



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 05:31 AM UTC

PDB ID : 5MPE / pdb_00005mpe
EMDB ID : EMD-3535
Title : 26S proteasome in presence of ATP (s2)
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 : 4.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

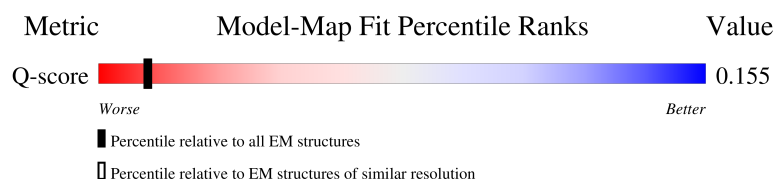
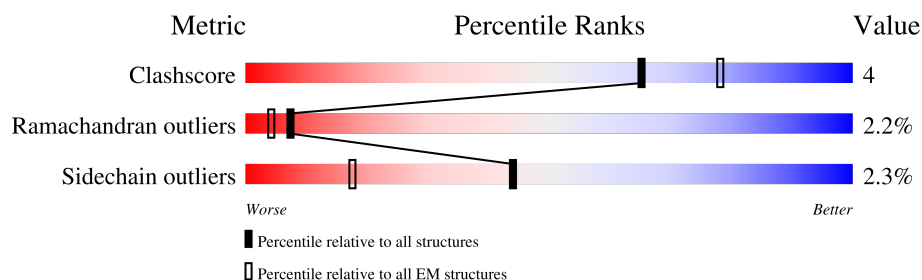
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.50 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	2937 (4.00 - 5.00)

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

Mol	Chain	Length	Quality of chain
1	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

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
1	W	197	Total	C	N	O	S	0	0
			1534	962	269	300	3		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

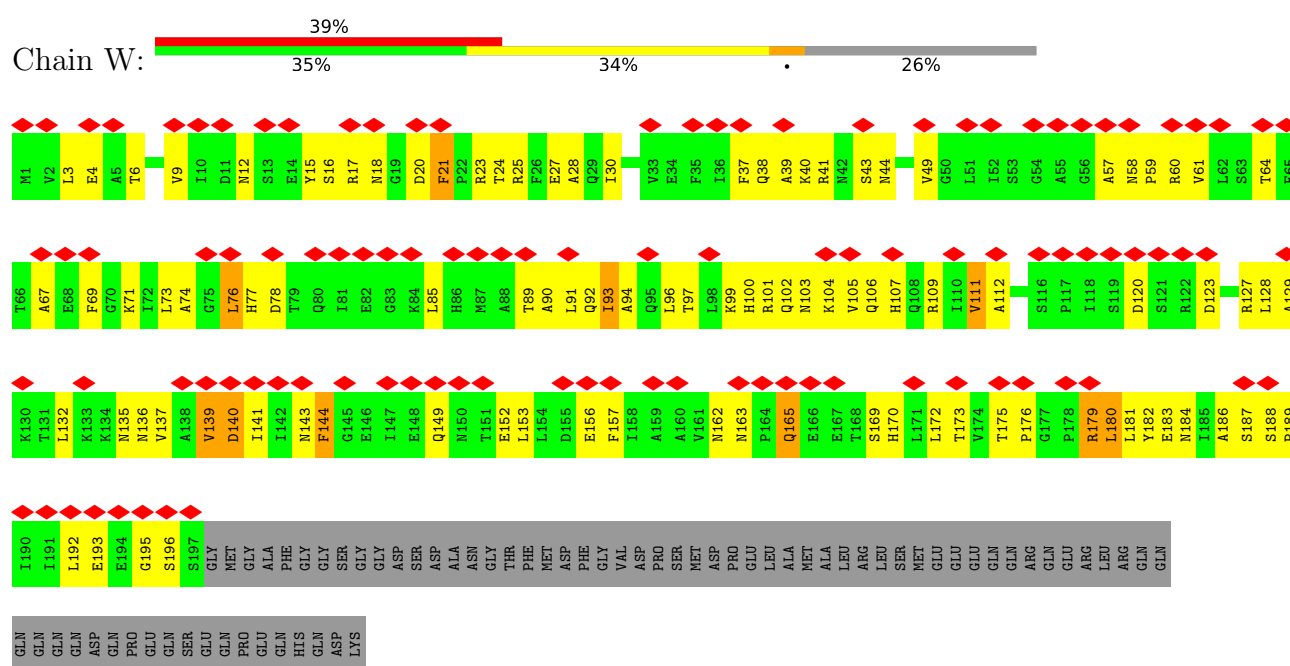
- Molecule 13 is a protein called 26S proteasome regulatory subunit RPN9.

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

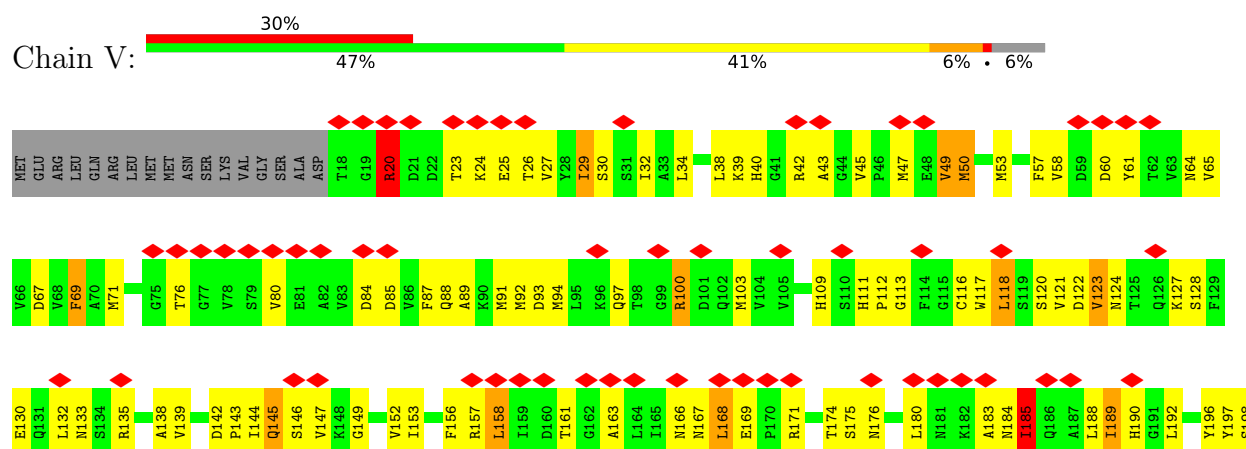
3 Residue-property plots [i](#)

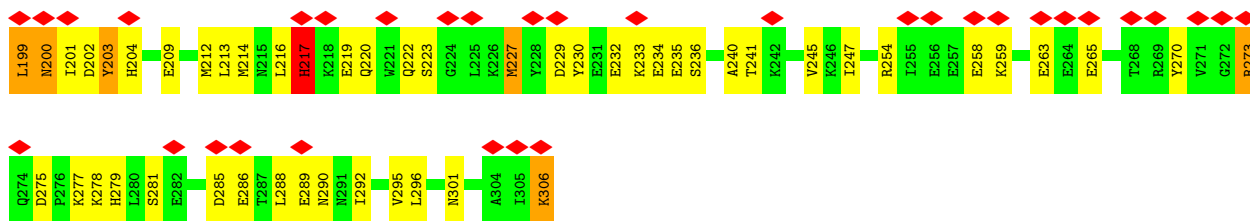
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

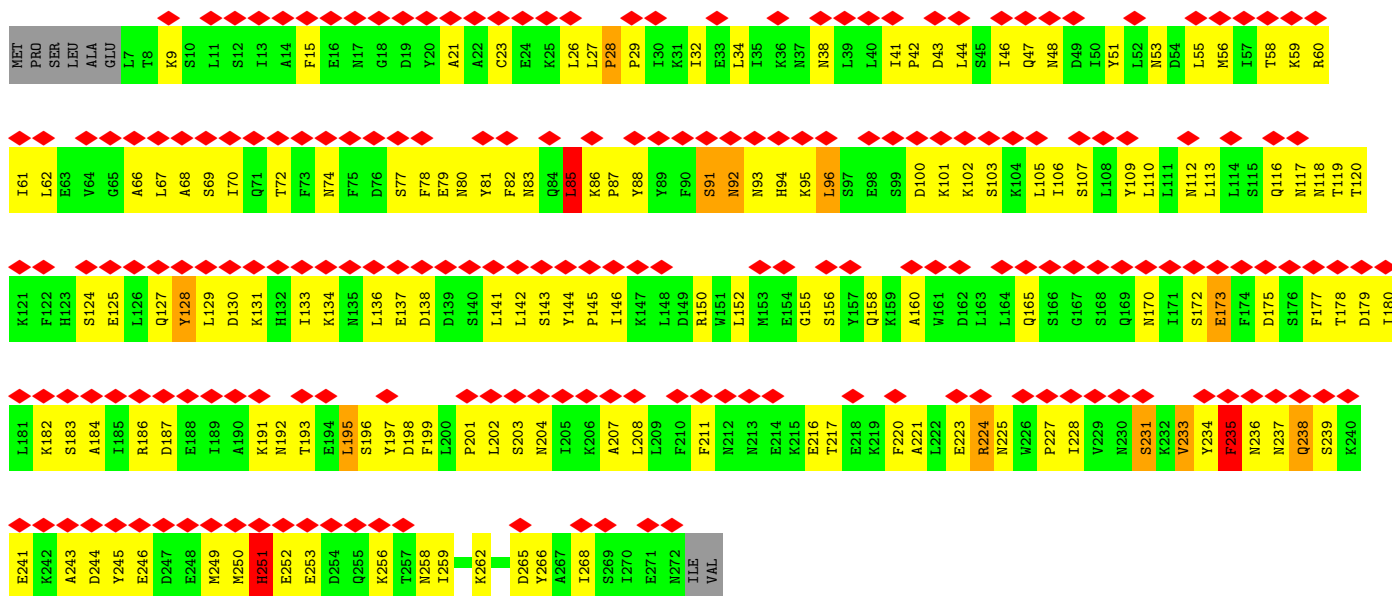
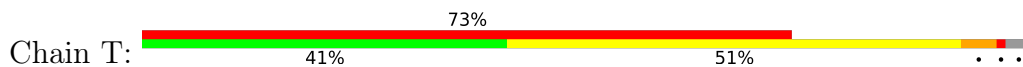


- Molecule 2: Ubiquitin carboxyl-terminal hydrolase RPN11

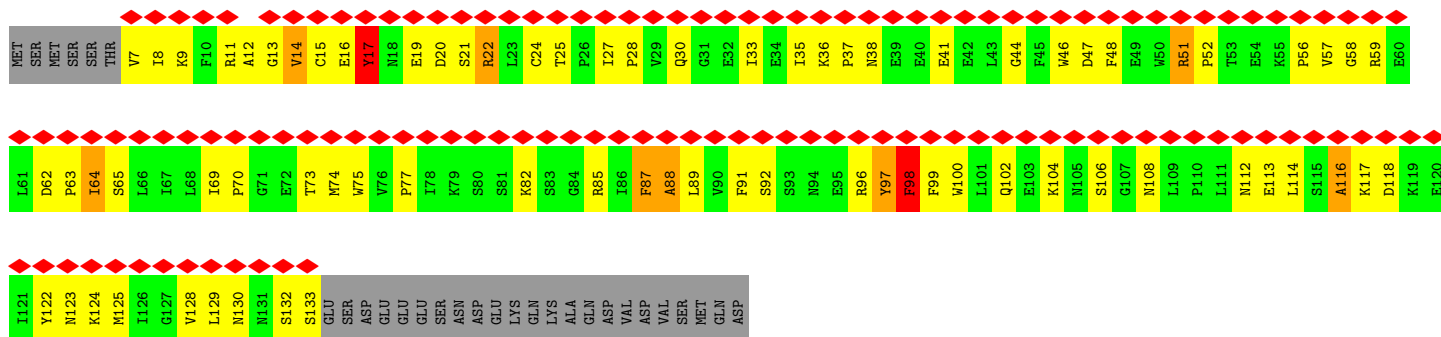
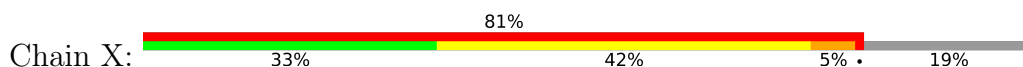




• Molecule 3: 26S proteasome regulatory subunit RPN12



• Molecule 4: 26S proteasome regulatory subunit RPN13

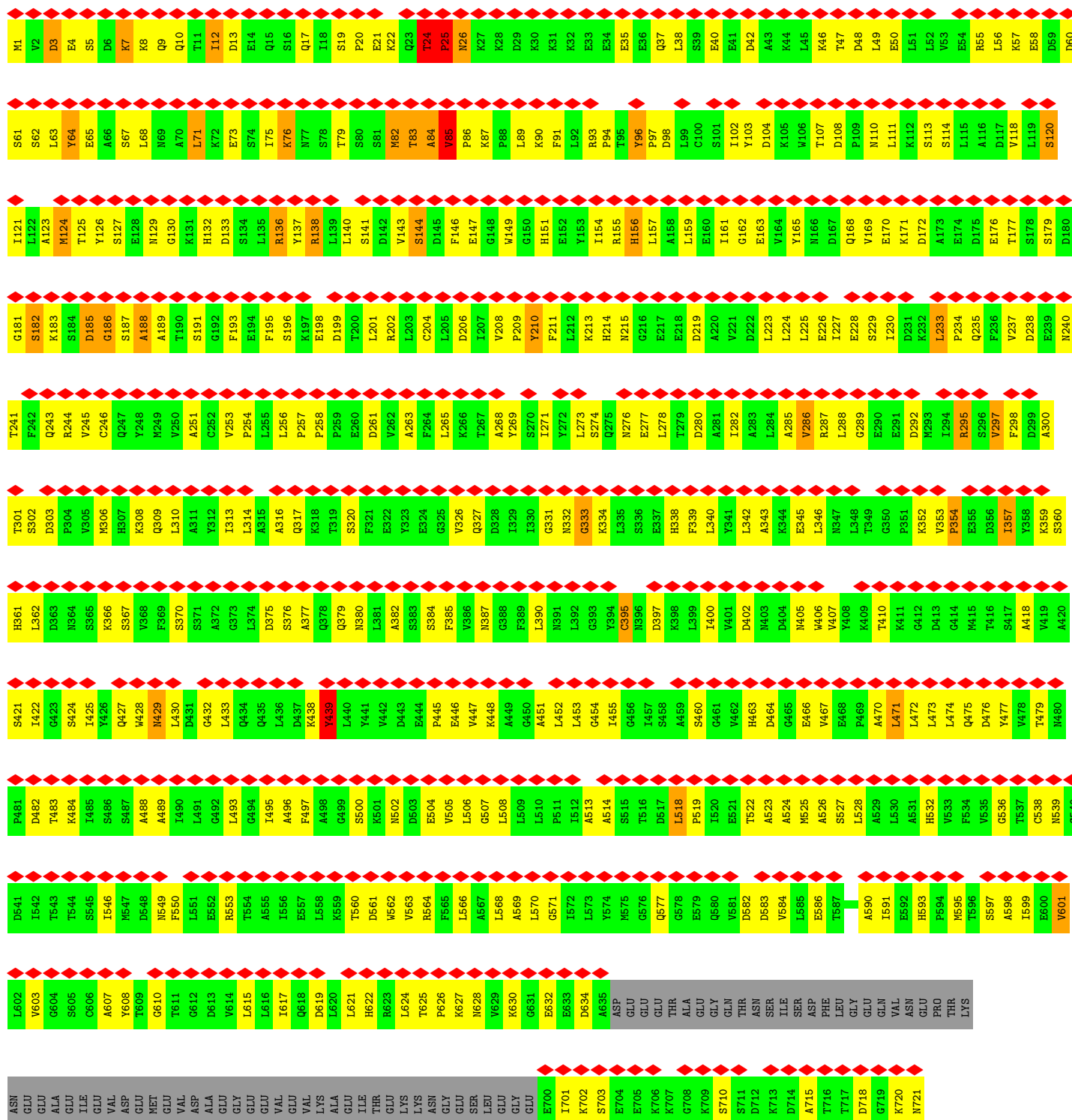
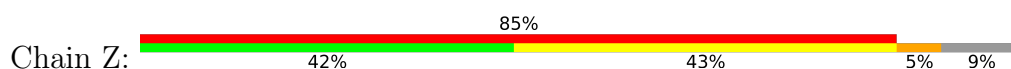


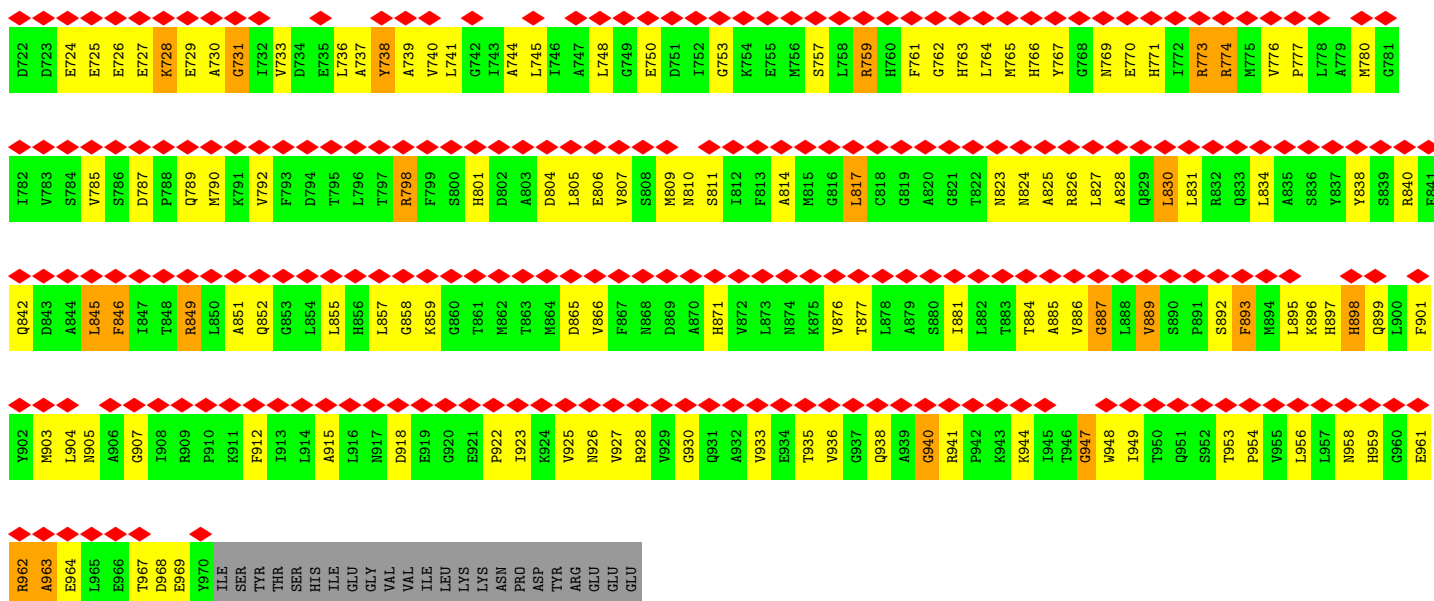
• Molecule 5: 26S proteasome complex subunit SEM1



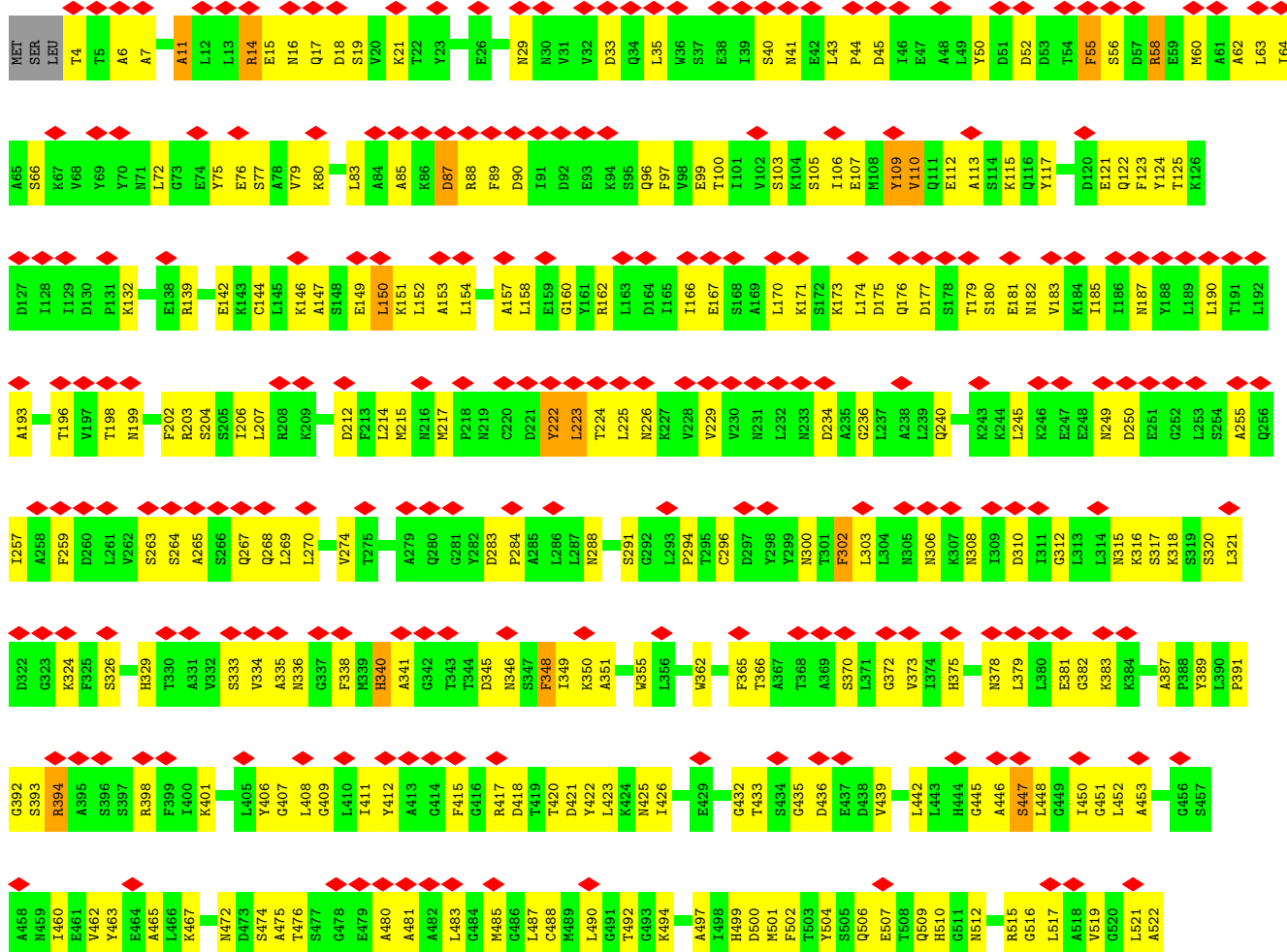
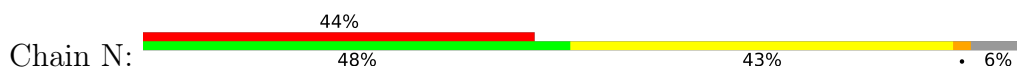


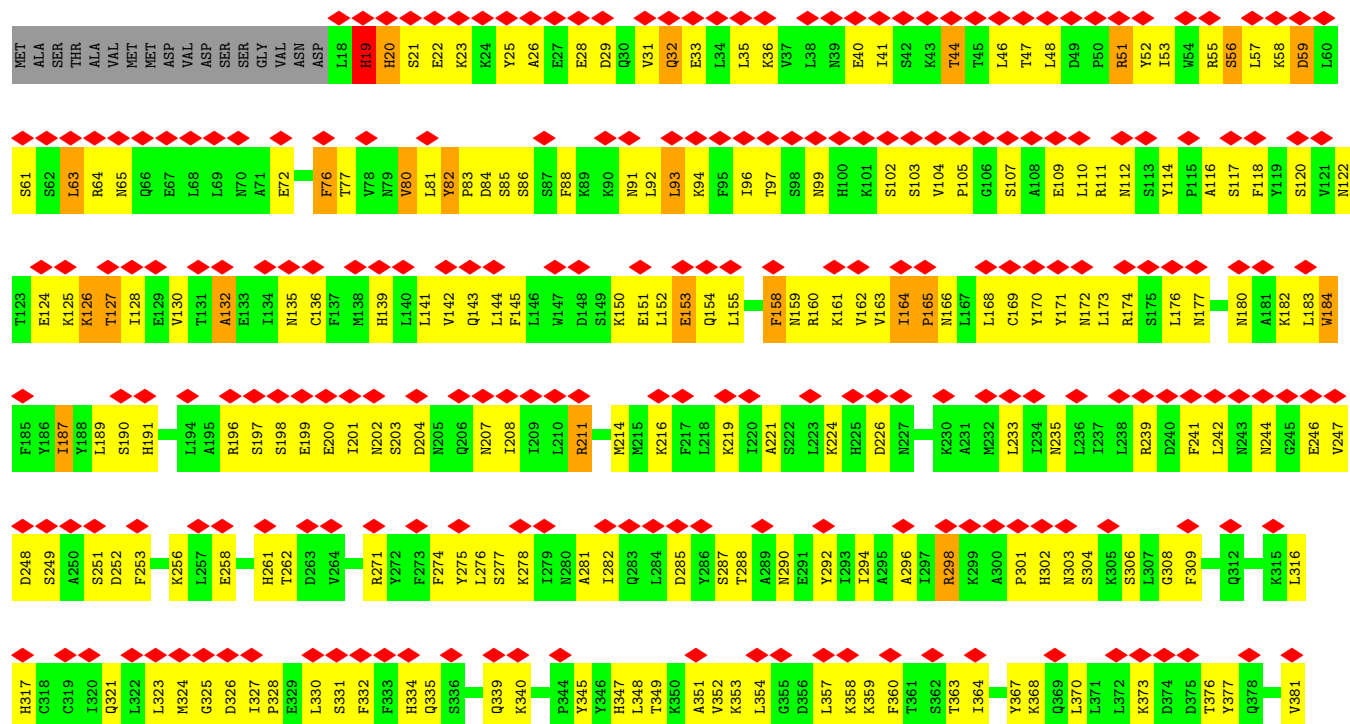
• Molecule 6: 26S proteasome regulatory subunit RPN1

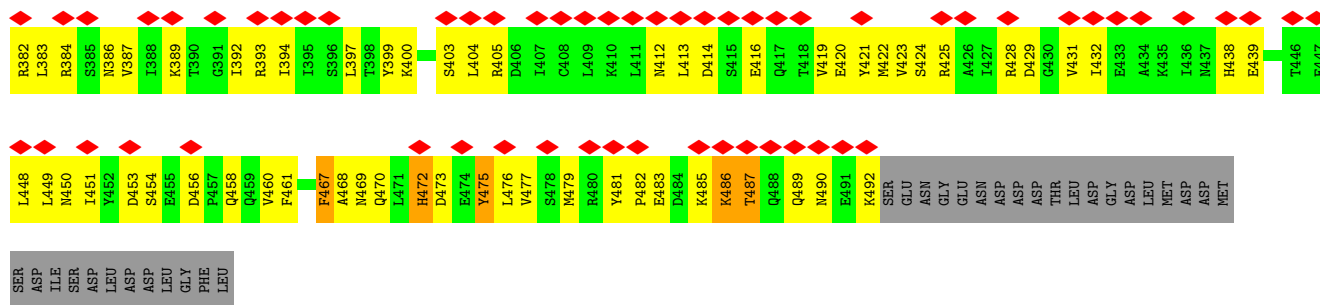




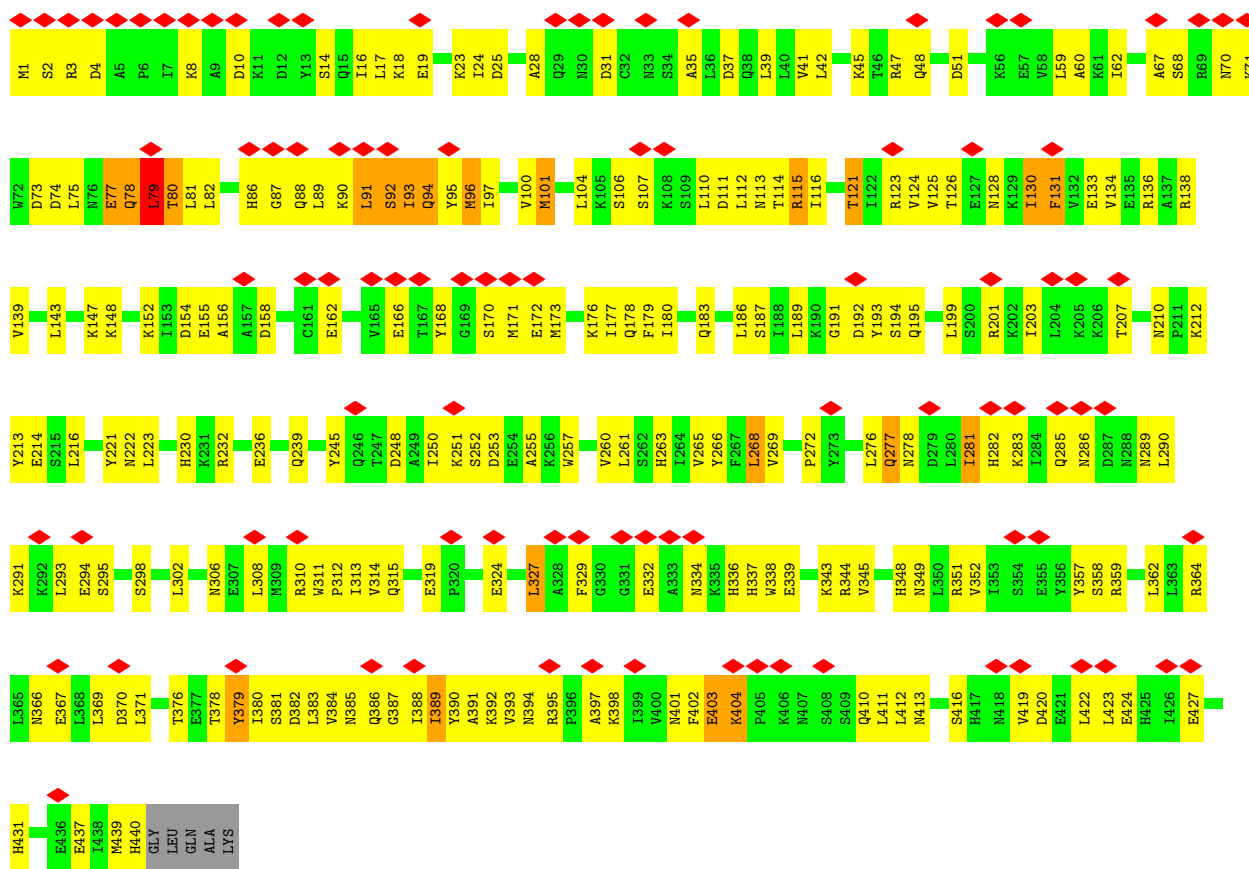
• Molecule 7: 26S proteasome regulatory subunit RPN2



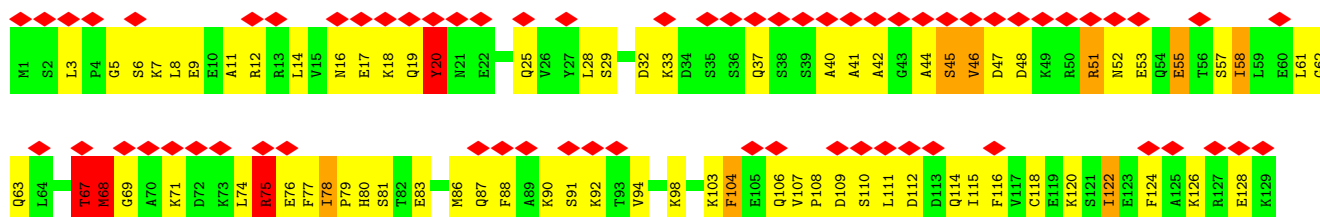
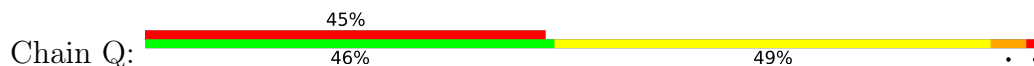


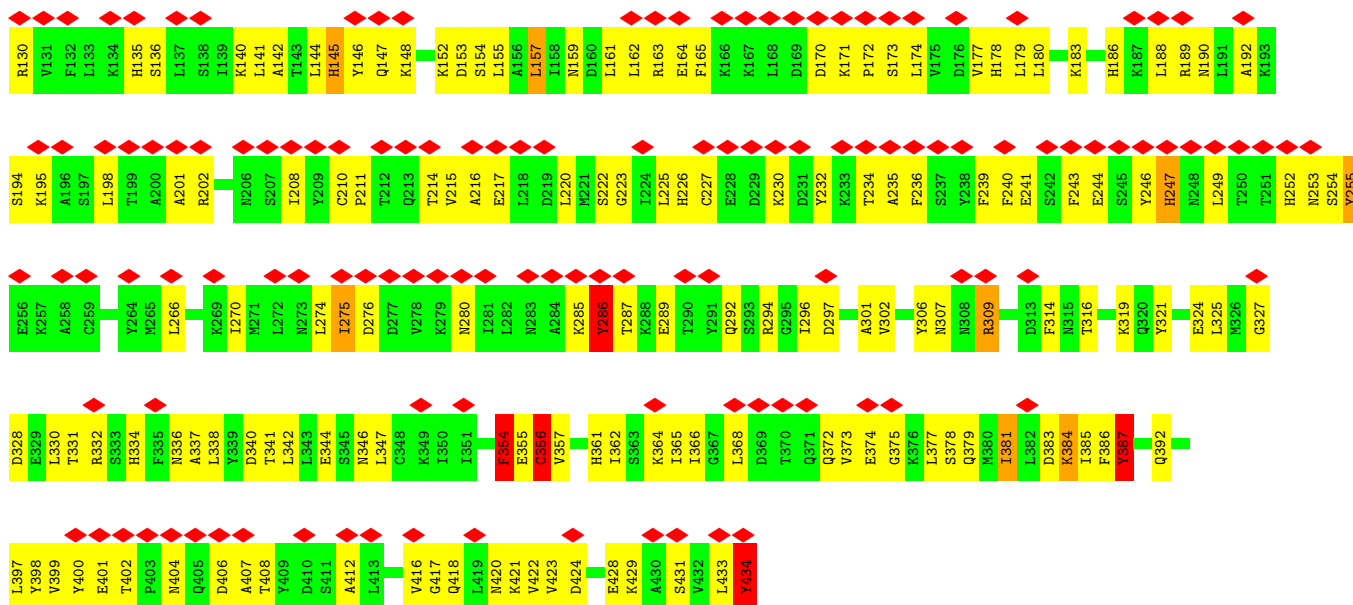


• Molecule 9: 26S proteasome regulatory subunit RPN5

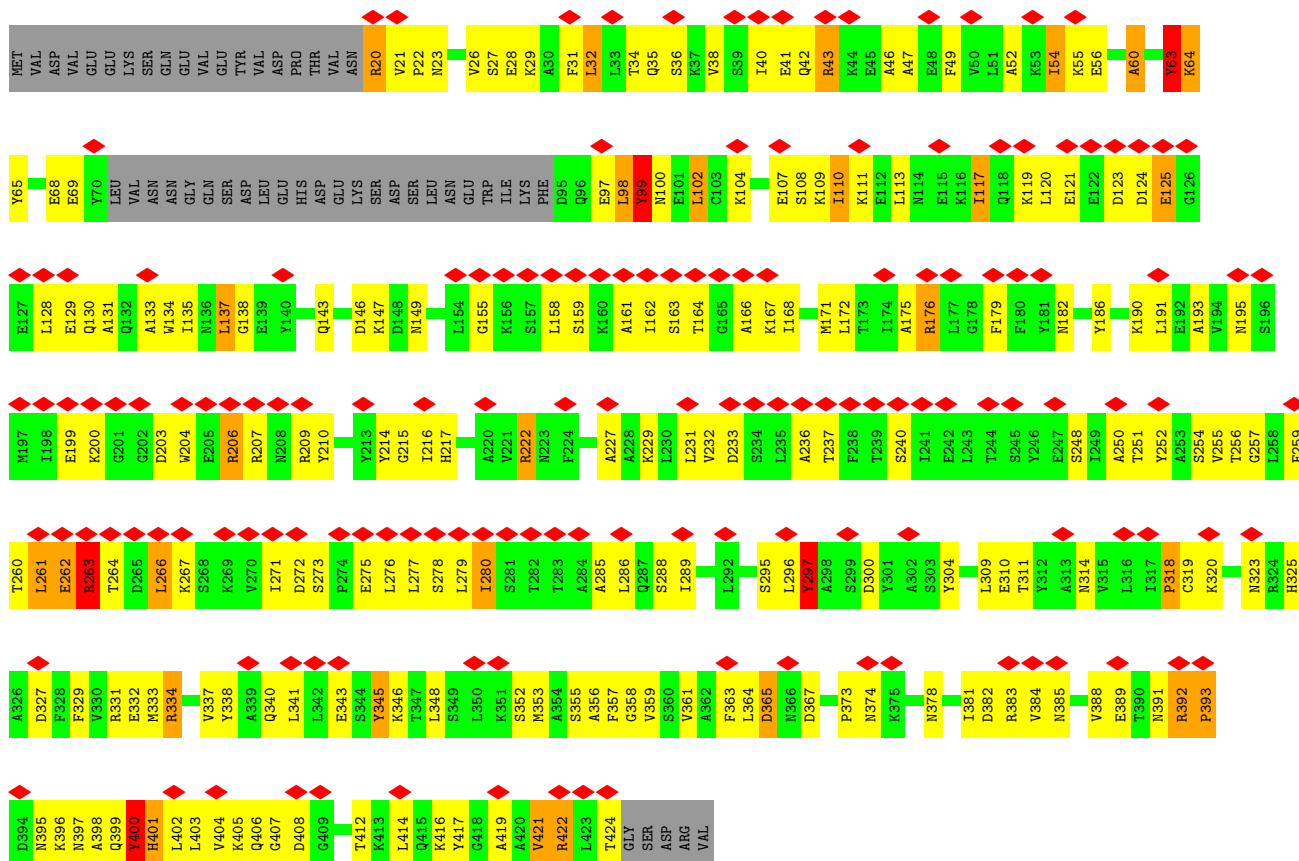


• Molecule 10: 26S proteasome regulatory subunit RPN6

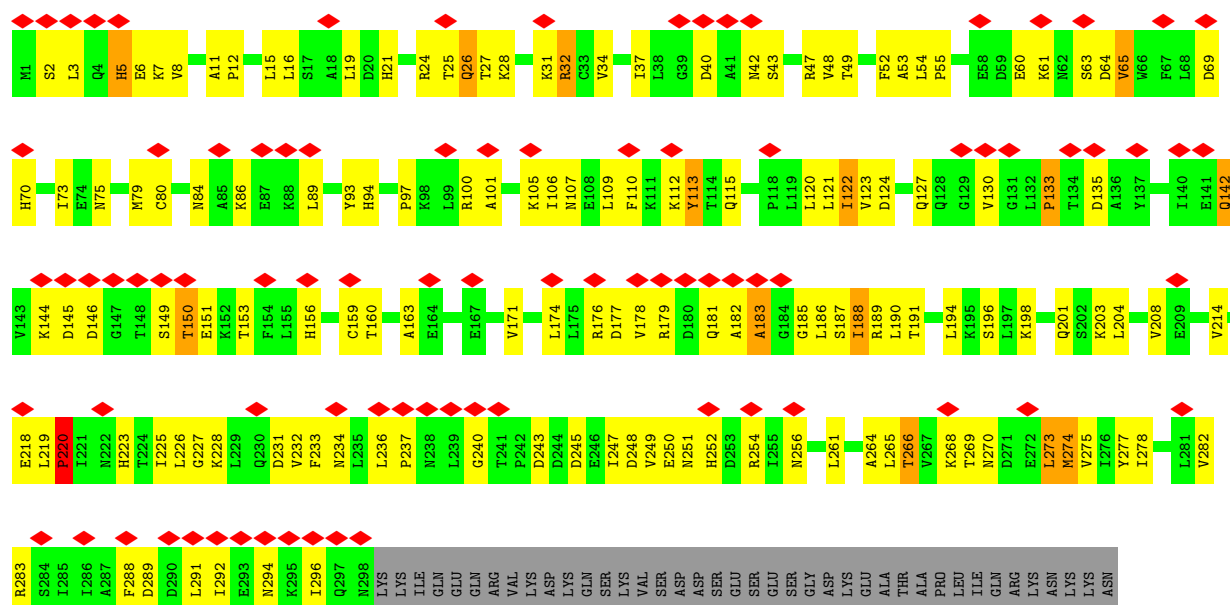
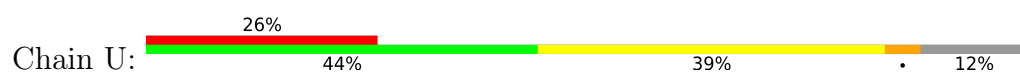




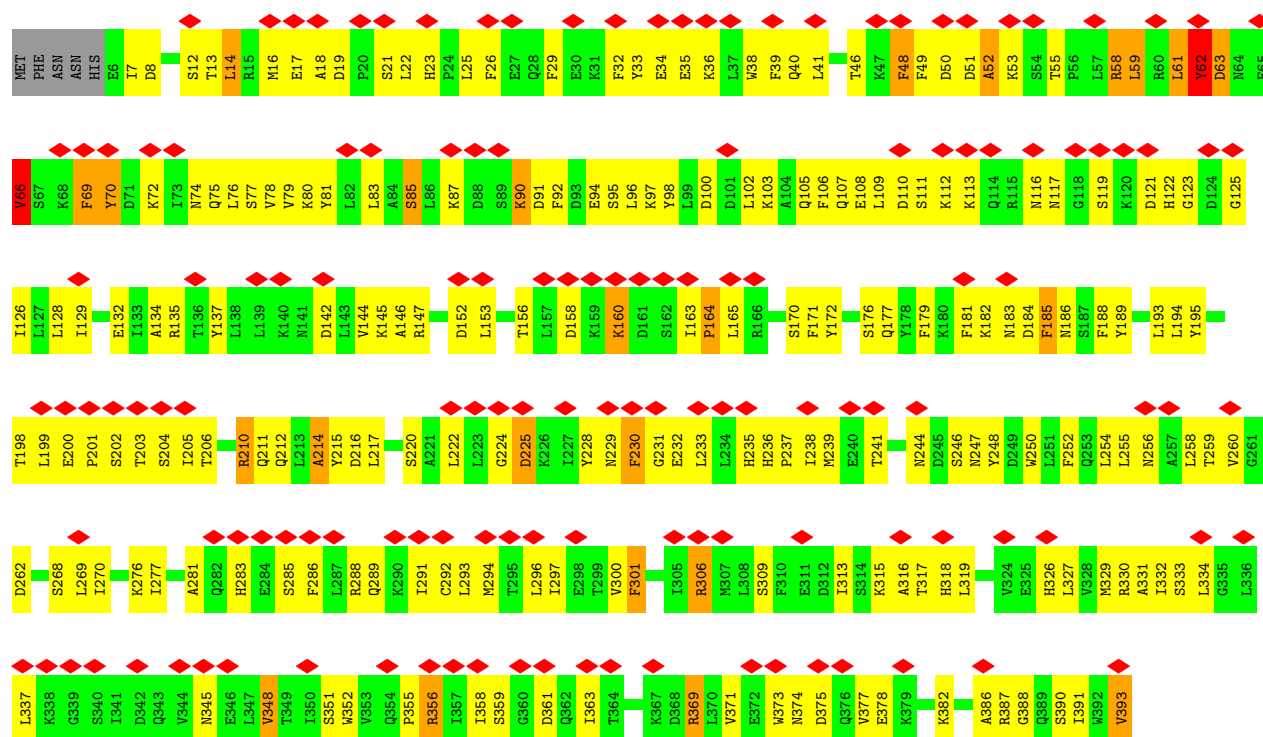
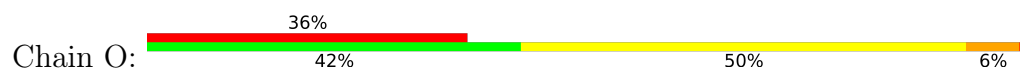
- Molecule 11: 26S proteasome regulatory subunit RPN7



- 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	193337	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 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.131	Depositor
Minimum map value	-0.092	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.017	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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	W	2.27	60/1557 (3.9%)	2.38	94/2111 (4.5%)
2	V	2.12	65/2309 (2.8%)	2.25	127/3115 (4.1%)
3	T	2.15	79/2235 (3.5%)	2.46	152/3017 (5.0%)
4	X	2.31	47/1058 (4.4%)	2.34	68/1432 (4.7%)
5	Y	2.27	18/438 (4.1%)	2.17	19/583 (3.3%)
6	Z	2.18	245/7122 (3.4%)	2.41	450/9645 (4.7%)
7	N	2.19	251/6994 (3.6%)	2.33	403/9455 (4.3%)
8	S	2.30	151/3966 (3.8%)	2.47	306/5355 (5.7%)
9	P	2.25	127/3663 (3.5%)	2.32	211/4940 (4.3%)
10	Q	2.20	120/3556 (3.4%)	2.43	234/4787 (4.9%)
11	R	2.33	106/3110 (3.4%)	2.41	186/4193 (4.4%)
12	U	2.17	89/2407 (3.7%)	2.36	137/3258 (4.2%)
13	O	2.17	113/3247 (3.5%)	2.33	179/4380 (4.1%)
All	All	2.21	1471/41662 (3.5%)	2.38	2566/56271 (4.6%)

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	2
2	V	0	7
3	T	0	9
4	X	0	7
5	Y	0	1
6	Z	0	19
7	N	0	13
8	S	0	10
9	P	0	5
10	Q	0	11
11	R	0	18
12	U	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	O	0	13
All	All	0	118

All (1471) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	99	TYR	CZ-OH	31.69	2.04	1.38
9	P	78	GLN	C-N	30.09	1.75	1.33
11	R	99	TYR	CE1-CZ	29.61	2.09	1.38
8	S	59	ASP	CA-CB	-27.78	1.10	1.53
8	S	127	THR	CA-CB	27.40	1.98	1.53
13	O	66	VAL	CA-CB	-15.89	1.34	1.54
13	O	393	VAL	C-OXT	-11.57	1.00	1.23
5	Y	89	GLN	C-O	-11.57	1.00	1.23
9	P	440	HIS	C-O	-11.56	1.00	1.23
8	S	492	LYS	C-O	-11.55	1.00	1.23
2	V	306	LYS	C-O	-11.55	1.00	1.23
5	Y	89	GLN	C-OXT	-11.55	1.00	1.23
10	Q	434	TYR	C-OXT	-11.55	1.00	1.23
2	V	306	LYS	C-OXT	-11.54	1.00	1.23
10	Q	434	TYR	C-O	-11.54	1.00	1.23
11	R	424	THR	C-O	-11.54	1.00	1.23
7	N	925	ASP	C-O	-11.53	1.00	1.23
13	O	393	VAL	C-O	-11.51	1.00	1.23
4	X	133	SER	C-O	-11.51	1.00	1.23
9	P	3	ARG	NE-CZ	11.13	1.45	1.33
6	Z	256	LEU	CA-C	-10.71	1.44	1.52
10	Q	211	PRO	CA-C	-10.11	1.40	1.52
10	Q	163	ARG	CD-NE	10.09	1.60	1.46
1	W	169	SER	N-CA	-10.06	1.34	1.45
9	P	401	ASN	CA-C	-9.86	1.40	1.52
6	Z	907	GLY	CA-C	-9.81	1.45	1.52
3	T	245	TYR	C-N	9.57	1.46	1.33
1	W	17	ARG	NE-CZ	9.49	1.43	1.33
7	N	590	ALA	CA-C	-9.47	1.40	1.52
11	R	392	ARG	CA-CB	9.42	1.66	1.53
6	Z	157	LEU	CA-C	-9.37	1.39	1.52
10	Q	108	PRO	CA-C	-9.36	1.43	1.52
8	S	450	ASN	CA-C	-9.28	1.44	1.53
3	T	251	HIS	ND1-CE1	9.22	1.41	1.32
6	Z	801	HIS	CD2-NE2	9.19	1.48	1.37
7	N	106	ILE	CA-C	-9.15	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	653	ARG	NE-CZ	9.15	1.43	1.33
9	P	337	HIS	ND1-CE1	9.11	1.41	1.32
8	S	224	LYS	CA-C	-9.10	1.40	1.52
13	O	41	LEU	CA-C	-9.09	1.41	1.52
8	S	382	ARG	NE-CZ	9.07	1.43	1.33
9	P	70	ASN	CA-C	-8.95	1.41	1.52
7	N	608	LEU	N-CA	-8.91	1.35	1.46
7	N	585	ARG	NE-CZ	8.91	1.42	1.33
4	X	22	ARG	CD-NE	8.90	1.58	1.46
2	V	265	GLU	CA-C	-8.89	1.41	1.52
5	Y	22	GLU	N-CA	-8.88	1.35	1.46
7	N	7	ALA	N-CA	-8.85	1.37	1.46
13	O	390	SER	N-CA	-8.82	1.35	1.46
1	W	195	GLY	C-O	8.77	1.31	1.23
6	Z	25	PRO	CG-CD	-8.74	1.21	1.50
8	S	84	ASP	C-N	8.72	1.45	1.33
6	Z	56	LEU	CA-CB	8.70	1.66	1.54
11	R	331	ARG	CD-NE	8.68	1.58	1.46
1	W	176	PRO	N-CA	-8.67	1.36	1.47
11	R	209	ARG	CD-NE	8.62	1.58	1.46
7	N	432	GLY	CA-C	-8.58	1.46	1.51
6	Z	410	THR	CA-C	-8.57	1.41	1.52
11	R	331	ARG	NE-CZ	8.55	1.42	1.33
6	Z	61	SER	CA-C	-8.53	1.41	1.52
9	P	364	ARG	CD-NE	8.53	1.58	1.46
9	P	138	ARG	NE-CZ	8.51	1.42	1.33
10	Q	232	TYR	CA-C	-8.50	1.42	1.52
7	N	406	TYR	N-CA	8.46	1.56	1.46
5	Y	72	ASP	N-CA	-8.42	1.35	1.46
12	U	97	PRO	C-N	8.39	1.43	1.33
6	Z	807	VAL	CA-C	-8.39	1.42	1.52
6	Z	430	LEU	N-CA	-8.36	1.36	1.46
8	S	241	PHE	CA-C	-8.36	1.42	1.52
9	P	192	ASP	CA-CB	8.33	1.63	1.52
10	Q	12	ARG	C-N	8.30	1.44	1.33
6	Z	136	ARG	NE-CZ	8.25	1.42	1.33
12	U	223	HIS	ND1-CE1	8.23	1.40	1.32
7	N	584	ARG	NE-CZ	8.22	1.42	1.33
7	N	907	ASP	CA-CB	8.21	1.64	1.53
7	N	460	ILE	N-CA	-8.19	1.35	1.46
4	X	33	ILE	C-N	8.19	1.44	1.33
7	N	583	VAL	CA-CB	-8.17	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	381	VAL	N-CA	-8.16	1.36	1.46
7	N	14	ARG	CZ-NH1	8.14	1.44	1.32
8	S	239	ARG	CD-NE	8.13	1.57	1.46
7	N	913	PRO	CA-C	-8.12	1.42	1.52
9	P	28	ALA	N-CA	-8.11	1.35	1.46
4	X	41	GLU	CA-C	-8.10	1.43	1.53
6	Z	826	ARG	NE-CZ	8.10	1.42	1.33
8	S	276	LEU	CA-CB	8.08	1.66	1.53
2	V	235	GLU	N-CA	-8.08	1.36	1.46
12	U	232	VAL	C-O	-8.06	1.15	1.24
13	O	62	TYR	CA-CB	8.04	1.66	1.53
4	X	75	TRP	CA-C	-8.04	1.42	1.52
7	N	150	LEU	CA-C	-8.03	1.41	1.52
11	R	43	ARG	N-CA	-8.02	1.36	1.46
7	N	762	ARG	NE-CZ	7.97	1.41	1.33
7	N	340	HIS	ND1-CE1	7.97	1.40	1.32
7	N	162	ARG	CA-C	-7.96	1.43	1.52
8	S	163	VAL	C-N	7.96	1.42	1.33
1	W	172	LEU	C-N	7.94	1.43	1.33
8	S	109	GLU	CA-C	-7.92	1.43	1.52
8	S	58	LYS	CA-C	-7.90	1.42	1.52
3	T	28	PRO	CA-C	7.90	1.59	1.52
13	O	387	ARG	C-N	7.89	1.42	1.33
11	R	419	ALA	N-CA	-7.86	1.36	1.46
8	S	155	LEU	CA-C	-7.86	1.42	1.52
9	P	364	ARG	NE-CZ	7.85	1.41	1.33
6	Z	715	ALA	N-CA	-7.83	1.36	1.46
7	N	653	ARG	C-N	7.83	1.43	1.33
7	N	483	LEU	CA-C	-7.82	1.43	1.52
11	R	32	LEU	N-CA	-7.81	1.36	1.46
10	Q	106	GLN	C-N	7.80	1.43	1.33
8	S	130	VAL	CA-C	7.80	1.63	1.52
6	Z	138	ARG	NE-CZ	7.78	1.41	1.33
2	V	57	PHE	CA-C	-7.77	1.43	1.52
7	N	151	LYS	N-CA	-7.76	1.36	1.46
8	S	174	ARG	CD-NE	7.73	1.57	1.46
7	N	535	LEU	N-CA	-7.71	1.36	1.46
2	V	100	ARG	CD-NE	7.71	1.57	1.46
7	N	542	SER	CA-C	-7.70	1.43	1.52
9	P	255	ALA	N-CA	-7.69	1.37	1.46
7	N	467	LYS	N-CA	-7.69	1.37	1.46
7	N	802	ALA	CA-CB	7.69	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	401	LYS	CA-C	-7.67	1.42	1.52
8	S	334	HIS	CA-C	-7.66	1.43	1.52
8	S	339	GLN	CA-C	-7.66	1.43	1.52
11	R	43	ARG	CZ-NH2	7.66	1.43	1.33
8	S	472	HIS	CE1-NE2	-7.65	1.24	1.32
6	Z	253	VAL	CA-C	7.65	1.59	1.52
6	Z	24	THR	CA-C	7.64	1.62	1.52
8	S	53	ILE	CA-C	7.63	1.62	1.52
8	S	127	THR	C-N	7.62	1.42	1.33
10	Q	177	VAL	CA-CB	-7.61	1.44	1.54
9	P	412	LEU	C-N	7.61	1.44	1.33
12	U	149	SER	CA-C	-7.60	1.44	1.53
3	T	60	ARG	CD-NE	7.60	1.56	1.46
6	Z	361	HIS	ND1-CE1	7.58	1.40	1.32
13	O	52	ALA	N-CA	-7.58	1.37	1.46
7	N	515	ARG	NE-CZ	7.58	1.41	1.33
3	T	175	ASP	N-CA	7.55	1.56	1.46
12	U	47	ARG	NE-CZ	7.54	1.41	1.33
3	T	231	SER	N-CA	-7.53	1.36	1.46
10	Q	107	VAL	N-CA	-7.53	1.39	1.47
3	T	228	ILE	CA-C	-7.53	1.43	1.52
2	V	133	ASN	CA-C	-7.52	1.43	1.52
12	U	70	HIS	ND1-CE1	7.52	1.40	1.32
6	Z	741	LEU	CA-C	-7.50	1.43	1.52
7	N	302	PHE	N-CA	-7.49	1.37	1.46
6	Z	334	LYS	CA-C	-7.49	1.43	1.52
7	N	668	THR	CA-C	-7.49	1.43	1.52
3	T	144	TYR	N-CA	-7.48	1.39	1.46
9	P	345	VAL	N-CA	-7.47	1.37	1.46
11	R	383	ARG	CD-NE	7.47	1.56	1.46
12	U	189	ARG	C-N	7.46	1.43	1.33
10	Q	254	SER	CA-C	-7.45	1.42	1.52
9	P	1	MET	C-N	7.44	1.44	1.33
11	R	121	GLU	CA-C	-7.44	1.43	1.52
7	N	873	ARG	NE-CZ	7.43	1.41	1.33
1	W	59	PRO	CA-C	-7.43	1.43	1.52
13	O	210	ARG	NE-CZ	7.42	1.41	1.33
11	R	400	TYR	C-N	7.41	1.43	1.33
7	N	499	HIS	ND1-CE1	7.41	1.40	1.32
8	S	298	ARG	CA-C	-7.41	1.43	1.52
7	N	460	ILE	CA-C	7.39	1.63	1.52
7	N	905	LEU	CA-C	7.37	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O	183	ASN	CA-C	7.37	1.62	1.53
9	P	68	SER	N-CA	-7.36	1.36	1.45
8	S	485	LYS	N-CA	-7.35	1.37	1.46
7	N	507	GLU	N-CA	-7.35	1.37	1.46
6	Z	538	CYS	CA-C	7.34	1.61	1.52
10	Q	330	LEU	CA-C	-7.33	1.43	1.52
9	P	94	GLN	N-CA	-7.31	1.36	1.46
9	P	123	ARG	NE-CZ	7.31	1.41	1.33
12	U	49	THR	CA-C	-7.31	1.43	1.52
6	Z	703	SER	CA-C	7.30	1.62	1.52
9	P	106	SER	CA-C	-7.30	1.42	1.52
13	O	164	PRO	C-N	7.30	1.43	1.33
6	Z	390	LEU	N-CA	-7.28	1.37	1.46
7	N	139	ARG	NE-CZ	7.27	1.41	1.33
5	Y	88	ASN	CA-CB	7.27	1.64	1.53
6	Z	104	ASP	CA-C	-7.27	1.45	1.52
7	N	214	LEU	CA-C	-7.27	1.43	1.52
7	N	62	ALA	N-CA	-7.26	1.37	1.46
7	N	105	SER	C-N	7.25	1.43	1.33
6	Z	64	TYR	CA-C	-7.25	1.45	1.52
10	Q	157	LEU	CA-C	-7.24	1.43	1.52
10	Q	189	ARG	NE-CZ	7.24	1.41	1.33
12	U	189	ARG	CD-NE	7.22	1.56	1.46
9	P	285	GLN	CA-C	-7.22	1.43	1.52
13	O	165	LEU	CA-CB	7.21	1.64	1.53
6	Z	840	ARG	NE-CZ	7.21	1.41	1.33
3	T	59	LYS	C-N	7.21	1.43	1.33
6	Z	316	ALA	N-CA	-7.21	1.37	1.46
3	T	124	SER	C-N	7.20	1.43	1.33
10	Q	91	SER	N-CA	-7.18	1.37	1.46
7	N	602	VAL	CA-C	7.18	1.59	1.52
9	P	16	ILE	N-CA	-7.18	1.37	1.46
11	R	334	ARG	NE-CZ	7.18	1.41	1.33
12	U	43	SER	CA-C	-7.18	1.43	1.52
7	N	58	ARG	CA-C	-7.17	1.43	1.52
1	W	41	ARG	CZ-NH2	7.17	1.42	1.33
11	R	108	SER	N-CA	7.17	1.55	1.46
11	R	240	SER	CA-C	-7.17	1.42	1.52
1	W	57	ALA	C-N	7.17	1.42	1.33
7	N	570	ARG	NE-CZ	7.16	1.41	1.33
12	U	151	GLU	N-CA	-7.16	1.37	1.46
10	Q	309	ARG	NE-CZ	7.15	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	U	49	THR	N-CA	-7.15	1.37	1.46
10	Q	148	LYS	N-CA	-7.14	1.36	1.46
6	Z	244	ARG	NE-CZ	7.14	1.41	1.33
10	Q	297	ASP	N-CA	-7.14	1.37	1.46
1	W	90	ALA	CA-C	-7.13	1.43	1.52
6	Z	58	GLU	C-N	7.13	1.43	1.33
9	P	134	VAL	CA-C	-7.12	1.44	1.52
12	U	185	GLY	C-O	7.12	1.31	1.23
7	N	585	ARG	CD-NE	7.11	1.56	1.46
6	Z	185	ASP	CA-C	-7.11	1.43	1.52
4	X	47	ASP	CA-C	-7.11	1.44	1.52
4	X	59	ARG	CD-NE	7.10	1.56	1.46
1	W	74	ALA	CA-C	-7.10	1.43	1.52
10	Q	6	SER	CA-CB	-7.10	1.42	1.53
10	Q	384	LYS	N-CA	-7.10	1.37	1.46
6	Z	42	ASP	C-O	-7.08	1.16	1.24
6	Z	448	LYS	N-CA	-7.08	1.37	1.46
7	N	899	ASN	CA-C	-7.08	1.43	1.52
8	S	164	ILE	CA-C	-7.08	1.45	1.52
7	N	447	SER	N-CA	-7.08	1.37	1.46
9	P	156	ALA	C-N	7.07	1.43	1.33
12	U	163	ALA	C-N	7.07	1.42	1.33
8	S	22	GLU	C-N	7.06	1.42	1.33
6	Z	806	GLU	N-CA	-7.05	1.37	1.46
9	P	389	ILE	C-N	7.05	1.42	1.33
6	Z	582	ASP	N-CA	-7.04	1.37	1.46
7	N	52	ASP	CA-C	-7.04	1.43	1.53
10	Q	246	TYR	CA-C	-7.04	1.43	1.52
7	N	767	ALA	C-N	7.03	1.40	1.33
12	U	282	VAL	CA-C	-7.02	1.44	1.52
10	Q	202	ARG	N-CA	-7.00	1.37	1.46
7	N	512	ASN	C-N	7.00	1.42	1.33
6	Z	884	THR	CA-C	-7.00	1.43	1.52
2	V	288	LEU	N-CA	-6.98	1.37	1.46
8	S	180	ASN	CA-CB	6.98	1.65	1.53
10	Q	421	LYS	C-N	6.95	1.42	1.33
6	Z	338	HIS	ND1-CE1	6.95	1.39	1.32
6	Z	384	SER	N-CA	-6.95	1.38	1.46
7	N	296	CYS	C-O	-6.94	1.15	1.24
6	Z	759	ARG	NE-CZ	6.94	1.40	1.33
9	P	310	ARG	NE-CZ	6.94	1.40	1.33
6	Z	798	ARG	NE-CZ	6.93	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	141	ILE	N-CA	-6.93	1.37	1.46
13	O	40	GLN	C-N	6.91	1.43	1.33
12	U	264	ALA	N-CA	-6.91	1.38	1.46
10	Q	429	LYS	N-CA	-6.91	1.37	1.46
6	Z	295	ARG	CD-NE	6.91	1.55	1.46
10	Q	45	SER	CA-C	-6.90	1.43	1.52
12	U	191	THR	CA-C	-6.90	1.44	1.52
12	U	3	LEU	N-CA	-6.90	1.37	1.46
10	Q	9	GLU	N-CA	-6.89	1.38	1.46
1	W	25	ARG	CZ-NH2	6.89	1.42	1.33
6	Z	570	LEU	CA-C	-6.89	1.44	1.52
7	N	597	ARG	NE-CZ	6.88	1.40	1.33
6	Z	151	HIS	CD2-NE2	6.88	1.45	1.37
7	N	146	LYS	C-O	-6.87	1.16	1.24
10	Q	57	SER	CA-C	-6.87	1.44	1.52
2	V	94	MET	CA-C	-6.87	1.44	1.52
7	N	366	THR	CA-C	-6.86	1.43	1.52
9	P	423	LEU	C-N	6.85	1.43	1.33
13	O	185	PHE	CA-CB	6.85	1.64	1.53
6	Z	359	LYS	CA-C	-6.85	1.43	1.52
7	N	421	ASP	CA-C	-6.85	1.44	1.52
7	N	40	SER	CA-C	-6.85	1.43	1.52
3	T	172	SER	CA-C	-6.84	1.43	1.52
13	O	233	LEU	N-CA	-6.84	1.38	1.46
11	R	357	PHE	CA-C	6.82	1.61	1.52
13	O	248	TYR	N-CA	-6.81	1.38	1.46
2	V	135	ARG	N-CA	-6.81	1.37	1.46
9	P	28	ALA	CA-C	-6.81	1.43	1.52
9	P	398	LYS	CA-C	-6.80	1.47	1.52
2	V	295	VAL	CA-C	-6.79	1.44	1.52
3	T	178	THR	CA-C	-6.79	1.44	1.52
10	Q	381	ILE	N-CA	-6.79	1.38	1.46
6	Z	454	GLY	CA-C	-6.79	1.44	1.52
6	Z	68	LEU	N-CA	-6.78	1.38	1.46
7	N	409	GLY	N-CA	-6.78	1.37	1.45
13	O	135	ARG	NE-CZ	6.78	1.40	1.33
7	N	308	ASN	N-CA	-6.78	1.37	1.46
6	Z	849	ARG	NE-CZ	6.77	1.40	1.33
1	W	188	SER	C-N	6.77	1.41	1.33
12	U	2	SER	N-CA	-6.77	1.37	1.46
3	T	106	ILE	C-N	6.77	1.42	1.33
3	T	69	SER	CA-C	-6.76	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	198	SER	CA-C	6.76	1.61	1.52
11	R	297	TYR	N-CA	-6.76	1.38	1.46
11	R	191	LEU	C-N	6.76	1.42	1.33
12	U	142	GLN	N-CA	-6.75	1.37	1.45
7	N	607	GLN	CA-C	-6.75	1.44	1.52
7	N	741	TYR	C-N	6.75	1.42	1.33
10	Q	225	LEU	CA-CB	6.74	1.64	1.53
10	Q	243	PHE	CA-C	-6.74	1.44	1.52
11	R	261	LEU	N-CA	6.74	1.53	1.45
6	Z	619	ASP	CA-C	-6.74	1.43	1.52
8	S	145	PHE	C-N	6.74	1.42	1.33
6	Z	57	LYS	CA-C	-6.73	1.43	1.52
12	U	179	ARG	CD-NE	6.73	1.55	1.46
4	X	73	THR	CA-C	-6.72	1.44	1.52
7	N	291	SER	N-CA	-6.72	1.38	1.46
6	Z	75	ILE	N-CA	-6.71	1.39	1.46
7	N	378	ASN	CA-C	-6.71	1.45	1.53
13	O	260	VAL	C-N	6.71	1.40	1.33
7	N	284	PRO	N-CD	-6.71	1.38	1.47
10	Q	364	LYS	N-CA	-6.71	1.38	1.46
11	R	161	ALA	CA-C	-6.70	1.44	1.52
10	Q	186	HIS	ND1-CE1	6.69	1.39	1.32
13	O	119	SER	CA-C	-6.69	1.44	1.52
1	W	17	ARG	C-O	-6.69	1.16	1.24
11	R	314	ASN	CA-C	-6.69	1.43	1.52
3	T	61	ILE	C-O	6.68	1.31	1.24
9	P	232	ARG	NE-CZ	6.68	1.40	1.33
7	N	474	SER	C-N	6.68	1.42	1.33
9	P	24	ILE	C-N	6.68	1.43	1.34
6	Z	361	HIS	CD2-NE2	-6.68	1.30	1.37
3	T	137	GLU	C-N	6.67	1.40	1.33
10	Q	252	HIS	N-CA	-6.67	1.37	1.46
3	T	91	SER	CA-C	-6.66	1.44	1.52
7	N	433	THR	N-CA	-6.66	1.37	1.46
9	P	82	LEU	C-N	6.66	1.42	1.33
9	P	41	VAL	CA-CB	-6.66	1.46	1.54
7	N	152	LEU	C-N	6.65	1.42	1.33
10	Q	3	LEU	C-O	-6.65	1.18	1.24
8	S	80	VAL	CA-C	6.65	1.58	1.52
2	V	152	VAL	CA-CB	-6.64	1.45	1.53
7	N	510	HIS	CA-C	-6.63	1.43	1.52
6	Z	466	GLU	C-N	6.63	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	U	32	ARG	CD-NE	6.63	1.55	1.46
9	P	136	ARG	CZ-NH1	6.62	1.42	1.32
2	V	118	LEU	CA-CB	6.62	1.62	1.53
6	Z	447	VAL	CA-C	-6.62	1.42	1.52
9	P	252	SER	CA-CB	6.61	1.63	1.53
6	Z	377	ALA	CA-C	-6.60	1.44	1.52
4	X	8	ILE	C-N	6.60	1.42	1.33
4	X	87	PHE	CA-C	-6.60	1.44	1.52
12	U	70	HIS	CE1-NE2	-6.60	1.25	1.32
7	N	510	HIS	CG-CD2	6.59	1.43	1.35
8	S	224	LYS	N-CA	-6.59	1.37	1.46
8	S	128	ILE	CA-C	-6.58	1.44	1.52
13	O	283	HIS	CB-CG	6.58	1.59	1.50
4	X	58	GLY	C-N	6.58	1.42	1.33
6	Z	514	ALA	CA-C	-6.58	1.44	1.52
10	Q	412	ALA	CA-C	-6.58	1.44	1.52
8	S	277	SER	C-N	6.58	1.42	1.33
4	X	128	VAL	N-CA	-6.57	1.38	1.46
11	R	36	SER	C-N	6.57	1.42	1.33
12	U	153	THR	CA-C	-6.57	1.44	1.52
4	X	22	ARG	CZ-NH2	6.56	1.42	1.33
7	N	521	LEU	CA-C	-6.56	1.44	1.52
9	P	332	GLU	N-CA	-6.56	1.38	1.46
8	S	190	SER	CA-CB	6.56	1.63	1.53
6	Z	774	ARG	CA-C	-6.56	1.45	1.53
7	N	372	GLY	C-N	6.55	1.42	1.33
10	Q	189	ARG	CA-C	-6.55	1.44	1.52
11	R	206	ARG	CZ-NH2	6.55	1.42	1.33
9	P	148	LYS	CA-CB	-6.55	1.43	1.53
7	N	55	PHE	CA-C	-6.54	1.44	1.52
7	N	562	THR	CA-C	-6.54	1.44	1.52
6	Z	948	TRP	N-CA	-6.53	1.38	1.46
2	V	124	ASN	CA-C	-6.52	1.44	1.52
13	O	109	LEU	N-CA	-6.52	1.38	1.46
4	X	24	CYS	C-N	6.52	1.39	1.33
6	Z	46	LYS	C-N	6.52	1.42	1.33
1	W	23	ARG	NE-CZ	6.51	1.40	1.33
11	R	346	LYS	CA-CB	6.51	1.63	1.53
1	W	104	LYS	N-CA	-6.51	1.38	1.46
2	V	26	THR	CA-CB	-6.51	1.43	1.53
6	Z	584	VAL	CA-C	-6.51	1.45	1.52
6	Z	896	LYS	CA-C	-6.50	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	925	VAL	N-CA	-6.50	1.39	1.46
7	N	618	ARG	NE-CZ	6.50	1.40	1.33
7	N	622	ALA	CA-C	-6.50	1.44	1.52
6	Z	339	PHE	CA-CB	6.50	1.63	1.53
12	U	2	SER	CA-C	-6.50	1.44	1.52
6	Z	42	ASP	CA-C	6.50	1.61	1.52
11	R	21	VAL	CA-CB	-6.49	1.50	1.54
7	N	451	GLY	CA-C	-6.49	1.44	1.51
8	S	281	ALA	C-N	6.49	1.41	1.34
11	R	400	TYR	CA-C	-6.49	1.44	1.52
11	R	99	TYR	C-N	6.48	1.42	1.33
10	Q	324	GLU	C-N	6.47	1.42	1.33
7	N	4	THR	N-CA	6.47	1.58	1.46
9	P	80	THR	CA-C	-6.47	1.43	1.52
7	N	900	ASN	C-N	6.47	1.43	1.33
1	W	41	ARG	NE-CZ	6.47	1.40	1.33
9	P	48	GLN	C-N	6.46	1.42	1.33
1	W	77	HIS	N-CA	-6.46	1.38	1.46
7	N	245	LEU	C-N	6.46	1.43	1.33
2	V	275	ASP	CA-C	6.45	1.61	1.53
13	O	144	VAL	CA-C	6.45	1.60	1.52
7	N	889	ARG	CA-C	-6.44	1.44	1.52
6	Z	332	ASN	N-CA	-6.44	1.37	1.46
11	R	167	LYS	CA-C	-6.43	1.44	1.52
7	N	7	ALA	CA-C	-6.42	1.44	1.52
6	Z	460	SER	N-CA	-6.42	1.38	1.46
8	S	287	SER	C-N	6.42	1.43	1.33
6	Z	114	SER	CA-C	-6.42	1.44	1.52
6	Z	603	VAL	C-O	-6.42	1.15	1.24
7	N	62	ALA	CA-C	-6.42	1.44	1.52
9	P	230	HIS	ND1-CE1	6.41	1.39	1.32
6	Z	962	ARG	CA-CB	6.41	1.63	1.53
6	Z	10	GLN	C-N	6.41	1.43	1.33
5	Y	86	ARG	NE-CZ	6.40	1.40	1.33
7	N	598	ASP	CA-C	-6.40	1.45	1.52
11	R	422	ARG	NE-CZ	6.40	1.40	1.33
5	Y	30	GLU	CA-C	-6.40	1.44	1.52
10	Q	179	LEU	CA-C	-6.40	1.44	1.52
6	Z	566	LEU	CA-C	-6.40	1.44	1.52
7	N	33	ASP	C-N	6.40	1.42	1.33
6	Z	138	ARG	C-N	6.39	1.42	1.33
9	P	124	VAL	CA-C	-6.38	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	224	ARG	CZ-NH1	6.37	1.41	1.32
13	O	210	ARG	CA-C	-6.37	1.44	1.52
4	X	74	MET	N-CA	-6.37	1.37	1.46
9	P	282	HIS	CB-CG	6.36	1.59	1.50
13	O	112	LYS	CA-C	-6.36	1.44	1.52
2	V	259	LYS	C-O	-6.36	1.19	1.23
12	U	294	ASN	C-N	6.36	1.42	1.33
3	T	179	ASP	N-CA	6.35	1.54	1.46
10	Q	365	ILE	C-N	6.35	1.41	1.33
1	W	181	LEU	CA-CB	6.34	1.63	1.53
13	O	231	GLY	N-CA	-6.34	1.38	1.45
8	S	199	GLU	C-N	6.34	1.41	1.33
11	R	171	MET	C-N	6.33	1.42	1.33
12	U	208	VAL	N-CA	-6.33	1.39	1.46
12	U	289	ASP	CA-C	-6.33	1.44	1.52
7	N	550	GLY	CA-C	6.33	1.59	1.51
12	U	254	ARG	CD-NE	6.33	1.55	1.46
8	S	428	ARG	NE-CZ	6.33	1.40	1.33
8	S	330	LEU	CA-C	6.32	1.61	1.52
10	Q	357	VAL	N-CA	-6.32	1.38	1.46
5	Y	39	PRO	CA-C	-6.32	1.42	1.52
12	U	226	LEU	CA-C	-6.32	1.44	1.52
6	Z	47	THR	CA-C	-6.31	1.44	1.52
10	Q	61	LEU	C-N	6.31	1.42	1.34
9	P	348	HIS	N-CA	-6.31	1.38	1.46
6	Z	75	ILE	C-N	6.31	1.42	1.33
6	Z	831	LEU	N-CA	-6.29	1.38	1.46
7	N	602	VAL	CA-CB	6.29	1.57	1.54
8	S	161	LYS	CA-C	-6.29	1.44	1.52
6	Z	475	GLN	CA-C	-6.29	1.44	1.52
8	S	23	LYS	CA-CB	6.29	1.63	1.53
3	T	160	ALA	CA-C	-6.29	1.44	1.52
6	Z	967	THR	N-CA	-6.29	1.38	1.45
2	V	220	GLN	C-N	6.28	1.42	1.33
11	R	217	HIS	ND1-CE1	6.28	1.38	1.32
6	Z	628	ASN	CA-CB	6.28	1.63	1.53
1	W	92	GLN	C-N	6.28	1.41	1.33
6	Z	483	THR	N-CA	-6.28	1.38	1.46
7	N	809	ARG	CZ-NH1	6.27	1.41	1.32
12	U	188	ILE	C-O	-6.27	1.16	1.24
13	O	361	ASP	C-N	6.27	1.42	1.34
13	O	111	SER	CA-C	-6.27	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	67	LEU	C-N	6.26	1.41	1.33
12	U	159	CYS	N-CA	-6.26	1.38	1.46
7	N	72	LEU	C-N	6.26	1.42	1.33
2	V	230	TYR	N-CA	-6.26	1.37	1.46
10	Q	189	ARG	CD-NE	6.26	1.55	1.46
13	O	176	SER	CA-C	-6.25	1.44	1.52
10	Q	46	VAL	C-N	6.25	1.42	1.33
4	X	36	LYS	CA-C	-6.25	1.44	1.52
12	U	5	HIS	CA-C	-6.25	1.44	1.52
2	V	93	ASP	CA-CB	6.24	1.63	1.53
6	Z	780	MET	N-CA	-6.24	1.38	1.46
8	S	126	LYS	CA-CB	6.24	1.64	1.53
9	P	420	ASP	CA-C	-6.24	1.44	1.52
2	V	67	ASP	CA-C	-6.24	1.45	1.52
6	Z	452	LEU	CA-C	-6.24	1.44	1.52
9	P	214	GLU	C-N	6.24	1.42	1.33
6	Z	340	LEU	CA-C	-6.24	1.45	1.52
11	R	176	ARG	NE-CZ	6.23	1.40	1.33
13	O	239	MET	N-CA	-6.23	1.38	1.46
6	Z	526	ALA	CA-C	-6.23	1.44	1.52
8	S	91	ASN	N-CA	-6.23	1.38	1.46
6	Z	17	GLN	C-N	6.23	1.41	1.33
6	Z	314	LEU	N-CA	-6.22	1.39	1.46
13	O	17	GLU	C-N	6.22	1.41	1.33
7	N	177	ASP	CA-C	6.22	1.60	1.52
8	S	451	ILE	CA-C	-6.21	1.44	1.52
6	Z	104	ASP	N-CA	-6.21	1.39	1.46
13	O	144	VAL	CA-CB	-6.21	1.47	1.54
7	N	110	VAL	C-N	6.21	1.42	1.33
11	R	276	LEU	CA-CB	6.21	1.63	1.53
6	Z	792	VAL	CA-CB	6.20	1.62	1.54
8	S	400	LYS	C-N	6.20	1.41	1.33
8	S	51	ARG	CD-NE	6.20	1.54	1.46
10	Q	397	LEU	CA-C	-6.19	1.45	1.52
7	N	875	LEU	CA-C	-6.19	1.45	1.53
11	R	391	ASN	N-CA	-6.19	1.38	1.46
10	Q	120	LYS	CA-C	6.19	1.60	1.52
6	Z	161	ILE	N-CA	-6.18	1.39	1.46
8	S	316	LEU	CB-CG	6.18	1.65	1.53
9	P	431	HIS	N-CA	-6.18	1.38	1.46
12	U	182	ALA	CA-C	6.18	1.60	1.52
8	S	309	PHE	CA-C	-6.17	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	254	SER	C-N	6.17	1.41	1.33
13	O	193	LEU	N-CA	-6.17	1.38	1.46
1	W	172	LEU	CA-C	6.17	1.59	1.52
2	V	53	MET	N-CA	-6.17	1.38	1.46
10	Q	172	PRO	C-N	6.17	1.42	1.33
8	S	171	TYR	CA-C	-6.17	1.44	1.53
7	N	66	SER	C-N	6.17	1.42	1.33
8	S	40	GLU	N-CA	-6.16	1.39	1.46
11	R	28	GLU	C-O	-6.16	1.17	1.24
4	X	51	ARG	CD-NE	6.16	1.54	1.46
9	P	23	LYS	CA-CB	6.16	1.63	1.53
11	R	414	LEU	C-O	-6.15	1.17	1.24
9	P	124	VAL	CA-CB	-6.15	1.46	1.54
4	X	21	SER	CA-C	-6.14	1.44	1.52
11	R	176	ARG	CD-NE	6.14	1.54	1.46
2	V	97	GLN	CA-C	-6.14	1.44	1.52
9	P	143	LEU	C-N	6.14	1.41	1.33
10	Q	47	ASP	N-CA	-6.14	1.38	1.46
10	Q	285	LYS	CA-CB	6.14	1.63	1.53
11	R	21	VAL	CA-C	-6.14	1.47	1.52
3	T	55	LEU	CA-CB	6.13	1.63	1.53
8	S	454	SER	CA-CB	6.13	1.62	1.53
7	N	813	ARG	CZ-NH1	6.13	1.41	1.32
9	P	223	LEU	CA-C	-6.13	1.44	1.52
4	X	7	VAL	N-CA	6.12	1.57	1.46
8	S	290	ASN	CA-C	-6.12	1.45	1.52
3	T	125	GLU	CA-C	-6.12	1.44	1.52
1	W	60	ARG	NE-CZ	6.12	1.39	1.33
13	O	16	MET	CA-C	-6.12	1.45	1.52
8	S	405	ARG	CD-NE	6.11	1.54	1.46
12	U	65	VAL	N-CA	-6.11	1.39	1.46
9	P	81	LEU	N-CA	-6.10	1.38	1.46
3	T	238	GLN	CA-CB	6.10	1.62	1.53
8	S	278	LYS	C-N	6.10	1.41	1.33
7	N	446	ALA	C-O	6.09	1.31	1.24
12	U	11	ALA	CA-C	-6.09	1.46	1.52
9	P	338	TRP	NE1-CE2	6.09	1.44	1.37
1	W	43	SER	N-CA	-6.09	1.38	1.46
9	P	387	GLY	N-CA	-6.09	1.36	1.45
11	R	56	GLU	C-N	6.08	1.43	1.33
12	U	100	ARG	CD-NE	6.08	1.54	1.46
6	Z	343	ALA	N-CA	-6.08	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	265	LEU	CA-C	-6.08	1.45	1.52
10	Q	392	GLN	N-CA	-6.08	1.38	1.46
8	S	335	GLN	CA-C	-6.08	1.44	1.52
8	S	88	PHE	CA-CB	6.07	1.62	1.53
8	S	130	VAL	N-CA	-6.07	1.38	1.46
7	N	60	MET	C-N	6.07	1.41	1.33
6	Z	563	VAL	CA-C	-6.07	1.44	1.52
7	N	640	VAL	CA-CB	-6.06	1.46	1.54
13	O	211	GLN	CA-C	-6.06	1.45	1.52
6	Z	50	GLU	C-N	6.06	1.42	1.34
6	Z	202	ARG	N-CA	6.06	1.53	1.46
10	Q	235	ALA	C-N	6.06	1.41	1.33
6	Z	90	LYS	CA-CB	6.06	1.64	1.53
10	Q	174	LEU	N-CA	-6.06	1.38	1.46
6	Z	308	LYS	CA-C	6.04	1.60	1.52
7	N	795	GLU	CA-C	-6.04	1.44	1.52
8	S	368	LYS	N-CA	-6.04	1.39	1.46
7	N	171	LYS	C-N	6.04	1.42	1.33
6	Z	268	ALA	N-CA	-6.04	1.38	1.46
3	T	201	PRO	C-N	6.04	1.41	1.33
11	R	128	LEU	N-CA	-6.04	1.38	1.46
7	N	606	VAL	CA-CB	6.03	1.62	1.54
7	N	875	LEU	CA-CB	6.03	1.62	1.53
10	Q	62	GLY	CA-C	-6.03	1.43	1.51
9	P	251	LYS	CA-CB	6.03	1.62	1.53
11	R	203	ASP	CA-C	-6.03	1.45	1.52
6	Z	136	ARG	C-N	6.02	1.42	1.33
13	O	48	PHE	CA-C	-6.02	1.44	1.52
6	Z	12	ILE	N-CA	6.02	1.53	1.46
6	Z	773	ARG	CZ-NH1	6.02	1.41	1.32
11	R	385	ASN	CA-C	-6.02	1.44	1.52
12	U	47	ARG	C-N	6.02	1.40	1.33
13	O	292	CYS	CA-C	-6.02	1.45	1.52
9	P	139	VAL	N-CA	-6.02	1.38	1.46
9	P	116	ILE	N-CA	-6.02	1.39	1.46
6	Z	826	ARG	C-N	6.01	1.41	1.33
7	N	724	THR	C-N	6.01	1.42	1.33
7	N	912	GLU	N-CA	-6.01	1.37	1.45
10	Q	55	GLU	CA-CB	6.01	1.62	1.53
4	X	59	ARG	NE-CZ	6.01	1.39	1.33
7	N	453	ALA	N-CA	-6.01	1.39	1.46
1	W	37	PHE	N-CA	-6.00	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	77	PRO	N-CA	-6.00	1.39	1.47
7	N	664	LEU	CA-CB	6.00	1.61	1.53
10	Q	128	GLU	N-CA	-6.00	1.38	1.46
2	V	227	MET	SD-CE	6.00	1.94	1.79
7	N	906	ARG	NE-CZ	6.00	1.39	1.33
10	Q	19	GLN	CA-C	-6.00	1.45	1.52
1	W	127	ARG	NE-CZ	6.00	1.39	1.33
7	N	439	VAL	CA-C	-5.99	1.45	1.52
6	Z	451	ALA	N-CA	-5.99	1.39	1.46
7	N	566	SER	CA-C	-5.99	1.45	1.52
7	N	649	VAL	C-N	5.99	1.41	1.33
7	N	162	ARG	N-CA	-5.99	1.38	1.46
2	V	29	ILE	C-O	-5.99	1.16	1.23
7	N	40	SER	CA-CB	5.99	1.63	1.53
2	V	278	LYS	CA-C	-5.99	1.45	1.52
7	N	755	PRO	C-N	5.99	1.41	1.33
2	V	71	MET	CA-C	-5.98	1.44	1.52
7	N	310	ASP	CA-CB	5.98	1.61	1.53
8	S	239	ARG	NE-CZ	5.98	1.39	1.33
8	S	112	ASN	C-N	5.98	1.41	1.33
7	N	179	THR	CA-C	-5.97	1.45	1.52
7	N	862	SER	N-CA	-5.97	1.38	1.45
8	S	35	LEU	C-O	-5.97	1.17	1.24
3	T	9	LYS	C-N	5.97	1.42	1.33
7	N	921	ARG	CZ-NH1	5.97	1.41	1.32
9	P	37	ASP	CA-CB	5.97	1.62	1.53
13	O	229	ASN	CA-C	-5.97	1.43	1.52
7	N	517	LEU	CA-C	-5.97	1.44	1.52
8	S	253	PHE	N-CA	-5.96	1.39	1.46
6	Z	790	MET	CA-C	-5.96	1.45	1.52
13	O	235	HIS	CE1-NE2	-5.96	1.26	1.32
6	Z	168	GLN	C-N	5.96	1.41	1.33
8	S	332	PHE	CA-C	-5.96	1.45	1.52
7	N	183	VAL	C-N	5.96	1.41	1.33
3	T	179	ASP	CA-C	-5.95	1.45	1.52
6	Z	482	ASP	N-CA	-5.95	1.38	1.46
8	S	128	ILE	N-CA	-5.95	1.39	1.46
12	U	2	SER	C-N	5.94	1.42	1.33
6	Z	553	ARG	CZ-NH1	5.94	1.41	1.32
10	Q	142	ALA	CA-C	-5.93	1.45	1.52
3	T	231	SER	C-N	5.93	1.41	1.33
7	N	124	TYR	C-O	-5.93	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	278	LEU	CB-CG	5.93	1.65	1.53
11	R	155	GLY	CA-C	-5.93	1.45	1.52
13	O	262	ASP	CA-CB	5.93	1.61	1.53
13	O	80	LYS	C-N	5.92	1.41	1.33
7	N	528	ARG	CA-C	-5.92	1.44	1.52
7	N	333	SER	CA-CB	5.91	1.62	1.53
10	Q	241	GLU	N-CA	-5.91	1.39	1.46
7	N	436	ASP	C-O	-5.91	1.16	1.24
10	Q	80	HIS	C-N	5.91	1.42	1.33
10	Q	178	HIS	ND1-CE1	5.91	1.38	1.32
7	N	895	LYS	C-N	5.90	1.41	1.33
12	U	291	LEU	C-N	5.90	1.41	1.33
6	Z	507	GLY	C-N	5.90	1.41	1.33
6	Z	188	ALA	CA-CB	-5.90	1.43	1.53
6	Z	287	ARG	NE-CZ	5.90	1.39	1.33
3	T	193	THR	N-CA	-5.89	1.38	1.46
13	O	356	ARG	NE-CZ	5.89	1.39	1.33
6	Z	196	SER	N-CA	5.89	1.53	1.46
6	Z	215	ASN	N-CA	-5.89	1.39	1.46
2	V	133	ASN	C-O	-5.89	1.17	1.23
3	T	221	ALA	C-N	5.89	1.41	1.33
12	U	34	VAL	CA-C	-5.89	1.45	1.52
6	Z	928	ARG	NE-CZ	5.88	1.39	1.33
6	Z	473	LEU	CA-C	-5.88	1.45	1.52
6	Z	634	ASP	CA-C	-5.88	1.45	1.52
2	V	273	ARG	N-CA	-5.88	1.38	1.45
6	Z	13	ASP	CA-CB	5.88	1.62	1.53
7	N	329	HIS	C-O	-5.88	1.17	1.24
8	S	174	ARG	N-CA	-5.88	1.39	1.46
3	T	250	MET	C-O	-5.87	1.17	1.24
7	N	881	TYR	CA-C	-5.87	1.44	1.52
10	Q	216	ALA	CA-CB	5.87	1.62	1.53
4	X	106	SER	CA-C	-5.87	1.45	1.52
8	S	176	LEU	C-O	-5.87	1.16	1.24
6	Z	763	HIS	ND1-CE1	5.86	1.38	1.32
7	N	620	GLY	CA-C	5.86	1.59	1.51
9	P	298	SER	N-CA	-5.86	1.39	1.46
1	W	40	LYS	CA-C	-5.86	1.45	1.52
8	S	469	ASN	CA-CB	5.86	1.62	1.53
11	R	207	ARG	CZ-NH2	5.86	1.41	1.33
11	R	229	LYS	N-CA	-5.86	1.39	1.46
11	R	172	LEU	CA-C	-5.85	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	889	VAL	CA-C	5.85	1.59	1.52
8	S	53	ILE	N-CA	-5.85	1.39	1.46
9	P	395	ARG	NE-CZ	5.85	1.39	1.33
6	Z	583	ASP	CA-C	5.85	1.60	1.52
1	W	179	ARG	CA-CB	5.84	1.63	1.53
6	Z	71	LEU	N-CA	5.84	1.53	1.46
6	Z	159	LEU	C-N	5.84	1.41	1.33
7	N	50	TYR	C-N	5.84	1.41	1.33
8	S	256	LYS	C-N	5.84	1.41	1.33
13	O	355	PRO	N-CD	-5.84	1.39	1.47
6	Z	764	LEU	CA-CB	5.84	1.62	1.53
7	N	29	ASN	CA-CB	5.84	1.63	1.53
13	O	40	GLN	N-CA	-5.84	1.38	1.46
13	O	121	ASP	CA-CB	5.83	1.61	1.53
6	Z	301	THR	N-CA	-5.83	1.39	1.46
1	W	183	GLU	N-CA	-5.83	1.39	1.46
13	O	33	TYR	CA-CB	5.83	1.62	1.53
2	V	259	LYS	CA-CB	5.83	1.65	1.53
7	N	867	LYS	C-O	-5.83	1.17	1.23
10	Q	344	GLU	C-O	-5.83	1.17	1.24
11	R	110	ILE	CA-CB	5.83	1.62	1.54
7	N	392	GLY	N-CA	-5.82	1.37	1.45
6	Z	429	ASN	CA-C	-5.82	1.45	1.52
13	O	309	SER	C-N	5.82	1.42	1.34
2	V	38	LEU	C-O	-5.82	1.17	1.24
6	Z	569	ALA	N-CA	5.82	1.53	1.46
7	N	207	LEU	CA-CB	5.81	1.62	1.53
13	O	309	SER	N-CA	-5.81	1.38	1.45
4	X	28	PRO	N-CA	-5.81	1.40	1.47
7	N	640	VAL	C-N	5.81	1.42	1.33
1	W	28	ALA	C-N	5.80	1.41	1.33
9	P	370	ASP	CA-CB	5.80	1.61	1.53
8	S	191	HIS	CD2-NE2	5.79	1.44	1.37
3	T	237	ASN	CA-C	-5.79	1.45	1.52
10	Q	58	ILE	C-N	5.79	1.41	1.33
6	Z	224	LEU	N-CA	-5.79	1.39	1.46
6	Z	500	SER	N-CA	-5.79	1.39	1.46
6	Z	527	SER	C-N	5.79	1.41	1.33
7	N	575	ALA	C-O	-5.79	1.17	1.24
10	Q	246	TYR	C-N	5.79	1.41	1.33
12	U	250	GLU	CA-C	-5.78	1.45	1.52
11	R	327	ASP	N-CA	-5.78	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	41	ILE	C-N	5.78	1.38	1.33
7	N	87	ASP	N-CA	-5.78	1.38	1.45
7	N	203	ARG	NE-CZ	5.78	1.39	1.33
7	N	412	TYR	CA-CB	5.78	1.62	1.53
7	N	665	ILE	N-CA	-5.77	1.39	1.46
7	N	921	ARG	NE-CZ	5.77	1.39	1.33
6	Z	277	GLU	CA-C	-5.77	1.45	1.52
9	P	183	GLN	N-CA	-5.77	1.39	1.46
6	Z	345	GLU	N-CA	-5.77	1.39	1.46
11	R	365	ASP	N-CA	-5.77	1.39	1.46
7	N	543	ASP	N-CA	-5.77	1.39	1.46
7	N	492	THR	CA-C	-5.77	1.45	1.52
10	Q	309	ARG	CZ-NH2	5.77	1.41	1.33
11	R	43	ARG	NE-CZ	5.76	1.39	1.33
10	Q	81	SER	C-N	5.76	1.41	1.33
13	O	270	ILE	N-CA	-5.76	1.39	1.46
8	S	403	SER	CA-C	-5.76	1.45	1.52
9	P	383	LEU	C-N	5.76	1.40	1.33
4	X	91	PHE	C-N	5.76	1.41	1.33
1	W	3	LEU	CA-C	-5.76	1.48	1.53
7	N	890	PHE	CA-C	-5.75	1.45	1.52
7	N	561	GLY	CA-C	5.75	1.59	1.51
12	U	150	THR	C-N	5.75	1.41	1.33
6	Z	124	MET	N-CA	-5.75	1.39	1.46
11	R	381	ILE	N-CA	-5.75	1.39	1.46
12	U	146	ASP	CA-CB	5.75	1.62	1.53
6	Z	810	ASN	CA-CB	5.75	1.62	1.53
13	O	289	GLN	CA-C	5.74	1.60	1.52
1	W	97	THR	N-CA	-5.74	1.39	1.46
8	S	103	SER	CA-C	-5.74	1.45	1.52
1	W	16	SER	N-CA	-5.74	1.38	1.46
11	R	356	ALA	CA-C	-5.74	1.45	1.52
12	U	32	ARG	CZ-NH1	5.74	1.40	1.32
6	Z	922	PRO	CA-C	-5.73	1.46	1.52
12	U	214	VAL	C-N	5.73	1.40	1.33
2	V	23	THR	N-CA	-5.73	1.38	1.46
2	V	92	MET	CA-C	-5.73	1.45	1.52
3	T	109	TYR	N-CA	-5.73	1.39	1.46
6	Z	171	LYS	C-N	5.73	1.41	1.33
8	S	233	LEU	CA-C	-5.73	1.45	1.52
12	U	228	LYS	C-O	-5.73	1.17	1.24
6	Z	20	PRO	N-CA	-5.72	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	180	ASN	N-CA	5.72	1.53	1.46
8	S	393	ARG	NE-CZ	5.72	1.39	1.33
9	P	39	LEU	C-N	5.72	1.41	1.33
5	Y	41	ASP	CA-C	-5.72	1.45	1.52
7	N	452	LEU	N-CA	-5.72	1.39	1.46
5	Y	75	ASN	C-N	-5.72	1.26	1.33
10	Q	192	ALA	CA-C	-5.72	1.45	1.52
8	S	61	SER	CA-CB	5.72	1.62	1.53
11	R	232	VAL	CA-C	-5.72	1.43	1.52
6	Z	969	GLU	CA-CB	5.72	1.60	1.53
11	R	207	ARG	CD-NE	5.71	1.54	1.46
4	X	62	ASP	N-CA	-5.71	1.41	1.45
6	Z	463	HIS	ND1-CE1	5.71	1.38	1.32
7	N	801	THR	C-N	5.70	1.41	1.33
11	R	406	GLN	C-N	5.70	1.40	1.33
2	V	132	LEU	CA-C	-5.70	1.45	1.52
7	N	355	TRP	NE1-CE2	5.70	1.43	1.37
9	P	178	GLN	N-CA	-5.70	1.39	1.46
8	S	40	GLU	C-N	5.70	1.40	1.33
6	Z	382	ALA	CA-C	-5.70	1.45	1.52
10	Q	179	LEU	C-O	-5.70	1.17	1.24
9	P	42	LEU	CB-CG	5.69	1.64	1.53
10	Q	202	ARG	CZ-NH1	5.69	1.40	1.32
6	Z	472	LEU	CA-C	-5.69	1.45	1.52
6	Z	471	LEU	N-CA	-5.69	1.39	1.46
10	Q	302	VAL	N-CA	-5.69	1.39	1.46
1	W	109	ARG	NE-CZ	5.68	1.39	1.33
10	Q	246	TYR	N-CA	-5.68	1.39	1.46
7	N	594	VAL	CA-C	-5.68	1.45	1.52
10	Q	178	HIS	N-CA	-5.68	1.39	1.46
7	N	157	ALA	C-N	5.68	1.41	1.33
7	N	113	ALA	N-CA	-5.68	1.39	1.46
10	Q	234	THR	C-N	5.68	1.41	1.33
8	S	211	ARG	CA-CB	-5.68	1.44	1.53
13	O	110	ASP	C-O	5.68	1.31	1.24
6	Z	21	GLU	N-CA	-5.67	1.41	1.46
6	Z	132	HIS	ND1-CE1	5.67	1.38	1.32
11	R	166	ALA	C-N	5.67	1.41	1.33
8	S	262	THR	CA-C	-5.67	1.46	1.53
8	S	363	THR	N-CA	-5.66	1.39	1.46
6	Z	202	ARG	CA-C	-5.66	1.45	1.52
1	W	71	LYS	C-O	-5.66	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	646	LYS	CA-C	-5.66	1.45	1.52
8	S	405	ARG	NE-CZ	5.66	1.39	1.33
9	P	115	ARG	CD-NE	5.66	1.54	1.46
12	U	100	ARG	CZ-NH1	5.66	1.40	1.32
12	U	182	ALA	N-CA	-5.66	1.39	1.46
12	U	201	GLN	CA-C	-5.66	1.45	1.52
2	V	147	VAL	CA-CB	-5.66	1.48	1.54
13	O	246	SER	CA-CB	5.66	1.62	1.53
6	Z	881	ILE	C-O	-5.66	1.17	1.24
10	Q	416	VAL	CA-CB	5.66	1.61	1.54
11	R	159	SER	CA-C	-5.66	1.45	1.52
6	Z	439	TYR	C-N	5.65	1.41	1.34
7	N	626	GLY	CA-C	-5.65	1.46	1.52
10	Q	416	VAL	CA-C	-5.65	1.45	1.52
3	T	48	ASN	C-N	5.64	1.42	1.33
6	Z	739	ALA	C-N	5.64	1.41	1.33
10	Q	80	HIS	ND1-CE1	5.64	1.38	1.32
10	Q	266	LEU	C-N	5.64	1.41	1.33
2	V	47	MET	C-N	5.64	1.41	1.33
9	P	403	GLU	C-O	5.64	1.30	1.23
10	Q	130	ARG	NE-CZ	5.64	1.39	1.33
10	Q	420	ASN	CA-CB	5.64	1.62	1.53
12	U	109	LEU	N-CA	-5.64	1.39	1.46
6	Z	787	ASP	CA-C	5.63	1.58	1.53
1	W	102	GLN	C-N	5.63	1.42	1.33
11	R	383	ARG	NE-CZ	5.63	1.39	1.33
6	Z	37	GLN	N-CA	-5.63	1.38	1.46
10	Q	249	LEU	C-N	5.63	1.41	1.33
7	N	249	ASN	CA-CB	5.62	1.62	1.53
2	V	254	ARG	CZ-NH1	5.62	1.40	1.32
8	S	258	GLU	CA-C	-5.62	1.45	1.52
1	W	135	ASN	N-CA	-5.62	1.39	1.46
10	Q	286	TYR	CA-CB	5.62	1.62	1.53
6	Z	858	GLY	CA-C	-5.62	1.44	1.51
8	S	468	ALA	CA-C	-5.61	1.45	1.52
7	N	423	LEU	C-N	5.61	1.41	1.34
8	S	36	LYS	C-N	5.61	1.40	1.33
11	R	158	LEU	CA-C	5.61	1.60	1.52
11	R	397	ASN	C-N	5.61	1.41	1.33
8	S	142	VAL	C-N	5.60	1.41	1.33
10	Q	80	HIS	CE1-NE2	-5.60	1.26	1.32
6	Z	263	ALA	CA-CB	5.60	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	504	GLU	CA-CB	5.60	1.62	1.53
8	S	302	HIS	ND1-CE1	5.60	1.38	1.32
6	Z	40	GLU	CA-C	-5.60	1.45	1.52
6	Z	246	CYS	N-CA	-5.59	1.39	1.46
8	S	177	ASN	N-CA	-5.59	1.39	1.46
13	O	386	ALA	N-CA	-5.59	1.39	1.46
6	Z	395	CYS	N-CA	-5.59	1.38	1.46
8	S	383	LEU	CA-CB	5.59	1.62	1.53
8	S	404	LEU	CA-CB	5.59	1.62	1.53
12	U	26	GLN	CA-C	-5.59	1.46	1.53
12	U	179	ARG	NE-CZ	5.59	1.39	1.33
10	Q	155	LEU	CA-C	-5.58	1.45	1.52
8	S	111	ARG	CA-C	-5.58	1.45	1.52
6	Z	798	ARG	CD-NE	5.58	1.54	1.46
6	Z	280	ASP	N-CA	-5.58	1.39	1.46
7	N	615	ALA	N-CA	-5.58	1.39	1.46
8	S	421	TYR	C-N	5.58	1.41	1.33
8	S	325	GLY	C-N	5.58	1.40	1.33
2	V	157	ARG	NE-CZ	5.57	1.39	1.33
9	P	398	LYS	CA-CB	5.57	1.60	1.53
3	T	47	GLN	C-N	5.57	1.40	1.33
13	O	216	ASP	CA-C	-5.57	1.45	1.52
6	Z	300	ALA	CA-C	-5.57	1.45	1.52
2	V	135	ARG	CZ-NH1	5.57	1.40	1.32
8	S	182	LYS	CA-CB	5.57	1.62	1.53
7	N	288	ASN	C-N	5.56	1.40	1.33
13	O	103	LYS	C-N	5.56	1.41	1.33
6	Z	375	ASP	CA-CB	5.56	1.63	1.53
12	U	203	LYS	N-CA	-5.56	1.39	1.46
13	O	247	ASN	C-N	5.56	1.40	1.33
2	V	20	ARG	CD-NE	5.56	1.54	1.46
9	P	39	LEU	CA-C	-5.56	1.45	1.52
11	R	63	TYR	CA-CB	5.56	1.61	1.53
7	N	573	HIS	C-N	5.56	1.41	1.33
9	P	96	MET	C-N	5.56	1.41	1.34
3	T	23	CYS	N-CA	5.55	1.52	1.46
7	N	35	LEU	N-CA	-5.55	1.39	1.46
6	Z	564	ARG	CZ-NH1	5.55	1.40	1.32
3	T	182	LYS	CA-C	-5.55	1.45	1.52
10	Q	78	ILE	CA-C	-5.55	1.47	1.52
7	N	776	TYR	CA-CB	5.55	1.59	1.52
9	P	4	ASP	CA-CB	5.55	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	220	GLN	CA-C	-5.54	1.45	1.52
4	X	62	ASP	CA-C	5.54	1.57	1.52
3	T	77	SER	C-N	5.54	1.41	1.33
8	S	373	LYS	CA-C	-5.54	1.45	1.52
10	Q	153	ASP	CA-C	-5.54	1.45	1.52
10	Q	372	GLN	C-N	5.54	1.40	1.33
3	T	186	ARG	CZ-NH1	5.54	1.40	1.32
7	N	222	TYR	N-CA	-5.54	1.38	1.46
13	O	94	GLU	CA-C	-5.54	1.45	1.52
7	N	326	SER	CA-C	-5.54	1.45	1.52
11	R	109	LYS	C-N	5.54	1.41	1.33
9	P	77	GLU	CA-CB	5.53	1.62	1.53
6	Z	233	LEU	CA-C	-5.53	1.45	1.52
6	Z	956	LEU	C-N	5.53	1.41	1.33
7	N	18	ASP	N-CA	-5.53	1.39	1.46
6	Z	710	SER	CA-CB	5.52	1.62	1.53
13	O	329	MET	CA-CB	5.52	1.61	1.53
2	V	30	SER	CA-C	-5.52	1.45	1.52
4	X	97	TYR	C-N	5.52	1.41	1.33
8	S	143	GLN	CA-C	-5.52	1.45	1.52
6	Z	922	PRO	C-N	5.52	1.40	1.33
8	S	126	LYS	N-CA	-5.52	1.39	1.46
6	Z	57	LYS	N-CA	-5.52	1.38	1.46
10	Q	91	SER	CA-C	-5.52	1.45	1.52
12	U	55	PRO	N-CA	-5.51	1.40	1.47
8	S	321	GLN	CA-C	-5.51	1.45	1.52
9	P	23	LYS	CA-C	-5.51	1.45	1.52
8	S	48	LEU	N-CA	-5.51	1.39	1.46
9	P	386	GLN	CA-CB	5.51	1.62	1.53
3	T	141	LEU	CA-C	-5.51	1.45	1.52
4	X	59	ARG	CZ-NH1	5.51	1.40	1.32
9	P	100	VAL	N-CA	5.51	1.53	1.46
9	P	395	ARG	CD-NE	5.51	1.53	1.46
11	R	60	ALA	CA-CB	-5.51	1.47	1.53
13	O	51	ASP	C-N	5.51	1.41	1.33
7	N	584	ARG	CZ-NH2	5.50	1.40	1.33
8	S	19	HIS	CA-C	-5.50	1.45	1.52
10	Q	71	LYS	C-N	5.50	1.41	1.33
6	Z	202	ARG	NE-CZ	5.50	1.39	1.33
12	U	21	HIS	CE1-NE2	5.50	1.38	1.32
13	O	259	THR	N-CA	-5.50	1.39	1.46
10	Q	327	GLY	C-O	-5.50	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	118	ASP	C-N	5.50	1.41	1.34
9	P	207	THR	C-N	5.50	1.41	1.33
7	N	321	LEU	N-CA	-5.49	1.39	1.46
11	R	222	ARG	CA-CB	5.49	1.62	1.53
2	V	100	ARG	NE-CZ	5.49	1.39	1.33
7	N	864	LYS	CA-C	5.49	1.59	1.52
4	X	117	LYS	N-CA	-5.49	1.39	1.46
6	Z	295	ARG	NE-CZ	5.49	1.39	1.33
8	S	448	LEU	N-CA	5.49	1.51	1.46
9	P	376	THR	C-N	5.49	1.41	1.33
12	U	63	SER	CA-C	-5.49	1.45	1.52
1	W	27	GLU	C-N	5.49	1.41	1.33
7	N	805	SER	N-CA	-5.49	1.39	1.46
6	Z	601	VAL	N-CA	5.48	1.53	1.46
7	N	11	ALA	CA-CB	-5.48	1.44	1.53
12	U	145	ASP	CA-C	5.48	1.60	1.52
13	O	206	THR	CA-C	-5.48	1.46	1.52
13	O	356	ARG	CZ-NH2	5.48	1.40	1.33
6	Z	79	THR	CA-C	-5.48	1.45	1.52
3	T	175	ASP	CA-CB	5.48	1.63	1.53
7	N	608	LEU	C-O	-5.48	1.17	1.24
7	N	727	THR	C-O	5.48	1.30	1.24
9	P	194	SER	N-CA	-5.48	1.39	1.46
13	O	337	LEU	CA-C	-5.48	1.45	1.52
1	W	38	GLN	N-CA	-5.47	1.39	1.46
4	X	62	ASP	CA-CB	5.47	1.60	1.54
6	Z	60	ASP	C-N	5.47	1.41	1.33
6	Z	214	HIS	ND1-CE1	5.47	1.38	1.32
8	S	298	ARG	NE-CZ	5.47	1.39	1.33
8	S	271	ARG	CD-NE	5.47	1.53	1.46
6	Z	925	VAL	CA-C	-5.47	1.46	1.52
9	P	344	ARG	NE-CZ	5.47	1.39	1.33
13	O	222	LEU	C-N	5.47	1.41	1.33
2	V	49	VAL	C-O	-5.47	1.17	1.23
7	N	607	GLN	CA-CB	5.47	1.61	1.53
11	R	179	PHE	N-CA	-5.47	1.39	1.46
6	Z	154	ILE	CA-C	-5.47	1.46	1.52
11	R	200	LYS	N-CA	-5.47	1.39	1.46
2	V	180	LEU	CA-C	-5.46	1.46	1.52
4	X	22	ARG	CZ-NH1	5.46	1.40	1.32
4	X	35	ILE	N-CA	-5.46	1.39	1.46
6	Z	161	ILE	C-O	-5.46	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	47	ALA	N-CA	-5.46	1.39	1.46
6	Z	525	MET	CA-CB	5.46	1.63	1.53
2	V	200	ASN	N-CA	-5.46	1.39	1.46
12	U	100	ARG	NE-CZ	5.45	1.39	1.33
1	W	170	HIS	ND1-CE1	5.45	1.38	1.32
7	N	586	ALA	C-O	-5.45	1.17	1.24
7	N	686	ILE	CA-C	-5.45	1.45	1.52
7	N	147	ALA	N-CA	-5.45	1.38	1.46
8	S	393	ARG	CA-C	-5.45	1.45	1.52
3	T	158	GLN	N-CA	5.45	1.52	1.46
13	O	388	GLY	C-O	-5.45	1.17	1.24
2	V	103	MET	CA-C	-5.44	1.46	1.52
6	Z	228	GLU	CA-C	-5.44	1.45	1.52
9	P	286	ASN	CA-CB	5.44	1.63	1.53
9	P	180	ILE	N-CA	-5.44	1.40	1.46
6	Z	333	GLY	N-CA	5.44	1.53	1.45
7	N	394	ARG	NE-CZ	5.44	1.39	1.33
7	N	549	TYR	CA-C	-5.44	1.46	1.52
9	P	155	GLU	N-CA	-5.44	1.39	1.46
3	T	42	PRO	CA-CB	-5.43	1.47	1.53
4	X	22	ARG	NE-CZ	5.43	1.39	1.33
6	Z	903	MET	C-O	-5.43	1.17	1.23
13	O	170	SER	CA-C	-5.43	1.45	1.52
6	Z	949	ILE	CA-C	5.43	1.59	1.52
12	U	179	ARG	CA-C	-5.43	1.45	1.52
7	N	519	VAL	N-CA	-5.43	1.39	1.46
13	O	128	LEU	N-CA	5.43	1.52	1.46
6	Z	225	LEU	CA-CB	5.43	1.62	1.53
13	O	222	LEU	C-O	-5.43	1.17	1.24
10	Q	244	GLU	C-N	5.43	1.40	1.33
5	Y	71	ASP	N-CA	-5.43	1.38	1.46
8	S	358	LYS	CA-CB	5.42	1.61	1.53
12	U	84	ASN	N-CA	-5.42	1.39	1.46
8	S	33	GLU	CA-C	-5.42	1.45	1.52
1	W	109	ARG	CA-C	-5.42	1.45	1.52
6	Z	379	GLN	C-N	5.42	1.41	1.33
13	O	125	GLY	N-CA	-5.42	1.39	1.45
11	R	233	ASP	C-N	5.42	1.41	1.33
3	T	94	HIS	CE1-NE2	-5.42	1.27	1.32
7	N	122	GLN	CA-C	5.42	1.59	1.53
9	P	121	THR	C-O	-5.42	1.17	1.24
12	U	16	LEU	N-CA	-5.42	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Q	336	ASN	C-N	5.42	1.41	1.33
11	R	129	GLU	CA-CB	-5.42	1.44	1.53
5	Y	81	LEU	CA-C	5.41	1.59	1.52
6	Z	476	ASP	CA-CB	5.41	1.61	1.53
6	Z	553	ARG	CZ-NH2	5.41	1.40	1.33
11	R	176	ARG	C-N	5.41	1.41	1.33
1	W	78	ASP	C-N	5.41	1.40	1.33
9	P	123	ARG	CZ-NH2	5.41	1.40	1.33
7	N	806	THR	CA-CB	-5.41	1.44	1.53
9	P	370	ASP	N-CA	-5.41	1.39	1.46
11	R	340	GLN	C-N	5.41	1.41	1.33
12	U	145	ASP	C-N	5.41	1.41	1.33
12	U	296	ILE	CA-C	-5.41	1.46	1.52
2	V	254	ARG	N-CA	-5.40	1.40	1.46
8	S	32	GLN	CA-C	-5.40	1.46	1.52
1	W	104	LYS	CA-CB	5.40	1.62	1.53
6	Z	470	ALA	C-N	5.40	1.40	1.33
9	P	357	TYR	N-CA	-5.40	1.39	1.46
7	N	335	ALA	CA-C	-5.40	1.45	1.52
7	N	407	GLY	C-N	5.40	1.41	1.33
6	Z	182	SER	C-N	5.39	1.41	1.33
13	O	224	GLY	N-CA	-5.39	1.39	1.45
7	N	180	SER	C-N	5.39	1.41	1.33
9	P	250	ILE	CA-C	-5.39	1.46	1.52
6	Z	774	ARG	CZ-NH2	5.39	1.40	1.33
12	U	176	ARG	CZ-NH2	5.39	1.40	1.33
3	T	81	TYR	N-CA	-5.39	1.40	1.46
4	X	70	PRO	N-CA	-5.39	1.40	1.47
13	O	210	ARG	CZ-NH1	5.39	1.40	1.32
13	O	369	ARG	NE-CZ	5.39	1.39	1.33
2	V	49	VAL	C-N	5.38	1.40	1.33
10	Q	309	ARG	N-CA	-5.38	1.39	1.46
13	O	215	TYR	CA-C	-5.38	1.46	1.52
6	Z	226	GLU	CA-C	-5.38	1.46	1.52
6	Z	597	SER	N-CA	5.38	1.53	1.46
12	U	69	ASP	N-CA	-5.38	1.39	1.46
6	Z	595	MET	N-CA	-5.38	1.39	1.46
7	N	72	LEU	N-CA	-5.38	1.39	1.46
6	Z	720	LYS	N-CA	-5.38	1.39	1.46
8	S	214	MET	CA-CB	5.38	1.61	1.53
9	P	199	LEU	N-CA	-5.37	1.39	1.46
8	S	489	GLN	C-N	5.37	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Q	356	CYS	CA-C	-5.37	1.45	1.52
12	U	60	GLU	CA-C	-5.37	1.45	1.52
7	N	810	ALA	CA-CB	5.37	1.62	1.53
3	T	62	LEU	C-N	5.36	1.40	1.33
6	Z	209	PRO	CA-CB	5.36	1.61	1.53
6	Z	421	SER	CA-C	5.36	1.60	1.52
9	P	338	TRP	C-O	-5.36	1.17	1.24
11	R	64	LYS	CA-CB	5.36	1.61	1.53
11	R	209	ARG	CZ-NH2	5.36	1.40	1.33
7	N	555	ILE	CA-C	-5.36	1.45	1.52
13	O	7	ILE	C-O	-5.36	1.18	1.24
13	O	199	LEU	CA-C	-5.36	1.45	1.52
4	X	98	PHE	C-N	5.36	1.41	1.33
6	Z	959	HIS	ND1-CE1	5.36	1.38	1.32
8	S	384	ARG	CD-NE	5.36	1.53	1.46
10	Q	8	LEU	CA-C	-5.36	1.45	1.52
11	R	325	HIS	CB-CG	5.36	1.57	1.50
3	T	101	LYS	C-N	5.35	1.40	1.33
3	T	198	ASP	C-N	5.35	1.40	1.33
3	T	246	GLU	C-N	5.35	1.41	1.33
4	X	51	ARG	NE-CZ	5.35	1.39	1.33
6	Z	568	LEU	C-N	5.35	1.41	1.33
12	U	106	ILE	N-CA	-5.35	1.40	1.46
7	N	97	PHE	C-N	5.35	1.40	1.33
7	N	345	ASP	CA-CB	5.35	1.62	1.53
7	N	916	LEU	CA-C	-5.35	1.46	1.52
9	P	35	ALA	CA-CB	-5.35	1.45	1.53
10	Q	307	ASN	CA-CB	5.35	1.61	1.53
10	Q	401	GLU	C-N	5.35	1.41	1.33
6	Z	380	ASN	CA-C	-5.34	1.46	1.52
7	N	666	GLN	CA-C	-5.34	1.46	1.53
7	N	394	ARG	CZ-NH2	5.34	1.40	1.33
11	R	401	HIS	ND1-CE1	5.34	1.37	1.32
6	Z	730	ALA	N-CA	-5.33	1.40	1.46
10	Q	195	LYS	CA-C	-5.33	1.46	1.52
10	Q	398	TYR	C-O	-5.33	1.17	1.24
8	S	472	HIS	CA-CB	5.33	1.61	1.53
13	O	117	ASN	CA-C	-5.33	1.45	1.52
13	O	202	SER	C-N	5.33	1.40	1.33
6	Z	528	LEU	CA-C	-5.33	1.45	1.52
8	S	387	VAL	CA-CB	5.33	1.60	1.54
1	W	192	LEU	CA-CB	5.33	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	221	ALA	C-N	5.33	1.40	1.33
11	R	359	VAL	CA-CB	-5.33	1.46	1.54
13	O	90	LYS	CA-C	-5.33	1.45	1.52
10	Q	6	SER	CA-C	-5.33	1.46	1.52
11	R	125	GLU	CA-CB	5.33	1.62	1.53
1	W	94	ALA	CA-C	5.32	1.59	1.52
9	P	315	GLN	C-N	5.32	1.40	1.33
4	X	17	TYR	CA-C	-5.32	1.45	1.52
9	P	203	ILE	N-CA	5.32	1.52	1.46
7	N	877	GLN	N-CA	-5.32	1.39	1.46
9	P	422	LEU	CA-CB	5.32	1.61	1.53
11	R	222	ARG	CZ-NH1	5.32	1.40	1.32
7	N	559	TYR	N-CA	-5.32	1.39	1.46
13	O	316	ALA	CA-C	-5.32	1.45	1.52
3	T	207	ALA	C-N	5.31	1.40	1.33
10	Q	340	ASP	CA-C	-5.31	1.45	1.52
8	S	277	SER	C-O	-5.31	1.18	1.24
12	U	187	SER	C-N	5.31	1.40	1.33
6	Z	445	PRO	N-CA	-5.30	1.40	1.47
7	N	312	GLY	CA-C	-5.30	1.44	1.51
6	Z	237	VAL	CA-C	-5.30	1.45	1.52
7	N	139	ARG	CZ-NH1	5.30	1.40	1.32
13	O	171	PHE	C-N	5.30	1.41	1.33
3	T	233	VAL	CA-C	-5.30	1.45	1.52
7	N	804	LEU	CA-C	-5.30	1.45	1.52
9	P	439	MET	CA-CB	5.30	1.61	1.53
11	R	200	LYS	CA-C	-5.30	1.46	1.52
13	O	186	ASN	CA-C	-5.30	1.45	1.52
5	Y	68	GLU	N-CA	5.29	1.52	1.46
7	N	351	ALA	C-O	5.29	1.30	1.24
8	S	174	ARG	CZ-NH2	5.29	1.40	1.33
9	P	397	ALA	N-CA	-5.29	1.39	1.46
1	W	25	ARG	NE-CZ	5.29	1.38	1.33
2	V	163	ALA	C-N	5.29	1.41	1.33
7	N	597	ARG	CZ-NH1	5.29	1.40	1.32
13	O	77	SER	CA-CB	5.29	1.61	1.53
6	Z	367	SER	C-N	5.29	1.38	1.33
7	N	105	SER	CA-C	-5.29	1.46	1.52
7	N	411	ILE	C-N	5.29	1.40	1.33
3	T	88	TYR	CA-CB	5.29	1.61	1.53
13	O	220	SER	CA-C	-5.29	1.46	1.52
1	W	91	LEU	C-N	5.28	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	531	LEU	CB-CG	5.28	1.64	1.53
8	S	145	PHE	CA-CB	5.28	1.61	1.53
7	N	11	ALA	C-N	-5.28	1.27	1.33
10	Q	375	GLY	C-N	5.28	1.41	1.33
11	R	403	LEU	C-N	5.28	1.40	1.33
7	N	601	THR	CA-C	5.28	1.60	1.52
7	N	786	ARG	CD-NE	5.28	1.53	1.46
11	R	295	SER	CA-C	5.28	1.59	1.52
6	Z	871	HIS	CD2-NE2	5.28	1.43	1.37
3	T	116	GLN	CA-C	5.28	1.60	1.52
7	N	858	LYS	CA-CB	5.28	1.60	1.52
3	T	105	LEU	N-CA	-5.27	1.39	1.46
9	P	230	HIS	CD2-NE2	5.27	1.43	1.37
8	S	277	SER	N-CA	-5.27	1.40	1.46
13	O	255	LEU	N-CA	-5.27	1.40	1.46
5	Y	84	TYR	C-O	-5.26	1.18	1.24
6	Z	327	GLN	C-N	5.26	1.41	1.33
7	N	448	LEU	CA-C	-5.26	1.46	1.52
1	W	99	LYS	CA-C	-5.26	1.45	1.52
3	T	236	ASN	N-CA	-5.26	1.39	1.46
8	S	144	LEU	N-CA	-5.26	1.40	1.46
9	P	166	GLU	C-N	5.26	1.40	1.33
13	O	97	LYS	CA-CB	5.26	1.61	1.53
6	Z	886	VAL	CA-CB	5.26	1.60	1.54
6	Z	405	ASN	N-CA	-5.25	1.40	1.46
11	R	325	HIS	CE1-NE2	-5.25	1.27	1.32
3	T	112	ASN	CA-C	-5.25	1.46	1.52
6	Z	345	GLU	CA-C	-5.25	1.46	1.52
11	R	143	GLN	CA-C	5.25	1.59	1.52
7	N	77	SER	N-CA	-5.25	1.39	1.46
12	U	121	LEU	C-N	5.25	1.39	1.33
3	T	68	ALA	N-CA	-5.25	1.40	1.46
7	N	650	ASP	CA-C	-5.25	1.46	1.52
7	N	672	ASN	C-O	-5.25	1.20	1.25
1	W	184	ASN	C-N	5.25	1.40	1.33
7	N	170	LEU	CA-C	5.25	1.59	1.52
8	S	48	LEU	CA-CB	5.25	1.61	1.53
9	P	131	PHE	C-N	5.25	1.40	1.33
10	Q	103	LYS	C-N	5.25	1.40	1.33
10	Q	148	LYS	CA-C	-5.25	1.45	1.52
6	Z	814	ALA	N-CA	-5.24	1.40	1.46
7	N	500	ASP	C-O	-5.24	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	185	ILE	CA-C	-5.24	1.46	1.52
3	T	102	LYS	CA-C	-5.24	1.46	1.52
4	X	20	ASP	CA-C	-5.24	1.45	1.52
11	R	117	ILE	C-N	5.24	1.40	1.33
12	U	178	VAL	CA-CB	-5.24	1.47	1.54
12	U	189	ARG	NE-CZ	5.24	1.38	1.33
2	V	84	ASP	N-CA	-5.24	1.39	1.46
6	Z	845	LEU	CB-CG	5.24	1.64	1.53
11	R	102	LEU	C-N	5.24	1.40	1.33
6	Z	718	ASP	CA-C	-5.24	1.46	1.52
4	X	73	THR	C-N	5.24	1.41	1.33
10	Q	408	THR	CA-C	5.23	1.59	1.52
6	Z	244	ARG	CD-NE	5.23	1.53	1.46
7	N	474	SER	CA-CB	5.23	1.62	1.53
12	U	5	HIS	ND1-CE1	5.23	1.37	1.32
6	Z	524	ALA	N-CA	-5.23	1.39	1.46
10	Q	25	GLN	CA-C	-5.23	1.45	1.52
8	S	135	ASN	C-O	-5.23	1.18	1.24
3	T	131	LYS	C-N	5.23	1.41	1.34
8	S	416	GLU	CA-CB	5.23	1.61	1.53
12	U	112	LYS	N-CA	-5.23	1.40	1.46
11	R	231	LEU	CB-CG	5.22	1.63	1.53
1	W	128	LEU	CA-C	-5.22	1.46	1.52
6	Z	295	ARG	CZ-NH2	5.22	1.40	1.33
6	Z	750	GLU	C-N	5.22	1.40	1.33
7	N	79	VAL	C-N	5.22	1.41	1.33
6	Z	12	ILE	C-N	5.22	1.41	1.33
2	V	116	CYS	N-CA	-5.22	1.40	1.46
9	P	410	GLN	CA-C	-5.22	1.46	1.52
6	Z	125	THR	CA-C	-5.21	1.45	1.52
6	Z	577	GLN	CA-C	-5.21	1.46	1.52
13	O	76	LEU	C-N	5.21	1.40	1.33
5	Y	41	ASP	CA-CB	5.21	1.61	1.53
8	S	473	ASP	N-CA	-5.21	1.40	1.46
7	N	728	LYS	CA-CB	5.21	1.61	1.53
8	S	41	ILE	CA-C	-5.21	1.45	1.52
3	T	192	ASN	CA-CB	5.21	1.61	1.53
4	X	100	TRP	N-CA	-5.21	1.39	1.46
7	N	665	ILE	C-O	-5.21	1.17	1.24
1	W	129	ALA	N-CA	-5.21	1.40	1.46
1	W	144	PHE	C-N	5.21	1.41	1.33
2	V	43	ALA	C-O	5.21	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	143	PRO	CA-CB	5.21	1.61	1.53
6	Z	73	GLU	C-O	-5.21	1.18	1.24
7	N	382	GLY	CA-C	-5.21	1.44	1.51
7	N	813	ARG	CA-C	-5.20	1.46	1.52
8	S	285	ASP	C-N	5.19	1.41	1.33
13	O	297	ILE	C-N	5.19	1.40	1.33
8	S	249	SER	CA-C	-5.19	1.46	1.52
9	P	187	SER	CA-C	5.19	1.59	1.52
11	R	163	SER	N-CA	5.19	1.52	1.46
12	U	47	ARG	CZ-NH1	5.19	1.40	1.32
6	Z	562	TRP	C-N	5.18	1.39	1.33
6	Z	792	VAL	N-CA	-5.18	1.40	1.46
8	S	298	ARG	CZ-NH2	5.18	1.40	1.33
8	S	453	ASP	N-CA	-5.18	1.39	1.46
4	X	27	ILE	C-N	5.18	1.40	1.33
9	P	147	LYS	CA-CB	5.18	1.61	1.53
9	P	266	TYR	C-O	-5.18	1.18	1.24
11	R	397	ASN	CA-C	-5.18	1.46	1.52
12	U	196	SER	CA-CB	5.18	1.61	1.53
2	V	139	VAL	N-CA	-5.18	1.40	1.46
6	Z	177	THR	CA-CB	-5.18	1.46	1.53
7	N	445	GLY	N-CA	-5.18	1.39	1.45
3	T	186	ARG	CA-C	-5.18	1.46	1.52
8	S	382	ARG	CA-CB	5.18	1.62	1.53
2	V	171	ARG	CZ-NH1	5.18	1.40	1.32
9	P	14	SER	CA-C	-5.18	1.46	1.52
9	P	286	ASN	C-N	5.18	1.40	1.33
10	Q	37	GLN	CA-CB	5.18	1.61	1.53
8	S	88	PHE	C-O	-5.17	1.18	1.24
8	S	170	TYR	CA-CB	5.17	1.61	1.53
7	N	776	TYR	C-N	5.17	1.39	1.33
7	N	462	VAL	C-N	5.17	1.40	1.33
7	N	666	GLN	CA-CB	5.17	1.61	1.53
13	O	281	ALA	C-N	5.17	1.41	1.33
13	O	317	THR	C-N	5.17	1.41	1.33
4	X	114	LEU	C-O	-5.17	1.17	1.23
7	N	535	LEU	C-N	5.17	1.40	1.33
8	S	116	ALA	N-CA	-5.17	1.40	1.46
3	T	183	SER	C-N	5.16	1.40	1.33
7	N	41	ASN	CA-C	-5.16	1.45	1.52
7	N	805	SER	CA-C	-5.16	1.45	1.52
9	P	201	ARG	CZ-NH2	5.16	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Q	103	LYS	C-O	-5.16	1.18	1.24
13	O	309	SER	CA-C	5.16	1.60	1.53
3	T	203	SER	CA-C	-5.16	1.46	1.52
7	N	154	LEU	N-CA	-5.16	1.40	1.46
7	N	917	ILE	CA-C	-5.16	1.46	1.52
8	S	399	TYR	CA-CB	5.16	1.61	1.53
10	Q	347	LEU	CA-CB	5.16	1.61	1.53
13	O	194	LEU	C-N	5.16	1.40	1.33
13	O	359	SER	C-N	5.16	1.40	1.33
6	Z	253	VAL	CA-CB	5.16	1.57	1.53
8	S	200	GLU	CA-C	-5.16	1.46	1.52
13	O	134	ALA	C-N	5.16	1.40	1.33
4	X	12	ALA	CA-CB	-5.16	1.44	1.53
6	Z	111	LEU	CA-C	5.16	1.59	1.52
8	S	422	MET	C-N	5.16	1.40	1.33
2	V	45	VAL	N-CA	-5.15	1.40	1.46
7	N	880	ARG	CD-NE	5.15	1.53	1.46
3	T	26	LEU	N-CA	-5.15	1.39	1.46
9	P	115	ARG	CZ-NH2	5.15	1.40	1.33
6	Z	532	HIS	CD2-NE2	5.15	1.43	1.37
6	Z	718	ASP	C-O	-5.15	1.18	1.24
13	O	356	ARG	C-N	5.15	1.40	1.34
13	O	369	ARG	CZ-NH2	5.15	1.40	1.33
9	P	162	GLU	CA-C	5.14	1.59	1.52
13	O	50	ASP	CA-C	-5.14	1.46	1.52
8	S	303	ASN	CA-C	-5.14	1.46	1.52
6	Z	549	ASN	N-CA	-5.14	1.40	1.46
12	U	223	HIS	CB-CG	-5.14	1.43	1.50
5	Y	86	ARG	CA-C	-5.14	1.46	1.52
8	S	142	VAL	CA-C	-5.14	1.46	1.52
8	S	485	LYS	C-N	5.14	1.40	1.33
13	O	330	ARG	CA-C	-5.13	1.46	1.52
13	O	382	LYS	N-CA	-5.13	1.40	1.46
6	Z	773	ARG	NE-CZ	5.13	1.38	1.33
8	S	204	ASP	CA-C	-5.13	1.46	1.52
9	P	154	ASP	C-N	5.13	1.40	1.33
9	P	385	ASN	CA-C	5.13	1.59	1.52
11	R	38	VAL	CA-C	-5.13	1.45	1.53
9	P	411	LEU	CA-CB	5.13	1.61	1.53
12	U	19	LEU	N-CA	-5.13	1.40	1.46
6	Z	627	LYS	N-CA	5.12	1.52	1.46
12	U	289	ASP	C-N	5.12	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	324	LYS	CA-CB	5.12	1.61	1.53
11	R	255	VAL	CA-CB	-5.12	1.48	1.54
10	Q	324	GLU	CA-C	-5.12	1.46	1.52
1	W	165	GLN	C-N	5.12	1.40	1.33
10	Q	51	ARG	CZ-NH1	5.12	1.40	1.32
10	Q	220	LEU	CB-CG	5.12	1.63	1.53
8	S	191	HIS	CB-CG	5.12	1.57	1.50
6	Z	493	LEU	CA-C	-5.11	1.46	1.52
4	X	11	ARG	CA-CB	5.11	1.60	1.53
6	Z	138	ARG	CZ-NH1	5.11	1.40	1.32
7	N	604	ARG	CZ-NH1	5.11	1.40	1.32
8	S	184	TRP	CZ2-CH2	5.11	1.47	1.37
7	N	684	SER	N-CA	-5.11	1.40	1.46
8	S	166	ASN	C-N	5.11	1.41	1.34
8	S	399	TYR	N-CA	-5.11	1.40	1.46
9	P	24	ILE	N-CA	-5.11	1.40	1.46
12	U	176	ARG	NE-CZ	5.11	1.38	1.33
13	O	119	SER	N-CA	-5.10	1.40	1.46
6	Z	55	ARG	CZ-NH1	5.10	1.39	1.32
9	P	391	ALA	C-N	-5.10	1.26	1.33
10	Q	152	LYS	N-CA	5.10	1.52	1.46
6	Z	313	ILE	N-CA	-5.10	1.40	1.46
9	P	276	LEU	CA-C	-5.10	1.46	1.52
13	O	132	GLU	C-N	5.10	1.40	1.33
6	Z	771	HIS	N-CA	-5.10	1.40	1.46
7	N	418	ASP	CA-C	5.10	1.59	1.52
10	Q	46	VAL	CA-C	-5.10	1.46	1.52
11	R	412	THR	C-O	-5.10	1.18	1.24
13	O	23	HIS	ND1-CE1	5.10	1.37	1.32
2	V	20	ARG	CZ-NH1	5.10	1.39	1.32
7	N	267	GLN	N-CA	-5.10	1.39	1.46
7	N	775	CYS	CA-CB	5.10	1.61	1.53
9	P	73	ASP	C-O	-5.10	1.18	1.24
1	W	170	HIS	CB-CG	-5.09	1.43	1.50
6	Z	204	CYS	CA-CB	5.09	1.61	1.53
7	N	15	GLU	CA-CB	5.09	1.61	1.53
7	N	606	VAL	N-CA	-5.09	1.39	1.46
12	U	268	LYS	CA-CB	5.09	1.61	1.53
7	N	731	VAL	C-N	5.09	1.40	1.33
13	O	390	SER	CA-C	-5.09	1.46	1.52
13	O	123	GLY	C-N	5.09	1.40	1.33
13	O	374	ASN	CA-CB	5.09	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	U	79	MET	N-CA	-5.09	1.40	1.46
1	W	152	GLU	CA-C	-5.09	1.46	1.52
8	S	414	ASP	C-N	5.09	1.40	1.33
11	R	209	ARG	NE-CZ	5.09	1.38	1.33
2	V	203	TYR	CA-C	-5.09	1.46	1.52
3	T	251	HIS	CD2-NE2	5.09	1.43	1.37
8	S	20	HIS	C-N	5.09	1.40	1.33
13	O	95	SER	C-O	-5.09	1.18	1.24
13	O	250	TRP	CA-C	-5.09	1.45	1.52
3	T	173	GLU	CA-C	-5.08	1.46	1.52
5	Y	27	LYS	CA-C	-5.08	1.46	1.52
9	P	404	LYS	N-CA	-5.08	1.40	1.46
1	W	101	ARG	NE-CZ	5.08	1.38	1.33
7	N	573	HIS	CB-CG	-5.08	1.43	1.50
8	S	28	GLU	CA-C	-5.08	1.46	1.52
11	R	137	LEU	CA-C	-5.08	1.46	1.52
13	O	177	GLN	N-CA	-5.08	1.40	1.46
7	N	121	GLU	N-CA	-5.08	1.39	1.46
7	N	222	TYR	C-N	5.08	1.40	1.33
7	N	688	ASN	CA-C	-5.08	1.46	1.52
9	P	86	HIS	N-CA	-5.07	1.39	1.46
3	T	113	LEU	C-N	5.07	1.40	1.33
1	W	109	ARG	CD-NE	5.07	1.53	1.46
7	N	106	ILE	C-N	5.07	1.40	1.33
7	N	870	ASN	N-CA	-5.07	1.39	1.46
9	P	289	ASN	CA-C	-5.07	1.45	1.52
13	O	296	LEU	CA-CB	5.07	1.61	1.53
9	P	395	ARG	CZ-NH1	5.07	1.39	1.32
11	R	38	VAL	C-O	5.07	1.30	1.24
3	T	107	SER	C-O	-5.07	1.18	1.24
9	P	193	TYR	N-CA	5.07	1.52	1.46
9	P	286	ASN	CG-ND2	5.07	1.43	1.33
10	Q	325	LEU	C-O	-5.07	1.18	1.24
2	V	24	LYS	C-N	5.07	1.40	1.33
4	X	88	ALA	CA-C	-5.07	1.46	1.52
7	N	730	VAL	CA-C	-5.07	1.46	1.52
9	P	293	LEU	CA-C	-5.07	1.46	1.52
10	Q	433	LEU	CA-C	5.07	1.59	1.52
2	V	167	ASN	CA-CB	5.06	1.61	1.53
3	T	47	GLN	CA-C	-5.06	1.46	1.52
8	S	326	ASP	C-N	5.06	1.38	1.33
2	V	20	ARG	NE-CZ	5.06	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O	222	LEU	CA-CB	5.06	1.61	1.53
13	O	301	PHE	CA-C	-5.06	1.46	1.52
6	Z	876	VAL	N-CA	-5.06	1.39	1.46
7	N	715	ILE	C-N	5.06	1.40	1.33
8	S	413	LEU	C-N	5.06	1.40	1.33
6	Z	766	HIS	CG-CD2	5.06	1.41	1.35
7	N	740	TRP	N-CA	-5.06	1.40	1.46
10	Q	402	THR	N-CA	5.06	1.52	1.46
12	U	21	HIS	CA-C	-5.06	1.45	1.52
13	O	231	GLY	C-N	5.06	1.40	1.33
1	W	4	GLU	CA-C	-5.06	1.46	1.52
6	Z	630	LYS	N-CA	-5.06	1.40	1.46
8	S	458	GLN	C-N	5.06	1.40	1.33
3	T	83	ASN	C-O	-5.05	1.18	1.24
6	Z	87	LYS	C-O	-5.05	1.20	1.24
7	N	696	LYS	N-CA	-5.05	1.40	1.46
8	S	125	LYS	CA-C	5.05	1.59	1.52
3	T	128	TYR	CA-C	-5.05	1.46	1.52
6	Z	489	ALA	CA-C	-5.05	1.46	1.52
7	N	255	ALA	CA-C	-5.05	1.46	1.52
7	N	506	GLN	N-CA	-5.05	1.40	1.46
7	N	812	ALA	CA-C	-5.05	1.46	1.52
7	N	897	LYS	CA-C	-5.05	1.46	1.52
6	Z	823	ASN	CA-C	-5.05	1.46	1.52
7	N	635	GLN	CA-CB	5.05	1.61	1.53
3	T	44	LEU	C-O	-5.05	1.16	1.23
6	Z	162	GLY	C-N	5.05	1.40	1.33
6	Z	925	VAL	CA-CB	-5.05	1.48	1.54
10	Q	280	ASN	N-CA	5.05	1.52	1.46
6	Z	169	VAL	C-N	5.04	1.39	1.33
1	W	97	THR	C-N	5.04	1.40	1.33
9	P	221	TYR	N-CA	-5.04	1.39	1.46
12	U	189	ARG	N-CA	-5.04	1.39	1.46
11	R	273	SER	C-N	5.04	1.40	1.33
13	O	146	ALA	C-O	-5.04	1.18	1.24
3	T	180	ILE	C-N	5.04	1.40	1.34
11	R	119	LYS	C-N	5.04	1.40	1.34
8	S	51	ARG	CZ-NH1	5.04	1.39	1.32
7	N	257	ILE	C-N	5.03	1.40	1.33
9	P	245	TYR	CZ-OH	5.03	1.48	1.38
11	R	263	ARG	NE-CZ	5.03	1.38	1.33
8	S	387	VAL	N-CA	-5.03	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	259	ILE	N-CA	-5.03	1.40	1.46
7	N	122	GLN	N-CA	-5.03	1.40	1.46
12	U	89	LEU	C-N	-5.03	1.29	1.33
6	Z	163	GLU	C-O	-5.03	1.18	1.24
12	U	283	ARG	CD-NE	5.03	1.53	1.46
1	W	69	PHE	CA-CB	5.03	1.61	1.53
3	T	227	PRO	C-N	5.03	1.40	1.33
11	R	23	ASN	CA-C	-5.03	1.46	1.52
11	R	131	ALA	C-N	5.03	1.40	1.33
6	Z	454	GLY	C-O	-5.02	1.17	1.23
7	N	296	CYS	CA-CB	5.02	1.61	1.53
8	S	477	VAL	CA-C	-5.02	1.46	1.52
6	Z	120	SER	N-CA	-5.02	1.40	1.46
6	Z	513	ALA	CA-CB	5.02	1.60	1.53
10	Q	86	MET	C-N	5.02	1.40	1.33
11	R	343	GLU	C-N	5.02	1.41	1.33
2	V	209	GLU	CA-C	-5.02	1.46	1.52
3	T	92	ASN	C-N	5.02	1.40	1.33
3	T	136	LEU	CA-C	5.02	1.59	1.52
6	Z	750	GLU	C-O	-5.02	1.18	1.23
12	U	80	CYS	C-N	5.02	1.40	1.34
13	O	55	THR	C-O	-5.02	1.17	1.24
6	Z	893	PHE	CA-C	-5.02	1.46	1.52
6	Z	8	LYS	C-N	5.01	1.40	1.33
7	N	198	THR	N-CA	-5.01	1.39	1.45
10	Q	289	GLU	N-CA	-5.01	1.40	1.46
4	X	70	PRO	CA-CB	-5.01	1.46	1.53
9	P	91	LEU	CA-CB	5.01	1.61	1.53
10	Q	87	GLN	C-O	5.01	1.29	1.24
12	U	240	GLY	C-N	5.01	1.40	1.33
13	O	38	TRP	CA-C	5.01	1.59	1.52
1	W	107	HIS	ND1-CE1	5.01	1.37	1.32
6	Z	292	ASP	C-O	-5.01	1.18	1.24
7	N	762	ARG	CZ-NH2	5.01	1.40	1.33
10	Q	399	VAL	C-N	5.01	1.40	1.33
11	R	405	LYS	CA-C	-5.01	1.46	1.52
2	V	286	GLU	CA-CB	5.01	1.61	1.53
3	T	27	LEU	C-N	5.01	1.39	1.33
7	N	868	VAL	CA-CB	-5.01	1.48	1.54
9	P	306	ASN	C-N	5.01	1.40	1.33
8	S	461	PHE	CA-C	-5.00	1.46	1.52
5	Y	86	ARG	CD-NE	5.00	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	383	LYS	CA-CB	5.00	1.61	1.53
9	P	291	LYS	N-CA	-5.00	1.39	1.46
11	R	378	ASN	CA-C	-5.00	1.47	1.53
12	U	79	MET	CA-C	-5.00	1.46	1.52
6	Z	76	LYS	N-CA	-5.00	1.40	1.46
9	P	136	ARG	N-CA	-5.00	1.40	1.46
11	R	352	SER	CA-C	-5.00	1.46	1.52

All (2566) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	99	TYR	CE1-CZ-OH	-22.86	51.30	119.90
13	O	62	TYR	CB-CA-C	-20.12	78.61	110.81
10	Q	77	PHE	CA-C-N	17.63	131.34	120.24
10	Q	77	PHE	C-N-CA	17.63	131.34	120.24
9	P	78	GLN	O-C-N	-17.38	99.48	122.59
6	Z	188	ALA	CB-CA-C	-16.53	82.62	110.56
6	Z	25	PRO	N-CA-CB	-15.22	87.27	103.25
8	S	59	ASP	CA-CB-CG	-14.94	97.66	112.60
6	Z	188	ALA	N-CA-CB	-13.79	90.43	110.56
6	Z	753	GLY	CA-C-N	12.13	136.20	120.44
6	Z	753	GLY	C-N-CA	12.13	136.20	120.44
9	P	329	PHE	CA-CB-CG	-11.52	102.28	113.80
11	R	373	PRO	CA-C-N	11.43	135.59	120.28
11	R	373	PRO	C-N-CA	11.43	135.59	120.28
3	T	170	ASN	CA-CB-CG	11.27	123.87	112.60
7	N	373	VAL	N-CA-C	-11.27	99.89	110.82
7	N	346	ASN	CA-CB-CG	-11.21	101.39	112.60
13	O	91	ASP	CA-CB-CG	-11.13	101.47	112.60
13	O	122	HIS	CA-CB-CG	-11.07	102.73	113.80
6	Z	532	HIS	N-CA-C	10.94	123.21	111.28
7	N	448	LEU	CA-C-N	10.91	132.31	119.99
7	N	448	LEU	C-N-CA	10.91	132.31	119.99
8	S	127	THR	N-CA-CB	10.86	127.38	110.44
9	P	313	ILE	N-CA-C	-10.81	102.26	111.56
11	R	21	VAL	O-C-N	-10.77	113.53	120.42
11	R	99	TYR	OH-CZ-CE2	10.76	152.16	119.90
9	P	370	ASP	N-CA-C	-10.66	98.44	110.91
4	X	91	PHE	CA-CB-CG	-10.48	103.32	113.80
10	Q	130	ARG	CA-C-N	10.32	135.08	120.53
10	Q	130	ARG	C-N-CA	10.32	135.08	120.53
6	Z	26	ASN	CA-CB-CG	-10.27	102.33	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	258	PRO	N-CA-C	10.25	123.21	110.70
10	Q	88	PHE	CA-CB-CG	-10.20	103.60	113.80
7	N	89	PHE	CA-C-N	10.14	133.87	120.28
7	N	89	PHE	C-N-CA	10.14	133.87	120.28
8	S	144	LEU	CA-C-N	10.13	133.86	120.28
8	S	144	LEU	C-N-CA	10.13	133.86	120.28
8	S	52	TYR	CA-C-N	10.09	133.27	120.56
8	S	52	TYR	C-N-CA	10.09	133.27	120.56
7	N	334	VAL	CA-C-O	-10.04	110.53	121.17
11	R	272	ASP	CA-CB-CG	-9.99	102.61	112.60
12	U	75	ASN	CA-CB-CG	-9.99	102.61	112.60
6	Z	84	ALA	N-CA-C	-9.75	101.06	113.16
6	Z	729	GLU	N-CA-C	-9.71	100.77	111.36
12	U	208	VAL	CA-C-O	-9.69	110.89	121.17
9	P	42	LEU	CA-C-O	-9.68	110.29	120.55
6	Z	518	LEU	CA-C-O	-9.62	108.58	120.23
13	O	230	PHE	CA-C-N	9.61	130.57	120.00
13	O	230	PHE	C-N-CA	9.61	130.57	120.00
9	P	78	GLN	CA-C-N	9.59	139.86	121.54
9	P	78	GLN	C-N-CA	9.59	139.86	121.54
8	S	364	ILE	CA-C-N	9.58	133.90	120.29
8	S	364	ILE	C-N-CA	9.58	133.90	120.29
13	O	313	ILE	N-CA-C	-9.58	100.56	111.00
6	Z	165	TYR	O-C-N	-9.57	111.98	122.12
10	Q	354	PHE	CB-CA-C	-9.51	91.22	109.66
3	T	53	ASN	CA-CB-CG	9.50	122.10	112.60
7	N	153	ALA	CA-C-N	9.50	133.78	120.29
7	N	153	ALA	C-N-CA	9.50	133.78	120.29
7	N	717	LEU	N-CA-C	-9.45	99.87	111.40
1	W	17	ARG	CA-C-N	9.41	134.17	120.90
1	W	17	ARG	C-N-CA	9.41	134.17	120.90
3	T	156	SER	CA-C-N	9.39	132.87	120.28
3	T	156	SER	C-N-CA	9.39	132.87	120.28
6	Z	737	ALA	CA-C-N	9.38	132.85	120.28
6	Z	737	ALA	C-N-CA	9.38	132.85	120.28
11	R	69	GLU	N-CA-C	9.37	124.52	113.18
10	Q	51	ARG	CA-C-N	9.35	133.16	120.54
10	Q	51	ARG	C-N-CA	9.35	133.16	120.54
7	N	87	ASP	CA-CB-CG	-9.34	103.27	112.60
8	S	65	ASN	CA-C-N	9.30	133.09	120.54
8	S	65	ASN	C-N-CA	9.30	133.09	120.54
8	S	419	VAL	CA-C-O	-9.27	111.02	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	260	THR	O-C-N	-9.27	109.79	122.30
7	N	602	VAL	N-CA-C	9.25	123.45	112.35
8	S	303	ASN	CA-C-N	9.25	133.05	120.38
8	S	303	ASN	C-N-CA	9.25	133.05	120.38
10	Q	94	VAL	CB-CA-C	-9.25	99.65	112.14
12	U	107	ASN	CA-C-N	9.24	134.35	120.31
12	U	107	ASN	C-N-CA	9.24	134.35	120.31
6	Z	405	ASN	CA-CB-CG	-9.21	103.39	112.60
11	R	68	GLU	O-C-N	-9.19	112.61	122.07
3	T	137	GLU	N-CA-C	-9.16	103.21	114.75
11	R	319	CYS	CA-C-N	9.16	132.55	120.28
11	R	319	CYS	C-N-CA	9.16	132.55	120.28
6	Z	26	ASN	CB-CA-C	-9.15	96.36	110.92
7	N	55	PHE	CA-CB-CG	-9.11	104.69	113.80
3	T	74	ASN	CA-C-N	9.05	132.76	120.54
3	T	74	ASN	C-N-CA	9.05	132.76	120.54
10	Q	11	ALA	CA-C-N	9.04	132.74	120.54
10	Q	11	ALA	C-N-CA	9.04	132.74	120.54
10	Q	334	HIS	CA-CB-CG	-9.03	104.77	113.80
12	U	177	ASP	CA-CB-CG	-9.03	103.57	112.60
11	R	261	LEU	CB-CA-C	9.02	125.62	109.83
8	S	414	ASP	CA-C-O	-8.99	111.38	120.82
3	T	117	ASN	OD1-CG-ND2	8.99	131.59	122.60
8	S	475	TYR	CA-C-N	8.98	132.31	120.28
8	S	475	TYR	C-N-CA	8.98	132.31	120.28
9	P	133	GLU	CA-C-N	8.96	131.85	120.56
9	P	133	GLU	C-N-CA	8.96	131.85	120.56
7	N	225	LEU	N-CA-C	8.95	121.04	111.28
7	N	548	ARG	CA-C-N	8.95	132.07	120.44
7	N	548	ARG	C-N-CA	8.95	132.07	120.44
7	N	125	THR	N-CA-C	-8.94	102.14	113.23
6	Z	811	SER	O-C-N	-8.91	112.67	122.12
13	O	216	ASP	CA-CB-CG	-8.91	103.69	112.60
9	P	402	PHE	CA-CB-CG	-8.86	104.94	113.80
3	T	92	ASN	N-CA-C	-8.84	91.97	110.80
9	P	327	LEU	N-CA-CB	8.82	125.40	110.49
11	R	325	HIS	ND1-CE1-NE2	8.81	117.21	108.40
6	Z	400	ILE	CA-C-N	8.78	132.49	120.46
6	Z	400	ILE	C-N-CA	8.78	132.49	120.46
8	S	490	ASN	CA-CB-CG	-8.78	103.82	112.60
12	U	247	ILE	N-CA-C	-8.76	102.30	110.53
8	S	326	ASP	CA-CB-CG	-8.76	103.84	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	204	SER	CA-C-O	-8.72	111.31	120.55
1	W	163	ASN	O-C-N	-8.71	116.14	121.71
8	S	317	HIS	N-CA-C	-8.71	101.87	111.36
7	N	678	ILE	N-CA-C	-8.69	102.08	110.42
8	S	23	LYS	N-CA-CB	8.69	122.61	110.01
8	S	33	GLU	CA-C-N	8.63	131.67	120.44
8	S	33	GLU	C-N-CA	8.63	131.67	120.44
6	Z	169	VAL	N-CA-CB	8.63	122.28	110.54
6	Z	418	ALA	CB-CA-C	-8.63	96.18	110.85
1	W	20	ASP	CA-CB-CG	-8.63	103.97	112.60
2	V	290	ASN	CA-CB-CG	-8.63	103.97	112.60
6	Z	625	THR	CA-C-N	8.62	128.21	119.24
6	Z	625	THR	C-N-CA	8.62	128.21	119.24
13	O	277	ILE	CA-C-O	-8.61	112.57	119.98
3	T	172	SER	N-CA-C	-8.59	103.92	114.75
9	P	420	ASP	CA-CB-CG	-8.59	104.01	112.60
6	Z	20	PRO	CA-C-O	-8.59	112.26	121.27
10	Q	365	ILE	N-CA-C	-8.58	102.19	110.42
6	Z	834	LEU	CA-C-N	8.57	131.77	120.28
6	Z	834	LEU	C-N-CA	8.57	131.77	120.28
12	U	288	PHE	CA-CB-CG	-8.57	105.23	113.80
7	N	483	LEU	CA-C-N	8.56	129.48	119.98
7	N	483	LEU	C-N-CA	8.56	129.48	119.98
13	O	156	THR	CA-C-O	8.55	129.79	120.82
6	Z	251	ALA	O-C-N	8.54	132.21	122.22
7	N	7	ALA	CA-C-N	8.53	128.12	119.24
7	N	7	ALA	C-N-CA	8.53	128.12	119.24
6	Z	297	VAL	O-C-N	8.52	130.76	121.90
11	R	374	ASN	OD1-CG-ND2	8.52	131.12	122.60
6	Z	8	LYS	N-CA-CB	8.52	122.56	110.04
7	N	158	LEU	N-CA-C	-8.51	101.95	111.14
6	Z	769	ASN	CA-CB-CG	-8.51	104.09	112.60
1	W	143	ASN	OD1-CG-ND2	-8.50	114.10	122.60
10	Q	220	LEU	N-CA-C	-8.50	102.10	111.36
9	P	398	LYS	N-CA-C	-8.49	98.69	111.34
7	N	99	GLU	CA-C-N	8.46	131.44	120.44
7	N	99	GLU	C-N-CA	8.46	131.44	120.44
7	N	432	GLY	O-C-N	8.46	126.59	121.85
8	S	162	VAL	CB-CA-C	8.46	122.38	111.81
10	Q	68	MET	N-CA-CB	8.45	124.86	110.50
8	S	72	GLU	CA-C-N	8.42	131.39	120.44
8	S	72	GLU	C-N-CA	8.42	131.39	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	348	VAL	CA-C-O	8.41	128.77	120.27
11	R	365	ASP	CA-CB-CG	-8.41	104.19	112.60
10	Q	67	THR	CA-C-N	8.41	136.84	121.70
10	Q	67	THR	C-N-CA	8.41	136.84	121.70
10	Q	171	LYS	CA-C-N	8.40	128.52	119.28
10	Q	171	LYS	C-N-CA	8.40	128.52	119.28
8	S	303	ASN	CA-CB-CG	-8.40	104.20	112.60
11	R	323	ASN	CA-C-O	8.40	129.64	120.82
6	Z	915	ALA	N-CA-C	-8.39	101.02	113.61
7	N	408	LEU	N-CA-C	-8.39	102.21	111.36
6	Z	285	ALA	N-CA-C	8.38	121.35	111.71
7	N	784	TYR	O-C-N	-8.37	112.67	121.30
8	S	274	PHE	CA-CB-CG	-8.37	105.43	113.80
7	N	596	LEU	CA-C-N	8.36	131.80	120.44
7	N	596	LEU	C-N-CA	8.36	131.80	120.44
8	S	323	LEU	CA-C-N	8.35	131.47	120.28
8	S	323	LEU	C-N-CA	8.35	131.47	120.28
9	P	18	LYS	N-CA-C	-8.35	100.85	112.45
3	T	239	SER	CA-C-N	8.35	131.29	120.44
3	T	239	SER	C-N-CA	8.35	131.29	120.44
10	Q	165	PHE	N-CA-C	-8.34	102.42	112.59
3	T	62	LEU	O-C-N	8.32	130.94	122.12
8	S	174	ARG	N-CA-CB	8.32	122.35	110.12
6	Z	76	LYS	N-CA-C	-8.31	104.28	114.75
7	N	640	VAL	N-CA-C	-8.31	102.15	110.62
6	Z	801	HIS	ND1-CE1-NE2	8.30	116.70	108.40
9	P	394	ASN	CA-CB-CG	8.30	120.90	112.60
3	T	251	HIS	CE1-NE2-CD2	-8.29	100.71	109.00
12	U	25	THR	N-CA-C	-8.28	103.19	113.38
1	W	157	PHE	CA-CB-CG	-8.28	105.52	113.80
10	Q	188	LEU	N-CA-C	-8.25	103.20	113.18
7	N	212	ASP	CA-CB-CG	-8.25	104.35	112.60
13	O	19	ASP	CA-C-O	-8.24	111.37	120.69
2	V	289	GLU	N-CA-CB	8.23	122.22	110.12
6	Z	865	ASP	CA-CB-CG	-8.21	104.39	112.60
11	R	255	VAL	CB-CA-C	-8.21	101.46	111.97
8	S	114	TYR	CA-C-O	-8.20	110.20	120.04
8	S	164	ILE	CA-C-N	8.20	127.92	119.56
8	S	164	ILE	C-N-CA	8.20	127.92	119.56
11	R	397	ASN	CA-C-O	-8.18	112.23	120.82
3	T	211	PHE	CA-CB-CG	-8.17	105.63	113.80
13	O	35	GLU	CA-C-N	8.17	137.14	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	35	GLU	C-N-CA	8.17	137.14	121.54
2	V	146	SER	N-CA-C	-8.15	103.05	113.16
4	X	27	ILE	CA-C-N	8.13	128.20	119.90
4	X	27	ILE	C-N-CA	8.13	128.20	119.90
8	S	360	PHE	CA-CB-CG	-8.13	105.67	113.80
12	U	183	ALA	O-C-N	8.13	132.63	122.55
11	R	146	ASP	CA-CB-CG	-8.13	104.47	112.60
6	Z	49	LEU	CA-C-N	8.12	131.15	120.28
6	Z	49	LEU	C-N-CA	8.12	131.15	120.28
11	R	260	THR	CA-C-N	-8.11	105.76	122.07
11	R	260	THR	C-N-CA	-8.11	105.76	122.07
7	N	499	HIS	CE1-NE2-CD2	-8.10	100.90	109.00
10	Q	177	VAL	N-CA-C	-8.09	102.55	110.72
10	Q	328	ASP	CA-CB-CG	-8.09	104.51	112.60
11	R	41	GLU	CA-C-N	8.08	131.11	120.28
11	R	41	GLU	C-N-CA	8.08	131.11	120.28
3	T	118	ASN	CA-C-N	8.08	132.59	120.31
3	T	118	ASN	C-N-CA	8.08	132.59	120.31
4	X	46	TRP	CE2-CD2-CE3	8.08	126.88	118.80
8	S	173	LEU	N-CA-C	-8.07	97.91	110.42
8	S	235	ASN	OD1-CG-ND2	8.07	130.68	122.60
12	U	144	LYS	CA-C-N	8.07	132.16	120.38
12	U	144	LYS	C-N-CA	8.07	132.16	120.38
11	R	54	ILE	N-CA-C	-8.05	102.96	110.53
6	Z	455	ILE	CA-C-O	-8.05	112.32	120.85
7	N	499	HIS	CG-CD2-NE2	8.05	115.25	107.20
8	S	429	ASP	CA-CB-CG	-8.05	104.55	112.60
13	O	230	PHE	CA-CB-CG	-8.04	105.76	113.80
2	V	124	ASN	CA-CB-CG	-8.04	104.56	112.60
7	N	485	MET	O-C-N	-8.03	113.80	122.07
3	T	62	LEU	CA-C-O	-8.03	112.04	120.55
7	N	591	LEU	CB-CA-C	-8.02	97.04	110.68
10	Q	381	ILE	N-CA-C	-8.02	102.72	110.42
11	R	296	LEU	N-CA-C	-8.02	102.48	111.14
2	V	265	GLU	CA-C-O	-8.01	112.06	120.55
12	U	266	THR	CA-C-N	8.01	131.43	120.46
12	U	266	THR	C-N-CA	8.01	131.43	120.46
2	V	189	ILE	N-CA-CB	8.00	121.42	110.54
6	Z	382	ALA	CB-CA-C	-7.99	97.52	110.79
11	R	99	TYR	CB-CA-C	7.97	123.49	110.90
7	N	539	MET	N-CA-C	-7.95	101.92	111.69
12	U	42	ASN	CA-CB-CG	-7.94	104.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	U	219	LEU	N-CA-C	-7.94	99.64	109.65
8	S	130	VAL	N-CA-C	-7.94	105.28	112.90
13	O	198	THR	CA-C-N	7.94	132.40	121.05
13	O	198	THR	C-N-CA	7.94	132.40	121.05
11	R	332	GLU	N-CA-C	-7.93	102.72	111.36
7	N	166	ILE	N-CA-C	-7.92	102.72	110.72
7	N	906	ARG	CA-C-N	7.92	133.00	122.30
7	N	906	ARG	C-N-CA	7.92	133.00	122.30
6	Z	801	HIS	CE1-NE2-CD2	-7.92	101.08	109.00
10	Q	420	ASN	CA-CB-CG	-7.91	104.69	112.60
12	U	101	ALA	N-CA-C	-7.91	103.21	113.17
8	S	469	ASN	CA-CB-CG	-7.91	104.69	112.60
6	Z	539	ASN	CA-CB-CG	-7.89	104.71	112.60
6	Z	761	PHE	O-C-N	-7.89	113.76	122.12
7	N	705	ILE	N-CA-C	-7.89	103.11	110.53
8	S	467	PHE	CA-CB-CG	-7.89	105.91	113.80
3	T	173	GLU	N-CA-CB	7.87	123.79	110.49
4	X	123	ASN	OD1-CG-ND2	7.87	130.47	122.60
3	T	130	ASP	N-CA-C	7.86	124.34	111.37
7	N	378	ASN	CA-CB-CG	-7.85	104.75	112.60
7	N	913	PRO	N-CA-CB	7.85	110.25	103.19
6	Z	433	LEU	CA-C-N	7.84	130.63	120.44
6	Z	433	LEU	C-N-CA	7.84	130.63	120.44
13	O	205	ILE	CA-C-N	7.84	131.84	120.71
13	O	205	ILE	C-N-CA	7.84	131.84	120.71
10	Q	314	PHE	CA-CB-CG	-7.82	105.98	113.80
9	P	413	ASN	OD1-CG-ND2	-7.81	114.79	122.60
6	Z	877	THR	CA-C-N	7.81	131.52	120.28
6	Z	877	THR	C-N-CA	7.81	131.52	120.28
1	W	156	GLU	CB-CG-CD	-7.79	99.35	112.60
6	Z	603	VAL	CA-C-N	7.78	128.62	119.98
6	Z	603	VAL	C-N-CA	7.78	128.62	119.98
8	S	184	TRP	CE2-CD2-CE3	7.76	126.56	118.80
7	N	614	ASN	CA-CB-CG	-7.76	104.84	112.60
7	N	19	SER	N-CA-CB	7.76	121.52	110.12
1	W	24	THR	N-CA-CB	7.75	125.48	111.37
3	T	56	MET	N-CA-C	7.75	119.73	111.28
10	Q	103	LYS	N-CA-CB	7.75	121.51	110.12
6	Z	7	LYS	N-CA-CB	7.75	122.07	110.53
10	Q	115	ILE	N-CA-C	7.74	117.85	110.42
10	Q	78	ILE	O-C-N	-7.74	114.57	120.07
8	S	48	LEU	CB-CA-C	-7.74	98.73	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	140	LEU	N-CA-C	-7.72	102.94	111.36
13	O	252	PHE	CA-C-O	7.72	128.74	120.55
3	T	66	ALA	CA-C-N	7.72	131.25	120.29
3	T	66	ALA	C-N-CA	7.72	131.25	120.29
3	T	155	GLY	N-CA-C	-7.72	104.06	115.72
6	Z	25	PRO	CB-CA-C	-7.72	98.82	111.56
12	U	127	GLN	OE1-CD-NE2	7.71	130.31	122.60
12	U	251	ASN	N-CA-CB	7.70	121.17	110.01
13	O	59	LEU	CB-CA-C	-7.69	98.50	110.81
8	S	334	HIS	CE1-NE2-CD2	-7.68	101.31	109.00
6	Z	342	LEU	N-CA-C	-7.68	103.52	113.12
6	Z	598	ALA	CA-C-N	7.68	130.98	120.46
6	Z	598	ALA	C-N-CA	7.68	130.98	120.46
7	N	880	ARG	N-CA-C	7.66	121.55	111.75
3	T	27	LEU	CA-C-O	-7.64	110.56	117.98
1	W	24	THR	N-CA-C	-7.64	97.43	109.50
10	Q	222	SER	CA-C-N	7.64	128.62	119.99
10	Q	222	SER	C-N-CA	7.64	128.62	119.99
7	N	415	PHE	CA-CB-CG	-7.64	106.16	113.80
11	R	26	VAL	N-CA-CB	7.63	119.48	110.55
8	S	456	ASP	CA-C-O	-7.63	111.61	118.63
6	Z	488	ALA	O-C-N	7.62	130.84	122.15
6	Z	288	LEU	N-CA-C	-7.62	102.92	111.07
10	Q	404	ASN	N-CA-C	7.62	120.14	110.24
11	R	215	GLY	CA-C-N	7.61	131.23	120.42
11	R	215	GLY	C-N-CA	7.61	131.23	120.42
8	S	139	HIS	CE1-NE2-CD2	-7.61	101.39	109.00
2	V	61	TYR	CB-CG-CD2	-7.61	109.39	120.80
7	N	761	ILE	CA-C-N	7.60	132.18	121.24
7	N	761	ILE	C-N-CA	7.60	132.18	121.24
8	S	277	SER	CA-C-N	7.60	130.32	120.44
8	S	277	SER	C-N-CA	7.60	130.32	120.44
4	X	37	PRO	N-CA-C	-7.59	101.84	114.75
11	R	295	SER	CA-C-N	7.59	130.76	120.44
11	R	295	SER	C-N-CA	7.59	130.76	120.44
8	S	48	LEU	N-CA-C	7.58	119.18	111.07
13	O	32	PHE	CA-CB-CG	-7.58	106.22	113.80
3	T	42	PRO	N-CA-C	-7.57	104.99	114.68
3	T	244	ASP	CA-CB-CG	7.56	120.16	112.60
6	Z	632	GLU	O-C-N	7.56	129.86	122.07
12	U	233	PHE	CA-CB-CG	-7.56	106.24	113.80
8	S	404	LEU	CA-C-N	7.55	130.74	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	404	LEU	C-N-CA	7.55	130.74	120.54
9	P	179	PHE	CA-CB-CG	-7.55	106.25	113.80
4	X	64	ILE	CA-C-O	7.54	127.30	120.96
6	Z	622	HIS	CB-CG-CD2	-7.54	121.40	131.20
3	T	258	ASN	CA-C-N	7.54	130.78	120.46
3	T	258	ASN	C-N-CA	7.54	130.78	120.46
4	X	102	GLN	N-CA-C	-7.52	103.56	112.89
3	T	116	GLN	N-CA-C	-7.52	103.56	112.89
3	T	48	ASN	OD1-CG-ND2	7.52	130.12	122.60
10	Q	180	LEU	CA-C-N	7.52	130.35	120.28
10	Q	180	LEU	C-N-CA	7.52	130.35	120.28
11	R	333	MET	CA-C-O	-7.52	112.45	120.42
3	T	109	TYR	N-CA-C	7.51	119.47	111.28
9	P	376	THR	N-CA-C	-7.50	103.04	111.07
8	S	152	LEU	CA-C-N	7.50	135.87	121.54
8	S	152	LEU	C-N-CA	7.50	135.87	121.54
12	U	201	GLN	OE1-CD-NE2	-7.50	115.10	122.60
13	O	212	GLN	OE1-CD-NE2	-7.49	115.11	122.60
8	S	351	ALA	CA-C-O	-7.48	112.62	120.55
6	Z	897	HIS	N-CA-C	-7.48	103.09	114.16
11	R	99	TYR	O-C-N	-7.48	114.02	122.09
9	P	381	SER	N-CA-C	-7.47	103.08	111.07
3	T	192	ASN	CA-CB-CG	-7.47	105.13	112.60
8	S	183	LEU	N-CA-CB	7.46	121.08	110.12
4	X	47	ASP	N-CA-CB	7.45	122.27	110.57
10	Q	252	HIS	CG-CD2-NE2	7.45	114.65	107.20
6	Z	935	THR	CA-C-O	7.44	128.55	120.58
7	N	387	ALA	CA-C-O	-7.44	111.12	118.34
6	Z	352	LYS	CA-C-N	7.44	126.28	120.33
6	Z	352	LYS	C-N-CA	7.44	126.28	120.33
3	T	113	LEU	CA-C-N	7.43	130.24	120.28
3	T	113	LEU	C-N-CA	7.43	130.24	120.28
3	T	152	LEU	CA-C-N	7.43	130.54	120.44
3	T	152	LEU	C-N-CA	7.43	130.54	120.44
10	Q	354	PHE	N-CA-C	7.43	121.58	109.85
9	P	431	HIS	O-C-N	7.42	130.61	122.15
11	R	217	HIS	N-CA-C	-7.42	103.13	111.07
13	O	108	GLU	CA-C-N	7.42	130.23	120.28
13	O	108	GLU	C-N-CA	7.42	130.23	120.28
4	X	47	ASP	CA-CB-CG	7.42	120.02	112.60
8	S	241	PHE	CA-CB-CG	-7.42	106.39	113.80
7	N	259	PHE	CA-CB-CG	-7.41	106.39	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	12	ASN	CA-C-N	7.41	134.14	120.95
1	W	12	ASN	C-N-CA	7.41	134.14	120.95
11	R	20	ARG	CA-C-N	7.41	126.26	120.33
11	R	20	ARG	C-N-CA	7.41	126.26	120.33
2	V	133	ASN	CA-CB-CG	7.41	120.01	112.60
7	N	250	ASP	CA-CB-CG	-7.41	105.19	112.60
7	N	263	SER	CA-C-N	7.40	130.51	120.44
7	N	263	SER	C-N-CA	7.40	130.51	120.44
3	T	177	PHE	CA-C-N	7.40	130.80	120.29
3	T	177	PHE	C-N-CA	7.40	130.80	120.29
12	U	275	VAL	N-CA-CB	7.40	119.21	110.55
10	Q	29	SER	CB-CA-C	7.40	122.64	110.81
7	N	726	ASP	CA-CB-CG	7.39	119.99	112.60
7	N	598	ASP	CA-CB-CG	-7.39	105.21	112.60
6	Z	892	SER	N-CA-C	7.38	120.94	110.23
1	W	153	LEU	N-CA-C	-7.38	103.32	111.36
9	P	101	MET	CA-C-N	7.38	130.50	120.54
9	P	101	MET	C-N-CA	7.38	130.50	120.54
12	U	106	ILE	O-C-N	7.37	129.02	121.87
12	U	223	HIS	CG-CD2-NE2	7.37	114.57	107.20
5	Y	78	LYS	CA-C-N	7.37	130.02	120.44
5	Y	78	LYS	C-N-CA	7.37	130.02	120.44
13	O	239	MET	N-CA-C	-7.37	104.82	113.88
13	O	23	HIS	CG-CD2-NE2	7.36	114.56	107.20
7	N	381	GLU	N-CA-C	-7.35	103.88	112.92
9	P	314	VAL	N-CA-C	-7.35	103.12	110.62
7	N	708	ALA	N-CA-C	7.34	120.63	110.35
6	Z	824	ASN	CA-CB-CG	-7.34	105.26	112.60
10	Q	421	LYS	CA-C-O	-7.34	112.64	120.42
6	Z	941	ARG	NE-CZ-NH2	7.34	125.81	119.20
6	Z	24	THR	CB-CA-C	7.33	124.61	110.17
7	N	425	ASN	CA-CB-CG	7.33	119.93	112.60
9	P	283	LYS	CA-C-O	7.33	128.19	120.42
9	P	431	HIS	CB-CA-C	-7.33	98.39	110.85
12	U	75	ASN	CB-CA-C	-7.33	98.39	110.85
7	N	100	THR	N-CA-C	-7.32	103.23	111.07
1	W	188	SER	CA-C-N	7.31	127.75	119.93
1	W	188	SER	C-N-CA	7.31	127.75	119.93
10	Q	190	ASN	CA-CB-CG	7.31	119.91	112.60
11	R	40	ILE	N-CA-C	-7.31	103.16	110.62
13	O	92	PHE	N-CA-C	-7.30	103.34	112.90
3	T	48	ASN	N-CA-C	-7.30	98.67	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	U	156	HIS	CE1-NE2-CD2	-7.29	101.71	109.00
7	N	900	ASN	O-C-N	-7.28	113.91	122.87
10	Q	354	PHE	CA-CB-CG	7.28	121.08	113.80
8	S	473	ASP	CA-CB-CG	7.28	119.88	112.60
13	O	142	ASP	N-CA-C	-7.27	95.31	110.80
6	Z	425	ILE	CA-C-O	7.27	128.35	120.57
6	Z	433	LEU	CA-C-O	7.26	128.25	120.55
1	W	170	HIS	ND1-CE1-NE2	7.26	115.66	108.40
7	N	488	CYS	O-C-N	7.26	129.93	122.09
8	S	367	TYR	CA-C-N	7.25	130.31	120.38
8	S	367	TYR	C-N-CA	7.25	130.31	120.38
9	P	352	VAL	O-C-N	7.25	129.30	121.83
13	O	286	PHE	CA-CB-CG	-7.25	106.55	113.80
8	S	394	ILE	N-CA-C	-7.25	103.47	110.42
1	W	152	GLU	CA-C-N	7.24	130.58	120.29
1	W	152	GLU	C-N-CA	7.24	130.58	120.29
9	P	260	VAL	O-C-N	7.24	129.00	121.91
3	T	82	PHE	CA-C-N	7.23	130.30	120.54
3	T	82	PHE	C-N-CA	7.23	130.30	120.54
5	Y	71	ASP	CA-CB-CG	-7.23	105.37	112.60
7	N	375	HIS	CB-CG-CD2	-7.23	121.80	131.20
11	R	27	SER	N-CA-CB	7.23	120.86	110.16
3	T	251	HIS	ND1-CE1-NE2	7.22	115.62	108.40
13	O	32	PHE	O-C-N	7.22	129.78	122.12
6	Z	593	HIS	N-CA-C	-7.21	101.73	108.22
7	N	50	TYR	O-C-N	7.20	130.36	122.15
3	T	43	ASP	CA-CB-CG	-7.20	105.40	112.60
8	S	239	ARG	N-CA-C	-7.20	103.47	111.82
2	V	285	ASP	N-CA-C	7.19	119.19	111.36
7	N	475	ALA	CA-C-O	-7.18	112.94	120.55
9	P	51	ASP	N-CA-CB	7.18	120.48	110.07
5	Y	31	GLU	N-CA-CB	7.17	122.60	110.49
6	Z	397	ASP	CA-CB-CG	7.17	119.77	112.60
9	P	162	GLU	CA-C-O	-7.17	112.83	120.42
6	Z	98	ASP	CA-C-O	-7.16	112.96	120.55
6	Z	507	GLY	O-C-N	-7.16	113.69	122.71
11	R	271	ILE	CA-C-O	-7.16	111.83	120.78
2	V	258	GLU	CB-CG-CD	-7.16	100.44	112.60
3	T	251	HIS	CG-CD2-NE2	7.16	114.36	107.20
11	R	216	ILE	N-CA-C	-7.15	103.50	110.72
11	R	199	GLU	N-CA-C	-7.14	104.60	113.38
13	O	66	VAL	CA-CB-CG2	-7.14	98.26	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	733	VAL	O-C-N	-7.14	114.95	121.87
2	V	273	ARG	NE-CZ-NH1	-7.13	114.37	121.50
6	Z	169	VAL	O-C-N	7.13	128.79	121.87
9	P	348	HIS	N-CA-C	-7.12	102.93	111.69
10	Q	398	TYR	N-CA-CB	7.12	122.04	110.43
13	O	348	VAL	N-CA-CB	7.12	121.50	111.82
7	N	329	HIS	O-C-N	7.11	129.66	122.12
8	S	423	VAL	N-CA-C	-7.11	103.59	110.42
6	Z	183	LYS	CA-C-N	7.11	132.80	122.36
6	Z	183	LYS	C-N-CA	7.11	132.80	122.36
3	T	107	SER	CA-C-N	7.10	129.79	120.28
3	T	107	SER	C-N-CA	7.10	129.79	120.28
6	Z	104	ASP	CA-CB-CG	7.10	119.70	112.60
6	Z	3	ASP	O-C-N	-7.10	114.94	123.10
3	T	202	LEU	O-C-N	7.09	129.47	122.09
6	Z	24	THR	CA-C-N	7.09	128.70	119.84
6	Z	24	THR	C-N-CA	7.09	128.70	119.84
10	Q	6	SER	CA-C-O	-7.09	113.38	120.82
3	T	265	ASP	N-CA-C	-7.08	103.49	111.14
6	Z	9	GLN	CA-C-O	-7.08	112.92	120.42
9	P	431	HIS	N-CA-CB	7.08	120.64	110.16
10	Q	296	ILE	CA-C-N	7.08	129.76	120.28
10	Q	296	ILE	C-N-CA	7.08	129.76	120.28
11	R	147	LYS	CA-C-N	7.08	129.76	120.28
11	R	147	LYS	C-N-CA	7.08	129.76	120.28
10	Q	331	THR	O-C-N	7.07	129.36	122.07
2	V	85	ASP	CA-CB-CG	-7.07	105.53	112.60
6	Z	930	GLY	CA-C-N	7.06	134.14	122.07
6	Z	930	GLY	C-N-CA	7.06	134.14	122.07
13	O	374	ASN	O-C-N	7.06	130.20	122.15
8	S	191	HIS	CA-C-N	7.05	129.73	120.28
8	S	191	HIS	C-N-CA	7.05	129.73	120.28
7	N	226	ASN	CA-CB-CG	-7.05	105.55	112.60
13	O	204	SER	N-CA-C	-7.05	103.60	111.28
6	Z	8	LYS	CA-C-N	7.05	130.30	120.29
6	Z	8	LYS	C-N-CA	7.05	130.30	120.29
6	Z	276	ASN	CA-CB-CG	7.04	119.64	112.60
8	S	128	ILE	N-CA-C	-7.04	98.36	108.42
12	U	27	THR	CA-CB-OG1	7.03	120.15	109.60
8	S	328	PRO	N-CA-CB	7.03	109.87	103.33
8	S	413	LEU	CA-C-O	7.03	129.03	121.16
13	O	181	PHE	N-CA-CB	7.03	120.20	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	113	LYS	CA-C-O	7.03	127.87	120.42
9	P	128	ASN	N-CA-CB	7.03	120.44	109.83
9	P	393	VAL	O-C-N	-7.02	115.98	123.14
7	N	636	SER	N-CA-C	-7.02	103.63	111.28
13	O	252	PHE	O-C-N	-7.02	114.68	122.12
11	R	143	GLN	N-CA-CB	7.02	120.44	110.12
2	V	161	THR	N-CA-C	-7.01	103.72	111.36
12	U	190	LEU	N-CA-C	-7.01	103.57	111.14
8	S	126	LYS	CB-CA-C	7.00	124.35	110.42
7	N	409	GLY	CA-C-O	-7.00	113.54	120.75
4	X	92	SER	CA-C-N	6.99	132.64	122.36
4	X	92	SER	C-N-CA	6.99	132.64	122.36
3	T	125	GLU	CA-C-N	6.99	129.64	120.28
3	T	125	GLU	C-N-CA	6.99	129.64	120.28
7	N	650	ASP	CA-CB-CG	-6.99	105.61	112.60
12	U	194	LEU	O-C-N	6.99	130.11	122.15
13	O	189	TYR	N-CA-C	6.98	118.68	111.14
13	O	244	ASN	CA-CB-CG	-6.98	105.62	112.60
9	P	378	THR	N-CA-C	6.98	118.89	111.28
12	U	64	ASP	CA-CB-CG	-6.97	105.63	112.60
6	Z	176	GLU	CA-C-O	-6.96	112.23	120.10
8	S	59	ASP	CA-C-N	6.96	129.49	120.44
8	S	59	ASP	C-N-CA	6.96	129.49	120.44
3	T	201	PRO	CA-C-N	6.96	129.94	120.54
3	T	201	PRO	C-N-CA	6.96	129.94	120.54
2	V	279	HIS	CA-CB-CG	-6.96	106.84	113.80
9	P	10	ASP	N-CA-CB	6.96	120.10	110.01
13	O	181	PHE	N-CA-C	-6.96	103.63	111.07
9	P	440	HIS	CA-C-O	-6.95	108.98	120.80
7	N	925	ASP	CA-C-O	-6.94	109.00	120.80
8	S	80	VAL	N-CA-C	-6.94	100.07	108.53
4	X	133	SER	CA-C-O	-6.93	109.01	120.80
11	R	424	THR	CA-C-O	-6.93	109.02	120.80
9	P	359	ARG	N-CA-C	-6.93	97.67	109.24
7	N	804	LEU	CB-CA-C	-6.93	99.29	110.79
8	S	324	MET	N-CA-C	-6.93	103.73	111.28
8	S	492	LYS	CA-C-O	-6.92	109.03	120.80
6	Z	855	LEU	CA-C-N	6.92	130.12	120.29
6	Z	855	LEU	C-N-CA	6.92	130.12	120.29
2	V	128	SER	CB-CA-C	-6.92	99.31	110.79
7	N	721	ASP	CA-CB-CG	-6.92	105.68	112.60
10	Q	270	ILE	CA-C-N	6.91	130.10	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	270	ILE	C-N-CA	6.91	130.10	120.29
8	S	477	VAL	O-C-N	-6.91	115.14	121.91
10	Q	378	SER	CA-C-N	6.91	129.53	120.28
10	Q	378	SER	C-N-CA	6.91	129.53	120.28
6	Z	583	ASP	CA-CB-CG	-6.90	105.70	112.60
7	N	580	ASN	N-CA-CB	6.89	120.24	109.83
8	S	392	ILE	N-CA-C	-6.89	102.63	112.35
8	S	432	ILE	N-CA-C	-6.89	104.13	110.82
13	O	236	HIS	CA-C-N	6.89	128.46	119.84
13	O	236	HIS	C-N-CA	6.89	128.46	119.84
8	S	110	LEU	N-CA-C	-6.89	102.14	113.50
6	Z	206	ASP	N-CA-C	-6.88	105.82	114.56
3	T	195	LEU	N-CA-C	-6.88	103.84	111.82
7	N	58	ARG	O-C-N	-6.87	114.83	122.12
6	Z	757	SER	CA-C-N	6.87	129.37	120.44
6	Z	757	SER	C-N-CA	6.87	129.37	120.44
13	O	348	VAL	O-C-N	-6.87	116.04	123.18
8	S	296	ALA	CA-C-N	6.86	129.34	120.56
8	S	296	ALA	C-N-CA	6.86	129.34	120.56
12	U	245	ASP	N-CA-CB	6.86	120.31	110.16
13	O	331	ALA	N-CA-C	6.86	118.83	111.36
5	Y	80	GLU	CB-CA-C	-6.85	100.07	110.90
8	S	486	LYS	CA-C-O	-6.85	113.29	120.55
6	Z	7	LYS	CB-CA-C	-6.84	97.74	109.65
7	N	202	PHE	CA-CB-CG	-6.84	106.95	113.80
8	S	370	LEU	CA-C-N	6.84	130.01	120.29
8	S	370	LEU	C-N-CA	6.84	130.01	120.29
8	S	420	GLU	CB-CG-CD	-6.84	100.96	112.60
7	N	147	ALA	CA-C-N	6.84	132.73	122.68
7	N	147	ALA	C-N-CA	6.84	132.73	122.68
8	S	203	SER	CB-CA-C	-6.84	99.44	110.79
10	Q	379	GLN	N-CA-CB	6.84	120.17	110.12
13	O	203	THR	N-CA-C	-6.84	104.51	112.92
11	R	327	ASP	CA-C-O	6.83	127.66	120.42
11	R	421	VAL	N-CA-CB	6.83	120.82	110.58
7	N	762	ARG	N-CA-C	-6.82	99.56	109.59
13	O	352	TRP	CD2-CE2-CZ2	-6.82	115.58	122.40
6	Z	451	ALA	CA-C-O	6.82	127.78	120.55
3	T	112	ASN	CA-CB-CG	6.82	119.42	112.60
10	Q	92	LYS	CA-C-N	6.82	129.74	120.54
10	Q	92	LYS	C-N-CA	6.82	129.74	120.54
11	R	391	ASN	N-CA-CB	6.81	119.98	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	650	ASP	N-CA-CB	6.81	120.13	110.12
3	T	249	MET	O-C-N	-6.81	114.85	122.75
7	N	740	TRP	N-CA-C	-6.80	103.10	111.40
10	Q	275	ILE	N-CA-C	-6.80	106.60	113.47
12	U	236	LEU	CA-C-N	6.80	128.34	119.84
12	U	236	LEU	C-N-CA	6.80	128.34	119.84
13	O	14	LEU	CA-C-O	-6.80	113.21	120.42
6	Z	904	LEU	CA-C-N	6.80	134.52	121.54
6	Z	904	LEU	C-N-CA	6.80	134.52	121.54
10	Q	234	THR	CA-C-O	-6.79	113.22	120.42
12	U	16	LEU	N-CA-CB	6.79	119.86	110.01
3	T	117	ASN	CA-CB-CG	6.79	119.39	112.60
7	N	630	ALA	CA-C-O	-6.79	113.30	120.63
10	Q	301	ALA	CA-C-N	6.79	129.76	120.46
10	Q	301	ALA	C-N-CA	6.79	129.76	120.46
7	N	268	GLN	CB-CG-CD	-6.79	101.07	112.60
9	P	125	VAL	CA-C-N	6.78	134.50	121.54
9	P	125	VAL	C-N-CA	6.78	134.50	121.54
7	N	685	VAL	O-C-N	6.78	128.44	121.87
10	Q	292	GLN	OE1-CD-NE2	-6.78	115.82	122.60
3	T	28	PRO	CA-C-N	6.78	126.29	119.24
3	T	28	PRO	C-N-CA	6.78	126.29	119.24
7	N	738	GLN	OE1-CD-NE2	6.78	129.38	122.60
2	V	89	ALA	O-C-N	6.77	129.04	122.07
9	P	176	LYS	CA-C-N	6.77	129.33	120.60
9	P	176	LYS	C-N-CA	6.77	129.33	120.60
13	O	23	HIS	O-C-N	-6.77	114.46	120.48
8	S	487	THR	CA-C-O	-6.76	113.25	120.42
11	R	358	GLY	N-CA-C	-6.76	104.92	116.01
1	W	9	VAL	N-CA-CB	6.76	119.97	111.46
7	N	338	PHE	CA-CB-CG	6.75	120.55	113.80
8	S	308	GLY	CA-C-O	-6.75	114.09	121.05
12	U	122	ILE	O-C-N	6.75	130.52	122.62
6	Z	224	LEU	CA-C-N	6.75	130.18	120.79
6	Z	224	LEU	C-N-CA	6.75	130.18	120.79
7	N	288	ASN	OD1-CG-ND2	6.75	129.35	122.60
8	S	153	GLU	CA-C-N	6.75	129.22	120.44
8	S	153	GLU	C-N-CA	6.75	129.22	120.44
9	P	343	LYS	N-CA-CB	6.75	120.00	109.94
7	N	190	LEU	N-CA-C	-6.75	104.01	111.36
11	R	227	ALA	CA-C-N	6.75	129.32	120.28
11	R	227	ALA	C-N-CA	6.75	129.32	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	413	LEU	CA-C-N	6.74	129.21	120.44
8	S	413	LEU	C-N-CA	6.74	129.21	120.44
10	Q	106	GLN	O-C-N	6.74	129.01	122.07
13	O	297	ILE	CA-C-O	6.74	127.75	120.47
6	Z	771	HIS	O-C-N	6.73	129.01	122.07
3	T	196	SER	N-CA-C	6.73	118.27	111.07
10	Q	428	GLU	N-CA-C	-6.73	104.02	111.36
13	O	144	VAL	N-CA-CB	6.73	119.19	110.57
6	Z	827	LEU	N-CA-C	-6.73	103.87	111.14
6	Z	246	CYS	CA-C-N	6.73	129.84	120.29
6	Z	246	CYS	C-N-CA	6.73	129.84	120.29
10	Q	71	LYS	CA-C-N	6.73	129.29	120.28
10	Q	71	LYS	C-N-CA	6.73	129.29	120.28
2	V	87	PHE	O-C-N	6.72	129.81	122.15
6	Z	901	PHE	N-CA-C	-6.72	105.06	112.72
6	Z	936	VAL	CA-C-N	6.72	134.58	121.41
6	Z	936	VAL	C-N-CA	6.72	134.58	121.41
9	P	130	ILE	O-C-N	-6.71	114.18	122.57
8	S	201	ILE	CA-C-N	6.71	130.51	120.31
8	S	201	ILE	C-N-CA	6.71	130.51	120.31
13	O	235	HIS	CA-CB-CG	6.71	120.51	113.80
8	S	189	LEU	CA-C-N	6.71	129.27	120.28
8	S	189	LEU	C-N-CA	6.71	129.27	120.28
6	Z	726	GLU	N-CA-C	6.71	118.67	111.36
10	Q	163	ARG	NE-CZ-NH2	-6.71	113.16	119.20
9	P	48	GLN	CA-C-O	6.71	127.86	120.82
7	N	796	VAL	N-CA-C	-6.70	103.95	110.72
6	Z	497	PHE	CA-CB-CG	-6.70	107.10	113.80
6	Z	64	TYR	N-CA-C	-6.70	104.15	112.72
7	N	515	ARG	CA-C-N	6.70	127.41	119.98
7	N	515	ARG	C-N-CA	6.70	127.41	119.98
2	V	23	THR	N-CA-C	-6.70	99.11	109.76
7	N	199	ASN	O-C-N	6.70	131.40	122.96
11	R	138	GLY	O-C-N	6.70	129.34	122.24
12	U	256	ASN	OD1-CG-ND2	-6.70	115.91	122.60
8	S	468	ALA	N-CA-C	6.69	118.57	111.28
9	P	47	ARG	CA-C-N	6.68	129.13	120.44
9	P	47	ARG	C-N-CA	6.68	129.13	120.44
3	T	225	ASN	CA-CB-CG	-6.68	105.92	112.60
6	Z	549	ASN	N-CA-C	-6.68	104.08	111.36
4	X	41	GLU	CA-C-N	6.68	129.12	120.44
4	X	41	GLU	C-N-CA	6.68	129.12	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	81	TYR	N-CA-CB	6.67	119.69	110.01
8	S	164	ILE	CA-C-O	-6.67	111.01	119.95
11	R	99	TYR	CA-C-N	6.67	129.54	120.54
11	R	99	TYR	C-N-CA	6.67	129.54	120.54
7	N	784	TYR	CA-C-N	6.67	128.17	119.84
7	N	784	TYR	C-N-CA	6.67	128.17	119.84
11	R	164	THR	CA-C-N	6.67	127.52	119.99
11	R	164	THR	C-N-CA	6.67	127.52	119.99
1	W	170	HIS	CE1-NE2-CD2	-6.66	102.34	109.00
12	U	252	HIS	CE1-NE2-CD2	-6.66	102.34	109.00
6	Z	615	LEU	N-CA-C	6.66	119.10	111.11
9	P	416	SER	N-CA-CB	6.66	119.67	110.01
7	N	318	LYS	CB-CA-C	-6.66	99.73	110.79
12	U	292	ILE	CA-C-O	6.66	127.87	120.95
12	U	181	GLN	N-CA-C	-6.65	104.74	112.92
8	S	26	ALA	CA-C-O	6.65	127.80	120.82
11	R	32	LEU	O-C-N	6.65	129.27	122.09
9	P	311	TRP	CA-C-O	-6.64	111.89	118.34
10	Q	252	HIS	CE1-NE2-CD2	-6.64	102.36	109.00
13	O	8	ASP	CA-CB-CG	-6.64	105.96	112.60
4	X	51	ARG	CB-CA-C	-6.64	99.82	109.45
6	Z	622	HIS	CA-CB-CG	6.64	120.44	113.80
6	Z	9	GLN	O-C-N	6.63	129.71	122.15
13	O	327	LEU	N-CA-C	6.63	118.51	111.28
8	S	376	THR	CA-C-N	6.63	129.16	120.28
8	S	376	THR	C-N-CA	6.63	129.16	120.28
9	P	193	TYR	CA-CB-CG	-6.63	101.97	113.90
7	N	613	HIS	CE1-NE2-CD2	-6.62	102.38	109.00
3	T	265	ASP	CA-CB-CG	-6.62	105.98	112.60
9	P	312	PRO	N-CA-C	-6.61	105.89	114.03
11	R	353	MET	O-C-N	6.61	129.69	122.15
1	W	187	SER	O-C-N	-6.61	112.78	122.43
6	Z	809	MET	O-C-N	6.61	129.23	122.09
6	Z	866	VAL	O-C-N	6.61	128.39	121.91
6	Z	432	GLY	CA-C-N	6.60	129.12	120.28
6	Z	432	GLY	C-N-CA	6.60	129.12	120.28
6	Z	961	GLU	CA-C-N	6.60	129.44	120.54
6	Z	961	GLU	C-N-CA	6.60	129.44	120.54
13	O	23	HIS	CE1-NE2-CD2	-6.60	102.40	109.00
7	N	21	LYS	CA-C-N	6.60	129.41	120.44
7	N	21	LYS	C-N-CA	6.60	129.41	120.44
11	R	361	VAL	O-C-N	-6.60	115.45	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	604	ARG	CA-C-N	6.59	129.00	120.56
7	N	604	ARG	C-N-CA	6.59	129.00	120.56
1	W	85	LEU	CA-C-O	-6.59	114.57	121.55
7	N	274	VAL	CB-CA-C	-6.58	103.25	112.14
7	N	453	ALA	CB-CA-C	-6.58	99.66	110.85
8	S	382	ARG	N-CA-C	-6.58	104.51	112.54
8	S	470	GLN	N-CA-C	-6.58	104.19	111.36
6	Z	352	LYS	N-CA-CB	6.58	119.89	110.16
7	N	174	LEU	N-CA-C	-6.58	99.19	109.25
6	Z	24	THR	C-N-CD	-6.58	98.04	125.00
6	Z	944	LYS	N-CA-CB	6.58	120.98	110.85
7	N	596	LEU	N-CA-CB	6.58	119.78	110.12
8	S	187	ILE	CA-C-O	6.57	128.14	121.17
6	Z	824	ASN	CA-C-O	6.57	126.22	118.79
7	N	870	ASN	CA-CB-CG	-6.57	106.03	112.60
11	R	345	TYR	CB-CA-C	-6.57	99.63	110.14
6	Z	817	LEU	N-CA-C	-6.57	103.81	110.97
8	S	352	VAL	O-C-N	-6.57	115.07	121.90
6	Z	954	PRO	CA-C-O	6.56	129.18	121.31
1	W	132	LEU	N-CA-C	6.56	118.51	111.36
7	N	154	LEU	O-C-N	6.56	129.63	122.15
13	O	306	ARG	N-CA-C	-6.56	103.89	112.41
4	X	62	ASP	CA-CB-CG	-6.56	106.04	112.60
13	O	48	PHE	CA-CB-CG	-6.55	107.25	113.80
7	N	502	PHE	CA-C-O	-6.55	113.48	120.42
11	R	159	SER	O-C-N	6.55	128.81	122.07
7	N	154	LEU	CA-C-O	-6.55	113.48	120.42
7	N	635	GLN	CA-C-N	6.55	129.05	120.28
7	N	635	GLN	C-N-CA	6.55	129.05	120.28
8	S	139	HIS	ND1-CE1-NE2	6.55	114.95	108.40
9	P	25	ASP	O-C-N	-6.55	114.56	122.22
1	W	120	ASP	CA-C-N	6.54	134.04	121.54
1	W	120	ASP	C-N-CA	6.54	134.04	121.54
6	Z	361	HIS	CG-CD2-NE2	6.54	113.74	107.20
10	Q	280	ASN	CA-C-N	6.54	128.80	120.56
10	Q	280	ASN	C-N-CA	6.54	128.80	120.56
12	U	243	ASP	CA-CB-CG	-6.54	106.06	112.60
8	S	99	ASN	CA-CB-CG	-6.54	106.06	112.60
6	Z	731	GLY	O-C-N	-6.54	115.15	122.28
7	N	16	ASN	CA-C-O	6.54	127.68	120.82
8	S	461	PHE	CA-CB-CG	-6.54	107.26	113.80
6	Z	199	ASP	N-CA-C	6.53	118.40	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	823	ASN	CA-C-O	6.53	127.42	120.36
6	Z	622	HIS	CB-CG-ND1	6.53	132.50	122.70
7	N	703	GLN	OE1-CD-NE2	6.53	129.13	122.60
9	P	45	LYS	CA-C-N	6.53	129.56	120.29
9	P	45	LYS	C-N-CA	6.53	129.56	120.29
3	T	204	ASN	CA-C-N	6.52	128.78	120.56
3	T	204	ASN	C-N-CA	6.52	128.78	120.56
8	S	103	SER	N-CA-C	-6.52	104.47	112.88
8	S	256	LYS	N-CA-C	-6.52	103.86	112.72
6	Z	502	ASN	OD1-CG-ND2	6.51	129.12	122.60
2	V	204	HIS	CA-CB-CG	6.51	120.31	113.80
7	N	174	LEU	O-C-N	6.51	131.03	123.02
9	P	419	VAL	CA-C-N	6.51	129.00	120.28
9	P	419	VAL	C-N-CA	6.51	129.00	120.28
5	Y	73	PHE	CA-CB-CG	-6.50	107.30	113.80
9	P	222	ASN	O-C-N	6.50	129.57	122.15
6	Z	340	LEU	N-CA-C	-6.50	102.85	111.24
7	N	804	LEU	CA-C-O	-6.50	113.66	120.55
8	S	461	PHE	N-CA-CB	6.50	120.36	110.28
10	Q	216	ALA	CA-C-N	6.50	128.99	120.28
10	Q	216	ALA	C-N-CA	6.50	128.99	120.28
13	O	152	ASP	N-CA-CB	6.50	119.44	110.01
10	Q	347	LEU	CA-C-O	-6.50	114.00	120.82
11	R	99	TYR	CD1-CE1-CZ	-6.50	107.91	119.60
6	Z	887	GLY	CA-C-N	6.49	130.99	121.31
6	Z	887	GLY	C-N-CA	6.49	130.99	121.31
6	Z	159	LEU	N-CA-CB	6.49	120.34	110.28
7	N	375	HIS	N-CA-C	-6.49	105.66	112.93
2	V	236	SER	N-CA-C	6.49	118.35	111.28
7	N	565	ASN	CA-C-N	6.49	128.88	120.44
7	N	565	ASN	C-N-CA	6.49	128.88	120.44
9	P	170	SER	CA-C-N	6.49	133.93	121.54
9	P	170	SER	C-N-CA	6.49	133.93	121.54
3	T	21	ALA	CA-C-N	6.48	128.96	120.28
3	T	21	ALA	C-N-CA	6.48	128.96	120.28
5	Y	21	ASN	N-CA-C	-6.48	104.22	111.28
2	V	149	GLY	N-CA-C	-6.48	106.63	114.66
7	N	676	ALA	O-C-N	-6.48	115.25	122.12
12	U	26	GLN	N-CA-C	6.48	120.59	111.52
3	T	186	ARG	CA-C-O	-6.47	113.69	120.55
8	S	424	SER	O-C-N	-6.47	115.26	122.12
10	Q	342	LEU	CA-C-N	6.47	128.86	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	342	LEU	C-N-CA	6.47	128.86	120.44
11	R	195	ASN	CA-CB-CG	-6.47	106.13	112.60
9	P	152	LYS	N-CA-C	-6.47	105.69	112.93
13	O	145	LYS	CB-CA-C	-6.47	100.05	110.79
7	N	340	HIS	CB-CA-C	-6.47	100.27	110.94
9	P	265	VAL	CA-CB-CG1	6.47	121.39	110.40
5	Y	38	PHE	CA-C-O	-6.46	112.39	118.73
6	Z	761	PHE	CA-C-O	6.46	127.40	120.55
8	S	104	VAL	CA-C-O	-6.46	114.08	119.76
3	T	245	TYR	N-CA-C	6.45	118.31	111.28
6	Z	303	ASP	CA-CB-CG	-6.45	106.15	112.60
7	N	821	LYS	CB-CA-C	-6.45	100.71	110.90
3	T	58	THR	N-CA-C	-6.45	104.18	111.14
7	N	881	TYR	N-CA-C	-6.44	105.57	113.50
9	P	278	ASN	CA-CB-CG	-6.44	106.16	112.60
8	S	483	GLU	CA-C-N	6.44	129.20	120.44
8	S	483	GLU	C-N-CA	6.44	129.20	120.44
12	U	86	LYS	O-C-N	6.44	129.04	122.09
6	Z	726	GLU	O-C-N	6.44	129.49	122.15
1	W	187	SER	CA-C-O	6.44	127.35	119.11
8	S	171	TYR	CA-C-N	6.43	133.83	121.54
8	S	171	TYR	C-N-CA	6.43	133.83	121.54
8	S	256	LYS	CA-C-N	6.43	131.60	121.56
8	S	256	LYS	C-N-CA	6.43	131.60	121.56
9	P	216	LEU	O-C-N	6.43	128.94	122.12
9	P	90	LYS	N-CA-C	-6.43	105.74	113.97
10	Q	111	LEU	CA-C-N	6.43	133.83	121.54
10	Q	111	LEU	C-N-CA	6.43	133.83	121.54
6	Z	195	PHE	N-CA-CB	6.43	119.57	110.12
9	P	324	GLU	N-CA-C	-6.43	104.20	111.14
1	W	111	VAL	N-CA-CB	6.42	119.55	111.46
7	N	181	GLU	CA-C-N	6.42	128.79	120.44
7	N	181	GLU	C-N-CA	6.42	128.79	120.44
7	N	578	ASP	O-C-N	6.42	130.58	123.01
7	N	225	LEU	CA-C-N	6.42	128.88	120.28
7	N	225	LEU	C-N-CA	6.42	128.88	120.28
7	N	675	VAL	CB-CA-C	-6.41	103.49	112.14
11	R	97	GLU	N-CA-C	6.41	119.08	111.33
8	S	354	LEU	CA-C-O	6.41	126.80	119.18
10	Q	104	PHE	CA-CB-CG	6.40	120.20	113.80
8	S	31	VAL	CA-C-O	-6.40	114.61	121.27
9	P	327	LEU	CA-C-N	6.40	133.76	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	327	LEU	C-N-CA	6.40	133.76	121.54
11	R	121	GLU	CA-C-O	-6.39	113.64	120.42
13	O	277	ILE	O-C-N	6.39	128.40	120.66
3	T	241	GLU	CA-C-N	6.39	129.17	120.54
3	T	241	GLU	C-N-CA	6.39	129.17	120.54
7	N	605	ILE	O-C-N	6.39	128.55	121.90
9	P	195	GLN	CA-C-N	6.39	130.02	120.31
9	P	195	GLN	C-N-CA	6.39	130.02	120.31
7	N	236	GLY	O-C-N	6.39	128.39	122.19
2	V	200	ASN	CA-CB-CG	-6.39	106.21	112.60
8	S	158	PHE	CA-C-N	6.39	128.74	120.44
8	S	158	PHE	C-N-CA	6.39	128.74	120.44
6	Z	593	HIS	O-C-N	-6.38	115.90	121.71
12	U	223	HIS	CE1-NE2-CD2	-6.38	102.62	109.00
7	N	283	ASP	CA-C-O	-6.38	111.42	120.16
11	R	124	ASP	CA-C-N	6.38	133.72	121.54
11	R	124	ASP	C-N-CA	6.38	133.72	121.54
13	O	297	ILE	N-CA-C	6.38	119.06	111.09
9	P	311	TRP	O-C-N	6.37	126.70	120.71
2	V	169	GLU	CA-C-O	-6.37	112.47	118.33
7	N	187	ASN	CA-C-N	6.37	128.81	120.28
7	N	187	ASN	C-N-CA	6.37	128.81	120.28
5	Y	76	GLU	CB-CA-C	-6.36	100.63	110.81
2	V	166	ASN	OD1-CG-ND2	6.36	128.96	122.60
7	N	912	GLU	CA-C-N	6.36	126.73	119.93
7	N	912	GLU	C-N-CA	6.36	126.73	119.93
13	O	391	ILE	CA-C-N	6.36	129.96	120.17
13	O	391	ILE	C-N-CA	6.36	129.96	120.17
6	Z	591	ILE	CA-C-O	-6.36	115.22	121.58
7	N	85	ALA	O-C-N	6.35	128.85	122.12
9	P	41	VAL	CA-C-O	-6.35	114.34	120.95
11	R	248	SER	O-C-N	6.35	129.39	122.15
8	S	348	LEU	N-CA-CB	6.35	119.21	110.01
4	X	17	TYR	CA-C-N	6.34	130.76	121.31
4	X	17	TYR	C-N-CA	6.34	130.76	121.31
6	Z	865	ASP	CA-C-N	6.34	128.55	120.56
6	Z	865	ASP	C-N-CA	6.34	128.55	120.56
8	S	85	SER	CA-C-N	6.34	128.68	120.44
8	S	85	SER	C-N-CA	6.34	128.68	120.44
11	R	135	ILE	CA-C-N	6.34	129.95	120.31
11	R	135	ILE	C-N-CA	6.34	129.95	120.31
10	Q	386	PHE	CA-C-N	6.34	133.65	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	386	PHE	C-N-CA	6.34	133.65	121.54
6	Z	380	ASN	N-CA-C	-6.34	104.45	111.36
13	O	23	HIS	ND1-CE1-NE2	6.33	114.73	108.40
8	S	288	THR	O-C-N	6.33	130.46	122.23
13	O	12	SER	CA-C-N	6.33	128.77	120.28
13	O	12	SER	C-N-CA	6.33	128.77	120.28
7	N	472	ASN	N-CA-C	-6.33	104.82	112.54
12	U	231	ASP	N-CA-CB	-6.33	100.47	110.22
6	Z	895	LEU	N-CA-C	-6.33	100.33	110.14
2	V	76	THR	O-C-N	-6.33	114.59	122.24
13	O	352	TRP	CE2-CD2-CE3	6.33	125.13	118.80
7	N	418	ASP	N-CA-C	-6.32	104.47	111.36
6	Z	621	LEU	CB-CA-C	-6.32	100.96	110.88
1	W	18	ASN	O-C-N	6.32	130.68	122.97
4	X	124	LYS	CA-C-N	6.32	129.26	120.29
4	X	124	LYS	C-N-CA	6.32	129.26	120.29
7	N	534	ASP	CA-CB-CG	6.32	118.92	112.60
9	P	106	SER	CA-C-N	6.32	128.74	120.28
9	P	106	SER	C-N-CA	6.32	128.74	120.28
2	V	71	MET	CA-C-N	6.31	127.73	119.84
2	V	71	MET	C-N-CA	6.31	127.73	119.84
1	W	128	LEU	CA-C-O	-6.31	113.87	120.55
3	T	268	ILE	CA-C-N	6.30	128.63	120.44
3	T	268	ILE	C-N-CA	6.30	128.63	120.44
9	P	337	HIS	N-CA-C	-6.30	106.22	114.04
10	Q	69	GLY	N-CA-C	-6.30	102.12	112.83
13	O	19	ASP	CA-C-N	6.30	125.98	119.56
13	O	19	ASP	C-N-CA	6.30	125.98	119.56
3	T	259	ILE	CA-C-N	6.29	128.49	120.56
3	T	259	ILE	C-N-CA	6.29	128.49	120.56
7	N	439	VAL	CA-C-N	6.29	128.71	120.28
7	N	439	VAL	C-N-CA	6.29	128.71	120.28
1	W	100	HIS	CA-CB-CG	-6.29	107.51	113.80
10	Q	226	HIS	ND1-CE1-NE2	6.29	114.69	108.40
11	R	46	ALA	O-C-N	6.29	129.58	122.22
2	V	189	ILE	CB-CA-C	-6.29	103.65	112.14
3	T	223	GLU	CB-CG-CD	-6.29	101.92	112.60
6	Z	923	ILE	CA-C-N	6.29	129.87	120.31
6	Z	923	ILE	C-N-CA	6.29	129.87	120.31
9	P	263	HIS	ND1-CE1-NE2	6.28	114.68	108.40
11	R	404	VAL	N-CA-CB	6.28	120.01	110.58
11	R	138	GLY	CA-C-O	-6.28	113.61	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	187	ILE	O-C-N	-6.28	115.76	121.91
11	R	323	ASN	O-C-N	-6.28	115.60	122.07
12	U	274	MET	CA-C-N	6.28	128.47	120.56
12	U	274	MET	C-N-CA	6.28	128.47	120.56
2	V	241	THR	CA-C-N	6.28	128.69	120.28
2	V	241	THR	C-N-CA	6.28	128.69	120.28
7	N	725	LEU	CA-C-N	6.28	130.82	121.72
7	N	725	LEU	C-N-CA	6.28	130.82	121.72
2	V	301	ASN	CB-CA-C	-6.28	101.02	110.88
11	R	278	SER	O-C-N	6.28	129.99	122.27
6	Z	488	ALA	CA-C-O	-6.27	113.77	120.42
7	N	602	VAL	CA-C-O	-6.27	114.49	118.69
6	Z	507	GLY	CA-C-O	6.27	126.85	119.45
12	U	130	VAL	CA-C-N	6.27	127.28	120.44
12	U	130	VAL	C-N-CA	6.27	127.28	120.44
2	V	145	GLN	CB-CG-CD	-6.27	101.94	112.60
6	Z	235	GLN	O-C-N	6.27	128.86	122.09
8	S	316	LEU	CA-C-N	6.27	129.19	120.29
8	S	316	LEU	C-N-CA	6.27	129.19	120.29
9	P	4	ASP	CA-CB-CG	-6.27	106.33	112.60
6	Z	617	ILE	N-CA-C	6.27	118.92	111.09
6	Z	346	LEU	CA-C-O	6.27	127.19	120.55
11	R	355	SER	CA-C-O	6.27	127.19	120.55
8	S	397	LEU	CA-C-N	6.26	128.58	120.44
8	S	397	LEU	C-N-CA	6.26	128.58	120.44
6	Z	828	ALA	N-CA-C	-6.26	104.37	111.07
1	W	106	GLN	CB-CA-C	-6.26	100.14	109.90
7	N	650	ASP	CB-CA-C	-6.26	100.40	110.79
10	Q	338	LEU	CA-C-N	6.26	129.49	120.79
10	Q	338	LEU	C-N-CA	6.26	129.49	120.79
9	P	392	LYS	N-CA-C	-6.26	97.62	108.69
4	X	69	ILE	CA-C-N	6.25	127.66	119.84
4	X	69	ILE	C-N-CA	6.25	127.66	119.84
7	N	56	SER	N-CA-C	-6.25	105.29	113.17
6	Z	546	ILE	N-CA-C	-6.25	104.41	110.72
6	Z	710	SER	O-C-N	6.25	129.28	122.15
2	V	39	LYS	N-CA-C	-6.25	104.47	111.28
6	Z	295	ARG	NE-CZ-NH2	-6.25	113.58	119.20
4	X	100	TRP	CE2-CD2-CE3	6.25	125.05	118.80
7	N	651	PHE	CA-C-O	6.25	127.05	119.31
10	Q	236	PHE	CA-C-O	-6.24	114.26	120.82
8	S	207	ASN	OD1-CG-ND2	6.24	128.84	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	177	THR	N-CA-C	-6.24	99.70	109.25
2	V	130	GLU	N-CA-C	-6.24	104.58	111.82
3	T	262	LYS	CA-C-O	-6.24	113.89	120.63
6	Z	724	GLU	CA-C-N	6.24	128.64	120.28
6	Z	724	GLU	C-N-CA	6.24	128.64	120.28
6	Z	549	ASN	CA-C-O	6.23	127.03	120.42
8	S	261	HIS	CA-CB-CG	-6.23	107.57	113.80
3	T	256	LYS	CG-CD-CE	6.23	125.63	111.30
6	Z	309	GLN	OE1-CD-NE2	-6.23	116.37	122.60
11	R	341	LEU	CA-C-N	6.23	129.78	120.31
11	R	341	LEU	C-N-CA	6.23	129.78	120.31
8	S	93	LEU	CD1-CG-CD2	6.22	124.49	110.80
6	Z	496	ALA	CA-C-O	-6.22	114.29	120.82
10	Q	5	GLY	CA-C-N	6.22	128.53	120.44
10	Q	5	GLY	C-N-CA	6.22	128.53	120.44
11	R	137	LEU	CA-C-N	6.22	127.91	120.14
11	R	137	LEU	C-N-CA	6.22	127.91	120.14
1	W	30	ILE	CA-C-N	6.21	128.60	120.28
1	W	30	ILE	C-N-CA	6.21	128.60	120.28
8	S	487	THR	O-C-N	6.21	129.23	122.15
6	Z	785	VAL	CA-C-O	-6.21	114.07	120.71
9	P	379	TYR	CA-CB-CG	-6.21	102.73	113.90
10	Q	280	ASN	OD1-CG-ND2	-6.21	116.39	122.60
8	S	76	PHE	CA-CB-CG	6.20	120.00	113.80
7	N	690	HIS	ND1-CE1-NE2	6.20	114.60	108.40
1	W	93	ILE	N-CA-C	-6.20	104.46	110.72
3	T	120	THR	CA-C-N	6.20	129.73	120.31
3	T	120	THR	C-N-CA	6.20	129.73	120.31
7	N	639	ASP	CA-C-N	6.20	128.96	120.46
7	N	639	ASP	C-N-CA	6.20	128.96	120.46
6	Z	170	GLU	CA-C-N	6.20	129.21	120.28
6	Z	170	GLU	C-N-CA	6.20	129.21	120.28
7	N	476	THR	N-CA-C	-6.20	107.56	114.62
9	P	248	ASP	CA-C-N	6.20	129.40	120.79
9	P	248	ASP	C-N-CA	6.20	129.40	120.79
13	O	156	THR	CA-C-N	6.20	128.58	120.28
13	O	156	THR	C-N-CA	6.20	128.58	120.28
8	S	21	SER	N-CA-C	6.19	118.57	111.02
11	R	250	ALA	O-C-N	6.19	128.44	122.07
13	O	126	ILE	CA-C-O	-6.19	114.98	121.41
13	O	334	LEU	N-CA-C	-6.19	104.64	111.82
2	V	111	HIS	CB-CA-C	-6.18	102.80	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	61	TYR	CB-CG-CD1	6.18	130.07	120.80
6	Z	933	VAL	N-CA-CB	6.18	119.12	112.07
7	N	730	VAL	N-CA-CB	6.18	117.78	110.55
7	N	871	MET	CB-CA-C	6.18	121.13	112.11
9	P	416	SER	CB-CA-C	-6.18	101.18	110.88
10	Q	69	GLY	CA-C-N	6.18	130.16	121.02
10	Q	69	GLY	C-N-CA	6.18	130.16	121.02
10	Q	285	LYS	N-CA-C	-6.17	104.47	111.14
7	N	270	LEU	CA-C-N	6.17	128.83	120.44
7	N	270	LEU	C-N-CA	6.17	128.83	120.44
9	P	336	HIS	N-CA-C	-6.17	106.02	112.93
9	P	104	LEU	N-CA-CB	6.17	118.95	110.01
6	Z	740	VAL	CA-C-N	6.17	128.54	120.28
6	Z	740	VAL	C-N-CA	6.17	128.54	120.28
11	R	68	GLU	N-CA-C	-6.17	104.47	111.07
7	N	543	ASP	CA-C-O	-6.16	114.02	120.55
9	P	207	THR	CA-C-O	-6.16	114.02	120.55
10	Q	306	TYR	N-CA-C	6.16	118.08	111.36
9	P	366	ASN	N-CA-C	6.16	118.00	111.28
7	N	345	ASP	O-C-N	6.16	130.78	122.59
7	N	465	ALA	CA-C-N	6.16	129.67	120.31
7	N	465	ALA	C-N-CA	6.16	129.67	120.31
7	N	522	ALA	N-CA-CB	6.16	118.94	110.01
13	O	18	ALA	CB-CA-C	-6.16	98.60	109.62
2	V	202	ASP	CA-CB-CG	-6.15	106.45	112.60
4	X	129	LEU	N-CA-CB	6.15	119.27	110.16
8	S	387	VAL	CA-C-N	6.15	128.43	120.56
8	S	387	VAL	C-N-CA	6.15	128.43	120.56
12	U	110	PHE	CA-CB-CG	-6.15	107.65	113.80
3	T	93	ASN	N-CA-C	-6.14	101.11	110.14
7	N	582	ASP	CA-CB-CG	-6.14	106.46	112.60
11	R	149	ASN	CA-CB-CG	-6.14	106.46	112.60
9	P	260	VAL	CA-C-O	-6.14	114.66	121.17
11	R	402	LEU	O-C-N	6.14	129.15	122.15
3	T	69	SER	N-CA-C	6.14	117.97	111.28
9	P	114	THR	N-CA-C	-6.14	104.50	111.07
6	Z	961	GLU	N-CA-CB	6.14	119.01	110.17
6	Z	424	SER	N-CA-C	6.13	119.86	112.38
6	Z	851	ALA	CA-C-O	-6.13	114.87	121.56
7	N	18	ASP	N-CA-C	-6.13	104.67	111.36
6	Z	214	HIS	CA-CB-CG	-6.13	107.67	113.80
7	N	75	TYR	CA-CB-CG	-6.13	102.87	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	532	HIS	CB-CA-C	-6.13	100.62	110.79
7	N	177	ASP	O-C-N	6.13	128.71	122.09
10	Q	289	GLU	O-C-N	-6.13	115.66	122.03
1	W	96	LEU	O-C-N	6.12	128.61	122.12
6	Z	725	GLU	N-CA-C	-6.12	104.61	111.28
2	V	89	ALA	CA-C-O	-6.12	114.39	120.82
9	P	266	TYR	CB-CG-CD2	-6.12	111.62	120.80
8	S	33	GLU	CA-C-O	-6.12	114.35	120.90
11	R	63	TYR	CA-C-N	6.12	128.48	120.28
11	R	63	TYR	C-N-CA	6.12	128.48	120.28
9	P	60	ALA	CA-C-O	6.12	126.91	120.42
9	P	252	SER	CB-CA-C	-6.12	100.45	110.85
2	V	174	THR	CA-C-N	6.12	133.22	121.54
2	V	174	THR	C-N-CA	6.12	133.22	121.54
10	Q	422	VAL	CA-C-O	-6.12	114.69	121.17
6	Z	765	MET	CA-C-N	6.11	128.75	120.44
6	Z	765	MET	C-N-CA	6.11	128.75	120.44
7	N	512	ASN	CA-CB-CG	-6.11	106.49	112.60
8	S	317	HIS	CE1-NE2-CD2	-6.11	102.89	109.00
9	P	51	ASP	N-CA-C	-6.11	104.54	111.14
3	T	86	LYS	O-C-N	-6.11	114.30	121.32
1	W	17	ARG	N-CA-C	6.11	118.44	111.11
9	P	315	GLN	CB-CG-CD	-6.11	102.22	112.60
12	U	124	ASP	CA-CB-CG	6.11	118.71	112.60
6	Z	522	THR	N-CA-C	-6.10	106.09	112.93
8	S	198	SER	N-CA-CB	6.10	120.80	110.49
8	S	294	ILE	N-CA-C	-6.10	104.39	110.62
2	V	88	GLN	O-C-N	6.10	128.68	122.09
8	S	168	LEU	CB-CA-C	-6.10	99.03	110.01
9	P	382	ASP	CA-CB-CG	6.10	118.70	112.60
13	O	46	THR	CA-C-N	6.10	128.37	120.44
13	O	46	THR	C-N-CA	6.10	128.37	120.44
6	Z	502	ASN	CA-C-O	-6.10	114.68	121.51
11	R	352	SER	N-CA-C	6.10	117.60	111.07
6	Z	963	ALA	CA-C-N	6.10	129.49	120.95
6	Z	963	ALA	C-N-CA	6.10	129.49	120.95
8	S	94	LYS	N-CA-C	6.09	117.92	111.28
1	W	192	LEU	CA-C-N	6.09	129.76	121.05
1	W	192	LEU	C-N-CA	6.09	129.76	121.05
6	Z	211	PHE	N-CA-C	-6.09	104.56	111.14
7	N	338	PHE	CA-C-O	-6.09	114.42	120.70
10	Q	88	PHE	CA-C-O	-6.09	114.43	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	U	234	ASN	OD1-CG-ND2	6.09	128.69	122.60
6	Z	241	THR	CA-C-N	6.09	128.44	120.28
6	Z	241	THR	C-N-CA	6.09	128.44	120.28
6	Z	776	VAL	O-C-N	-6.09	115.75	120.07
13	O	333	SER	CB-CA-C	-6.08	100.51	110.85
6	Z	63	LEU	N-CA-CB	6.08	119.76	110.70
3	T	253	GLU	CB-CG-CD	-6.08	102.26	112.60
6	Z	938	GLN	CA-C-O	-6.08	114.46	121.15
7	N	149	GLU	N-CA-C	-6.08	98.99	108.90
2	V	138	ALA	CA-C-N	-6.08	115.18	123.14
2	V	138	ALA	C-N-CA	-6.08	115.18	123.14
13	O	351	SER	N-CA-C	-6.08	104.67	114.09
6	Z	621	LEU	N-CA-C	-6.08	104.57	111.07
1	W	135	ASN	CA-CB-CG	-6.08	106.53	112.60
6	Z	110	ASN	OD1-CG-ND2	-6.07	116.53	122.60
11	R	396	LYS	CA-C-N	6.07	128.33	120.44
11	R	396	LYS	C-N-CA	6.07	128.33	120.44
12	U	294	ASN	CA-CB-CG	-6.07	106.53	112.60
6	Z	302	SER	N-CA-C	6.07	117.69	111.14
7	N	274	VAL	N-CA-CB	6.07	118.79	110.54
10	Q	424	ASP	CA-C-O	6.07	126.98	120.55
11	R	190	LYS	CA-C-O	-6.07	114.12	120.55
1	W	73	LEU	O-C-N	-6.06	115.69	122.12
4	X	16	GLU	CA-C-O	6.06	129.18	120.51
8	S	244	ASN	N-CA-C	-6.06	105.92	113.38
11	R	155	GLY	N-CA-C	-6.06	105.01	112.77
2	V	233	LYS	N-CA-C	-6.06	104.75	111.36
7	N	801	THR	N-CA-C	-6.06	104.75	111.36
6	Z	310	LEU	CA-C-N	6.06	128.68	120.44
6	Z	310	LEU	C-N-CA	6.06	128.68	120.44
7	N	657	MET	N-CA-C	-6.06	104.76	111.36
6	Z	271	ILE	CA-C-N	6.06	128.31	120.44
6	Z	271	ILE	C-N-CA	6.06	128.31	120.44
9	P	378	THR	CB-CA-C	-6.05	100.74	110.79
9	P	282	HIS	CE1-NE2-CD2	-6.05	102.95	109.00
6	Z	626	PRO	CA-C-N	6.05	128.39	120.28
6	Z	626	PRO	C-N-CA	6.05	128.39	120.28
6	Z	223	LEU	N-CA-C	-6.05	104.81	111.82
7	N	509	GLN	CA-C-N	6.05	129.97	121.02
7	N	509	GLN	C-N-CA	6.05	129.97	121.02
11	R	133	ALA	CA-C-N	6.04	128.87	120.29
11	R	133	ALA	C-N-CA	6.04	128.87	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	327	ASP	CA-CB-CG	6.04	118.64	112.60
8	S	25	TYR	CA-C-N	6.04	128.29	120.44
8	S	25	TYR	C-N-CA	6.04	128.29	120.44
6	Z	206	ASP	CA-CB-CG	6.03	118.63	112.60
6	Z	254	PRO	CB-CA-C	6.03	119.36	110.85
1	W	180	LEU	CA-C-N	6.03	128.64	120.44
1	W	180	LEU	C-N-CA	6.03	128.64	120.44
7	N	234	ASP	CA-CB-CG	-6.03	106.57	112.60
1	W	186	ALA	N-CA-CB	6.03	118.81	110.07
6	Z	859	LYS	CA-C-N	6.03	127.01	120.44
6	Z	859	LYS	C-N-CA	6.03	127.01	120.44
7	N	115	LYS	N-CA-C	-6.03	104.71	111.28
5	Y	82	ASP	N-CA-CB	6.02	118.97	110.12
6	Z	9	GLN	N-CA-C	-6.02	104.80	111.36
7	N	97	PHE	N-CA-C	-6.02	106.10	113.50
8	S	405	ARG	CD-NE-CZ	-6.02	115.97	124.40
12	U	26	GLN	OE1-CD-NE2	6.02	128.62	122.60
2	V	53	MET	CA-C-O	6.01	126.99	120.43
6	Z	571	GLY	CA-C-N	6.01	129.97	120.47
6	Z	571	GLY	C-N-CA	6.01	129.97	120.47
7	N	502	PHE	N-CA-C	-6.01	104.81	111.36
10	Q	7	LYS	CA-C-N	6.01	128.65	120.54
10	Q	7	LYS	C-N-CA	6.01	128.65	120.54
3	T	69	SER	CA-C-N	6.00	128.13	120.56
3	T	69	SER	C-N-CA	6.00	128.13	120.56
11	R	214	TYR	O-C-N	-6.00	115.30	122.15
3	T	208	LEU	N-CA-CB	6.00	118.94	110.12
2	V	212	MET	CA-C-N	6.00	128.32	120.28
2	V	212	MET	C-N-CA	6.00	128.32	120.28
3	T	38	ASN	OD1-CG-ND2	6.00	128.60	122.60
6	Z	172	ASP	O-C-N	6.00	128.25	122.07
7	N	863	SER	O-C-N	6.00	128.48	122.12
6	Z	851	ALA	CA-C-N	5.99	128.80	120.29
6	Z	851	ALA	C-N-CA	5.99	128.80	120.29
7	N	490	LEU	CB-CA-C	-5.99	102.43	109.80
8	S	472	HIS	N-CA-CB	5.99	118.69	110.01
6	Z	238	ASP	CA-C-O	-5.99	114.21	120.92
8	S	126	LYS	CA-C-N	5.99	132.20	121.66
8	S	126	LYS	C-N-CA	5.99	132.20	121.66
2	V	91	MET	N-CA-C	5.99	117.80	111.28
6	Z	762	GLY	N-CA-C	-5.99	106.92	114.16
11	R	325	HIS	O-C-N	5.98	129.37	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	154	ASP	CA-CB-CG	-5.98	106.62	112.60
10	Q	17	GLU	N-CA-C	-5.98	107.80	114.62
10	Q	316	THR	O-C-N	5.98	128.97	122.15
2	V	198	SER	N-CA-CB	5.98	120.03	110.16
10	Q	77	PHE	N-CA-C	5.98	117.88	111.36
4	X	82	LYS	CG-CD-CE	5.98	125.05	111.30
6	Z	376	SER	N-CA-CB	5.98	120.59	110.49
6	Z	938	GLN	O-C-N	5.98	130.26	122.97
10	Q	78	ILE	CB-CA-C	-5.98	108.01	114.35
13	O	332	ILE	N-CA-C	-5.97	104.69	110.72
1	W	6	THR	N-CA-CB	5.97	120.72	110.68
2	V	109	HIS	ND1-CE1-NE2	5.97	114.37	108.40
6	Z	133	ASP	N-CA-CB	5.97	118.90	110.12
10	Q	153	ASP	N-CA-C	-5.97	104.85	111.36
3	T	70	ILE	N-CA-C	5.97	116.15	110.42
13	O	318	HIS	CE1-NE2-CD2	-5.97	103.03	109.00
3	T	138	ASP	CA-CB-CG	-5.97	106.63	112.60
12	U	232	VAL	CA-C-O	-5.96	114.43	121.05
6	Z	582	ASP	CA-CB-CG	-5.96	106.64	112.60
10	Q	67	THR	N-CA-C	-5.96	98.10	110.80
12	U	73	ILE	CA-C-N	5.96	128.27	120.28
12	U	73	ILE	C-N-CA	5.96	128.27	120.28
4	X	52	PRO	N-CA-CB	5.96	109.17	102.67
7	N	365	PHE	N-CA-C	-5.96	104.70	111.07
7	N	599	TYR	CA-C-N	5.96	128.54	120.44
7	N	599	TYR	C-N-CA	5.96	128.54	120.44
7	N	804	LEU	N-CA-CB	5.96	118.88	110.12
11	R	310	GLU	O-C-N	-5.96	115.81	122.12
9	P	413	ASN	CB-CA-C	-5.96	100.73	110.85
7	N	662	MET	N-CA-CB	5.95	119.47	110.30
8	S	334	HIS	CG-CD2-NE2	5.95	113.15	107.20
12	U	270	ASN	CA-CB-CG	-5.95	106.65	112.60
13	O	91	ASP	N-CA-CB	5.95	119.05	110.06
13	O	185	PHE	CA-CB-CG	-5.95	107.85	113.80
9	P	80	THR	N-CA-C	5.95	121.19	111.37
10	Q	374	GLU	CA-C-O	-5.95	114.20	120.63
8	S	481	TYR	N-CA-C	5.95	120.84	112.75
13	O	256	ASN	N-CA-C	-5.95	105.28	112.54
8	S	159	ASN	CA-C-N	5.95	128.17	120.44
8	S	159	ASN	C-N-CA	5.95	128.17	120.44
10	Q	12	ARG	CA-C-N	5.95	128.57	120.54
10	Q	12	ARG	C-N-CA	5.95	128.57	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	U	28	LYS	CA-C-O	5.95	127.75	121.33
12	U	183	ALA	CA-C-O	-5.94	114.94	121.84
2	V	123	VAL	N-CA-C	-5.94	104.72	110.72
6	Z	118	VAL	CA-C-N	5.94	128.24	120.28
6	Z	118	VAL	C-N-CA	5.94	128.24	120.28
11	R	179	PHE	CA-C-O	-5.94	113.38	120.10
4	X	69	ILE	CA-C-O	-5.94	113.92	119.62
3	T	199	PHE	CA-C-O	5.94	126.77	120.36
12	U	252	HIS	ND1-CE1-NE2	5.94	114.34	108.40
9	P	437	GLU	N-CA-CB	5.93	119.48	110.28
13	O	98	TYR	CA-C-N	5.93	128.16	120.44
13	O	98	TYR	C-N-CA	5.93	128.16	120.44
7	N	485	MET	N-CA-C	5.93	117.42	111.07
7	N	690	HIS	CE1-NE2-CD2	-5.93	103.07	109.00
13	O	105	GLN	CA-C-N	5.93	128.82	120.28
13	O	105	GLN	C-N-CA	5.93	128.82	120.28
13	O	206	THR	N-CA-CB	5.93	118.79	109.83
13	O	373	TRP	CE2-CD2-CE3	5.93	124.73	118.80
12	U	220	PRO	O-C-N	5.93	130.64	122.64
1	W	103	ASN	N-CA-CB	5.92	121.72	111.00
9	P	334	ASN	CA-CB-CG	-5.92	106.67	112.60
11	R	363	PHE	CA-CB-CG	-5.92	107.88	113.80
2	V	217	HIS	CE1-NE2-CD2	-5.92	103.08	109.00
7	N	613	HIS	N-CA-C	-5.92	105.97	112.72
2	V	168	LEU	CA-C-N	5.92	128.40	120.58
2	V	168	LEU	C-N-CA	5.92	128.40	120.58
11	R	310	GLU	CB-CA-C	-5.92	100.97	110.79
4	X	22	ARG	N-CA-CB	5.92	121.75	112.46
7	N	45	ASP	CA-CB-CG	-5.92	106.68	112.60
9	P	289	ASN	CA-C-N	5.92	128.80	120.28
9	P	289	ASN	C-N-CA	5.92	128.80	120.28
6	Z	496	ALA	O-C-N	5.91	128.16	122.07
11	R	310	GLU	CA-C-O	5.91	126.82	120.55
6	Z	132	HIS	CG-CD2-NE2	5.91	113.11	107.20
8	S	187	ILE	CA-C-N	5.91	129.00	120.79
8	S	187	ILE	C-N-CA	5.91	129.00	120.79
2	V	87	PHE	N-CA-CB	5.91	118.91	110.16
7	N	917	ILE	N-CA-C	-5.91	98.63	107.37
10	Q	145	HIS	CB-CA-C	-5.91	99.33	110.67
6	Z	320	SER	N-CA-CB	5.91	119.43	110.28
8	S	353	LYS	N-CA-C	5.90	118.47	111.33
7	N	803	VAL	N-CA-C	5.90	116.64	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	358	ILE	N-CA-C	-5.90	96.11	106.61
3	T	252	GLU	CA-C-O	5.90	125.91	119.24
1	W	123	ASP	CA-CB-CG	-5.89	106.71	112.60
3	T	133	ILE	CA-C-O	5.89	125.74	119.91
6	Z	453	LEU	CA-C-N	5.89	126.52	119.98
6	Z	453	LEU	C-N-CA	5.89	126.52	119.98
9	P	158	ASP	CA-CB-CG	-5.89	106.71	112.60
7	N	890	PHE	CA-CB-CG	-5.89	107.91	113.80
6	Z	138	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	W	162	ASN	CA-CB-CG	-5.89	106.71	112.60
4	X	116	ALA	N-CA-C	-5.89	98.26	110.80
9	P	272	PRO	CA-C-N	5.89	129.20	120.90
9	P	272	PRO	C-N-CA	5.89	129.20	120.90
4	X	65	SER	N-CA-CB	5.88	119.95	110.65
10	Q	274	LEU	N-CA-C	-5.88	97.72	108.02
11	R	325	HIS	CE1-NE2-CD2	-5.88	103.12	109.00
9	P	371	LEU	CA-C-O	5.88	128.04	121.40
7	N	223	LEU	N-CA-C	-5.88	104.88	111.28
8	S	127	THR	CB-CA-C	-5.88	97.62	109.55
10	Q	53	GLU	N-CA-C	5.88	118.16	111.11
11	R	168	ILE	CA-C-N	5.88	128.47	120.54
11	R	168	ILE	C-N-CA	5.88	128.47	120.54
12	U	251	ASN	CB-CA-C	-5.88	101.65	110.88
7	N	906	ARG	NH1-CZ-NH2	-5.88	111.66	119.30
10	Q	202	ARG	NH1-CZ-NH2	-5.88	111.66	119.30
6	Z	766	HIS	ND1-CE1-NE2	5.87	114.27	108.40
6	Z	886	VAL	N-CA-CB	5.87	118.00	110.13
6	Z	55	ARG	NH1-CZ-NH2	-5.87	111.67	119.30
10	Q	385	ILE	CA-C-O	5.87	128.12	120.78
1	W	101	ARG	CA-C-N	5.87	128.14	120.28
1	W	101	ARG	C-N-CA	5.87	128.14	120.28
7	N	442	LEU	N-CA-C	-5.87	104.07	111.11
1	W	189	PRO	N-CA-CB	5.87	108.47	103.19
8	S	486	LYS	CB-CG-CD	5.87	124.79	111.30
11	R	398	ALA	N-CA-CB	5.86	118.51	110.01
12	U	223	HIS	CA-CB-CG	-5.86	107.94	113.80
7	N	375	HIS	ND1-CE1-NE2	5.86	114.26	108.40
11	R	256	THR	O-C-N	5.86	128.33	122.12
11	R	367	ASP	CA-CB-CG	5.86	118.46	112.60
7	N	743	PHE	CA-CB-CG	-5.86	107.94	113.80
8	S	292	TYR	CA-C-O	-5.85	114.34	120.55
6	Z	506	LEU	CA-C-O	-5.85	114.67	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	67	ALA	N-CA-C	-5.85	105.72	112.92
3	T	246	GLU	N-CA-C	-5.85	104.90	111.28
7	N	593	PHE	CA-CB-CG	-5.85	107.95	113.80
8	S	431	VAL	N-CA-CB	5.85	116.99	110.62
11	R	193	ALA	CA-C-N	5.85	129.71	120.47
11	R	193	ALA	C-N-CA	5.85	129.71	120.47
13	O	283	HIS	N-CA-C	-5.85	102.81	111.81
7	N	264	SER	CB-CA-C	-5.84	101.67	110.90
9	P	100	VAL	CA-C-N	5.84	128.11	120.28
9	P	100	VAL	C-N-CA	5.84	128.11	120.28
13	O	326	HIS	CG-CD2-NE2	5.84	113.05	107.20
12	U	12	PRO	CA-C-N	5.84	128.11	120.28
12	U	12	PRO	C-N-CA	5.84	128.11	120.28
9	P	3	ARG	CG-CD-NE	-5.84	99.15	112.00
13	O	129	ILE	CA-C-O	-5.84	115.20	121.27
10	Q	383	ASP	CA-CB-CG	-5.84	106.76	112.60
7	N	217	MET	CA-C-N	5.84	125.38	119.19
7	N	217	MET	C-N-CA	5.84	125.38	119.19
3	T	251	HIS	O-C-N	-5.83	114.83	122.59
6	Z	132	HIS	CE1-NE2-CD2	-5.83	103.17	109.00
6	Z	5	SER	N-CA-C	-5.83	105.93	113.16
7	N	715	ILE	N-CA-C	-5.83	99.48	107.99
2	V	135	ARG	N-CA-C	-5.83	105.36	112.88
12	U	130	VAL	CA-C-O	5.83	125.38	119.20
12	U	251	ASN	CA-C-N	5.83	128.09	120.28
12	U	251	ASN	C-N-CA	5.83	128.09	120.28
12	U	278	ILE	N-CA-C	-5.83	104.68	110.62
7	N	401	LYS	CB-CA-C	-5.82	101.12	110.79
1	W	107	HIS	CE1-NE2-CD2	-5.82	103.18	109.00
4	X	44	GLY	O-C-N	-5.82	115.00	122.39
8	S	122	ASN	CA-C-O	-5.82	114.25	120.42
9	P	338	TRP	N-CA-C	-5.82	104.93	111.28
6	Z	406	TRP	CA-C-N	5.82	127.89	120.56
6	Z	406	TRP	C-N-CA	5.82	127.89	120.56
10	Q	332	ARG	N-CA-C	5.82	117.70	111.36
12	U	8	VAL	CB-CA-C	-5.82	103.42	110.99
6	Z	191	SER	CB-CA-C	-5.82	99.87	110.63
8	S	394	ILE	CA-C-N	5.82	128.43	120.46
8	S	394	ILE	C-N-CA	5.82	128.43	120.46
11	R	117	ILE	CA-C-O	-5.82	114.90	120.95
6	Z	718	ASP	CB-CA-C	-5.81	101.14	110.79
7	N	621	THR	N-CA-C	-5.81	105.03	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	107	HIS	CG-CD2-NE2	5.81	113.01	107.20
3	T	87	PRO	N-CA-C	5.81	122.23	113.81
7	N	310	ASP	N-CA-CB	5.81	119.34	109.87
9	P	263	HIS	CE1-NE2-CD2	-5.81	103.19	109.00
11	R	28	GLU	N-CA-C	-5.81	104.86	111.14
6	Z	227	ILE	O-C-N	5.81	127.50	121.87
7	N	187	ASN	O-C-N	-5.81	116.09	122.07
11	R	34	THR	N-CA-CB	5.81	118.59	109.94
9	P	19	GLU	N-CA-C	-5.80	105.70	112.89
4	X	15	CYS	CA-C-O	5.80	127.48	120.99
8	S	347	HIS	CE1-NE2-CD2	-5.80	103.20	109.00
2	V	203	TYR	CA-CB-CG	-5.80	103.47	113.90
6	Z	346	LEU	CA-C-N	5.80	128.05	120.28
6	Z	346	LEU	C-N-CA	5.80	128.05	120.28
12	U	121	LEU	N-CA-C	-5.80	97.73	107.99
13	O	58	ARG	CB-CG-CD	5.80	124.63	111.30
13	O	156	THR	N-CA-CB	5.80	118.41	110.01
6	Z	561	ASP	CA-CB-CG	-5.79	106.81	112.60
10	Q	384	LYS	N-CA-CB	5.79	120.28	110.49
2	V	42	ARG	N-CA-C	-5.79	105.05	111.36
8	S	345	TYR	CA-C-O	5.79	126.69	120.55
12	U	123	VAL	N-CA-C	-5.79	98.70	107.73
2	V	120	SER	O-C-N	5.79	128.26	122.12
8	S	386	ASN	CA-CB-CG	-5.79	106.81	112.60
4	X	62	ASP	CA-C-N	5.79	127.07	119.84
4	X	62	ASP	C-N-CA	5.79	127.07	119.84
6	Z	361	HIS	CE1-NE2-CD2	-5.79	103.22	109.00
6	Z	947	GLY	CA-C-N	5.79	128.03	120.28
6	Z	947	GLY	C-N-CA	5.79	128.03	120.28
4	X	30	GLN	CA-C-N	5.78	127.56	120.51
4	X	30	GLN	C-N-CA	5.78	127.56	120.51
7	N	107	GLU	O-C-N	5.78	128.25	122.12
7	N	762	ARG	CA-C-O	-5.78	113.87	120.58
2	V	80	VAL	N-CA-C	-5.78	104.88	110.72
6	Z	130	GLY	N-CA-C	-5.78	107.20	115.64
5	Y	21	ASN	N-CA-CB	5.78	118.61	110.12
7	N	103	SER	CA-C-N	5.78	128.02	120.28
7	N	103	SER	C-N-CA	5.78	128.02	120.28
1	W	136	ASN	CA-CB-CG	-5.77	106.83	112.60
3	T	96	LEU	N-CA-CB	5.77	120.24	110.49
6	Z	479	THR	O-C-N	5.77	128.73	122.15
7	N	501	MET	CA-C-N	5.77	128.48	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	501	MET	C-N-CA	5.77	128.48	120.29
13	O	58	ARG	CA-CB-CG	5.77	125.64	114.10
7	N	613	HIS	ND1-CE1-NE2	5.77	114.17	108.40
13	O	7	ILE	CA-C-N	5.77	128.01	120.28
13	O	7	ILE	C-N-CA	5.77	128.01	120.28
6	Z	201	LEU	N-CA-CB	5.76	118.79	110.20
9	P	79	LEU	CA-C-O	-5.76	112.27	120.51
8	S	419	VAL	N-CA-C	-5.76	104.90	110.72
10	Q	202	ARG	N-CA-CB	5.76	118.59	110.12
11	R	262	GLU	N-CA-CB	5.76	118.68	110.44
8	S	301	PRO	N-CA-CB	5.76	108.45	103.27
9	P	113	ASN	CA-C-N	5.76	127.93	120.44
9	P	113	ASN	C-N-CA	5.76	127.93	120.44
1	W	120	ASP	CA-CB-CG	-5.76	106.84	112.60
9	P	23	LYS	N-CA-CB	5.76	118.68	110.16
11	R	60	ALA	N-CA-C	5.75	120.73	113.25
7	N	504	TYR	CA-CB-CG	-5.75	103.54	113.90
7	N	516	GLY	N-CA-C	-5.75	105.83	112.73
10	Q	201	ALA	N-CA-C	-5.75	105.09	111.36
9	P	173	MET	N-CA-C	-5.75	104.21	111.11
6	Z	295	ARG	O-C-N	5.75	128.22	122.12
6	Z	590	ALA	CA-C-N	5.75	128.34	120.35
6	Z	590	ALA	C-N-CA	5.75	128.34	120.35
11	R	236	ALA	CB-CA-C	-5.75	101.86	110.88
13	O	77	SER	CA-C-N	5.75	127.80	120.56
13	O	77	SER	C-N-CA	5.75	127.80	120.56
13	O	378	GLU	CA-C-O	-5.75	114.79	120.82
13	O	22	LEU	CB-CA-C	-5.74	100.50	110.09
2	V	113	GLY	O-C-N	5.74	128.33	122.24
6	Z	446	GLU	CB-CG-CD	-5.74	102.84	112.60
7	N	637	ALA	N-CA-C	5.74	117.21	111.07
11	R	98	LEU	O-C-N	5.74	128.06	122.09
8	S	165	PRO	N-CA-C	5.74	121.30	113.84
3	T	146	ILE	O-C-N	5.73	127.43	121.87
6	Z	518	LEU	O-C-N	5.73	127.34	121.72
7	N	350	LYS	CA-C-N	5.73	127.89	120.44
7	N	350	LYS	C-N-CA	5.73	127.89	120.44
8	S	20	HIS	CA-C-O	5.73	126.84	120.82
9	P	422	LEU	N-CA-CB	5.73	118.64	110.16
10	Q	194	SER	N-CA-C	-5.73	105.17	111.82
12	U	240	GLY	N-CA-C	-5.73	107.42	115.32
7	N	862	SER	CA-C-N	5.73	127.95	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	862	SER	C-N-CA	5.73	127.95	120.28
13	O	391	ILE	N-CA-C	5.72	116.11	107.75
6	Z	331	GLY	CA-C-O	-5.72	114.22	120.40
9	P	67	ALA	CB-CA-C	-5.72	101.89	110.88
9	P	95	TYR	CA-C-N	5.72	127.88	120.44
9	P	95	TYR	C-N-CA	5.72	127.88	120.44
12	U	15	LEU	N-CA-CB	5.72	118.37	110.07
8	S	56	SER	CA-C-N	5.72	127.95	120.28
8	S	56	SER	C-N-CA	5.72	127.95	120.28
10	Q	110	SER	CA-C-N	5.72	132.47	121.54
10	Q	110	SER	C-N-CA	5.72	132.47	121.54
11	R	111	LYS	N-CA-C	5.72	117.97	111.11
7	N	306	ASN	CA-C-N	5.72	129.47	121.24
7	N	306	ASN	C-N-CA	5.72	129.47	121.24
9	P	376	THR	CA-CB-OG1	5.72	118.18	109.60
10	Q	321	TYR	CA-C-N	5.72	128.73	120.38
10	Q	321	TYR	C-N-CA	5.72	128.73	120.38
6	Z	107	THR	N-CA-CB	5.72	119.89	110.69
8	S	88	PHE	N-CA-C	5.72	117.19	111.07
6	Z	156	HIS	CB-CG-CD2	-5.71	123.77	131.20
6	Z	240	ASN	OD1-CG-ND2	-5.71	116.89	122.60
9	P	100	VAL	N-CA-CB	5.71	117.89	110.57
9	P	424	GLU	N-CA-C	-5.71	105.13	111.36
10	Q	362	ILE	N-CA-C	-5.71	104.79	110.62
6	Z	953	THR	CA-C-N	5.71	125.47	119.76
6	Z	953	THR	C-N-CA	5.71	125.47	119.76
8	S	332	PHE	N-CA-CB	5.71	118.51	110.12
11	R	388	VAL	O-C-N	-5.71	115.40	122.88
11	R	338	TYR	CB-CG-CD1	5.70	129.36	120.80
11	R	285	ALA	CB-CA-C	-5.70	101.32	110.79
13	O	319	LEU	CA-C-N	5.70	126.49	120.11
13	O	319	LEU	C-N-CA	5.70	126.49	120.11
2	V	65	VAL	N-CA-C	-5.70	99.02	107.51
3	T	28	PRO	N-CA-C	5.70	117.65	110.70
8	S	476	LEU	N-CA-C	-5.70	105.07	111.28
13	O	232	GLU	CA-C-N	5.70	127.92	120.28
13	O	232	GLU	C-N-CA	5.70	127.92	120.28
7	N	362	TRP	N-CA-C	-5.70	106.29	113.18
11	R	288	SER	CA-C-O	5.69	126.45	120.42
12	U	156	HIS	N-CA-CB	5.69	118.42	109.83
9	P	178	GLN	N-CA-C	5.68	117.15	111.07
10	Q	33	LYS	CA-C-N	5.68	128.69	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	33	LYS	C-N-CA	5.68	128.69	120.79
10	Q	247	HIS	CG-CD2-NE2	5.68	112.89	107.20
12	U	160	THR	N-CA-C	-5.68	100.85	108.86
2	V	296	LEU	N-CA-C	-5.68	104.99	111.07
7	N	551	GLY	N-CA-C	-5.68	105.77	112.64
8	S	154	GLN	CA-C-N	5.68	127.82	120.44
8	S	154	GLN	C-N-CA	5.68	127.82	120.44
10	Q	309	ARG	N-CA-CB	5.68	120.08	110.49
12	U	3	LEU	N-CA-C	-5.68	105.47	112.90
4	X	13	GLY	O-C-N	-5.67	116.42	123.12
7	N	543	ASP	CB-CA-C	-5.67	101.37	110.79
6	Z	62	SER	CA-CB-OG	-5.67	99.75	111.10
7	N	582	ASP	N-CA-C	-5.67	105.10	111.28
6	Z	479	THR	CA-C-O	-5.67	114.41	120.42
7	N	348	PHE	O-C-N	5.67	128.21	122.09
9	P	319	GLU	O-C-N	-5.67	115.43	120.48
2	V	273	ARG	NH1-CZ-NH2	5.67	126.67	119.30
7	N	76	GLU	N-CA-C	-5.67	105.18	111.36
7	N	300	ASN	OD1-CG-ND2	5.67	128.27	122.60
7	N	308	ASN	CA-CB-CG	-5.67	106.93	112.60
7	N	340	HIS	ND1-CE1-NE2	5.67	114.07	108.40
11	R	162	ILE	CA-C-N	5.67	129.31	120.75
11	R	162	ILE	C-N-CA	5.67	129.31	120.75
2	V	109	HIS	CE1-NE2-CD2	-5.67	103.33	109.00
12	U	273	LEU	N-CA-CB	5.67	118.22	110.01
6	Z	219	ASP	CA-CB-CG	-5.66	106.94	112.60
8	S	252	ASP	CA-C-O	-5.66	114.42	120.42
10	Q	128	GLU	N-CA-C	-5.66	106.04	113.12
3	T	78	PHE	CA-C-O	-5.66	114.88	120.82
6	Z	944	LYS	CA-C-N	5.66	130.14	122.90
6	Z	944	LYS	C-N-CA	5.66	130.14	122.90
9	P	390	TYR	CA-CB-CG	-5.66	103.72	113.90
10	Q	147	GLN	CA-C-N	5.66	132.61	121.58
10	Q	147	GLN	C-N-CA	5.66	132.61	121.58
8	S	168	LEU	N-CA-C	-5.66	106.14	113.16
8	S	352	VAL	CA-C-O	5.66	127.33	121.05
8	S	384	ARG	NE-CZ-NH1	5.66	127.16	121.50
7	N	494	LYS	CA-C-N	5.65	125.01	118.85
7	N	494	LYS	C-N-CA	5.65	125.01	118.85
7	N	662	MET	N-CA-C	-5.65	105.11	112.23
7	N	805	SER	N-CA-C	5.65	118.38	111.82
12	U	80	CYS	N-CA-CB	5.65	119.04	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	U	232	VAL	N-CA-C	-5.65	105.22	110.53
9	P	177	ILE	N-CA-C	-5.65	104.43	110.36
6	Z	246	CYS	O-C-N	-5.64	115.33	122.27
12	U	100	ARG	NE-CZ-NH2	5.64	124.28	119.20
13	O	375	ASP	CA-CB-CG	-5.64	106.96	112.60
2	V	111	HIS	CE1-NE2-CD2	-5.64	103.36	109.00
6	Z	129	ASN	N-CA-C	-5.64	105.21	111.36
10	Q	52	ASN	N-CA-CB	5.64	118.34	109.94
11	R	329	PHE	CA-C-O	5.64	126.74	120.82
13	O	63	ASP	N-CA-CB	5.64	118.34	109.94
1	W	100	HIS	CB-CA-C	-5.64	100.45	109.75
1	W	96	LEU	CB-CA-C	-5.64	101.43	110.79
3	T	165	GLN	O-C-N	5.64	128.57	122.15
12	U	31	LYS	CA-C-N	5.64	128.87	120.87
12	U	31	LYS	C-N-CA	5.64	128.87	120.87
8	S	196	ARG	CA-C-O	5.63	125.88	119.18
8	S	224	LYS	CA-C-N	5.63	130.58	122.35
8	S	224	LYS	C-N-CA	5.63	130.58	122.35
9	P	257	TRP	CA-CB-CG	5.63	124.31	113.60
10	Q	14	LEU	CA-C-N	5.63	127.66	120.56
10	Q	14	LEU	C-N-CA	5.63	127.66	120.56
10	Q	214	THR	O-C-N	-5.63	115.63	122.22
13	O	185	PHE	N-CA-C	-5.63	104.76	111.69
2	V	209	GLU	CA-C-N	5.63	127.83	120.28
2	V	209	GLU	C-N-CA	5.63	127.83	120.28
6	Z	958	ASN	N-CA-C	-5.63	100.00	109.07
7	N	658	ILE	CA-C-N	5.63	127.83	120.28
7	N	658	ILE	C-N-CA	5.63	127.83	120.28
9	P	367	GLU	N-CA-C	5.63	117.42	111.28
6	Z	448	LYS	N-CA-CB	5.63	118.49	110.16
10	Q	162	LEU	N-CA-C	-5.63	105.19	112.68
3	T	60	ARG	CA-C-N	5.63	127.76	120.56
3	T	60	ARG	C-N-CA	5.63	127.76	120.56
3	T	258	ASN	N-CA-C	-5.63	100.53	109.59
11	R	416	LYS	N-CA-C	-5.63	105.06	111.14
2	V	58	VAL	CA-C-O	-5.62	116.13	121.64
10	Q	280	ASN	N-CA-C	-5.62	105.23	111.36
13	O	330	ARG	NE-CZ-NH2	-5.62	114.14	119.20
6	Z	48	ASP	CA-CB-CG	-5.62	106.98	112.60
6	Z	736	LEU	N-CA-C	5.62	117.40	111.28
8	S	169	CYS	N-CA-C	-5.62	105.23	111.36
7	N	900	ASN	CA-C-O	5.62	127.37	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	229	SER	N-CA-C	-5.62	105.93	112.89
11	R	334	ARG	NE-CZ-NH2	-5.62	114.14	119.20
6	Z	159	LEU	CB-CA-C	-5.61	99.89	110.67
7	N	891	VAL	CA-C-N	5.61	125.52	119.85
7	N	891	VAL	C-N-CA	5.61	125.52	119.85
3	T	15	PHE	CB-CA-C	-5.61	102.07	110.88
9	P	172	GLU	N-CA-CB	5.61	118.25	110.17
8	S	182	LYS	N-CA-C	-5.61	106.48	113.55
8	S	208	ILE	CA-C-N	5.61	128.15	120.46
8	S	208	ILE	C-N-CA	5.61	128.15	120.46
11	R	263	ARG	CA-C-O	-5.61	112.49	120.51
1	W	64	THR	N-CA-C	-5.61	101.70	110.17
6	Z	834	LEU	N-CA-CB	5.61	118.30	109.94
2	V	122	ASP	N-CA-CB	5.61	119.70	110.39
9	P	339	GLU	CB-CG-CD	-5.61	103.07	112.60
7	N	613	HIS	N-CA-CB	5.60	119.05	110.70
7	N	771	PHE	N-CA-CB	5.60	120.98	111.57
13	O	100	ASP	CA-CB-CG	-5.60	107.00	112.60
1	W	41	ARG	NE-CZ-NH1	5.60	127.10	121.50
4	X	25	THR	N-CA-C	-5.60	96.64	108.73
7	N	373	VAL	CA-C-N	5.60	127.61	120.56
7	N	373	VAL	C-N-CA	5.60	127.61	120.56
8	S	202	ASN	N-CA-C	-5.60	105.33	111.82
2	V	168	LEU	N-CA-C	-5.59	105.22	113.61
8	S	111	ARG	CA-C-N	5.59	130.76	122.82
8	S	111	ARG	C-N-CA	5.59	130.76	122.82
1	W	189	PRO	CB-CA-C	5.59	118.74	111.64
3	T	100	ASP	CA-C-N	5.59	127.77	120.28
3	T	100	ASP	C-N-CA	5.59	127.77	120.28
10	Q	372	GLN	N-CA-CB	-5.59	101.89	110.16
4	X	11	ARG	NE-CZ-NH1	5.59	127.09	121.50
6	Z	357	ILE	CA-C-N	5.59	128.23	120.29
6	Z	357	ILE	C-N-CA	5.59	128.23	120.29
6	Z	912	PHE	CA-C-O	5.59	124.84	119.08
8	S	57	LEU	CA-C-N	5.59	127.71	120.44
8	S	57	LEU	C-N-CA	5.59	127.71	120.44
8	S	304	SER	CA-C-O	-5.59	114.59	120.63
7	N	174	LEU	CA-C-O	-5.59	114.01	120.49
7	N	375	HIS	CE1-NE2-CD2	-5.59	103.41	109.00
10	Q	341	THR	N-CA-C	-5.59	105.19	112.23
9	P	74	ASP	N-CA-C	-5.58	105.34	111.82
2	V	32	ILE	CB-CA-C	-5.58	104.82	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	94	VAL	O-C-N	-5.58	116.45	121.87
8	S	382	ARG	NE-CZ-NH2	-5.58	114.18	119.20
12	U	223	HIS	N-CA-C	-5.58	105.73	112.54
13	O	371	VAL	N-CA-C	-5.58	105.06	110.42
10	Q	421	LYS	N-CA-C	-5.58	105.28	111.36
13	O	98	TYR	N-CA-CB	5.58	118.42	110.16
13	O	382	LYS	CA-C-O	-5.58	114.51	120.42
6	Z	766	HIS	CA-C-O	-5.58	114.96	120.70
12	U	250	GLU	N-CA-C	5.58	117.36	111.28
6	Z	141	SER	N-CA-C	-5.58	106.48	113.28
7	N	151	LYS	N-CA-C	5.58	118.12	111.71
12	U	123	VAL	CA-C-N	5.58	128.75	120.95
12	U	123	VAL	C-N-CA	5.58	128.75	120.95
6	Z	352	LYS	CB-CA-C	-5.57	101.38	110.85
8	S	63	LEU	N-CA-C	5.57	117.35	111.28
9	P	310	ARG	N-CA-CB	5.57	119.32	110.57
3	T	85	LEU	N-CA-CB	5.57	118.24	109.94
7	N	115	LYS	CA-C-O	-5.57	114.65	120.55
7	N	315	ASN	N-CA-C	-5.57	105.29	111.36
10	Q	68	MET	CB-CA-C	-5.57	99.52	110.10
1	W	175	THR	CA-C-O	-5.57	112.53	120.16
6	Z	826	ARG	N-CA-C	-5.57	105.36	111.82
7	N	15	GLU	N-CA-C	5.57	118.09	110.24
7	N	411	ILE	O-C-N	5.57	127.51	121.94
7	N	420	THR	CA-C-N	5.57	127.68	120.44
7	N	420	THR	C-N-CA	5.57	127.68	120.44
10	Q	136	SER	N-CA-C	-5.57	105.13	111.14
13	O	345	ASN	CA-C-N	5.57	130.26	122.36
13	O	345	ASN	C-N-CA	5.57	130.26	122.36
2	V	245	VAL	CB-CA-C	-5.57	104.63	112.14
10	Q	373	VAL	CA-C-O	-5.57	115.27	121.17
3	T	91	SER	N-CA-CB	5.56	118.64	110.35
2	V	216	LEU	CA-C-N	5.56	132.16	121.54
2	V	216	LEU	C-N-CA	5.56	132.16	121.54
11	R	275	GLU	CA-C-O	5.56	126.31	120.42
6	Z	132	HIS	CA-CB-CG	-5.56	108.24	113.80
7	N	123	PHE	CG-CD1-CE1	5.56	130.15	120.70
13	O	326	HIS	CE1-NE2-CD2	-5.56	103.44	109.00
3	T	220	PHE	O-C-N	5.56	129.10	122.27
6	Z	251	ALA	CA-C-O	-5.56	113.82	120.10
13	O	377	VAL	O-C-N	5.56	127.36	121.91
1	W	140	ASP	CA-CB-CG	-5.55	107.05	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	809	MET	CA-C-O	-5.55	114.98	120.70
8	S	277	SER	CB-CA-C	-5.55	102.16	110.88
8	S	482	PRO	N-CA-CB	5.55	109.39	103.39
3	T	143	SER	N-CA-C	5.55	118.86	111.75
8	S	92	LEU	CA-C-N	5.55	127.72	120.28
8	S	92	LEU	C-N-CA	5.55	127.72	120.28
5	Y	83	ARG	NE-CZ-NH1	5.55	127.05	121.50
6	Z	151	HIS	O-C-N	5.55	129.80	122.36
8	S	352	VAL	CA-C-N	5.55	127.99	120.38
8	S	352	VAL	C-N-CA	5.55	127.99	120.38
9	P	345	VAL	CB-CA-C	5.55	119.29	112.02
9	P	349	ASN	CA-C-O	-5.55	114.99	120.82
6	Z	224	LEU	CA-C-O	5.55	126.37	120.10
7	N	167	GLU	N-CA-C	5.55	117.01	111.07
7	N	488	CYS	CA-C-O	-5.55	114.98	120.70
7	N	519	VAL	O-C-N	5.55	128.07	121.80
7	N	902	VAL	N-CA-C	-5.55	102.36	109.30
8	S	216	LYS	CA-C-N	5.55	128.27	120.28
8	S	216	LYS	C-N-CA	5.55	128.27	120.28
12	U	146	ASP	CA-CB-CG	5.55	118.15	112.60
7	N	681	ASN	N-CA-C	-5.55	105.31	111.36
9	P	154	ASP	CA-C-N	5.54	127.71	120.28
9	P	154	ASP	C-N-CA	5.54	127.71	120.28
10	Q	226	HIS	CE1-NE2-CD2	-5.54	103.45	109.00
7	N	435	GLY	CA-C-N	5.54	129.43	121.50
7	N	435	GLY	C-N-CA	5.54	129.43	121.50
9	P	427	GLU	CA-C-N	5.54	128.16	120.29
9	P	427	GLU	C-N-CA	5.54	128.16	120.29
13	O	225	ASP	N-CA-CB	5.54	119.86	110.49
1	W	193	GLU	N-CA-CB	5.54	118.07	109.48
3	T	92	ASN	N-CA-CB	5.54	119.86	110.49
8	S	251	SER	N-CA-CB	5.54	118.36	110.16
10	Q	214	THR	CA-C-N	5.54	128.29	120.42
10	Q	214	THR	C-N-CA	5.54	128.29	120.42
11	R	416	LYS	O-C-N	5.54	128.07	122.09
7	N	621	THR	O-C-N	5.54	128.46	122.15
13	O	74	ASN	CA-C-O	-5.54	115.68	121.55
8	S	141	LEU	CA-C-N	5.54	127.54	120.56
8	S	141	LEU	C-N-CA	5.54	127.54	120.56
6	Z	195	PHE	CA-CB-CG	-5.54	108.26	113.80
6	Z	87	LYS	CA-C-O	-5.53	113.82	119.08
10	Q	247	HIS	CE1-NE2-CD2	-5.53	103.47	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	23	LYS	CA-C-N	5.53	127.69	120.28
8	S	23	LYS	C-N-CA	5.53	127.69	120.28
9	P	70	ASN	CA-CB-CG	-5.53	107.07	112.60
6	Z	40	GLU	CB-CG-CD	-5.53	103.20	112.60
7	N	229	VAL	CA-C-N	5.53	128.27	120.42
7	N	229	VAL	C-N-CA	5.53	128.27	120.42
11	R	99	TYR	CB-CG-CD2	-5.53	112.51	120.80
12	U	277	TYR	N-CA-C	5.53	118.23	111.82
1	W	186	ALA	CB-CA-C	-5.53	102.17	110.90
8	S	127	THR	N-CA-C	-5.53	106.38	113.23
2	V	234	GLU	O-C-N	5.52	127.97	122.12
4	X	46	TRP	O-C-N	-5.52	116.49	123.12
1	W	23	ARG	NE-CZ-NH2	-5.52	114.23	119.20
6	Z	230	ILE	N-CA-C	-5.52	105.46	110.82
7	N	144	CYS	O-C-N	-5.52	115.86	122.15
9	P	337	HIS	CE1-NE2-CD2	-5.52	103.48	109.00
11	R	204	TRP	N-CA-C	-5.52	106.05	112.89
8	S	136	CYS	CA-C-N	5.51	127.67	120.28
8	S	136	CYS	C-N-CA	5.51	127.67	120.28
9	P	194	SER	CB-CA-C	-5.51	101.48	110.85
3	T	250	MET	CA-C-N	5.51	132.07	121.54
3	T	250	MET	C-N-CA	5.51	132.07	121.54
6	Z	210	TYR	CA-C-N	5.51	127.93	120.44
6	Z	210	TYR	C-N-CA	5.51	127.93	120.44
11	R	29	LYS	CA-C-O	-5.51	114.71	120.55
8	S	331	SER	CA-C-N	5.51	127.66	120.28
8	S	331	SER	C-N-CA	5.51	127.66	120.28
6	Z	814	ALA	CA-C-O	-5.50	115.04	120.82
10	Q	416	VAL	O-C-N	5.50	127.20	121.87
13	O	87	LYS	N-CA-C	-5.50	105.30	112.23
6	Z	721	ASN	N-CA-CB	5.50	117.98	110.01
3	T	9	LYS	CG-CD-CE	5.50	123.94	111.30
3	T	34	LEU	CA-C-N	5.50	129.31	120.30
3	T	34	LEU	C-N-CA	5.50	129.31	120.30
12	U	243	ASP	CA-C-N	5.50	127.65	120.28
12	U	243	ASP	C-N-CA	5.50	127.65	120.28
8	S	412	ASN	OD1-CG-ND2	5.50	128.09	122.60
9	P	380	ILE	O-C-N	5.50	127.20	121.87
4	X	82	LYS	N-CA-CB	5.49	117.95	109.98
6	Z	198	GLU	N-CA-C	5.49	116.95	111.07
6	Z	622	HIS	CE1-NE2-CD2	-5.49	103.51	109.00
7	N	52	ASP	N-CA-C	5.49	117.62	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	379	LEU	CA-C-N	5.49	127.58	120.44
7	N	379	LEU	C-N-CA	5.49	127.58	120.44
9	P	266	TYR	CB-CG-CD1	5.49	129.04	120.80
10	Q	225	LEU	N-CA-C	-5.49	104.81	112.45
4	X	89	LEU	CA-C-N	5.49	129.23	122.37
4	X	89	LEU	C-N-CA	5.49	129.23	122.37
7	N	497	ALA	CA-C-N	5.49	127.98	120.46
7	N	497	ALA	C-N-CA	5.49	127.98	120.46
7	N	918	GLU	N-CA-CB	5.49	118.35	110.06
9	P	93	ILE	O-C-N	5.49	127.20	121.87
10	Q	316	THR	CA-C-O	-5.49	114.60	120.42
13	O	146	ALA	CB-CA-C	-5.49	101.52	110.85
13	O	293	LEU	N-CA-CB	5.49	118.19	110.12
8	S	413	LEU	N-CA-CB	5.49	118.04	109.97
9	P	189	LEU	O-C-N	5.49	128.41	122.15
9	P	294	GLU	N-CA-CB	5.49	118.93	110.81
10	Q	53	GLU	N-CA-CB	5.49	118.12	109.94
6	Z	810	ASN	CB-CA-C	-5.48	101.53	110.85
12	U	122	ILE	CA-C-O	-5.48	114.62	121.04
6	Z	113	SER	CA-C-N	5.48	127.89	120.44
6	Z	113	SER	C-N-CA	5.48	127.89	120.44
8	S	204	ASP	CA-C-N	5.48	127.90	120.44
8	S	204	ASP	C-N-CA	5.48	127.90	120.44
10	Q	80	HIS	ND1-CE1-NE2	5.48	113.88	108.40
13	O	214	ALA	CA-C-N	5.48	127.57	120.44
13	O	214	ALA	C-N-CA	5.48	127.57	120.44
6	Z	103	TYR	CA-C-O	-5.48	114.16	120.24
6	Z	179	SER	O-C-N	-5.48	116.31	122.12
9	P	82	LEU	CB-CA-C	5.48	119.58	110.81
11	R	159	SER	N-CA-CB	5.48	117.96	110.01
6	Z	823	ASN	O-C-N	-5.48	116.78	123.30
7	N	452	LEU	CA-C-N	5.48	128.07	120.29
7	N	452	LEU	C-N-CA	5.48	128.07	120.29
7	N	492	THR	O-C-N	5.48	128.40	122.15
1	W	181	LEU	N-CA-C	-5.48	105.22	111.14
10	Q	29	SER	CA-C-N	5.47	128.40	120.79
10	Q	29	SER	C-N-CA	5.47	128.40	120.79
9	P	82	LEU	CA-C-N	5.47	127.93	120.54
9	P	82	LEU	C-N-CA	5.47	127.93	120.54
3	T	216	GLU	N-CA-C	-5.47	105.48	111.82
7	N	90	ASP	CA-C-N	5.47	127.95	120.46
7	N	90	ASP	C-N-CA	5.47	127.95	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	797	GLU	O-C-N	-5.47	115.92	122.15
2	V	263	GLU	N-CA-C	5.47	116.92	111.07
6	Z	38	LEU	N-CA-CB	5.47	118.75	110.28
7	N	649	VAL	N-CA-CB	5.47	116.49	110.53
7	N	154	LEU	CA-C-N	5.47	126.01	120.00
7	N	154	LEU	C-N-CA	5.47	126.01	120.00
10	Q	252	HIS	CA-CB-CG	5.46	119.26	113.80
10	Q	337	ALA	CA-C-N	5.46	127.55	120.44
10	Q	337	ALA	C-N-CA	5.46	127.55	120.44
7	N	112	GLU	CA-C-O	-5.46	114.76	120.55
9	P	295	SER	CB-CA-C	5.46	119.46	110.88
6	Z	830	LEU	CA-C-O	-5.46	115.09	120.82
7	N	312	GLY	N-CA-C	-5.46	107.89	114.66
7	N	877	GLN	N-CA-CB	5.46	118.33	110.20
8	S	357	LEU	O-C-N	5.46	127.99	122.09
6	Z	306	MET	N-CA-C	-5.46	105.42	113.61
7	N	719	ASN	N-CA-CB	5.46	118.07	109.83
6	Z	181	GLY	CA-C-O	5.46	126.67	119.58
6	Z	744	ALA	O-C-N	5.46	127.90	122.12
11	R	272	ASP	N-CA-C	-5.46	106.70	113.19
6	Z	61	SER	N-CA-C	5.45	119.10	112.23
6	Z	243	GLN	OE1-CD-NE2	5.45	128.05	122.60
10	Q	83	GLU	N-CA-C	-5.45	105.25	111.14
10	Q	226	HIS	CA-CB-CG	-5.45	108.35	113.80
11	R	236	ALA	N-CA-CB	5.45	117.92	110.01
2	V	50	MET	CA-C-O	5.45	127.14	121.31
3	T	103	SER	CB-CA-C	-5.45	102.32	110.88
11	R	47	ALA	N-CA-C	5.45	117.98	111.71
13	O	80	LYS	N-CA-C	-5.45	105.50	111.82
11	R	215	GLY	CA-C-O	-5.45	115.44	121.05
12	U	160	THR	CA-CB-OG1	5.45	117.77	109.60
2	V	199	LEU	CA-C-N	5.45	131.94	121.54
2	V	199	LEU	C-N-CA	5.45	131.94	121.54
7	N	593	PHE	CA-C-N	5.45	127.92	120.46
7	N	593	PHE	C-N-CA	5.45	127.92	120.46
9	P	155	GLU	N-CA-C	-5.44	105.35	111.28
9	P	263	HIS	CG-CD2-NE2	5.44	112.64	107.20
12	U	79	MET	O-C-N	5.44	128.35	122.15
12	U	105	LYS	CA-C-O	-5.44	114.65	120.42
6	Z	97	PRO	CA-C-N	5.44	127.57	120.28
6	Z	97	PRO	C-N-CA	5.44	127.57	120.28
6	Z	303	ASP	CA-C-O	-5.44	112.70	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	464	ASP	CA-C-O	-5.44	113.36	120.00
6	Z	745	LEU	CB-CA-C	-5.44	101.76	110.79
7	N	300	ASN	CB-CG-OD1	-5.44	109.92	120.80
7	N	409	GLY	O-C-N	5.44	127.41	122.19
7	N	539	MET	N-CA-CB	5.44	118.31	110.20
12	U	61	LYS	O-C-N	5.44	127.97	122.09
7	N	202	PHE	CA-C-N	5.44	127.51	120.44
7	N	202	PHE	C-N-CA	5.44	127.51	120.44
9	P	358	SER	N-CA-CB	5.44	118.67	110.30
6	Z	634	ASP	N-CA-C	5.44	117.28	111.36
8	S	282	ILE	N-CA-C	5.43	119.65	112.04
6	Z	497	PHE	N-CA-C	-5.43	106.16	112.89
10	Q	361	HIS	CA-C-N	5.43	127.90	120.46
10	Q	361	HIS	C-N-CA	5.43	127.90	120.46
2	V	64	ASN	N-CA-C	-5.43	99.67	108.52
8	S	64	ARG	CA-C-N	5.43	131.91	121.54
8	S	64	ARG	C-N-CA	5.43	131.91	121.54
12	U	248	ASP	CA-C-O	-5.43	114.80	120.55
13	O	363	ILE	N-CA-C	-5.43	105.09	110.62
6	Z	144	SER	CA-C-O	5.42	128.27	120.51
6	Z	838	TYR	CA-C-N	5.42	127.86	120.54
6	Z	838	TYR	C-N-CA	5.42	127.86	120.54
6	Z	918	ASP	N-CA-C	-5.42	107.21	113.88
11	R	186	TYR	CA-C-N	5.42	127.89	120.46
11	R	186	TYR	C-N-CA	5.42	127.89	120.46
13	O	285	SER	N-CA-CB	5.42	117.88	110.01
13	O	345	ASN	CA-C-O	5.42	125.16	119.03
13	O	107	GLN	CA-C-O	-5.42	115.13	120.82
3	T	116	GLN	N-CA-CB	5.42	119.23	110.40
6	Z	258	PRO	N-CA-CB	5.42	108.34	103.08
6	Z	536	GLY	CA-C-N	5.42	131.89	121.54
6	Z	536	GLY	C-N-CA	5.42	131.89	121.54
12	U	113	TYR	CB-CG-CD2	5.42	128.93	120.80
6	Z	55	ARG	NE-CZ-NH2	5.42	124.08	119.20
10	Q	183	LYS	N-CA-CB	5.42	118.08	110.12
7	N	303	LEU	N-CA-C	-5.41	105.54	111.82
7	N	580	ASN	CA-C-N	5.41	127.80	120.44
7	N	580	ASN	C-N-CA	5.41	127.80	120.44
7	N	798	LYS	CA-C-N	5.41	128.10	120.42
7	N	798	LYS	C-N-CA	5.41	128.10	120.42
6	Z	146	PHE	O-C-N	-5.41	117.58	123.26
7	N	535	LEU	CA-C-N	5.41	127.87	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	535	LEU	C-N-CA	5.41	127.87	120.46
8	S	201	ILE	O-C-N	5.41	127.91	121.80
10	Q	8	LEU	CA-C-N	5.41	127.47	120.44
10	Q	8	LEU	C-N-CA	5.41	127.47	120.44
2	V	43	ALA	CA-C-O	5.40	126.15	120.42
6	Z	842	GLN	O-C-N	5.40	129.65	122.95
10	Q	289	GLU	N-CA-C	5.40	116.86	110.97
13	O	172	TYR	N-CA-C	5.40	119.13	112.54
8	S	114	TYR	N-CA-C	-5.40	101.99	110.14
10	Q	154	SER	CA-C-N	5.40	127.46	120.44
10	Q	154	SER	C-N-CA	5.40	127.46	120.44
7	N	50	TYR	CA-C-O	-5.40	114.70	120.42
13	O	293	LEU	CA-C-O	5.40	126.27	120.55
10	Q	110	SER	N-CA-CB	5.40	119.61	110.49
12	U	236	LEU	CB-CA-C	5.40	118.57	109.67
7	N	650	ASP	CA-C-O	-5.39	114.83	120.55
8	S	32	GLN	CA-C-N	5.39	127.82	120.54
8	S	32	GLN	C-N-CA	5.39	127.82	120.54
8	S	425	ARG	O-C-N	-5.39	116.00	122.15
12	U	186	LEU	CA-C-O	-5.39	115.16	120.82
6	Z	852	GLN	CA-C-O	5.39	126.14	120.42
7	N	202	PHE	O-C-N	5.39	127.62	122.07
10	Q	18	LYS	N-CA-C	-5.39	99.31	110.80
10	Q	195	LYS	N-CA-CB	5.39	117.83	110.01
11	R	277	LEU	O-C-N	-5.39	116.40	122.12
6	Z	202	ARG	N-CA-C	5.39	116.84	111.07
6	Z	463	HIS	CA-CB-CG	5.39	119.19	113.80
10	Q	136	SER	N-CA-CB	5.39	117.88	110.07
3	T	72	THR	N-CA-C	-5.39	106.30	112.92
6	Z	370	SER	CA-C-N	5.39	128.50	120.90
6	Z	370	SER	C-N-CA	5.39	128.50	120.90
6	Z	505	VAL	CB-CA-C	5.39	119.08	112.02
13	O	193	LEU	N-CA-CB	5.39	118.04	110.12
2	V	277	LYS	CA-C-N	5.38	127.94	120.29
2	V	277	LYS	C-N-CA	5.38	127.94	120.29
6	Z	550	PHE	CA-C-N	5.38	127.44	120.44
6	Z	550	PHE	C-N-CA	5.38	127.44	120.44
4	X	123	ASN	N-CA-CB	5.38	118.03	110.12
8	S	26	ALA	CA-C-N	5.38	127.44	120.44
8	S	26	ALA	C-N-CA	5.38	127.44	120.44
12	U	133	PRO	N-CA-C	-5.38	101.39	112.47
5	Y	23	GLU	CA-C-O	5.38	126.25	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	28	LEU	N-CA-CB	5.38	117.81	110.01
2	V	214	MET	N-CA-C	-5.38	105.50	111.36
7	N	789	GLU	CB-CG-CD	-5.38	103.46	112.60
3	T	251	HIS	N-CA-CB	5.37	119.57	110.49
6	Z	927	VAL	CA-C-N	5.37	129.77	122.19
6	Z	927	VAL	C-N-CA	5.37	129.77	122.19
8	S	469	ASN	CA-C-O	5.37	126.25	120.55
1	W	76	LEU	N-CA-C	-5.37	105.59	111.82
6	Z	387	ASN	CA-C-N	5.37	125.90	119.94
6	Z	387	ASN	C-N-CA	5.37	125.90	119.94
9	P	172	GLU	CA-C-N	5.37	127.79	120.54
9	P	172	GLU	C-N-CA	5.37	127.79	120.54
6	Z	744	ALA	N-CA-CB	5.37	118.01	110.12
11	R	130	GLN	O-C-N	-5.37	116.43	122.12
7	N	591	LEU	N-CA-CB	5.37	118.11	110.06
8	S	330	LEU	CA-C-N	5.37	127.47	120.28
8	S	330	LEU	C-N-CA	5.37	127.47	120.28
9	P	437	GLU	CA-C-N	5.37	127.43	120.56
9	P	437	GLU	C-N-CA	5.37	127.43	120.56
10	Q	208	ILE	N-CA-C	-5.37	107.52	112.83
13	O	201	PRO	N-CA-C	-5.37	107.15	113.86
4	X	125	MET	CA-C-O	-5.37	114.73	120.42
7	N	540	LEU	N-CA-CB	5.37	118.60	110.28
7	N	64	ILE	O-C-N	5.37	127.07	121.87
7	N	265	ALA	CB-CA-C	-5.37	100.47	109.65
6	Z	455	ILE	O-C-N	5.36	127.35	121.83
12	U	54	LEU	O-C-N	-5.36	116.79	121.35
6	Z	771	HIS	CA-C-O	-5.36	115.19	120.82
8	S	271	ARG	CB-CA-C	-5.36	101.89	110.79
2	V	69	PHE	CA-CB-CG	-5.36	108.44	113.80
6	Z	67	SER	CB-CA-C	-5.36	100.90	110.70
7	N	467	LYS	N-CA-C	5.36	117.12	111.28
12	U	245	ASP	CA-C-N	5.36	127.46	120.28
12	U	245	ASP	C-N-CA	5.36	127.46	120.28
6	Z	624	LEU	N-CA-CB	5.36	117.99	110.12
8	S	247	VAL	O-C-N	5.36	127.06	121.87
8	S	306	SER	CA-C-N	5.36	127.46	120.28
8	S	306	SER	C-N-CA	5.36	127.46	120.28
11	R	203	ASP	O-C-N	-5.36	116.69	123.01
8	S	285	ASP	N-CA-C	-5.35	100.45	108.96
11	R	36	SER	N-CA-C	-5.35	106.12	113.30
2	V	45	VAL	CA-CB-CG1	5.35	119.50	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	397	LEU	CA-C-O	-5.35	115.20	120.82
12	U	156	HIS	CA-C-O	-5.35	115.30	121.19
4	X	69	ILE	N-CA-C	-5.35	101.63	107.73
8	S	348	LEU	CB-CA-C	-5.35	102.48	110.88
10	Q	287	THR	CA-C-O	5.35	126.21	120.70
10	Q	159	ASN	CA-C-N	5.35	127.88	120.29
10	Q	159	ASN	C-N-CA	5.35	127.88	120.29
13	O	46	THR	CA-CB-OG1	5.35	117.62	109.60
6	Z	286	VAL	N-CA-CB	5.35	119.49	110.56
2	V	197	TYR	CA-CB-CG	5.34	123.52	113.90
6	Z	261	ASP	O-C-N	5.34	127.86	122.09
9	P	306	ASN	CA-CB-CG	-5.34	107.26	112.60
11	R	214	TYR	N-CA-C	-5.34	105.53	111.36
11	R	333	MET	O-C-N	5.34	128.24	122.15
6	Z	632	GLU	CA-C-O	-5.34	115.21	120.82
7	N	480	ALA	O-C-N	5.34	128.24	122.15
10	Q	418	GLN	N-CA-CB	5.34	117.97	110.12
7	N	507	GLU	CA-C-N	5.34	129.32	120.94
7	N	507	GLU	C-N-CA	5.34	129.32	120.94
8	S	359	LYS	CA-C-N	5.34	127.38	120.44
8	S	359	LYS	C-N-CA	5.34	127.38	120.44
4	X	130	ASN	OD1-CG-ND2	-5.34	117.26	122.60
2	V	76	THR	N-CA-C	-5.34	106.15	113.30
4	X	100	TRP	CG-CD2-CE3	-5.34	128.56	133.90
6	Z	418	ALA	N-CA-CB	5.34	118.06	110.16
10	Q	217	GLU	N-CA-CB	5.34	117.96	110.12
12	U	218	GLU	N-CA-CB	5.34	120.19	112.13
2	V	176	ASN	CA-C-N	5.33	129.14	120.60
2	V	176	ASN	C-N-CA	5.33	129.14	120.60
9	P	221	TYR	CA-C-O	5.33	126.11	119.97
13	O	177	GLN	CA-C-O	5.33	126.20	120.55
12	U	196	SER	N-CA-C	5.33	117.17	111.36
2	V	139	VAL	O-C-N	-5.33	117.50	123.26
2	V	232	GLU	O-C-N	-5.33	115.71	122.27
6	Z	474	LEU	CA-C-N	5.33	127.42	120.28
6	Z	474	LEU	C-N-CA	5.33	127.42	120.28
13	O	147	ARG	N-CA-C	5.33	116.77	111.07
1	W	196	SER	CA-C-O	5.33	124.54	118.47
6	Z	484	LYS	O-C-N	5.33	127.77	122.12
12	U	225	ILE	CA-C-N	5.33	127.42	120.28
12	U	225	ILE	C-N-CA	5.33	127.42	120.28
6	Z	246	CYS	N-CA-C	-5.33	105.64	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	290	LEU	N-CA-C	5.33	117.84	111.71
4	X	57	VAL	CA-C-O	-5.33	114.80	120.39
6	Z	96	TYR	N-CA-C	-5.33	105.51	112.75
12	U	53	ALA	N-CA-CB	5.33	117.84	110.17
2	V	217	HIS	CA-C-N	5.32	129.73	120.68
2	V	217	HIS	C-N-CA	5.32	129.73	120.68
8	S	451	ILE	CA-C-N	5.32	127.68	120.44
8	S	451	ILE	C-N-CA	5.32	127.68	120.44
9	P	107	SER	N-CA-CB	5.32	117.95	110.12
10	Q	227	CYS	CA-C-N	5.32	127.95	120.28
10	Q	227	CYS	C-N-CA	5.32	127.95	120.28
4	X	108	ASN	CA-CB-CG	-5.32	107.28	112.60
6	Z	899	GLN	N-CA-CB	5.32	120.77	112.25
7	N	903	VAL	N-CA-C	-5.32	99.89	107.77
1	W	172	LEU	N-CA-CB	5.32	118.95	110.65
10	Q	406	ASP	CA-C-N	5.32	127.68	120.44
10	Q	406	ASP	C-N-CA	5.32	127.68	120.44
2	V	27	VAL	N-CA-C	-5.32	100.09	108.23
6	Z	733	VAL	N-CA-CB	5.32	117.77	110.54
8	S	349	THR	CB-CA-C	-5.32	102.53	110.88
10	Q	83	GLU	CA-C-N	5.32	127.94	120.28
10	Q	83	GLU	C-N-CA	5.32	127.94	120.28
12	U	15	LEU	N-CA-C	-5.32	105.40	111.14
2	V	118	LEU	CB-CA-C	-5.32	102.12	110.79
2	V	241	THR	CB-CA-C	-5.32	102.53	110.88
7	N	96	GLN	N-CA-C	-5.32	106.47	113.17
8	S	57	LEU	O-C-N	-5.32	116.48	122.12
2	V	281	SER	N-CA-C	-5.32	105.40	111.14
6	Z	261	ASP	CA-CB-CG	5.32	117.92	112.60
11	R	104	LYS	CA-C-N	5.32	128.18	120.79
11	R	104	LYS	C-N-CA	5.32	128.18	120.79
7	N	204	SER	CA-C-O	5.31	126.40	120.82
7	N	772	GLN	N-CA-C	-5.31	100.74	109.40
8	S	308	GLY	O-C-N	5.31	127.39	122.13
9	P	71	LYS	N-CA-CB	5.31	118.51	110.28
8	S	72	GLU	CA-CB-CG	5.31	124.72	114.10
13	O	200	GLU	CA-C-O	-5.31	114.65	120.17
7	N	740	TRP	CB-CG-CD2	-5.31	119.37	126.80
7	N	747	HIS	ND1-CE1-NE2	5.31	113.71	108.40
8	S	304	SER	O-C-N	5.31	127.75	122.12
3	T	129	LEU	CA-C-N	5.31	128.78	120.82
3	T	129	LEU	C-N-CA	5.31	128.78	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	215	MET	CA-C-O	-5.31	113.87	119.97
8	S	244	ASN	CA-C-N	5.30	129.57	121.51
8	S	244	ASN	C-N-CA	5.30	129.57	121.51
13	O	160	LYS	CB-CA-C	5.30	117.80	110.16
10	Q	374	GLU	O-C-N	5.30	127.74	122.12
3	T	44	LEU	O-C-N	5.30	128.66	122.67
3	T	127	GLN	CA-C-O	-5.30	115.25	120.82
6	Z	438	LYS	CA-C-O	-5.30	115.24	121.07
7	N	500	ASP	CA-C-O	5.30	126.04	120.42
11	R	346	LYS	N-CA-CB	5.30	117.65	109.91
12	U	171	VAL	CB-CA-C	-5.30	105.08	112.02
11	R	364	LEU	CA-C-O	-5.30	114.93	120.55
7	N	729	SER	N-CA-CB	5.30	117.91	110.12
12	U	236	LEU	O-C-N	-5.30	115.98	121.28
13	O	182	LYS	CA-C-N	5.30	129.66	122.19
13	O	182	LYS	C-N-CA	5.30	129.66	122.19
8	S	139	HIS	CA-C-N	5.29	127.32	120.44
8	S	139	HIS	C-N-CA	5.29	127.32	120.44
2	V	40	HIS	ND1-CE1-NE2	5.29	113.69	108.40
12	U	243	ASP	O-C-N	-5.29	116.51	122.12
1	W	40	LYS	CG-CD-CE	5.29	123.47	111.30
1	W	77	HIS	N-CA-C	5.29	117.05	111.28
3	T	258	ASN	CA-C-O	5.29	126.32	120.71
1	W	40	LYS	CA-C-N	5.29	127.36	120.28
1	W	40	LYS	C-N-CA	5.29	127.36	120.28
7	N	481	ALA	O-C-N	5.29	127.73	122.12
10	Q	6	SER	O-C-N	5.29	127.52	122.07
7	N	907	ASP	N-CA-CB	5.29	119.05	110.17
6	Z	427	GLN	CA-C-N	5.29	130.33	122.82
6	Z	427	GLN	C-N-CA	5.29	130.33	122.82
9	P	268	LEU	CB-CA-C	-5.29	101.86	110.85
9	P	338	TRP	CA-C-N	5.29	127.36	120.28
9	P	338	TRP	C-N-CA	5.29	127.36	120.28
11	R	52	ALA	N-CA-CB	5.29	117.67	110.01
6	Z	586	GLU	N-CA-C	5.28	117.04	111.28
9	P	369	LEU	CA-C-N	5.28	130.91	122.93
9	P	369	LEU	C-N-CA	5.28	130.91	122.93
7	N	349	ILE	O-C-N	5.28	127.38	121.94
8	S	184	TRP	O-C-N	-5.28	115.77	122.27
7	N	335	ALA	CA-C-O	5.28	126.15	120.55
11	R	32	LEU	CA-C-O	-5.28	115.26	120.70
13	O	239	MET	O-C-N	5.28	129.44	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	348	VAL	CB-CA-C	-5.28	103.29	110.42
7	N	346	ASN	N-CA-C	-5.27	106.08	112.88
2	V	230	TYR	CA-CB-CG	-5.27	104.41	113.90
6	Z	823	ASN	N-CA-CB	5.27	119.54	110.68
10	Q	223	GLY	O-C-N	5.27	127.35	122.13
11	R	382	ASP	CA-C-N	5.27	127.29	120.44
11	R	382	ASP	C-N-CA	5.27	127.29	120.44
13	O	91	ASP	CA-C-N	5.27	131.22	121.52
13	O	91	ASP	C-N-CA	5.27	131.22	121.52
2	V	71	MET	N-CA-CB	5.27	118.81	110.11
4	X	21	SER	CA-C-O	5.27	125.37	119.41
6	Z	959	HIS	ND1-CE1-NE2	5.27	113.67	108.40
13	O	179	PHE	CB-CA-C	-5.27	102.04	110.79
1	W	179	ARG	N-CA-CB	5.27	119.40	110.49
1	W	73	LEU	N-CA-CB	5.27	117.86	110.12
2	V	275	ASP	CA-C-N	5.27	124.77	119.19
2	V	275	ASP	C-N-CA	5.27	124.77	119.19
9	P	87	GLY	CA-C-N	5.27	131.60	121.54
9	P	87	GLY	C-N-CA	5.27	131.60	121.54
4	X	70	PRO	N-CA-CB	5.26	108.78	103.25
6	Z	360	SER	N-CA-C	-5.26	105.54	111.28
11	R	311	THR	CA-CB-OG1	5.26	117.50	109.60
6	Z	147	GLU	N-CA-C	-5.26	106.36	112.89
12	U	113	TYR	CB-CG-CD1	-5.26	112.91	120.80
6	Z	125	THR	CA-C-O	-5.26	113.92	119.97
11	R	134	TRP	N-CA-CB	5.26	117.94	110.16
6	Z	298	PHE	CA-C-N	5.26	127.75	120.29
6	Z	298	PHE	C-N-CA	5.26	127.75	120.29
9	P	207	THR	O-C-N	5.25	127.69	122.12
10	Q	155	LEU	N-CA-C	-5.25	105.45	111.07
4	X	64	ILE	N-CA-C	-5.25	100.63	107.88
6	Z	930	GLY	O-C-N	5.25	126.81	122.71
8	S	242	LEU	CB-CA-C	-5.25	102.07	110.79
3	T	110	LEU	CA-C-N	5.25	127.32	120.28
3	T	110	LEU	C-N-CA	5.25	127.32	120.28
4	X	99	PHE	CA-CB-CG	-5.25	108.55	113.80
8	S	117	SER	CA-C-N	5.25	131.57	121.54
8	S	117	SER	C-N-CA	5.25	131.57	121.54
8	S	294	ILE	O-C-N	-5.25	116.78	121.87
1	W	102	GLN	N-CA-C	-5.25	105.56	111.28
10	Q	417	GLY	CA-C-O	-5.25	115.64	121.05
7	N	485	MET	CA-C-N	5.25	126.89	120.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	485	MET	C-N-CA	5.25	126.89	120.22
7	N	808	ALA	CA-C-N	5.25	130.32	121.14
7	N	808	ALA	C-N-CA	5.25	130.32	121.14
10	Q	215	VAL	N-CA-C	-5.25	105.42	110.72
1	W	173	THR	CA-C-N	5.25	129.94	123.12
1	W	173	THR	C-N-CA	5.25	129.94	123.12
6	Z	169	VAL	CB-CA-C	-5.25	105.06	112.14
7	N	182	ASN	N-CA-C	-5.25	105.46	111.07
7	N	370	SER	CA-C-N	5.25	127.57	120.38
7	N	370	SER	C-N-CA	5.25	127.57	120.38
11	R	175	ALA	CA-C-N	5.25	127.84	120.28
11	R	175	ALA	C-N-CA	5.25	127.84	120.28
13	O	158	ASP	CA-CB-CG	-5.25	107.35	112.60
13	O	294	MET	N-CA-C	-5.25	105.47	111.14
7	N	283	ASP	CA-C-N	5.25	125.33	119.87
7	N	283	ASP	C-N-CA	5.25	125.33	119.87
3	T	83	ASN	CA-C-N	5.24	127.26	120.44
3	T	83	ASN	C-N-CA	5.24	127.26	120.44
11	R	318	PRO	CA-C-N	5.24	129.59	121.26
11	R	318	PRO	C-N-CA	5.24	129.59	121.26
6	Z	710	SER	CA-C-O	-5.24	114.86	120.42
6	Z	940	GLY	CA-C-N	5.24	127.28	120.26
6	Z	940	GLY	C-N-CA	5.24	127.28	120.26
7	N	566	SER	CA-C-O	-5.24	115.32	120.82
8	S	120	SER	CA-C-O	-5.24	115.32	120.82
8	S	248	ASP	O-C-N	5.24	127.68	122.12
10	Q	53	GLU	CA-C-N	5.24	127.25	120.44
10	Q	53	GLU	C-N-CA	5.24	127.25	120.44
6	Z	463	HIS	CB-CG-CD2	-5.24	124.39	131.20
7	N	796	VAL	CB-CA-C	-5.24	104.99	112.22
8	S	226	ASP	N-CA-C	-5.24	98.85	108.02
10	Q	122	ILE	CA-C-N	5.24	127.30	120.28
10	Q	122	ILE	C-N-CA	5.24	127.30	120.28
13	O	241	THR	CA-CB-OG1	5.24	117.46	109.60
8	S	211	ARG	CA-C-N	5.24	127.25	120.44
8	S	211	ARG	C-N-CA	5.24	127.25	120.44
11	R	300	ASP	CA-C-N	5.23	131.31	122.26
11	R	300	ASP	C-N-CA	5.23	131.31	122.26
9	P	8	LYS	CA-C-N	5.23	127.60	120.54
9	P	8	LYS	C-N-CA	5.23	127.60	120.54
9	P	253	ASP	N-CA-C	-5.23	101.91	109.59
9	P	269	VAL	CA-C-N	5.23	129.45	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	269	VAL	C-N-CA	5.23	129.45	120.72
9	P	424	GLU	CA-C-O	-5.23	114.88	120.42
6	Z	418	ALA	CA-C-N	5.23	127.84	120.42
6	Z	418	ALA	C-N-CA	5.23	127.84	120.42
6	Z	65	GLU	N-CA-CB	5.22	119.32	110.49
6	Z	91	PHE	N-CA-C	-5.22	106.49	112.92
7	N	481	ALA	N-CA-C	5.22	116.97	111.28
8	S	31	VAL	CA-C-N	5.22	127.23	120.44
8	S	31	VAL	C-N-CA	5.22	127.23	120.44
13	O	229	ASN	CA-CB-CG	-5.22	107.38	112.60
3	T	172	SER	CA-C-N	5.22	131.52	121.54
3	T	172	SER	C-N-CA	5.22	131.52	121.54
6	Z	549	ASN	O-C-N	-5.22	116.20	122.15
9	P	94	GLN	O-C-N	5.22	129.67	122.46
9	P	166	GLU	CA-CB-CG	5.22	124.55	114.10
9	P	345	VAL	CA-C-N	5.22	127.84	120.42
9	P	345	VAL	C-N-CA	5.22	127.84	120.42
9	P	384	VAL	CA-C-N	5.22	127.71	120.29
9	P	384	VAL	C-N-CA	5.22	127.71	120.29
13	O	217	LEU	CA-C-O	5.22	126.08	120.55
13	O	62	TYR	CB-CG-CD2	-5.22	112.97	120.80
11	R	309	LEU	CB-CA-C	-5.22	101.98	110.85
6	Z	245	VAL	CA-C-N	5.22	128.24	120.31
6	Z	245	VAL	C-N-CA	5.22	128.24	120.31
6	Z	766	HIS	CE1-NE2-CD2	-5.22	103.78	109.00
12	U	94	HIS	N-CA-C	-5.21	100.41	108.90
2	V	219	GLU	N-CA-C	-5.21	106.70	113.16
4	X	104	LYS	N-CA-C	-5.21	105.26	113.02
10	Q	306	TYR	CB-CA-C	-5.21	102.00	110.85
6	Z	828	ALA	O-C-N	-5.21	116.71	122.07
7	N	463	TYR	CA-C-O	-5.21	115.03	120.55
10	Q	135	HIS	CG-CD2-NE2	5.21	112.41	107.20
2	V	34	LEU	CA-C-N	5.20	127.25	120.28
2	V	34	LEU	C-N-CA	5.20	127.25	120.28
2	V	92	MET	N-CA-C	-5.20	105.61	111.28
6	Z	769	ASN	OD1-CG-ND2	5.20	127.80	122.60
9	P	177	ILE	CA-C-O	-5.20	115.86	121.27
6	Z	523	ALA	N-CA-C	-5.20	105.81	113.61
6	Z	897	HIS	CG-CD2-NE2	5.20	112.40	107.20
9	P	16	ILE	CA-C-N	5.20	131.79	122.38
9	P	16	ILE	C-N-CA	5.20	131.79	122.38
12	U	250	GLU	CB-CA-C	-5.20	102.16	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	42	GLN	CG-CD-NE2	-5.20	108.60	116.40
7	N	632	LYS	CB-CG-CD	5.20	123.25	111.30
6	Z	958	ASN	CA-C-N	5.20	130.70	122.60
6	Z	958	ASN	C-N-CA	5.20	130.70	122.60
7	N	910	PRO	N-CA-CB	5.20	108.58	102.76
8	S	460	VAL	O-C-N	5.20	127.00	121.91
13	O	34	GLU	O-C-N	5.20	127.63	122.12
6	Z	701	ILE	CA-C-N	5.19	127.24	120.28
6	Z	701	ILE	C-N-CA	5.19	127.24	120.28
8	S	389	LYS	CA-C-N	5.19	127.24	120.28
8	S	389	LYS	C-N-CA	5.19	127.24	120.28
11	R	60	ALA	CA-C-O	-5.19	113.85	118.63
9	P	31	ASP	CA-C-N	5.19	127.76	120.28
9	P	31	ASP	C-N-CA	5.19	127.76	120.28
9	P	75	LEU	O-C-N	5.19	127.62	122.12
1	W	61	VAL	O-C-N	5.19	128.64	122.83
13	O	39	PHE	CB-CA-C	-5.19	102.70	110.90
13	O	306	ARG	CA-C-O	-5.19	113.67	119.95
6	Z	964	GLU	CA-C-N	-5.19	112.78	121.39
6	Z	964	GLU	C-N-CA	-5.19	112.78	121.39
1	W	135	ASN	CB-CA-C	-5.19	102.38	110.94
10	Q	16	ASN	CB-CA-C	-5.18	101.14	110.37
12	U	174	LEU	O-C-N	5.18	128.65	122.27
13	O	116	ASN	OD1-CG-ND2	5.18	127.78	122.60
2	V	279	HIS	ND1-CE1-NE2	5.18	113.58	108.40
6	Z	522	THR	CA-C-O	-5.18	113.22	119.59
6	Z	766	HIS	CA-C-N	5.18	127.18	120.44
6	Z	766	HIS	C-N-CA	5.18	127.18	120.44
7	N	6	ALA	O-C-N	5.18	129.77	122.41
7	N	89	PHE	N-CA-C	-5.18	106.73	113.16
7	N	614	ASN	CA-C-O	-5.18	115.01	120.92
7	N	618	ARG	N-CA-CB	5.18	117.74	110.12
7	N	743	PHE	N-CA-CB	5.18	119.59	110.37
6	Z	21	GLU	CB-CG-CD	-5.18	103.79	112.60
5	Y	24	ILE	N-CA-C	-5.18	105.49	110.72
7	N	17	GLN	CA-C-N	5.18	127.64	120.29
7	N	17	GLN	C-N-CA	5.18	127.64	120.29
8	S	384	ARG	NE-CZ-NH2	-5.18	114.54	119.20
11	R	204	TRP	CG-CD2-CE3	-5.18	128.72	133.90
13	O	195	TYR	O-C-N	5.18	127.61	122.12
13	O	329	MET	CA-C-N	5.18	127.22	120.28
13	O	329	MET	C-N-CA	5.18	127.22	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	184	ASP	CA-C-O	5.18	126.59	120.69
6	Z	702	LYS	CG-CD-CE	5.18	123.21	111.30
8	S	340	LYS	N-CA-C	5.18	117.83	111.82
2	V	121	VAL	N-CA-C	-5.17	105.50	110.72
6	Z	738	TYR	CA-CB-CG	-5.17	104.59	113.90
6	Z	876	VAL	CA-C-N	5.17	127.64	120.29
6	Z	876	VAL	C-N-CA	5.17	127.64	120.29
1	W	49	VAL	CB-CA-C	-5.17	101.76	110.71
6	Z	405	ASN	O-C-N	-5.17	116.55	122.08
7	N	658	ILE	O-C-N	-5.17	116.84	121.91
12	U	100	ARG	N-CA-C	-5.17	101.43	109.24
11	R	399	GLN	CB-CA-C	-5.17	100.74	110.67
13	O	246	SER	CA-C-N	5.17	128.17	120.31
13	O	246	SER	C-N-CA	5.17	128.17	120.31
3	T	32	ILE	N-CA-C	-5.17	105.50	110.72
6	Z	733	VAL	CA-C-O	5.17	126.33	120.95
7	N	274	VAL	N-CA-C	5.17	115.89	110.62
11	R	111	LYS	CB-CA-C	-5.17	102.54	110.81
4	X	129	LEU	N-CA-C	5.17	116.99	111.36
8	S	86	SER	CA-C-N	5.17	127.20	120.28
8	S	86	SER	C-N-CA	5.17	127.20	120.28
8	S	353	LYS	CA-C-O	5.17	126.21	120.63
9	P	191	GLY	N-CA-C	-5.17	108.19	115.32
10	Q	75	ARG	CA-C-N	5.17	131.41	121.54
10	Q	75	ARG	C-N-CA	5.17	131.41	121.54
11	R	107	GLU	N-CA-C	5.17	117.31	111.11
13	O	52	ALA	O-C-N	-5.17	115.50	122.22
10	Q	120	LYS	CA-C-N	5.17	127.15	120.44
10	Q	120	LYS	C-N-CA	5.17	127.15	120.44
2	V	127	LYS	N-CA-CB	5.16	117.80	110.16
4	X	73	THR	CA-C-O	5.16	125.82	120.40
6	Z	463	HIS	CB-CG-ND1	5.16	130.44	122.70
7	N	801	THR	OG1-CB-CG2	-5.16	98.98	109.30
6	Z	110	ASN	N-CA-C	-5.16	105.55	111.07
7	N	317	SER	O-C-N	5.16	127.59	122.12
7	N	375	HIS	CB-CG-ND1	5.16	130.44	122.70
1	W	89	THR	N-CA-CB	5.16	118.28	110.28
2	V	254	ARG	NE-CZ-NH1	5.16	126.66	121.50
5	Y	37	ASP	CA-CB-CG	-5.16	107.44	112.60
6	Z	273	LEU	O-C-N	5.16	127.38	122.07
6	Z	785	VAL	CA-C-N	5.16	127.46	120.44
6	Z	785	VAL	C-N-CA	5.16	127.46	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	U	174	LEU	CA-C-O	-5.16	114.04	119.97
4	X	130	ASN	O-C-N	5.16	127.38	122.07
10	Q	140	LYS	CA-C-N	5.16	127.19	120.28
10	Q	140	LYS	C-N-CA	5.16	127.19	120.28
7	N	562	THR	N-CA-C	-5.16	99.94	108.75
8	S	306	SER	N-CA-C	-5.15	106.68	113.17
9	P	261	LEU	N-CA-CB	5.15	117.79	110.16
12	U	227	GLY	N-CA-C	-5.15	106.52	112.50
12	U	265	LEU	CA-C-N	5.15	127.61	120.29
12	U	265	LEU	C-N-CA	5.15	127.61	120.29
13	O	315	LYS	CA-CB-CG	5.15	124.41	114.10
2	V	204	HIS	ND1-CE1-NE2	5.15	113.55	108.40
2	V	213	LEU	N-CA-C	-5.15	105.67	111.28
6	Z	274	SER	CA-C-N	5.15	128.16	120.90
6	Z	274	SER	C-N-CA	5.15	128.16	120.90
10	Q	225	LEU	N-CA-CB	5.15	117.94	110.26
6	Z	295	ARG	CB-CG-CD	5.15	123.14	111.30
9	P	94	GLN	CA-C-O	-5.15	112.36	119.05
2	V	143	PRO	N-CA-CB	5.15	108.66	103.25
2	V	223	SER	N-CA-C	5.15	119.03	112.34
7	N	176	GLN	O-C-N	5.15	128.76	122.58
8	S	55	ARG	CA-C-N	5.15	127.18	120.28
8	S	55	ARG	C-N-CA	5.15	127.18	120.28
9	P	8	LYS	CA-CB-CG	5.15	124.39	114.10
3	T	184	ALA	CA-C-N	5.15	127.04	120.56
3	T	184	ALA	C-N-CA	5.15	127.04	120.56
7	N	122	GLN	CA-C-N	5.15	127.17	120.28
7	N	122	GLN	C-N-CA	5.15	127.17	120.28
4	X	14	VAL	CG1-CB-CG2	5.14	122.12	110.80
10	Q	342	LEU	N-CA-C	-5.14	105.75	111.36
1	W	58	ASN	CA-CB-CG	5.14	117.74	112.60
6	Z	181	GLY	O-C-N	-5.14	116.07	122.34
8	S	327	ILE	CA-C-N	5.14	125.04	119.85
8	S	327	ILE	C-N-CA	5.14	125.04	119.85
6	Z	495	ILE	CA-C-O	-5.14	115.40	120.85
1	W	21	PHE	CA-C-N	5.14	125.05	119.76
1	W	21	PHE	C-N-CA	5.14	125.05	119.76
9	P	2	SER	O-C-N	-5.14	115.54	122.43
7	N	350	LYS	CB-CG-CD	5.14	123.11	111.30
11	R	259	PHE	O-C-N	-5.14	116.78	122.07
1	W	112	ALA	CB-CA-C	-5.13	100.31	109.71
3	T	196	SER	CB-CA-C	-5.13	102.82	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	203	ARG	CD-NE-CZ	5.13	131.59	124.40
7	N	719	ASN	N-CA-C	-5.13	102.78	110.23
3	T	266	TYR	CB-CG-CD1	5.13	128.50	120.80
7	N	566	SER	N-CA-C	-5.13	105.58	111.07
7	N	624	ALA	CB-CA-C	-5.13	102.82	110.88
7	N	320	SER	N-CA-C	-5.13	105.38	111.69
12	U	274	MET	CA-C-O	-5.13	115.11	120.55
7	N	341	ALA	N-CA-C	5.13	116.91	110.24
7	N	407	GLY	CA-C-N	5.13	127.57	120.29
7	N	407	GLY	C-N-CA	5.13	127.57	120.29
11	R	149	ASN	OD1-CG-ND2	5.13	127.73	122.60
13	O	247	ASN	OD1-CG-ND2	5.13	127.73	122.60
4	X	87	PHE	N-CA-C	-5.13	100.81	108.96
9	P	112	LEU	N-CA-C	5.13	116.56	111.07
11	R	391	ASN	CB-CG-ND2	-5.13	108.71	116.40
13	O	108	GLU	CB-CG-CD	-5.13	103.89	112.60
7	N	80	LYS	CA-C-N	5.12	128.10	120.31
7	N	80	LYS	C-N-CA	5.12	128.10	120.31
7	N	910	PRO	N-CA-C	-5.12	106.04	114.75
5	Y	29	LEU	N-CA-CB	5.12	118.22	110.28
6	Z	467	VAL	N-CA-CB	5.12	117.81	111.41
6	Z	208	VAL	N-CA-CB	5.12	113.73	110.50
7	N	207	LEU	CB-CA-C	-5.12	102.84	110.88
13	O	374	ASN	OD1-CG-ND2	5.12	127.72	122.60
7	N	423	LEU	CA-C-N	5.12	127.65	120.28
7	N	423	LEU	C-N-CA	5.12	127.65	120.28
3	T	145	PRO	N-CD-CG	5.12	110.88	103.20
6	Z	17	GLN	O-C-N	5.12	127.55	122.12
6	Z	379	GLN	CA-C-N	5.12	127.56	120.29
6	Z	379	GLN	C-N-CA	5.12	127.56	120.29
10	Q	20	TYR	CA-C-N	5.12	127.14	120.28
10	Q	20	TYR	C-N-CA	5.12	127.14	120.28
7	N	240	GLN	N-CA-CB	5.12	117.64	110.12
9	P	329	PHE	N-CA-C	-5.12	101.91	109.18
1	W	182	TYR	N-CA-C	-5.12	105.89	111.82
6	Z	123	ALA	O-C-N	5.12	127.34	122.07
6	Z	488	ALA	N-CA-C	-5.12	105.78	111.36
6	Z	956	LEU	CA-C-O	5.12	125.77	120.40
11	R	277	LEU	CA-C-O	5.12	125.97	120.55
13	O	85	SER	N-CA-CB	5.12	118.21	110.28
3	T	134	LYS	N-CA-C	-5.11	105.62	111.14
2	V	258	GLU	N-CA-CB	5.11	119.13	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	217	THR	N-CA-CB	5.11	117.42	110.01
6	Z	256	LEU	CA-C-N	5.11	125.64	120.38
6	Z	256	LEU	C-N-CA	5.11	125.64	120.38
7	N	417	ARG	CA-C-O	-5.11	115.13	120.55
10	Q	128	GLU	N-CA-CB	5.11	118.24	110.42
2	V	185	ILE	CB-CA-C	5.11	119.67	111.29
7	N	487	LEU	N-CA-CB	5.11	117.63	110.12
7	N	580	ASN	CB-CA-C	-5.11	101.24	109.72
9	P	201	ARG	CA-C-O	5.11	125.65	119.11
1	W	111	VAL	CA-CB-CG1	5.11	119.08	110.40
7	N	817	THR	N-CA-CB	5.11	117.37	109.91
7	N	426	ILE	CA-C-O	-5.11	115.25	120.71
12	U	52	PHE	CA-C-N	5.11	128.95	120.94
12	U	52	PHE	C-N-CA	5.11	128.95	120.94
13	O	236	HIS	CA-C-O	-5.11	114.18	120.05
2	V	23	THR	N-CA-CB	5.10	117.86	109.95
8	S	451	ILE	N-CA-C	-5.10	107.32	112.17
10	Q	63	GLN	N-CA-C	-5.10	107.05	113.28
8	S	29	ASP	CA-C-N	5.10	127.07	120.44
8	S	29	ASP	C-N-CA	5.10	127.07	120.44
6	Z	625	THR	O-C-N	-5.10	115.94	120.48
4	X	22	ARG	CB-CA-C	-5.10	104.69	111.63
6	Z	85	VAL	CA-C-N	5.10	124.71	119.05
6	Z	85	VAL	C-N-CA	5.10	124.71	119.05
7	N	574	VAL	CB-CA-C	5.10	119.02	112.14
7	N	762	ARG	NE-CZ-NH1	5.10	126.60	121.50
12	U	135	ASP	N-CA-C	-5.10	101.84	109.95
8	S	107	SER	N-CA-C	-5.10	107.06	113.28
9	P	376	THR	CA-C-N	5.10	127.11	120.28
9	P	376	THR	C-N-CA	5.10	127.11	120.28
10	Q	14	LEU	N-CA-C	5.10	116.83	111.28
13	O	276	LYS	N-CA-C	-5.09	105.73	111.28
6	Z	10	GLN	O-C-N	5.09	127.52	122.12
3	T	109	TYR	CB-CA-C	-5.09	102.34	110.79
7	N	321	LEU	N-CA-CB	5.09	118.69	110.65
11	R	407	GLY	N-CA-C	-5.09	106.25	112.77
12	U	7	LYS	CB-CA-C	-5.09	98.74	109.38
13	O	107	GLN	CA-C-N	5.09	127.52	120.29
13	O	107	GLN	C-N-CA	5.09	127.52	120.29
2	V	111	HIS	CG-CD2-NE2	5.09	112.29	107.20
5	Y	29	LEU	N-CA-C	-5.09	105.92	111.82
7	N	196	THR	CA-C-N	5.09	127.90	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	196	THR	C-N-CA	5.09	127.90	120.98
10	Q	210	CYS	CA-C-O	-5.09	114.97	119.75
7	N	291	SER	CA-C-N	5.09	130.17	121.07
7	N	291	SER	C-N-CA	5.09	130.17	121.07
8	S	124	GLU	CA-C-O	-5.09	115.03	120.42
6	Z	313	ILE	CA-C-N	5.08	127.05	120.44
6	Z	313	ILE	C-N-CA	5.08	127.05	120.44
6	Z	771	HIS	CE1-NE2-CD2	-5.08	103.92	109.00
10	Q	98	LYS	CA-C-N	5.08	127.09	120.28
10	Q	98	LYS	C-N-CA	5.08	127.09	120.28
6	Z	102	ILE	N-CA-C	-5.08	107.89	113.43
9	P	42	LEU	O-C-N	5.08	127.51	122.12
9	P	239	GLN	CA-C-O	5.08	125.94	120.55
13	O	21	SER	CA-C-O	5.08	125.82	119.97
3	T	59	LYS	N-CA-C	5.08	116.82	111.28
7	N	724	THR	CA-C-N	5.08	131.25	121.54
7	N	724	THR	C-N-CA	5.08	131.25	121.54
11	R	417	TYR	CA-C-N	5.08	125.73	119.99
11	R	417	TYR	C-N-CA	5.08	125.73	119.99
10	Q	116	PHE	N-CA-C	5.08	116.51	111.07
6	Z	289	GLY	CA-C-O	-5.08	113.48	118.96
6	Z	317	GLN	CA-C-O	-5.08	114.13	119.97
8	S	334	HIS	N-CA-CB	5.08	117.64	110.13
8	S	404	LEU	N-CA-C	-5.08	105.93	111.82
9	P	95	TYR	N-CA-C	5.08	116.62	111.14
6	Z	55	ARG	CD-NE-CZ	5.07	131.50	124.40
6	Z	214	HIS	N-CA-C	-5.07	105.84	112.23
6	Z	209	PRO	O-C-N	5.07	129.12	122.27
10	Q	239	PHE	O-C-N	-5.07	115.46	122.46
11	R	229	LYS	N-CA-C	5.07	116.89	111.36
8	S	414	ASP	O-C-N	5.07	127.29	122.07
13	O	14	LEU	CB-CA-C	-5.07	102.23	110.85
6	Z	280	ASP	CA-C-N	5.07	127.07	120.28
6	Z	280	ASP	C-N-CA	5.07	127.07	120.28
7	N	902	VAL	O-C-N	5.07	128.19	122.67
10	Q	145	HIS	N-CA-CB	5.07	118.14	110.28
8	S	46	LEU	CA-C-N	5.07	131.22	121.54
8	S	46	LEU	C-N-CA	5.07	131.22	121.54
8	S	160	ARG	CA-C-N	5.07	127.38	120.54
8	S	160	ARG	C-N-CA	5.07	127.38	120.54
11	R	137	LEU	CB-CA-C	-5.07	102.24	110.85
11	R	389	GLU	CA-C-N	-5.07	115.62	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	389	GLU	C-N-CA	-5.07	115.62	122.77
3	T	60	ARG	N-CA-CB	5.07	117.57	110.12
8	S	479	MET	CA-C-N	5.07	128.01	120.31
8	S	479	MET	C-N-CA	5.07	128.01	120.31
9	P	236	GLU	CA-C-N	5.07	127.40	120.46
9	P	236	GLU	C-N-CA	5.07	127.40	120.46
2	V	204	HIS	CG-CD2-NE2	5.06	112.26	107.20
10	Q	346	ASN	O-C-N	5.06	127.49	122.12
1	W	165	GLN	O-C-N	-5.06	115.86	122.59
8	S	450	ASN	N-CA-C	-5.06	104.99	110.91
11	R	251	THR	CA-C-N	5.06	127.47	120.29
11	R	251	THR	C-N-CA	5.06	127.47	120.29
2	V	127	LYS	CB-CA-C	-5.06	102.25	110.85
2	V	222	GLN	CA-C-N	5.06	128.77	120.63
2	V	222	GLN	C-N-CA	5.06	128.77	120.63
10	Q	37	GLN	CA-C-N	5.06	127.31	120.38
10	Q	37	GLN	C-N-CA	5.06	127.31	120.38
9	P	277	GLN	CA-C-N	5.06	127.01	120.44
9	P	277	GLN	C-N-CA	5.06	127.01	120.44
12	U	198	LYS	CA-C-N	5.06	125.70	119.99
12	U	198	LYS	C-N-CA	5.06	125.70	119.99
12	U	178	VAL	CB-CA-C	-5.05	104.07	112.26
7	N	625	LEU	CA-C-N	5.05	125.55	119.94
7	N	625	LEU	C-N-CA	5.05	125.55	119.94
10	Q	141	LEU	N-CA-CB	5.05	117.55	110.12
10	Q	145	HIS	ND1-CE1-NE2	5.05	113.45	108.40
13	O	374	ASN	N-CA-C	-5.05	105.85	111.36
12	U	204	LEU	CA-C-N	5.05	127.05	120.28
12	U	204	LEU	C-N-CA	5.05	127.05	120.28
6	Z	422	ILE	N-CA-C	-5.05	105.78	110.53
7	N	146	LYS	CA-C-N	5.05	129.98	121.14
7	N	146	LYS	C-N-CA	5.05	129.98	121.14
8	S	151	GLU	CA-C-O	-5.05	114.83	120.54
10	Q	404	ASN	CA-C-N	5.05	131.19	121.54
10	Q	404	ASN	C-N-CA	5.05	131.19	121.54
10	Q	407	ALA	CB-CA-C	-5.05	102.92	110.90
2	V	240	ALA	O-C-N	5.05	127.91	122.15
7	N	492	THR	N-CA-CB	5.05	117.63	110.16
1	W	39	ALA	CB-CA-C	-5.05	102.41	110.79
6	Z	168	GLN	CG-CD-NE2	-5.04	108.83	116.40
8	S	423	VAL	CA-C-N	5.04	127.04	120.28
8	S	423	VAL	C-N-CA	5.04	127.04	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	362	LEU	CA-C-O	5.04	125.90	120.55
10	Q	301	ALA	O-C-N	5.04	127.90	122.15
11	R	400	TYR	N-CA-C	5.04	116.47	111.07
3	T	191	LYS	CA-C-N	5.04	127.04	120.28
3	T	191	LYS	C-N-CA	5.04	127.04	120.28
5	Y	25	ASN	N-CA-CB	5.04	117.62	110.16
6	Z	476	ASP	O-C-N	-5.04	116.88	122.07
7	N	224	THR	O-C-N	5.04	127.54	122.09
7	N	544	GLU	N-CA-CB	5.04	117.06	109.34
8	S	377	TYR	CG-CD1-CE1	-5.04	113.64	121.20
9	P	104	LEU	CA-C-N	5.04	127.04	120.28
9	P	104	LEU	C-N-CA	5.04	127.04	120.28
12	U	249	VAL	CA-C-O	-5.04	115.82	121.17
1	W	89	THR	CA-C-N	5.04	127.44	120.29
1	W	89	THR	C-N-CA	5.04	127.44	120.29
4	X	82	LYS	CA-C-O	5.04	126.09	120.90
5	Y	79	ALA	N-CA-C	-5.04	105.68	111.07
9	P	358	SER	N-CA-C	-5.04	105.88	112.23
8	S	132	ALA	CA-C-N	5.04	127.53	120.28
8	S	132	ALA	C-N-CA	5.04	127.53	120.28
3	T	119	THR	O-C-N	-5.03	116.08	122.27
3	T	142	LEU	CA-C-N	5.03	127.73	120.38
3	T	142	LEU	C-N-CA	5.03	127.73	120.38
6	Z	968	ASP	N-CA-C	-5.03	100.20	108.41
10	Q	174	LEU	CA-C-N	5.03	127.36	120.46
10	Q	174	LEU	C-N-CA	5.03	127.36	120.46
10	Q	240	PHE	CA-C-N	5.03	127.44	120.29
10	Q	240	PHE	C-N-CA	5.03	127.44	120.29
1	W	139	VAL	N-CA-C	-5.03	100.87	108.12
7	N	792	SER	CA-C-O	-5.03	115.22	120.55
6	Z	599	ILE	O-C-N	-5.03	116.99	121.87
7	N	870	ASN	CB-CG-OD1	5.03	130.86	120.80
13	O	96	LEU	CA-C-N	5.03	127.28	120.44
13	O	96	LEU	C-N-CA	5.03	127.28	120.44
4	X	9	LYS	N-CA-C	-5.03	101.51	109.76
6	Z	422	ILE	CA-C-O	-5.03	115.47	121.05
1	W	137	VAL	N-CA-C	-5.03	100.88	108.12
6	Z	402	ASP	CA-C-O	-5.03	114.57	120.20
7	N	64	ILE	CA-C-O	-5.03	115.72	120.95
10	Q	179	LEU	N-CA-CB	5.03	117.30	110.01
4	X	85	ARG	CA-C-N	5.03	129.78	123.10
4	X	85	ARG	C-N-CA	5.03	129.78	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	598	ALA	CA-C-O	5.03	125.88	120.55
8	S	51	ARG	NE-CZ-NH1	-5.03	116.47	121.50
8	S	487	THR	N-CA-CB	5.03	117.60	110.16
13	O	268	SER	CA-C-O	-5.03	115.52	120.70
7	N	62	ALA	O-C-N	5.02	127.44	122.12
3	T	243	ALA	CA-C-N	5.02	126.97	120.44
3	T	243	ALA	C-N-CA	5.02	126.97	120.44
7	N	193	ALA	CB-CA-C	-5.02	102.31	110.85
8	S	64	ARG	O-C-N	5.02	127.45	122.08
6	Z	108	ASP	CA-C-N	5.02	125.04	119.32
6	Z	108	ASP	C-N-CA	5.02	125.04	119.32
7	N	704	GLY	CA-C-N	5.02	126.99	120.56
7	N	704	GLY	C-N-CA	5.02	126.99	120.56
10	Q	32	ASP	CA-C-N	5.02	126.97	120.44
10	Q	32	ASP	C-N-CA	5.02	126.97	120.44
12	U	203	LYS	N-CA-CB	5.02	117.59	110.16
1	W	44	ASN	CA-CB-CG	-5.02	107.58	112.60
8	S	183	LEU	CB-CA-C	-5.02	102.46	110.79
8	S	468	ALA	O-C-N	5.02	127.44	122.12
9	P	385	ASN	OD1-CG-ND2	5.02	127.62	122.60
12	U	294	ASN	OD1-CG-ND2	5.02	127.62	122.60
2	V	292	ILE	CA-C-O	-5.02	115.34	120.71
4	X	56	PRO	N-CA-C	5.02	119.44	111.26
6	Z	553	ARG	CD-NE-CZ	5.02	131.42	124.40
6	Z	168	GLN	N-CA-C	-5.01	105.48	112.45
6	Z	451	ALA	CA-C-N	5.01	127.41	120.29
6	Z	451	ALA	C-N-CA	5.01	127.41	120.29
7	N	109	TYR	N-CA-C	-5.01	105.71	111.07
7	N	336	ASN	O-C-N	5.01	127.50	122.09
6	Z	607	ALA	CA-C-N	-5.01	113.31	122.38
6	Z	607	ALA	C-N-CA	-5.01	113.31	122.38
7	N	550	GLY	CA-C-N	5.01	125.65	119.99
7	N	550	GLY	C-N-CA	5.01	125.65	119.99
10	Q	90	LYS	CA-C-N	5.01	127.41	120.29
10	Q	90	LYS	C-N-CA	5.01	127.41	120.29
10	Q	135	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
10	Q	178	HIS	ND1-CE1-NE2	5.01	113.41	108.40
11	R	408	ASP	O-C-N	5.01	127.43	122.12
12	U	6	GLU	N-CA-C	5.01	116.82	111.36
6	Z	353	VAL	CA-C-N	5.01	125.28	119.47
6	Z	353	VAL	C-N-CA	5.01	125.28	119.47
7	N	229	VAL	CA-C-O	-5.01	115.54	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	161	LYS	N-CA-C	5.01	117.12	111.11
10	Q	135	HIS	CA-C-N	5.01	127.25	120.44
10	Q	135	HIS	C-N-CA	5.01	127.25	120.44
10	Q	423	VAL	N-CA-C	5.01	115.78	110.72
12	U	40	ASP	N-CA-C	5.01	117.31	110.55
6	Z	513	ALA	CB-CA-C	-5.01	102.91	111.02
2	V	60	ASP	N-CA-C	-5.01	107.30	113.41
6	Z	561	ASP	O-C-N	5.00	127.30	122.09
7	N	581	ASP	N-CA-C	5.00	116.55	111.14
6	Z	149	TRP	CB-CA-C	-5.00	101.06	110.67
6	Z	475	GLN	CA-C-N	5.00	126.94	120.44
6	Z	475	GLN	C-N-CA	5.00	126.94	120.44
8	S	438	HIS	CA-CB-CG	-5.00	108.80	113.80
11	R	100	ASN	CA-C-N	5.00	129.15	121.19
11	R	100	ASN	C-N-CA	5.00	129.15	121.19

There are no chirality outliers.

All (118) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	N	117	TYR	Sidechain
7	N	14	ARG	Sidechain
7	N	222	TYR	Sidechain
7	N	302	PHE	Sidechain
7	N	389	TYR	Sidechain
7	N	394	ARG	Sidechain
7	N	398	ARG	Sidechain
7	N	422	TYR	Sidechain
7	N	553	PHE	Sidechain
7	N	597	ARG	Sidechain
7	N	613	HIS	Sidechain
7	N	788	TYR	Sidechain
7	N	813	ARG	Sidechain
13	O	106	PHE	Sidechain
13	O	137	TYR	Sidechain
13	O	185	PHE	Sidechain
13	O	188	PHE	Sidechain
13	O	210	ARG	Sidechain
13	O	288	ARG	Sidechain
13	O	301	PHE	Sidechain
13	O	306	ARG	Sidechain
13	O	356	ARG	Sidechain

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Mol	Chain	Res	Type	Group
13	O	369	ARG	Sidechain
13	O	48	PHE	Sidechain
13	O	62	TYR	Sidechain
13	O	70	TYR	Sidechain
9	P	110	LEU	Mainchain
9	P	115	ARG	Sidechain
9	P	168	TYR	Sidechain
9	P	379	TYR	Sidechain
9	P	79	LEU	Mainchain
10	Q	124	PHE	Peptide
10	Q	145	HIS	Sidechain
10	Q	146	TYR	Sidechain
10	Q	161	LEU	Peptide
10	Q	20	TYR	Sidechain
10	Q	255	TYR	Sidechain
10	Q	309	ARG	Sidechain
10	Q	387	TYR	Sidechain
10	Q	400	TYR	Sidechain
10	Q	434	TYR	Sidechain
10	Q	67	THR	Peptide
11	R	176	ARG	Sidechain
11	R	20	ARG	Sidechain
11	R	206	ARG	Sidechain
11	R	210	TYR	Sidechain
11	R	222	ARG	Sidechain
11	R	252	TYR	Sidechain
11	R	297	TYR	Sidechain
11	R	334	ARG	Sidechain
11	R	345	TYR	Sidechain
11	R	392	ARG	Sidechain
11	R	400	TYR	Sidechain
11	R	401	HIS	Sidechain
11	R	422	ARG	Sidechain
11	R	43	ARG	Sidechain
11	R	49	PHE	Sidechain
11	R	63	TYR	Sidechain
11	R	65	TYR	Sidechain
11	R	99	TYR	Sidechain
8	S	158	PHE	Sidechain
8	S	197	SER	Mainchain,Peptide
8	S	275	TYR	Sidechain
8	S	298	ARG	Sidechain

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Mol	Chain	Res	Type	Group
8	S	467	PHE	Sidechain
8	S	486	LYS	Mainchain
8	S	51	ARG	Sidechain
8	S	76	PHE	Sidechain
8	S	82	TYR	Sidechain
3	T	128	TYR	Sidechain
3	T	150	ARG	Sidechain
3	T	197	TYR	Sidechain
3	T	224	ARG	Sidechain
3	T	234	TYR	Sidechain
3	T	235	PHE	Sidechain
3	T	251	HIS	Peptide
3	T	51	TYR	Sidechain
3	T	91	SER	Peptide
12	U	113	TYR	Sidechain
12	U	24	ARG	Sidechain
12	U	32	ARG	Sidechain
2	V	100	ARG	Sidechain
2	V	156	PHE	Sidechain
2	V	20	ARG	Sidechain
2	V	217	HIS	Sidechain
2	V	229	ASP	Peptide
2	V	270	TYR	Sidechain
2	V	273	ARG	Sidechain
1	W	15	TYR	Sidechain
1	W	21	PHE	Sidechain
4	X	122	TYR	Sidechain
4	X	17	TYR	Sidechain
4	X	22	ARG	Sidechain
4	X	48	PHE	Sidechain
4	X	51	ARG	Sidechain
4	X	87	PHE	Sidechain
4	X	98	PHE	Sidechain
5	Y	38	PHE	Sidechain
6	Z	136	ARG	Sidechain
6	Z	137	TYR	Sidechain
6	Z	138	ARG	Sidechain
6	Z	155	ARG	Sidechain
6	Z	210	TYR	Sidechain
6	Z	269	TYR	Sidechain
6	Z	295	ARG	Sidechain
6	Z	439	TYR	Sidechain

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Mol	Chain	Res	Type	Group
6	Z	477	TYR	Sidechain
6	Z	608	TYR	Sidechain
6	Z	64	TYR	Sidechain
6	Z	738	TYR	Sidechain
6	Z	759	ARG	Sidechain
6	Z	774	ARG	Sidechain
6	Z	798	ARG	Sidechain
6	Z	849	ARG	Sidechain
6	Z	893	PHE	Sidechain
6	Z	898	HIS	Sidechain
6	Z	962	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	1534	0	1542	1	0
2	V	2274	0	2273	25	0
3	T	2192	0	2161	7	0
4	X	1032	0	1017	4	0
5	Y	435	0	393	10	0
6	Z	7005	0	6932	75	0
7	N	6882	0	6959	25	0
8	S	3894	0	3938	23	0
9	P	3608	0	3693	21	0
10	Q	3499	0	3524	25	0
11	R	3060	0	3083	51	0
12	U	2373	0	2403	17	0
13	O	3186	0	3213	58	0
All	All	40974	0	41131	328	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 (328) 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)
9:P:78:GLN:C	9:P:79:LEU:N	1.75	1.41
11:R:99:TYR:CE1	11:R:99:TYR:CZ	2.09	1.39
8:S:127:THR:CB	8:S:127:THR:CA	1.98	1.37
11:R:99:TYR:CE1	11:R:99:TYR:OH	1.79	1.32
9:P:212:LYS:O	9:P:213:TYR:CD1	1.92	1.22
11:R:64:LYS:NZ	11:R:99:TYR:CZ	2.10	1.18
6:Z:84:ALA:O	6:Z:86:PRO:HD3	1.45	1.16
6:Z:35:GLU:OE2	6:Z:83:THR:HG21	1.46	1.13
11:R:99:TYR:CZ	11:R:99:TYR:OH	2.04	1.10
11:R:60:ALA:O	11:R:99:TYR:CZ	2.04	1.09
11:R:60:ALA:HB1	11:R:99:TYR:CE1	1.89	1.07
11:R:60:ALA:HB1	11:R:99:TYR:CZ	1.88	1.06
13:O:69:PHE:HD1	13:O:72:LYS:HB2	1.18	1.02
11:R:60:ALA:CB	11:R:99:TYR:CE1	2.44	1.01
11:R:60:ALA:C	11:R:99:TYR:CZ	2.39	1.00
11:R:64:LYS:NZ	11:R:99:TYR:CE1	2.29	0.99
13:O:69:PHE:CD1	13:O:72:LYS:CB	2.36	0.99
13:O:69:PHE:CD1	13:O:72:LYS:HB2	1.99	0.97
12:U:37:ILE:CG2	12:U:48:VAL:CG1	2.44	0.94
6:Z:26:ASN:OD1	6:Z:26:ASN:C	2.08	0.93
13:O:69:PHE:HD1	13:O:72:LYS:CB	1.59	0.93
11:R:99:TYR:HH	11:R:99:TYR:HE1	1.00	0.89
8:S:219:LYS:HE2	8:S:219:LYS:HA	1.56	0.87
12:U:37:ILE:CG2	12:U:48:VAL:HG11	2.03	0.86
13:O:70:TYR:C	13:O:70:TYR:CD2	2.52	0.86
13:O:70:TYR:CD2	13:O:70:TYR:O	2.29	0.86
6:Z:26:ASN:OD1	6:Z:26:ASN:O	1.95	0.84
9:P:212:LYS:O	9:P:213:TYR:HD1	1.55	0.84
11:R:60:ALA:HB1	11:R:99:TYR:CE2	2.11	0.84
13:O:49:PHE:CZ	13:O:62:TYR:HB2	2.12	0.82
6:Z:84:ALA:O	6:Z:86:PRO:CD	2.27	0.81
12:U:37:ILE:HG21	12:U:48:VAL:HG11	1.64	0.80
13:O:49:PHE:CE1	13:O:62:TYR:HB2	2.19	0.78
6:Z:127:SER:OG	6:Z:188:ALA:HA	1.83	0.78
13:O:49:PHE:CD1	13:O:58:ARG:HG2	2.18	0.78
9:P:212:LYS:C	9:P:213:TYR:CD1	2.62	0.78
13:O:14:LEU:HD21	13:O:61:LEU:HB2	1.66	0.76
11:R:60:ALA:CA	11:R:99:TYR:CE1	2.68	0.76
12:U:37:ILE:CG2	12:U:48:VAL:HG13	2.13	0.76
6:Z:124:MET:CA	6:Z:188:ALA:HB1	2.16	0.76
11:R:60:ALA:HB1	11:R:99:TYR:CD1	2.21	0.76
11:R:60:ALA:O	11:R:99:TYR:OH	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:62:TYR:CD1	13:O:62:TYR:C	2.62	0.73
11:R:64:LYS:NZ	11:R:99:TYR:CD1	2.56	0.73
2:V:29:ILE:HD12	2:V:201:ILE:HG21	1.71	0.72
6:Z:1:MET:HA	6:Z:25:PRO:HG3	1.70	0.72
11:R:60:ALA:CB	11:R:99:TYR:CZ	2.71	0.72
13:O:14:LEU:CD2	13:O:61:LEU:HB2	2.19	0.72
2:V:185:ILE:HA	2:V:189:ILE:HB	1.73	0.71
5:Y:17:THR:O	8:S:59:ASP:CB	2.38	0.71
12:U:37:ILE:HG22	12:U:48:VAL:HG13	1.72	0.71
11:R:60:ALA:CB	11:R:99:TYR:CD1	2.75	0.69
6:Z:1:MET:C	6:Z:25:PRO:HB3	2.17	0.68
5:Y:17:THR:O	8:S:59:ASP:HB2	1.93	0.68
8:S:127:THR:CB	8:S:127:THR:C	2.67	0.68
11:R:64:LYS:NZ	11:R:99:TYR:OH	2.21	0.68
11:R:60:ALA:HB1	11:R:99:TYR:CD2	2.30	0.67
6:Z:93:ARG:HB3	6:Z:94:PRO:HD3	1.76	0.67
6:Z:124:MET:HA	6:Z:188:ALA:HB1	1.77	0.67
6:Z:35:GLU:CD	6:Z:83:THR:HG21	2.19	0.67
13:O:62:TYR:CD1	13:O:62:TYR:O	2.48	0.66
13:O:62:TYR:CG	13:O:63:ASP:N	2.48	0.66
6:Z:124:MET:O	6:Z:188:ALA:CA	2.44	0.66
11:R:64:LYS:NZ	11:R:99:TYR:CG	2.64	0.66
13:O:26:PHE:HE1	13:O:61:LEU:HD22	1.62	0.65
2:V:69:PHE:C	2:V:69:PHE:CD1	2.73	0.65
6:Z:1:MET:CA	6:Z:25:PRO:HG3	2.25	0.65
13:O:70:TYR:C	13:O:70:TYR:HD2	2.04	0.65
10:Q:157:LEU:C	10:Q:157:LEU:HD23	2.22	0.64
10:Q:275:ILE:C	10:Q:275:ILE:HD12	2.21	0.64
6:Z:124:MET:SD	6:Z:182:SER:HB3	2.37	0.64
10:Q:55:GLU:O	10:Q:58:ILE:HG22	1.97	0.64
5:Y:89:GLN:OXT	5:Y:89:GLN:CG	2.45	0.64
10:Q:366:ILE:HG23	10:Q:368:LEU:H	1.63	0.64
11:R:55:LYS:HA	11:R:98:LEU:HD13	1.78	0.64
2:V:29:ILE:HD12	2:V:201:ILE:CG2	2.28	0.63
6:Z:1:MET:O	6:Z:25:PRO:HB3	1.99	0.63
6:Z:1:MET:O	6:Z:25:PRO:CB	2.46	0.63
6:Z:7:LYS:HB3	6:Z:26:ASN:ND2	2.13	0.63
11:R:64:LYS:NZ	11:R:99:TYR:CE2	2.52	0.63
2:V:142:ASP:OD1	2:V:144:ILE:HG22	1.99	0.62
13:O:70:TYR:CE1	13:O:78:VAL:HG11	2.34	0.62
6:Z:35:GLU:OE2	6:Z:83:THR:CG2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:60:ALA:HA	11:R:99:TYR:CE1	2.35	0.61
13:O:70:TYR:O	13:O:70:TYR:HD2	1.83	0.61
12:U:37:ILE:HG23	12:U:48:VAL:CG1	2.27	0.61
6:Z:124:MET:CB	6:Z:188:ALA:HB1	2.31	0.60
6:Z:1:MET:O	6:Z:25:PRO:HG3	2.01	0.60
13:O:66:VAL:HG13	13:O:78:VAL:HG13	1.84	0.60
3:T:80:ASN:HA	7:N:11:ALA:HB1	1.84	0.60
9:P:78:GLN:O	9:P:79:LEU:N	2.29	0.60
6:Z:24:THR:HB	6:Z:25:PRO:HD3	1.83	0.59
6:Z:84:ALA:C	6:Z:86:PRO:HD3	2.25	0.59
6:Z:185:ASP:O	6:Z:186:GLY:C	2.45	0.59
13:O:52:ALA:O	13:O:58:ARG:HB2	2.02	0.59
13:O:66:VAL:CG1	13:O:78:VAL:HG13	2.32	0.59
9:P:93:ILE:O	9:P:96:MET:HB3	2.03	0.58
11:R:32:LEU:HA	11:R:35:GLN:HE21	1.69	0.58
11:R:257:GLY:O	11:R:266:LEU:HD13	2.04	0.58
6:Z:3:ASP:O	6:Z:26:ASN:HB2	2.04	0.58
11:R:113:LEU:HD13	11:R:137:LEU:HD22	1.86	0.58
13:O:49:PHE:HD1	13:O:58:ARG:HG2	1.69	0.57
5:Y:89:GLN:OXT	5:Y:89:GLN:HG2	2.05	0.57
11:R:64:LYS:NZ	11:R:99:TYR:CD2	2.72	0.57
9:P:59:LEU:O	9:P:62:ILE:HG12	2.04	0.57
6:Z:124:MET:O	6:Z:188:ALA:CB	2.52	0.57
10:Q:355:GLU:O	10:Q:356:CYS:CB	2.53	0.56
13:O:214:ALA:HB2	13:O:238:ILE:HG13	1.86	0.56
10:Q:118:CYS:SG	10:Q:144:LEU:HD13	2.45	0.56
9:P:101:MET:HE1	9:P:121:THR:HG21	1.88	0.56
6:Z:24:THR:CB	6:Z:25:PRO:CD	2.84	0.56
6:Z:82:MET:HG3	6:Z:82:MET:O	2.05	0.56
5:Y:18:LYS:HA	8:S:56:SER:HA	1.86	0.56
7:N:773:MET:HG2	7:N:884:PHE:CD1	2.41	0.55
13:O:258:LEU:HD23	13:O:291:ILE:HD13	1.88	0.55
13:O:70:TYR:OH	13:O:75:GLN:HG3	2.07	0.55
2:V:142:ASP:OD1	2:V:142:ASP:C	2.49	0.54
13:O:258:LEU:HD23	13:O:291:ILE:CD1	2.37	0.54
6:Z:124:MET:HB3	6:Z:188:ALA:CB	2.37	0.54
8:S:164:ILE:HB	8:S:165:PRO:CD	2.37	0.54
9:P:94:GLN:HB3	9:P:131:PHE:CD2	2.43	0.54
13:O:163:ILE:HG22	13:O:164:PRO:O	2.07	0.54
6:Z:82:MET:HA	6:Z:85:VAL:HA	1.88	0.54
7:N:43:LEU:N	7:N:44:PRO:CD	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:59:LEU:C	13:O:59:LEU:HD23	2.31	0.54
12:U:37:ILE:HD11	12:U:93:TYR:HB3	1.89	0.54
6:Z:24:THR:HB	6:Z:25:PRO:CD	2.37	0.54
2:V:306:LYS:OXT	2:V:306:LYS:HG3	2.07	0.53
8:S:19:HIS:CD2	8:S:19:HIS:H	2.26	0.53
6:Z:84:ALA:C	6:Z:86:PRO:CD	2.82	0.53
3:T:28:PRO:HB2	3:T:29:PRO:HD3	1.89	0.53
6:Z:24:THR:N	6:Z:25:PRO:HD2	2.20	0.52
9:P:212:LYS:C	9:P:213:TYR:CG	2.86	0.52
6:Z:124:MET:C	6:Z:188:ALA:CB	2.83	0.52
8:S:219:LYS:HE2	8:S:219:LYS:CA	2.34	0.52
7:N:665:ILE:HG23	7:N:665:ILE:O	2.10	0.52
10:Q:78:ILE:HB	10:Q:79:PRO:HD3	1.90	0.52
8:S:184:TRP:HA	8:S:187:ILE:HD12	1.92	0.52
9:P:268:LEU:HD21	9:P:281:ILE:HG13	1.92	0.52
2:V:117:TRP:HB3	2:V:188:LEU:HG	1.92	0.51
11:R:279:LEU:O	11:R:280:ILE:HG12	2.10	0.51
8:S:472:HIS:CE1	12:U:266:THR:HA	2.45	0.51
6:Z:124:MET:CA	6:Z:188:ALA:CB	2.88	0.51
8:S:439:GLU:OE1	8:S:439:GLU:N	2.33	0.51
6:Z:354:PRO:HA	6:Z:357:ILE:HG12	1.93	0.51
12:U:37:ILE:HG21	12:U:48:VAL:CG1	2.26	0.51
7:N:773:MET:HG3	7:N:884:PHE:HD1	1.76	0.51
11:R:286:LEU:O	11:R:289:ILE:HG22	2.11	0.50
12:U:120:LEU:CD2	12:U:122:ILE:HG13	2.41	0.50
13:O:49:PHE:CZ	13:O:62:TYR:CB	2.92	0.50
6:Z:845:LEU:HG	6:Z:846:PHE:CE1	2.47	0.50
12:U:37:ILE:HG23	12:U:48:VAL:HG11	1.86	0.50
13:O:26:PHE:CE1	13:O:61:LEU:HD22	2.44	0.50
2:V:192:LEU:HA	2:V:196:TYR:CZ	2.47	0.50
6:Z:1:MET:C	6:Z:25:PRO:HG3	2.36	0.50
13:O:58:ARG:O	13:O:62:TYR:HB3	2.12	0.49
6:Z:124:MET:SD	6:Z:182:SER:CB	3.00	0.49
11:R:60:ALA:HB1	11:R:99:TYR:CG	2.47	0.49
10:Q:20:TYR:CZ	10:Q:68:MET:HG2	2.47	0.49
13:O:393:VAL:OXT	13:O:393:VAL:HG12	2.11	0.49
7:N:150:LEU:HD22	7:N:173:LYS:HG3	1.95	0.49
10:Q:74:LEU:C	10:Q:74:LEU:HD23	2.37	0.49
2:V:144:ILE:HG23	2:V:145:GLN:HG3	1.95	0.49
6:Z:728:LYS:HB2	6:Z:731:GLY:H	1.78	0.49
7:N:110:VAL:HG13	7:N:160:GLY:CA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:77:THR:O	8:S:80:VAL:HG22	2.13	0.49
6:Z:1:MET:O	6:Z:25:PRO:CG	2.60	0.49
13:O:49:PHE:CE1	13:O:58:ARG:HG2	2.48	0.49
7:N:110:VAL:HG13	7:N:160:GLY:HA2	1.95	0.48
7:N:773:MET:CG	7:N:884:PHE:CD1	2.95	0.48
6:Z:428:TRP:CD1	6:Z:428:TRP:O	2.66	0.48
6:Z:767:TYR:C	6:Z:767:TYR:CD2	2.91	0.48
5:Y:20:LYS:NZ	8:S:63:LEU:HD13	2.28	0.48
10:Q:377:LEU:O	10:Q:381:ILE:HG13	2.14	0.48
13:O:254:LEU:HG	13:O:269:LEU:HD13	1.96	0.48
10:Q:275:ILE:HD12	10:Q:276:ASP:N	2.29	0.48
2:V:29:ILE:CD1	2:V:201:ILE:HG21	2.41	0.48
13:O:258:LEU:HA	13:O:291:ILE:CD1	2.44	0.48
11:R:261:LEU:CA	11:R:266:LEU:HB2	2.43	0.48
13:O:59:LEU:O	13:O:63:ASP:CB	2.62	0.48
2:V:117:TRP:CB	2:V:188:LEU:HG	2.44	0.47
2:V:188:LEU:C	2:V:188:LEU:HD23	2.39	0.47
10:Q:247:HIS:CE1	10:Q:286:TYR:CE2	3.02	0.47
2:V:183:ALA:O	2:V:184:ASN:HB2	2.14	0.47
6:Z:4:GLU:O	6:Z:26:ASN:ND2	2.47	0.47
3:T:80:ASN:CA	7:N:11:ALA:HB1	2.43	0.47
13:O:70:TYR:CE1	13:O:102:LEU:HD11	2.50	0.47
11:R:262:GLU:O	11:R:266:LEU:HB3	2.15	0.47
11:R:64:LYS:HG2	11:R:99:TYR:CZ	2.50	0.47
10:Q:255:TYR:H	10:Q:255:TYR:HD1	1.62	0.46
3:T:233:VAL:HG21	3:T:235:PHE:CE1	2.50	0.46
5:Y:32:ASP:HB3	5:Y:33:ASP:H	1.51	0.46
13:O:59:LEU:CG	13:O:85:SER:HB3	2.45	0.46
6:Z:124:MET:O	6:Z:188:ALA:HA	2.15	0.46
10:Q:67:THR:H	10:Q:68:MET:HG3	1.80	0.46
13:O:62:TYR:HE1	13:O:66:VAL:HG21	1.81	0.46
6:Z:124:MET:CB	6:Z:188:ALA:CB	2.94	0.46
9:P:59:LEU:CG	9:P:96:MET:HG2	2.46	0.46
2:V:118:LEU:HB2	2:V:196:TYR:CE2	2.51	0.46
8:S:475:TYR:CE2	12:U:269:THR:HB	2.51	0.46
11:R:113:LEU:HD13	11:R:137:LEU:CD2	2.46	0.46
3:T:80:ASN:HA	7:N:11:ALA:CB	2.46	0.46
7:N:773:MET:CG	7:N:884:PHE:HD1	2.28	0.45
3:T:85:LEU:HD13	3:T:85:LEU:HA	1.88	0.45
11:R:60:ALA:HB2	11:R:99:TYR:CD1	2.49	0.45
8:S:211:ARG:NH2	8:S:246:GLU:OE1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:258:LEU:HA	13:O:291:ILE:HD12	1.98	0.45
2:V:25:GLU:CD	2:V:25:GLU:H	2.24	0.45
2:V:29:ILE:CD1	2:V:201:ILE:CG2	2.95	0.45
6:Z:385:PHE:N	6:Z:385:PHE:CD1	2.81	0.45
7:N:55:PHE:O	7:N:58:ARG:HG3	2.17	0.45
9:P:89:LEU:HD12	9:P:92:SER:HB2	1.98	0.45
13:O:214:ALA:HB2	13:O:238:ILE:CG1	2.47	0.45
10:Q:109:ASP:HB2	10:Q:114:GLN:HE22	1.82	0.44
10:Q:157:LEU:C	10:Q:157:LEU:CD2	2.90	0.44
11:R:304:TYR:CE2	11:R:337:VAL:HG11	2.52	0.44
2:V:247:ILE:O	2:V:247:ILE:HG22	2.17	0.44
13:O:58:ARG:O	13:O:62:TYR:CB	2.65	0.44
6:Z:7:LYS:HB3	6:Z:26:ASN:CG	2.42	0.44
11:R:60:ALA:CA	11:R:99:TYR:CZ	2.99	0.44
3:T:80:ASN:CB	7:N:11:ALA:HB1	2.48	0.44
6:Z:185:ASP:O	6:Z:186:GLY:O	2.35	0.44
6:Z:189:ALA:O	6:Z:193:PHE:CG	2.70	0.44
10:Q:431:SER:HA	10:Q:434:TYR:CD2	2.53	0.44
6:Z:124:MET:C	6:Z:188:ALA:HB2	2.42	0.44
6:Z:362:LEU:HD13	6:Z:395:CYS:HA	2.00	0.44
9:P:59:LEU:HD21	9:P:96:MET:HG2	2.00	0.44
13:O:25:LEU:HB3	13:O:29:PHE:CZ	2.53	0.44
11:R:60:ALA:HB3	11:R:102:LEU:HD22	1.98	0.44
6:Z:407:VAL:HG11	6:Z:439:TYR:CE1	2.53	0.43
6:Z:898:HIS:CD2	6:Z:898:HIS:H	2.36	0.43
7:N:83:LEU:HG	7:N:132:LYS:HG2	2.00	0.43
8:S:81:LEU:N	8:S:81:LEU:HD22	2.32	0.43
9:P:77:GLU:O	9:P:80:THR:HB	2.18	0.43
13:O:62:TYR:CD2	13:O:63:ASP:N	2.86	0.43
2:V:189:ILE:O	2:V:189:ILE:HG13	2.17	0.43
5:Y:21:ASN:N	8:S:59:ASP:OD2	2.51	0.43
6:Z:124:MET:HB3	6:Z:188:ALA:HB2	2.00	0.43
11:R:261:LEU:HB2	11:R:266:LEU:HB2	2.00	0.43
12:U:274:MET:HB3	12:U:274:MET:HE2	1.49	0.43
13:O:49:PHE:HZ	13:O:62:TYR:HB2	1.76	0.43
4:X:17:TYR:CE1	4:X:96:ARG:HB2	2.53	0.43
7:N:83:LEU:HG	7:N:132:LYS:CG	2.49	0.43
9:P:93:ILE:HG22	9:P:97:ILE:HG13	2.00	0.43
13:O:160:LYS:HD3	13:O:163:ILE:CD1	2.48	0.43
6:Z:120:SER:O	6:Z:124:MET:HG3	2.18	0.43
11:R:279:LEU:O	11:R:280:ILE:CG1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:196:TYR:CD2	2:V:196:TYR:N	2.86	0.43
5:Y:21:ASN:HB2	8:S:59:ASP:OD2	2.19	0.43
7:N:447:SER:O	7:N:450:ILE:HG22	2.18	0.43
9:P:388:ILE:HG22	9:P:389:ILE:HG23	1.99	0.43
11:R:99:TYR:O	11:R:102:LEU:HB3	2.18	0.43
6:Z:24:THR:CB	6:Z:25:PRO:HD3	2.46	0.43
7:N:711:ARG:NH1	7:N:786:ARG:O	2.52	0.43
12:U:120:LEU:HD22	12:U:122:ILE:HG13	2.01	0.43
2:V:153:ILE:HG21	2:V:203:TYR:OH	2.19	0.43
9:P:89:LEU:HB3	9:P:91:LEU:H	1.84	0.42
6:Z:1:MET:CA	6:Z:25:PRO:CG	2.95	0.42
6:Z:4:GLU:C	6:Z:26:ASN:ND2	2.78	0.42
13:O:53:LYS:O	13:O:58:ARG:NH1	2.52	0.42
2:V:123:VAL:HG13	2:V:158:LEU:HD11	2.01	0.42
5:Y:33:ASP:OD1	5:Y:33:ASP:C	2.63	0.42
7:N:316:LYS:HD2	7:N:316:LYS:C	2.44	0.42
6:Z:25:PRO:HB2	6:Z:26:ASN:H	1.43	0.42
6:Z:124:MET:O	6:Z:188:ALA:HB2	2.19	0.42
9:P:351:ARG:HD3	9:P:388:ILE:CG2	2.49	0.42
10:Q:67:THR:H	10:Q:68:MET:CG	2.33	0.42
10:Q:78:ILE:N	10:Q:79:PRO:CD	2.83	0.42
11:R:257:GLY:O	11:R:266:LEU:CD1	2.67	0.42
11:R:400:TYR:CD1	11:R:400:TYR:C	2.98	0.42
4:X:17:TYR:HE1	4:X:96:ARG:HB2	1.84	0.42
4:X:88:ALA:HA	4:X:98:PHE:HD1	1.85	0.42
13:O:62:TYR:CE1	13:O:81:TYR:CB	3.03	0.42
6:Z:93:ARG:HB3	6:Z:94:PRO:CD	2.48	0.42
13:O:62:TYR:CE1	13:O:81:TYR:HB2	2.55	0.42
6:Z:127:SER:OG	6:Z:188:ALA:CA	2.60	0.42
6:Z:82:MET:HB2	6:Z:85:VAL:HG22	2.01	0.41
7:N:710:GLY:O	7:N:711:ARG:HB2	2.20	0.41
13:O:49:PHE:HZ	13:O:62:TYR:CB	2.33	0.41
4:X:64:ILE:HD13	4:X:97:TYR:CE1	2.54	0.41
6:Z:24:THR:HG23	6:Z:71:LEU:HB2	2.02	0.41
8:S:475:TYR:CD1	12:U:273:LEU:HB2	2.55	0.41
6:Z:518:LEU:HD23	6:Z:518:LEU:HA	1.92	0.41
12:U:183:ALA:H	12:U:188:ILE:HG21	1.85	0.41
8:S:219:LYS:HA	8:S:219:LYS:CE	2.32	0.41
10:Q:354:PHE:N	10:Q:354:PHE:CD1	2.88	0.41
13:O:79:VAL:O	13:O:83:LEU:HG	2.20	0.41
6:Z:1:MET:C	6:Z:25:PRO:CB	2.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:31:PHE:CE2	11:R:320:LYS:HA	2.54	0.41
13:O:228:TYR:HA	13:O:230:PHE:CE2	2.55	0.41
9:P:59:LEU:HG	9:P:96:MET:HG2	2.03	0.41
6:Z:89:LEU:O	6:Z:126:TYR:CD1	2.74	0.41
9:P:17:LEU:HD23	9:P:17:LEU:HA	1.82	0.41
2:V:69:PHE:CD1	2:V:69:PHE:O	2.73	0.41
7:N:109:TYR:CD1	7:N:109:TYR:C	2.99	0.41
10:Q:67:THR:N	10:Q:68:MET:HG3	2.35	0.41
10:Q:75:ARG:NH1	10:Q:76:GLU:OE2	2.54	0.41
11:R:60:ALA:O	11:R:99:TYR:CE1	2.73	0.41
13:O:66:VAL:HG11	13:O:78:VAL:HG13	2.03	0.41
13:O:70:TYR:HE1	13:O:102:LEU:HD11	1.86	0.41
2:V:49:VAL:HG12	2:V:50:MET:N	2.37	0.41
2:V:192:LEU:O	2:V:196:TYR:O	2.39	0.41
6:Z:804:ASP:O	6:Z:805:LEU:HB2	2.21	0.41
13:O:393:VAL:OXT	13:O:393:VAL:CG1	2.69	0.41
6:Z:76:LYS:HE2	6:Z:121:ILE:HG21	2.02	0.40
7:N:340:HIS:HE1	7:N:348:PHE:HB2	1.85	0.40
11:R:267:LYS:HG3	11:R:297:TYR:CD1	2.56	0.40
11:R:267:LYS:HG3	11:R:297:TYR:CE1	2.56	0.40
13:O:53:LYS:O	13:O:58:ARG:CZ	2.69	0.40
1:W:93:ILE:HG13	12:U:65:VAL:HG13	2.04	0.40
6:Z:83:THR:HB	6:Z:84:ALA:H	1.76	0.40
7:N:43:LEU:H	7:N:44:PRO:CD	2.35	0.40
11:R:117:ILE:HA	11:R:120:LEU:HD12	2.02	0.40
13:O:58:ARG:CD	13:O:59:LEU:N	2.84	0.40
6:Z:354:PRO:O	6:Z:357:ILE:HG12	2.21	0.40
8:S:164:ILE:HB	8:S:165:PRO:HD3	2.03	0.40
10:Q:118:CYS:O	10:Q:122:ILE:HG13	2.21	0.40
7:N:87:ASP:O	7:N:88:ARG:HB2	2.21	0.40
7:N:206:ILE:HD13	7:N:206:ILE:HA	1.88	0.40
10:Q:355:GLU:O	10:Q:356:CYS:HB3	2.22	0.40
11:R:261:LEU:CB	11:R:266:LEU:HB2	2.52	0.40
6:Z:12:ILE:CG1	6:Z:22:LYS:HE3	2.51	0.40
6:Z:96:TYR:HE1	6:Z:156:HIS:CE1	2.40	0.40
6:Z:282:ILE:HB	6:Z:297:VAL:HG11	2.03	0.40
8:S:19:HIS:CG	8:S:20:HIS:N	2.90	0.40
10:Q:356:CYS:SG	10:Q:356:CYS:O	2.79	0.40
11:R:54:ILE:HD13	11:R:63:TYR:CE1	2.57	0.40
13:O:59:LEU:HG	13:O:85:SER:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	195/268 (73%)	179 (92%)	12 (6%)	4 (2%)	5	30
2	V	287/306 (94%)	263 (92%)	18 (6%)	6 (2%)	5	30
3	T	264/274 (96%)	236 (89%)	21 (8%)	7 (3%)	4	25
4	X	125/156 (80%)	107 (86%)	12 (10%)	6 (5%)	2	16
5	Y	47/89 (53%)	43 (92%)	3 (6%)	1 (2%)	5	30
6	Z	902/993 (91%)	820 (91%)	55 (6%)	27 (3%)	3	22
7	N	886/945 (94%)	849 (96%)	30 (3%)	7 (1%)	16	53
8	S	473/523 (90%)	436 (92%)	24 (5%)	13 (3%)	4	25
9	P	438/445 (98%)	408 (93%)	22 (5%)	8 (2%)	6	33
10	Q	432/434 (100%)	388 (90%)	26 (6%)	18 (4%)	2	17
11	R	377/429 (88%)	352 (93%)	17 (4%)	8 (2%)	5	30
12	U	296/338 (88%)	280 (95%)	11 (4%)	5 (2%)	7	35
13	O	386/393 (98%)	368 (95%)	16 (4%)	2 (0%)	24	63
All	All	5108/5593 (91%)	4729 (93%)	267 (5%)	112 (2%)	7	29

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	200	ASN
3	T	92	ASN
3	T	96	LEU
3	T	173	GLU
4	X	116	ALA
5	Y	34	GLU
6	Z	24	THR
6	Z	25	PRO
6	Z	85	VAL
6	Z	519	PRO

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Mol	Chain	Res	Type
6	Z	728	LYS
8	S	47	THR
8	S	83	PRO
8	S	172	ASN
9	P	88	GLN
10	Q	42	ALA
10	Q	75	ARG
10	Q	356	CYS
11	R	125	GLU
11	R	263	ARG
13	O	36	LYS
1	W	165	GLN
2	V	175	SER
4	X	38	ASN
6	Z	186	GLY
6	Z	187	SER
6	Z	727	GLU
6	Z	926	ASN
6	Z	963	ALA
7	N	175	ASP
8	S	44	THR
8	S	102	SER
8	S	126	LYS
8	S	132	ALA
8	S	150	LYS
8	S	153	GLU
9	P	79	LEU
9	P	111	ASP
9	P	126	THR
10	Q	51	ARG
10	Q	68	MET
10	Q	170	ASP
10	Q	387	TYR
11	R	123	ASP
11	R	280	ILE
1	W	179	ARG
3	T	95	LYS
3	T	235	PHE
3	T	251	HIS
4	X	112	ASN
6	Z	234	PRO
6	Z	773	ARG

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Mol	Chain	Res	Type
6	Z	885	ALA
6	Z	887	GLY
6	Z	905	ASN
6	Z	947	GLY
7	N	725	LEU
7	N	757	THR
7	N	786	ARG
8	S	118	PHE
9	P	130	ILE
9	P	171	MET
10	Q	44	ALA
10	Q	48	ASP
10	Q	230	LYS
10	Q	253	ASN
10	Q	286	TYR
12	U	133	PRO
1	W	144	PHE
2	V	112	PRO
2	V	217	HIS
4	X	19	GLU
4	X	63	PRO
6	Z	82	MET
6	Z	143	VAL
6	Z	144	SER
6	Z	770	GLU
6	Z	825	ALA
7	N	391	PRO
10	Q	46	VAL
10	Q	384	LYS
11	R	395	ASN
12	U	5	HIS
12	U	237	PRO
13	O	225	ASP
1	W	180	LEU
2	V	20	ARG
6	Z	789	GLN
7	N	393	SER
8	S	82	TYR
8	S	97	THR
9	P	92	SER
9	P	327	LEU
10	Q	41	ALA

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Mol	Chain	Res	Type
11	R	264	THR
12	U	150	THR
4	X	113	GLU
7	N	888	ASP
10	Q	40	ALA
10	Q	45	SER
10	Q	126	LYS
11	R	393	PRO
2	V	185	ILE
3	T	46	ILE
6	Z	940	GLY
11	R	110	ILE
12	U	220	PRO
6	Z	19	SER
6	Z	610	GLY
6	Z	233	LEU
6	Z	333	GLY
8	S	96	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	171/230 (74%)	165 (96%)	6 (4%)	32	53
2	V	253/268 (94%)	248 (98%)	5 (2%)	48	65
3	T	249/256 (97%)	243 (98%)	6 (2%)	43	63
4	X	116/144 (81%)	114 (98%)	2 (2%)	53	67
5	Y	50/81 (62%)	49 (98%)	1 (2%)	48	65
6	Z	773/850 (91%)	754 (98%)	19 (2%)	42	62
7	N	745/797 (94%)	731 (98%)	14 (2%)	50	66
8	S	447/489 (91%)	440 (98%)	7 (2%)	55	69
9	P	412/415 (99%)	404 (98%)	8 (2%)	50	66
10	Q	391/391 (100%)	382 (98%)	9 (2%)	44	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	R	333/379 (88%)	322 (97%)	11 (3%)	33	55
12	U	271/308 (88%)	266 (98%)	5 (2%)	51	67
13	O	363/368 (99%)	353 (97%)	10 (3%)	38	59
All	All	4574/4976 (92%)	4471 (98%)	103 (2%)	44	63

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	76	LEU
1	W	105	VAL
1	W	111	VAL
1	W	139	VAL
1	W	140	ASP
1	W	149	GLN
2	V	158	LEU
2	V	168	LEU
2	V	190	HIS
2	V	199	LEU
2	V	227	MET
3	T	79	GLU
3	T	85	LEU
3	T	187	ASP
3	T	195	LEU
3	T	231	SER
3	T	238	GLN
4	X	14	VAL
4	X	132	SER
5	Y	32	ASP
6	Z	83	THR
6	Z	213	LYS
6	Z	257	PRO
6	Z	286	VAL
6	Z	326	VAL
6	Z	354	PRO
6	Z	366	LYS
6	Z	429	ASN
6	Z	471	LEU
6	Z	508	LEU
6	Z	560	THR
6	Z	601	VAL
6	Z	748	LEU

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Mol	Chain	Res	Type
6	Z	777	PRO
6	Z	817	LEU
6	Z	830	LEU
6	Z	846	PHE
6	Z	857	LEU
6	Z	889	VAL
7	N	63	LEU
7	N	142	GLU
7	N	223	LEU
7	N	269	LEU
7	N	294	PRO
7	N	739	PHE
7	N	765	ASP
7	N	773	MET
7	N	785	PRO
7	N	790	GLU
7	N	861	TYR
7	N	868	VAL
7	N	873	ARG
7	N	893	VAL
8	S	19	HIS
8	S	32	GLN
8	S	44	THR
8	S	93	LEU
8	S	105	PRO
8	S	449	LEU
8	S	487	THR
9	P	186	LEU
9	P	210	ASN
9	P	277	GLN
9	P	281	ILE
9	P	302	LEU
9	P	308	LEU
9	P	403	GLU
9	P	404	LYS
10	Q	104	PHE
10	Q	112	ASP
10	Q	164	GLU
10	Q	173	SER
10	Q	198	LEU
10	Q	294	ARG
10	Q	319	LYS

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Mol	Chain	Res	Type
10	Q	354	PHE
10	Q	387	TYR
11	R	22	PRO
11	R	182	ASN
11	R	237	THR
11	R	263	ARG
11	R	266	LEU
11	R	318	PRO
11	R	348	LEU
11	R	365	ASP
11	R	384	VAL
11	R	393	PRO
11	R	421	VAL
12	U	26	GLN
12	U	115	GLN
12	U	142	GLN
12	U	220	PRO
12	U	261	LEU
13	O	13	THR
13	O	61	LEU
13	O	62	TYR
13	O	66	VAL
13	O	69	PHE
13	O	90	LYS
13	O	153	LEU
13	O	237	PRO
13	O	300	VAL
13	O	348	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	W	44	ASN
1	W	95	GLN
1	W	107	HIS
1	W	149	GLN
1	W	184	ASN
2	V	73	GLN
2	V	131	GLN
2	V	145	GLN
2	V	167	ASN
2	V	274	GLN

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Mol	Chain	Res	Type
2	V	279	HIS
2	V	290	ASN
3	T	48	ASN
3	T	84	GLN
3	T	93	ASN
3	T	127	GLN
3	T	135	ASN
3	T	170	ASN
3	T	213	ASN
3	T	238	GLN
4	X	38	ASN
4	X	105	ASN
6	Z	15	GLN
6	Z	17	GLN
6	Z	129	ASN
6	Z	156	HIS
6	Z	215	ASN
6	Z	275	GLN
6	Z	327	GLN
6	Z	380	ASN
6	Z	405	ASN
6	Z	429	ASN
6	Z	435	GLN
6	Z	502	ASN
6	Z	622	HIS
6	Z	721	ASN
6	Z	763	HIS
6	Z	766	HIS
6	Z	769	ASN
6	Z	771	HIS
6	Z	829	GLN
6	Z	833	GLN
6	Z	842	GLN
6	Z	871	HIS
6	Z	897	HIS
6	Z	898	HIS
6	Z	899	GLN
6	Z	926	ASN
7	N	176	GLN
7	N	233	ASN
7	N	288	ASN
7	N	306	ASN

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Mol	Chain	Res	Type
7	N	340	HIS
7	N	378	ASN
7	N	614	ASN
7	N	635	GLN
7	N	716	GLN
7	N	719	ASN
7	N	772	GLN
8	S	19	HIS
8	S	20	HIS
8	S	39	ASN
8	S	159	ASN
8	S	166	ASN
8	S	225	HIS
8	S	235	ASN
8	S	303	ASN
8	S	317	HIS
8	S	334	HIS
8	S	347	HIS
8	S	378	GLN
8	S	458	GLN
8	S	472	HIS
9	P	178	GLN
9	P	239	GLN
9	P	277	GLN
9	P	285	GLN
9	P	306	ASN
9	P	315	GLN
9	P	323	ASN
9	P	337	HIS
9	P	366	ASN
9	P	418	ASN
10	Q	19	GLN
10	Q	21	ASN
10	Q	80	HIS
10	Q	114	GLN
10	Q	247	HIS
10	Q	248	ASN
10	Q	307	ASN
10	Q	361	HIS
11	R	35	GLN
11	R	42	GLN
11	R	195	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	R	314	ASN
11	R	325	HIS
11	R	374	ASN
11	R	376	GLN
11	R	378	ASN
11	R	395	ASN
11	R	406	GLN
12	U	21	HIS
12	U	70	HIS
12	U	75	ASN
12	U	115	GLN
12	U	117	ASN
12	U	127	GLN
12	U	128	GLN
12	U	173	HIS
12	U	192	ASN
12	U	201	GLN
12	U	230	GLN
12	U	251	ASN
13	O	23	HIS
13	O	105	GLN
13	O	116	ASN
13	O	117	ASN
13	O	175	ASN
13	O	177	GLN
13	O	289	GLN
13	O	343	GLN
13	O	345	ASN
13	O	389	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	78:GLN	C	79:LEU	N	1.75

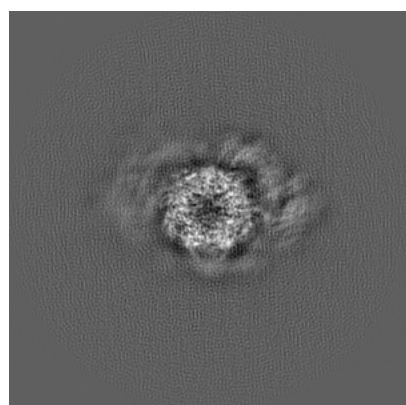
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3535. These allow visual inspection of the internal detail of the map and identification of artifacts.

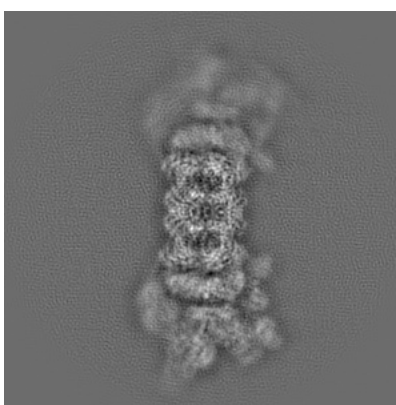
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

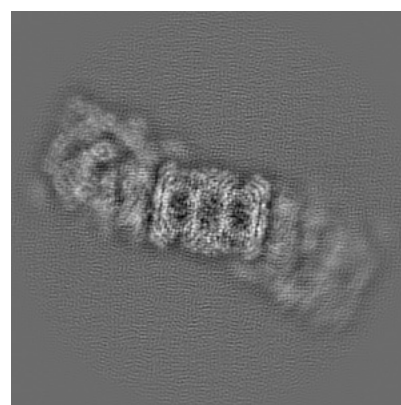
6.1.1 Primary map



X



Y

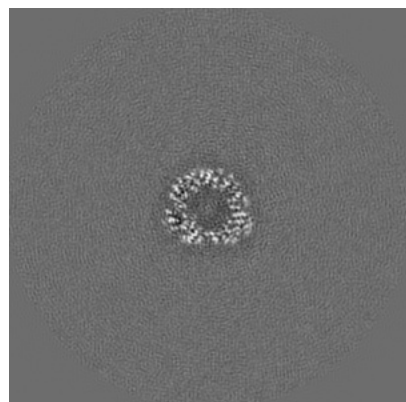


Z

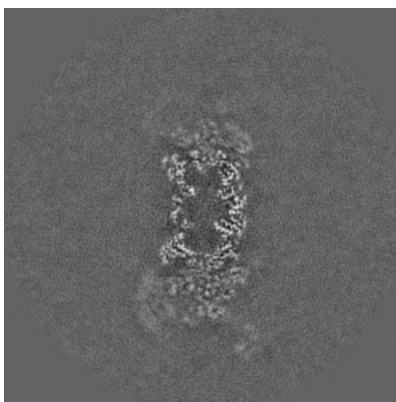
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

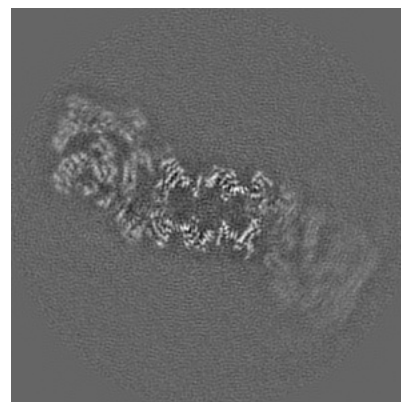
6.2.1 Primary map



X Index: 192



Y Index: 192

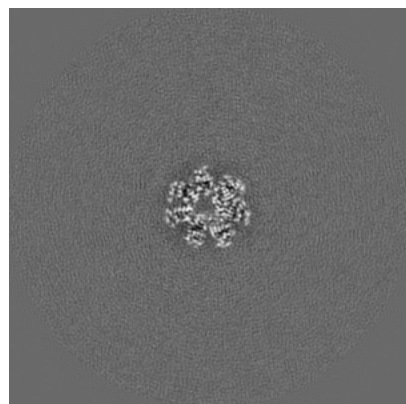


Z Index: 192

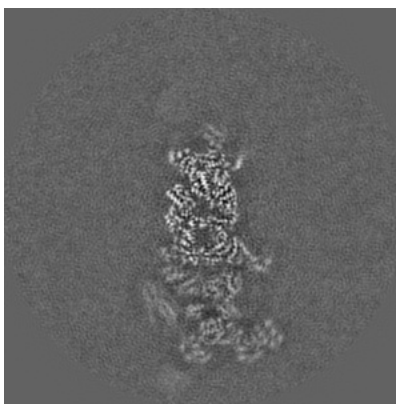
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

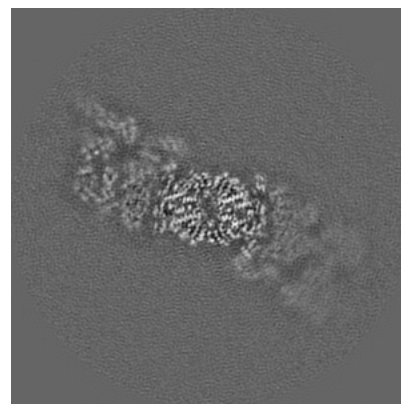
6.3.1 Primary map



X Index: 206



Y Index: 210

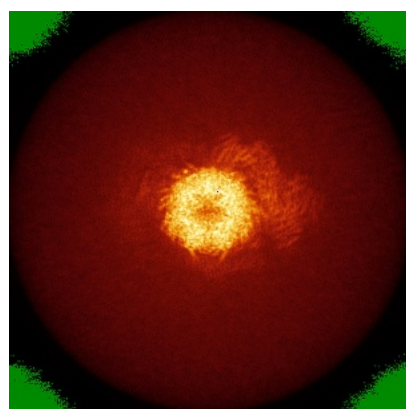


Z Index: 210

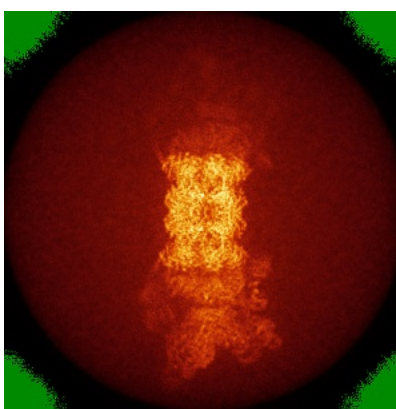
The images above show the largest variance slices of the map in three orthogonal directions.

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

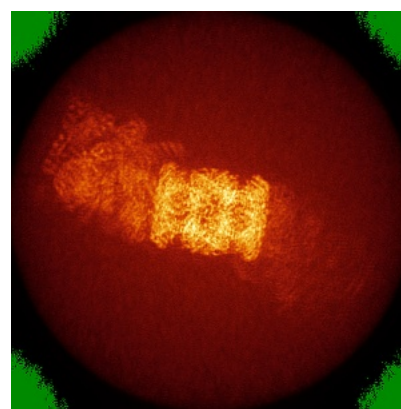
6.4.1 Primary map



X



Y

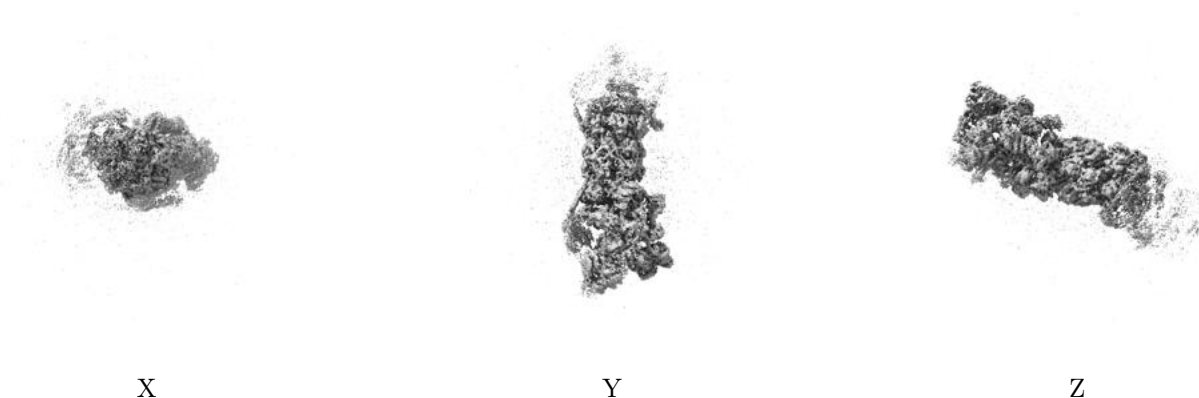


Z

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 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

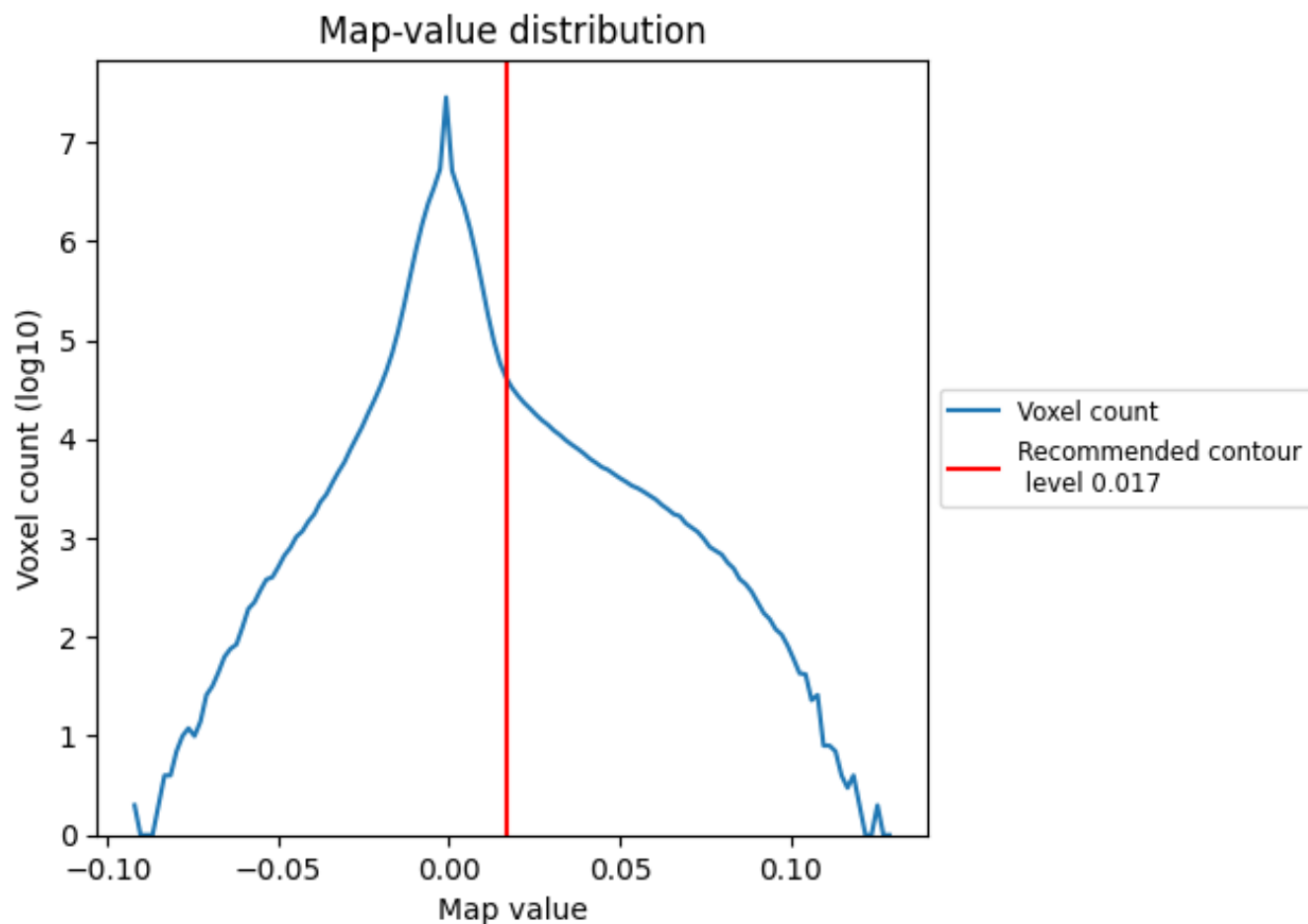
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

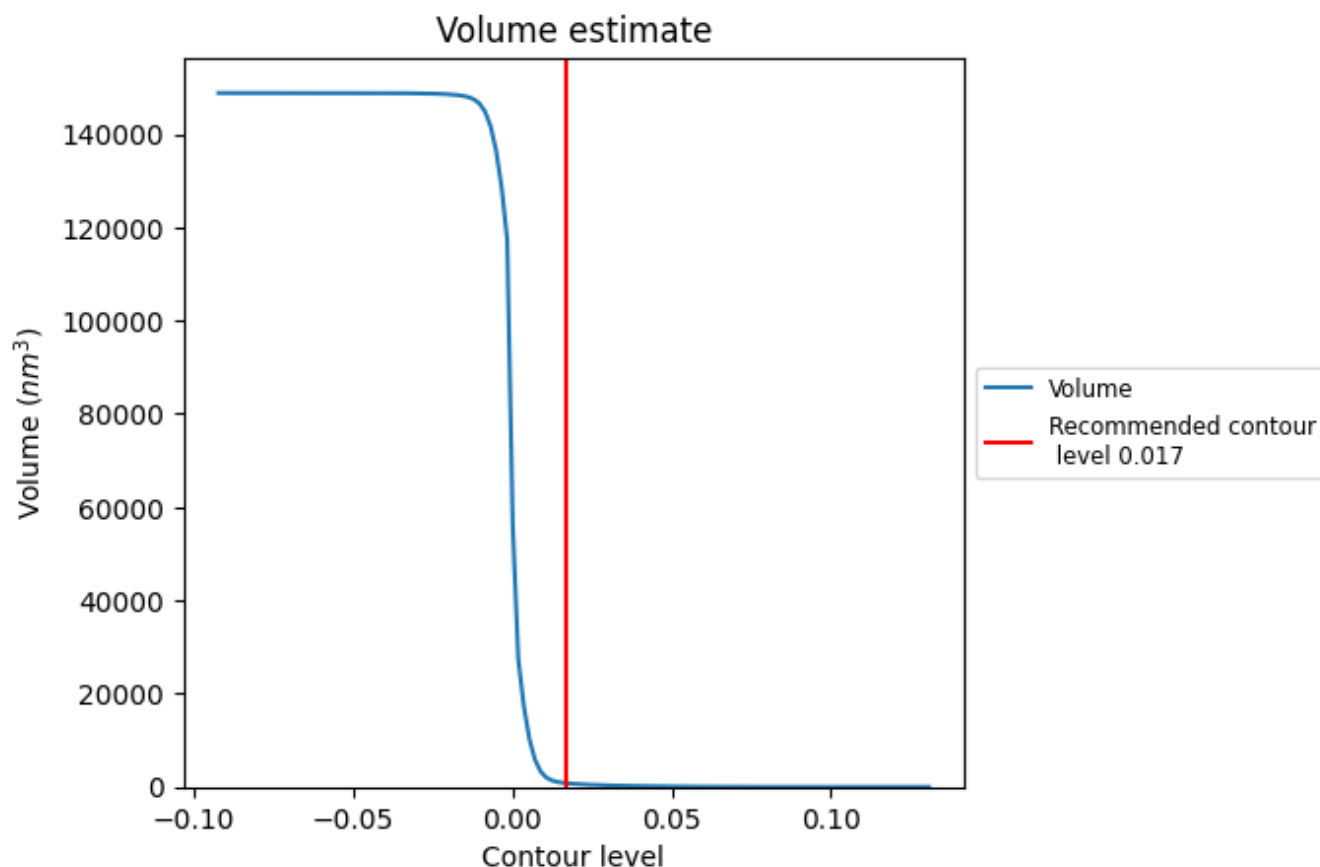
This section contains the results of statistical analysis of the map.

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.

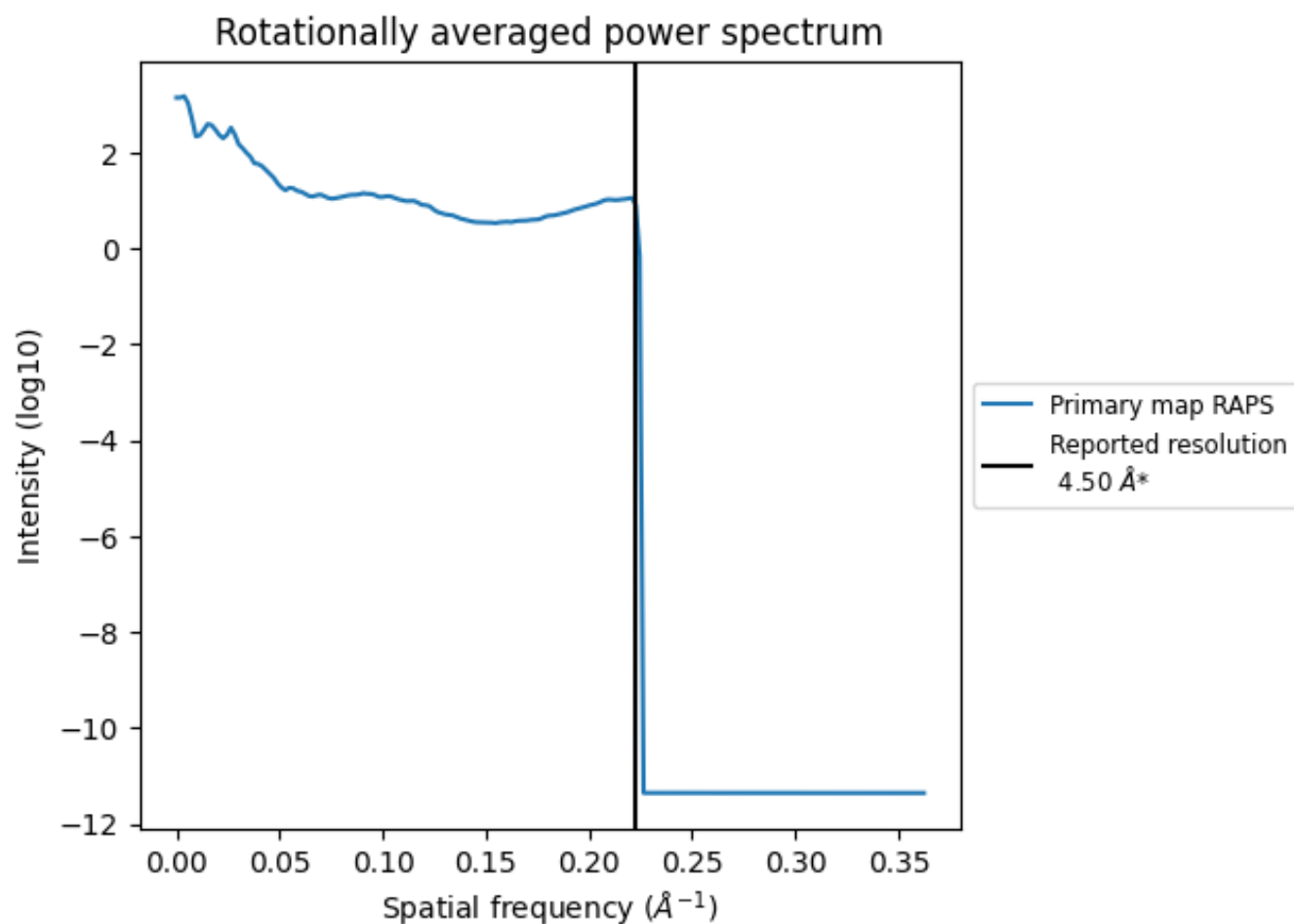
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 813 nm^3 ; this corresponds to an approximate mass of 734 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

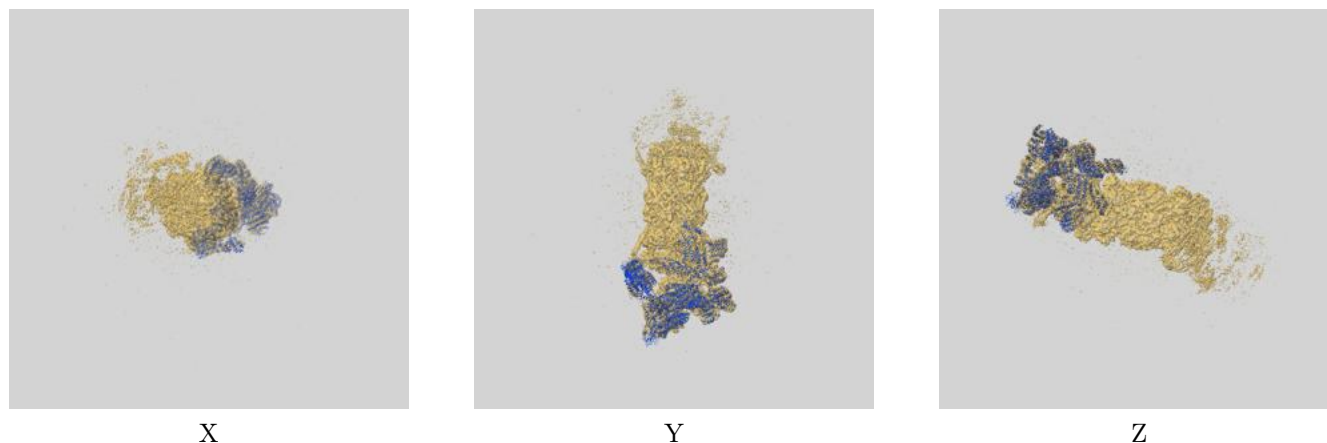
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

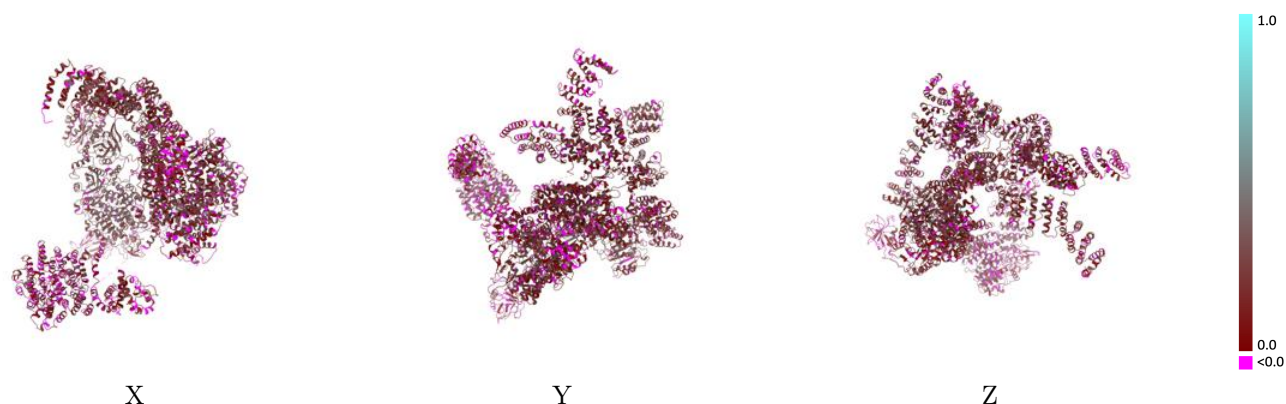
This section contains information regarding the fit between EMDB map EMD-3535 and PDB model 5MPE. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



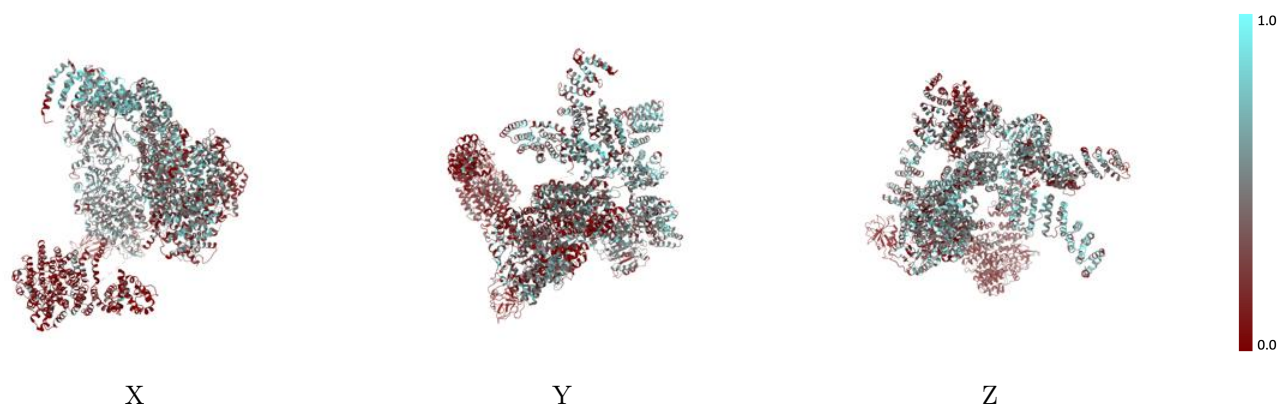
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



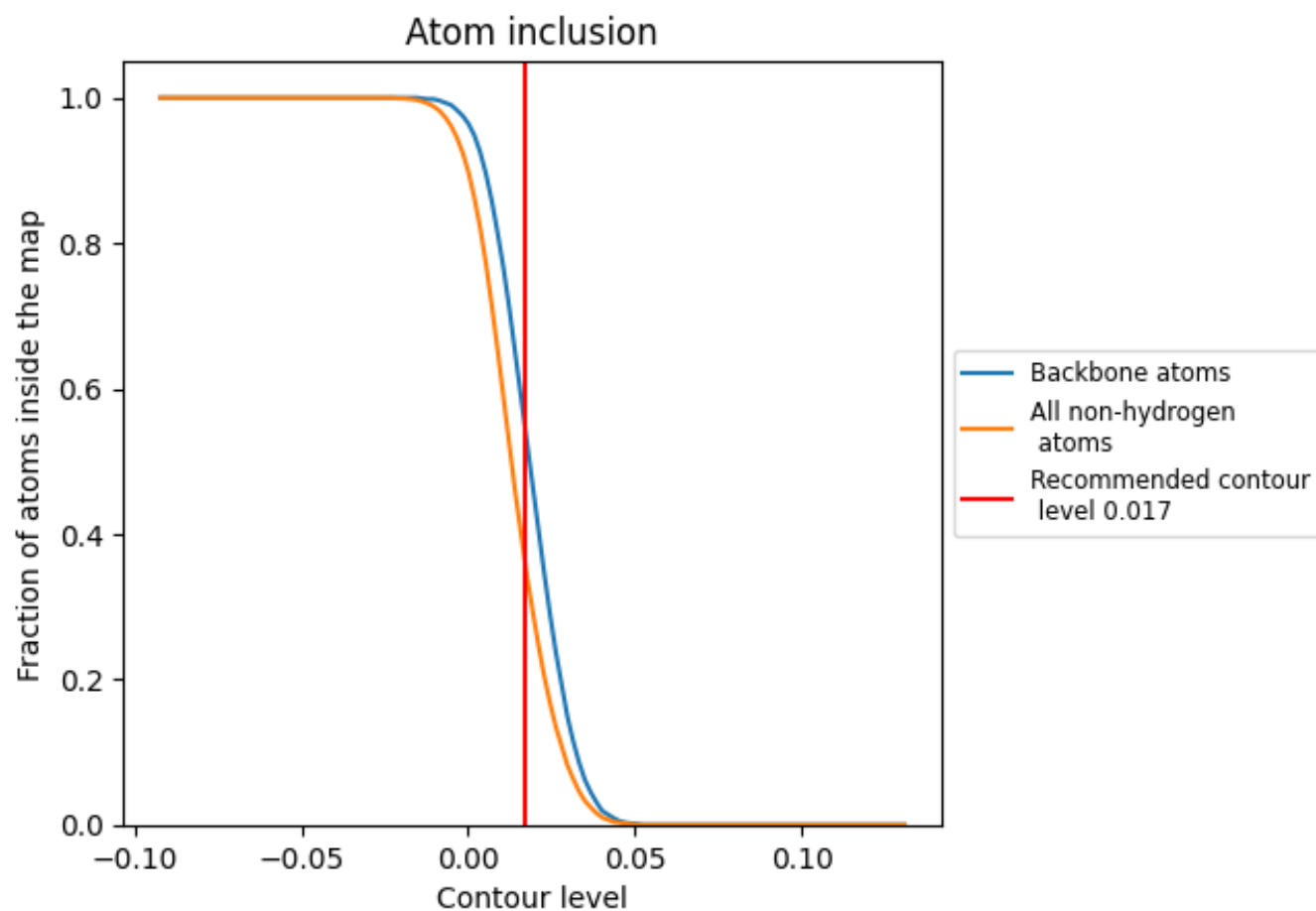
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 36% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3630	 0.1550
N	 0.4280	 0.1860
O	 0.4690	 0.1680
P	 0.5630	 0.1960
Q	 0.4330	 0.1430
R	 0.4580	 0.1670
S	 0.3410	 0.1390
T	 0.2140	 0.1130
U	 0.4780	 0.2160
V	 0.4870	 0.2080
W	 0.3990	 0.1820
X	 0.0170	 0.0660
Y	 0.2810	 0.1360
Z	 0.0980	 0.0930

