.20	101.24	109.76
10	Q	236	PHE	CA-C-N	5.20	127.67	120.29
10	Q	236	PHE	C-N-CA	5.20	127.67	120.29
2	V	255	ILE	N-CA-C	-5.20	107.41	112.29
7	N	433	THR	N-CA-CB	5.20	120.73	111.69
8	S	438	HIS	N-CA-C	-5.20	105.26	111.03
10	Q	323	LYS	CB-CA-C	-5.20	99.13	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	398	TYR	N-CA-CB	5.20	118.65	110.23
3	T	63	GLU	CA-C-O	-5.19	114.92	120.42
11	R	403	LEU	CA-C-O	-5.19	114.91	120.42
12	U	93	TYR	CA-C-N	5.19	130.31	122.99
12	U	93	TYR	C-N-CA	5.19	130.31	122.99
7	N	810	ALA	CA-C-N	5.19	130.56	121.52
7	N	810	ALA	C-N-CA	5.19	130.56	121.52
10	Q	117	VAL	N-CA-C	-5.19	105.44	110.42
11	R	24	TYR	CA-C-N	5.19	127.66	120.29
11	R	24	TYR	C-N-CA	5.19	127.66	120.29
12	U	33	CYS	N-CA-C	-5.19	100.23	109.06
1	W	82	GLU	CB-CG-CD	-5.19	103.78	112.60
3	T	106	ILE	CA-C-O	-5.19	115.67	121.17
4	X	72	GLU	N-CA-C	-5.19	105.82	113.61
6	Z	634	ASP	N-CA-C	-5.19	105.70	111.36
10	Q	340	ASP	N-CA-C	5.19	117.02	111.36
6	Z	856	HIS	ND1-CE1-NE2	5.19	113.59	108.40
7	N	349	ILE	CA-C-N	5.19	127.23	120.28
7	N	349	ILE	C-N-CA	5.19	127.23	120.28
10	Q	386	PHE	CA-C-N	5.19	131.45	121.54
10	Q	386	PHE	C-N-CA	5.19	131.45	121.54
11	R	337	VAL	O-C-N	5.19	127.17	121.83
8	S	131	THR	N-CA-C	5.19	117.84	111.82
9	P	333	ALA	CA-C-O	5.19	125.92	120.42
7	N	274	VAL	CA-C-N	5.19	127.54	120.54
7	N	274	VAL	C-N-CA	5.19	127.54	120.54
12	U	140	ILE	N-CA-C	-5.19	101.01	108.89
13	O	300	VAL	CA-CB-CG1	5.18	119.21	110.40
8	S	114	TYR	CA-C-O	-5.18	115.31	120.96
10	Q	132	PHE	CA-CB-CG	5.18	118.98	113.80
13	O	204	SER	O-C-N	5.18	128.06	122.15
4	X	10	PHE	N-CA-C	-5.18	100.86	108.99
7	N	523	LEU	O-C-N	5.18	127.41	122.07
7	N	719	ASN	CA-CB-CG	5.18	117.78	112.60
8	S	487	THR	N-CA-CB	5.18	117.74	110.12
7	N	318	LYS	CB-CA-C	-5.18	102.19	110.79
7	N	690	HIS	ND1-CE1-NE2	5.18	113.58	108.40
1	W	170	HIS	CB-CA-C	-5.18	99.32	110.45
2	V	68	VAL	O-C-N	5.18	128.87	123.02
6	Z	2	VAL	O-C-N	-5.18	117.14	122.63
3	T	88	TYR	O-C-N	-5.17	116.74	122.07
7	N	676	ALA	CA-C-N	5.17	127.64	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	676	ALA	C-N-CA	5.17	127.64	120.29
10	Q	318	LEU	CB-CA-C	5.17	120.80	109.99
2	V	249	GLU	CB-CA-C	-5.17	102.20	110.79
6	Z	211	PHE	O-C-N	5.17	127.60	122.12
11	R	101	GLU	N-CA-CB	5.17	118.21	109.78
2	V	194	ARG	CB-CA-C	-5.17	102.54	110.81
12	U	242	PRO	CA-C-N	5.17	127.52	120.54
12	U	242	PRO	C-N-CA	5.17	127.52	120.54
1	W	31	ASP	CA-CB-CG	-5.17	107.43	112.60
7	N	714	THR	O-C-N	5.17	130.02	122.94
8	S	93	LEU	N-CA-C	-5.17	105.64	111.28
9	P	385	ASN	CA-C-O	5.17	126.03	120.55
10	Q	220	LEU	N-CA-C	-5.17	105.73	111.36
7	N	152	LEU	CA-C-N	5.17	127.16	120.44
7	N	152	LEU	C-N-CA	5.17	127.16	120.44
8	S	120	SER	CA-C-N	5.17	127.07	120.56
8	S	120	SER	C-N-CA	5.17	127.07	120.56
8	S	119	TYR	N-CA-C	-5.17	101.71	109.15
9	P	222	ASN	N-CA-CB	5.17	117.71	110.12
2	V	68	VAL	N-CA-C	-5.16	100.33	108.90
3	T	48	ASN	CA-CB-CG	5.16	117.76	112.60
6	Z	217	GLU	CA-C-O	5.16	127.37	121.28
7	N	140	MET	CA-C-N	5.16	127.75	120.42
7	N	140	MET	C-N-CA	5.16	127.75	120.42
9	P	36	LEU	N-CA-C	5.16	116.59	111.07
13	O	373	TRP	CB-CG-CD2	-5.16	119.57	126.80
6	Z	149	TRP	N-CA-CB	5.16	119.09	110.32
10	Q	75	ARG	NE-CZ-NH1	-5.16	116.34	121.50
8	S	446	THR	CA-C-N	5.16	128.43	121.05
8	S	446	THR	C-N-CA	5.16	128.43	121.05
9	P	30	ASN	N-CA-CB	5.16	117.89	110.20
10	Q	318	LEU	O-C-N	-5.16	115.34	122.46
1	W	28	ALA	N-CA-CB	5.16	118.27	110.28
6	Z	292	ASP	CB-CA-C	5.16	118.97	110.88
7	N	352	ASN	OD1-CG-ND2	5.15	127.75	122.60
3	T	195	LEU	CA-C-N	5.15	127.45	120.65
3	T	195	LEU	C-N-CA	5.15	127.45	120.65
6	Z	387	ASN	CB-CG-ND2	-5.15	108.67	116.40
6	Z	565	PHE	N-CA-CB	5.15	117.69	110.12
7	N	387	ALA	N-CA-CB	5.15	118.42	110.43
9	P	38	GLN	OE1-CD-NE2	5.15	127.75	122.60
10	Q	400	TYR	N-CA-CB	5.15	119.55	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	50	GLU	CB-CA-C	-5.15	102.24	110.79
7	N	136	ILE	O-C-N	-5.15	116.87	121.87
8	S	474	GLU	CA-C-O	-5.15	115.09	120.55
9	P	18	LYS	CB-CA-C	-5.15	101.27	110.70
9	P	111	ASP	CA-C-N	5.15	127.49	120.54
9	P	111	ASP	C-N-CA	5.15	127.49	120.54
10	Q	118	CYS	CA-C-N	5.15	127.14	120.44
10	Q	118	CYS	C-N-CA	5.15	127.14	120.44
6	Z	286	VAL	N-CA-CB	-5.15	103.54	110.54
7	N	282	TYR	N-CA-CB	5.15	117.88	109.69
10	Q	120	LYS	N-CA-C	5.15	116.58	111.07
2	V	114	PHE	CB-CG-CD1	5.15	129.45	120.70
6	Z	49	LEU	CB-CA-C	-5.15	102.80	110.88
7	N	817	THR	O-C-N	5.15	127.38	122.03
8	S	290	ASN	OD1-CG-ND2	5.15	127.75	122.60
9	P	353	ILE	CA-C-O	-5.15	115.39	120.85
3	T	177	PHE	O-C-N	5.14	129.84	122.13
10	Q	25	GLN	OE1-CD-NE2	5.14	127.75	122.60
11	R	204	TRP	CA-C-N	5.14	127.17	120.28
11	R	204	TRP	C-N-CA	5.14	127.17	120.28
11	R	322	LEU	O-C-N	-5.14	115.27	122.37
11	R	63	TYR	CA-C-N	5.14	127.17	120.28
11	R	63	TYR	C-N-CA	5.14	127.17	120.28
6	Z	582	ASP	CA-CB-CG	5.14	117.74	112.60
6	Z	565	PHE	CA-CB-CG	-5.14	108.66	113.80
11	R	218	CYS	CA-C-O	5.14	125.88	119.97
12	U	222	ASN	CA-CB-CG	-5.14	107.46	112.60
7	N	548	ARG	CA-C-N	5.14	127.12	120.44
7	N	548	ARG	C-N-CA	5.14	127.12	120.44
7	N	669	GLU	N-CA-C	-5.14	107.01	113.28
8	S	76	PHE	N-CA-C	-5.14	105.68	111.28
8	S	154	GLN	CA-C-O	-5.14	115.43	120.82
9	P	374	SER	O-C-N	-5.14	116.78	122.07
9	P	434	THR	O-C-N	5.14	127.57	122.12
2	V	138	ALA	CB-CA-C	-5.13	101.92	110.14
7	N	634	LEU	CA-C-N	5.13	129.41	120.68
7	N	634	LEU	C-N-CA	5.13	129.41	120.68
10	Q	316	THR	N-CA-C	-5.13	105.76	111.36
2	V	226	LYS	N-CA-CB	5.13	117.50	109.85
10	Q	14	LEU	CA-C-N	5.13	127.49	120.46
10	Q	14	LEU	C-N-CA	5.13	127.49	120.46
11	R	275	GLU	CA-C-N	5.13	127.58	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	275	GLU	C-N-CA	5.13	127.58	120.29
1	W	110	ILE	N-CA-C	-5.13	100.93	108.11
7	N	442	LEU	CA-C-N	5.13	130.12	121.14
7	N	442	LEU	C-N-CA	5.13	130.12	121.14
9	P	293	LEU	N-CA-CB	5.13	117.58	110.04
10	Q	120	LYS	O-C-N	5.13	127.36	122.07
12	U	251	ASN	CA-CB-CG	-5.13	107.47	112.60
13	O	165	LEU	CB-CA-C	-5.13	102.27	110.79
5	Y	67	VAL	CA-C-N	5.13	128.38	121.05
5	Y	67	VAL	C-N-CA	5.13	128.38	121.05
12	U	171	VAL	N-CA-CB	5.13	117.14	110.57
1	W	42	ASN	CA-C-N	5.13	127.10	120.44
1	W	42	ASN	C-N-CA	5.13	127.10	120.44
2	V	183	ALA	O-C-N	5.13	128.56	122.46
6	Z	69	ASN	N-CA-CB	5.13	117.75	110.16
6	Z	484	LYS	CB-CA-C	-5.13	102.28	110.79
7	N	717	LEU	CA-C-O	5.13	125.86	120.42
8	S	320	ILE	CA-C-N	5.13	127.15	120.28
8	S	320	ILE	C-N-CA	5.13	127.15	120.28
3	T	43	ASP	CA-C-N	5.12	131.33	121.54
3	T	43	ASP	C-N-CA	5.12	131.33	121.54
6	Z	103	TYR	CB-CG-CD1	5.12	128.49	120.80
7	N	95	SER	N-CA-CB	5.12	118.61	110.57
9	P	94	GLN	CA-C-O	-5.12	112.39	119.05
9	P	95	TYR	N-CA-C	5.12	116.67	111.14
1	W	9	VAL	CA-CB-CG1	5.12	119.11	110.40
9	P	144	VAL	O-C-N	5.12	126.84	121.87
11	R	224	PHE	CA-CB-CG	-5.12	108.68	113.80
7	N	45	ASP	CA-CB-CG	-5.12	107.48	112.60
9	P	121	THR	N-CA-CB	5.12	117.83	110.20
6	Z	760	HIS	CE1-NE2-CD2	-5.12	103.88	109.00
7	N	106	ILE	O-C-N	-5.12	116.89	121.91
9	P	11	LYS	CA-C-O	5.12	126.19	120.82
11	R	224	PHE	CB-CG-CD1	-5.12	112.00	120.70
5	Y	80	GLU	CA-CB-CG	5.12	124.33	114.10
7	N	248	GLU	CB-CA-C	-5.12	102.78	111.02
8	S	476	LEU	CA-C-O	5.12	125.97	120.70
10	Q	90	LYS	O-C-N	5.12	130.26	122.94
1	W	146	GLU	O-C-N	5.12	127.61	122.09
6	Z	357	ILE	CA-C-O	5.12	126.00	120.47
8	S	411	LEU	N-CA-C	-5.12	106.63	112.92
1	W	128	LEU	N-CA-C	5.11	116.85	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	179	LEU	CA-C-O	5.11	125.97	120.55
10	Q	410	ASP	CA-C-N	5.11	129.37	120.68
10	Q	410	ASP	C-N-CA	5.11	129.37	120.68
7	N	310	ASP	CA-CB-CG	-5.11	107.49	112.60
13	O	326	HIS	CB-CG-CD2	-5.11	124.56	131.20
6	Z	850	LEU	CD1-CG-CD2	5.11	122.05	110.80
13	O	317	THR	N-CA-C	-5.11	107.09	113.38
6	Z	343	ALA	O-C-N	5.11	127.53	122.12
3	T	175	ASP	N-CA-CB	5.11	118.87	110.39
6	Z	254	PRO	CA-C-O	-5.11	111.81	118.86
6	Z	295	ARG	CD-NE-CZ	5.11	131.55	124.40
7	N	330	THR	O-C-N	5.11	127.33	122.07
7	N	76	GLU	CA-C-N	5.10	128.07	120.31
7	N	76	GLU	C-N-CA	5.10	128.07	120.31
11	R	179	PHE	N-CA-CB	5.10	118.08	110.22
2	V	39	LYS	O-C-N	5.10	127.33	122.07
3	T	212	ASN	CA-CB-CG	-5.10	107.50	112.60
6	Z	179	SER	CA-C-O	5.10	125.81	119.79
6	Z	463	HIS	CE1-NE2-CD2	-5.10	103.90	109.00
6	Z	560	THR	CA-CB-OG1	5.10	117.25	109.60
10	Q	14	LEU	O-C-N	-5.10	116.71	122.12
3	T	192	ASN	N-CA-C	-5.10	105.61	111.07
6	Z	203	LEU	CD1-CG-CD2	-5.10	99.58	110.80
2	V	162	GLY	CA-C-N	5.10	127.11	120.28
2	V	162	GLY	C-N-CA	5.10	127.11	120.28
7	N	523	LEU	N-CA-C	-5.10	105.61	111.07
9	P	238	ALA	CA-C-O	-5.10	115.02	120.42
2	V	240	ALA	O-C-N	-5.10	116.34	122.15
7	N	261	LEU	N-CA-C	5.10	116.92	111.36
12	U	252	HIS	CE1-NE2-CD2	-5.10	103.90	109.00
1	W	169	SER	O-C-N	-5.09	116.60	122.87
6	Z	460	SER	N-CA-CB	5.09	118.07	110.22
8	S	48	LEU	CB-CA-C	-5.09	102.88	110.88
2	V	176	ASN	CA-C-N	5.09	127.10	120.28
2	V	176	ASN	C-N-CA	5.09	127.10	120.28
6	Z	123	ALA	N-CA-C	-5.09	105.81	111.36
6	Z	470	ALA	O-C-N	5.09	128.53	122.27
7	N	899	ASN	CA-C-N	5.09	128.10	120.87
7	N	899	ASN	C-N-CA	5.09	128.10	120.87
10	Q	402	THR	CA-C-O	-5.09	114.71	119.80
1	W	106	GLN	N-CA-CB	5.09	117.78	109.69
7	N	887	ASP	CA-CB-CG	-5.09	107.51	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	142	ASP	CA-C-O	-5.09	113.62	119.32
3	T	177	PHE	CA-C-O	-5.09	113.82	119.67
6	Z	343	ALA	CA-C-O	-5.09	115.16	120.55
2	V	114	PHE	N-CA-CB	5.09	119.86	111.62
13	O	10	ILE	CA-C-N	5.09	127.09	120.28
13	O	10	ILE	C-N-CA	5.09	127.09	120.28
6	Z	532	HIS	CA-CB-CG	5.08	118.89	113.80
6	Z	842	GLN	N-CA-CB	5.08	117.43	109.85
12	U	28	LYS	CA-C-O	-5.08	115.99	121.38
6	Z	46	LYS	O-C-N	5.08	127.51	122.12
6	Z	155	ARG	CD-NE-CZ	5.08	131.52	124.40
7	N	583	VAL	O-C-N	5.08	127.07	121.83
8	S	139	HIS	ND1-CE1-NE2	5.08	113.48	108.40
9	P	136	ARG	CA-C-O	5.08	125.94	120.55
9	P	154	ASP	CA-C-N	5.08	127.09	120.28
9	P	154	ASP	C-N-CA	5.08	127.09	120.28
12	U	75	ASN	CA-C-N	5.08	127.09	120.28
12	U	75	ASN	C-N-CA	5.08	127.09	120.28
3	T	46	ILE	O-C-N	-5.08	117.19	123.09
6	Z	151	HIS	CA-CB-CG	5.08	118.88	113.80
7	N	237	LEU	CA-C-N	5.08	127.09	120.28
7	N	237	LEU	C-N-CA	5.08	127.09	120.28
8	S	321	GLN	CB-CG-CD	-5.08	103.96	112.60
11	R	187	VAL	CB-CA-C	-5.08	105.28	112.14
12	U	22	TYR	CB-CG-CD1	5.08	128.42	120.80
13	O	25	LEU	N-CA-C	-5.08	105.01	111.11
13	O	210	ARG	CA-C-N	5.08	127.51	120.29
13	O	210	ARG	C-N-CA	5.08	127.51	120.29
6	Z	898	HIS	CE1-NE2-CD2	-5.08	103.92	109.00
7	N	206	ILE	CA-C-N	5.08	127.08	120.28
7	N	206	ILE	C-N-CA	5.08	127.08	120.28
9	P	288	ASN	N-CA-CB	5.08	117.68	110.16
10	Q	162	LEU	CB-CA-C	5.08	120.08	112.31
8	S	406	ASP	CA-C-O	-5.08	115.04	120.42
8	S	195	ALA	O-C-N	5.08	128.16	122.22
2	V	254	ARG	NE-CZ-NH1	5.07	126.57	121.50
9	P	162	GLU	CA-C-N	5.07	127.39	120.54
9	P	162	GLU	C-N-CA	5.07	127.39	120.54
13	O	352	TRP	CE2-CD2-CE3	5.07	123.87	118.80
11	R	196	SER	N-CA-C	-5.07	105.83	111.36
8	S	380	CYS	CA-C-N	5.07	127.41	120.46
8	S	380	CYS	C-N-CA	5.07	127.41	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	865	ASP	CA-CB-CG	-5.07	107.53	112.60
7	N	10	LEU	CA-C-O	-5.07	115.50	120.82
6	Z	593	HIS	ND1-CE1-NE2	5.07	113.47	108.40
10	Q	206	ASN	N-CA-CB	5.07	117.57	110.12
10	Q	361	HIS	ND1-CE1-NE2	5.07	113.47	108.40
11	R	146	ASP	CA-CB-CG	-5.07	107.53	112.60
4	X	90	VAL	CA-CB-CG2	-5.07	101.79	110.40
6	Z	549	ASN	CA-C-O	5.06	125.79	120.42
8	S	40	GLU	N-CA-C	5.06	116.49	111.07
7	N	158	LEU	CA-C-N	5.06	127.57	120.28
7	N	158	LEU	C-N-CA	5.06	127.57	120.28
7	N	38	GLU	CB-CG-CD	-5.06	104.00	112.60
9	P	78	GLN	CA-C-O	-5.06	115.06	120.42
12	U	107	ASN	N-CA-C	5.06	117.45	111.33
12	U	165	GLU	CB-CG-CD	-5.06	104.00	112.60
13	O	343	GLN	CB-CA-C	5.06	119.83	109.55
3	T	217	THR	N-CA-CB	5.06	117.35	110.01
7	N	615	ALA	CA-C-N	5.06	127.47	120.29
7	N	615	ALA	C-N-CA	5.06	127.47	120.29
13	O	381	GLY	CA-C-O	5.06	125.50	120.09
9	P	24	ILE	O-C-N	-5.06	116.62	121.83
9	P	280	LEU	CA-C-O	-5.06	114.63	120.24
1	W	72	ILE	O-C-N	5.06	126.77	121.87
6	Z	317	GLN	N-CA-C	-5.06	105.66	111.07
3	T	194	GLU	N-CA-C	5.05	116.48	111.07
6	Z	739	ALA	O-C-N	5.05	127.48	122.12
8	S	135	ASN	CA-C-O	-5.05	115.51	120.82
6	Z	839	SER	CA-C-O	-5.05	115.19	120.55
11	R	316	LEU	N-CA-CB	5.05	117.64	110.16
13	O	142	ASP	N-CA-C	-5.05	97.11	107.67
2	V	125	THR	CA-C-N	5.05	127.05	120.28
2	V	125	THR	C-N-CA	5.05	127.05	120.28
6	Z	907	GLY	N-CA-C	-5.05	102.21	111.25
8	S	421	TYR	CB-CA-C	-5.05	99.43	109.99
8	S	435	LYS	N-CA-C	-5.05	100.11	108.75
13	O	292	CYS	CA-C-N	5.05	127.05	120.28
13	O	292	CYS	C-N-CA	5.05	127.05	120.28
6	Z	265	LEU	CB-CA-C	-5.05	99.76	110.31
8	S	252	ASP	CA-C-N	5.05	127.05	120.28
8	S	252	ASP	C-N-CA	5.05	127.05	120.28
13	O	164	PRO	CA-N-CD	5.05	119.07	112.00
13	O	220	SER	N-CA-CB	5.05	117.54	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	95	GLN	CB-CA-C	-5.05	102.41	110.79
4	X	43	LEU	N-CA-C	-5.05	106.27	114.09
7	N	40	SER	CB-CA-C	-5.05	102.41	110.79
3	T	269	SER	CA-C-N	5.05	127.58	120.42
3	T	269	SER	C-N-CA	5.05	127.58	120.42
5	Y	81	LEU	CB-CA-C	-5.05	102.41	110.79
6	Z	510	LEU	CA-C-O	-5.05	113.25	120.16
8	S	277	SER	O-C-N	5.05	127.47	122.12
10	Q	162	LEU	O-C-N	5.05	126.73	121.79
11	R	118	GLN	CB-CA-C	-5.05	102.41	110.79
11	R	351	LYS	CA-C-N	5.05	127.00	120.44
11	R	351	LYS	C-N-CA	5.05	127.00	120.44
13	O	170	SER	N-CA-C	5.05	116.78	111.28
13	O	227	ILE	CA-C-N	5.05	130.49	121.15
13	O	227	ILE	C-N-CA	5.05	130.49	121.15
13	O	318	HIS	CG-CD2-NE2	5.04	112.25	107.20
3	T	164	LEU	N-CA-CB	5.04	117.53	110.12
6	Z	316	ALA	N-CA-CB	5.04	117.53	110.12
7	N	818	LYS	CG-CD-CE	5.04	122.90	111.30
9	P	114	THR	N-CA-C	-5.04	105.67	111.07
1	W	48	THR	CA-C-O	5.04	127.10	121.40
6	Z	224	LEU	CA-C-N	5.04	127.34	120.54
6	Z	224	LEU	C-N-CA	5.04	127.34	120.54
8	S	409	LEU	N-CA-C	5.04	116.86	111.36
10	Q	36	SER	CA-C-N	5.04	127.03	120.28
10	Q	36	SER	C-N-CA	5.04	127.03	120.28
10	Q	297	ASP	CB-CA-C	-5.04	102.93	110.90
12	U	220	PRO	O-C-N	5.04	129.15	123.10
6	Z	502	ASN	CB-CG-ND2	5.04	123.96	116.40
1	W	107	HIS	CE1-NE2-CD2	-5.04	103.96	109.00
2	V	89	ALA	CA-C-O	5.04	125.89	120.55
6	Z	487	SER	O-C-N	5.04	127.46	122.12
7	N	66	SER	CA-C-O	-5.04	115.53	120.82
7	N	915	ALA	N-CA-C	-5.04	101.75	109.76
9	P	257	TRP	N-CA-C	-5.04	105.88	112.23
10	Q	12	ARG	NE-CZ-NH2	-5.04	114.67	119.20
10	Q	106	GLN	O-C-N	-5.04	116.79	122.03
11	R	340	GLN	N-CA-CB	5.04	117.62	110.16
13	O	302	VAL	CA-C-N	-5.04	115.68	123.14
13	O	302	VAL	C-N-CA	-5.04	115.68	123.14
7	N	449	GLY	O-C-N	-5.04	117.14	122.13
7	N	511	GLY	O-C-N	5.04	127.03	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	U	114	THR	O-C-N	5.04	128.65	122.96
6	Z	269	TYR	CB-CG-CD2	-5.04	113.25	120.80
7	N	877	GLN	N-CA-CB	5.03	117.91	110.56
10	Q	112	ASP	CA-C-N	5.03	127.33	120.54
10	Q	112	ASP	C-N-CA	5.03	127.33	120.54
7	N	466	LEU	N-CA-CB	5.03	117.61	110.16
8	S	275	TYR	CA-C-O	-5.03	115.54	120.82
12	U	135	ASP	O-C-N	5.03	129.50	123.16
6	Z	738	TYR	CB-CG-CD1	5.03	128.35	120.80
9	P	5	ALA	CA-C-O	-5.03	113.46	118.34
9	P	86	HIS	ND1-CE1-NE2	5.03	113.43	108.40
13	O	251	LEU	CA-C-N	5.03	127.95	120.31
13	O	251	LEU	C-N-CA	5.03	127.95	120.31
6	Z	909	ARG	CA-C-N	5.03	124.47	119.24
6	Z	909	ARG	C-N-CA	5.03	124.47	119.24
8	S	183	LEU	CA-C-N	5.03	127.95	120.31
8	S	183	LEU	C-N-CA	5.03	127.95	120.31
7	N	255	ALA	N-CA-C	-5.03	105.88	111.36
8	S	101	LYS	CA-C-N	5.03	131.14	121.54
8	S	101	LYS	C-N-CA	5.03	131.14	121.54
8	S	122	ASN	CA-C-O	-5.03	115.09	120.42
11	R	335	ARG	CB-CA-C	-5.03	102.30	110.85
7	N	438	ASP	N-CA-CB	5.03	117.30	110.01
11	R	264	THR	O-C-N	-5.03	116.79	122.12
6	Z	526	ALA	CA-C-O	-5.02	115.72	121.00
11	R	251	THR	CA-C-O	-5.02	114.19	119.97
6	Z	156	HIS	O-C-N	5.02	127.24	122.07
6	Z	714	ASP	CA-CB-CG	5.02	117.62	112.60
13	O	232	GLU	O-C-N	5.02	127.44	122.12
2	V	251	TYR	CA-CB-CG	-5.02	104.87	113.90
2	V	263	GLU	CA-C-O	5.02	125.87	120.55
13	O	206	THR	O-C-N	5.02	128.57	122.85
13	O	376	GLN	CB-CG-CD	-5.02	104.07	112.60
6	Z	240	ASN	CA-CB-CG	-5.02	107.58	112.60
3	T	102	LYS	CB-CA-C	-5.01	102.95	110.92
7	N	548	ARG	CA-CB-CG	5.01	124.13	114.10
3	T	178	THR	N-CA-CB	5.01	117.41	109.94
11	R	340	GLN	CB-CG-CD	-5.01	104.08	112.60
1	W	134	LYS	CA-C-O	5.01	125.73	120.42
2	V	132	LEU	O-C-N	5.01	127.44	122.08
6	Z	785	VAL	N-CA-C	-5.01	105.82	110.53
8	S	199	GLU	CA-C-N	5.01	130.68	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	199	GLU	C-N-CA	5.01	130.68	122.81
10	Q	347	LEU	CB-CA-C	-5.01	102.33	110.85
6	Z	1	MET	CG-SD-CE	-5.01	89.88	100.90
12	U	34	VAL	CA-CB-CG1	5.01	118.92	110.40
7	N	652	VAL	N-CA-C	-5.01	105.66	110.72
11	R	29	LYS	CA-C-N	5.01	126.99	120.28
11	R	29	LYS	C-N-CA	5.01	126.99	120.28
13	O	27	GLU	N-CA-C	-5.01	105.71	111.07
13	O	299	THR	N-CA-C	5.01	116.74	111.28
2	V	40	HIS	ND1-CE1-NE2	5.00	113.41	108.40
7	N	268	GLN	N-CA-CB	5.00	117.48	110.12
1	W	50	GLY	CA-C-N	5.00	130.74	122.33
1	W	50	GLY	C-N-CA	5.00	130.74	122.33
6	Z	295	ARG	O-C-N	-5.00	116.36	122.22
6	Z	322	GLU	CA-C-N	5.00	130.65	122.65
6	Z	322	GLU	C-N-CA	5.00	130.65	122.65
9	P	263	HIS	CA-C-N	5.00	127.06	120.60
9	P	263	HIS	C-N-CA	5.00	127.06	120.60
12	U	96	GLY	O-C-N	-5.00	116.77	121.77
12	U	217	LYS	CA-C-N	5.00	129.84	122.63
12	U	217	LYS	C-N-CA	5.00	129.84	122.63
3	T	29	PRO	CA-C-N	5.00	128.84	120.64
3	T	29	PRO	C-N-CA	5.00	128.84	120.64
6	Z	463	HIS	CA-CB-CG	5.00	118.80	113.80
6	Z	718	ASP	N-CA-CB	-5.00	102.77	110.12
9	P	48	GLN	CB-CA-C	-5.00	100.47	110.42

There are no chirality outliers.

All (123) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	N	123	PHE	Sidechain
7	N	139	ARG	Sidechain
7	N	188	TYR	Sidechain
7	N	298	TYR	Sidechain
7	N	328	PHE	Sidechain
7	N	398	ARG	Sidechain
7	N	417	ARG	Sidechain
7	N	471	TYR	Sidechain
7	N	50	TYR	Sidechain
7	N	502	PHE	Sidechain
7	N	504	TYR	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
7	N	510	HIS	Sidechain
7	N	58	ARG	Sidechain
7	N	584	ARG	Sidechain
7	N	585	ARG	Sidechain
7	N	593	PHE	Sidechain
7	N	599	TYR	Sidechain
7	N	618	ARG	Sidechain
7	N	70	TYR	Sidechain
7	N	743	PHE	Sidechain
7	N	813	ARG	Sidechain
7	N	873	ARG	Sidechain
7	N	98	VAL	Peptide
13	O	228	TYR	Sidechain
13	O	248	TYR	Sidechain
13	O	252	PHE	Sidechain
13	O	310	PHE	Sidechain
13	O	356	ARG	Sidechain
13	O	58	ARG	Sidechain
13	O	60	ARG	Sidechain
13	O	62	TYR	Sidechain
13	O	70	TYR	Sidechain
13	O	81	TYR	Sidechain
13	O	98	TYR	Sidechain
9	P	115	ARG	Sidechain
9	P	201	ARG	Sidechain
9	P	234	TYR	Sidechain
9	P	240	TYR	Sidechain
9	P	273	TYR	Sidechain
9	P	310	ARG	Sidechain
9	P	351	ARG	Sidechain
9	P	79	LEU	Mainchain
10	Q	104	PHE	Sidechain
10	Q	127	ARG	Sidechain
10	Q	151	TYR	Sidechain
10	Q	161	LEU	Mainchain,Peptide
10	Q	163	ARG	Sidechain
10	Q	185	TYR	Sidechain
10	Q	20	TYR	Sidechain
10	Q	202	ARG	Sidechain
10	Q	255	TYR	Sidechain
10	Q	291	TYR	Sidechain
10	Q	294	ARG	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
10	Q	306	TYR	Sidechain
10	Q	309	ARG	Sidechain
10	Q	354	PHE	Peptide
10	Q	387	TYR	Sidechain
10	Q	400	TYR	Sidechain
10	Q	409	TYR	Sidechain
10	Q	84	TYR	Sidechain
11	R	123	ASP	Peptide
11	R	186	TYR	Sidechain
11	R	207	ARG	Sidechain
11	R	210	TYR	Sidechain
11	R	305	PHE	Sidechain
11	R	331	ARG	Sidechain
11	R	334	ARG	Sidechain
11	R	335	ARG	Sidechain
11	R	357	PHE	Sidechain
11	R	417	TYR	Sidechain
11	R	63	TYR	Sidechain
11	R	70	TYR	Sidechain
8	S	119	TYR	Sidechain
8	S	145	PHE	Sidechain
8	S	188	TYR	Sidechain
8	S	197	SER	Mainchain,Peptide
8	S	261	HIS	Peptide
8	S	275	TYR	Sidechain
8	S	377	TYR	Sidechain
8	S	393	ARG	Sidechain
8	S	428	ARG	Sidechain
8	S	452	TYR	Sidechain
8	S	472	HIS	Sidechain
8	S	480	ARG	Sidechain
8	S	82	TYR	Sidechain
3	T	157	TYR	Sidechain
3	T	177	PHE	Sidechain
3	T	211	PHE	Sidechain
3	T	51	TYR	Sidechain
3	T	81	TYR	Sidechain
3	T	89	TYR	Sidechain
12	U	176	ARG	Sidechain
12	U	24	ARG	Sidechain
12	U	32	ARG	Sidechain
12	U	52	PHE	Sidechain

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Mol	Chain	Res	Type	Group
2	V	157	ARG	Sidechain
2	V	171	ARG	Sidechain
2	V	229	ASP	Peptide
2	V	270	TYR	Sidechain
2	V	61	TYR	Sidechain
1	W	122	ARG	Sidechain
1	W	127	ARG	Sidechain
1	W	182	TYR	Sidechain
1	W	23	ARG	Sidechain
1	W	25	ARG	Sidechain
1	W	77	HIS	Sidechain
4	X	51	ARG	Sidechain
4	X	99	PHE	Sidechain
5	Y	86	ARG	Sidechain
6	Z	132	HIS	Sidechain
6	Z	210	TYR	Sidechain
6	Z	269	TYR	Sidechain
6	Z	312	TYR	Sidechain
6	Z	323	TYR	Sidechain
6	Z	385	PHE	Sidechain
6	Z	394	TYR	Sidechain
6	Z	426	TYR	Sidechain
6	Z	477	TYR	Sidechain
6	Z	773	ARG	Sidechain
6	Z	774	ARG	Sidechain
6	Z	849	ARG	Sidechain

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	1534	0	1542	17	0
2	V	2274	0	2272	53	0
3	T	2192	0	2157	13	0
4	X	1032	0	1017	5	0
5	Y	435	0	394	17	0
6	Z	7005	0	6932	87	0
7	N	6882	0	6959	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	S	3894	0	3937	33	0
9	P	3608	0	3694	15	0
10	Q	3499	0	3524	18	0
11	R	3060	0	3083	12	0
12	U	2373	0	2403	7	0
13	O	3186	0	3213	12	0
All	All	40974	0	41127	313	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 (313) 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)
8:S:127:THR:CB	8:S:127:THR:CA	1.80	1.58
6:Z:30:LYS:CG	6:Z:37:GLN:HB3	1.22	1.55
6:Z:24:THR:HB	6:Z:25:PRO:CD	1.36	1.51
2:V:118:LEU:HB2	2:V:195:HIS:CD2	1.47	1.49
2:V:118:LEU:CB	2:V:195:HIS:NE2	1.80	1.44
5:Y:21:ASN:CG	8:S:55:ARG:NH1	1.68	1.44
6:Z:30:LYS:CG	6:Z:37:GLN:CB	2.03	1.34
6:Z:85:VAL:CG1	6:Z:86:PRO:HD3	1.60	1.28
6:Z:30:LYS:CD	6:Z:37:GLN:HB3	1.64	1.26
5:Y:21:ASN:ND2	8:S:55:ARG:CZ	1.99	1.24
6:Z:30:LYS:HG3	6:Z:37:GLN:CB	1.63	1.24
6:Z:85:VAL:HG12	6:Z:86:PRO:CD	1.67	1.24
2:V:118:LEU:HB2	2:V:195:HIS:NE2	0.92	1.23
6:Z:85:VAL:CG1	6:Z:86:PRO:CD	2.18	1.19
7:N:36:TRP:CE3	7:N:36:TRP:O	1.95	1.19
6:Z:24:THR:CB	6:Z:25:PRO:CD	2.22	1.17
6:Z:85:VAL:CB	6:Z:86:PRO:HD2	1.69	1.17
6:Z:85:VAL:CB	6:Z:86:PRO:CD	2.22	1.17
6:Z:30:LYS:HG2	6:Z:37:GLN:HB3	1.23	1.15
7:N:856:PHE:O	7:N:857:TYR:O	1.64	1.14
6:Z:24:THR:HB	6:Z:25:PRO:HD2	1.20	1.14
6:Z:85:VAL:HB	6:Z:86:PRO:CD	1.77	1.13
7:N:708:ALA:HB1	7:N:713:VAL:HG22	1.30	1.13
1:W:126:ILE:HA	1:W:157:PHE:HZ	1.10	1.12
1:W:155:ASP:HB2	1:W:171:LEU:HD22	1.28	1.12
7:N:8:PRO:CB	7:N:8:PRO:CA	2.17	1.10
2:V:118:LEU:HD12	2:V:195:HIS:HD2	1.12	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:126:ILE:HA	1:W:157:PHE:CZ	1.86	1.09
6:Z:30:LYS:HG3	6:Z:37:GLN:CG	1.82	1.09
6:Z:30:LYS:HG3	6:Z:37:GLN:CD	1.78	1.08
5:Y:65:ASP:HB2	11:R:331:ARG:CD	1.84	1.08
6:Z:85:VAL:HG12	6:Z:86:PRO:HD3	1.15	1.07
6:Z:24:THR:HB	6:Z:25:PRO:HD3	1.12	1.06
6:Z:282:ILE:HG13	6:Z:318:LYS:HD2	1.38	1.06
6:Z:85:VAL:O	6:Z:88:PRO:HD2	1.55	1.05
2:V:118:LEU:CB	2:V:195:HIS:CD2	2.32	1.04
2:V:118:LEU:O	2:V:195:HIS:CE1	2.11	1.02
6:Z:282:ILE:HD11	6:Z:297:VAL:CG1	1.89	1.02
6:Z:24:THR:CB	6:Z:25:PRO:HD3	1.84	1.01
7:N:339:MET:HA	7:N:709:GLY:N	1.77	0.99
7:N:708:ALA:CB	7:N:713:VAL:HG22	1.93	0.97
7:N:36:TRP:O	7:N:36:TRP:CD2	2.17	0.97
6:Z:282:ILE:CD1	6:Z:297:VAL:HB	1.95	0.97
5:Y:65:ASP:HB2	11:R:331:ARG:HD3	1.47	0.95
6:Z:85:VAL:HB	6:Z:86:PRO:HD2	0.95	0.94
6:Z:49:LEU:HD21	6:Z:93:ARG:HG2	1.49	0.93
2:V:118:LEU:HD12	2:V:195:HIS:CD2	2.02	0.93
1:W:155:ASP:CB	1:W:171:LEU:HD22	1.98	0.93
2:V:118:LEU:CD1	2:V:195:HIS:HD2	1.83	0.92
6:Z:282:ILE:CD1	6:Z:297:VAL:CG1	2.49	0.91
8:S:127:THR:CB	8:S:127:THR:N	2.34	0.91
5:Y:65:ASP:HB2	11:R:331:ARG:HD2	1.51	0.90
7:N:707:ASN:O	7:N:709:GLY:N	2.05	0.88
6:Z:85:VAL:HG12	6:Z:86:PRO:N	1.84	0.88
6:Z:282:ILE:CD1	6:Z:297:VAL:HG11	2.05	0.87
7:N:6:ALA:HB2	7:N:35:LEU:CD1	2.06	0.86
2:V:157:ARG:O	2:V:196:TYR:CA	2.24	0.86
6:Z:282:ILE:CD1	6:Z:297:VAL:CB	2.54	0.85
5:Y:21:ASN:HD21	8:S:55:ARG:CZ	1.77	0.85
5:Y:21:ASN:CG	8:S:55:ARG:CZ	2.45	0.84
2:V:159:ILE:HD11	2:V:196:TYR:O	1.78	0.83
1:W:158:ILE:HG23	1:W:169:SER:HB2	1.61	0.82
2:V:159:ILE:HD11	2:V:196:TYR:CD1	2.15	0.82
7:N:708:ALA:HB1	7:N:713:VAL:CG2	2.10	0.82
2:V:24:LYS:HG3	2:V:196:TYR:CD1	2.14	0.81
6:Z:30:LYS:HD3	6:Z:37:GLN:HB3	1.61	0.81
2:V:157:ARG:H	2:V:196:TYR:HB2	1.46	0.81
2:V:118:LEU:O	2:V:195:HIS:HE1	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:282:ILE:HD13	6:Z:297:VAL:CB	2.12	0.78
7:N:6:ALA:HB2	7:N:35:LEU:HD13	1.64	0.78
2:V:157:ARG:O	2:V:196:TYR:CB	2.32	0.76
2:V:24:LYS:HG3	2:V:196:TYR:CE1	2.20	0.76
2:V:158:LEU:HA	2:V:195:HIS:O	1.86	0.76
5:Y:33:ASP:C	5:Y:35:PHE:H	1.93	0.76
6:Z:30:LYS:HG2	6:Z:37:GLN:CB	1.91	0.75
11:R:280:ILE:HG13	11:R:281:SER:N	2.01	0.75
2:V:118:LEU:CG	2:V:195:HIS:CD2	2.70	0.75
6:Z:24:THR:CG2	6:Z:25:PRO:HD3	2.16	0.74
6:Z:282:ILE:HD11	6:Z:297:VAL:CB	2.18	0.73
6:Z:30:LYS:CD	6:Z:37:GLN:CB	2.53	0.73
6:Z:282:ILE:HD13	6:Z:297:VAL:HB	1.69	0.71
13:O:393:VAL:OXT	13:O:393:VAL:HG12	1.90	0.70
7:N:35:LEU:C	7:N:37:SER:H	1.98	0.69
8:S:127:THR:CA	8:S:127:THR:HB	2.14	0.69
3:T:84:GLN:OE1	7:N:8:PRO:CB	2.41	0.69
7:N:6:ALA:HB2	7:N:35:LEU:HD12	1.74	0.69
2:V:196:TYR:HD1	2:V:197:TYR:HB3	1.59	0.68
6:Z:93:ARG:HB3	6:Z:94:PRO:CD	2.24	0.68
2:V:196:TYR:HD1	2:V:197:TYR:CB	2.07	0.68
6:Z:49:LEU:CD2	6:Z:93:ARG:HG2	2.22	0.68
3:T:84:GLN:NE2	7:N:8:PRO:CB	2.57	0.68
2:V:159:ILE:HD11	2:V:196:TYR:CE1	2.29	0.67
2:V:118:LEU:CD1	2:V:195:HIS:CD2	2.68	0.67
6:Z:30:LYS:HD3	6:Z:37:GLN:CB	2.21	0.67
7:N:444:HIS:CD2	7:N:480:ALA:HB2	2.29	0.67
1:W:155:ASP:CG	1:W:171:LEU:HD22	2.20	0.67
8:S:127:THR:CB	8:S:127:THR:C	2.65	0.67
13:O:32:PHE:HB2	13:O:41:LEU:HD13	1.75	0.67
1:W:155:ASP:HB2	1:W:171:LEU:CD2	2.16	0.67
4:X:18:ASN:HD21	4:X:21:SER:H	1.43	0.66
6:Z:85:VAL:HG11	6:Z:86:PRO:HD3	1.69	0.66
7:N:36:TRP:CD2	7:N:36:TRP:C	2.71	0.65
8:S:345:TYR:CD1	8:S:345:TYR:N	2.61	0.65
5:Y:21:ASN:ND2	8:S:55:ARG:NH1	0.66	0.65
8:S:339:GLN:HA	8:S:339:GLN:OE1	1.96	0.65
6:Z:282:ILE:HD11	6:Z:297:VAL:HB	1.73	0.64
5:Y:33:ASP:C	5:Y:35:PHE:N	2.56	0.64
2:V:157:ARG:O	2:V:196:TYR:HB2	1.96	0.64
9:P:93:ILE:HG22	9:P:97:ILE:HG13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:84:GLN:OE1	7:N:8:PRO:HB3	1.98	0.63
1:W:126:ILE:CA	1:W:157:PHE:HZ	1.98	0.62
3:T:80:ASN:ND2	7:N:11:ALA:O	2.19	0.62
7:N:35:LEU:O	7:N:37:SER:N	2.33	0.62
6:Z:282:ILE:HD11	6:Z:297:VAL:HG12	1.77	0.61
8:S:127:THR:CB	8:S:127:THR:H	2.12	0.61
11:R:241:ILE:HG23	11:R:241:ILE:O	1.99	0.61
5:Y:21:ASN:HD22	8:S:55:ARG:HH11	0.61	0.60
13:O:266:PHE:CZ	13:O:270:ILE:HG13	2.35	0.60
8:S:127:THR:N	8:S:127:THR:HB	2.17	0.60
10:Q:3:LEU:C	10:Q:3:LEU:HD23	2.26	0.60
6:Z:93:ARG:HB3	6:Z:94:PRO:HD3	1.83	0.60
5:Y:21:ASN:HD22	8:S:55:ARG:NH1	1.25	0.60
2:V:117:TRP:CH2	2:V:184:ASN:ND2	2.70	0.59
7:N:707:ASN:C	7:N:709:GLY:N	2.59	0.59
7:N:856:PHE:O	7:N:857:TYR:C	2.41	0.59
6:Z:509:LEU:HA	6:Z:512:ILE:HD11	1.83	0.59
10:Q:78:ILE:CG2	10:Q:117:VAL:HG21	2.32	0.59
2:V:157:ARG:O	2:V:196:TYR:HA	2.00	0.59
6:Z:329:ILE:HD13	6:Z:464:ASP:OD1	2.02	0.59
1:W:158:ILE:HG23	1:W:169:SER:CB	2.31	0.59
7:N:447:SER:O	7:N:450:ILE:HG22	2.02	0.58
7:N:707:ASN:C	7:N:709:GLY:H	2.10	0.58
6:Z:30:LYS:HA	6:Z:37:GLN:OE1	2.03	0.58
6:Z:31:LYS:HD2	6:Z:79:THR:HG23	1.86	0.57
13:O:393:VAL:OXT	13:O:393:VAL:CG1	2.53	0.56
2:V:118:LEU:CA	2:V:195:HIS:NE2	2.67	0.56
6:Z:24:THR:CB	6:Z:25:PRO:HD2	2.07	0.56
2:V:183:ALA:N	2:V:188:LEU:CD1	2.69	0.56
3:T:84:GLN:CD	7:N:8:PRO:CB	2.79	0.56
5:Y:21:ASN:HD21	8:S:55:ARG:NH1	0.65	0.56
7:N:35:LEU:C	7:N:37:SER:N	2.60	0.55
6:Z:294:ILE:HD13	6:Z:327:GLN:HG2	1.89	0.55
2:V:196:TYR:CD1	2:V:197:TYR:HB3	2.39	0.55
6:Z:282:ILE:HD13	6:Z:297:VAL:CG2	2.37	0.55
2:V:183:ALA:C	2:V:188:LEU:HD12	2.32	0.54
8:S:164:ILE:HB	8:S:165:PRO:CD	2.37	0.54
8:S:427:ILE:HG22	8:S:427:ILE:O	2.07	0.54
6:Z:85:VAL:O	6:Z:88:PRO:CD	2.43	0.54
6:Z:282:ILE:HD13	6:Z:297:VAL:CG1	2.37	0.54
7:N:708:ALA:CB	7:N:713:VAL:CG2	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:303:VAL:O	2:V:306:LYS:O	2.24	0.54
8:S:481:TYR:HB2	8:S:482:PRO:HD3	1.89	0.54
10:Q:119:GLU:O	10:Q:122:ILE:HG22	2.07	0.54
12:U:14:VAL:HG21	12:U:48:VAL:HG12	1.90	0.54
6:Z:282:ILE:HD13	6:Z:297:VAL:HG21	1.89	0.54
10:Q:71:LYS:HG3	10:Q:73:LYS:H	1.74	0.53
2:V:157:ARG:N	2:V:196:TYR:HB2	2.20	0.53
2:V:159:ILE:CD1	2:V:196:TYR:O	2.55	0.53
1:W:30:ILE:HG23	1:W:76:LEU:HD21	1.89	0.53
6:Z:157:LEU:HB3	6:Z:207:ILE:HD12	1.91	0.53
1:W:126:ILE:CA	1:W:157:PHE:CZ	2.76	0.53
2:V:118:LEU:HB3	2:V:195:HIS:NE2	2.08	0.52
3:T:152:LEU:HD21	3:T:185:ILE:HD12	1.92	0.52
2:V:193:ASN:C	2:V:193:ASN:HD22	2.17	0.52
4:X:36:LYS:C	4:X:38:ASN:H	2.17	0.52
7:N:860:LYS:O	7:N:861:TYR:C	2.54	0.52
9:P:203:ILE:HG12	9:P:208:PHE:CZ	2.45	0.51
11:R:280:ILE:HG13	11:R:281:SER:H	1.76	0.51
2:V:117:TRP:CH2	2:V:184:ASN:CG	2.88	0.51
7:N:6:ALA:CB	7:N:35:LEU:HD13	2.39	0.51
8:S:123:THR:HG22	8:S:130:VAL:HG22	1.93	0.51
10:Q:275:ILE:C	10:Q:275:ILE:HD12	2.36	0.51
6:Z:282:ILE:HD13	6:Z:297:VAL:HG11	1.91	0.51
11:R:137:LEU:HB3	11:R:153:THR:HG21	1.91	0.51
2:V:250:GLN:HB3	2:V:276:PRO:HB3	1.92	0.51
6:Z:30:LYS:HG2	6:Z:37:GLN:HB2	1.87	0.51
9:P:48:GLN:HE22	9:P:89:LEU:HB3	1.76	0.50
6:Z:945:ILE:CG1	6:Z:965:LEU:HD21	2.41	0.50
6:Z:9:GLN:HA	6:Z:12:ILE:HD12	1.94	0.50
8:S:127:THR:HB	8:S:127:THR:H	1.74	0.50
2:V:143:PRO:HG2	2:V:144:ILE:HG23	1.93	0.50
6:Z:79:THR:O	6:Z:83:THR:HG23	2.12	0.50
7:N:7:ALA:HB3	7:N:8:PRO:HD2	1.94	0.50
8:S:345:TYR:H	8:S:345:TYR:HD1	1.51	0.50
10:Q:78:ILE:HG21	10:Q:117:VAL:HG21	1.93	0.50
6:Z:161:ILE:HD11	6:Z:207:ILE:HG13	1.95	0.49
5:Y:33:ASP:O	5:Y:35:PHE:N	2.46	0.49
1:W:158:ILE:CG2	1:W:169:SER:HB2	2.40	0.49
6:Z:542:ILE:HG12	6:Z:544:THR:H	1.76	0.49
8:S:164:ILE:HB	8:S:165:PRO:HD3	1.94	0.49
2:V:118:LEU:O	2:V:195:HIS:NE2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:65:ASP:CB	11:R:331:ARG:HD2	2.35	0.49
7:N:856:PHE:C	7:N:857:TYR:O	2.50	0.49
9:P:94:GLN:OE1	9:P:94:GLN:N	2.42	0.49
6:Z:556:ILE:HD12	6:Z:556:ILE:C	2.38	0.48
9:P:399:ILE:HG21	9:P:401:ASN:HD21	1.77	0.48
2:V:24:LYS:HG3	2:V:196:TYR:CZ	2.47	0.48
8:S:81:LEU:HD22	8:S:123:THR:HB	1.95	0.48
6:Z:88:PRO:HA	6:Z:91:PHE:HB2	1.95	0.48
13:O:169:ASN:HD22	13:O:198:THR:HG23	1.78	0.48
2:V:24:LYS:HG3	2:V:196:TYR:CG	2.48	0.48
2:V:183:ALA:N	2:V:188:LEU:HD12	2.29	0.48
2:V:159:ILE:HG12	2:V:196:TYR:CE2	2.48	0.48
13:O:41:LEU:O	13:O:45:LEU:CD2	2.62	0.48
10:Q:95:LYS:HD3	10:Q:95:LYS:C	2.39	0.48
2:V:172:GLN:HB3	2:V:196:TYR:OH	2.13	0.48
6:Z:354:PRO:HA	6:Z:357:ILE:HG12	1.96	0.48
6:Z:424:SER:HA	6:Z:457:ILE:HG21	1.94	0.48
2:V:184:ASN:HB2	2:V:188:LEU:HB2	1.95	0.47
7:N:7:ALA:N	7:N:8:PRO:HD2	2.28	0.47
6:Z:20:PRO:HB2	6:Z:24:THR:OG1	2.15	0.47
7:N:707:ASN:O	7:N:708:ALA:C	2.58	0.47
13:O:291:ILE:HD13	13:O:291:ILE:HA	1.66	0.47
2:V:157:ARG:O	2:V:196:TYR:CD2	2.68	0.47
2:V:193:ASN:C	2:V:193:ASN:ND2	2.73	0.47
2:V:217:HIS:CE1	2:V:219:GLU:C	2.93	0.47
7:N:860:LYS:O	7:N:861:TYR:O	2.32	0.47
9:P:349:ASN:O	9:P:353:ILE:HG13	2.15	0.47
8:S:399:TYR:CD2	8:S:402:ILE:HD13	2.50	0.47
10:Q:78:ILE:HG22	10:Q:117:VAL:CG2	2.44	0.47
3:T:181:LEU:O	3:T:185:ILE:HG12	2.14	0.47
4:X:77:PRO:C	4:X:78:ILE:HG13	2.40	0.47
6:Z:542:ILE:HG23	6:Z:545:SER:H	1.80	0.47
7:N:778:LYS:HB2	7:N:860:LYS:O	2.15	0.47
2:V:196:TYR:HB3	2:V:197:TYR:O	2.15	0.46
6:Z:471:LEU:HD13	6:Z:471:LEU:C	2.41	0.46
10:Q:359:ILE:HD11	10:Q:390:LEU:HD21	1.97	0.46
1:W:10:ILE:HG22	1:W:33:VAL:HG22	1.98	0.46
6:Z:81:SER:O	6:Z:82:MET:HB3	2.16	0.46
6:Z:30:LYS:CG	6:Z:37:GLN:HB2	2.28	0.45
6:Z:282:ILE:CG1	6:Z:297:VAL:HG11	2.45	0.45
1:W:154:LEU:H	1:W:154:LEU:HG	1.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:266:TYR:CD1	9:P:329:PHE:HE2	2.35	0.45
5:Y:21:ASN:OD1	8:S:55:ARG:NH2	2.50	0.45
5:Y:21:ASN:OD1	8:S:55:ARG:NH1	2.35	0.45
11:R:280:ILE:CG1	11:R:281:SER:H	2.30	0.45
6:Z:945:ILE:HG12	6:Z:965:LEU:HD21	1.99	0.45
2:V:182:LYS:C	2:V:188:LEU:HD13	2.42	0.45
13:O:37:LEU:O	13:O:41:LEU:HB2	2.17	0.45
9:P:89:LEU:HG	9:P:90:LYS:H	1.82	0.44
10:Q:130:ARG:HG3	10:Q:133:LEU:H	1.82	0.44
12:U:161:ILE:C	12:U:161:ILE:HD12	2.41	0.44
9:P:193:TYR:CD1	9:P:230:HIS:CD2	3.06	0.44
6:Z:535:VAL:HG12	6:Z:536:GLY:N	2.32	0.44
6:Z:614:VAL:O	6:Z:617:ILE:HG12	2.17	0.44
6:Z:802:ASP:CG	6:Z:803:ALA:H	2.25	0.44
1:W:143:ASN:OD1	1:W:147:ILE:HG23	2.17	0.44
6:Z:298:PHE:CE1	6:Z:315:ALA:HB1	2.53	0.44
3:T:79:GLU:O	3:T:82:PHE:HB3	2.18	0.43
3:T:84:GLN:CD	7:N:8:PRO:HB3	2.43	0.43
8:S:427:ILE:O	8:S:427:ILE:CG2	2.65	0.43
10:Q:3:LEU:HB3	10:Q:4:PRO:HD3	2.00	0.43
10:Q:11:ALA:HB1	10:Q:27:TYR:CZ	2.54	0.43
2:V:159:ILE:HD11	2:V:196:TYR:CG	2.51	0.43
9:P:177:ILE:HG12	9:P:203:ILE:CD1	2.48	0.43
6:Z:581:VAL:HG12	6:Z:581:VAL:O	2.17	0.43
13:O:189:TYR:CD2	13:O:189:TYR:C	2.97	0.43
7:N:861:TYR:CG	7:N:862:SER:N	2.86	0.43
6:Z:701:ILE:HG13	6:Z:702:LYS:N	2.33	0.43
8:S:126:LYS:HD2	8:S:129:GLU:OE2	2.19	0.43
8:S:337:ASN:C	8:S:339:GLN:H	2.25	0.43
12:U:37:ILE:CG2	12:U:48:VAL:HG13	2.49	0.43
6:Z:419:VAL:HA	6:Z:422:ILE:HD12	2.01	0.43
7:N:6:ALA:C	7:N:8:PRO:HG2	2.44	0.43
7:N:450:ILE:CG2	7:N:451:GLY:N	2.82	0.43
1:W:15:TYR:CE1	13:O:39:PHE:CE2	3.07	0.42
2:V:247:ILE:HG22	2:V:280:LEU:HG	2.01	0.42
6:Z:30:LYS:HB2	6:Z:30:LYS:HE2	1.48	0.42
7:N:5:THR:O	7:N:8:PRO:HG3	2.19	0.42
10:Q:264:TYR:N	10:Q:264:TYR:CD1	2.87	0.42
9:P:7:ILE:HG22	9:P:8:LYS:N	2.34	0.42
2:V:118:LEU:C	2:V:195:HIS:NE2	2.78	0.42
7:N:918:GLU:CD	7:N:918:GLU:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:93:ILE:O	9:P:96:MET:HB2	2.20	0.42
3:T:70:ILE:HD11	3:T:78:PHE:CE1	2.53	0.42
4:X:78:ILE:HG12	4:X:114:LEU:O	2.19	0.42
10:Q:154:SER:O	10:Q:158:ILE:HG13	2.19	0.42
12:U:8:VAL:HG22	12:U:46:ILE:HD12	2.01	0.42
2:V:72:PRO:HA	12:U:83:ILE:HG12	2.01	0.42
6:Z:451:ALA:O	6:Z:455:ILE:HG13	2.19	0.42
13:O:41:LEU:HD12	13:O:41:LEU:HA	1.87	0.42
7:N:450:ILE:HG23	7:N:451:GLY:N	2.34	0.42
6:Z:30:LYS:CG	6:Z:37:GLN:CD	2.69	0.42
13:O:62:TYR:CE1	13:O:82:LEU:HD13	2.55	0.42
7:N:124:TYR:CD1	7:N:124:TYR:N	2.88	0.42
7:N:161:TYR:HA	7:N:202:PHE:CZ	2.54	0.42
10:Q:66:VAL:HG12	10:Q:66:VAL:O	2.20	0.41
7:N:859:ASN:C	7:N:861:TYR:N	2.77	0.41
8:S:78:VAL:HA	8:S:105:PRO:HA	2.02	0.41
9:P:433:ILE:HD13	12:U:210:TYR:HB2	2.01	0.41
10:Q:3:LEU:HD22	10:Q:33:LYS:HG2	2.02	0.41
7:N:523:LEU:HA	7:N:557:LEU:HD13	2.02	0.41
10:Q:129:LYS:HB3	10:Q:130:ARG:H	1.74	0.41
4:X:64:ILE:HG12	4:X:65:SER:N	2.36	0.41
3:T:205:ILE:HG22	3:T:217:THR:HG21	2.03	0.41
11:R:198:ILE:CG2	11:R:207:ARG:HG3	2.51	0.41
3:T:31:LYS:HZ1	3:T:81:TYR:HE1	1.66	0.41
6:Z:282:ILE:HG12	6:Z:297:VAL:HG11	2.02	0.41
9:P:177:ILE:HG12	9:P:203:ILE:HD13	2.02	0.41
11:R:198:ILE:HG23	11:R:207:ARG:HG3	2.03	0.41
1:W:26:PHE:O	1:W:30:ILE:HG13	2.21	0.41
12:U:37:ILE:HG23	12:U:48:VAL:CG1	2.51	0.41
3:T:70:ILE:HD11	3:T:78:PHE:CZ	2.56	0.40
6:Z:31:LYS:HB2	6:Z:31:LYS:HE2	1.95	0.40
6:Z:88:PRO:O	6:Z:92:LEU:HG	2.21	0.40
6:Z:945:ILE:HG13	6:Z:965:LEU:HD21	2.04	0.40
8:S:81:LEU:HD12	8:S:81:LEU:HA	1.93	0.40
10:Q:129:LYS:HD2	10:Q:129:LYS:N	2.36	0.40
6:Z:354:PRO:O	6:Z:357:ILE:HG12	2.21	0.40
11:R:387:ILE:HG22	11:R:388:VAL:N	2.36	0.40
7:N:7:ALA:N	7:N:8:PRO:CD	2.84	0.40
8:S:119:TYR:O	8:S:123:THR:HG23	2.21	0.40
9:P:48:GLN:NE2	9:P:89:LEU:HD23	2.36	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	W	195/268 (73%)	175 (90%)	13 (7%)	7 (4%)	2	22
2	V	287/306 (94%)	262 (91%)	15 (5%)	10 (4%)	3	23
3	T	264/274 (96%)	240 (91%)	20 (8%)	4 (2%)	8	39
4	X	125/156 (80%)	105 (84%)	19 (15%)	1 (1%)	16	52
5	Y	47/89 (53%)	39 (83%)	6 (13%)	2 (4%)	2	20
6	Z	902/993 (91%)	813 (90%)	66 (7%)	23 (2%)	4	29
7	N	886/945 (94%)	842 (95%)	31 (4%)	13 (2%)	8	39
8	S	473/523 (90%)	441 (93%)	17 (4%)	15 (3%)	3	24
9	P	438/445 (98%)	405 (92%)	22 (5%)	11 (2%)	4	29
10	Q	432/434 (100%)	392 (91%)	32 (7%)	8 (2%)	6	34
11	R	377/429 (88%)	353 (94%)	16 (4%)	8 (2%)	5	32
12	U	296/338 (88%)	282 (95%)	12 (4%)	2 (1%)	18	55
13	O	386/393 (98%)	366 (95%)	17 (4%)	3 (1%)	16	52
All	All	5108/5593 (91%)	4715 (92%)	286 (6%)	107 (2%)	8	32

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	184	ASN
2	V	197	TYR
2	V	274	GLN
4	X	116	ALA
6	Z	24	THR
6	Z	82	MET
6	Z	85	VAL
7	N	36	TRP
7	N	708	ALA
7	N	857	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	S	47	THR
8	S	102	SER
8	S	150	LYS
8	S	449	LEU
9	P	126	THR
9	P	397	ALA
10	Q	75	ARG
10	Q	170	ASP
1	W	13	SER
1	W	144	PHE
1	W	149	GLN
1	W	165	GLN
3	T	94	HIS
3	T	173	GLU
6	Z	142	ASP
6	Z	233	LEU
6	Z	802	ASP
6	Z	870	ALA
7	N	123	PHE
7	N	345	ASP
7	N	378	ASN
7	N	436	ASP
7	N	861	TYR
7	N	895	LYS
8	S	44	THR
8	S	118	PHE
8	S	132	ALA
8	S	153	GLU
8	S	433	GLU
9	P	89	LEU
9	P	327	LEU
10	Q	253	ASN
11	R	238	PHE
11	R	393	PRO
1	W	3	LEU
2	V	185	ILE
2	V	262	THR
5	Y	70	ASP
6	Z	377	ALA
6	Z	513	ALA
6	Z	578	GLY
6	Z	887	GLY

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	Z	926	ASN
6	Z	940	GLY
6	Z	947	GLY
7	N	33	ASP
7	N	765	ASP
7	N	858	LYS
8	S	83	PRO
8	S	84	ASP
8	S	258	GLU
9	P	6	PRO
9	P	7	ILE
10	Q	18	LYS
10	Q	42	ALA
10	Q	51	ARG
10	Q	110	SER
11	R	124	ASP
13	O	226	LYS
1	W	179	ARG
2	V	143	PRO
2	V	196	TYR
2	V	257	GLU
5	Y	34	GLU
6	Z	25	PRO
6	Z	237	VAL
6	Z	366	LYS
6	Z	557	GLU
6	Z	825	ALA
7	N	859	ASN
8	S	65	ASN
8	S	97	THR
9	P	85	LYS
9	P	150	GLU
9	P	171	MET
11	R	280	ILE
11	R	375	LYS
11	R	395	ASN
12	U	41	ALA
13	O	346	GLU
1	W	190	ILE
2	V	78	VAL
3	T	132	HIS
3	T	257	THR

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Mol	Chain	Res	Type
6	Z	65	GLU
6	Z	463	HIS
9	P	92	SER
10	Q	387	TYR
11	R	376	GLN
12	U	150	THR
6	Z	728	LYS
11	R	106	ASN
2	V	112	PRO
6	Z	86	PRO
8	S	96	ILE
9	P	132	VAL
13	O	205	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	171/230 (74%)	165 (96%)	6 (4%)	32	54
2	V	253/268 (94%)	242 (96%)	11 (4%)	26	49
3	T	249/256 (97%)	237 (95%)	12 (5%)	23	46
4	X	116/144 (81%)	112 (97%)	4 (3%)	32	55
5	Y	50/81 (62%)	48 (96%)	2 (4%)	28	50
6	Z	773/850 (91%)	748 (97%)	25 (3%)	34	56
7	N	745/797 (94%)	726 (97%)	19 (3%)	40	61
8	S	447/489 (91%)	439 (98%)	8 (2%)	51	67
9	P	412/415 (99%)	404 (98%)	8 (2%)	50	67
10	Q	391/391 (100%)	380 (97%)	11 (3%)	38	59
11	R	333/379 (88%)	326 (98%)	7 (2%)	47	65
12	U	271/308 (88%)	267 (98%)	4 (2%)	57	70
13	O	363/368 (99%)	354 (98%)	9 (2%)	42	62
All	All	4574/4976 (92%)	4448 (97%)	126 (3%)	38	59

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	3	LEU
1	W	59	PRO
1	W	139	VAL
1	W	154	LEU
1	W	157	PHE
1	W	183	GLU
2	V	27	VAL
2	V	47	MET
2	V	71	MET
2	V	109	HIS
2	V	173	THR
2	V	185	ILE
2	V	190	HIS
2	V	192	LEU
2	V	199	LEU
2	V	219	GLU
2	V	227	MET
3	T	34	LEU
3	T	58	THR
3	T	64	VAL
3	T	76	ASP
3	T	82	PHE
3	T	85	LEU
3	T	105	LEU
3	T	130	ASP
3	T	201	PRO
3	T	214	GLU
3	T	242	LYS
3	T	257	THR
4	X	14	VAL
4	X	21	SER
4	X	28	PRO
4	X	62	ASP
5	Y	66	ASP
5	Y	72	ASP
6	Z	27	LYS
6	Z	29	ASP
6	Z	30	LYS
6	Z	81	SER
6	Z	83	THR
6	Z	171	LYS
6	Z	185	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	Z	222	ASP
6	Z	284	LEU
6	Z	354	PRO
6	Z	386	VAL
6	Z	402	ASP
6	Z	434	GLN
6	Z	445	PRO
6	Z	548	ASP
6	Z	563	VAL
6	Z	566	LEU
6	Z	609	THR
6	Z	703	SER
6	Z	797	THR
6	Z	842	GLN
6	Z	874	ASN
6	Z	878	LEU
6	Z	910	PRO
6	Z	955	VAL
7	N	105	SER
7	N	124	TYR
7	N	219	ASN
7	N	318	LYS
7	N	381	GLU
7	N	412	TYR
7	N	417	ARG
7	N	419	THR
7	N	455	MET
7	N	534	ASP
7	N	574	VAL
7	N	717	LEU
7	N	739	PHE
7	N	754	THR
7	N	771	PHE
7	N	792	SER
7	N	858	LYS
7	N	886	LYS
7	N	919	THR
8	S	60	LEU
8	S	133	GLU
8	S	242	LEU
8	S	247	VAL
8	S	264	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	S	326	ASP
8	S	456	ASP
8	S	475	TYR
9	P	121	THR
9	P	133	GLU
9	P	140	THR
9	P	309	MET
9	P	312	PRO
9	P	368	LEU
9	P	400	VAL
9	P	403	GLU
10	Q	4	PRO
10	Q	75	ARG
10	Q	104	PHE
10	Q	114	GLN
10	Q	138	SER
10	Q	149	LYS
10	Q	157	LEU
10	Q	166	LYS
10	Q	180	LEU
10	Q	250	THR
10	Q	318	LEU
11	R	51	LEU
11	R	110	ILE
11	R	204	TRP
11	R	293	THR
11	R	306	PRO
11	R	352	SER
11	R	376	GLN
12	U	13	LEU
12	U	26	GLN
12	U	180	ASP
12	U	261	LEU
13	O	41	LEU
13	O	45	LEU
13	O	66	VAL
13	O	70	TYR
13	O	91	ASP
13	O	100	ASP
13	O	161	ASP
13	O	294	MET
13	O	307	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

Mol	Chain	Res	Type
1	W	77	HIS
1	W	106	GLN
1	W	135	ASN
1	W	136	ASN
2	V	145	GLN
2	V	176	ASN
2	V	195	HIS
2	V	217	HIS
2	V	220	GLN
3	T	48	ASN
3	T	127	GLN
3	T	170	ASN
3	T	272	ASN
4	X	18	ASN
4	X	123	ASN
4	X	130	ASN
5	Y	89	GLN
6	Z	15	GLN
6	Z	23	GLN
6	Z	156	HIS
6	Z	215	ASN
6	Z	243	GLN
6	Z	275	GLN
6	Z	276	ASN
6	Z	307	HIS
6	Z	309	GLN
6	Z	317	GLN
6	Z	380	ASN
6	Z	396	ASN
6	Z	429	ASN
6	Z	480	ASN
6	Z	532	HIS
6	Z	539	ASN
6	Z	593	HIS
6	Z	622	HIS
6	Z	769	ASN
6	Z	789	GLN
6	Z	823	ASN
6	Z	824	ASN
6	Z	829	GLN
6	Z	842	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	Z	856	HIS
6	Z	874	ASN
6	Z	905	ASN
6	Z	926	ASN
7	N	71	ASN
7	N	116	GLN
7	N	122	GLN
7	N	231	ASN
7	N	240	GLN
7	N	256	GLN
7	N	280	GLN
7	N	300	ASN
7	N	306	ASN
7	N	315	ASN
7	N	346	ASN
7	N	375	HIS
7	N	430	ASN
7	N	444	HIS
7	N	580	ASN
7	N	613	HIS
7	N	707	ASN
7	N	747	HIS
8	S	19	HIS
8	S	91	ASN
8	S	100	HIS
8	S	112	ASN
8	S	139	HIS
8	S	172	ASN
8	S	225	HIS
8	S	280	ASN
8	S	283	GLN
8	S	290	ASN
8	S	312	GLN
8	S	314	ASN
8	S	317	HIS
8	S	334	HIS
8	S	412	ASN
8	S	417	GLN
8	S	437	ASN
8	S	469	ASN
8	S	470	GLN
9	P	70	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	P	98	GLN
9	P	230	HIS
9	P	289	ASN
9	P	323	ASN
9	P	348	HIS
9	P	385	ASN
9	P	386	GLN
9	P	401	ASN
9	P	425	HIS
10	Q	37	GLN
10	Q	54	GLN
10	Q	135	HIS
10	Q	190	ASN
10	Q	226	HIS
10	Q	247	HIS
10	Q	248	ASN
10	Q	273	ASN
10	Q	280	ASN
10	Q	283	ASN
10	Q	292	GLN
10	Q	315	ASN
10	Q	425	GLN
11	R	100	ASN
11	R	106	ASN
11	R	287	GLN
11	R	340	GLN
11	R	385	ASN
11	R	399	GLN
12	U	4	GLN
12	U	30	ASN
12	U	50	ASN
12	U	77	ASN
12	U	116	ASN
12	U	156	HIS
12	U	222	ASN
12	U	230	GLN
13	O	64	ASN
13	O	117	ASN
13	O	122	HIS
13	O	169	ASN
13	O	177	GLN
13	O	244	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	O	326	HIS
13	O	376	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

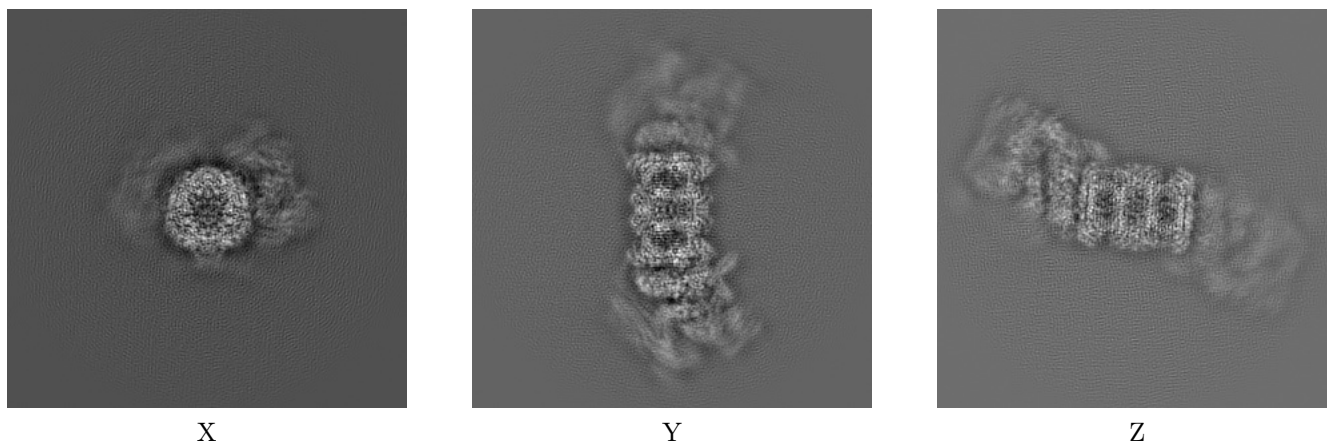
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3534. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

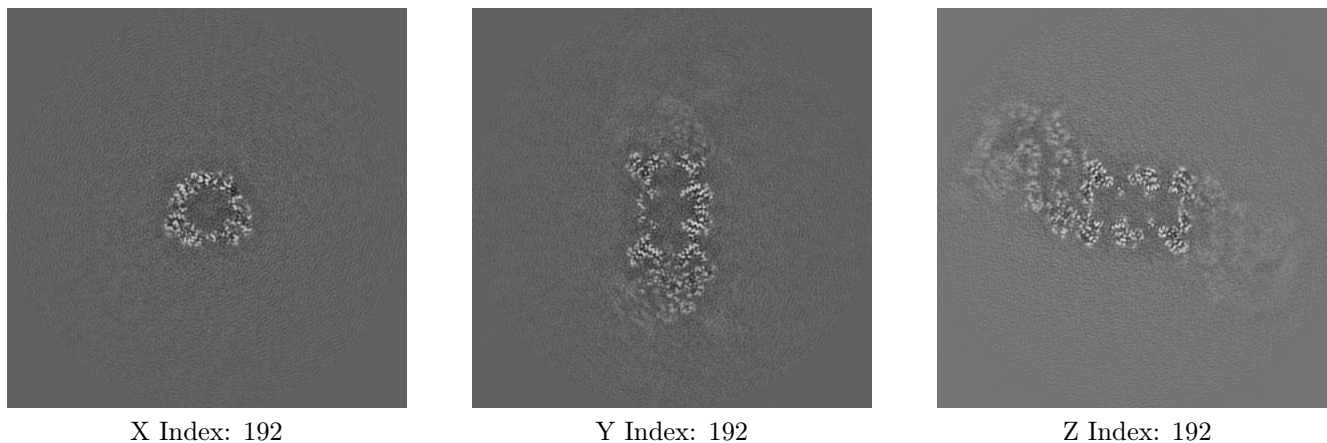
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

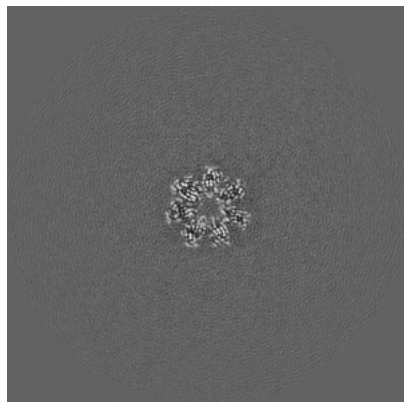
#### 6.2.1 Primary map



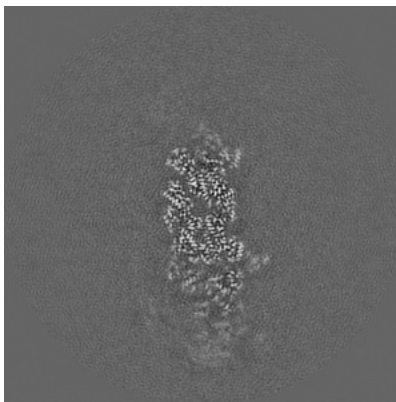
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

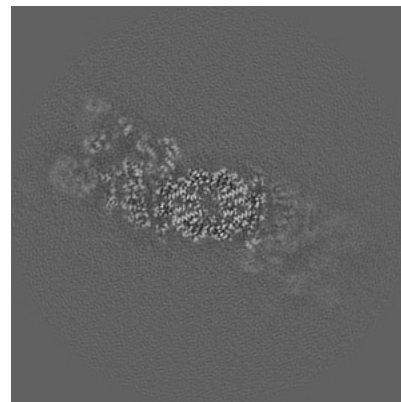
### 6.3.1 Primary map



X Index: 177



Y Index: 212

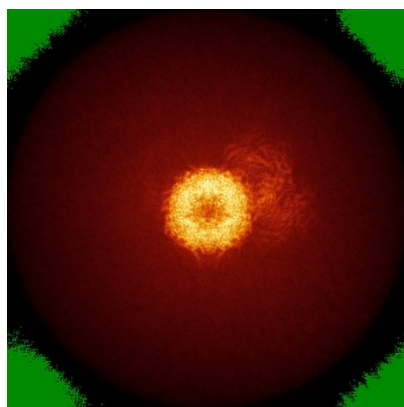


Z Index: 208

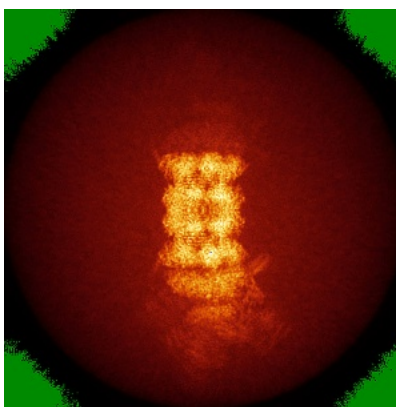
The images above show the largest variance slices of the map in three orthogonal directions.

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

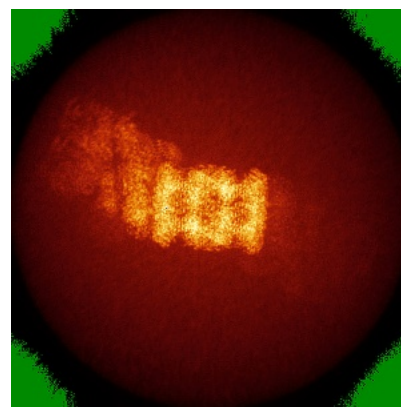
### 6.4.1 Primary map



X



Y

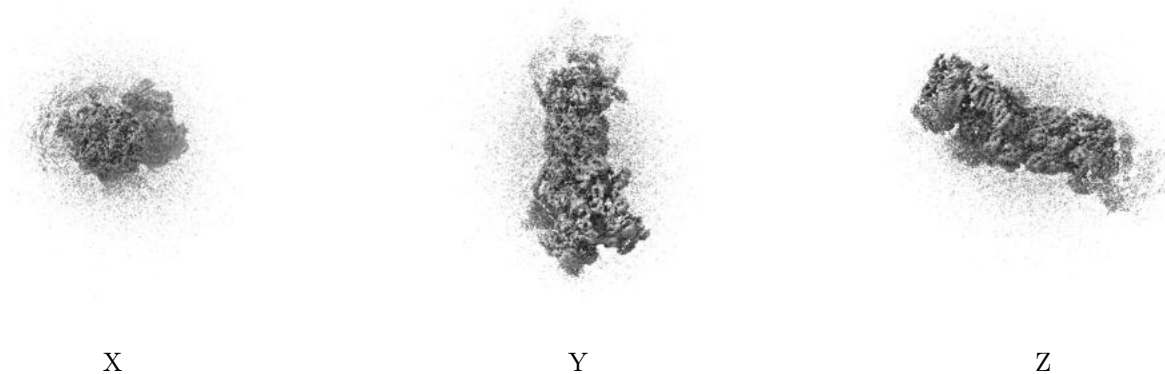


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

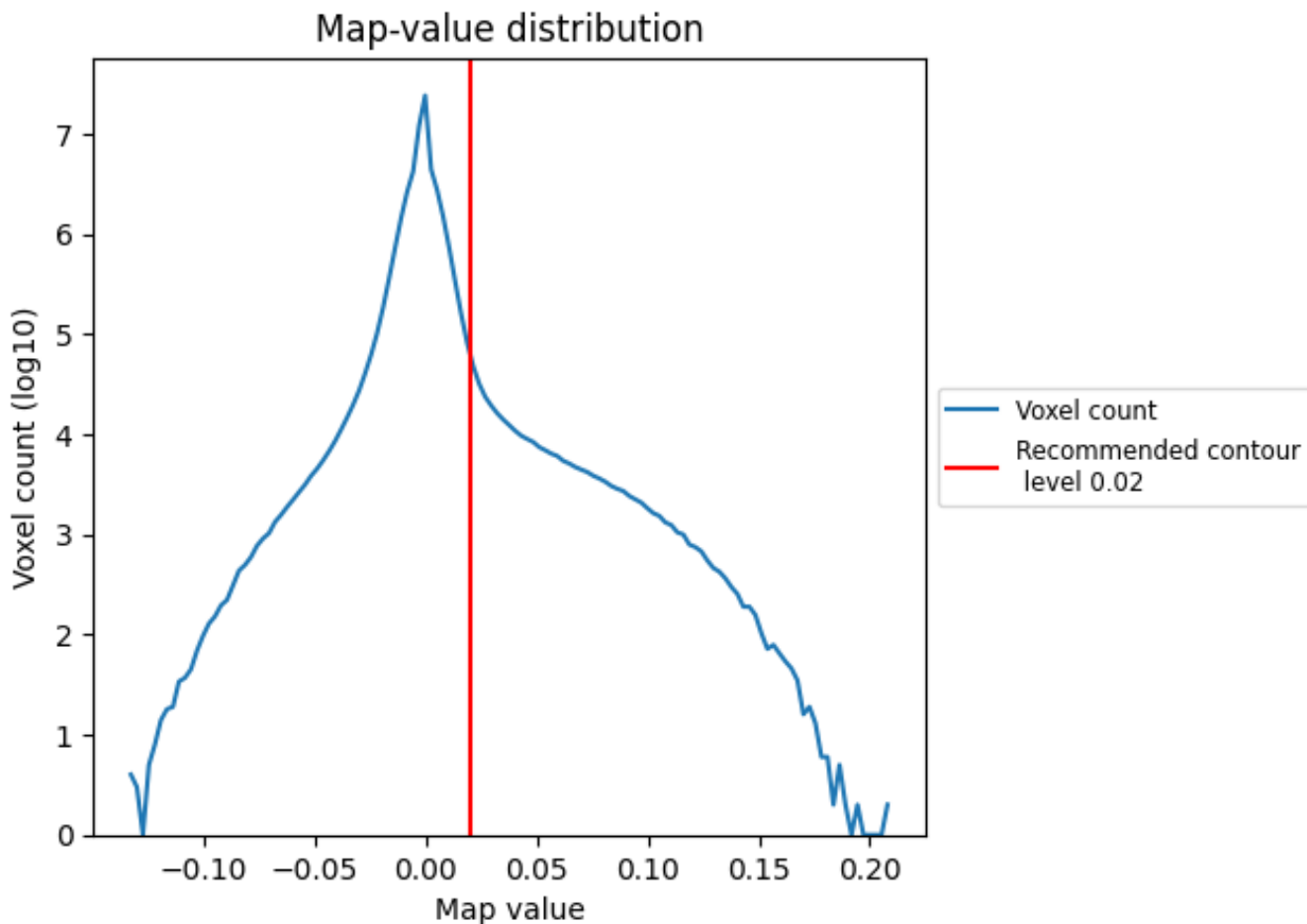
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

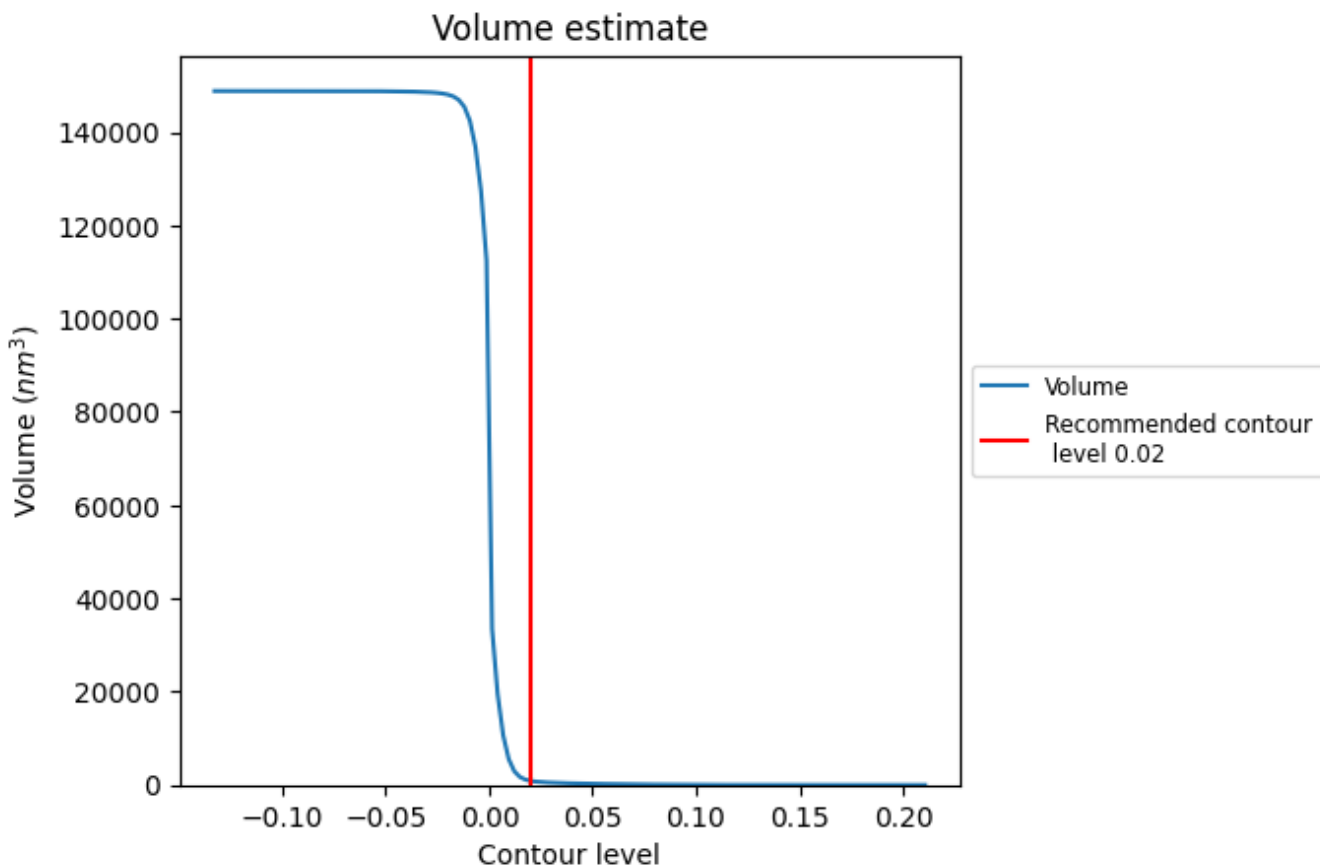
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

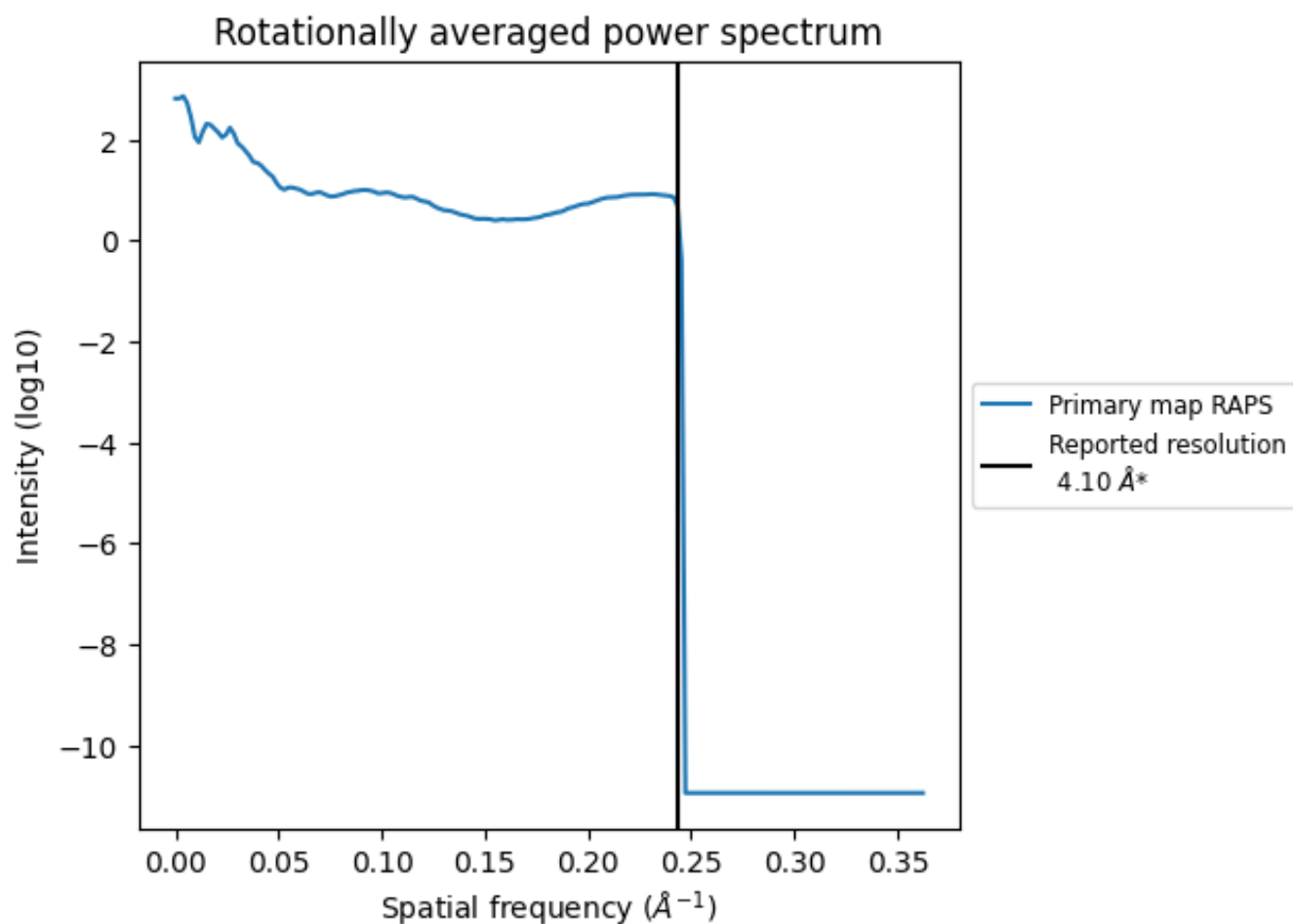
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 881  $\text{nm}^3$ ; this corresponds to an approximate mass of 796 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 [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>

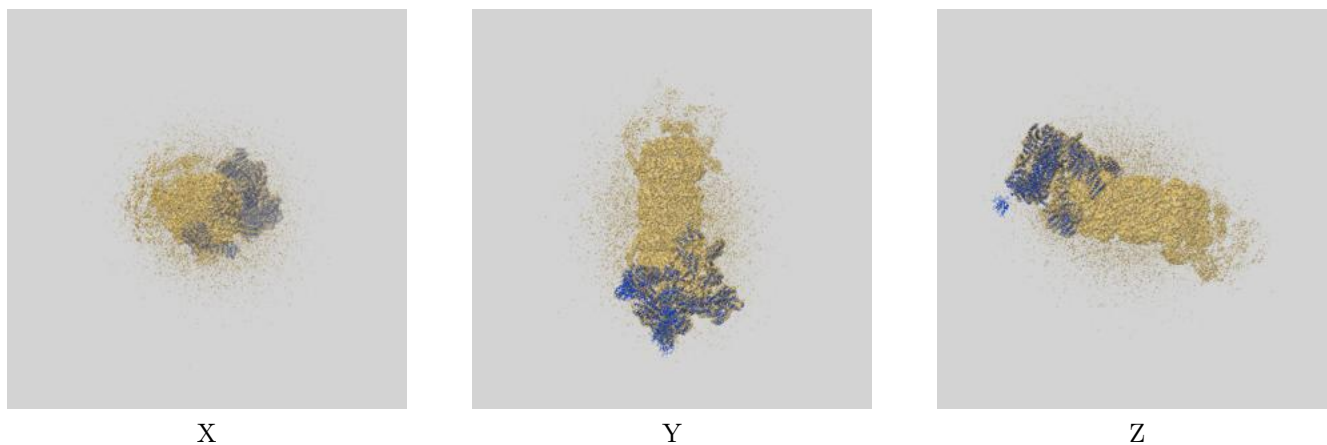
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

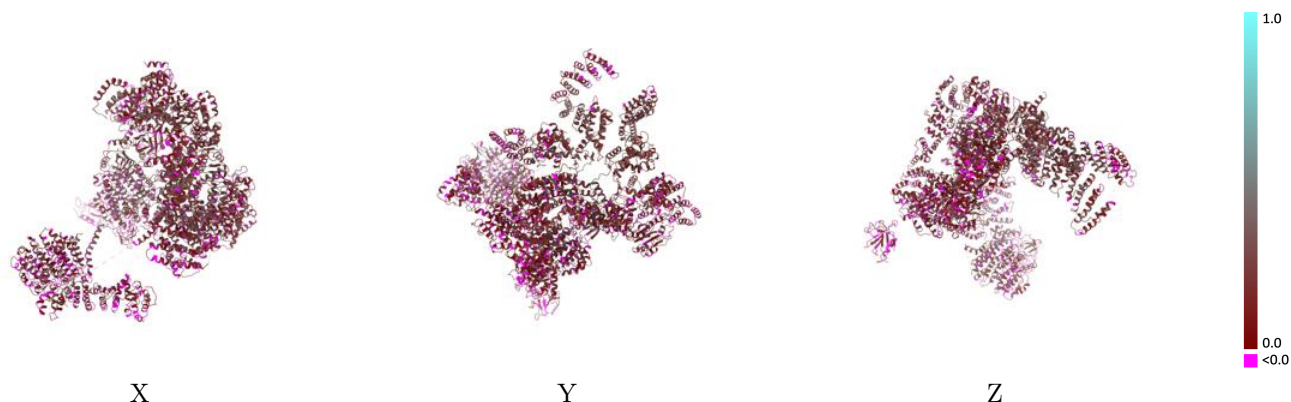
This section contains information regarding the fit between EMDB map EMD-3534 and PDB model 5MPD. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



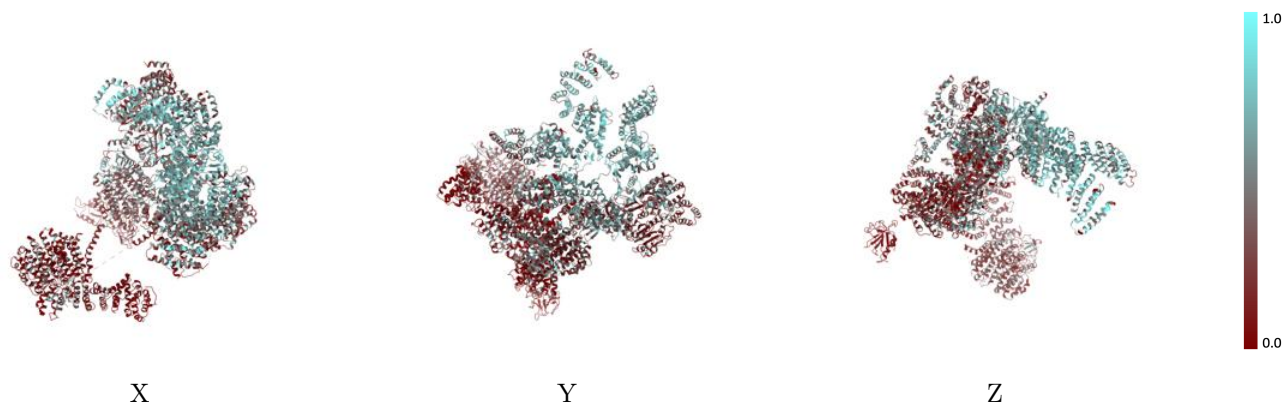
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



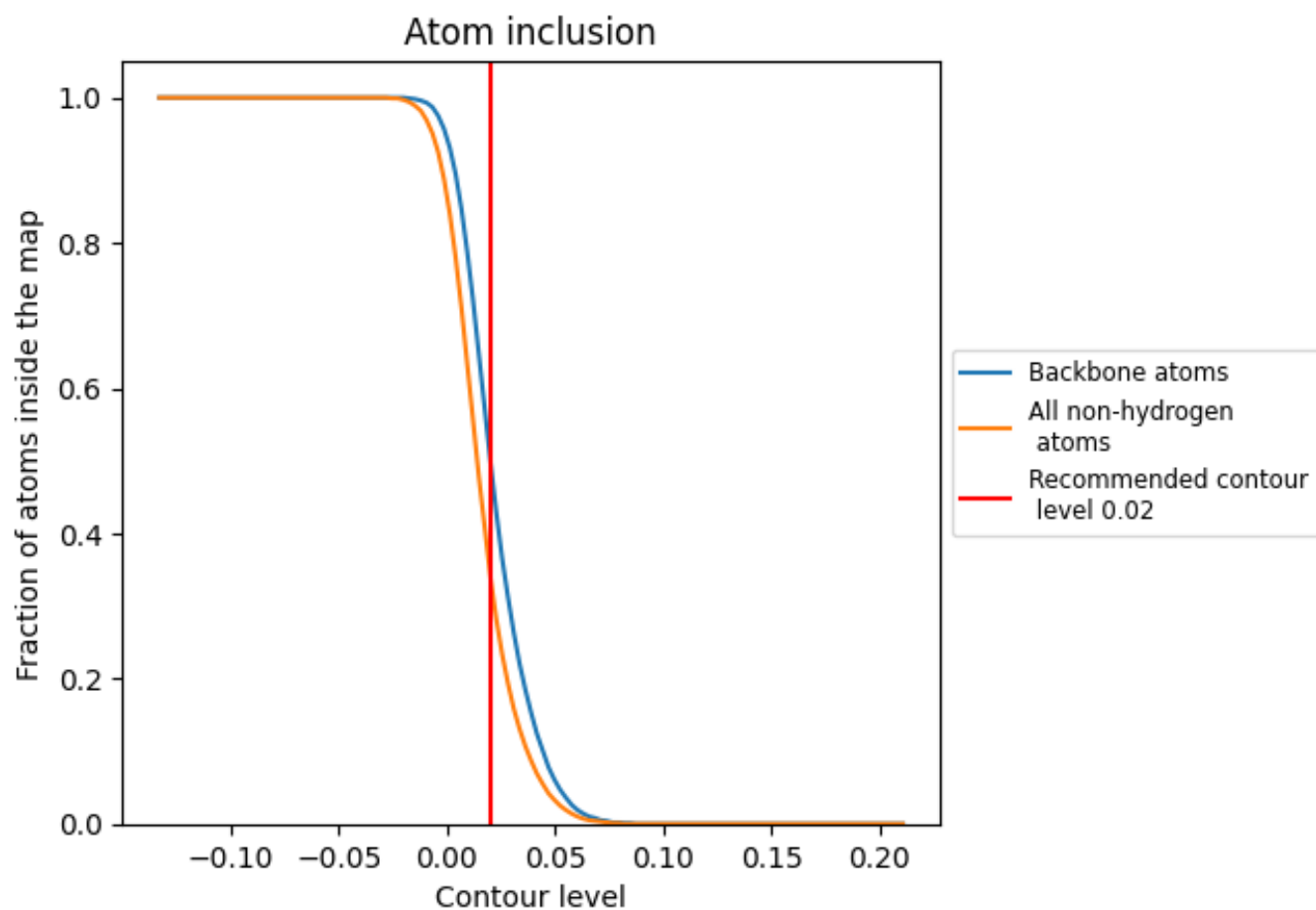
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).





























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 34% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3440	 0.1690
N	 0.2120	 0.1430
O	 0.3940	 0.1720
P	 0.6350	 0.2450
Q	 0.6210	 0.2300
R	 0.5310	 0.2040
S	 0.3550	 0.1570
T	 0.2900	 0.1490
U	 0.4070	 0.1900
V	 0.4420	 0.2060
W	 0.1740	 0.1320
X	 0.0050	 0.0660
Y	 0.3160	 0.1370
Z	 0.1290	 0.1250

