



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:32 AM UTC

PDB ID : 3J9U / pdb_00003j9u
EMDB ID : EMD-6285
Title : Yeast V-ATPase state 2
Authors : Zhao, J.; Benlekbir, S.; Rubinstein, J.L.
Deposited on : 2015-02-23
Resolution : 7.60 Å(reported)
Based on initial models : 1U7L, 1HO8, 4RND, 4DL0

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:

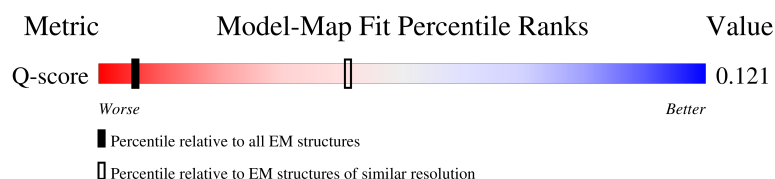
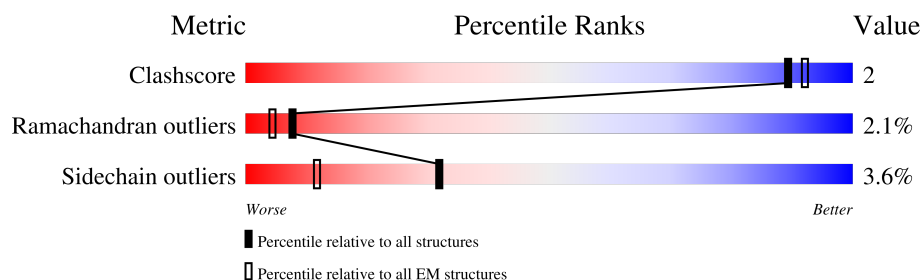
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 7.60 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.



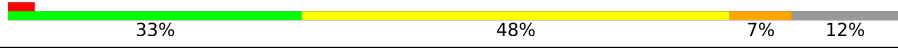
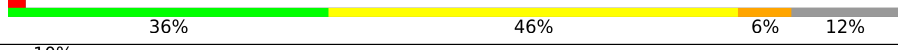
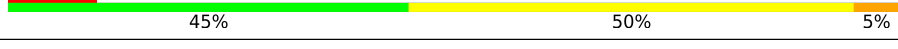
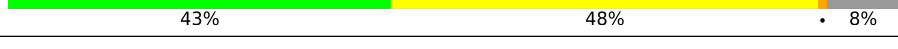
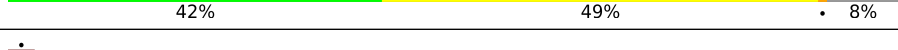
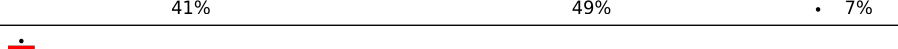
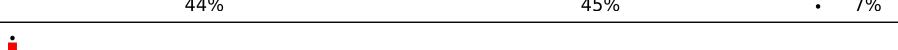
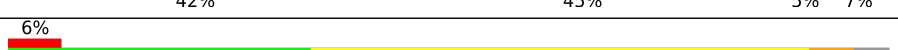
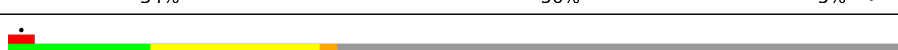
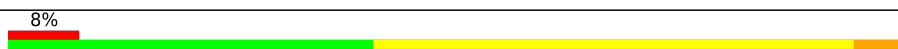
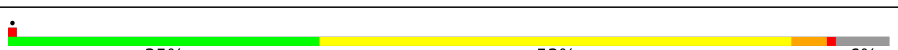
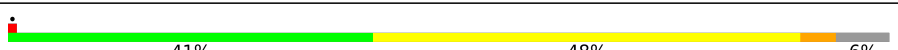
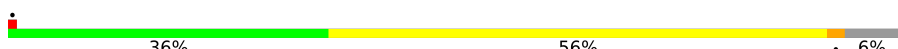
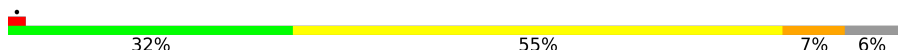
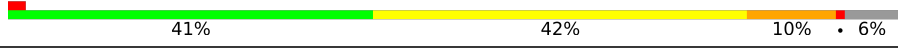
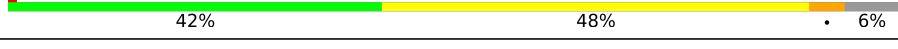
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	389 (7.10 - 8.10)

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	M	256	
2	N	118	
3	A	616	
3	C	616	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	616	
4	B	517	
4	D	517	
4	F	517	
5	Q	345	
6	H	114	
6	J	114	
6	L	114	
7	G	233	
7	I	233	
7	K	233	
8	P	478	
9	b	840	
10	O	392	
11	R	160	
11	S	160	
11	T	160	
11	U	160	
11	V	160	
11	W	160	
11	X	160	
11	Y	160	
11	Z	160	
11	a	160	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 57659 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 V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	210	Total	C	N	O	S	0	0
			1691	1061	305	321	4		

- Molecule 2 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	N	115	Total	C	N	O	0	0
			928	589	157	182		

- Molecule 3 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	593	Total	C	N	O	S	0	0
			4578	2904	760	894	20		
3	E	593	Total	C	N	O	S	0	0
			4578	2904	760	894	20		
3	A	593	Total	C	N	O	S	0	0
			4578	2904	760	894	20		

- Molecule 4 is a protein called V-type proton ATPase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	457	Total	C	N	O	S	0	0
			3585	2266	612	695	12		
4	F	457	Total	C	N	O	S	0	0
			3585	2266	612	695	12		
4	B	457	Total	C	N	O	S	0	0
			3585	2266	612	695	12		

- Molecule 5 is a protein called V-type proton ATPase subunit d.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	345	Total	C	N	O	S	0	0
			2802	1779	454	555	14		

- Molecule 6 is a protein called V-type proton ATPase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	105	Total	C	N	O		0	0
			824	517	144	163			
6	H	105	Total	C	N	O		0	0
			824	517	144	163			
6	J	105	Total	C	N	O		0	0
			824	517	144	163			

- Molecule 7 is a protein called V-type proton ATPase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	217	Total	C	N	O	S	0	0
			1731	1083	296	347	5		
7	G	217	Total	C	N	O	S	0	0
			1731	1083	296	347	5		
7	I	217	Total	C	N	O	S	0	0
			1731	1083	296	347	5		

- Molecule 8 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	461	Total	C	N	O	S	0	0
			3712	2373	623	704	12		

- Molecule 9 is a protein called V-type proton ATPase subunit a, vacuolar isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	b	312	Total	C	N	O	S	0	0
			2540	1614	434	489	3		

- Molecule 10 is a protein called V-type proton ATPase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	392	Total	C	N	O	S	0	0
			3122	2005	516	596	5		

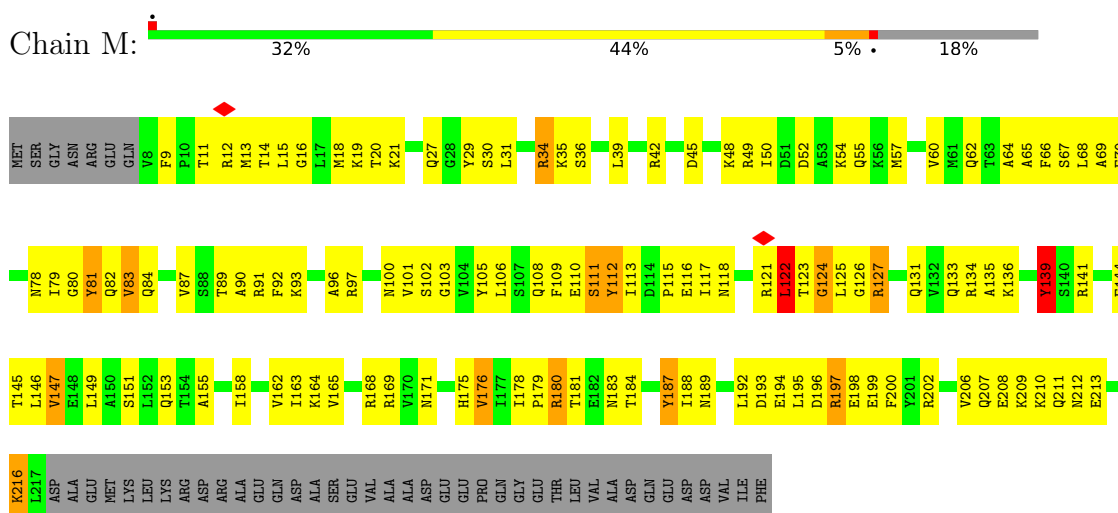
- Molecule 11 is a protein called V-type proton ATPase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	X	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	a	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	R	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	Z	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	S	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	Y	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	T	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	V	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	W	150	Total 1071	C 704	N 173	O 187	S 7	0	0

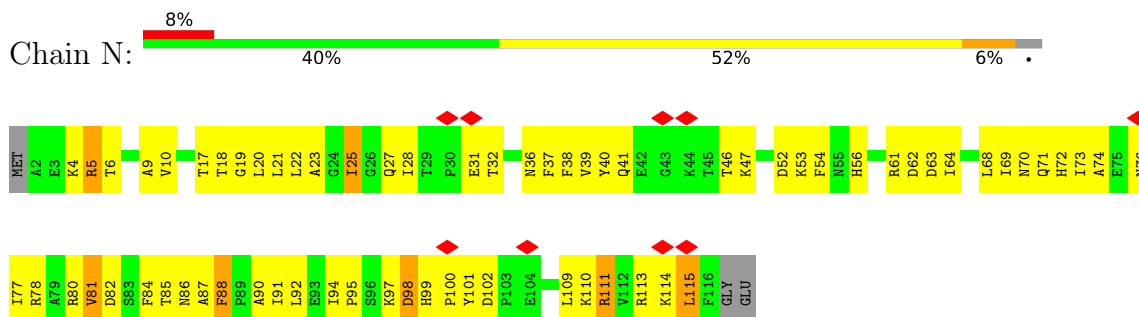
3 Residue-property plots

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

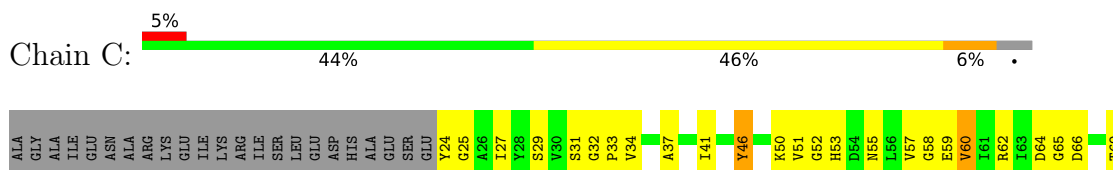
• Molecule 1: V-type proton ATPase subunit D

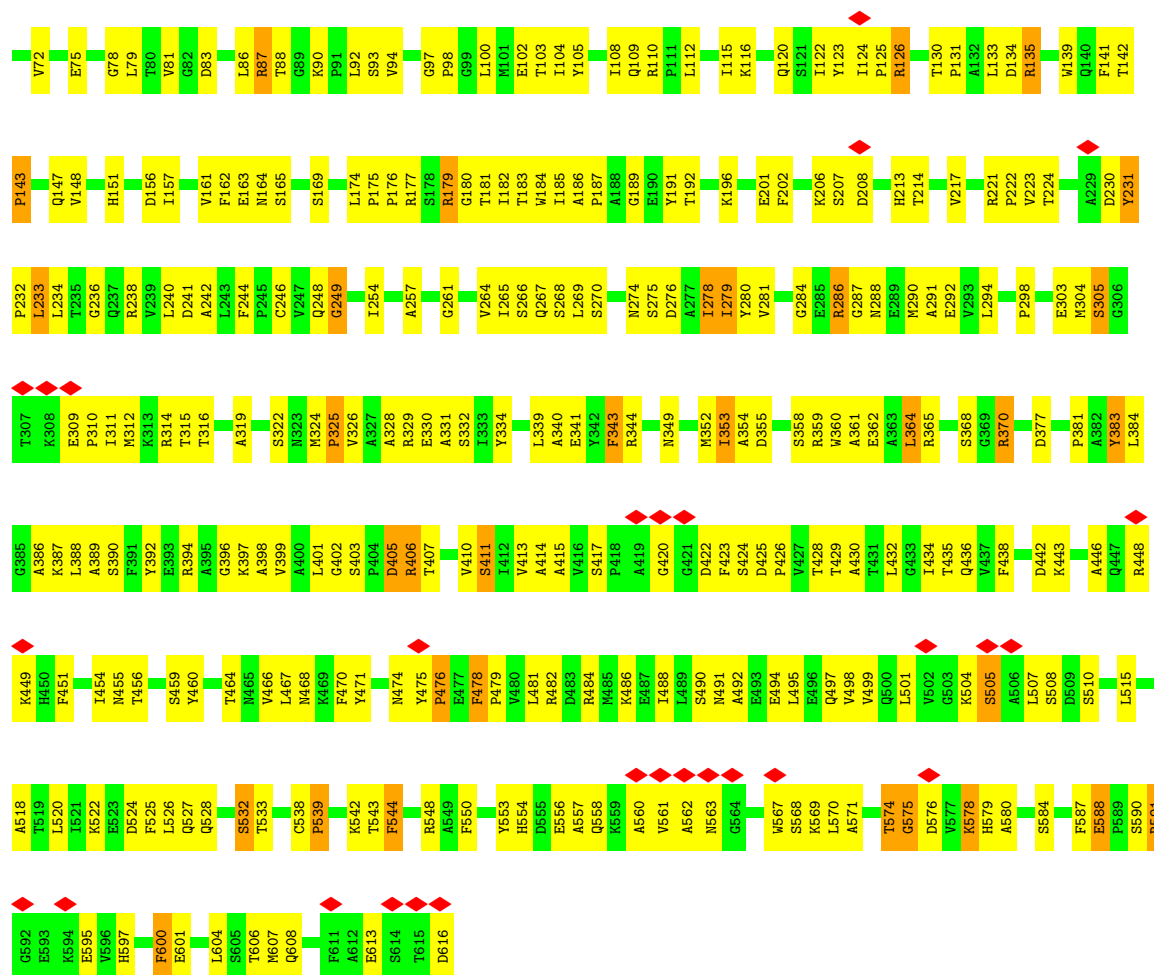


• Molecule 2: V-type proton ATPase subunit F



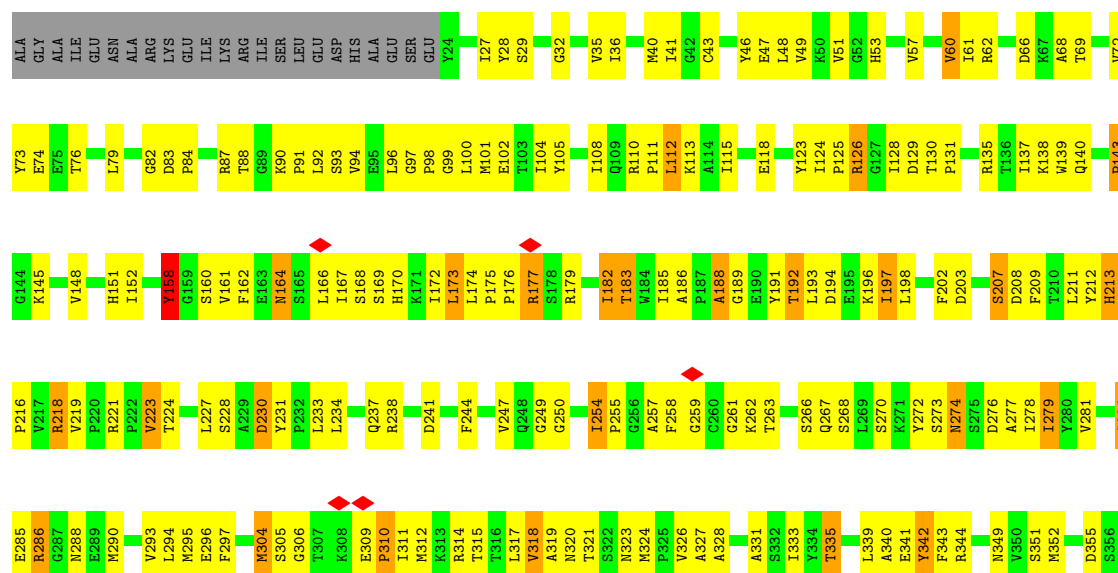
• Molecule 3: V-type proton ATPase catalytic subunit A

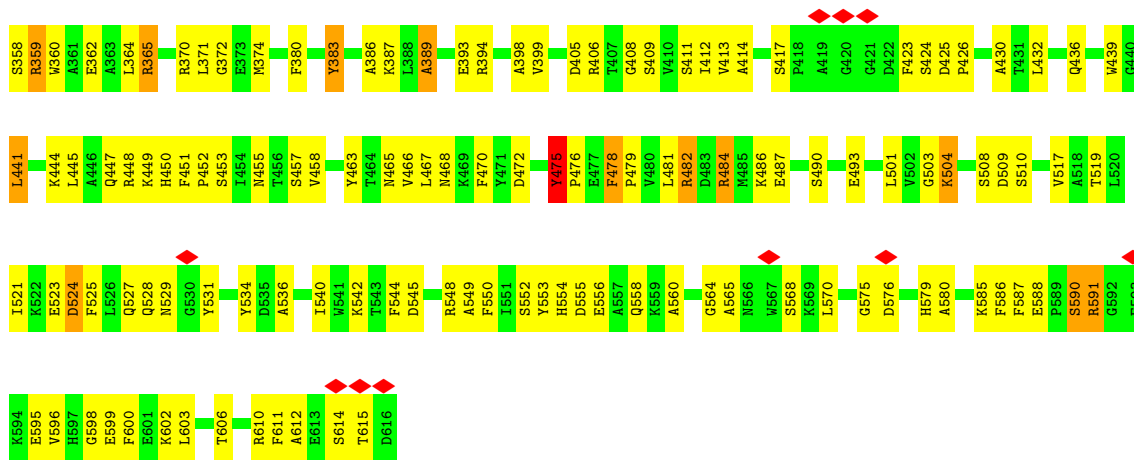




• Molecule 3: V-type proton ATPase catalytic subunit A

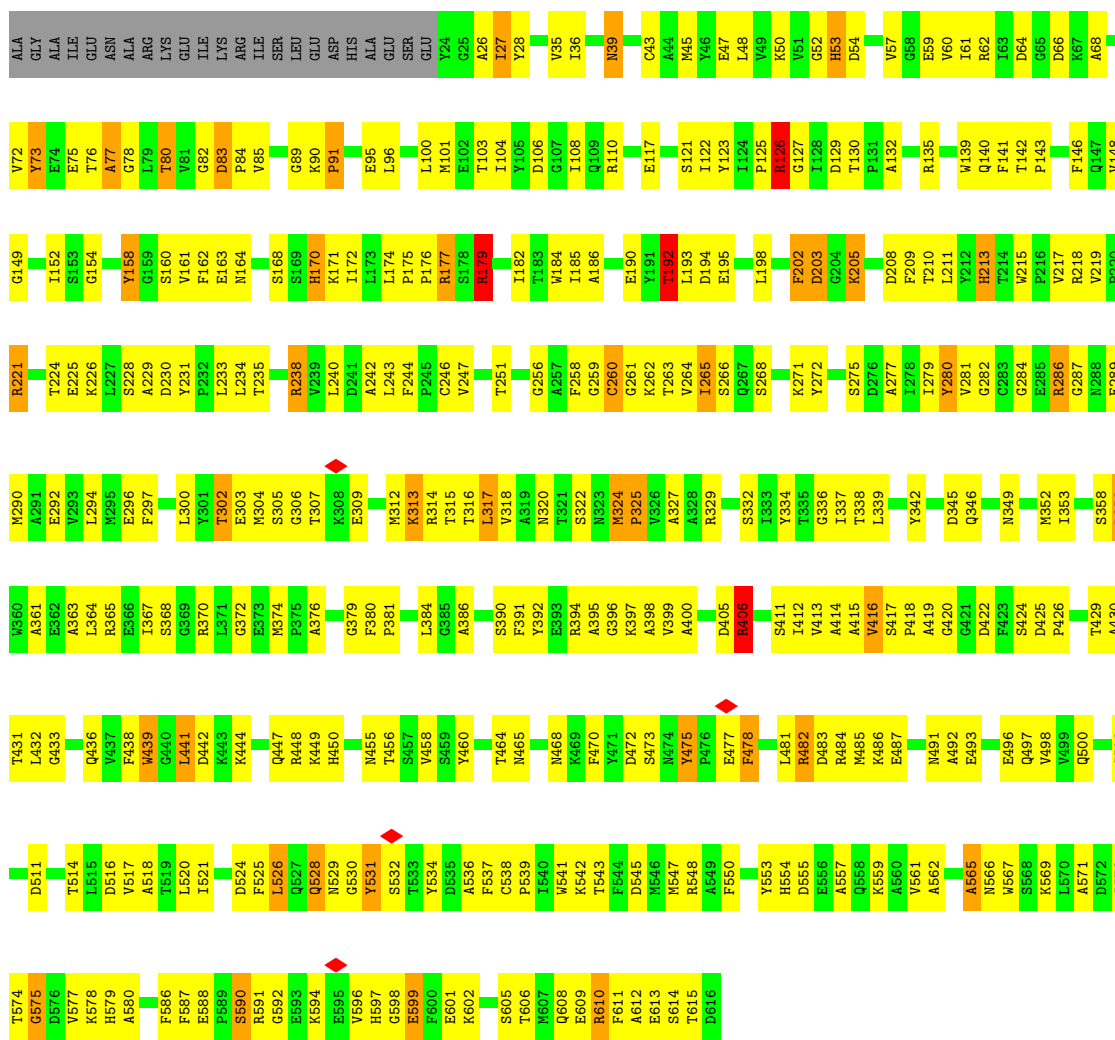
Chain E: 45% 45% 6% •





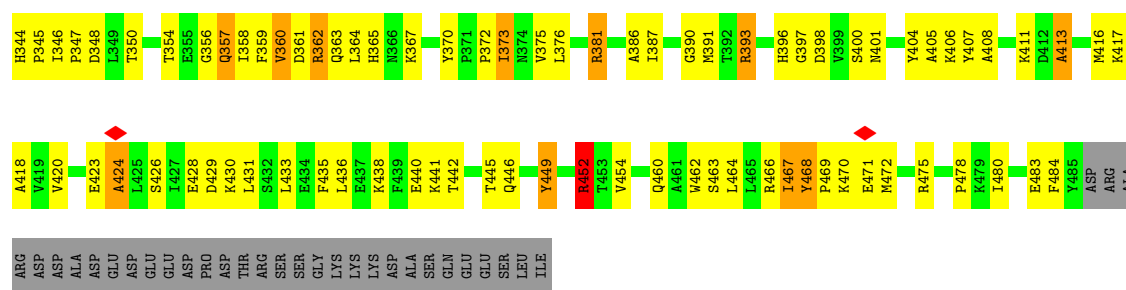
• Molecule 3: V-type proton ATPase catalytic subunit A

Chain A: 41% 48% 7%

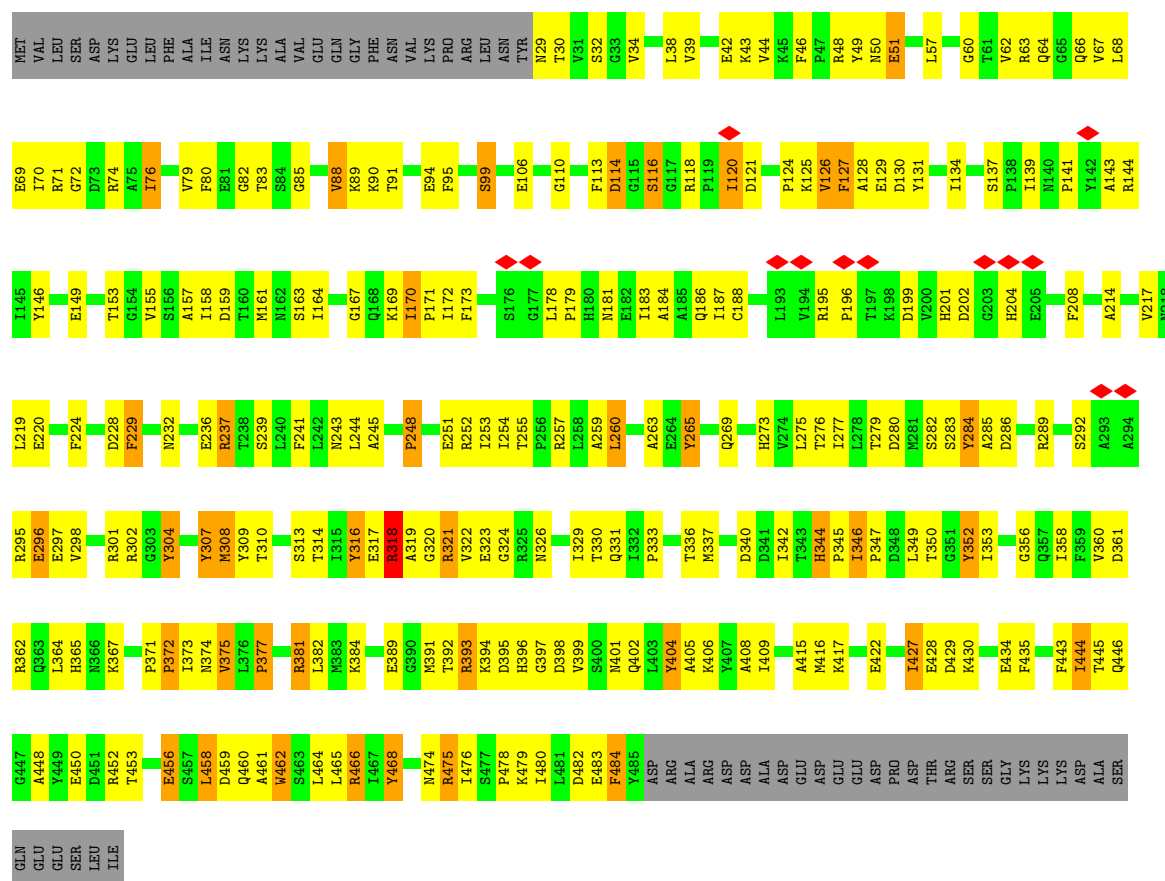


• Molecule 4: V-type proton ATPase subunit B

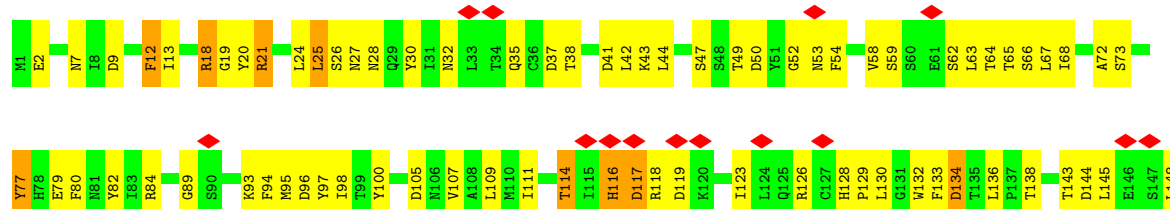


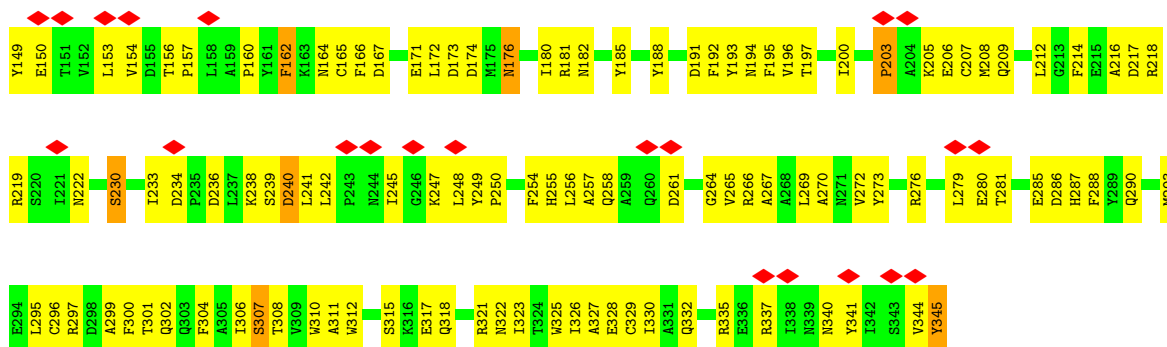


• Molecule 4: V-type proton ATPase subunit B

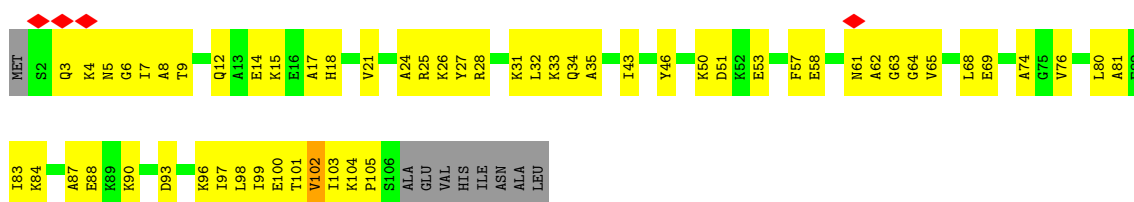


• Molecule 5: V-type proton ATPase subunit d

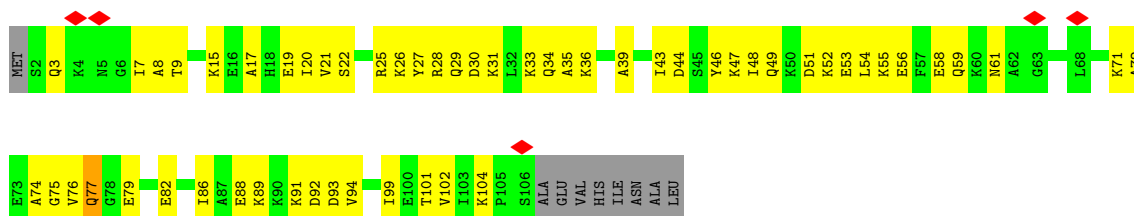




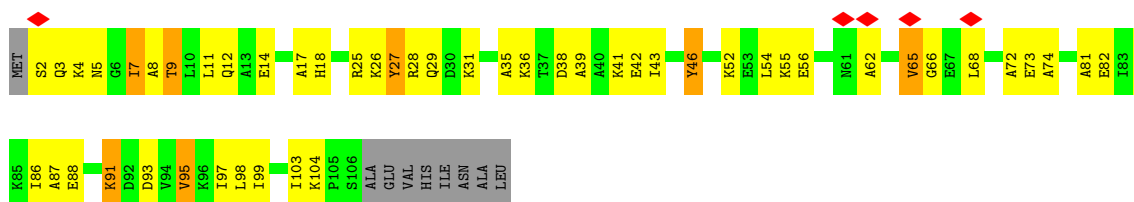
• Molecule 6: V-type proton ATPase subunit G



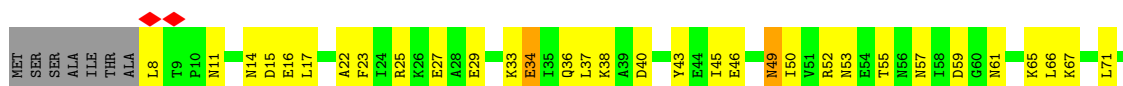
• Molecule 6: V-type proton ATPase subunit G

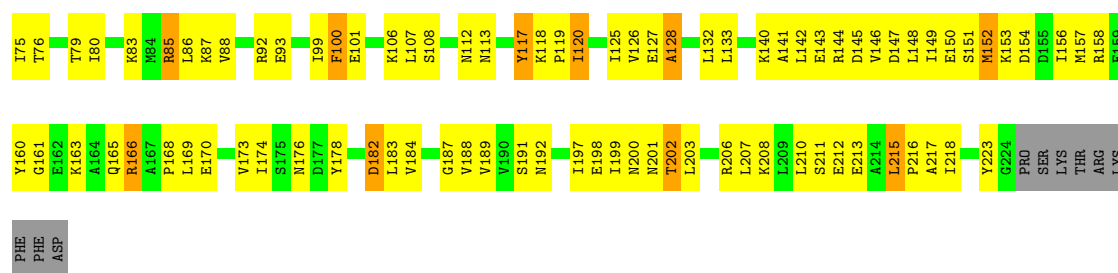


• Molecule 6: V-type proton ATPase subunit G

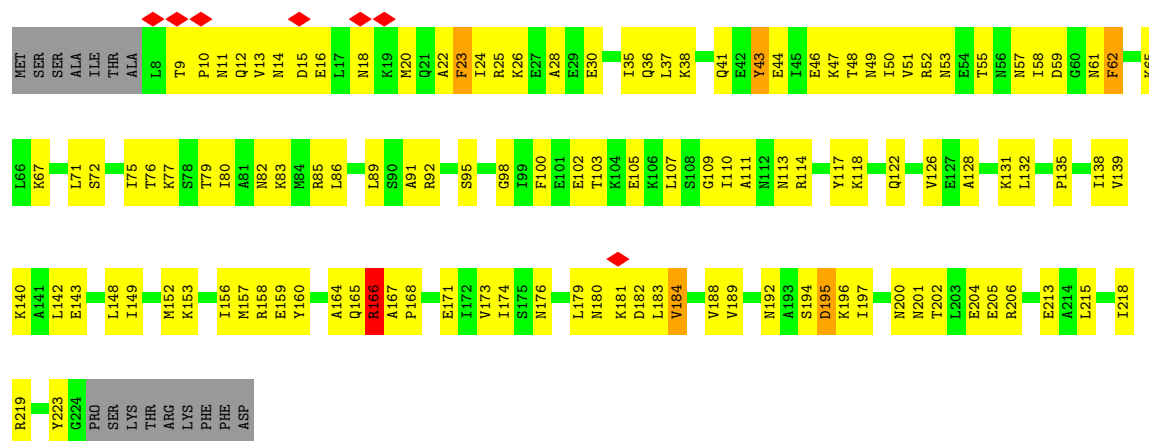


• Molecule 7: V-type proton ATPase subunit E

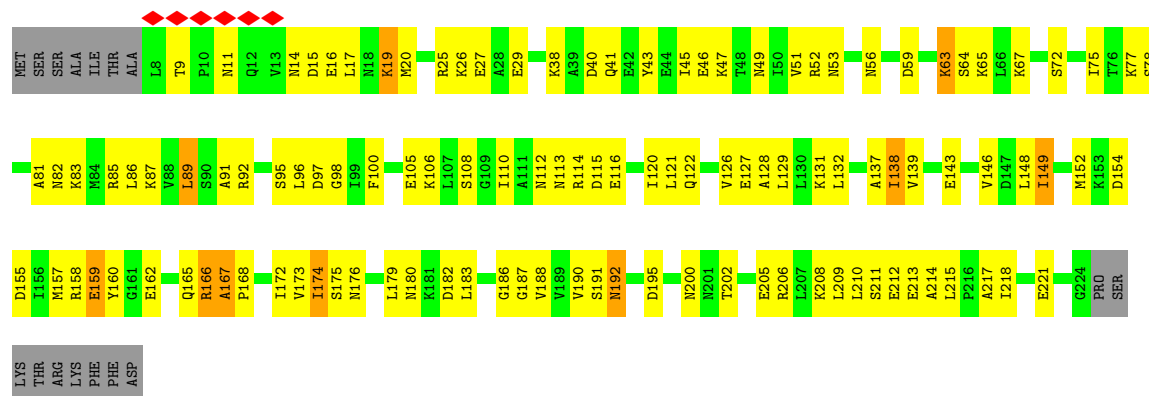




• Molecule 7: V-type proton ATPase subunit E

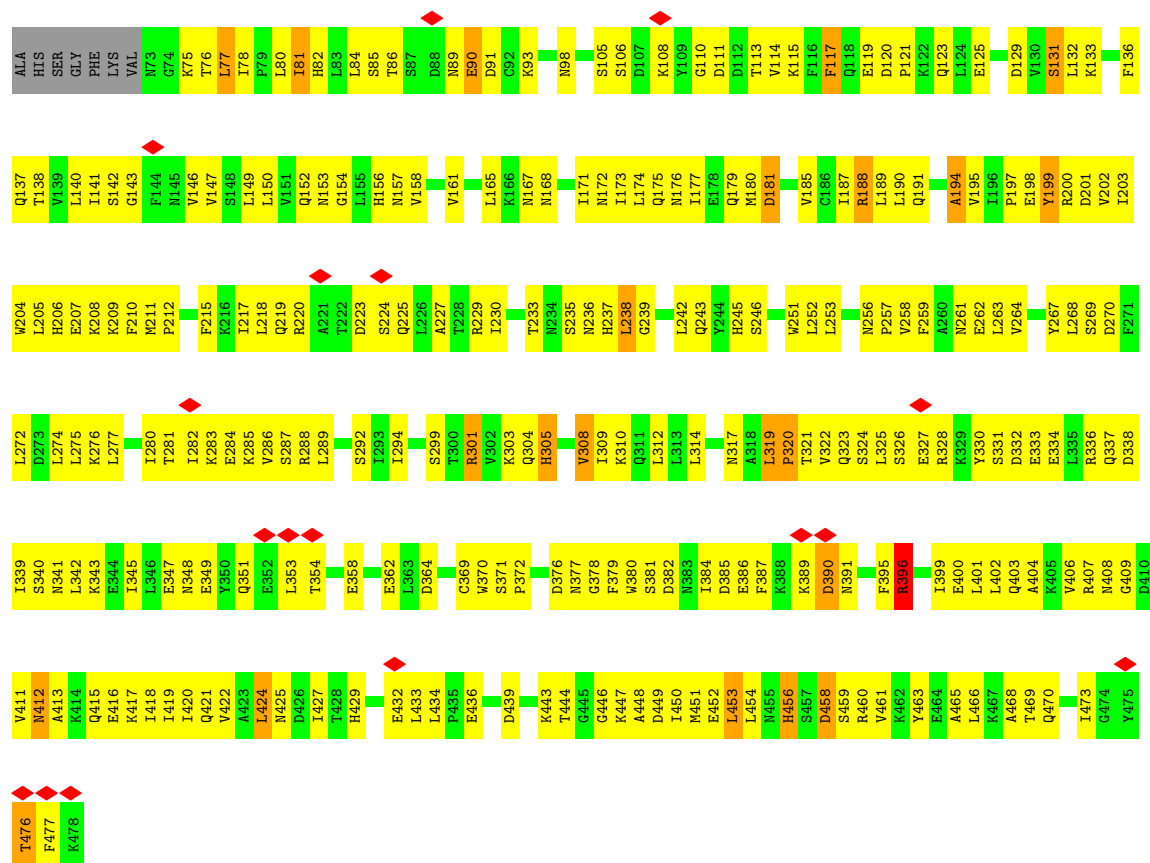


• Molecule 7: V-type proton ATPase subunit E

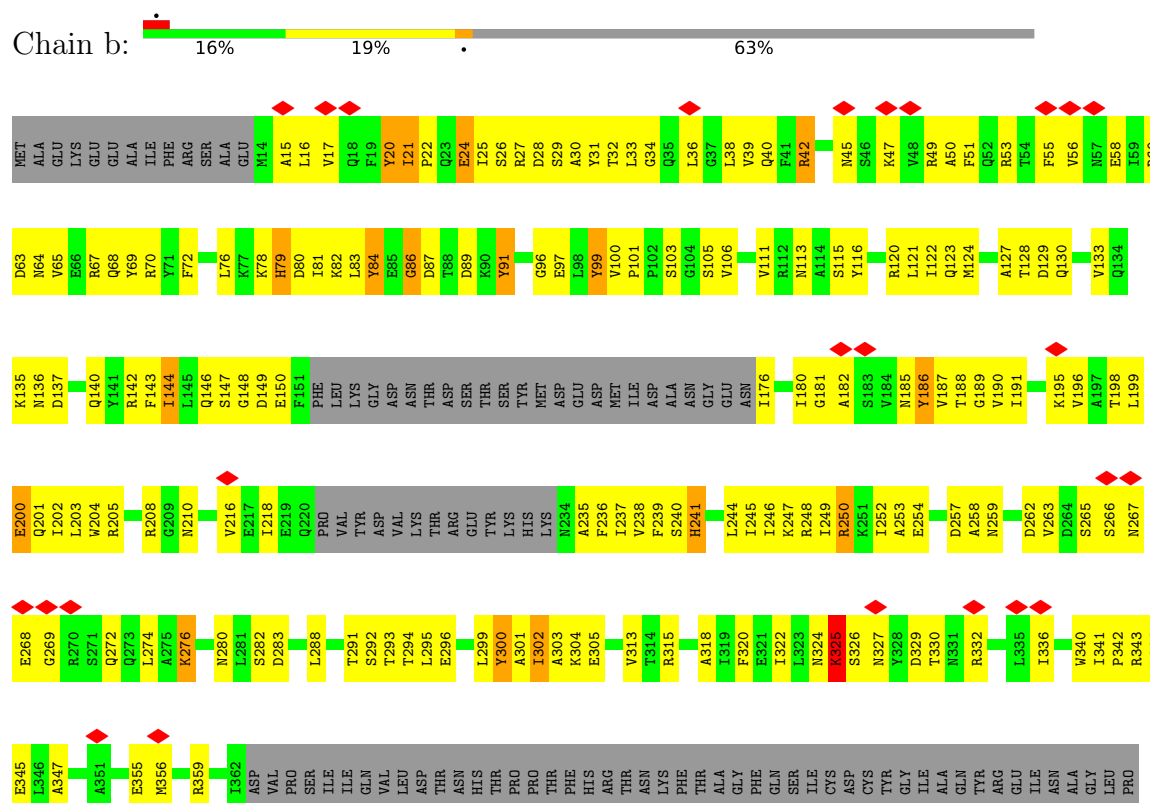


• Molecule 8: V-type proton ATPase subunit H



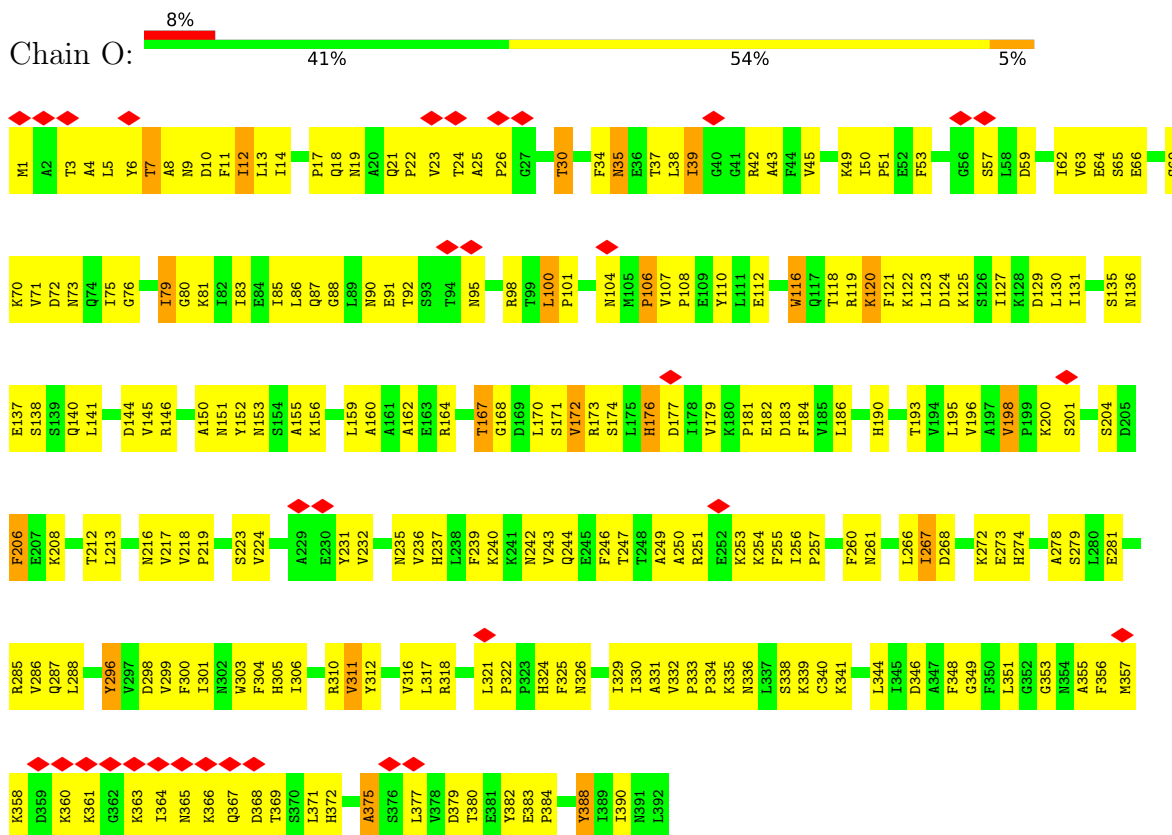


• Molecule 9: V-type proton ATPase subunit a, vacuolar isoform



[illegible]

- Molecule 10: V-type proton ATPase subunit C

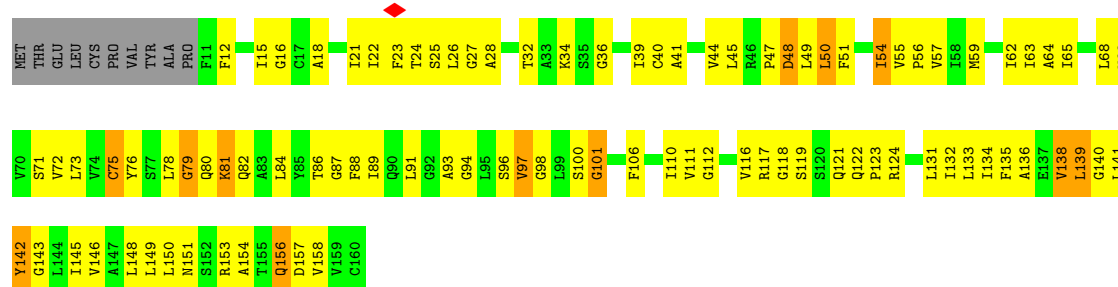


- Molecule 11: V-type proton ATPase subunit c

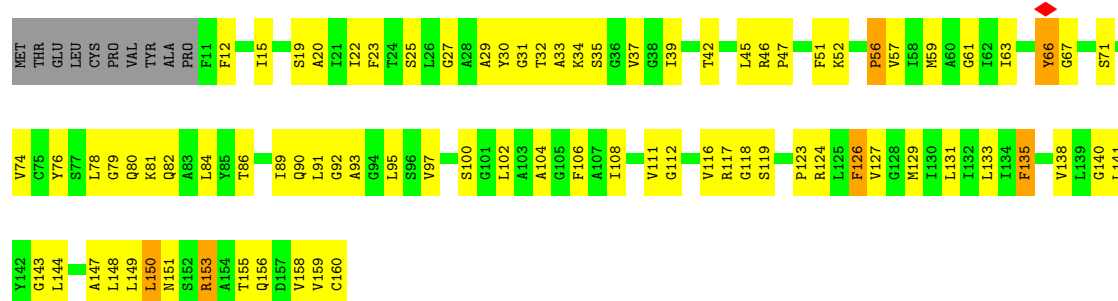




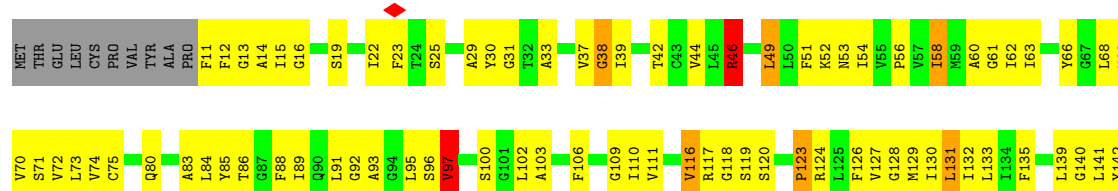
- Molecule 11: V-type proton ATPase subunit c



- Molecule 11: V-type proton ATPase subunit c



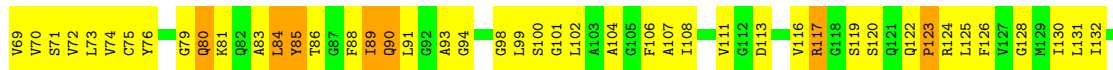
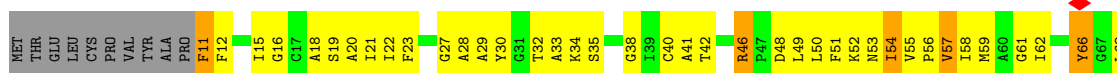
- Molecule 11: V-type proton ATPase subunit c





- Molecule 11: V-type proton ATPase subunit c

Chain Z: 31% 55% 8% 6%



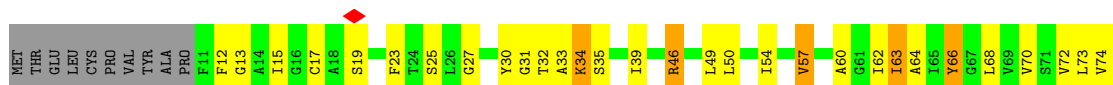
- Molecule 11: V-type proton ATPase subunit c

Chain S: 41% 48% 6%



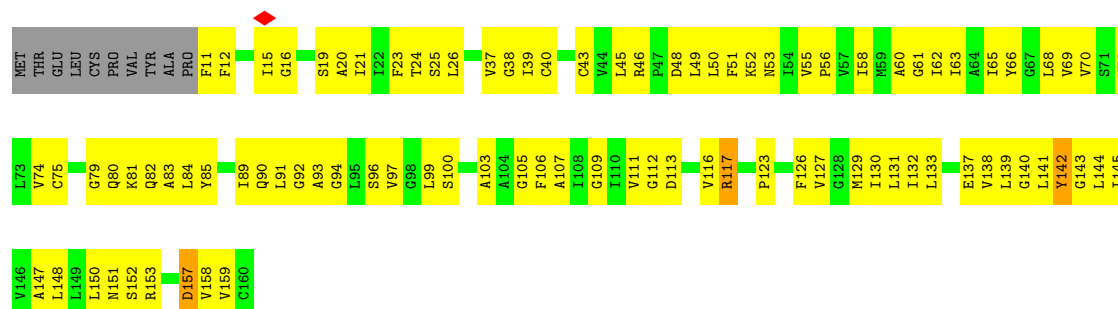
- Molecule 11: V-type proton ATPase subunit c

Chain Y: 41% 42% 10% 6%

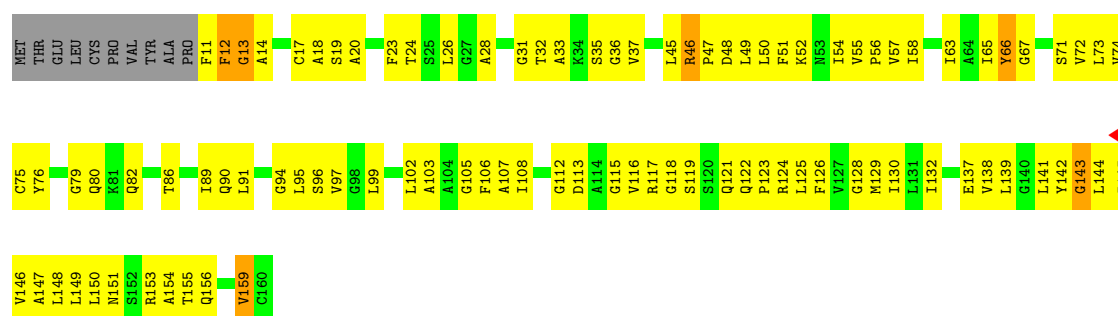
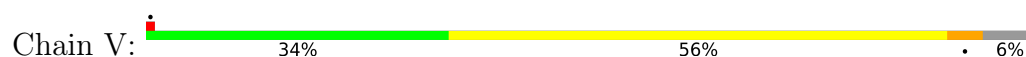


- Molecule 11: V-type proton ATPase subunit c

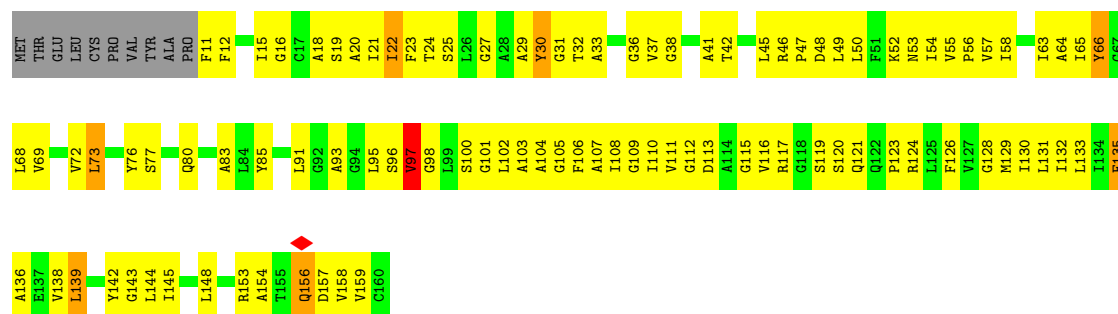
Chain T: 36% 56% 6%



- Molecule 11: V-type proton ATPase subunit c



- Molecule 11: V-type proton ATPase subunit c



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38347	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	7000	Depositor
Magnification	34483	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.131	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	371.2, 371.2, 371.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.45, 1.45, 1.45	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	M	2.32	73/1710 (4.3%)	2.63	156/2295 (6.8%)
2	N	2.38	47/944 (5.0%)	2.38	57/1277 (4.5%)
3	A	2.29	184/4677 (3.9%)	2.50	305/6339 (4.8%)
3	C	2.24	170/4677 (3.6%)	2.46	307/6339 (4.8%)
3	E	2.25	157/4677 (3.4%)	2.43	291/6339 (4.6%)
4	B	2.23	124/3654 (3.4%)	2.43	243/4953 (4.9%)
4	D	2.29	146/3654 (4.0%)	2.50	281/4953 (5.7%)
4	F	2.34	158/3654 (4.3%)	2.51	263/4953 (5.3%)
5	Q	2.22	101/2861 (3.5%)	2.55	225/3880 (5.8%)
6	H	2.10	19/828 (2.3%)	2.49	62/1098 (5.6%)
6	J	2.12	22/828 (2.7%)	2.42	50/1098 (4.6%)
6	L	2.18	30/828 (3.6%)	2.49	60/1098 (5.5%)
7	G	2.24	60/1743 (3.4%)	2.56	140/2338 (6.0%)
7	I	2.26	71/1743 (4.1%)	2.49	124/2338 (5.3%)
7	K	2.30	77/1743 (4.4%)	2.42	114/2338 (4.9%)
8	P	2.29	148/3766 (3.9%)	2.73	383/5087 (7.5%)
9	b	2.27	92/2578 (3.6%)	2.51	198/3479 (5.7%)
10	O	2.26	115/3185 (3.6%)	2.55	254/4314 (5.9%)
11	R	2.27	38/1086 (3.5%)	2.64	103/1472 (7.0%)
11	S	2.22	32/1086 (2.9%)	2.72	101/1472 (6.9%)
11	T	2.26	38/1086 (3.5%)	2.75	123/1472 (8.4%)
11	U	2.25	37/1086 (3.4%)	2.75	119/1472 (8.1%)
11	V	2.36	45/1086 (4.1%)	2.76	122/1472 (8.3%)
11	W	2.33	46/1086 (4.2%)	2.75	117/1472 (7.9%)
11	X	2.25	41/1086 (3.8%)	2.76	126/1472 (8.6%)
11	Y	2.30	41/1086 (3.8%)	2.62	90/1472 (6.1%)
11	Z	2.38	55/1086 (5.1%)	2.77	125/1472 (8.5%)
11	a	2.39	44/1086 (4.1%)	2.80	112/1472 (7.6%)
All	All	2.27	2211/58610 (3.8%)	2.55	4651/79236 (5.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	9
2	N	0	4
3	A	0	12
3	C	0	13
3	E	0	15
4	B	0	17
4	D	0	13
4	F	0	14
5	Q	0	8
6	J	0	3
6	L	0	1
7	G	0	1
7	I	0	3
7	K	0	6
8	P	0	5
9	b	0	6
10	O	0	8
11	R	0	1
11	S	0	2
11	T	0	4
11	U	0	4
11	V	0	3
11	W	0	2
11	X	0	2
11	Y	0	2
11	Z	0	3
11	a	0	2
All	All	0	163

All (2211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	335	ARG	CA-C	-12.70	1.36	1.52
4	D	346	ILE	CA-CB	-12.40	1.47	1.54
8	P	372	PRO	CA-C	-12.23	1.40	1.52
11	Z	101	GLY	CA-C	-11.32	1.39	1.51
11	a	20	ALA	C-N	10.98	1.46	1.33
4	F	431	LEU	CA-C	-10.62	1.39	1.52
3	E	94	VAL	CA-C	-10.50	1.40	1.52
4	F	139	ILE	CA-CB	-10.22	1.48	1.55
3	E	36	ILE	CA-C	-10.20	1.40	1.52
11	X	36	GLY	CA-C	-10.19	1.40	1.51
3	A	185	ILE	CA-C	-10.09	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	137	ALA	CA-C	-9.97	1.40	1.52
3	E	72	VAL	CA-CB	-9.89	1.42	1.54
5	Q	206	GLU	CA-C	-9.87	1.44	1.52
11	V	45	LEU	C-N	9.83	1.42	1.33
3	A	219	VAL	CA-C	9.83	1.60	1.53
3	A	397	LYS	C-N	9.79	1.46	1.33
11	U	27	GLY	CA-C	-9.72	1.41	1.52
11	a	112	GLY	CA-C	-9.65	1.40	1.51
8	P	351	GLN	CA-C	9.61	1.65	1.52
11	V	141	LEU	N-CA	-9.58	1.34	1.46
11	W	121	GLN	C-N	9.55	1.42	1.33
10	O	190	HIS	ND1-CE1	9.52	1.42	1.32
11	Y	85	TYR	CA-C	-9.52	1.40	1.52
11	R	49	LEU	N-CA	-9.48	1.34	1.46
4	D	424	ALA	CA-C	-9.42	1.40	1.52
3	E	482	ARG	CD-NE	9.30	1.59	1.46
4	F	43	LYS	N-CA	-9.29	1.35	1.46
4	F	420	VAL	C-N	9.30	1.40	1.33
4	D	302	ARG	NE-CZ	9.26	1.43	1.33
1	M	178	ILE	CA-CB	-9.21	1.49	1.54
3	E	554	HIS	ND1-CE1	9.15	1.41	1.32
11	T	20	ALA	C-N	9.11	1.44	1.34
11	W	57	VAL	C-N	9.08	1.43	1.34
3	C	436	GLN	CA-C	9.04	1.64	1.52
3	A	215	TRP	CA-CB	9.03	1.67	1.53
3	A	352	MET	CA-C	-8.99	1.41	1.52
7	I	85	ARG	NE-CZ	8.99	1.43	1.33
10	O	181	PRO	N-CA	-8.96	1.35	1.47
11	Z	76	TYR	CA-CB	8.94	1.67	1.53
11	W	103	ALA	C-N	8.92	1.45	1.33
9	b	136	ASN	CA-CB	8.86	1.67	1.53
3	C	428	THR	CA-C	-8.83	1.41	1.52
3	E	231	TYR	CA-CB	8.80	1.65	1.53
8	P	349	GLU	N-CA	-8.80	1.35	1.46
4	F	252	ARG	CD-NE	8.80	1.58	1.46
7	I	174	ILE	CA-C	-8.73	1.43	1.53
3	A	64	ASP	CA-C	-8.71	1.42	1.53
4	D	301	ARG	CD-NE	8.71	1.58	1.46
10	O	112	GLU	C-N	8.71	1.45	1.33
4	B	374	ASN	CA-CB	8.68	1.65	1.53
4	D	393	ARG	NE-CZ	8.64	1.42	1.33
3	E	508	SER	CA-C	-8.62	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	359	ARG	CD-NE	8.56	1.58	1.46
3	A	45	MET	CA-C	-8.55	1.42	1.52
4	D	320	GLY	CA-C	-8.55	1.43	1.52
10	O	367	GLN	N-CA	-8.51	1.38	1.46
10	O	213	LEU	CA-C	-8.51	1.41	1.52
11	U	155	THR	C-N	8.50	1.43	1.33
4	D	112	ILE	CA-CB	8.49	1.64	1.54
3	A	358	SER	N-CA	-8.49	1.35	1.46
4	B	257	ARG	NE-CZ	8.48	1.42	1.33
3	A	281	VAL	C-N	8.48	1.38	1.33
4	F	373	ILE	CA-C	-8.46	1.42	1.52
3	C	436	GLN	N-CA	-8.45	1.34	1.45
3	C	344	ARG	NE-CZ	8.44	1.42	1.33
3	A	394	ARG	CD-NE	8.44	1.58	1.46
4	B	304	TYR	CA-C	-8.44	1.41	1.52
2	N	6	THR	N-CA	-8.42	1.35	1.46
4	D	195	ARG	NE-CZ	8.41	1.42	1.33
4	F	128	ALA	CA-C	-8.40	1.42	1.52
3	A	430	ALA	CA-C	-8.40	1.41	1.52
11	S	153	ARG	CD-NE	8.40	1.58	1.46
4	D	104	VAL	CA-C	-8.40	1.42	1.52
2	N	76	ASN	CA-C	-8.39	1.42	1.52
3	C	133	LEU	CA-C	-8.39	1.42	1.52
3	C	59	GLU	CA-C	-8.37	1.42	1.52
8	P	417	LYS	C-N	8.36	1.44	1.33
11	V	151	ASN	CA-C	-8.36	1.41	1.52
11	R	130	ILE	CA-CB	-8.36	1.44	1.54
11	X	139	LEU	CA-C	-8.32	1.42	1.52
10	O	71	VAL	CA-CB	-8.32	1.44	1.54
3	A	336	GLY	N-CA	-8.27	1.35	1.45
3	A	574	THR	C-N	8.26	1.45	1.33
3	A	542	LYS	N-CA	-8.24	1.36	1.46
1	M	163	ILE	CA-CB	-8.23	1.44	1.54
11	T	23	PHE	CA-C	-8.23	1.42	1.52
6	H	7	ILE	CA-CB	-8.22	1.44	1.54
3	C	411	SER	CA-C	-8.21	1.42	1.52
4	B	284	TYR	CA-C	-8.17	1.42	1.52
11	X	51	PHE	C-N	8.15	1.45	1.33
7	K	174	ILE	C-N	8.10	1.44	1.33
3	E	321	THR	CA-C	-8.10	1.42	1.53
4	D	41	LEU	CA-C	-8.10	1.43	1.52
3	A	406	ARG	NE-CZ	8.08	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	W	102	LEU	C-N	8.07	1.45	1.33
1	M	200	PHE	C-N	8.05	1.44	1.33
4	D	289	ARG	CA-CB	8.04	1.65	1.53
7	G	182	ASP	CA-C	8.04	1.63	1.52
3	A	455	ASN	CA-C	-8.03	1.42	1.52
5	Q	68	ILE	N-CA	-8.03	1.36	1.46
11	Z	51	PHE	CA-CB	8.03	1.65	1.53
9	b	79	HIS	ND1-CE1	8.02	1.40	1.32
3	A	57	VAL	CA-C	-8.02	1.43	1.52
11	Y	68	LEU	CA-CB	8.01	1.65	1.53
11	X	117	ARG	CD-NE	8.00	1.57	1.46
3	A	184	TRP	C-N	7.98	1.43	1.33
11	a	76	TYR	N-CA	-7.98	1.36	1.46
11	W	101	GLY	CA-C	-7.97	1.43	1.52
3	C	37	ALA	CA-C	-7.97	1.42	1.52
10	O	372	HIS	ND1-CE1	7.96	1.40	1.32
3	A	194	ASP	C-N	7.94	1.43	1.33
9	b	60	ARG	NE-CZ	7.94	1.41	1.33
4	F	318	ARG	CD-NE	7.94	1.57	1.46
3	E	258	PHE	CA-C	-7.94	1.46	1.53
11	Z	100	SER	C-N	7.92	1.43	1.33
11	W	36	GLY	C-N	7.92	1.43	1.33
7	G	166	ARG	CD-NE	7.90	1.57	1.46
3	A	370	ARG	C-N	7.89	1.44	1.34
4	F	81	GLU	CA-C	-7.89	1.43	1.52
8	P	336	ARG	CD-NE	7.89	1.57	1.46
4	F	362	ARG	CD-NE	7.89	1.57	1.46
7	K	67	LYS	C-N	7.88	1.44	1.34
11	Y	151	ASN	CA-CB	7.88	1.65	1.53
4	F	118	ARG	CZ-NH1	7.87	1.43	1.32
4	F	103	PRO	CA-C	-7.87	1.45	1.52
5	Q	207	CYS	CA-CB	7.86	1.65	1.53
3	E	221	ARG	NE-CZ	7.86	1.41	1.33
3	A	325	PRO	N-CA	-7.85	1.37	1.47
1	M	135	ALA	C-N	7.83	1.44	1.33
11	R	95	LEU	C-N	7.83	1.43	1.33
1	M	21	LYS	CA-C	-7.82	1.42	1.52
1	M	184	THR	N-CA	-7.81	1.36	1.46
7	G	152	MET	CA-C	-7.80	1.41	1.52
4	B	74	ARG	CD-NE	7.80	1.57	1.46
3	E	602	LYS	CA-C	-7.80	1.42	1.52
11	X	153	ARG	NE-CZ	7.80	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	148	VAL	CA-C	-7.79	1.43	1.52
3	E	258	PHE	CA-CB	7.79	1.64	1.53
4	B	172	ILE	CA-CB	-7.78	1.45	1.54
5	Q	209	GLN	N-CA	-7.77	1.37	1.46
8	P	404	ALA	C-N	7.77	1.44	1.33
11	W	37	VAL	CA-CB	7.77	1.64	1.54
9	b	16	LEU	N-CA	-7.77	1.36	1.46
11	V	36	GLY	CA-C	-7.76	1.43	1.51
4	F	160	THR	N-CA	7.75	1.55	1.46
11	R	30	TYR	N-CA	-7.75	1.36	1.46
4	F	376	LEU	C-N	7.75	1.41	1.33
4	D	208	PHE	CA-C	-7.75	1.43	1.52
3	E	237	GLN	C-N	7.74	1.44	1.33
6	H	56	GLU	CA-C	-7.74	1.42	1.52
11	Y	107	ALA	C-N	7.74	1.43	1.33
4	D	263	ALA	CA-C	-7.72	1.42	1.52
7	K	33	LYS	N-CA	-7.72	1.36	1.46
4	F	170	ILE	N-CA	-7.71	1.40	1.45
3	E	92	LEU	CA-CB	7.71	1.63	1.53
11	U	62	ILE	CA-CB	-7.71	1.44	1.54
8	P	140	LEU	CA-CB	7.71	1.65	1.53
9	b	263	VAL	CA-CB	-7.71	1.44	1.54
4	F	55	LEU	CA-CB	7.70	1.63	1.53
3	A	190	GLU	C-N	7.70	1.43	1.33
1	M	179	PRO	N-CA	-7.69	1.37	1.47
6	J	52	LYS	CA-C	7.69	1.62	1.52
1	M	96	ALA	CA-C	-7.69	1.42	1.52
5	Q	261	ASP	CA-C	-7.68	1.43	1.53
8	P	267	TYR	CA-C	-7.68	1.41	1.52
3	A	161	VAL	N-CA	-7.68	1.37	1.46
10	O	22	PRO	CA-C	-7.66	1.44	1.52
4	D	226	LYS	C-N	7.66	1.44	1.33
3	C	201	GLU	CA-CB	7.66	1.63	1.53
7	I	110	ILE	N-CA	-7.66	1.37	1.46
7	K	143	GLU	C-N	7.66	1.43	1.33
4	D	190	GLN	C-N	7.65	1.43	1.33
11	Z	80	GLN	CA-C	-7.65	1.43	1.52
7	K	203	LEU	CA-C	-7.64	1.43	1.52
9	b	120	ARG	NE-CZ	7.64	1.41	1.33
8	P	201	ASP	C-N	7.64	1.43	1.33
4	F	233	GLY	CA-C	-7.64	1.41	1.51
3	C	505	SER	CA-C	-7.63	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	U	42	THR	C-N	7.63	1.44	1.34
11	a	25	SER	CA-C	-7.63	1.43	1.52
6	L	18	HIS	CA-C	-7.63	1.43	1.52
3	C	104	ILE	CA-CB	-7.62	1.45	1.54
10	O	216	ASN	CA-C	-7.62	1.44	1.53
2	N	27	GLN	CA-C	-7.62	1.43	1.52
3	A	534	TYR	CA-C	-7.62	1.43	1.52
8	P	245	HIS	C-N	7.61	1.44	1.33
7	I	190	VAL	CA-CB	-7.61	1.45	1.54
7	I	47	LYS	N-CA	-7.61	1.37	1.46
6	H	49	GLN	N-CA	-7.61	1.37	1.46
3	E	365	ARG	CZ-NH2	7.60	1.43	1.33
1	M	97	ARG	CZ-NH2	7.59	1.43	1.33
3	E	49	VAL	CA-C	-7.59	1.43	1.52
5	Q	72	ALA	CA-CB	7.58	1.65	1.53
9	b	127	ALA	N-CA	-7.58	1.37	1.46
5	Q	321	ARG	CD-NE	7.58	1.56	1.46
2	N	5	ARG	NE-CZ	7.56	1.41	1.33
8	P	84	LEU	N-CA	-7.55	1.37	1.46
5	Q	209	GLN	CA-C	7.55	1.62	1.52
11	V	46	ARG	NE-CZ	7.55	1.41	1.33
9	b	15	ALA	C-N	7.55	1.43	1.33
4	D	47	PRO	CA-C	-7.54	1.44	1.52
11	Z	117	ARG	NE-CZ	7.54	1.41	1.33
7	I	126	VAL	CA-CB	-7.54	1.45	1.54
10	O	195	LEU	CA-C	-7.53	1.43	1.52
11	S	16	GLY	CA-C	-7.53	1.43	1.52
4	B	356	GLY	N-CA	-7.53	1.37	1.45
5	Q	72	ALA	C-N	7.53	1.44	1.33
4	B	321	ARG	NE-CZ	7.53	1.41	1.33
11	S	133	LEU	C-N	7.53	1.43	1.33
5	Q	296	CYS	CA-C	-7.52	1.43	1.52
7	K	140	LYS	CA-C	-7.52	1.43	1.52
3	E	599	GLU	CA-CB	7.51	1.65	1.53
4	F	217	VAL	CA-CB	-7.50	1.46	1.54
8	P	147	VAL	N-CA	-7.50	1.37	1.46
7	K	52	ARG	NE-CZ	7.49	1.41	1.33
7	I	51	VAL	CA-CB	-7.46	1.45	1.54
11	W	47	PRO	CA-CB	7.46	1.64	1.53
3	C	90	LYS	N-CA	-7.45	1.38	1.46
4	D	174	SER	CA-C	-7.45	1.42	1.52
10	O	21	GLN	N-CA	-7.45	1.38	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	405	ALA	C-N	7.43	1.44	1.34
11	Z	22	ILE	N-CA	-7.42	1.37	1.46
4	D	286	ASP	CA-CB	7.42	1.65	1.53
11	W	142	TYR	CA-C	-7.41	1.43	1.52
10	O	379	ASP	CA-C	-7.40	1.43	1.52
11	R	14	ALA	C-N	7.40	1.42	1.34
8	P	429	HIS	ND1-CE1	7.38	1.40	1.32
7	G	92	ARG	N-CA	-7.37	1.36	1.46
3	C	270	SER	N-CA	-7.37	1.37	1.46
10	O	254	LYS	N-CA	-7.37	1.34	1.46
11	R	46	ARG	C-N	7.37	1.39	1.33
8	P	204	TRP	NE1-CE2	7.36	1.45	1.37
3	A	152	ILE	CA-C	-7.36	1.44	1.52
11	X	78	LEU	CA-CB	7.36	1.65	1.53
11	Y	91	LEU	CA-C	-7.36	1.43	1.52
2	N	92	LEU	CA-C	-7.34	1.43	1.52
11	V	139	LEU	CA-C	-7.34	1.43	1.52
7	G	57	ASN	C-N	7.34	1.43	1.33
11	U	123	PRO	CA-C	-7.34	1.45	1.52
1	M	31	LEU	C-N	7.33	1.44	1.34
10	O	123	LEU	CA-CB	7.32	1.65	1.53
4	B	393	ARG	NE-CZ	7.31	1.41	1.33
9	b	67	ARG	NE-CZ	7.31	1.41	1.33
11	U	101	GLY	C-N	7.31	1.43	1.33
9	b	216	VAL	N-CA	-7.30	1.37	1.46
8	P	301	ARG	N-CA	-7.29	1.37	1.46
4	D	118	ARG	CA-C	-7.29	1.44	1.53
11	U	123	PRO	N-CA	-7.28	1.41	1.47
3	E	595	GLU	CA-C	-7.28	1.43	1.52
8	P	108	LYS	C-N	7.28	1.43	1.33
7	G	50	ILE	C-N	7.28	1.43	1.33
4	F	206	GLU	CA-C	-7.28	1.43	1.52
7	I	115	ASP	N-CA	-7.28	1.36	1.46
11	X	117	ARG	NE-CZ	7.26	1.41	1.33
3	C	481	LEU	C-N	7.26	1.43	1.33
4	F	118	ARG	CA-C	7.26	1.59	1.52
7	K	166	ARG	NE-CZ	7.25	1.41	1.33
7	I	182	ASP	CA-C	-7.25	1.44	1.53
2	N	87	ALA	N-CA	-7.25	1.36	1.46
11	U	123	PRO	N-CD	7.25	1.57	1.47
4	F	117	GLY	C-N	7.25	1.42	1.32
9	b	205	ARG	NE-CZ	7.24	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	155	THR	CA-CB	7.24	1.62	1.53
8	P	408	ASN	CA-C	-7.23	1.43	1.52
11	W	136	ALA	N-CA	-7.23	1.36	1.46
3	E	417	SER	CA-CB	7.23	1.64	1.54
10	O	273	GLU	C-O	7.23	1.32	1.24
9	b	50	ALA	CA-CB	7.22	1.64	1.53
3	A	205	LYS	C-N	7.21	1.43	1.33
3	A	521	ILE	CA-CB	-7.21	1.45	1.54
4	B	214	ALA	CA-C	-7.21	1.44	1.52
4	F	170	ILE	CA-C	7.20	1.58	1.52
1	M	16	GLY	N-CA	7.20	1.54	1.45
11	a	153	ARG	N-CA	-7.19	1.37	1.46
1	M	89	THR	C-N	7.19	1.43	1.33
2	N	111	ARG	CD-NE	7.18	1.56	1.46
10	O	223	SER	C-N	7.18	1.41	1.33
3	E	123	TYR	CA-C	-7.18	1.43	1.52
11	V	13	GLY	CA-C	-7.18	1.44	1.52
4	B	125	LYS	CA-C	-7.17	1.43	1.52
4	D	30	THR	CA-C	-7.17	1.43	1.53
8	P	235	SER	N-CA	-7.17	1.36	1.46
8	P	415	GLN	CA-C	-7.16	1.43	1.52
3	A	229	ALA	CA-C	-7.16	1.43	1.52
1	M	108	GLN	C-N	7.16	1.44	1.33
4	B	331	GLN	CA-C	-7.15	1.44	1.52
7	G	58	ILE	CA-CB	-7.15	1.45	1.54
4	D	245	ALA	C-N	7.14	1.43	1.33
7	I	46	GLU	CA-C	-7.14	1.43	1.52
3	A	380	PHE	C-N	7.14	1.42	1.33
11	Y	109	GLY	C-N	7.14	1.42	1.33
11	a	30	TYR	CA-C	-7.13	1.43	1.52
7	K	170	GLU	N-CA	-7.13	1.37	1.46
6	J	46	TYR	N-CA	-7.13	1.36	1.46
11	a	131	LEU	C-N	7.12	1.42	1.33
4	D	201	HIS	CG-ND1	-7.12	1.30	1.38
5	Q	212	LEU	CA-C	7.12	1.61	1.52
3	E	309	GLU	C-O	-7.12	1.20	1.23
11	S	145	ILE	CA-CB	-7.12	1.46	1.54
4	D	325	ARG	NE-CZ	7.11	1.40	1.33
10	O	135	SER	CA-C	7.11	1.61	1.52
3	C	587	PHE	CA-CB	7.11	1.64	1.53
3	A	353	ILE	CA-C	-7.10	1.43	1.52
4	F	341	ASP	CA-C	-7.09	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	25	LEU	CA-C	-7.09	1.44	1.52
11	Y	60	ALA	C-N	7.09	1.42	1.33
7	G	53	ASN	CA-CB	7.09	1.64	1.53
11	Z	42	THR	N-CA	-7.09	1.37	1.46
11	Z	46	ARG	NE-CZ	7.08	1.40	1.33
11	V	102	LEU	CA-CB	7.08	1.64	1.53
3	A	538	CYS	CA-CB	7.08	1.62	1.53
11	W	20	ALA	C-N	7.08	1.42	1.33
3	E	177	ARG	CZ-NH2	7.08	1.42	1.33
10	O	138	SER	CA-C	-7.08	1.43	1.52
10	O	363	LYS	CA-C	-7.07	1.43	1.52
11	V	150	LEU	C-N	7.07	1.42	1.33
8	P	187	ILE	CA-CB	-7.07	1.45	1.54
9	b	241	HIS	ND1-CE1	7.06	1.39	1.32
3	E	172	ILE	CA-C	-7.06	1.44	1.52
11	W	41	ALA	C-N	7.06	1.43	1.33
4	D	379	LEU	CA-C	-7.06	1.43	1.52
10	O	174	SER	N-CA	-7.06	1.37	1.46
4	D	178	LEU	CA-CB	7.05	1.64	1.54
4	D	157	ALA	C-N	7.05	1.42	1.33
10	O	330	ILE	C-O	-7.05	1.16	1.24
7	K	169	LEU	CA-C	-7.05	1.44	1.52
10	O	324	HIS	N-CA	-7.05	1.37	1.45
1	M	144	GLU	N-CA	-7.04	1.37	1.46
11	X	149	LEU	C-N	7.04	1.42	1.33
3	C	482	ARG	CA-C	-7.03	1.43	1.52
3	A	433	GLY	CA-C	-7.02	1.44	1.52
11	S	15	ILE	CA-C	7.02	1.63	1.52
4	F	252	ARG	NE-CZ	7.00	1.40	1.33
7	G	180	ASN	CA-C	-7.00	1.44	1.52
3	C	424	SER	C-N	7.00	1.43	1.33
8	P	39	ILE	C-N	7.00	1.43	1.33
11	W	117	ARG	CD-NE	7.00	1.56	1.46
6	L	74	ALA	C-N	6.99	1.42	1.33
11	V	32	THR	C-N	6.99	1.42	1.33
4	B	169	LYS	C-N	6.98	1.41	1.33
3	A	314	ARG	CD-NE	6.96	1.55	1.46
4	B	301	ARG	CZ-NH1	6.96	1.42	1.32
7	K	49	ASN	CA-C	-6.95	1.44	1.52
8	P	199	TYR	C-N	6.95	1.43	1.33
6	J	41	LYS	N-CA	6.95	1.55	1.46
11	T	150	LEU	C-N	6.95	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	156	ASP	N-CA	-6.94	1.37	1.45
3	C	238	ARG	CD-NE	6.94	1.55	1.46
5	Q	44	LEU	CA-C	-6.93	1.44	1.52
9	b	22	PRO	CA-C	-6.93	1.43	1.52
11	W	52	LYS	CA-C	-6.93	1.44	1.52
7	I	89	LEU	CA-C	-6.92	1.43	1.52
3	A	363	ALA	CA-C	-6.92	1.43	1.52
7	G	149	ILE	N-CA	6.92	1.54	1.46
4	F	362	ARG	NE-CZ	6.91	1.40	1.33
9	b	258	ALA	CA-C	-6.91	1.44	1.52
5	Q	166	PHE	N-CA	-6.90	1.38	1.46
10	O	298	ASP	C-N	6.90	1.42	1.33
11	Z	106	PHE	N-CA	-6.90	1.38	1.46
6	J	66	GLY	CA-C	-6.89	1.42	1.51
11	U	54	ILE	C-O	-6.89	1.15	1.24
3	C	134	ASP	CA-C	-6.89	1.43	1.52
4	F	468	TYR	CA-C	-6.89	1.44	1.52
3	A	104	ILE	C-N	6.88	1.42	1.33
11	S	147	ALA	N-CA	-6.88	1.38	1.46
5	Q	266	ARG	CZ-NH1	6.88	1.42	1.32
10	O	49	LYS	C-N	6.88	1.41	1.33
4	B	289	ARG	N-CA	-6.87	1.38	1.46
8	P	12	HIS	C-N	6.86	1.43	1.33
8	P	439	ASP	N-CA	6.86	1.54	1.46
10	O	130	LEU	C-N	6.86	1.42	1.33
6	L	99	ILE	N-CA	6.85	1.54	1.46
11	X	51	PHE	CA-C	6.85	1.61	1.52
3	E	209	PHE	CA-C	-6.85	1.44	1.52
5	Q	150	GLU	CA-C	-6.85	1.44	1.52
8	P	120	ASP	CA-CB	6.84	1.61	1.53
1	M	207	GLN	N-CA	6.84	1.54	1.46
7	I	187	GLY	CA-C	-6.83	1.42	1.52
3	A	309	GLU	C-O	6.83	1.27	1.23
3	C	579	HIS	ND1-CE1	6.83	1.39	1.32
8	P	387	PHE	CA-CB	6.83	1.64	1.53
11	Z	102	LEU	N-CA	-6.82	1.38	1.46
7	G	200	ASN	CA-CB	6.82	1.61	1.52
3	A	85	VAL	C-N	6.81	1.42	1.33
4	B	237	ARG	CZ-NH1	6.80	1.42	1.32
3	C	353	ILE	CA-CB	-6.79	1.45	1.54
7	K	108	SER	CA-CB	6.79	1.64	1.53
11	X	26	LEU	N-CA	6.79	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	b	47	LYS	N-CA	-6.79	1.38	1.46
4	D	252	ARG	C-N	6.79	1.41	1.33
10	O	69	SER	N-CA	-6.78	1.38	1.46
11	V	46	ARG	CA-CB	6.78	1.61	1.53
3	C	162	PHE	CA-C	-6.78	1.44	1.52
4	D	449	TYR	CA-C	-6.78	1.44	1.52
4	F	440	GLU	CA-CB	6.78	1.64	1.53
3	E	286	ARG	NE-CZ	6.78	1.40	1.33
8	P	294	ILE	N-CA	6.78	1.54	1.46
7	G	197	ILE	CA-C	-6.77	1.44	1.52
11	Z	124	ARG	CZ-NH2	6.77	1.42	1.33
4	D	354	THR	C-N	6.77	1.42	1.33
11	Y	120	SER	CA-C	-6.77	1.43	1.52
3	E	524	ASP	CA-CB	6.76	1.64	1.53
9	b	142	ARG	NE-CZ	6.76	1.40	1.33
7	I	96	LEU	N-CA	-6.76	1.38	1.46
4	F	55	LEU	N-CA	-6.76	1.37	1.46
4	F	166	ARG	CA-C	-6.76	1.43	1.52
3	A	441	LEU	N-CA	-6.75	1.37	1.46
11	R	25	SER	C-N	6.75	1.42	1.33
11	V	121	GLN	CA-C	-6.75	1.44	1.52
1	M	141	ARG	CD-NE	6.75	1.55	1.46
3	E	186	ALA	CA-C	6.75	1.61	1.52
7	G	113	ASN	CA-C	-6.75	1.44	1.52
4	D	475	ARG	NE-CZ	6.75	1.40	1.33
3	E	606	THR	CA-CB	-6.74	1.42	1.53
4	B	452	ARG	CD-NE	6.74	1.55	1.46
9	b	140	GLN	C-N	6.74	1.43	1.33
3	A	537	PHE	CA-CB	6.74	1.65	1.53
8	P	236	ASN	CA-C	-6.74	1.44	1.52
2	N	17	THR	N-CA	6.73	1.54	1.46
3	E	189	GLY	N-CA	-6.73	1.39	1.45
11	W	23	PHE	CA-CB	6.73	1.63	1.53
11	V	156	GLN	C-N	6.73	1.43	1.33
3	C	398	ALA	C-N	6.72	1.42	1.33
3	C	368	SER	CA-C	-6.72	1.44	1.52
11	V	147	ALA	CA-C	-6.72	1.44	1.52
3	C	75	GLU	CA-C	-6.72	1.44	1.52
3	C	116	LYS	N-CA	-6.71	1.38	1.46
3	C	103	THR	C-N	6.71	1.42	1.33
11	Z	15	ILE	C-N	6.71	1.41	1.33
7	K	184	VAL	CA-C	-6.71	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Z	139	LEU	C-N	6.71	1.42	1.33
3	A	238	ARG	NE-CZ	6.70	1.40	1.33
9	b	42	ARG	CA-C	-6.70	1.44	1.52
9	b	113	ASN	N-CA	-6.70	1.37	1.46
10	O	118	THR	CA-C	-6.69	1.44	1.52
11	S	117	ARG	N-CA	6.69	1.54	1.46
11	X	68	LEU	CA-C	6.68	1.61	1.52
11	W	97	VAL	C-N	6.68	1.41	1.33
5	Q	241	LEU	CA-CB	6.68	1.63	1.53
7	K	25	ARG	CD-NE	6.67	1.55	1.46
11	T	123	PRO	CA-C	-6.67	1.45	1.52
7	K	133	LEU	N-CA	-6.67	1.36	1.46
4	B	360	VAL	C-N	6.66	1.42	1.33
4	B	204	HIS	ND1-CE1	6.66	1.39	1.32
4	D	437	GLU	C-N	6.65	1.43	1.33
3	A	433	GLY	N-CA	-6.65	1.37	1.45
3	A	458	VAL	N-CA	-6.65	1.38	1.46
7	K	145	ASP	CA-CB	6.65	1.64	1.54
5	Q	315	SER	CA-C	-6.64	1.44	1.52
11	T	97	VAL	C-N	6.64	1.41	1.33
11	Y	12	PHE	N-CA	-6.64	1.37	1.46
3	E	255	PRO	C-N	6.64	1.43	1.33
4	F	354	THR	CA-C	-6.64	1.44	1.52
11	W	128	GLY	CA-C	-6.64	1.43	1.51
2	N	53	LYS	C-N	6.63	1.42	1.33
3	C	179	ARG	CZ-NH2	6.63	1.42	1.33
3	C	401	LEU	CA-C	-6.63	1.44	1.52
9	b	149	ASP	CA-C	-6.63	1.44	1.52
3	A	322	SER	CA-CB	6.63	1.64	1.53
7	G	72	SER	C-N	6.63	1.43	1.34
10	O	145	VAL	N-CA	-6.62	1.38	1.46
8	P	288	ARG	NE-CZ	6.62	1.40	1.33
6	H	104	LYS	C-N	6.62	1.41	1.33
7	I	217	ALA	CA-C	-6.62	1.44	1.52
11	a	39	ILE	CA-CB	-6.62	1.46	1.54
11	Z	23	PHE	N-CA	-6.61	1.38	1.46
3	C	222	PRO	N-CA	-6.61	1.39	1.46
3	A	160	SER	C-N	6.61	1.42	1.33
4	B	67	VAL	N-CA	-6.61	1.38	1.46
4	B	444	ILE	C-N	6.61	1.42	1.33
9	b	299	LEU	CA-C	-6.61	1.44	1.52
3	C	510	SER	C-N	6.60	1.43	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	27	GLN	C-N	6.60	1.42	1.33
9	b	135	LYS	C-N	6.59	1.42	1.33
2	N	97	LYS	CA-CB	6.59	1.61	1.53
4	B	289	ARG	CD-NE	6.59	1.55	1.46
3	E	139	TRP	NE1-CE2	-6.59	1.30	1.37
4	B	295	ARG	CD-NE	6.58	1.55	1.46
4	B	295	ARG	CZ-NH1	6.58	1.42	1.32
11	X	140	GLY	C-N	6.58	1.42	1.33
4	D	118	ARG	NE-CZ	6.58	1.40	1.33
3	E	111	PRO	CA-C	-6.58	1.46	1.52
11	R	15	ILE	CA-CB	-6.58	1.45	1.54
9	b	341	ILE	CA-C	-6.58	1.47	1.52
3	A	567	TRP	CA-C	-6.58	1.44	1.52
4	D	289	ARG	CD-NE	6.58	1.55	1.46
6	L	5	ASN	CA-C	-6.58	1.44	1.52
11	Y	153	ARG	CD-NE	6.58	1.55	1.46
3	E	162	PHE	CA-CB	6.57	1.61	1.53
5	Q	326	ILE	CA-CB	6.57	1.62	1.54
3	C	402	GLY	N-CA	-6.57	1.39	1.45
2	N	69	ILE	CA-CB	-6.57	1.45	1.54
3	C	478	PHE	CA-CB	6.57	1.60	1.54
10	O	190	HIS	CG-CD2	6.57	1.43	1.35
7	K	150	GLU	N-CA	-6.56	1.38	1.46
3	A	521	ILE	C-N	6.56	1.42	1.33
7	G	160	TYR	CA-C	-6.56	1.44	1.52
7	G	192	ASN	CA-C	-6.55	1.44	1.53
3	A	179	ARG	NE-CZ	6.55	1.40	1.33
11	S	16	GLY	N-CA	6.54	1.53	1.45
2	N	68	LEU	CA-C	-6.54	1.44	1.52
3	E	203	ASP	CA-CB	6.54	1.63	1.53
11	U	27	GLY	C-N	6.53	1.42	1.33
3	E	475	TYR	CA-C	-6.53	1.44	1.52
4	F	166	ARG	CD-NE	6.53	1.55	1.46
3	A	548	ARG	CD-NE	6.53	1.55	1.46
4	F	223	ARG	CZ-NH1	6.53	1.41	1.32
10	O	250	ALA	N-CA	-6.53	1.38	1.46
9	b	208	ARG	CZ-NH2	6.52	1.42	1.33
6	H	76	VAL	C-N	6.52	1.42	1.33
3	A	272	TYR	N-CA	-6.52	1.37	1.46
4	B	172	ILE	CA-C	-6.52	1.44	1.52
3	C	507	LEU	CA-C	-6.52	1.44	1.52
7	G	44	GLU	C-N	6.52	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	U	84	LEU	CA-C	-6.52	1.44	1.52
3	E	152	ILE	C-N	6.52	1.41	1.33
3	E	166	LEU	C-N	6.51	1.39	1.33
4	B	144	ARG	CZ-NH1	6.51	1.41	1.32
3	C	560	ALA	C-N	6.51	1.41	1.33
1	M	116	GLU	CA-C	-6.50	1.44	1.52
8	P	459	SER	N-CA	-6.50	1.38	1.46
2	N	90	ALA	C-O	-6.50	1.16	1.23
3	C	443	LYS	CA-C	-6.50	1.44	1.52
9	b	237	ILE	C-N	6.50	1.42	1.33
10	O	236	VAL	N-CA	-6.50	1.38	1.46
11	V	108	ILE	CA-CB	6.49	1.64	1.54
4	B	304	TYR	CA-CB	6.49	1.62	1.53
10	O	37	THR	C-N	6.49	1.43	1.33
2	N	77	ILE	C-O	-6.48	1.16	1.24
4	F	242	LEU	C-N	6.48	1.42	1.33
11	W	133	LEU	CA-C	-6.48	1.44	1.52
5	Q	261	ASP	CA-CB	6.47	1.63	1.53
4	F	334	ILE	CA-CB	-6.47	1.46	1.54
11	Y	13	GLY	N-CA	-6.47	1.37	1.45
3	A	195	GLU	CA-C	6.47	1.61	1.52
8	P	23	ARG	CD-NE	6.47	1.55	1.46
3	C	27	ILE	CA-C	6.46	1.59	1.52
4	B	74	ARG	NE-CZ	6.46	1.40	1.33
11	T	93	ALA	CA-C	-6.46	1.44	1.52
4	D	297	GLU	C-N	6.46	1.38	1.33
10	O	344	LEU	CA-CB	6.45	1.63	1.53
8	P	324	SER	C-N	6.45	1.42	1.33
4	D	349	LEU	CA-C	-6.45	1.44	1.52
3	C	116	LYS	C-N	6.45	1.42	1.33
11	Y	107	ALA	CA-C	-6.45	1.44	1.52
4	B	417	LYS	C-N	6.44	1.42	1.33
4	B	409	ILE	N-CA	-6.44	1.38	1.46
4	B	344	HIS	ND1-CE1	6.43	1.39	1.32
10	O	170	LEU	CA-C	-6.43	1.44	1.52
6	H	58	GLU	C-N	6.43	1.42	1.34
4	D	33	GLY	C-N	6.43	1.42	1.33
8	P	46	ALA	C-N	6.43	1.42	1.33
4	F	52	ILE	C-N	6.42	1.42	1.33
4	D	308	MET	CA-C	-6.42	1.44	1.52
3	C	34	VAL	CA-C	6.42	1.60	1.52
3	E	295	MET	CA-C	-6.42	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	544	PHE	C-N	6.41	1.42	1.33
9	b	245	ILE	C-N	6.41	1.42	1.33
7	I	205	GLU	CA-C	-6.41	1.44	1.52
11	V	51	PHE	C-N	6.41	1.42	1.33
3	E	57	VAL	C-N	6.41	1.42	1.33
7	I	122	GLN	N-CA	-6.41	1.38	1.46
3	A	146	PHE	CA-CB	6.41	1.62	1.53
3	A	172	ILE	C-N	6.41	1.42	1.33
3	C	147	GLN	C-N	6.41	1.41	1.33
3	C	520	LEU	CA-C	6.40	1.61	1.52
5	Q	321	ARG	CA-C	-6.40	1.44	1.52
10	O	24	THR	N-CA	6.40	1.54	1.46
3	E	588	GLU	CA-C	-6.40	1.44	1.52
2	N	114	LYS	CA-CB	6.40	1.62	1.53
3	C	490	SER	CA-C	-6.40	1.44	1.52
11	V	118	GLY	N-CA	6.40	1.53	1.45
11	U	124	ARG	CD-NE	6.40	1.55	1.46
1	M	15	LEU	CA-C	-6.39	1.44	1.52
4	B	365	HIS	ND1-CE1	6.39	1.39	1.32
3	C	92	LEU	C-O	-6.39	1.16	1.24
11	R	109	GLY	N-CA	-6.39	1.37	1.45
1	M	180	ARG	CZ-NH2	6.39	1.41	1.33
7	G	52	ARG	NE-CZ	6.39	1.40	1.33
4	F	189	ARG	NE-CZ	6.38	1.40	1.33
11	a	74	VAL	C-N	6.38	1.41	1.33
4	D	284	TYR	CA-C	6.38	1.61	1.52
11	Z	70	VAL	CA-C	-6.38	1.45	1.52
3	A	282	GLY	CA-C	-6.38	1.46	1.51
11	Z	55	VAL	CA-CB	6.38	1.57	1.54
11	V	71	SER	CA-C	-6.37	1.44	1.52
6	J	41	LYS	CA-CB	6.37	1.64	1.53
6	J	42	GLU	N-CA	-6.37	1.37	1.46
3	C	281	VAL	CA-C	-6.37	1.44	1.52
1	M	12	ARG	NE-CZ	6.37	1.40	1.33
4	F	69	GLU	C-N	6.37	1.42	1.33
3	C	501	LEU	N-CA	-6.36	1.38	1.46
3	C	87	ARG	CA-CB	6.36	1.63	1.53
4	D	333	PRO	C-N	6.36	1.41	1.33
4	B	130	ASP	CA-C	6.36	1.60	1.52
11	Z	61	GLY	CA-C	6.36	1.60	1.51
3	C	527	GLN	CA-C	-6.36	1.46	1.53
3	C	29	SER	CA-C	-6.35	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	454	ILE	CA-C	-6.35	1.45	1.52
4	F	58	PRO	N-CA	-6.35	1.40	1.47
11	X	124	ARG	NE-CZ	6.35	1.40	1.33
3	A	117	GLU	N-CA	-6.35	1.38	1.46
4	B	253	ILE	C-N	6.35	1.41	1.33
1	M	55	GLN	C-N	6.35	1.42	1.33
11	Z	69	VAL	CA-C	-6.35	1.45	1.52
4	D	269	GLN	N-CA	-6.34	1.38	1.46
11	W	143	GLY	CA-C	-6.34	1.45	1.52
8	P	25	VAL	CA-C	-6.34	1.44	1.52
11	Z	137	GLU	C-N	6.34	1.42	1.33
4	F	212	PHE	CA-C	-6.34	1.45	1.52
5	Q	171	GLU	C-N	6.34	1.42	1.33
1	M	163	ILE	N-CA	-6.33	1.39	1.46
3	C	189	GLY	N-CA	-6.33	1.39	1.45
8	P	129	ASP	C-N	6.33	1.40	1.34
5	Q	322	ASN	C-N	6.33	1.41	1.33
7	K	202	THR	CA-C	-6.33	1.44	1.53
11	T	90	GLN	N-CA	-6.33	1.38	1.46
7	G	128	ALA	N-CA	-6.33	1.38	1.46
11	W	24	THR	C-N	6.33	1.42	1.33
3	C	528	GLN	N-CA	-6.33	1.38	1.45
4	F	464	LEU	CA-C	-6.33	1.44	1.52
7	G	95	SER	CA-C	-6.33	1.44	1.52
4	F	180	HIS	ND1-CE1	6.32	1.38	1.32
4	F	256	PRO	N-CA	-6.32	1.39	1.47
7	G	16	GLU	N-CA	-6.32	1.38	1.46
4	F	56	THR	CA-CB	-6.32	1.44	1.53
8	P	171	ILE	C-N	6.32	1.42	1.33
2	N	20	LEU	CA-CB	6.32	1.63	1.53
11	Z	147	ALA	CA-C	-6.32	1.44	1.52
3	A	484	ARG	CZ-NH1	6.31	1.41	1.32
11	V	20	ALA	C-N	6.31	1.41	1.33
3	A	126	ARG	CD-NE	6.31	1.55	1.46
7	K	25	ARG	NE-CZ	6.31	1.40	1.33
3	C	65	GLY	CA-C	-6.30	1.44	1.52
4	B	79	VAL	CA-C	-6.30	1.45	1.52
4	D	466	ARG	CZ-NH1	6.30	1.41	1.32
3	A	202	PHE	CA-CB	6.30	1.64	1.53
4	F	59	ASP	C-N	6.29	1.42	1.33
8	P	341	ASN	CA-C	6.29	1.60	1.52
11	Z	132	ILE	CA-CB	6.29	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	84	SER	C-N	6.29	1.43	1.33
8	P	105	SER	CA-CB	6.29	1.63	1.53
8	P	380	TRP	CA-C	-6.29	1.44	1.52
5	Q	321	ARG	NE-CZ	6.28	1.40	1.33
9	b	22	PRO	N-CD	6.28	1.56	1.47
1	M	208	GLU	CA-CB	6.28	1.63	1.53
3	A	312	MET	CA-C	-6.28	1.43	1.52
4	B	265	TYR	N-CA	-6.28	1.38	1.46
4	B	333	PRO	CA-C	-6.28	1.44	1.52
10	O	42	ARG	CZ-NH1	6.28	1.41	1.32
7	I	53	ASN	CA-C	-6.28	1.44	1.52
11	W	105	GLY	N-CA	6.28	1.54	1.45
7	G	215	LEU	N-CA	-6.28	1.40	1.46
1	M	49	ARG	CD-NE	6.27	1.55	1.46
3	C	361	ALA	CA-C	-6.27	1.44	1.52
3	A	342	TYR	C-N	6.27	1.42	1.34
8	P	268	LEU	CA-C	-6.26	1.44	1.52
4	F	148	GLU	C-N	6.26	1.41	1.33
4	B	482	ASP	CA-CB	6.26	1.63	1.53
7	I	167	ALA	CA-CB	6.26	1.63	1.53
10	O	164	ARG	CZ-NH1	6.26	1.41	1.32
4	D	182	GLU	CA-C	-6.26	1.44	1.52
4	F	466	ARG	NE-CZ	6.26	1.40	1.33
3	A	449	LYS	CA-C	-6.26	1.44	1.52
2	N	98	ASP	CA-CB	6.26	1.64	1.53
8	P	407	ARG	N-CA	-6.26	1.38	1.46
4	B	188	CYS	CA-C	-6.25	1.44	1.52
10	O	156	LYS	N-CA	-6.25	1.38	1.46
5	Q	279	LEU	C-O	-6.25	1.15	1.24
7	G	75	ILE	N-CA	-6.25	1.38	1.46
9	b	254	GLU	N-CA	-6.25	1.38	1.46
10	O	288	LEU	N-CA	-6.25	1.38	1.46
11	U	53	ASN	C-N	6.25	1.41	1.34
5	Q	340	ASN	CA-CB	6.25	1.63	1.53
7	I	128	ALA	CA-C	-6.25	1.44	1.52
8	P	119	GLU	CA-C	-6.24	1.45	1.52
3	E	177	ARG	CD-NE	6.24	1.54	1.46
8	P	452	GLU	CA-CB	6.24	1.63	1.53
9	b	244	LEU	C-N	6.24	1.41	1.33
7	I	202	THR	CA-C	-6.24	1.44	1.53
4	B	239	SER	CA-C	-6.24	1.45	1.52
7	K	113	ASN	N-CA	-6.23	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Z	52	LYS	C-N	6.23	1.41	1.33
1	M	121	ARG	CD-NE	6.23	1.54	1.46
1	M	212	ASN	C-N	6.23	1.42	1.33
2	N	39	VAL	N-CA	-6.23	1.39	1.46
7	G	86	LEU	CA-CB	6.23	1.63	1.53
7	I	16	GLU	C-N	6.23	1.42	1.33
11	Y	87	GLY	CA-C	6.23	1.60	1.51
3	A	539	PRO	C-N	6.23	1.41	1.33
3	A	123	TYR	CA-CB	6.23	1.63	1.53
3	E	179	ARG	NE-CZ	6.23	1.39	1.33
11	X	45	LEU	C-N	6.23	1.40	1.33
4	F	182	GLU	N-CA	-6.22	1.38	1.46
8	P	301	ARG	CD-NE	6.22	1.54	1.46
10	O	355	ALA	CA-CB	6.22	1.63	1.53
11	W	158	VAL	CA-CB	-6.22	1.46	1.54
4	D	189	ARG	NE-CZ	6.22	1.39	1.33
11	a	46	ARG	CZ-NH1	6.22	1.41	1.32
3	E	92	LEU	N-CA	-6.22	1.38	1.46
1	M	55	GLN	CA-C	-6.22	1.44	1.52
3	E	521	ILE	CA-C	-6.22	1.44	1.52
3	A	139	TRP	N-CA	-6.22	1.38	1.45
4	B	269	GLN	C-N	6.22	1.42	1.33
4	B	323	GLU	C-N	6.22	1.40	1.34
7	G	35	ILE	N-CA	-6.22	1.39	1.46
3	E	244	PHE	CA-C	-6.22	1.45	1.52
9	b	359	ARG	NE-CZ	6.22	1.39	1.33
11	U	47	PRO	CA-CB	6.21	1.62	1.53
3	E	529	ASN	N-CA	-6.21	1.38	1.46
4	D	250	ILE	CA-C	-6.21	1.44	1.52
11	T	15	ILE	C-N	6.21	1.41	1.33
7	G	10	PRO	N-CA	-6.21	1.39	1.47
11	Z	117	ARG	C-N	6.21	1.41	1.33
5	Q	109	LEU	CA-CB	6.20	1.63	1.53
11	Z	126	PHE	N-CA	-6.20	1.38	1.46
11	T	60	ALA	C-N	6.20	1.41	1.33
3	A	171	LYS	CA-C	-6.20	1.45	1.52
7	K	27	GLU	C-N	6.20	1.42	1.33
10	O	72	ASP	N-CA	-6.20	1.38	1.46
11	Y	88	PHE	N-CA	-6.20	1.38	1.46
4	F	272	ARG	CD-NE	6.20	1.54	1.46
11	W	139	LEU	N-CA	-6.20	1.38	1.46
3	C	394	ARG	C-N	6.20	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	O	303	TRP	CA-CB	6.20	1.63	1.53
3	E	174	LEU	C-N	6.19	1.40	1.33
5	Q	230	SER	N-CA	-6.19	1.38	1.46
3	E	48	LEU	CA-C	-6.19	1.44	1.52
8	P	76	THR	N-CA	-6.19	1.38	1.46
3	E	158	TYR	C-N	6.19	1.40	1.32
4	B	458	LEU	N-CA	-6.18	1.38	1.46
10	O	274	HIS	CA-C	-6.18	1.45	1.52
3	C	330	GLU	CA-CB	6.17	1.63	1.53
4	F	71	ARG	CA-C	-6.17	1.44	1.52
9	b	25	ILE	C-N	6.17	1.42	1.33
9	b	124	MET	N-CA	-6.17	1.39	1.46
4	F	132	LEU	C-N	6.17	1.41	1.33
4	B	347	PRO	C-N	6.17	1.42	1.33
7	K	117	TYR	CZ-OH	6.17	1.51	1.38
3	A	72	VAL	CA-CB	-6.17	1.46	1.54
8	P	32	ARG	NE-CZ	6.17	1.39	1.33
8	P	285	LYS	CA-C	-6.17	1.44	1.52
3	C	53	HIS	CE1-NE2	6.17	1.38	1.32
8	P	312	LEU	CA-C	-6.17	1.45	1.52
10	O	129	ASP	CA-C	-6.16	1.44	1.52
7	K	192	ASN	CA-CB	6.16	1.63	1.53
7	I	19	LYS	CA-CB	6.16	1.63	1.53
11	S	117	ARG	NE-CZ	6.16	1.39	1.33
3	A	246	CYS	C-N	6.16	1.42	1.33
9	b	304	LYS	N-CA	-6.16	1.39	1.46
5	Q	287	HIS	ND1-CE1	6.15	1.38	1.32
3	E	211	LEU	C-N	6.15	1.41	1.33
3	E	394	ARG	CD-NE	6.15	1.54	1.46
3	E	470	PHE	N-CA	-6.15	1.39	1.46
4	F	54	ASN	N-CA	-6.15	1.38	1.46
11	U	89	ILE	C-N	6.15	1.42	1.33
4	F	40	ILE	CA-CB	6.15	1.61	1.54
7	K	217	ALA	C-N	6.14	1.41	1.33
2	N	69	ILE	CA-C	-6.14	1.44	1.52
10	O	177	ASP	CA-C	-6.14	1.44	1.52
7	K	61	ASN	C-N	6.14	1.42	1.33
4	D	50	ASN	CA-CB	6.14	1.63	1.53
4	F	390	GLY	C-N	6.13	1.42	1.33
4	F	454	VAL	CA-C	6.13	1.61	1.52
3	A	602	LYS	C-N	6.13	1.42	1.34
5	Q	195	PHE	CA-CB	6.13	1.62	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Z	73	LEU	C-N	6.13	1.41	1.33
6	L	68	LEU	CA-CB	6.13	1.63	1.53
6	L	32	LEU	N-CA	-6.13	1.38	1.46
3	C	183	THR	C-N	6.13	1.41	1.33
3	E	568	SER	N-CA	-6.13	1.38	1.46
10	O	153	ASN	C-N	6.13	1.42	1.33
11	V	95	LEU	CA-C	-6.12	1.44	1.52
3	C	248	GLN	C-O	-6.12	1.16	1.24
10	O	217	VAL	CA-CB	-6.12	1.46	1.54
10	O	92	THR	CA-C	-6.12	1.44	1.52
3	C	192	THR	CA-C	-6.12	1.44	1.53
7	K	206	ARG	N-CA	-6.12	1.39	1.46
7	I	40	ASP	C-N	6.12	1.42	1.33
11	W	64	ALA	CA-C	-6.12	1.44	1.52
11	Y	46	ARG	C-N	6.12	1.39	1.33
1	M	124	GLY	CA-C	-6.11	1.43	1.51
3	A	215	TRP	CA-C	6.11	1.58	1.52
1	M	12	ARG	CZ-NH2	6.11	1.41	1.33
7	G	153	LYS	CA-CB	6.11	1.62	1.53
5	Q	167	ASP	CA-C	-6.11	1.45	1.52
9	b	265	SER	C-N	6.11	1.41	1.33
3	E	570	LEU	C-O	-6.10	1.16	1.24
4	D	484	PHE	CA-C	-6.10	1.45	1.52
9	b	266	SER	C-N	6.10	1.40	1.33
11	X	106	PHE	N-CA	-6.09	1.38	1.46
3	E	579	HIS	CE1-NE2	-6.09	1.26	1.32
6	J	14	GLU	C-O	-6.09	1.17	1.24
7	K	107	LEU	C-N	6.09	1.42	1.33
11	R	153	ARG	CA-C	6.09	1.60	1.52
11	T	74	VAL	CA-C	-6.09	1.45	1.52
6	L	6	GLY	N-CA	-6.09	1.38	1.45
3	C	478	PHE	C-N	6.08	1.43	1.33
7	I	179	LEU	CA-CB	6.08	1.62	1.53
2	N	95	PRO	CA-CB	-6.08	1.45	1.53
2	N	77	ILE	N-CA	-6.08	1.38	1.46
3	C	286	ARG	CZ-NH2	6.08	1.41	1.33
7	I	158	ARG	CZ-NH2	6.08	1.41	1.33
11	Y	25	SER	C-N	6.08	1.41	1.33
5	Q	245	ILE	CA-CB	6.08	1.62	1.54
11	T	140	GLY	N-CA	-6.08	1.38	1.45
4	F	431	LEU	C-O	-6.07	1.17	1.24
3	A	565	ALA	C-N	6.07	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	270	ASP	CA-C	6.07	1.60	1.52
8	P	305	HIS	CE1-NE2	-6.07	1.26	1.32
3	E	393	GLU	C-N	6.07	1.42	1.34
3	E	414	ALA	N-CA	-6.07	1.38	1.46
3	A	610	ARG	NE-CZ	6.07	1.39	1.33
8	P	322	VAL	CA-CB	-6.07	1.46	1.54
4	F	167	GLY	C-N	6.07	1.42	1.33
3	A	384	LEU	N-CA	-6.07	1.39	1.46
8	P	407	ARG	C-N	6.07	1.42	1.33
11	Z	157	ASP	CA-CB	6.07	1.62	1.53
2	N	53	LYS	CA-C	-6.06	1.45	1.52
4	F	190	GLN	N-CA	-6.06	1.38	1.46
3	A	234	LEU	CA-CB	6.06	1.61	1.53
9	b	20	TYR	C-N	6.06	1.40	1.33
3	C	274	ASN	CA-CB	6.06	1.61	1.53
1	M	158	ILE	CA-CB	6.06	1.62	1.54
4	F	367	LYS	C-N	6.06	1.42	1.33
3	A	231	TYR	CA-C	-6.06	1.45	1.52
11	U	101	GLY	CA-C	-6.06	1.45	1.52
11	Z	138	VAL	N-CA	-6.06	1.39	1.46
4	F	436	LEU	N-CA	-6.05	1.39	1.46
3	E	183	THR	CA-C	6.05	1.60	1.52
4	F	452	ARG	CZ-NH2	6.05	1.41	1.33
3	E	315	THR	C-N	6.05	1.42	1.33
3	A	110	ARG	CZ-NH1	6.05	1.41	1.32
11	S	140	GLY	C-N	6.05	1.41	1.33
3	E	43	CYS	CA-C	-6.05	1.45	1.52
7	K	61	ASN	N-CA	-6.05	1.38	1.46
11	U	74	VAL	CA-CB	-6.05	1.47	1.54
3	E	213	HIS	CE1-NE2	-6.05	1.26	1.32
9	b	143	PHE	C-N	6.04	1.41	1.33
3	A	266	SER	CA-C	-6.04	1.45	1.52
5	Q	95	MET	CA-CB	6.04	1.62	1.53
9	b	133	VAL	N-CA	6.04	1.53	1.46
7	I	92	ARG	CD-NE	6.04	1.54	1.46
3	E	74	GLU	CA-C	-6.04	1.45	1.52
1	M	42	ARG	CA-C	-6.04	1.45	1.52
3	E	90	LYS	N-CA	6.04	1.51	1.45
4	D	213	ALA	CA-C	-6.04	1.45	1.52
4	B	321	ARG	CZ-NH2	6.04	1.41	1.33
6	L	102	VAL	N-CA	-6.04	1.38	1.46
9	b	267	ASN	N-CA	-6.04	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	182	GLU	CA-CB	6.03	1.62	1.53
4	B	302	ARG	C-N	6.03	1.41	1.33
8	P	326	SER	CA-C	-6.03	1.45	1.52
1	M	115	PRO	CA-C	-6.03	1.48	1.53
3	E	409	SER	N-CA	-6.03	1.38	1.46
4	B	39	VAL	CA-CB	-6.03	1.47	1.54
4	B	483	GLU	C-N	6.03	1.41	1.33
9	b	135	LYS	CA-C	-6.03	1.45	1.52
11	V	153	ARG	NE-CZ	6.03	1.39	1.33
4	F	381	ARG	CZ-NH2	6.03	1.41	1.33
4	B	252	ARG	CD-NE	6.02	1.54	1.46
9	b	113	ASN	CA-C	-6.02	1.44	1.52
9	b	144	ILE	CA-C	-6.02	1.45	1.52
9	b	313	VAL	CA-C	-6.02	1.45	1.52
3	A	53	HIS	N-CA	-6.02	1.38	1.46
5	Q	171	GLU	CA-C	-6.02	1.46	1.53
4	F	257	ARG	CA-CB	6.02	1.62	1.53
5	Q	327	ALA	CA-C	-6.02	1.44	1.52
4	F	438	LYS	C-N	6.01	1.41	1.33
3	A	141	PHE	N-CA	-6.01	1.38	1.46
10	O	124	ASP	CA-CB	6.01	1.63	1.53
7	G	140	LYS	CA-C	-6.01	1.45	1.52
7	I	215	LEU	N-CA	-6.01	1.40	1.46
3	A	543	THR	N-CA	-6.01	1.39	1.46
4	F	261	THR	CA-C	-6.01	1.45	1.52
4	B	90	LYS	CA-C	-6.01	1.44	1.52
7	G	65	LYS	CA-C	-6.01	1.45	1.52
11	R	124	ARG	NE-CZ	6.01	1.39	1.33
7	G	118	LYS	N-CA	-6.01	1.41	1.46
3	E	293	VAL	C-N	6.01	1.41	1.33
11	U	74	VAL	C-N	6.01	1.41	1.33
3	A	106	ASP	N-CA	-6.00	1.39	1.45
5	Q	27	ASN	CA-CB	6.00	1.62	1.53
8	P	229	ARG	CZ-NH1	6.00	1.41	1.32
7	I	209	LEU	N-CA	-6.00	1.39	1.46
8	P	402	LEU	CA-CB	6.00	1.62	1.53
9	b	120	ARG	C-N	6.00	1.42	1.33
6	J	36	LYS	CA-CB	6.00	1.62	1.53
4	D	272	ARG	CZ-NH2	6.00	1.41	1.33
4	F	370	TYR	CA-CB	6.00	1.63	1.53
3	E	309	GLU	CA-CB	6.00	1.57	1.52
4	F	375	VAL	CA-C	-6.00	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	O	71	VAL	N-CA	-6.00	1.39	1.46
11	Y	64	ALA	C-N	5.99	1.41	1.33
4	D	215	MET	CA-C	-5.99	1.45	1.52
3	A	182	ILE	N-CA	-5.99	1.39	1.46
8	P	195	VAL	C-O	-5.99	1.16	1.24
10	O	160	ALA	C-N	5.99	1.41	1.33
11	a	106	PHE	N-CA	-5.99	1.39	1.46
4	B	116	SER	C-N	5.99	1.42	1.33
11	Y	54	ILE	C-N	5.98	1.40	1.33
4	F	244	LEU	N-CA	-5.98	1.38	1.45
5	Q	143	THR	CA-CB	-5.98	1.45	1.54
9	b	235	ALA	N-CA	-5.98	1.38	1.46
1	M	52	ASP	CA-C	-5.98	1.45	1.52
11	Z	86	THR	N-CA	-5.98	1.39	1.46
5	Q	240	ASP	CA-CB	5.98	1.63	1.53
1	M	178	ILE	CA-C	5.97	1.58	1.52
7	K	154	ASP	CA-C	-5.97	1.45	1.52
11	a	133	LEU	CA-C	-5.97	1.45	1.52
3	E	41	ILE	C-N	5.97	1.41	1.33
8	P	280	ILE	C-N	5.97	1.41	1.33
8	P	407	ARG	CD-NE	5.97	1.54	1.46
7	G	30	GLU	N-CA	-5.97	1.39	1.46
4	D	170	ILE	N-CA	-5.97	1.40	1.46
8	P	264	VAL	C-O	-5.97	1.17	1.24
8	P	336	ARG	CA-CB	5.97	1.62	1.53
3	E	370	ARG	CZ-NH2	5.96	1.41	1.33
6	L	34	GLN	C-O	-5.96	1.17	1.24
11	X	150	LEU	CA-CB	5.96	1.62	1.53
11	S	99	LEU	C-N	5.96	1.42	1.33
11	T	65	ILE	C-N	5.96	1.42	1.33
4	F	442	THR	C-N	5.96	1.41	1.33
7	I	208	LYS	N-CA	5.96	1.53	1.46
11	U	124	ARG	CA-CB	5.96	1.64	1.53
3	E	339	LEU	CA-C	-5.96	1.45	1.52
4	D	407	TYR	CA-CB	5.96	1.63	1.53
4	B	364	LEU	C-N	5.96	1.41	1.33
3	E	40	MET	CA-C	-5.96	1.45	1.52
4	F	59	ASP	N-CA	-5.95	1.38	1.46
3	A	158	TYR	C-N	5.95	1.39	1.33
5	Q	79	GLU	CA-C	-5.95	1.44	1.52
11	X	98	GLY	CA-C	-5.95	1.45	1.52
3	C	169	SER	CA-C	-5.95	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	201	HIS	ND1-CE1	5.95	1.38	1.32
5	Q	264	GLY	C-N	5.95	1.41	1.33
7	K	152	MET	C-N	5.95	1.41	1.33
8	P	470	GLN	C-N	5.95	1.41	1.33
4	D	261	THR	N-CA	-5.95	1.39	1.46
3	E	161	VAL	C-N	5.95	1.41	1.33
6	L	14	GLU	CA-CB	5.95	1.62	1.53
8	P	459	SER	C-N	5.94	1.42	1.33
4	D	63	ARG	CD-NE	5.94	1.54	1.46
7	K	29	GLU	CA-C	5.94	1.60	1.52
8	P	207	GLU	CA-C	-5.94	1.45	1.52
3	E	457	SER	N-CA	-5.94	1.39	1.46
2	N	115	LEU	N-CA	-5.94	1.38	1.46
4	B	38	LEU	N-CA	-5.94	1.38	1.46
11	X	69	VAL	C-N	5.94	1.41	1.33
11	T	83	ALA	N-CA	5.94	1.53	1.45
7	I	180	ASN	CA-C	-5.94	1.45	1.53
4	F	255	THR	CA-C	5.93	1.59	1.52
11	U	46	ARG	NE-CZ	5.93	1.39	1.33
8	P	9	ASP	C-N	5.93	1.41	1.33
8	P	141	ILE	CA-C	-5.93	1.45	1.52
11	a	149	LEU	CA-C	5.93	1.60	1.52
1	M	169	ARG	CA-CB	5.92	1.62	1.53
4	F	40	ILE	CA-C	5.92	1.60	1.52
4	D	362	ARG	CZ-NH1	5.92	1.41	1.32
11	Z	75	CYS	C-N	5.92	1.41	1.33
4	F	411	LYS	N-CA	-5.92	1.39	1.46
11	U	25	SER	N-CA	5.91	1.53	1.46
3	C	236	GLY	C-N	5.91	1.41	1.33
1	M	112	TYR	CZ-OH	5.91	1.50	1.38
3	A	329	ARG	NE-CZ	5.91	1.39	1.33
10	O	318	ARG	CD-NE	5.91	1.54	1.46
7	G	89	LEU	C-N	5.91	1.42	1.33
7	I	52	ARG	NE-CZ	5.91	1.39	1.33
8	P	12	HIS	CA-CB	5.91	1.62	1.53
10	O	91	GLU	CA-C	-5.90	1.45	1.52
3	A	525	PHE	CA-CB	5.90	1.62	1.53
5	Q	285	GLU	C-N	5.90	1.41	1.33
11	a	46	ARG	NE-CZ	5.90	1.39	1.33
11	Y	68	LEU	CA-C	-5.90	1.45	1.52
3	C	360	TRP	NE1-CE2	-5.90	1.30	1.37
4	F	277	ILE	CA-CB	-5.90	1.47	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	219	ARG	NE-CZ	5.90	1.39	1.33
11	T	45	LEU	CA-C	-5.90	1.45	1.52
4	F	101	ARG	N-CA	-5.90	1.38	1.45
3	E	610	ARG	CZ-NH1	5.89	1.41	1.32
4	D	211	VAL	CA-CB	-5.89	1.47	1.54
8	P	340	SER	C-N	5.89	1.41	1.33
8	P	305	HIS	ND1-CE1	5.89	1.38	1.32
10	O	369	THR	C-N	5.89	1.41	1.33
1	M	180	ARG	NE-CZ	5.89	1.39	1.33
3	C	352	MET	CA-C	-5.89	1.45	1.52
4	F	363	GLN	C-N	5.89	1.41	1.33
3	E	126	ARG	CZ-NH2	5.88	1.41	1.33
3	A	599	GLU	CA-CB	5.88	1.62	1.53
6	L	104	LYS	C-N	5.88	1.41	1.33
3	A	591	ARG	NE-CZ	5.88	1.39	1.33
8	P	403	GLN	CA-CB	5.88	1.62	1.53
10	O	330	ILE	CA-C	-5.88	1.45	1.52
3	C	34	VAL	CA-CB	-5.88	1.47	1.54
7	I	188	VAL	N-CA	-5.88	1.40	1.46
1	M	42	ARG	NE-CZ	5.88	1.39	1.33
3	E	288	ASN	CA-C	5.88	1.60	1.52
4	F	129	GLU	C-N	5.88	1.41	1.33
11	R	117	ARG	CD-NE	5.88	1.54	1.46
3	A	275	SER	CA-C	-5.88	1.45	1.52
10	O	155	ALA	N-CA	-5.88	1.38	1.46
11	a	92	GLY	CA-C	-5.88	1.44	1.52
4	F	435	PHE	N-CA	-5.88	1.39	1.46
3	E	196	LYS	C-O	-5.87	1.16	1.23
2	N	84	PHE	N-CA	5.87	1.53	1.46
3	C	142	THR	CA-C	-5.87	1.46	1.52
3	E	166	LEU	N-CA	-5.87	1.38	1.46
11	U	99	LEU	N-CA	-5.87	1.38	1.46
4	B	170	ILE	N-CA	-5.87	1.39	1.46
3	C	27	ILE	N-CA	-5.87	1.39	1.46
4	B	171	PRO	C-N	5.87	1.41	1.33
4	B	461	ALA	N-CA	-5.87	1.39	1.46
11	Z	107	ALA	C-N	5.87	1.41	1.34
3	E	62	ARG	CD-NE	5.86	1.54	1.46
4	B	452	ARG	C-N	5.86	1.41	1.33
11	R	160	CYS	CA-CB	5.86	1.65	1.53
11	S	31	GLY	C-O	-5.86	1.17	1.23
4	D	299	PRO	CA-CB	-5.86	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	430	LYS	C-N	5.86	1.41	1.33
2	N	32	THR	N-CA	-5.86	1.38	1.46
6	L	4	LYS	C-N	5.86	1.41	1.33
11	R	89	ILE	C-N	5.86	1.41	1.33
11	V	112	GLY	C-N	5.86	1.40	1.33
3	A	380	PHE	CA-CB	5.85	1.61	1.53
10	O	5	LEU	N-CA	-5.85	1.38	1.46
3	C	100	LEU	CA-C	-5.85	1.45	1.52
5	Q	26	SER	N-CA	5.85	1.52	1.45
10	O	122	LYS	N-CA	-5.85	1.38	1.46
4	D	469	PRO	C-N	5.85	1.42	1.33
6	L	24	ALA	C-N	5.85	1.41	1.33
4	D	137	SER	C-N	-5.85	1.28	1.33
4	D	357	GLN	C-N	5.85	1.40	1.33
3	C	72	VAL	CA-C	-5.84	1.45	1.52
4	D	111	ARG	NE-CZ	5.84	1.39	1.33
3	C	57	VAL	C-N	5.84	1.41	1.33
3	E	598	GLY	C-N	5.84	1.41	1.33
11	T	117	ARG	NE-CZ	5.84	1.39	1.33
5	Q	234	ASP	CA-CB	5.84	1.61	1.53
9	b	96	GLY	CA-C	-5.84	1.45	1.52
10	O	326	ASN	CA-C	-5.84	1.45	1.52
4	F	359	PHE	CA-CB	5.83	1.62	1.53
4	D	106	GLU	N-CA	-5.83	1.39	1.46
11	X	133	LEU	C-N	5.83	1.40	1.34
8	P	409	GLY	C-N	5.83	1.39	1.33
11	a	102	LEU	C-N	5.83	1.41	1.33
3	E	486	LYS	C-N	5.83	1.41	1.33
8	P	106	SER	C-N	5.83	1.41	1.33
3	A	482	ARG	CZ-NH1	5.82	1.41	1.32
6	L	88	GLU	CA-C	-5.82	1.44	1.52
11	R	13	GLY	C-O	5.82	1.31	1.23
3	C	456	THR	N-CA	-5.82	1.38	1.46
3	E	482	ARG	CA-C	-5.82	1.45	1.52
4	F	346	ILE	C-O	-5.82	1.19	1.24
1	M	83	VAL	C-N	5.82	1.41	1.33
3	A	542	LYS	CA-C	-5.82	1.45	1.52
6	H	27	TYR	N-CA	-5.82	1.39	1.46
4	F	79	VAL	CA-C	-5.82	1.46	1.52
3	A	349	ASN	C-N	5.82	1.41	1.33
4	B	273	HIS	CG-CD2	-5.82	1.29	1.35
6	J	35	ALA	C-N	5.82	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	106	PHE	N-CA	-5.82	1.39	1.46
4	D	295	ARG	NE-CZ	5.82	1.39	1.33
4	D	435	PHE	CA-CB	5.82	1.62	1.53
7	K	198	GLU	CA-C	-5.82	1.45	1.52
1	M	164	LYS	CA-C	-5.81	1.45	1.52
3	C	413	VAL	CA-CB	-5.81	1.46	1.54
3	C	448	ARG	CA-C	5.81	1.60	1.52
4	F	132	LEU	CA-C	-5.81	1.45	1.52
3	C	330	GLU	CA-C	5.81	1.60	1.52
3	C	340	ALA	C-N	5.81	1.41	1.33
4	B	350	THR	N-CA	-5.81	1.39	1.46
9	b	31	TYR	CA-C	-5.81	1.45	1.52
8	P	277	LEU	N-CA	-5.81	1.39	1.46
5	Q	84	ARG	CD-NE	5.81	1.54	1.46
4	F	240	LEU	CA-C	-5.81	1.45	1.52
3	E	504	LYS	N-CA	-5.80	1.39	1.46
7	I	139	VAL	CA-C	-5.80	1.45	1.52
11	V	145	ILE	CA-C	5.80	1.60	1.52
11	W	100	SER	CA-C	-5.80	1.45	1.52
3	E	277	ALA	CA-C	-5.79	1.45	1.52
3	A	414	ALA	CA-C	5.79	1.59	1.52
10	O	286	VAL	N-CA	-5.79	1.39	1.46
3	C	518	ALA	CA-C	-5.79	1.45	1.52
9	b	198	THR	CA-CB	5.79	1.62	1.53
11	a	63	ILE	CA-C	-5.79	1.45	1.52
10	O	372	HIS	C-N	5.79	1.40	1.33
2	N	80	ARG	CD-NE	5.79	1.54	1.46
3	C	213	HIS	CA-C	-5.79	1.45	1.52
4	F	240	LEU	CA-CB	5.79	1.62	1.53
3	A	127	GLY	C-N	5.78	1.41	1.33
4	B	475	ARG	CZ-NH1	5.78	1.40	1.32
4	F	418	ALA	CA-C	-5.78	1.45	1.52
4	F	475	ARG	CZ-NH1	5.78	1.40	1.32
11	W	130	ILE	C-N	5.78	1.41	1.33
1	M	183	ASN	C-N	5.78	1.41	1.33
5	Q	2	GLU	CA-C	-5.78	1.45	1.52
9	b	29	SER	C-N	5.78	1.41	1.33
3	A	419	ALA	C-N	5.78	1.41	1.33
7	I	149	ILE	C-N	5.77	1.41	1.33
3	E	286	ARG	N-CA	-5.77	1.39	1.46
6	H	15	LYS	CA-C	5.77	1.60	1.52
3	C	464	THR	CA-C	-5.77	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	17	LEU	N-CA	-5.77	1.39	1.46
11	V	79	GLY	CA-C	-5.77	1.43	1.51
3	C	62	ARG	NE-CZ	5.77	1.39	1.33
3	A	412	ILE	CA-C	-5.77	1.45	1.52
7	G	98	GLY	C-N	5.77	1.41	1.33
4	D	274	VAL	N-CA	-5.77	1.39	1.46
3	A	224	THR	N-CA	-5.77	1.39	1.46
4	D	140	ASN	CA-C	5.76	1.60	1.52
3	E	323	ASN	C-N	5.76	1.41	1.33
4	B	361	ASP	C-N	5.76	1.41	1.33
5	Q	171	GLU	CA-CB	5.76	1.62	1.53
10	O	11	PHE	CA-C	-5.76	1.45	1.52
11	Y	27	GLY	N-CA	5.76	1.52	1.45
1	M	169	ARG	CZ-NH1	5.76	1.40	1.32
2	N	61	ARG	NE-CZ	5.76	1.39	1.33
9	b	332	ARG	N-CA	-5.76	1.39	1.46
7	G	173	VAL	C-N	5.76	1.40	1.33
7	I	59	ASP	CA-C	-5.76	1.45	1.52
7	K	192	ASN	CA-C	-5.76	1.45	1.52
5	Q	53	ASN	CA-C	-5.75	1.45	1.52
8	P	199	TYR	CA-CB	5.75	1.62	1.53
9	b	142	ARG	C-N	5.75	1.41	1.33
11	R	103	ALA	C-N	5.75	1.41	1.33
11	S	66	TYR	CA-C	-5.75	1.45	1.52
4	D	463	SER	C-N	5.75	1.41	1.33
3	A	376	ALA	C-N	5.75	1.41	1.33
9	b	82	LYS	CA-CB	5.75	1.61	1.53
8	P	330	TYR	CA-C	-5.75	1.46	1.52
11	S	46	ARG	CZ-NH2	5.75	1.41	1.33
3	C	314	ARG	CZ-NH1	5.75	1.40	1.32
3	A	48	LEU	CA-CB	5.74	1.62	1.53
4	F	471	GLU	CA-C	-5.74	1.44	1.52
5	Q	312	TRP	CA-C	-5.74	1.45	1.52
4	D	248	PRO	CA-C	-5.74	1.46	1.52
8	P	17	ARG	CZ-NH2	5.74	1.41	1.33
8	P	345	ILE	C-N	5.74	1.41	1.33
3	E	69	THR	CB-OG1	-5.74	1.34	1.43
7	K	120	ILE	CA-CB	-5.74	1.47	1.54
11	X	110	ILE	CA-C	-5.74	1.46	1.52
3	E	145	LYS	CA-C	-5.73	1.45	1.52
4	F	309	TYR	CA-CB	5.73	1.62	1.53
11	Z	128	GLY	CA-C	-5.73	1.44	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	W	109	GLY	C-N	5.73	1.40	1.33
2	N	63	ASP	CA-CB	5.73	1.62	1.53
5	Q	311	ALA	N-CA	-5.73	1.39	1.46
11	T	24	THR	CA-C	-5.73	1.45	1.52
3	A	221	ARG	CZ-NH1	5.73	1.40	1.32
4	B	391	MET	C-N	5.73	1.40	1.33
9	b	274	LEU	C-N	5.73	1.41	1.33
10	O	120	LYS	CA-C	-5.73	1.45	1.52
5	Q	332	GLN	N-CA	-5.73	1.39	1.46
11	W	73	LEU	CA-C	-5.73	1.45	1.52
9	b	218	ILE	CA-CB	-5.73	1.47	1.54
4	D	193	LEU	CA-CB	5.72	1.63	1.53
4	F	400	SER	CA-C	-5.72	1.45	1.52
6	H	71	LYS	N-CA	-5.72	1.38	1.46
4	D	146	TYR	CA-CB	5.72	1.61	1.53
10	O	301	ILE	CB-CG1	5.72	1.64	1.53
4	B	63	ARG	NE-CZ	5.72	1.39	1.33
11	V	146	VAL	C-N	5.71	1.41	1.33
3	E	591	ARG	NE-CZ	5.71	1.39	1.33
11	U	75	CYS	CA-CB	5.71	1.62	1.53
3	C	248	GLN	C-N	5.71	1.40	1.33
4	F	413	ALA	C-N	5.71	1.41	1.33
3	C	459	SER	C-N	5.71	1.40	1.33
3	A	579	HIS	CA-C	-5.71	1.45	1.52
4	F	357	GLN	N-CA	-5.71	1.38	1.46
4	F	131	TYR	CA-CB	5.71	1.62	1.53
7	K	50	ILE	C-N	5.70	1.41	1.33
11	R	88	PHE	C-N	5.70	1.41	1.33
7	G	102	GLU	N-CA	-5.70	1.39	1.46
3	E	125	PRO	CA-C	-5.70	1.46	1.52
5	Q	153	LEU	C-N	5.70	1.41	1.33
7	K	53	ASN	C-O	5.70	1.30	1.24
8	P	111	ASP	C-N	5.70	1.41	1.33
8	P	276	LYS	C-N	5.70	1.41	1.33
8	P	282	ILE	C-N	5.70	1.41	1.33
8	P	343	LYS	N-CA	-5.70	1.39	1.46
10	O	7	THR	N-CA	-5.70	1.38	1.46
3	C	554	HIS	CA-CB	5.70	1.62	1.53
11	a	153	ARG	C-N	5.70	1.41	1.33
11	T	132	ILE	CA-CB	-5.70	1.47	1.54
3	C	484	ARG	CD-NE	5.70	1.54	1.46
3	A	224	THR	C-N	5.70	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	62	SER	C-N	5.69	1.41	1.33
8	P	286	VAL	C-N	5.69	1.41	1.33
4	B	66	GLN	C-N	5.69	1.40	1.33
11	a	93	ALA	N-CA	-5.69	1.39	1.46
4	F	470	LYS	CA-CB	5.69	1.62	1.53
4	B	195	ARG	C-N	-5.69	1.27	1.34
3	A	431	THR	C-N	5.69	1.41	1.34
5	Q	180	ILE	N-CA	-5.69	1.40	1.46
8	P	36	LEU	N-CA	-5.69	1.39	1.46
3	A	62	ARG	NE-CZ	5.69	1.39	1.33
1	M	100	ASN	C-N	5.68	1.40	1.33
3	A	170	HIS	CE1-NE2	-5.68	1.26	1.32
4	B	57	LEU	CA-C	-5.68	1.45	1.52
11	T	40	CYS	N-CA	-5.68	1.39	1.46
4	F	86	ILE	N-CA	-5.68	1.40	1.46
4	F	114	ASP	N-CA	-5.68	1.38	1.45
7	K	144	ARG	CZ-NH1	5.68	1.40	1.32
7	G	46	GLU	N-CA	-5.68	1.39	1.46
3	C	143	PRO	CA-C	5.67	1.59	1.52
3	E	590	SER	N-CA	-5.67	1.38	1.46
4	D	206	GLU	CA-C	-5.67	1.45	1.52
1	M	19	LYS	CA-CB	5.67	1.62	1.53
11	a	35	SER	CA-CB	5.67	1.62	1.53
4	F	76	ILE	CA-C	5.67	1.59	1.52
4	F	246	ASN	CA-CB	5.67	1.62	1.54
3	A	317	LEU	CA-C	-5.67	1.45	1.52
7	I	92	ARG	CA-CB	5.67	1.62	1.53
3	C	217	VAL	CA-CB	-5.67	1.47	1.54
3	C	304	MET	C-N	5.66	1.41	1.33
6	J	18	HIS	CA-CB	5.66	1.62	1.53
3	C	241	ASP	CA-CB	5.66	1.62	1.53
4	B	408	ALA	C-N	5.66	1.41	1.33
4	D	361	ASP	CA-CB	5.66	1.61	1.53
3	E	96	LEU	CA-C	-5.66	1.46	1.52
4	F	311	ASP	CA-C	-5.66	1.45	1.52
4	B	362	ARG	CZ-NH1	5.66	1.40	1.32
11	a	76	TYR	C-O	-5.66	1.17	1.24
4	F	34	VAL	N-CA	-5.65	1.39	1.46
7	G	80	ILE	CA-C	-5.65	1.46	1.52
11	V	126	PHE	CA-CB	5.65	1.62	1.53
3	A	400	ALA	C-N	5.65	1.41	1.33
11	V	90	GLN	C-N	5.65	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	59	GLU	N-CA	-5.65	1.38	1.45
9	b	81	ILE	C-N	5.65	1.41	1.33
7	I	160	TYR	CA-C	-5.65	1.45	1.52
9	b	305	GLU	CA-CB	5.65	1.62	1.53
8	P	136	PHE	C-N	5.65	1.41	1.33
9	b	359	ARG	CA-CB	5.65	1.60	1.53
11	a	86	THR	C-N	5.65	1.41	1.33
11	R	85	TYR	C-N	5.65	1.41	1.33
4	F	445	THR	N-CA	-5.64	1.39	1.46
8	P	362	GLU	CA-C	-5.64	1.45	1.52
3	E	517	VAL	C-N	5.64	1.41	1.34
11	a	126	PHE	CA-CB	5.64	1.62	1.53
2	N	54	PHE	CA-C	-5.64	1.45	1.52
3	C	125	PRO	C-N	5.64	1.40	1.33
3	C	467	LEU	N-CA	-5.64	1.39	1.46
5	Q	321	ARG	N-CA	-5.64	1.39	1.46
7	G	184	VAL	CA-CB	-5.64	1.46	1.55
7	G	25	ARG	NE-CZ	5.64	1.39	1.33
4	F	364	LEU	CA-C	-5.63	1.45	1.52
4	F	405	ALA	C-N	5.63	1.41	1.33
10	O	150	ALA	CA-CB	5.63	1.62	1.53
4	D	88	VAL	CA-CB	-5.63	1.48	1.54
11	X	134	ILE	CA-CB	5.63	1.64	1.54
11	V	51	PHE	CA-C	-5.63	1.45	1.52
3	E	314	ARG	NE-CZ	5.63	1.39	1.33
3	A	400	ALA	CA-CB	5.63	1.62	1.53
7	I	172	ILE	CA-CB	-5.63	1.47	1.54
4	F	95	PHE	C-N	5.63	1.42	1.33
9	b	359	ARG	N-CA	-5.63	1.39	1.46
7	G	153	LYS	CA-C	-5.63	1.45	1.52
11	Z	70	VAL	N-CA	-5.63	1.40	1.46
11	Y	114	ALA	N-CA	-5.63	1.39	1.46
1	M	91	ARG	C-N	5.63	1.41	1.33
3	C	184	TRP	CA-C	-5.63	1.46	1.52
5	Q	181	ARG	CD-NE	5.63	1.54	1.46
2	N	99	HIS	ND1-CE1	5.62	1.38	1.32
3	E	224	THR	C-N	5.62	1.40	1.33
4	D	96	THR	C-N	5.62	1.42	1.33
11	a	155	THR	C-N	5.62	1.41	1.33
11	Z	57	VAL	CA-CB	-5.62	1.47	1.54
3	C	532	SER	C-N	5.62	1.42	1.33
7	I	183	LEU	N-CA	-5.62	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	81	TYR	C-N	5.62	1.41	1.33
7	G	219	ARG	CZ-NH1	5.62	1.40	1.32
3	E	208	ASP	N-CA	-5.61	1.38	1.45
8	P	453	LEU	CA-CB	5.61	1.63	1.53
3	C	484	ARG	CZ-NH2	5.61	1.40	1.33
7	I	154	ASP	N-CA	-5.61	1.39	1.46
4	D	318	ARG	CD-NE	5.61	1.54	1.46
4	B	48	ARG	NE-CZ	5.61	1.39	1.33
4	F	165	ALA	C-N	5.61	1.41	1.33
3	A	438	PHE	CA-C	-5.61	1.45	1.52
6	H	31	LYS	C-N	5.60	1.41	1.33
11	X	136	ALA	C-N	5.60	1.41	1.33
1	M	111	SER	N-CA	-5.60	1.38	1.46
4	F	362	ARG	CA-C	-5.60	1.45	1.52
5	Q	89	GLY	N-CA	-5.60	1.35	1.45
2	N	102	ASP	N-CA	-5.60	1.39	1.46
3	C	429	THR	C-O	-5.60	1.17	1.24
3	A	500	GLN	CA-CB	5.60	1.62	1.53
11	T	58	ILE	C-N	5.60	1.41	1.33
3	A	520	LEU	C-N	5.60	1.41	1.33
4	D	166	ARG	CZ-NH2	5.60	1.40	1.33
4	D	189	ARG	CA-C	-5.60	1.45	1.52
6	H	47	LYS	CA-C	-5.60	1.46	1.52
3	A	161	VAL	C-N	5.59	1.41	1.33
11	T	90	GLN	CA-CB	5.59	1.62	1.53
4	F	136	GLY	C-N	5.59	1.41	1.33
6	L	43	ILE	N-CA	-5.59	1.39	1.46
7	I	14	ASN	CG-ND2	5.59	1.45	1.33
3	C	276	ASP	CA-C	-5.59	1.45	1.52
3	E	596	VAL	CA-CB	-5.59	1.47	1.54
3	A	152	ILE	N-CA	-5.59	1.40	1.46
4	B	118	ARG	C-N	-5.59	1.27	1.33
9	b	241	HIS	CG-CD2	5.59	1.42	1.35
11	R	38	GLY	N-CA	-5.59	1.39	1.45
11	Z	75	CYS	CA-CB	5.59	1.62	1.53
9	b	189	GLY	CA-C	-5.59	1.44	1.51
7	I	127	GLU	CA-CB	5.58	1.62	1.53
11	S	85	TYR	CA-C	5.58	1.60	1.52
11	T	43	CYS	N-CA	5.58	1.53	1.46
3	E	527	GLN	CA-C	-5.58	1.45	1.52
8	P	85	SER	CA-CB	5.58	1.62	1.53
11	X	122	GLN	CA-CB	5.58	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	V	13	GLY	C-N	5.58	1.41	1.34
11	Z	89	ILE	N-CA	-5.58	1.39	1.46
4	F	265	TYR	C-N	5.58	1.41	1.33
4	F	417	LYS	CA-CB	5.58	1.62	1.53
5	Q	32	ASN	CA-CB	5.58	1.62	1.53
3	E	35	VAL	N-CA	-5.58	1.39	1.46
6	L	80	LEU	CA-C	-5.58	1.44	1.52
7	I	206	ARG	CD-NE	5.58	1.54	1.46
1	M	64	ALA	CA-C	-5.57	1.45	1.52
7	G	205	GLU	CA-C	-5.57	1.45	1.52
11	T	152	SER	N-CA	5.57	1.53	1.46
7	K	14	ASN	CA-C	-5.57	1.45	1.52
9	b	53	ARG	CZ-NH1	5.57	1.40	1.32
3	C	548	ARG	CZ-NH1	5.57	1.40	1.32
3	E	126	ARG	CD-NE	5.57	1.54	1.46
3	A	218	ARG	CZ-NH1	5.57	1.40	1.32
4	B	149	GLU	CA-C	-5.57	1.46	1.52
11	W	76	TYR	CA-CB	5.57	1.61	1.53
11	U	147	ALA	C-O	-5.57	1.17	1.24
3	A	244	PHE	C-N	-5.56	1.26	1.33
11	V	117	ARG	CD-NE	5.56	1.54	1.46
3	E	351	SER	CA-C	-5.56	1.45	1.52
3	A	121	SER	CA-CB	-5.56	1.45	1.52
9	b	182	ALA	CA-C	-5.56	1.46	1.53
11	Y	126	PHE	C-N	5.56	1.40	1.34
3	E	221	ARG	CA-C	-5.56	1.46	1.53
5	Q	315	SER	C-N	5.56	1.41	1.34
11	V	56	PRO	C-N	5.56	1.40	1.33
8	P	85	SER	N-CA	-5.56	1.39	1.46
3	A	162	PHE	CA-C	-5.55	1.45	1.52
6	L	57	PHE	CA-CB	5.55	1.62	1.53
7	K	128	ALA	CA-C	-5.55	1.45	1.52
8	P	470	GLN	N-CA	5.55	1.53	1.46
3	C	606	THR	N-CA	-5.55	1.39	1.46
3	E	370	ARG	NE-CZ	5.55	1.39	1.33
3	A	539	PRO	CA-C	-5.55	1.46	1.53
3	E	101	MET	CA-C	-5.55	1.45	1.52
3	A	562	ALA	C-O	-5.55	1.17	1.24
8	P	267	TYR	CA-CB	5.55	1.61	1.53
11	U	120	SER	N-CA	-5.55	1.39	1.46
4	B	42	GLU	CA-C	-5.55	1.46	1.52
5	Q	136	LEU	N-CA	5.55	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	64	SER	N-CA	-5.55	1.39	1.46
3	A	436	GLN	N-CA	-5.54	1.38	1.45
11	Z	111	VAL	CA-C	-5.54	1.45	1.52
2	N	80	ARG	C-N	5.54	1.40	1.33
3	E	409	SER	CA-C	-5.54	1.45	1.52
3	A	294	LEU	CA-C	-5.54	1.45	1.52
4	B	392	THR	C-N	5.54	1.40	1.33
11	a	84	LEU	C-N	5.54	1.41	1.33
8	P	436	GLU	C-N	-5.54	1.26	1.33
10	O	384	PRO	CA-C	-5.54	1.44	1.52
11	Y	137	GLU	C-N	5.54	1.40	1.33
1	M	207	GLN	CA-C	-5.54	1.45	1.52
9	b	248	ARG	C-N	5.54	1.40	1.33
7	G	82	ASN	CA-CB	5.54	1.62	1.53
3	E	481	LEU	CB-CG	5.54	1.64	1.53
10	O	122	LYS	CA-C	-5.54	1.45	1.52
2	N	37	PHE	N-CA	-5.54	1.39	1.45
11	R	97	VAL	C-O	-5.54	1.17	1.24
1	M	91	ARG	CA-CB	5.53	1.62	1.53
3	A	205	LYS	N-CA	5.53	1.53	1.46
4	B	118	ARG	NE-CZ	5.53	1.39	1.33
9	b	39	VAL	CA-C	-5.53	1.46	1.52
7	G	117	TYR	CA-CB	5.53	1.62	1.53
11	T	56	PRO	C-N	5.53	1.40	1.33
3	C	180	GLY	N-CA	-5.53	1.38	1.45
3	A	39	ASN	CA-C	-5.53	1.45	1.52
7	K	67	LYS	CA-C	-5.53	1.45	1.52
7	K	118	LYS	CA-CB	5.53	1.60	1.53
7	G	158	ARG	CZ-NH2	5.53	1.40	1.33
11	S	157	ASP	C-N	5.53	1.41	1.33
3	C	449	LYS	C-N	5.53	1.41	1.33
7	I	108	SER	CA-C	-5.53	1.45	1.52
3	C	423	PHE	N-CA	-5.53	1.40	1.46
3	A	264	VAL	C-N	5.53	1.40	1.33
8	P	412	ASN	CA-CB	5.53	1.62	1.53
11	V	58	ILE	N-CA	5.53	1.53	1.46
4	F	135	ASN	C-N	5.52	1.40	1.33
8	P	246	SER	N-CA	-5.52	1.39	1.46
11	V	115	GLY	CA-C	-5.52	1.44	1.51
4	B	320	GLY	CA-C	-5.52	1.44	1.51
6	J	26	LYS	CA-C	-5.52	1.45	1.52
1	M	175	HIS	CD2-NE2	5.52	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	420	VAL	CA-C	-5.52	1.45	1.52
4	D	362	ARG	CA-C	-5.52	1.45	1.52
4	B	82	GLY	CA-C	-5.52	1.44	1.51
8	P	292	SER	CA-CB	5.52	1.61	1.53
11	Y	95	LEU	C-O	-5.52	1.17	1.24
9	b	101	PRO	C-N	-5.52	1.28	1.34
1	M	195	LEU	C-O	-5.51	1.17	1.24
4	D	396	HIS	CA-C	-5.51	1.45	1.52
6	L	34	GLN	N-CA	-5.51	1.39	1.46
10	O	321	LEU	CA-CB	5.51	1.62	1.53
11	S	92	GLY	C-N	5.51	1.41	1.33
3	A	80	THR	N-CA	-5.51	1.39	1.45
11	Z	98	GLY	C-N	5.51	1.42	1.33
3	C	329	ARG	NE-CZ	5.51	1.39	1.33
3	C	562	ALA	C-N	5.51	1.42	1.33
4	F	408	ALA	CA-CB	5.51	1.61	1.53
5	Q	205	LYS	CA-C	-5.51	1.46	1.52
11	Z	147	ALA	C-N	5.51	1.40	1.33
11	V	143	GLY	C-N	5.51	1.40	1.33
4	B	298	VAL	N-CA	-5.51	1.41	1.46
11	R	58	ILE	CA-CB	-5.51	1.47	1.54
4	F	257	ARG	CZ-NH1	5.50	1.40	1.32
4	F	424	ALA	C-N	5.50	1.41	1.33
8	P	16	ILE	CA-C	5.50	1.59	1.52
8	P	181	ASP	CA-C	-5.50	1.45	1.52
8	P	259	PHE	CA-C	-5.50	1.45	1.52
3	C	579	HIS	N-CA	-5.50	1.39	1.46
6	J	104	LYS	CA-C	-5.50	1.45	1.52
11	T	16	GLY	N-CA	5.50	1.52	1.45
1	M	141	ARG	CZ-NH2	5.50	1.40	1.33
3	A	424	SER	CA-C	-5.50	1.45	1.52
9	b	190	VAL	CA-C	-5.50	1.46	1.52
3	A	411	SER	C-N	5.49	1.40	1.33
9	b	327	ASN	C-N	5.49	1.41	1.34
11	a	150	LEU	C-N	5.49	1.40	1.33
4	D	158	ILE	C-O	-5.49	1.18	1.24
4	D	413	ALA	CA-C	-5.49	1.45	1.52
11	T	26	LEU	N-CA	5.49	1.53	1.46
8	P	154	GLY	C-N	5.49	1.40	1.33
4	F	44	VAL	N-CA	-5.49	1.38	1.46
7	K	182	ASP	C-N	5.49	1.40	1.33
11	V	17	CYS	C-N	5.49	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	W	48	ASP	CA-C	-5.49	1.45	1.52
11	V	118	GLY	CA-C	-5.49	1.46	1.52
4	B	237	ARG	NE-CZ	5.48	1.39	1.33
7	G	20	MET	N-CA	-5.48	1.39	1.46
7	I	95	SER	N-CA	-5.48	1.39	1.46
3	E	476	PRO	CA-C	-5.48	1.46	1.52
7	K	188	VAL	N-CA	-5.48	1.40	1.46
6	J	54	LEU	CA-C	-5.48	1.45	1.52
3	C	344	ARG	N-CA	5.48	1.53	1.46
4	F	269	GLN	N-CA	5.48	1.53	1.46
8	P	239	GLY	CA-C	-5.48	1.46	1.52
8	P	283	LYS	CA-C	-5.48	1.45	1.52
9	b	252	ILE	C-N	5.48	1.40	1.33
6	H	52	LYS	CA-CB	5.48	1.61	1.53
6	L	28	ARG	CD-NE	5.48	1.53	1.46
4	F	398	ASP	CA-C	-5.47	1.45	1.52
4	B	475	ARG	C-N	5.47	1.40	1.33
11	S	116	VAL	CA-C	-5.47	1.45	1.53
11	V	50	LEU	N-CA	5.47	1.52	1.46
3	C	607	MET	N-CA	5.47	1.52	1.46
9	b	34	GLY	CA-C	-5.47	1.45	1.51
11	Y	34	LYS	C-N	5.47	1.40	1.33
4	D	304	TYR	CA-CB	5.47	1.62	1.52
4	F	462	TRP	CA-C	-5.47	1.45	1.52
3	A	559	LYS	CA-CB	5.47	1.61	1.53
10	O	184	PHE	CA-CB	5.47	1.63	1.53
5	Q	107	VAL	N-CA	-5.47	1.40	1.46
11	T	26	LEU	C-N	5.47	1.40	1.33
4	D	71	ARG	CD-NE	5.46	1.53	1.46
3	E	355	ASP	N-CA	-5.46	1.39	1.46
3	A	569	LYS	CA-C	-5.46	1.45	1.52
6	L	64	GLY	CA-C	-5.46	1.44	1.51
10	O	167	THR	C-N	5.46	1.38	1.33
6	H	3	GLN	N-CA	-5.46	1.39	1.46
11	R	96	SER	CA-CB	5.46	1.61	1.53
7	K	76	THR	CB-OG1	-5.46	1.35	1.43
11	Z	20	ALA	CA-C	-5.46	1.45	1.52
3	C	151	HIS	CG-ND1	-5.46	1.32	1.38
4	D	353	ILE	CA-C	-5.46	1.45	1.52
3	E	586	PHE	CA-CB	5.46	1.60	1.53
1	M	90	ALA	CA-C	-5.46	1.46	1.52
4	F	184	ALA	CA-CB	5.46	1.61	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	O	361	LYS	CA-CB	5.46	1.62	1.53
6	H	28	ARG	NE-CZ	5.46	1.39	1.33
3	E	241	ASP	C-N	5.46	1.40	1.33
3	A	247	VAL	C-N	5.46	1.41	1.33
4	F	147	PRO	CA-C	-5.45	1.46	1.52
10	O	204	SER	N-CA	5.45	1.53	1.46
11	a	12	PHE	C-N	5.45	1.40	1.33
7	K	191	SER	CA-C	-5.45	1.45	1.52
4	D	287	ALA	C-N	5.45	1.41	1.33
1	M	202	ARG	CZ-NH2	5.44	1.40	1.33
4	B	118	ARG	N-CA	-5.44	1.40	1.46
4	F	184	ALA	C-N	5.44	1.40	1.33
3	A	448	ARG	CD-NE	5.44	1.53	1.46
4	B	452	ARG	CZ-NH2	5.44	1.40	1.33
7	K	16	GLU	C-N	5.44	1.40	1.33
8	P	219	GLN	CA-CB	5.44	1.61	1.53
3	E	168	SER	CA-C	-5.44	1.45	1.52
3	C	417	SER	C-N	5.44	1.40	1.33
3	E	138	LYS	CA-CB	5.44	1.61	1.53
5	Q	335	ARG	CD-NE	5.44	1.53	1.46
3	C	182	ILE	CA-C	-5.44	1.46	1.52
11	X	79	GLY	N-CA	5.44	1.49	1.44
6	J	73	GLU	N-CA	-5.43	1.39	1.46
4	D	48	ARG	CD-NE	5.43	1.53	1.46
4	D	74	ARG	NE-CZ	5.43	1.39	1.33
3	E	450	HIS	ND1-CE1	5.43	1.38	1.32
7	G	91	ALA	N-CA	-5.43	1.39	1.46
4	D	255	THR	CA-C	5.43	1.58	1.52
7	I	190	VAL	C-N	5.43	1.40	1.33
4	D	337	MET	CA-C	5.43	1.59	1.52
7	K	85	ARG	NE-CZ	5.43	1.39	1.33
11	Y	35	SER	CA-CB	5.43	1.61	1.53
4	D	237	ARG	CZ-NH2	5.42	1.40	1.33
4	F	407	TYR	C-N	5.42	1.40	1.33
11	Z	76	TYR	CA-C	-5.42	1.45	1.52
3	C	280	TYR	C-N	5.42	1.40	1.33
3	C	53	HIS	ND1-CE1	5.42	1.38	1.32
7	I	78	SER	C-N	5.42	1.41	1.33
3	C	311	ILE	N-CA	-5.42	1.39	1.46
4	D	320	GLY	N-CA	-5.42	1.39	1.45
7	I	221	GLU	CA-C	-5.42	1.45	1.52
4	D	278	LEU	N-CA	-5.42	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	472	ASP	C-N	5.42	1.40	1.33
7	K	151	SER	CA-CB	5.42	1.61	1.53
11	T	52	LYS	CA-CB	5.42	1.61	1.53
3	C	314	ARG	CD-NE	5.41	1.53	1.46
3	A	211	LEU	CA-C	-5.41	1.45	1.52
8	P	167	ASN	N-CA	-5.41	1.39	1.46
10	O	140	GLN	CA-C	-5.41	1.45	1.52
4	F	295	ARG	N-CA	5.41	1.52	1.45
6	L	101	THR	CA-C	5.41	1.59	1.52
11	R	106	PHE	CA-CB	5.41	1.61	1.53
5	Q	272	VAL	N-CA	5.41	1.53	1.46
10	O	124	ASP	C-N	5.41	1.40	1.33
7	G	85	ARG	CZ-NH2	5.41	1.40	1.33
6	J	38	ASP	C-N	5.41	1.41	1.33
11	R	61	GLY	N-CA	-5.41	1.38	1.45
4	F	214	ALA	CA-C	-5.41	1.46	1.52
4	B	450	GLU	C-N	5.41	1.40	1.33
6	L	98	LEU	CA-CB	5.41	1.61	1.53
7	I	206	ARG	CA-C	-5.41	1.45	1.52
7	K	188	VAL	C-N	5.41	1.40	1.33
11	T	62	ILE	CA-CB	5.41	1.61	1.54
4	D	327	GLY	CA-C	-5.41	1.45	1.51
3	E	140	GLN	N-CA	-5.41	1.39	1.46
3	A	226	LYS	CA-CB	5.41	1.61	1.53
4	B	446	GLN	CA-C	-5.41	1.45	1.52
4	B	245	ALA	C-N	5.40	1.41	1.34
2	N	109	LEU	C-N	5.40	1.40	1.33
3	C	79	LEU	N-CA	-5.40	1.39	1.46
7	K	36	GLN	C-N	5.40	1.41	1.33
11	X	44	VAL	C-N	5.40	1.41	1.33
11	S	149	LEU	CA-CB	5.40	1.61	1.53
11	a	90	GLN	CA-CB	5.40	1.61	1.53
3	C	498	VAL	C-O	-5.40	1.17	1.24
4	D	49	TYR	CA-C	-5.40	1.45	1.52
10	O	8	ALA	CA-CB	5.40	1.60	1.53
11	X	122	GLN	CA-C	-5.40	1.46	1.52
11	W	120	SER	CA-C	-5.40	1.45	1.52
4	D	282	SER	C-N	5.39	1.41	1.33
4	D	287	ALA	CA-CB	5.39	1.61	1.53
3	A	192	THR	CA-CB	-5.39	1.45	1.53
11	T	79	GLY	C-N	5.39	1.42	1.33
1	M	82	GLN	C-O	-5.39	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	O	66	GLU	CA-C	-5.39	1.46	1.52
11	R	12	PHE	N-CA	5.39	1.53	1.46
3	C	557	ALA	N-CA	-5.39	1.40	1.46
8	P	476	THR	C-N	5.39	1.40	1.33
2	N	78	ARG	NE-CZ	5.39	1.39	1.33
11	Z	46	ARG	CD-NE	5.39	1.53	1.46
3	C	315	THR	CA-C	-5.39	1.46	1.52
4	D	98	GLU	C-N	5.39	1.40	1.33
4	B	282	SER	N-CA	5.39	1.53	1.46
5	Q	328	GLU	N-CA	-5.38	1.39	1.46
11	Z	104	ALA	N-CA	5.38	1.52	1.46
11	S	83	ALA	CA-C	-5.38	1.46	1.52
11	W	69	VAL	CA-C	-5.38	1.46	1.52
8	P	476	THR	N-CA	5.38	1.52	1.46
11	Y	148	LEU	CA-CB	5.38	1.61	1.53
3	E	610	ARG	CA-CB	5.38	1.61	1.53
10	O	281	GLU	CA-CB	5.38	1.61	1.53
7	I	168	PRO	CA-CB	5.38	1.61	1.53
2	N	64	ILE	N-CA	-5.37	1.39	1.46
3	A	297	PHE	CA-C	5.37	1.59	1.52
4	B	128	ALA	CA-C	-5.37	1.45	1.52
6	H	26	LYS	N-CA	-5.37	1.39	1.46
6	L	31	LYS	C-N	5.37	1.41	1.33
4	B	69	GLU	CA-C	-5.37	1.45	1.52
2	N	99	HIS	CD2-NE2	5.37	1.43	1.37
3	E	128	ILE	CA-CB	-5.37	1.47	1.54
11	Z	35	SER	N-CA	5.37	1.52	1.46
11	Z	88	PHE	C-N	5.37	1.40	1.33
3	C	362	GLU	C-O	-5.36	1.17	1.24
11	U	53	ASN	CA-C	-5.36	1.45	1.52
11	U	71	SER	C-N	5.36	1.40	1.34
11	S	18	ALA	N-CA	-5.36	1.40	1.46
3	E	374	MET	C-N	5.36	1.40	1.33
4	F	105	SER	CA-C	-5.36	1.46	1.52
10	O	298	ASP	N-CA	-5.36	1.39	1.46
7	I	45	ILE	N-CA	-5.36	1.40	1.46
7	I	186	GLY	CA-C	-5.36	1.45	1.51
6	J	18	HIS	C-N	5.36	1.41	1.33
3	E	174	LEU	CA-C	5.36	1.59	1.52
4	F	48	ARG	NE-CZ	5.36	1.39	1.33
5	Q	24	LEU	C-O	-5.36	1.17	1.23
5	Q	185	TYR	C-N	5.36	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	255	HIS	ND1-CE1	5.36	1.38	1.32
9	b	332	ARG	C-N	5.36	1.40	1.33
10	O	317	LEU	N-CA	-5.36	1.39	1.46
3	C	578	LYS	N-CA	-5.36	1.39	1.46
10	O	125	LYS	C-N	5.36	1.40	1.33
4	B	283	SER	CA-C	-5.35	1.45	1.52
2	N	78	ARG	CZ-NH1	5.35	1.40	1.32
4	F	484	PHE	N-CA	-5.35	1.39	1.46
4	B	125	LYS	C-N	5.35	1.40	1.33
4	B	316	TYR	CA-C	5.35	1.59	1.52
8	P	333	GLU	CA-C	-5.35	1.45	1.52
3	E	130	THR	CA-CB	5.35	1.60	1.53
7	K	76	THR	N-CA	-5.35	1.39	1.46
8	P	389	LYS	CA-CB	5.35	1.62	1.53
3	A	244	PHE	N-CA	-5.35	1.38	1.46
8	P	208	LYS	CA-C	-5.35	1.45	1.52
11	Z	123	PRO	C-O	5.35	1.31	1.24
11	W	157	ASP	CA-CB	5.35	1.62	1.53
11	U	84	LEU	C-N	5.35	1.41	1.34
11	X	121	GLN	N-CA	-5.35	1.39	1.46
11	X	26	LEU	CA-C	-5.34	1.45	1.52
4	D	434	GLU	C-N	5.34	1.41	1.33
5	Q	38	THR	CA-C	-5.34	1.45	1.52
5	Q	327	ALA	C-N	5.34	1.41	1.33
8	P	288	ARG	CD-NE	5.34	1.53	1.46
10	O	358	LYS	CA-CB	5.34	1.64	1.53
11	X	59	MET	CA-CB	5.34	1.61	1.53
11	W	110	ILE	C-N	5.34	1.40	1.33
3	C	526	LEU	CB-CG	5.34	1.64	1.53
8	P	108	LYS	N-CA	-5.34	1.39	1.46
9	b	72	PHE	C-N	5.34	1.40	1.33
11	U	94	GLY	C-N	5.34	1.40	1.33
7	G	109	GLY	C-N	5.34	1.40	1.33
11	R	74	VAL	C-O	-5.34	1.18	1.24
3	A	215	TRP	CZ2-CH2	5.33	1.47	1.37
5	Q	84	ARG	CZ-NH2	5.33	1.40	1.33
3	C	504	LYS	C-N	5.33	1.41	1.33
3	A	176	PRO	CA-C	-5.33	1.45	1.52
8	P	251	TRP	CA-C	-5.33	1.45	1.52
10	O	332	VAL	C-N	5.33	1.39	1.33
11	R	11	PHE	C-N	5.33	1.41	1.33
4	B	285	ALA	C-N	5.33	1.41	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	256	LEU	N-CA	-5.33	1.39	1.46
10	O	246	PHE	C-N	5.33	1.40	1.33
3	C	397	LYS	C-N	5.33	1.40	1.33
3	A	185	ILE	CA-CB	5.33	1.60	1.54
3	A	550	PHE	CA-CB	5.33	1.61	1.53
4	B	313	SER	CA-CB	5.33	1.61	1.53
3	A	554	HIS	N-CA	-5.32	1.40	1.46
4	B	208	PHE	CA-C	-5.32	1.46	1.52
11	Y	79	GLY	C-O	-5.32	1.19	1.24
4	D	195	ARG	CA-CB	5.32	1.61	1.53
3	E	29	SER	CA-C	-5.32	1.45	1.52
3	E	115	ILE	CA-CB	5.32	1.61	1.54
9	b	31	TYR	CA-CB	5.32	1.61	1.53
11	W	31	GLY	CA-C	5.32	1.58	1.51
3	C	179	ARG	NE-CZ	5.32	1.39	1.33
4	F	426	SER	C-N	5.32	1.40	1.33
7	I	143	GLU	C-N	5.32	1.41	1.33
1	M	171	ASN	N-CA	-5.32	1.40	1.46
9	b	69	TYR	C-N	5.32	1.41	1.33
7	G	71	LEU	CA-C	-5.32	1.45	1.52
11	a	84	LEU	CA-CB	5.32	1.61	1.53
11	Y	105	GLY	C-N	5.32	1.41	1.33
4	B	344	HIS	CG-ND1	-5.32	1.32	1.38
11	R	92	GLY	CA-C	-5.32	1.45	1.52
11	W	143	GLY	N-CA	5.32	1.52	1.45
10	O	357	MET	C-N	5.31	1.41	1.33
11	X	138	VAL	N-CA	-5.31	1.40	1.46
8	P	384	ILE	N-CA	5.31	1.52	1.46
3	C	290	MET	CA-C	-5.31	1.46	1.52
3	C	396	GLY	CA-C	-5.31	1.46	1.51
4	F	424	ALA	CA-CB	-5.31	1.44	1.53
3	A	68	ALA	CA-C	-5.31	1.46	1.52
3	E	68	ALA	C-N	5.31	1.40	1.33
4	F	302	ARG	NE-CZ	5.31	1.38	1.33
3	A	280	TYR	CA-C	-5.31	1.46	1.52
6	H	9	THR	CA-C	5.31	1.59	1.52
6	H	93	ASP	CA-CB	-5.31	1.44	1.53
3	C	524	ASP	N-CA	-5.31	1.40	1.46
3	E	177	ARG	CA-C	-5.31	1.45	1.53
8	P	347	GLU	C-N	5.31	1.40	1.33
2	N	91	ILE	CA-CB	-5.31	1.47	1.54
8	P	263	LEU	CA-C	-5.30	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	V	72	VAL	C-N	5.30	1.40	1.33
3	E	510	SER	C-O	-5.30	1.18	1.24
1	M	108	GLN	CA-C	-5.30	1.46	1.52
3	A	315	THR	CA-CB	-5.30	1.44	1.53
5	Q	245	ILE	N-CA	-5.30	1.39	1.46
9	b	146	GLN	CA-C	5.30	1.59	1.52
6	J	3	GLN	N-CA	-5.30	1.40	1.46
7	I	179	LEU	N-CA	-5.30	1.39	1.45
10	O	253	LYS	C-N	5.30	1.41	1.33
4	D	242	LEU	N-CA	-5.30	1.39	1.46
10	O	159	LEU	CA-CB	5.30	1.61	1.53
4	D	462	TRP	CA-CB	5.30	1.61	1.53
3	A	289	GLU	N-CA	5.30	1.52	1.46
4	B	275	LEU	CA-C	-5.30	1.46	1.52
3	C	186	ALA	CA-C	-5.29	1.47	1.53
3	A	26	ALA	N-CA	-5.29	1.39	1.46
3	A	91	PRO	N-CA	-5.29	1.40	1.47
3	A	414	ALA	N-CA	5.29	1.52	1.46
9	b	216	VAL	C-N	5.29	1.41	1.33
3	E	448	ARG	CD-NE	5.29	1.53	1.46
4	F	127	PHE	C-N	5.29	1.40	1.33
3	A	302	THR	C-N	5.29	1.41	1.33
3	A	346	GLN	C-N	5.29	1.40	1.33
1	M	187	TYR	CZ-OH	5.29	1.49	1.38
10	O	304	PHE	CA-C	5.29	1.59	1.52
5	Q	58	VAL	CA-CB	5.29	1.61	1.54
8	P	17	ARG	C-N	5.29	1.40	1.33
10	O	85	ILE	CA-C	5.29	1.59	1.52
3	C	442	ASP	N-CA	-5.29	1.39	1.46
7	I	52	ARG	CZ-NH1	5.29	1.40	1.32
11	Y	54	ILE	N-CA	-5.29	1.39	1.46
11	S	73	LEU	N-CA	5.28	1.52	1.46
4	D	311	ASP	CA-C	-5.28	1.46	1.52
4	B	159	ASP	CA-CB	5.28	1.61	1.53
5	Q	25	LEU	CB-CG	5.28	1.64	1.53
11	a	46	ARG	CD-NE	5.28	1.53	1.46
4	F	113	PHE	C-N	5.28	1.40	1.33
5	Q	59	SER	CA-C	-5.28	1.46	1.52
8	P	137	GLN	CA-C	5.28	1.59	1.52
3	E	87	ARG	CZ-NH1	5.28	1.40	1.32
11	R	149	LEU	CA-C	-5.28	1.46	1.52
3	C	370	ARG	CD-NE	5.28	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	145	ILE	CA-C	-5.28	1.45	1.52
7	I	97	ASP	N-CA	-5.28	1.38	1.46
11	Y	126	PHE	C-O	-5.28	1.17	1.24
4	B	459	ASP	N-CA	-5.28	1.39	1.46
8	P	323	GLN	C-N	5.28	1.40	1.33
11	Z	80	GLN	CA-CB	5.28	1.61	1.53
4	D	391	MET	C-N	5.27	1.40	1.33
3	E	339	LEU	CA-CB	5.27	1.61	1.53
7	K	156	ILE	C-N	5.27	1.41	1.34
11	R	147	ALA	CA-C	-5.27	1.46	1.52
2	N	101	TYR	CB-CG	5.27	1.63	1.51
5	Q	315	SER	CA-CB	5.27	1.61	1.53
8	P	203	ILE	C-N	5.27	1.41	1.34
3	A	561	VAL	C-N	5.27	1.40	1.33
4	D	301	ARG	NE-CZ	5.27	1.38	1.33
4	D	325	ARG	CA-C	5.27	1.59	1.52
3	A	530	GLY	CA-C	-5.27	1.44	1.52
3	C	316	THR	N-CA	-5.27	1.39	1.46
3	C	525	PHE	CA-CB	5.27	1.62	1.53
4	B	29	ASN	C-N	5.27	1.40	1.33
10	O	251	ARG	C-N	5.27	1.40	1.33
6	L	105	PRO	CA-C	5.27	1.59	1.52
3	C	291	ALA	N-CA	-5.26	1.39	1.46
4	D	344	HIS	ND1-CE1	5.26	1.37	1.32
11	V	48	ASP	CA-CB	5.26	1.62	1.53
1	M	27	GLN	C-N	5.26	1.40	1.33
3	C	455	ASN	CA-C	-5.26	1.46	1.52
4	F	111	ARG	NE-CZ	5.26	1.38	1.33
4	D	83	THR	N-CA	-5.26	1.39	1.46
4	D	361	ASP	CA-C	-5.26	1.46	1.52
3	C	83	ASP	N-CA	5.26	1.53	1.45
4	D	67	VAL	CA-C	5.26	1.58	1.52
5	Q	217	ASP	CA-CB	5.26	1.61	1.53
8	P	413	ALA	CA-C	-5.26	1.46	1.52
3	C	334	TYR	CA-C	-5.25	1.46	1.52
9	b	38	LEU	N-CA	-5.25	1.39	1.46
3	E	458	VAL	N-CA	-5.25	1.39	1.46
3	A	307	THR	C-O	-5.25	1.17	1.24
5	Q	13	ILE	CA-CB	-5.25	1.47	1.54
5	Q	18	ARG	CD-NE	5.25	1.53	1.46
4	B	95	PHE	N-CA	5.25	1.52	1.46
7	K	126	VAL	CA-C	-5.25	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	137	GLU	C-N	5.25	1.40	1.34
10	O	112	GLU	CA-C	-5.25	1.45	1.52
4	D	396	HIS	CG-CD2	5.25	1.41	1.35
4	B	397	GLY	CA-C	-5.25	1.45	1.51
3	A	395	ALA	C-N	5.25	1.39	1.32
3	A	395	ALA	CA-C	-5.25	1.45	1.52
4	B	244	LEU	CA-CB	5.25	1.61	1.53
11	a	45	LEU	CB-CG	5.25	1.64	1.53
11	V	46	ARG	CD-NE	5.25	1.53	1.46
11	R	129	MET	C-N	5.25	1.40	1.33
8	P	310	LYS	N-CA	5.24	1.52	1.46
10	O	318	ARG	CZ-NH1	5.24	1.40	1.32
11	X	96	SER	C-N	5.24	1.40	1.33
5	Q	41	ASP	CA-C	-5.24	1.46	1.52
7	K	147	ASP	C-N	5.24	1.41	1.33
8	P	376	ASP	CA-C	5.24	1.59	1.52
4	D	388	GLY	CA-C	-5.24	1.44	1.51
11	a	29	ALA	C-N	5.24	1.40	1.33
11	a	59	MET	CA-C	5.24	1.59	1.52
5	Q	286	ASP	C-N	5.24	1.41	1.33
7	G	11	ASN	CA-C	-5.24	1.46	1.52
9	b	70	ARG	CD-NE	5.24	1.53	1.46
10	O	70	LYS	CA-CB	5.24	1.61	1.53
11	a	81	LYS	CA-C	-5.24	1.46	1.52
3	E	194	ASP	CA-C	-5.24	1.45	1.52
4	B	131	TYR	CA-CB	5.24	1.61	1.53
8	P	80	LEU	C-O	-5.24	1.17	1.24
10	O	88	GLY	CA-C	-5.24	1.46	1.52
11	a	104	ALA	CA-CB	5.24	1.61	1.53
11	R	23	PHE	CB-CG	5.24	1.62	1.50
3	A	514	THR	N-CA	5.23	1.52	1.46
3	C	177	ARG	N-CA	-5.23	1.39	1.46
7	K	132	LEU	CA-C	-5.23	1.48	1.53
7	I	214	ALA	CA-C	-5.23	1.46	1.52
3	E	318	VAL	CA-C	5.23	1.59	1.52
9	b	359	ARG	CZ-NH2	5.23	1.40	1.33
7	G	25	ARG	CZ-NH1	5.23	1.40	1.32
11	R	44	VAL	CA-C	-5.23	1.46	1.53
11	X	18	ALA	CA-C	-5.23	1.46	1.52
11	R	102	LEU	C-N	5.23	1.41	1.33
11	Y	50	LEU	C-N	5.23	1.40	1.33
3	C	574	THR	CA-C	5.23	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	359	ARG	CZ-NH1	5.22	1.40	1.32
3	A	425	ASP	N-CA	-5.22	1.38	1.45
4	B	127	PHE	CA-C	5.22	1.59	1.52
5	Q	21	ARG	N-CA	-5.22	1.40	1.46
7	K	80	ILE	CB-CG1	5.22	1.63	1.53
11	Z	79	GLY	CA-C	-5.22	1.44	1.52
3	C	426	PRO	N-CD	5.22	1.55	1.47
3	E	359	ARG	NE-CZ	5.22	1.38	1.33
8	P	180	MET	C-N	5.22	1.40	1.33
7	I	210	LEU	CA-CB	5.22	1.61	1.53
4	B	134	ILE	CA-C	-5.22	1.45	1.52
7	I	56	ASN	CA-C	5.22	1.59	1.52
4	F	232	ASN	C-O	-5.22	1.17	1.24
5	Q	149	TYR	N-CA	-5.22	1.40	1.46
11	X	21	ILE	CA-C	-5.22	1.46	1.52
3	A	225	GLU	CA-C	-5.22	1.45	1.52
11	U	72	VAL	C-N	5.22	1.40	1.33
3	E	218	ARG	CZ-NH1	5.21	1.40	1.32
4	B	353	ILE	C-N	5.21	1.40	1.33
8	P	44	ALA	CA-C	5.21	1.59	1.52
11	Z	81	LYS	N-CA	-5.21	1.39	1.46
4	D	218	ASN	CA-C	-5.21	1.45	1.53
3	A	493	GLU	CA-CB	5.21	1.61	1.53
8	P	34	GLU	CA-C	-5.21	1.45	1.52
7	I	106	LYS	CA-C	-5.21	1.46	1.52
11	S	39	ILE	C-N	5.21	1.40	1.33
3	C	515	LEU	CA-CB	5.21	1.61	1.53
9	b	122	ILE	CA-CB	-5.21	1.47	1.54
7	G	59	ASP	CA-CB	5.21	1.61	1.53
4	F	266	LEU	CA-C	-5.21	1.46	1.52
8	P	4	THR	C-N	5.21	1.41	1.33
4	F	121	ASP	N-CA	-5.21	1.39	1.46
3	A	130	THR	CA-C	5.21	1.58	1.52
11	W	85	TYR	N-CA	5.21	1.52	1.46
4	F	224	PHE	CA-CB	5.21	1.61	1.53
4	B	51	GLU	C-N	5.21	1.40	1.33
9	b	121	LEU	CA-C	-5.21	1.46	1.52
4	D	458	LEU	N-CA	-5.20	1.40	1.46
3	E	319	ALA	N-CA	-5.20	1.40	1.46
10	O	135	SER	C-N	5.20	1.40	1.33
6	H	35	ALA	CA-C	-5.20	1.46	1.52
3	E	614	SER	CA-C	-5.20	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	122	ILE	C-O	-5.20	1.17	1.24
3	A	303	GLU	C-N	5.20	1.41	1.33
4	B	346	ILE	C-N	5.20	1.41	1.34
5	Q	118	ARG	NE-CZ	5.20	1.38	1.33
2	N	28	ILE	CA-C	5.20	1.59	1.52
3	C	86	LEU	CA-C	-5.20	1.46	1.52
3	C	275	SER	C-N	5.20	1.40	1.33
7	G	132	LEU	C-N	5.20	1.40	1.33
3	C	550	PHE	CA-CB	5.20	1.61	1.53
4	D	207	ASN	C-N	5.20	1.41	1.33
4	F	47	PRO	CA-CB	5.20	1.60	1.53
11	R	118	GLY	C-N	5.20	1.40	1.33
11	a	104	ALA	N-CA	-5.19	1.40	1.46
4	D	154	GLY	CA-C	-5.19	1.44	1.51
7	K	34	GLU	CA-C	5.19	1.59	1.52
1	M	90	ALA	N-CA	-5.19	1.40	1.46
3	C	392	TYR	CZ-OH	5.19	1.49	1.38
3	E	160	SER	CA-CB	5.19	1.62	1.53
3	E	549	ALA	N-CA	-5.19	1.40	1.46
7	K	148	LEU	C-N	5.19	1.40	1.33
9	b	84	TYR	CA-CB	5.19	1.61	1.53
11	R	12	PHE	C-N	5.19	1.40	1.33
11	Y	156	GLN	CA-C	-5.19	1.45	1.52
3	C	429	THR	CA-C	5.18	1.59	1.52
3	C	135	ARG	CZ-NH1	5.18	1.40	1.32
4	D	63	ARG	NE-CZ	5.18	1.38	1.33
7	K	92	ARG	C-N	5.18	1.41	1.33
8	P	175	GLN	C-N	5.18	1.40	1.33
11	X	153	ARG	CA-CB	5.18	1.61	1.53
5	Q	156	THR	CA-CB	5.18	1.61	1.53
6	L	53	GLU	CA-CB	5.18	1.62	1.53
10	O	7	THR	CA-CB	5.18	1.62	1.53
11	U	46	ARG	CA-C	-5.18	1.47	1.53
1	M	139	TYR	C-N	5.18	1.40	1.33
4	D	335	LEU	C-O	-5.18	1.17	1.24
3	E	481	LEU	CA-C	-5.18	1.45	1.52
11	S	94	GLY	CA-C	-5.18	1.46	1.52
1	M	211	GLN	CA-C	5.17	1.59	1.52
3	C	27	ILE	C-O	-5.17	1.19	1.24
3	C	597	HIS	CA-C	-5.17	1.46	1.52
4	F	460	GLN	N-CA	-5.17	1.40	1.46
9	b	300	TYR	N-CA	5.17	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	14	ASN	C-O	-5.17	1.17	1.24
5	Q	72	ALA	C-O	5.17	1.30	1.24
11	S	93	ALA	N-CA	-5.17	1.40	1.46
7	I	27	GLU	CA-C	-5.17	1.45	1.52
3	E	560	ALA	CA-C	-5.17	1.46	1.52
3	A	234	LEU	CA-C	-5.17	1.46	1.52
10	O	42	ARG	C-N	5.17	1.40	1.33
7	I	53	ASN	CA-CB	5.17	1.61	1.53
11	Y	78	LEU	C-N	5.17	1.40	1.33
5	Q	337	ARG	NE-CZ	5.16	1.38	1.33
10	O	365	ASN	N-CA	-5.16	1.39	1.46
6	L	84	LYS	CA-CB	5.16	1.62	1.53
7	K	8	LEU	N-CA	5.16	1.56	1.46
7	K	144	ARG	CA-C	-5.16	1.45	1.52
11	a	118	GLY	C-N	5.16	1.40	1.33
11	W	115	GLY	C-N	5.16	1.40	1.33
4	B	201	HIS	CB-CG	-5.16	1.43	1.50
6	J	97	ILE	CA-C	-5.16	1.46	1.52
4	F	365	HIS	CG-ND1	5.16	1.44	1.38
3	A	450	HIS	CE1-NE2	-5.16	1.27	1.32
7	K	206	ARG	CZ-NH1	5.16	1.40	1.32
11	Z	89	ILE	CA-CB	-5.16	1.47	1.54
5	Q	194	ASN	C-O	-5.15	1.18	1.24
8	P	194	ALA	N-CA	5.15	1.52	1.46
11	W	18	ALA	CA-C	-5.15	1.46	1.52
3	E	191	TYR	CA-CB	5.15	1.63	1.54
3	E	509	ASP	CA-C	-5.15	1.45	1.52
7	G	48	THR	CA-C	-5.15	1.46	1.52
3	C	177	ARG	CA-CB	5.15	1.61	1.53
4	D	362	ARG	CD-NE	5.15	1.53	1.46
3	A	314	ARG	N-CA	-5.15	1.39	1.46
11	S	74	VAL	C-N	5.15	1.40	1.33
3	C	86	LEU	C-N	5.15	1.40	1.33
8	P	110	GLY	CA-C	5.15	1.59	1.51
4	F	393	ARG	CD-NE	5.15	1.53	1.46
6	L	27	TYR	CA-CB	5.15	1.61	1.53
4	D	218	ASN	N-CA	-5.14	1.39	1.45
3	E	194	ASP	C-N	5.14	1.40	1.33
3	A	329	ARG	N-CA	-5.14	1.40	1.46
4	B	308	MET	C-N	5.14	1.40	1.33
11	X	154	ALA	C-N	5.14	1.40	1.33
4	F	118	ARG	N-CA	-5.14	1.41	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	367	LYS	N-CA	-5.14	1.39	1.46
4	D	429	ASP	C-O	-5.14	1.17	1.24
4	F	252	ARG	CZ-NH1	5.14	1.40	1.32
3	A	148	VAL	CA-C	-5.14	1.47	1.52
6	J	14	GLU	C-N	5.14	1.41	1.33
11	T	113	ASP	CA-CB	5.14	1.61	1.53
1	M	81	TYR	CA-C	-5.14	1.46	1.52
3	C	325	PRO	N-CA	-5.14	1.41	1.47
4	D	56	THR	CA-C	-5.14	1.46	1.52
4	F	88	VAL	CA-C	-5.14	1.46	1.52
9	b	191	ILE	CA-C	-5.14	1.46	1.52
11	T	130	ILE	N-CA	-5.14	1.40	1.46
4	D	214	ALA	CA-C	-5.13	1.46	1.52
3	A	261	GLY	CA-C	-5.13	1.44	1.51
5	Q	340	ASN	N-CA	-5.13	1.40	1.46
8	P	305	HIS	CA-CB	5.13	1.61	1.53
11	X	56	PRO	C-N	5.13	1.40	1.33
11	X	148	LEU	C-N	5.13	1.40	1.33
4	D	321	ARG	CA-CB	5.13	1.61	1.53
3	A	384	LEU	CB-CG	5.13	1.63	1.53
6	L	99	ILE	C-N	5.13	1.40	1.33
9	b	332	ARG	CA-C	-5.13	1.47	1.52
11	Y	141	LEU	C-N	5.13	1.40	1.33
4	D	72	GLY	CA-C	-5.13	1.44	1.51
10	O	251	ARG	CA-CB	5.13	1.61	1.53
7	G	114	ARG	CZ-NH1	5.13	1.40	1.32
11	U	117	ARG	CZ-NH1	5.13	1.40	1.32
10	O	53	PHE	CA-C	-5.13	1.46	1.52
10	O	288	LEU	C-N	5.13	1.40	1.33
7	G	100	PHE	CA-C	-5.13	1.45	1.52
11	Y	125	LEU	C-N	5.13	1.41	1.33
1	M	158	ILE	CA-C	5.13	1.59	1.52
4	F	228	ASP	CA-C	-5.13	1.46	1.52
8	P	177	ILE	N-CA	-5.13	1.41	1.46
10	O	53	PHE	C-N	5.13	1.40	1.33
10	O	306	ILE	N-CA	-5.12	1.40	1.46
7	I	77	LYS	CA-CB	5.12	1.61	1.53
11	R	44	VAL	CA-CB	-5.12	1.47	1.54
1	M	210	LYS	C-N	5.12	1.40	1.33
4	D	244	LEU	N-CA	-5.12	1.39	1.45
3	A	338	THR	C-N	5.12	1.40	1.33
5	Q	118	ARG	CA-C	-5.12	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	267	GLN	CA-C	-5.11	1.46	1.52
4	D	131	TYR	N-CA	5.11	1.52	1.46
5	Q	105	ASP	C-N	5.11	1.40	1.33
2	N	18	THR	CA-CB	-5.11	1.45	1.53
4	D	48	ARG	CZ-NH1	5.11	1.40	1.32
4	F	400	SER	CA-CB	5.11	1.61	1.53
8	P	177	ILE	CA-CB	-5.11	1.48	1.54
11	V	49	LEU	CA-C	-5.11	1.45	1.52
3	E	357	SER	CA-C	-5.11	1.45	1.52
3	C	208	ASP	CA-CB	5.11	1.61	1.53
7	K	161	GLY	CA-C	5.11	1.58	1.51
8	P	331	SER	CA-CB	5.11	1.61	1.53
7	I	25	ARG	CZ-NH1	5.11	1.39	1.32
11	U	99	LEU	CA-CB	5.11	1.61	1.53
11	V	159	VAL	CA-CB	5.11	1.61	1.54
2	N	85	THR	CA-CB	-5.11	1.46	1.54
4	D	403	LEU	CA-C	-5.11	1.46	1.52
4	B	478	PRO	C-N	5.11	1.40	1.33
11	V	132	ILE	C-N	5.11	1.40	1.33
4	D	54	ASN	CA-C	-5.10	1.46	1.52
4	F	333	PRO	CA-CB	-5.10	1.47	1.53
11	W	27	GLY	C-N	5.10	1.40	1.33
8	P	331	SER	N-CA	-5.10	1.40	1.46
10	O	251	ARG	CZ-NH1	5.10	1.39	1.32
11	S	72	VAL	CA-CB	-5.10	1.48	1.54
2	N	22	LEU	N-CA	5.10	1.52	1.46
3	C	303	GLU	N-CA	-5.10	1.40	1.46
3	C	309	GLU	CA-CB	5.10	1.61	1.53
4	B	317	GLU	C-N	5.10	1.40	1.33
8	P	447	LYS	CA-CB	5.10	1.61	1.53
9	b	21	ILE	CB-CG1	5.10	1.63	1.53
6	J	39	ALA	C-N	5.10	1.40	1.34
7	I	15	ASP	N-CA	5.10	1.52	1.46
11	Z	46	ARG	N-CA	-5.10	1.41	1.46
11	Z	124	ARG	CA-CB	5.10	1.61	1.53
4	B	404	TYR	N-CA	-5.10	1.40	1.46
3	C	597	HIS	CA-CB	5.09	1.60	1.53
3	E	262	LYS	CA-CB	5.09	1.61	1.53
7	K	153	LYS	CA-C	-5.09	1.46	1.52
11	X	78	LEU	N-CA	-5.09	1.40	1.45
3	A	103	THR	CA-C	-5.09	1.46	1.52
4	B	220	GLU	C-N	5.09	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	138	PRO	N-CA	-5.09	1.41	1.47
3	A	392	TYR	CA-C	-5.09	1.46	1.52
8	P	320	PRO	N-CA	-5.09	1.40	1.47
8	P	328	ARG	CD-NE	5.09	1.53	1.46
7	K	59	ASP	CA-CB	5.09	1.61	1.53
7	K	183	LEU	CA-C	-5.09	1.47	1.52
1	M	65	ALA	C-N	-5.09	1.27	1.33
3	A	60	VAL	N-CA	-5.09	1.40	1.46
3	A	275	SER	N-CA	5.09	1.52	1.46
5	Q	160	PRO	C-N	5.09	1.40	1.33
7	K	206	ARG	C-N	5.09	1.40	1.33
11	W	19	SER	C-O	-5.09	1.18	1.24
3	C	97	GLY	CA-C	-5.08	1.44	1.51
5	Q	254	PHE	CA-CB	5.08	1.61	1.53
7	K	85	ARG	CZ-NH1	5.08	1.39	1.32
3	A	397	LYS	CA-CB	5.08	1.60	1.53
5	Q	197	THR	CA-CB	-5.08	1.45	1.53
9	b	293	THR	CA-C	-5.08	1.46	1.52
11	T	66	TYR	C-O	-5.08	1.18	1.24
1	M	216	LYS	C-N	5.08	1.40	1.33
3	C	544	PHE	CG-CD2	5.08	1.49	1.38
4	F	302	ARG	CA-CB	-5.08	1.45	1.53
7	I	47	LYS	CA-CB	5.08	1.61	1.53
11	Y	46	ARG	NE-CZ	5.08	1.38	1.33
1	M	183	ASN	CA-CB	5.08	1.61	1.53
3	C	278	ILE	N-CA	-5.08	1.40	1.46
4	D	393	ARG	CD-NE	5.08	1.53	1.46
4	F	244	LEU	C-N	5.08	1.40	1.33
11	R	139	LEU	C-N	5.08	1.41	1.33
4	D	412	ASP	N-CA	5.08	1.52	1.46
8	P	206	HIS	ND1-CE1	5.08	1.37	1.32
4	F	88	VAL	CA-CB	-5.08	1.49	1.55
7	K	43	TYR	CA-CB	5.08	1.61	1.53
9	b	111	VAL	CA-C	-5.08	1.46	1.52
11	S	87	GLY	C-N	5.08	1.40	1.34
3	C	570	LEU	CA-CB	5.07	1.61	1.53
4	D	117	GLY	CA-C	-5.07	1.44	1.51
5	Q	21	ARG	NE-CZ	5.07	1.38	1.33
8	P	336	ARG	CZ-NH2	5.07	1.40	1.33
6	H	82	GLU	C-N	5.07	1.40	1.33
7	G	110	ILE	CA-CB	-5.07	1.48	1.54
4	D	385	SER	N-CA	-5.07	1.41	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	V	47	PRO	CA-C	-5.07	1.47	1.52
3	A	27	ILE	CA-CB	-5.07	1.47	1.53
3	C	108	ILE	C-N	5.07	1.40	1.33
4	D	332	ILE	N-CA	-5.07	1.41	1.46
4	F	152	SER	CA-CB	5.07	1.61	1.53
11	S	101	GLY	C-N	5.07	1.40	1.33
4	D	316	TYR	N-CA	-5.06	1.39	1.46
3	C	58	GLY	CA-C	-5.06	1.46	1.51
7	G	95	SER	C-N	5.06	1.40	1.33
11	a	20	ALA	CA-C	-5.06	1.46	1.52
3	E	389	ALA	C-N	5.06	1.40	1.33
3	A	95	GLU	C-N	5.06	1.40	1.33
11	Y	140	GLY	N-CA	5.06	1.52	1.45
4	F	163	SER	CA-CB	5.06	1.60	1.53
4	B	375	VAL	N-CA	5.06	1.52	1.46
7	K	85	ARG	CZ-NH2	5.06	1.40	1.33
3	C	249	GLY	N-CA	-5.06	1.37	1.44
3	E	88	THR	CA-C	-5.06	1.45	1.52
10	O	104	ASN	C-O	5.06	1.30	1.23
10	O	151	ASN	N-CA	-5.06	1.39	1.46
11	a	63	ILE	N-CA	-5.06	1.40	1.46
2	N	101	TYR	C-N	5.05	1.39	1.33
4	D	75	ALA	C-N	5.05	1.39	1.33
4	D	219	LEU	C-N	5.05	1.40	1.33
3	E	576	ASP	CA-CB	5.05	1.61	1.53
4	B	279	THR	C-N	5.05	1.40	1.33
8	P	432	GLU	CA-C	5.05	1.59	1.52
11	U	117	ARG	CD-NE	5.05	1.53	1.46
3	A	89	GLY	CA-C	5.05	1.58	1.51
4	B	183	ILE	C-N	5.05	1.40	1.33
7	I	20	MET	CA-CB	5.05	1.61	1.53
11	Z	12	PHE	N-CA	-5.05	1.39	1.46
11	T	99	LEU	CA-C	-5.05	1.45	1.52
3	E	479	PRO	C-O	-5.05	1.17	1.24
10	O	172	VAL	CA-C	-5.05	1.46	1.52
6	J	86	ILE	N-CA	-5.05	1.39	1.46
11	a	79	GLY	CA-C	-5.05	1.46	1.52
4	D	100	LEU	CA-CB	5.05	1.61	1.53
3	E	219	VAL	CA-C	5.05	1.57	1.52
7	K	197	ILE	CA-C	5.05	1.58	1.52
9	b	24	GLU	CA-C	-5.05	1.46	1.52
9	b	283	ASP	C-N	5.05	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	267	ALA	C-N	5.05	1.40	1.33
4	D	454	VAL	CA-CB	-5.05	1.47	1.54
5	Q	98	ILE	CA-C	-5.05	1.46	1.52
11	W	119	SER	CA-C	-5.05	1.46	1.52
11	Z	107	ALA	CA-C	-5.04	1.46	1.52
4	D	334	ILE	N-CA	5.04	1.52	1.46
9	b	121	LEU	C-N	-5.04	1.27	1.33
11	U	119	SER	C-N	5.04	1.40	1.33
11	a	34	LYS	C-O	-5.04	1.18	1.24
3	C	590	SER	C-N	5.04	1.40	1.33
3	A	586	PHE	CA-CB	5.04	1.61	1.53
7	K	55	THR	C-N	5.04	1.40	1.33
8	P	11	THR	N-CA	-5.04	1.40	1.46
8	P	150	LEU	CA-C	-5.04	1.46	1.52
10	O	43	ALA	CA-C	-5.04	1.46	1.52
10	O	390	ILE	CA-CB	5.04	1.60	1.54
11	U	60	ALA	CA-CB	5.04	1.61	1.53
4	F	272	ARG	CA-C	-5.04	1.46	1.52
6	L	90	LYS	C-N	5.04	1.40	1.33
8	P	432	GLU	CA-CB	5.04	1.61	1.53
11	Y	32	THR	C-N	5.04	1.40	1.33
3	A	358	SER	C-N	5.04	1.41	1.33
5	Q	233	ILE	CA-CB	5.04	1.60	1.54
8	P	47	LEU	N-CA	-5.04	1.40	1.46
11	a	27	GLY	CA-C	-5.04	1.46	1.51
9	b	340	TRP	N-CA	-5.04	1.39	1.46
10	O	17	PRO	CA-CB	-5.04	1.46	1.53
11	W	108	ILE	C-N	5.04	1.40	1.34
4	B	195	ARG	NE-CZ	5.03	1.38	1.33
7	K	34	GLU	N-CA	-5.03	1.40	1.46
6	L	26	LYS	CA-CB	5.03	1.61	1.53
1	M	42	ARG	C-N	5.03	1.40	1.33
4	F	301	ARG	CD-NE	5.03	1.53	1.46
4	F	463	SER	C-N	5.03	1.40	1.33
7	K	223	TYR	N-CA	-5.03	1.38	1.46
10	O	371	LEU	CA-CB	5.03	1.61	1.53
4	B	466	ARG	CD-NE	5.03	1.53	1.46
7	K	88	VAL	CA-C	-5.03	1.46	1.52
8	P	323	GLN	CA-C	-5.03	1.46	1.52
5	Q	67	LEU	C-N	5.03	1.40	1.33
11	T	107	ALA	N-CA	-5.03	1.40	1.46
11	W	42	THR	C-N	5.03	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	W	153	ARG	NE-CZ	5.03	1.38	1.33
11	W	158	VAL	C-O	-5.03	1.18	1.24
3	E	261	GLY	CA-C	-5.03	1.44	1.51
11	a	143	GLY	CA-C	5.03	1.57	1.52
3	C	31	SER	CA-C	-5.02	1.47	1.53
11	Y	131	LEU	N-CA	-5.02	1.40	1.46
8	P	411	VAL	CA-C	-5.02	1.46	1.52
11	S	82	GLN	CA-C	-5.02	1.46	1.52
1	M	192	LEU	CA-CB	5.02	1.61	1.53
3	E	333	ILE	CA-CB	-5.02	1.48	1.54
3	E	430	ALA	CA-C	5.02	1.59	1.52
3	A	518	ALA	C-O	-5.02	1.18	1.24
4	B	373	ILE	C-N	5.02	1.40	1.33
11	T	116	VAL	CA-CB	-5.02	1.47	1.54
11	T	141	LEU	C-N	5.02	1.40	1.33
3	E	135	ARG	NE-CZ	5.02	1.38	1.33
4	F	438	LYS	CA-C	-5.02	1.46	1.52
11	X	87	GLY	C-N	5.02	1.40	1.34
3	A	77	ALA	CA-C	-5.02	1.46	1.52
10	O	13	LEU	N-CA	-5.02	1.40	1.46
11	S	101	GLY	CA-C	-5.02	1.46	1.51
4	D	173	PHE	CA-CB	5.01	1.60	1.53
4	D	331	GLN	C-N	5.01	1.37	1.33
3	E	238	ARG	NE-CZ	5.01	1.38	1.33
3	E	472	ASP	CA-C	-5.01	1.46	1.52
4	F	321	ARG	CA-C	-5.01	1.46	1.52
3	A	154	GLY	C-N	5.01	1.41	1.33
8	P	312	LEU	C-N	5.01	1.40	1.33
7	I	75	ILE	CA-CB	-5.01	1.48	1.54
3	E	126	ARG	NE-CZ	5.01	1.38	1.33
3	E	556	GLU	N-CA	5.01	1.52	1.46
1	M	91	ARG	NE-CZ	5.01	1.38	1.33
1	M	210	LYS	CA-CB	5.01	1.61	1.53
4	B	318	ARG	CA-C	-5.01	1.47	1.53
10	O	310	ARG	CZ-NH1	5.01	1.39	1.32
11	a	76	TYR	CA-C	-5.01	1.46	1.52
3	C	267	GLN	CA-CB	5.01	1.61	1.53
3	E	365	ARG	CZ-NH1	5.01	1.39	1.32
8	P	220	ARG	CZ-NH2	5.01	1.40	1.33
2	N	47	LYS	CA-CB	5.01	1.61	1.53
5	Q	154	VAL	C-N	5.01	1.40	1.33
11	U	107	ALA	N-CA	-5.01	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	371	LEU	N-CA	5.01	1.52	1.46
4	B	228	ASP	C-N	5.01	1.40	1.33
4	B	243	ASN	C-N	5.01	1.40	1.33
8	P	199	TYR	CA-C	-5.01	1.46	1.52
8	P	433	LEU	CB-CG	5.01	1.63	1.53
10	O	146	ARG	CZ-NH1	5.01	1.39	1.32
7	G	122	GLN	N-CA	5.01	1.52	1.46
11	Z	53	ASN	CA-C	-5.01	1.46	1.52
4	D	206	GLU	N-CA	-5.00	1.39	1.46
11	X	27	GLY	CA-C	-5.00	1.46	1.51
11	S	97	VAL	CA-CB	5.00	1.60	1.54
11	V	138	VAL	N-CA	-5.00	1.40	1.46
7	K	46	GLU	CA-C	-5.00	1.46	1.52
10	O	255	PHE	C-N	5.00	1.39	1.33
6	J	97	ILE	C-N	5.00	1.40	1.33
11	X	50	LEU	CA-C	-5.00	1.45	1.52

All (4651) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	109	PHE	CA-CB-CG	-14.01	99.80	113.80
4	F	180	HIS	CA-CB-CG	12.23	126.03	113.80
11	a	124	ARG	N-CA-C	-11.94	101.01	114.62
11	Z	46	ARG	O-C-N	-11.65	111.77	121.44
4	D	346	ILE	CA-C-O	-11.50	110.98	118.69
7	G	165	GLN	CA-C-N	11.50	137.17	120.38
7	G	165	GLN	C-N-CA	11.50	137.17	120.38
8	P	153	ASN	CA-CB-CG	-11.46	101.14	112.60
11	T	45	LEU	N-CA-C	-11.36	99.12	113.43
8	P	211	MET	CA-C-O	-11.11	107.56	118.34
11	W	12	PHE	N-CA-C	-11.05	99.91	113.50
3	C	425	ASP	CA-C-N	11.02	132.25	119.47
3	C	425	ASP	C-N-CA	11.02	132.25	119.47
10	O	331	ALA	CA-C-N	10.94	133.11	123.04
10	O	331	ALA	C-N-CA	10.94	133.11	123.04
6	H	79	GLU	N-CA-C	-10.82	98.73	112.90
4	F	156	SER	CA-C-N	10.73	134.66	120.28
4	F	156	SER	C-N-CA	10.73	134.66	120.28
3	E	290	MET	N-CA-C	-10.60	99.52	111.82
6	L	61	ASN	CA-CB-CG	-10.56	102.04	112.60
7	I	15	ASP	CA-CB-CG	-10.40	102.20	112.60
3	A	432	LEU	CA-C-N	10.36	131.44	119.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	432	LEU	C-N-CA	10.36	131.44	119.94
5	Q	332	GLN	CA-C-N	10.35	136.73	122.34
5	Q	332	GLN	C-N-CA	10.35	136.73	122.34
4	B	134	ILE	CA-CB-CG1	10.32	127.94	110.40
5	Q	191	ASP	CA-CB-CG	10.32	122.92	112.60
9	b	344	ASP	CA-CB-CG	-10.28	102.32	112.60
3	A	209	PHE	CA-CB-CG	-10.28	103.52	113.80
3	E	304	MET	N-CA-C	-10.26	99.46	112.90
11	V	126	PHE	CA-CB-CG	10.20	124.00	113.80
7	K	176	ASN	OD1-CG-ND2	10.16	132.76	122.60
10	O	183	ASP	N-CA-C	-10.16	101.95	114.75
9	b	302	ILE	N-CA-C	-10.12	103.25	113.47
7	I	165	GLN	CA-C-N	10.05	137.50	120.71
7	I	165	GLN	C-N-CA	10.05	137.50	120.71
3	A	470	PHE	CA-CB-CG	-9.98	103.82	113.80
11	V	113	ASP	CA-CB-CG	9.97	122.57	112.60
10	O	198	VAL	CA-C-N	9.96	130.04	119.78
10	O	198	VAL	C-N-CA	9.96	130.04	119.78
11	T	139	LEU	CA-C-N	9.96	130.99	119.94
11	T	139	LEU	C-N-CA	9.96	130.99	119.94
4	B	324	GLY	N-CA-C	-9.95	102.93	113.58
3	A	542	LYS	CA-C-N	9.95	133.61	120.28
3	A	542	LYS	C-N-CA	9.95	133.61	120.28
1	M	15	LEU	CA-C-O	-9.89	110.44	120.82
3	E	612	ALA	CA-C-N	9.81	133.43	120.28
3	E	612	ALA	C-N-CA	9.81	133.43	120.28
3	E	331	ALA	CA-C-N	9.80	133.77	120.54
3	E	331	ALA	C-N-CA	9.80	133.77	120.54
8	P	282	ILE	N-CA-C	-9.78	101.98	113.42
11	V	35	SER	CA-C-N	9.78	131.04	119.99
11	V	35	SER	C-N-CA	9.78	131.04	119.99
7	K	45	ILE	N-CA-C	9.76	119.79	110.42
8	P	429	HIS	CG-CD2-NE2	9.76	116.96	107.20
11	R	54	ILE	O-C-N	-9.70	112.07	121.87
7	G	53	ASN	CA-C-N	9.70	137.17	120.68
7	G	53	ASN	C-N-CA	9.70	137.17	120.68
7	I	176	ASN	CA-CB-CG	-9.68	102.92	112.60
3	C	468	ASN	CA-CB-CG	9.68	122.28	112.60
3	A	66	ASP	CA-CB-CG	-9.63	102.97	112.60
10	O	62	ILE	CA-C-N	9.63	133.66	120.46
10	O	62	ILE	C-N-CA	9.63	133.66	120.46
11	U	90	GLN	CA-C-N	9.60	133.50	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	U	90	GLN	C-N-CA	9.60	133.50	120.54
6	H	29	GLN	CA-C-N	9.57	132.88	120.44
6	H	29	GLN	C-N-CA	9.57	132.88	120.44
8	P	143	GLY	CA-C-N	9.56	133.44	120.54
8	P	143	GLY	C-N-CA	9.56	133.44	120.54
11	Y	132	ILE	O-C-N	9.52	131.24	121.91
11	S	69	VAL	CA-C-N	9.51	133.23	120.77
11	S	69	VAL	C-N-CA	9.51	133.23	120.77
11	a	37	VAL	CA-C-N	9.49	130.44	120.00
11	a	37	VAL	C-N-CA	9.49	130.44	120.00
4	B	462	TRP	CA-C-N	9.46	132.96	120.28
4	B	462	TRP	C-N-CA	9.46	132.96	120.28
11	a	95	LEU	CA-C-N	9.45	133.30	120.54
11	a	95	LEU	C-N-CA	9.45	133.30	120.54
8	P	8	MET	N-CA-C	-9.40	103.90	114.62
4	F	111	ARG	NE-CZ-NH2	9.39	127.65	119.20
4	F	179	PRO	CA-C-N	9.39	133.80	120.28
4	F	179	PRO	C-N-CA	9.39	133.80	120.28
10	O	322	PRO	CA-C-N	9.38	129.59	119.28
10	O	322	PRO	C-N-CA	9.38	129.59	119.28
3	E	453	SER	CA-C-N	9.37	134.37	120.69
3	E	453	SER	C-N-CA	9.37	134.37	120.69
11	a	129	MET	CA-C-N	9.35	132.66	120.60
11	a	129	MET	C-N-CA	9.35	132.66	120.60
10	O	349	GLY	CA-C-N	9.31	133.68	120.28
10	O	349	GLY	C-N-CA	9.31	133.68	120.28
11	X	15	ILE	CA-C-N	9.28	130.48	119.99
11	X	15	ILE	C-N-CA	9.28	130.48	119.99
11	U	11	PHE	CA-CB-CG	9.25	123.05	113.80
8	P	82	HIS	CA-CB-CG	-9.23	104.56	113.80
7	I	91	ALA	CA-C-N	9.23	132.65	120.28
7	I	91	ALA	C-N-CA	9.23	132.65	120.28
7	K	112	ASN	CA-CB-CG	-9.22	103.38	112.60
3	C	434	ILE	CA-C-N	9.21	134.65	120.75
3	C	434	ILE	C-N-CA	9.21	134.65	120.75
1	M	178	ILE	CA-C-O	-9.21	112.52	118.69
4	D	74	ARG	N-CA-CB	9.20	126.03	110.49
8	P	434	LEU	CA-C-N	9.19	128.93	119.64
8	P	434	LEU	C-N-CA	9.19	128.93	119.64
9	b	45	ASN	N-CA-C	-9.19	95.36	109.24
7	I	154	ASP	CA-C-N	9.18	132.58	120.28
7	I	154	ASP	C-N-CA	9.18	132.58	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	b	291	THR	CA-C-N	9.17	133.31	120.29
9	b	291	THR	C-N-CA	9.17	133.31	120.29
8	P	12	HIS	CE1-NE2-CD2	-9.16	99.84	109.00
11	W	93	ALA	CA-C-N	9.16	130.14	119.98
11	W	93	ALA	C-N-CA	9.16	130.14	119.98
3	C	377	ASP	CA-C-N	9.15	137.42	123.05
3	C	377	ASP	C-N-CA	9.15	137.42	123.05
5	Q	172	LEU	N-CA-C	-9.15	101.04	113.30
11	S	24	THR	CA-C-N	9.13	132.31	120.44
11	S	24	THR	C-N-CA	9.13	132.31	120.44
4	D	453	THR	N-CA-C	-9.11	96.57	109.69
3	E	185	ILE	CA-C-O	9.10	130.27	120.53
7	K	210	LEU	CA-C-N	9.10	132.47	120.28
7	K	210	LEU	C-N-CA	9.10	132.47	120.28
11	S	52	LYS	CA-C-N	9.10	132.27	120.44
11	S	52	LYS	C-N-CA	9.10	132.27	120.44
4	F	158	ILE	CA-C-N	9.10	132.26	120.44
4	F	158	ILE	C-N-CA	9.10	132.26	120.44
11	U	52	LYS	CA-C-N	9.07	132.79	120.54
11	U	52	LYS	C-N-CA	9.07	132.79	120.54
7	I	213	GLU	N-CA-C	-9.05	102.39	113.97
3	E	194	ASP	N-CA-C	-9.04	101.22	112.88
4	F	344	HIS	CA-C-O	-9.04	111.33	120.64
6	J	93	ASP	CA-CB-CG	-9.02	103.58	112.60
7	K	100	PHE	CA-CB-CG	-9.01	104.79	113.80
4	B	120	ILE	N-CA-C	-9.01	103.61	112.17
4	D	114	ASP	CA-CB-CG	-9.00	103.60	112.60
9	b	355	GLU	N-CA-C	-9.00	100.06	112.30
3	E	278	ILE	CB-CA-C	9.00	123.47	110.33
8	P	26	ALA	CA-C-N	9.00	132.34	120.28
8	P	26	ALA	C-N-CA	9.00	132.34	120.28
11	S	41	ALA	CA-C-N	8.99	133.98	120.31
11	S	41	ALA	C-N-CA	8.99	133.98	120.31
4	D	257	ARG	CA-C-N	8.97	133.03	120.29
4	D	257	ARG	C-N-CA	8.97	133.03	120.29
7	G	196	LYS	N-CA-C	-8.97	101.91	113.12
4	B	110	GLY	CA-C-N	8.96	135.36	122.09
4	B	110	GLY	C-N-CA	8.96	135.36	122.09
11	R	135	PHE	CA-CB-CG	-8.96	104.84	113.80
4	F	350	THR	CA-C-N	8.96	131.34	120.14
4	F	350	THR	C-N-CA	8.96	131.34	120.14
8	P	418	ILE	CA-C-N	8.96	132.73	120.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	418	ILE	C-N-CA	8.96	132.73	120.46
11	X	119	SER	CA-C-N	8.95	132.63	120.54
11	X	119	SER	C-N-CA	8.95	132.63	120.54
8	P	450	ILE	CA-C-O	-8.95	111.64	120.95
1	M	199	GLU	CA-C-N	8.94	132.99	120.29
1	M	199	GLU	C-N-CA	8.94	132.99	120.29
4	B	352	TYR	CA-C-N	8.94	133.11	120.42
4	B	352	TYR	C-N-CA	8.94	133.11	120.42
11	X	72	VAL	O-C-N	8.94	130.67	121.91
11	W	73	LEU	CA-C-N	8.93	131.82	120.56
11	W	73	LEU	C-N-CA	8.93	131.82	120.56
10	O	250	ALA	N-CA-C	8.93	121.01	111.28
3	A	399	VAL	CA-C-N	8.92	133.38	120.71
3	A	399	VAL	C-N-CA	8.92	133.38	120.71
11	Y	81	LYS	N-CA-C	-8.88	95.02	108.52
8	P	197	PRO	CA-C-N	8.88	132.18	120.28
8	P	197	PRO	C-N-CA	8.88	132.18	120.28
7	I	46	GLU	CA-C-N	8.86	131.96	120.44
7	I	46	GLU	C-N-CA	8.86	131.96	120.44
3	C	46	TYR	CA-C-N	8.85	133.71	121.05
3	C	46	TYR	C-N-CA	8.85	133.71	121.05
4	F	249	THR	N-CA-C	8.85	120.92	111.28
8	P	267	TYR	CA-C-N	8.83	132.46	120.54
8	P	267	TYR	C-N-CA	8.83	132.46	120.54
3	A	529	ASN	CA-CB-CG	-8.83	103.77	112.60
11	S	54	ILE	N-CA-C	8.82	122.08	111.05
4	B	130	ASP	N-CA-C	-8.78	95.98	109.24
5	Q	330	ILE	CA-C-N	8.77	132.03	120.28
5	Q	330	ILE	C-N-CA	8.77	132.03	120.28
8	P	114	VAL	CA-C-N	8.75	132.01	120.28
8	P	114	VAL	C-N-CA	8.75	132.01	120.28
11	Y	39	ILE	N-CA-C	8.74	118.81	110.42
5	Q	273	TYR	N-CA-CB	8.74	123.58	110.29
11	U	111	VAL	CA-C-N	8.74	129.87	119.99
11	U	111	VAL	C-N-CA	8.74	129.87	119.99
10	O	341	LYS	CA-C-N	8.74	131.80	120.44
10	O	341	LYS	C-N-CA	8.74	131.80	120.44
5	Q	281	THR	CA-C-N	8.74	129.68	119.98
5	Q	281	THR	C-N-CA	8.74	129.68	119.98
4	D	162	ASN	CA-CB-CG	-8.72	103.88	112.60
8	P	81	ILE	CA-C-N	8.72	131.77	120.44
8	P	81	ILE	C-N-CA	8.72	131.77	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	432	LEU	O-C-N	8.71	131.35	122.12
11	a	97	VAL	CB-CA-C	-8.71	100.57	112.24
4	D	129	GLU	N-CA-C	-8.71	103.08	114.31
4	B	232	ASN	CA-CB-CG	-8.70	103.90	112.60
11	W	66	TYR	CA-C-O	8.70	129.95	120.82
11	X	86	THR	CA-C-N	8.69	129.81	119.99
11	X	86	THR	C-N-CA	8.69	129.81	119.99
11	T	53	ASN	CA-C-O	8.69	130.20	120.90
11	W	30	TYR	CA-C-N	8.69	129.81	119.99
11	W	30	TYR	C-N-CA	8.69	129.81	119.99
10	O	242	ASN	CA-CB-CG	-8.68	103.92	112.60
10	O	35	ASN	OD1-CG-ND2	8.67	131.27	122.60
6	L	87	ALA	CA-C-O	8.67	129.86	120.24
11	V	37	VAL	CA-C-N	8.66	129.38	119.94
11	V	37	VAL	C-N-CA	8.66	129.38	119.94
4	D	206	GLU	CA-C-N	8.64	133.05	120.95
4	D	206	GLU	C-N-CA	8.64	133.05	120.95
1	M	100	ASN	CA-CB-CG	8.62	121.22	112.60
1	M	18	MET	N-CA-C	8.61	121.62	111.71
3	C	616	ASP	CA-CB-CG	-8.61	103.99	112.60
4	F	153	THR	N-CA-C	-8.61	102.52	113.72
3	A	442	ASP	CA-CB-CG	-8.61	103.99	112.60
3	A	260	CYS	CA-C-O	8.61	128.18	118.97
4	F	219	LEU	N-CA-C	8.61	120.66	111.28
8	P	274	LEU	CA-C-N	8.60	131.81	120.28
8	P	274	LEU	C-N-CA	8.60	131.81	120.28
8	P	321	THR	CA-C-N	8.60	132.64	120.42
8	P	321	THR	C-N-CA	8.60	132.64	120.42
4	F	212	PHE	CA-CB-CG	8.59	122.39	113.80
4	F	30	THR	CA-C-N	8.58	132.66	120.98
4	F	30	THR	C-N-CA	8.58	132.66	120.98
5	Q	269	LEU	CA-C-N	8.57	133.82	122.42
5	Q	269	LEU	C-N-CA	8.57	133.82	122.42
3	A	508	SER	N-CA-CB	8.57	123.47	110.70
11	X	93	ALA	CA-C-O	-8.57	111.87	120.70
11	X	123	PRO	CA-C-N	8.57	131.76	120.28
11	X	123	PRO	C-N-CA	8.57	131.76	120.28
4	D	57	LEU	N-CA-C	-8.56	99.25	110.39
11	X	93	ALA	O-C-N	8.56	131.34	122.09
11	a	51	PHE	N-CA-C	8.56	120.61	111.28
11	Z	137	GLU	CA-C-N	8.56	132.19	120.46
11	Z	137	GLU	C-N-CA	8.56	132.19	120.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	84	LEU	CA-C-N	8.55	131.74	120.28
11	T	84	LEU	C-N-CA	8.55	131.74	120.28
11	V	122	GLN	CA-C-N	8.55	130.53	119.84
11	V	122	GLN	C-N-CA	8.55	130.53	119.84
3	C	553	TYR	CA-C-O	-8.55	111.36	120.42
4	F	133	ASP	CA-CB-CG	-8.54	104.06	112.60
11	V	91	LEU	CA-C-N	8.54	130.81	120.14
11	V	91	LEU	C-N-CA	8.54	130.81	120.14
9	b	272	GLN	CA-C-N	8.53	131.71	120.28
9	b	272	GLN	C-N-CA	8.53	131.71	120.28
7	G	195	ASP	N-CA-CB	8.53	124.90	110.49
8	P	209	LYS	N-CA-C	8.52	121.80	111.40
11	Y	88	PHE	CA-CB-CG	-8.52	105.28	113.80
11	V	66	TYR	CA-C-N	8.52	129.62	119.99
11	V	66	TYR	C-N-CA	8.52	129.62	119.99
11	a	93	ALA	CA-C-N	8.51	129.38	119.94
11	a	93	ALA	C-N-CA	8.51	129.38	119.94
7	K	59	ASP	CA-CB-CG	-8.50	104.10	112.60
4	F	228	ASP	CA-CB-CG	8.49	121.09	112.60
8	P	179	GLN	CA-C-N	8.49	131.47	120.44
8	P	179	GLN	C-N-CA	8.49	131.47	120.44
4	D	334	ILE	N-CA-C	-8.48	96.24	108.11
5	Q	318	GLN	CA-C-N	8.48	132.33	120.29
5	Q	318	GLN	C-N-CA	8.48	132.33	120.29
4	D	201	HIS	CE1-NE2-CD2	-8.47	100.53	109.00
11	a	52	LYS	CA-C-N	8.47	131.45	120.44
11	a	52	LYS	C-N-CA	8.47	131.45	120.44
11	V	153	ARG	CA-C-N	8.47	131.45	120.44
11	V	153	ARG	C-N-CA	8.47	131.45	120.44
4	D	94	GLU	N-CA-C	-8.46	96.12	109.23
3	A	272	TYR	CA-C-N	8.46	133.14	121.05
3	A	272	TYR	C-N-CA	8.46	133.14	121.05
4	B	282	SER	CA-C-N	8.46	132.30	120.29
4	B	282	SER	C-N-CA	8.46	132.30	120.29
3	C	390	SER	CA-C-N	8.45	131.94	120.44
3	C	390	SER	C-N-CA	8.45	131.94	120.44
11	U	55	VAL	O-C-N	-8.45	111.47	121.10
5	Q	111	ILE	CA-C-N	8.45	131.60	120.28
5	Q	111	ILE	C-N-CA	8.45	131.60	120.28
11	X	110	ILE	N-CA-CB	8.44	120.19	110.65
1	M	146	LEU	CA-C-N	8.43	131.35	120.56
1	M	146	LEU	C-N-CA	8.43	131.35	120.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	324	MET	CA-C-O	-8.43	111.16	120.69
10	O	10	ASP	N-CA-C	-8.43	97.07	110.14
8	P	269	SER	CA-C-N	8.43	131.58	120.28
8	P	269	SER	C-N-CA	8.43	131.58	120.28
3	C	213	HIS	CE1-NE2-CD2	-8.43	100.57	109.00
5	Q	82	TYR	CB-CG-CD1	8.43	133.44	120.80
11	W	72	VAL	N-CA-CB	8.43	119.86	110.51
7	G	55	THR	CA-C-O	8.41	129.34	120.42
3	C	181	THR	N-CA-C	-8.41	95.69	109.40
6	J	18	HIS	ND1-CE1-NE2	8.40	116.80	108.40
8	P	348	ASN	CA-C-N	8.39	131.52	120.28
8	P	348	ASN	C-N-CA	8.39	131.52	120.28
11	S	39	ILE	CA-C-N	8.39	131.52	120.28
11	S	39	ILE	C-N-CA	8.39	131.52	120.28
7	G	153	LYS	N-CA-C	8.38	120.41	111.28
3	A	309	GLU	CA-C-O	-8.38	114.03	120.48
3	A	101	MET	CA-C-N	8.37	133.99	122.19
3	A	101	MET	C-N-CA	8.37	133.99	122.19
11	U	17	CYS	CA-C-N	8.37	132.42	120.79
11	U	17	CYS	C-N-CA	8.37	132.42	120.79
11	S	48	ASP	N-CA-C	-8.35	101.80	114.16
10	O	137	GLU	CA-C-N	8.35	132.15	120.29
10	O	137	GLU	C-N-CA	8.35	132.15	120.29
3	A	36	ILE	N-CA-C	-8.35	96.10	108.12
3	A	359	ARG	CA-C-N	8.33	132.12	120.29
3	A	359	ARG	C-N-CA	8.33	132.12	120.29
11	T	53	ASN	OD1-CG-ND2	-8.32	114.28	122.60
11	V	26	LEU	CA-C-N	8.32	129.39	119.99
11	V	26	LEU	C-N-CA	8.32	129.39	119.99
11	X	72	VAL	CA-C-O	-8.32	112.35	121.17
6	J	18	HIS	CE1-NE2-CD2	-8.31	100.69	109.00
3	C	100	LEU	N-CA-C	8.31	121.54	111.40
9	b	106	VAL	CA-C-N	8.31	131.84	120.46
9	b	106	VAL	C-N-CA	8.31	131.84	120.46
9	b	341	ILE	CB-CA-C	8.31	118.55	110.16
11	T	37	VAL	CA-C-N	8.30	129.13	120.00
11	T	37	VAL	C-N-CA	8.30	129.13	120.00
3	A	287	GLY	CA-C-N	8.29	132.91	120.31
3	A	287	GLY	C-N-CA	8.29	132.91	120.31
11	S	132	ILE	CA-C-N	8.28	131.38	120.28
11	S	132	ILE	C-N-CA	8.28	131.38	120.28
3	E	476	PRO	N-CA-C	8.28	124.23	111.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	322	VAL	N-CA-C	-8.28	96.56	108.48
8	P	78	ILE	CA-C-O	-8.27	113.15	118.69
8	P	113	THR	CA-C-N	8.26	132.15	120.42
8	P	113	THR	C-N-CA	8.26	132.15	120.42
3	E	341	GLU	CA-C-N	8.26	131.18	120.44
3	E	341	GLU	C-N-CA	8.26	131.18	120.44
8	P	420	ILE	CA-CB-CG1	-8.26	96.36	110.40
4	F	195	ARG	CA-C-O	-8.26	110.33	118.34
2	N	36	ASN	N-CA-C	-8.25	100.33	110.88
11	V	52	LYS	CA-C-N	8.25	131.67	120.54
11	V	52	LYS	C-N-CA	8.25	131.67	120.54
5	Q	32	ASN	CA-C-N	8.23	131.31	120.28
5	Q	32	ASN	C-N-CA	8.23	131.31	120.28
7	I	217	ALA	CA-C-N	8.23	132.11	120.42
7	I	217	ALA	C-N-CA	8.23	132.11	120.42
8	P	400	GLU	CA-C-N	8.22	131.29	120.28
8	P	400	GLU	C-N-CA	8.22	131.29	120.28
4	B	72	GLY	O-C-N	8.21	130.05	122.99
10	O	339	LYS	N-CA-C	-8.21	102.41	111.36
8	P	152	GLN	N-CA-CB	8.20	122.02	109.97
4	D	374	ASN	CA-CB-CG	8.19	120.79	112.60
8	P	191	GLN	OE1-CD-NE2	-8.18	114.42	122.60
3	C	246	CYS	N-CA-C	-8.17	96.44	109.59
4	F	483	GLU	CA-C-O	8.17	129.08	120.42
5	Q	28	ASN	CA-C-N	8.17	131.06	120.44
5	Q	28	ASN	C-N-CA	8.17	131.06	120.44
7	K	215	LEU	CA-C-O	-8.16	110.73	118.73
11	R	63	ILE	CA-C-N	8.16	131.22	120.28
11	R	63	ILE	C-N-CA	8.16	131.22	120.28
4	B	322	VAL	CA-C-N	8.15	132.71	121.05
4	B	322	VAL	C-N-CA	8.15	132.71	121.05
11	X	39	ILE	CA-C-N	8.15	131.21	120.28
11	X	39	ILE	C-N-CA	8.15	131.21	120.28
11	W	27	GLY	CA-C-N	8.15	131.87	120.29
11	W	27	GLY	C-N-CA	8.15	131.87	120.29
3	A	345	ASP	N-CA-CB	8.15	123.92	110.39
11	a	35	SER	N-CA-CB	8.14	121.81	110.01
11	U	146	VAL	N-CA-CB	8.13	119.54	110.51
3	A	391	PHE	CA-CB-CG	8.13	121.93	113.80
4	B	126	VAL	N-CA-C	8.12	118.92	110.72
11	Y	83	ALA	CA-C-N	8.12	131.16	120.28
11	Y	83	ALA	C-N-CA	8.12	131.16	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	104	ALA	CA-C-N	8.12	128.99	119.98
11	a	104	ALA	C-N-CA	8.12	128.99	119.98
7	G	103	THR	CA-C-O	-8.11	111.95	120.55
4	F	400	SER	O-C-N	8.11	130.71	122.12
8	P	41	ALA	CA-C-N	8.09	131.12	120.28
8	P	41	ALA	C-N-CA	8.09	131.12	120.28
10	O	244	GLN	CA-C-N	8.08	131.11	120.28
10	O	244	GLN	C-N-CA	8.08	131.11	120.28
5	Q	182	ASN	CA-C-N	8.08	131.10	120.28
5	Q	182	ASN	C-N-CA	8.08	131.10	120.28
9	b	55	PHE	CA-C-N	8.08	133.23	120.47
9	b	55	PHE	C-N-CA	8.08	133.23	120.47
11	T	12	PHE	N-CA-C	-8.07	103.57	113.50
4	D	383	MET	N-CA-C	-8.07	104.58	114.75
4	D	409	ILE	CA-C-N	8.07	128.88	120.00
4	D	409	ILE	C-N-CA	8.07	128.88	120.00
8	P	120	ASP	CB-CA-C	-8.07	98.83	110.13
4	D	155	VAL	CA-C-N	8.06	131.09	120.28
4	D	155	VAL	C-N-CA	8.06	131.09	120.28
11	W	15	ILE	CA-C-N	8.06	128.89	119.94
11	W	15	ILE	C-N-CA	8.06	128.89	119.94
4	F	365	HIS	ND1-CE1-NE2	8.05	116.45	108.40
4	F	354	THR	N-CA-CB	8.05	122.52	110.29
4	D	261	THR	O-C-N	-8.04	112.98	122.15
3	E	553	TYR	O-C-N	8.04	130.65	122.12
11	a	52	LYS	N-CA-C	8.04	119.83	111.14
11	a	79	GLY	CA-C-N	8.04	131.38	120.44
11	a	79	GLY	C-N-CA	8.04	131.38	120.44
8	P	270	ASP	CA-C-N	8.04	131.05	120.28
8	P	270	ASP	C-N-CA	8.04	131.05	120.28
9	b	82	LYS	O-C-N	8.04	132.49	123.16
10	O	267	ILE	CA-C-N	8.03	131.70	120.29
10	O	267	ILE	C-N-CA	8.03	131.70	120.29
11	W	124	ARG	N-CA-C	8.03	120.03	111.28
4	D	401	ASN	N-CA-C	8.03	119.66	111.07
7	K	173	VAL	N-CA-CB	8.01	120.58	111.21
7	G	49	ASN	CA-C-O	-8.01	112.59	121.00
7	K	66	LEU	N-CA-C	-8.00	102.50	111.14
11	X	68	LEU	N-CA-C	7.99	119.99	111.28
11	W	129	MET	CA-C-N	7.99	130.91	120.60
11	W	129	MET	C-N-CA	7.99	130.91	120.60
3	E	296	GLU	CB-CG-CD	-7.98	99.03	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	182	ILE	N-CA-CB	7.98	120.10	111.00
11	R	74	VAL	CA-C-O	-7.98	112.71	121.17
3	E	424	SER	N-CA-C	-7.98	100.15	112.99
3	C	185	ILE	CB-CA-C	7.97	121.36	110.99
3	E	266	SER	CB-CA-C	-7.97	97.30	110.85
11	U	35	SER	N-CA-CB	7.97	121.62	110.07
4	D	46	PHE	O-C-N	-7.96	113.23	120.71
11	V	73	LEU	CA-C-N	7.96	130.59	120.56
11	V	73	LEU	C-N-CA	7.96	130.59	120.56
3	E	360	TRP	CA-C-N	7.96	131.59	120.29
3	E	360	TRP	C-N-CA	7.96	131.59	120.29
4	D	113	PHE	CA-CB-CG	-7.95	105.85	113.80
6	H	54	LEU	N-CA-C	-7.94	101.92	111.69
9	b	148	GLY	CA-C-N	7.94	130.92	120.28
9	b	148	GLY	C-N-CA	7.94	130.92	120.28
3	E	209	PHE	CA-CB-CG	-7.94	105.86	113.80
9	b	299	LEU	CA-C-N	7.93	130.91	120.28
9	b	299	LEU	C-N-CA	7.93	130.91	120.28
7	K	36	GLN	CA-C-N	7.93	131.55	120.29
7	K	36	GLN	C-N-CA	7.93	131.55	120.29
4	F	234	SER	N-CA-C	-7.92	102.92	112.59
8	P	284	GLU	CA-C-N	7.92	131.54	120.29
8	P	284	GLU	C-N-CA	7.92	131.54	120.29
3	C	97	GLY	CA-C-N	7.92	129.74	119.84
3	C	97	GLY	C-N-CA	7.92	129.74	119.84
8	P	243	GLN	CA-C-N	7.92	130.89	120.28
8	P	243	GLN	C-N-CA	7.92	130.89	120.28
10	O	353	GLY	O-C-N	7.92	132.99	122.70
11	R	126	PHE	N-CA-CB	7.92	121.75	110.12
7	K	67	LYS	CA-C-O	-7.91	112.17	120.55
10	O	196	VAL	N-CA-C	-7.91	96.73	108.12
11	Z	54	ILE	CA-C-N	7.91	126.66	120.33
11	Z	54	ILE	C-N-CA	7.91	126.66	120.33
3	C	98	PRO	N-CA-CB	7.90	111.55	103.25
4	F	255	THR	CA-C-O	-7.90	110.99	118.73
9	b	236	PHE	CA-CB-CG	7.89	121.69	113.80
3	A	259	GLY	N-CA-C	-7.89	103.13	115.67
11	U	145	ILE	CA-C-N	7.89	130.78	120.60
11	U	145	ILE	C-N-CA	7.89	130.78	120.60
9	b	130	GLN	CA-C-N	7.88	130.49	120.56
9	b	130	GLN	C-N-CA	7.88	130.49	120.56
7	I	215	LEU	CA-C-O	-7.88	111.38	118.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	490	SER	CA-C-N	7.88	130.84	120.28
3	C	490	SER	C-N-CA	7.88	130.84	120.28
8	P	12	HIS	CG-CD2-NE2	7.88	115.08	107.20
8	P	75	LYS	CA-C-N	7.88	134.93	121.14
8	P	75	LYS	C-N-CA	7.88	134.93	121.14
7	I	11	ASN	CA-C-N	7.88	130.84	120.28
7	I	11	ASN	C-N-CA	7.88	130.84	120.28
6	J	12	GLN	CA-C-N	7.87	130.67	120.44
6	J	12	GLN	C-N-CA	7.87	130.67	120.44
11	T	66	TYR	N-CA-C	-7.87	102.78	111.36
4	B	46	PHE	CA-CB-CG	-7.86	105.94	113.80
11	X	57	VAL	N-CA-C	7.86	118.61	110.36
9	b	292	SER	N-CA-CB	7.85	121.78	110.16
11	a	149	LEU	N-CA-C	7.85	119.53	110.97
8	P	189	LEU	CA-C-N	7.84	130.63	120.44
8	P	189	LEU	C-N-CA	7.84	130.63	120.44
3	C	141	PHE	O-C-N	7.83	132.15	123.22
4	D	183	ILE	N-CA-C	-7.83	102.81	110.72
3	A	90	LYS	O-C-N	-7.83	115.93	121.65
4	D	474	ASN	OD1-CG-ND2	-7.83	114.77	122.60
3	A	575	GLY	CA-C-N	7.83	131.41	120.29
3	A	575	GLY	C-N-CA	7.83	131.41	120.29
8	P	337	GLN	OE1-CD-NE2	7.83	130.43	122.60
8	P	429	HIS	CE1-NE2-CD2	-7.83	101.17	109.00
5	Q	20	TYR	CA-C-N	7.83	131.10	120.38
5	Q	20	TYR	C-N-CA	7.83	131.10	120.38
4	B	63	ARG	CA-C-O	-7.83	111.95	121.11
9	b	51	PHE	CA-CB-CG	-7.83	105.97	113.80
3	A	297	PHE	O-C-N	-7.82	113.52	120.48
11	Z	15	ILE	CA-C-N	7.82	128.46	119.94
11	Z	15	ILE	C-N-CA	7.82	128.46	119.94
11	U	148	LEU	CA-C-N	7.80	131.07	120.54
11	U	148	LEU	C-N-CA	7.80	131.07	120.54
4	D	407	TYR	CA-C-N	7.80	131.36	120.29
4	D	407	TYR	C-N-CA	7.80	131.36	120.29
9	b	180	ILE	N-CA-C	-7.80	105.16	112.96
5	Q	218	ARG	CA-C-O	-7.78	112.66	120.82
3	E	270	SER	CB-CA-C	-7.77	97.89	110.79
4	F	348	ASP	CA-CB-CG	7.77	120.37	112.60
4	F	475	ARG	N-CA-C	-7.77	102.86	112.88
6	H	46	TYR	CA-C-N	7.76	131.19	120.63
6	H	46	TYR	C-N-CA	7.76	131.19	120.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	b	33	LEU	CA-C-N	7.76	128.76	119.99
9	b	33	LEU	C-N-CA	7.76	128.76	119.99
8	P	281	THR	CA-C-N	7.76	131.08	121.85
8	P	281	THR	C-N-CA	7.76	131.08	121.85
8	P	343	LYS	CA-C-N	7.76	130.99	120.44
8	P	343	LYS	C-N-CA	7.76	130.99	120.44
11	Z	126	PHE	N-CA-CB	7.76	122.17	110.22
8	P	404	ALA	CA-C-N	7.76	130.67	120.28
8	P	404	ALA	C-N-CA	7.76	130.67	120.28
3	E	137	ILE	N-CA-CB	7.75	120.30	110.99
3	E	326	VAL	CA-C-N	7.75	130.66	120.28
3	E	326	VAL	C-N-CA	7.75	130.66	120.28
6	H	22	SER	N-CA-CB	7.74	121.50	110.12
11	X	49	LEU	CA-C-N	7.74	132.43	120.82
11	X	49	LEU	C-N-CA	7.74	132.43	120.82
11	Y	74	VAL	CA-C-O	-7.74	113.23	121.27
6	H	99	ILE	CA-C-O	-7.73	112.97	121.17
3	C	322	SER	CA-C-N	7.73	131.27	120.29
3	C	322	SER	C-N-CA	7.73	131.27	120.29
4	D	201	HIS	CA-CB-CG	7.73	121.53	113.80
3	E	399	VAL	CA-C-N	7.73	131.80	120.90
3	E	399	VAL	C-N-CA	7.73	131.80	120.90
11	Y	33	ALA	N-CA-C	7.73	120.45	111.02
4	B	314	THR	O-C-N	7.73	130.31	122.12
4	D	216	GLY	O-C-N	7.72	129.60	122.57
7	G	167	ALA	CA-C-N	7.72	128.18	119.92
7	G	167	ALA	C-N-CA	7.72	128.18	119.92
7	G	189	VAL	CA-C-N	7.71	133.94	122.91
7	G	189	VAL	C-N-CA	7.71	133.94	122.91
11	W	96	SER	N-CA-C	7.71	120.36	111.11
8	P	342	LEU	CA-C-N	7.71	130.61	120.28
8	P	342	LEU	C-N-CA	7.71	130.61	120.28
4	D	133	ASP	CA-CB-CG	-7.70	104.90	112.60
8	P	185	VAL	CA-C-N	7.70	130.60	120.28
8	P	185	VAL	C-N-CA	7.70	130.60	120.28
11	R	19	SER	O-C-N	-7.70	114.14	122.07
3	A	45	MET	CA-C-O	7.70	129.05	120.43
3	A	478	PHE	CA-C-O	-7.69	111.21	118.44
9	b	326	SER	CA-C-N	7.68	133.55	120.72
9	b	326	SER	C-N-CA	7.68	133.55	120.72
4	F	113	PHE	CA-CB-CG	-7.68	106.12	113.80
4	F	423	GLU	CA-C-O	-7.68	112.79	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	340	ASN	CA-C-O	7.68	128.69	120.55
11	V	129	MET	CA-C-N	7.68	130.50	120.60
11	V	129	MET	C-N-CA	7.68	130.50	120.60
5	Q	126	ARG	CA-C-N	7.67	131.60	120.71
5	Q	126	ARG	C-N-CA	7.67	131.60	120.71
4	B	415	ALA	CA-C-N	7.67	131.18	120.29
4	B	415	ALA	C-N-CA	7.67	131.18	120.29
11	S	18	ALA	CA-C-N	7.67	130.89	120.54
11	S	18	ALA	C-N-CA	7.67	130.89	120.54
1	M	39	LEU	CA-C-N	7.66	131.96	120.31
1	M	39	LEU	C-N-CA	7.66	131.96	120.31
3	C	157	ILE	CA-C-N	7.66	133.70	120.68
3	C	157	ILE	C-N-CA	7.66	133.70	120.68
8	P	413	ALA	N-CA-C	-7.65	96.93	109.40
4	D	417	LYS	CA-C-O	7.64	128.85	120.82
11	X	101	GLY	O-C-N	7.64	129.52	122.18
11	T	111	VAL	CA-C-N	7.64	128.63	119.99
11	T	111	VAL	C-N-CA	7.64	128.63	119.99
11	W	153	ARG	CA-C-N	7.64	130.85	120.54
11	W	153	ARG	C-N-CA	7.64	130.85	120.54
3	A	132	ALA	N-CA-C	7.63	119.60	111.28
10	O	151	ASN	CA-CB-CG	-7.63	104.97	112.60
5	Q	265	VAL	CA-C-N	7.63	130.50	120.28
5	Q	265	VAL	C-N-CA	7.63	130.50	120.28
3	C	563	ASN	OD1-CG-ND2	7.62	130.22	122.60
2	N	74	ALA	CA-C-N	7.62	130.49	120.28
2	N	74	ALA	C-N-CA	7.62	130.49	120.28
11	R	129	MET	CA-C-N	7.62	130.15	120.56
11	R	129	MET	C-N-CA	7.62	130.15	120.56
3	C	518	ALA	CA-C-N	7.61	130.48	120.28
3	C	518	ALA	C-N-CA	7.61	130.48	120.28
7	K	75	ILE	N-CA-C	-7.61	103.03	110.72
6	H	102	VAL	CA-CB-CG1	7.61	123.34	110.40
11	a	15	ILE	CA-C-N	7.61	128.24	119.94
11	a	15	ILE	C-N-CA	7.61	128.24	119.94
9	b	336	ILE	N-CA-C	-7.61	97.06	108.17
11	Y	66	TYR	CA-C-N	7.61	128.59	119.99
11	Y	66	TYR	C-N-CA	7.61	128.59	119.99
4	B	304	TYR	N-CA-C	-7.60	99.82	110.31
5	Q	123	ILE	N-CA-C	-7.60	97.38	108.71
11	S	98	GLY	O-C-N	-7.60	114.90	122.19
1	M	151	SER	CA-C-N	7.60	131.22	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	151	SER	C-N-CA	7.60	131.22	120.28
3	C	399	VAL	N-CA-C	-7.59	96.61	108.23
3	A	464	THR	CA-C-N	7.59	130.67	120.65
3	A	464	THR	C-N-CA	7.59	130.67	120.65
8	P	385	ASP	CA-C-N	7.59	130.45	120.28
8	P	385	ASP	C-N-CA	7.59	130.45	120.28
4	D	455	PHE	CA-CB-CG	-7.59	106.21	113.80
11	T	83	ALA	O-C-N	-7.59	114.14	122.79
11	T	141	LEU	CA-C-N	7.59	130.78	120.38
11	T	141	LEU	C-N-CA	7.59	130.78	120.38
3	E	284	GLY	N-CA-C	-7.59	95.20	113.18
11	a	118	GLY	CA-C-N	7.59	130.66	120.65
11	a	118	GLY	C-N-CA	7.59	130.66	120.65
11	a	147	ALA	CA-C-N	7.59	133.25	121.19
11	a	147	ALA	C-N-CA	7.59	133.25	121.19
11	Y	105	GLY	O-C-N	7.59	129.47	122.19
11	R	80	GLN	OE1-CD-NE2	7.57	130.17	122.60
11	W	33	ALA	N-CA-C	7.57	120.26	111.02
6	L	81	ALA	N-CA-C	-7.57	104.18	113.41
8	P	152	GLN	N-CA-C	-7.56	99.09	110.28
3	C	430	ALA	N-CA-C	7.56	119.52	111.28
4	B	113	PHE	O-C-N	-7.56	113.44	122.96
9	b	176	ILE	CA-CB-CG1	7.56	123.25	110.40
10	O	304	PHE	CA-CB-CG	7.56	121.36	113.80
7	I	86	LEU	CA-C-N	7.55	130.25	120.44
7	I	86	LEU	C-N-CA	7.55	130.25	120.44
4	F	435	PHE	CA-CB-CG	-7.55	106.25	113.80
10	O	141	LEU	CA-C-N	7.55	130.25	120.44
10	O	141	LEU	C-N-CA	7.55	130.25	120.44
7	I	157	MET	CA-C-N	7.54	130.61	120.65
7	I	157	MET	C-N-CA	7.54	130.61	120.65
3	A	170	HIS	CA-CB-CG	-7.54	106.26	113.80
4	F	67	VAL	O-C-N	-7.54	114.46	122.68
8	P	77	LEU	CA-C-N	7.54	126.36	120.33
8	P	77	LEU	C-N-CA	7.54	126.36	120.33
3	E	46	TYR	CB-CA-C	-7.54	96.93	110.35
3	E	118	GLU	N-CA-C	7.54	119.39	111.03
10	O	316	VAL	O-C-N	-7.53	114.56	121.87
4	F	151	ILE	CA-C-N	7.53	132.19	121.42
4	F	151	ILE	C-N-CA	7.53	132.19	121.42
11	R	133	LEU	N-CA-C	7.53	119.48	111.28
7	G	102	GLU	CA-C-N	7.52	130.36	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	102	GLU	C-N-CA	7.52	130.36	120.28
7	I	113	ASN	CA-C-N	7.52	131.11	120.28
7	I	113	ASN	C-N-CA	7.52	131.11	120.28
6	J	5	ASN	N-CA-C	-7.52	102.00	112.45
1	M	122	LEU	CB-CA-C	-7.51	98.81	110.37
3	A	468	ASN	CB-CA-C	7.51	123.25	110.79
3	C	185	ILE	CA-C-N	7.50	130.81	120.39
3	C	185	ILE	C-N-CA	7.50	130.81	120.39
4	F	92	THR	N-CA-C	-7.50	97.92	109.24
4	F	308	MET	CA-C-N	7.50	130.33	120.28
4	F	308	MET	C-N-CA	7.50	130.33	120.28
11	Y	97	VAL	CA-C-N	7.50	128.46	119.99
11	Y	97	VAL	C-N-CA	7.50	128.46	119.99
3	C	533	THR	N-CA-C	-7.50	103.98	113.72
3	A	263	THR	CA-C-N	7.49	129.99	120.56
3	A	263	THR	C-N-CA	7.49	129.99	120.56
10	O	306	ILE	N-CA-CB	7.48	119.31	110.55
4	B	42	GLU	N-CA-C	-7.48	96.54	108.73
6	J	65	VAL	N-CA-C	-7.48	104.02	113.22
4	D	480	ILE	CA-C-N	7.48	130.30	120.28
4	D	480	ILE	C-N-CA	7.48	130.30	120.28
3	E	164	ASN	N-CA-CB	7.47	123.12	110.49
2	N	73	ILE	CA-C-N	7.47	130.29	120.28
2	N	73	ILE	C-N-CA	7.47	130.29	120.28
4	D	477	SER	CA-C-N	7.47	127.18	119.56
4	D	477	SER	C-N-CA	7.47	127.18	119.56
4	F	255	THR	CA-C-N	7.47	127.50	119.28
4	F	255	THR	C-N-CA	7.47	127.50	119.28
7	G	215	LEU	O-C-N	-7.47	113.45	120.55
5	Q	126	ARG	N-CA-C	-7.47	97.17	108.52
7	G	49	ASN	CA-CB-CG	7.47	120.07	112.60
6	J	88	GLU	CA-C-N	7.46	130.78	120.63
6	J	88	GLU	C-N-CA	7.46	130.78	120.63
4	D	40	ILE	CA-C-N	7.46	133.75	122.93
4	D	40	ILE	C-N-CA	7.46	133.75	122.93
3	C	51	VAL	N-CA-CB	7.46	122.79	110.86
11	Z	83	ALA	CA-C-N	7.46	130.27	120.28
11	Z	83	ALA	C-N-CA	7.46	130.27	120.28
3	C	93	SER	N-CA-C	-7.46	98.59	109.18
11	Y	145	ILE	CA-C-N	7.46	129.96	120.56
11	Y	145	ILE	C-N-CA	7.46	129.96	120.56
11	R	116	VAL	CA-C-O	7.45	128.30	120.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	56	ASN	CA-CB-CG	-7.45	105.15	112.60
11	V	154	ALA	CB-CA-C	-7.45	99.19	110.88
7	I	200	ASN	CA-CB-CG	-7.45	105.16	112.60
11	R	83	ALA	CA-C-O	7.44	129.44	121.55
11	Y	151	ASN	CA-CB-CG	-7.44	105.16	112.60
6	L	8	ALA	CA-C-N	7.43	130.85	120.29
6	L	8	ALA	C-N-CA	7.43	130.85	120.29
10	O	298	ASP	CA-CB-CG	7.43	120.03	112.60
3	A	511	ASP	O-C-N	-7.43	113.13	122.27
11	W	103	ALA	CA-C-N	7.43	130.10	120.44
11	W	103	ALA	C-N-CA	7.43	130.10	120.44
3	E	285	GLU	CA-C-N	7.43	130.23	120.28
3	E	285	GLU	C-N-CA	7.43	130.23	120.28
11	Z	126	PHE	N-CA-C	-7.42	103.18	111.71
3	C	478	PHE	O-C-N	-7.42	113.61	120.51
10	O	135	SER	CA-C-N	7.42	130.22	120.28
10	O	135	SER	C-N-CA	7.42	130.22	120.28
7	I	17	LEU	N-CA-C	-7.42	103.28	111.36
7	G	182	ASP	N-CA-C	-7.41	102.50	113.61
3	C	355	ASP	CB-CA-C	-7.41	100.50	110.79
4	F	156	SER	CA-C-O	-7.40	112.58	120.42
10	O	206	PHE	CA-CB-CG	-7.40	106.40	113.80
11	Z	104	ALA	N-CA-C	-7.40	103.22	111.28
11	X	138	VAL	N-CA-CB	7.40	119.72	110.47
8	P	129	ASP	N-CA-CB	7.39	120.73	110.01
11	U	57	VAL	CA-C-O	-7.39	113.26	120.95
5	Q	266	ARG	CA-C-N	7.39	130.79	120.29
5	Q	266	ARG	C-N-CA	7.39	130.79	120.29
8	P	256	ASN	CA-CB-CG	-7.39	105.21	112.60
8	P	305	HIS	CA-CB-CG	-7.39	106.41	113.80
7	G	23	PHE	CA-C-N	7.39	129.87	120.56
7	G	23	PHE	C-N-CA	7.39	129.87	120.56
3	E	161	VAL	N-CA-C	-7.39	97.45	108.46
11	Z	27	GLY	CA-C-N	7.38	130.48	120.44
11	Z	27	GLY	C-N-CA	7.38	130.48	120.44
4	F	250	ILE	N-CA-CB	7.38	121.64	110.58
4	B	422	GLU	N-CA-C	-7.38	103.37	112.88
11	R	73	LEU	CA-C-N	7.38	129.85	120.56
11	R	73	LEU	C-N-CA	7.38	129.85	120.56
3	E	452	PRO	N-CA-CB	7.37	110.71	102.60
11	V	32	THR	N-CA-C	-7.37	103.18	111.07
1	M	149	LEU	CA-C-N	7.37	130.89	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	149	LEU	C-N-CA	7.37	130.89	120.28
8	P	384	ILE	O-C-N	7.37	129.02	121.87
11	W	119	SER	N-CA-CB	7.37	120.92	109.94
4	D	102	ILE	CA-C-N	7.37	129.05	119.84
4	D	102	ILE	C-N-CA	7.37	129.05	119.84
5	Q	98	ILE	O-C-N	-7.37	114.24	121.83
6	L	83	ILE	N-CA-CB	-7.37	99.53	110.58
11	R	100	SER	CA-C-N	7.36	128.31	119.99
11	R	100	SER	C-N-CA	7.36	128.31	119.99
3	C	389	ALA	CA-C-N	7.36	130.14	120.28
3	C	389	ALA	C-N-CA	7.36	130.14	120.28
8	P	411	VAL	CB-CA-C	7.36	122.03	111.80
10	O	9	ASN	N-CA-C	-7.36	98.59	108.74
11	S	158	VAL	O-C-N	7.36	131.77	122.57
4	B	365	HIS	CA-C-N	7.35	130.13	120.28
4	B	365	HIS	C-N-CA	7.35	130.13	120.28
7	G	158	ARG	N-CA-C	7.35	119.08	111.14
6	L	76	VAL	CA-C-N	7.35	130.73	120.29
6	L	76	VAL	C-N-CA	7.35	130.73	120.29
3	E	212	TYR	N-CA-CB	7.35	120.75	110.17
4	F	387	ILE	O-C-N	7.35	130.19	122.62
4	B	353	ILE	N-CA-C	7.35	118.14	110.72
10	O	332	VAL	N-CA-C	-7.35	99.38	108.05
7	I	214	ALA	N-CA-C	-7.34	103.35	111.36
3	E	294	LEU	O-C-N	-7.34	114.51	122.07
3	C	164	ASN	N-CA-C	-7.34	98.16	109.24
4	F	293	ALA	N-CA-C	-7.34	104.36	112.72
4	F	234	SER	CA-C-O	-7.34	111.29	119.95
3	A	279	ILE	CA-C-O	7.34	128.02	120.39
11	U	53	ASN	OD1-CG-ND2	7.34	129.94	122.60
11	W	95	LEU	N-CA-CB	7.34	120.87	109.94
7	I	85	ARG	NE-CZ-NH2	-7.33	112.60	119.20
3	E	97	GLY	CA-C-N	7.33	127.09	119.76
3	E	97	GLY	C-N-CA	7.33	127.09	119.76
8	P	406	VAL	CA-C-O	-7.33	112.91	121.05
11	S	14	ALA	N-CA-C	7.33	119.27	111.28
11	T	138	VAL	N-CA-CB	7.33	123.19	110.65
3	C	435	THR	CB-CA-C	7.33	122.74	109.62
11	a	111	VAL	CA-C-N	7.33	128.27	119.99
11	a	111	VAL	C-N-CA	7.33	128.27	119.99
11	W	58	ILE	CA-C-N	7.32	130.41	120.38
11	W	58	ILE	C-N-CA	7.32	130.41	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	455	ASN	CA-C-N	7.32	130.09	120.28
3	E	455	ASN	C-N-CA	7.32	130.09	120.28
11	T	58	ILE	CA-C-N	7.32	130.09	120.28
11	T	58	ILE	C-N-CA	7.32	130.09	120.28
3	A	143	PRO	CA-C-N	7.32	132.57	122.04
3	A	143	PRO	C-N-CA	7.32	132.57	122.04
11	S	55	VAL	CA-C-N	7.32	126.85	119.24
11	S	55	VAL	C-N-CA	7.32	126.85	119.24
4	B	60	GLY	N-CA-C	-7.31	105.12	115.43
6	H	72	ALA	CA-C-N	7.31	132.92	120.71
6	H	72	ALA	C-N-CA	7.31	132.92	120.71
11	Y	63	ILE	CA-C-N	7.31	130.08	120.28
11	Y	63	ILE	C-N-CA	7.31	130.08	120.28
11	W	45	LEU	N-CA-C	-7.31	104.88	114.31
4	D	279	THR	N-CA-C	-7.30	97.04	109.24
7	I	180	ASN	CA-CB-CG	-7.30	105.30	112.60
3	E	173	LEU	N-CA-C	-7.30	98.04	109.72
11	Z	120	SER	CA-C-O	-7.30	113.16	120.82
4	F	108	MET	CA-C-N	7.29	131.76	120.75
4	F	108	MET	C-N-CA	7.29	131.76	120.75
5	Q	192	PHE	O-C-N	-7.29	114.39	122.12
11	T	148	LEU	N-CA-CB	7.28	120.79	109.94
3	E	270	SER	CA-C-N	7.28	130.03	120.28
3	E	270	SER	C-N-CA	7.28	130.03	120.28
3	E	423	PHE	N-CA-C	-7.28	101.49	113.50
4	B	248	PRO	CA-C-N	7.28	130.63	120.29
4	B	248	PRO	C-N-CA	7.28	130.63	120.29
3	E	138	LYS	O-C-N	-7.28	114.91	123.06
3	E	174	LEU	CA-C-N	7.28	127.88	120.38
3	E	174	LEU	C-N-CA	7.28	127.88	120.38
4	B	79	VAL	N-CA-CB	7.28	118.65	110.72
11	a	102	LEU	N-CA-C	7.28	119.21	111.28
9	b	347	ALA	CA-C-N	7.27	132.85	120.72
9	b	347	ALA	C-N-CA	7.27	132.85	120.72
11	Y	12	PHE	N-CA-C	-7.27	104.56	113.50
8	P	76	THR	CA-C-N	7.27	129.88	120.44
8	P	76	THR	C-N-CA	7.27	129.88	120.44
4	B	429	ASP	CA-CB-CG	7.26	119.86	112.60
1	M	165	VAL	O-C-N	7.26	128.91	121.87
8	P	156	HIS	CA-CB-CG	-7.26	106.54	113.80
11	Y	73	LEU	CA-C-N	7.26	129.97	120.60
11	Y	73	LEU	C-N-CA	7.26	129.97	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	279	ILE	CA-CB-CG1	7.26	122.74	110.40
3	E	97	GLY	O-C-N	-7.26	114.51	121.77
6	J	27	TYR	N-CA-CB	7.25	120.53	110.01
11	T	66	TYR	CA-C-N	7.25	128.19	119.99
11	T	66	TYR	C-N-CA	7.25	128.19	119.99
3	C	597	HIS	CG-CD2-NE2	7.25	114.45	107.20
3	A	477	GLU	CA-C-N	7.25	133.01	121.62
3	A	477	GLU	C-N-CA	7.25	133.01	121.62
11	Z	34	LYS	CA-C-O	-7.25	112.86	120.55
3	C	27	ILE	N-CA-CB	7.24	118.86	110.82
11	T	112	GLY	O-C-N	7.24	129.29	122.13
3	E	224	THR	N-CA-C	-7.23	103.33	111.14
8	P	91	ASP	CA-CB-CG	-7.23	105.37	112.60
11	Z	76	TYR	N-CA-C	7.23	119.16	111.28
4	F	180	HIS	CA-C-N	7.23	129.97	120.28
4	F	180	HIS	C-N-CA	7.23	129.97	120.28
9	b	241	HIS	CE1-NE2-CD2	-7.23	101.77	109.00
11	U	88	PHE	CA-CB-CG	-7.23	106.57	113.80
3	E	615	THR	N-CA-C	7.22	118.80	111.07
11	Y	132	ILE	CA-C-O	-7.22	113.52	121.17
4	D	111	ARG	CA-C-N	7.22	132.02	122.93
4	D	111	ARG	C-N-CA	7.22	132.02	122.93
4	F	256	PRO	N-CA-CB	7.22	111.18	103.39
3	E	380	PHE	CA-CB-CG	-7.21	106.59	113.80
3	C	274	ASN	OD1-CG-ND2	7.21	129.81	122.60
9	b	89	ASP	CA-C-O	7.21	126.77	118.55
7	I	182	ASP	N-CA-C	-7.21	101.39	112.99
8	P	206	HIS	CA-C-N	7.20	130.27	120.54
8	P	206	HIS	C-N-CA	7.20	130.27	120.54
4	D	95	PHE	O-C-N	-7.20	115.13	123.27
5	Q	82	TYR	CB-CG-CD2	-7.20	110.00	120.80
11	Z	16	GLY	CA-C-O	7.20	128.96	120.90
11	Z	48	ASP	O-C-N	-7.20	114.49	122.12
3	C	434	ILE	N-CA-C	-7.20	103.16	111.00
8	P	174	LEU	CA-C-N	7.20	129.80	120.44
8	P	174	LEU	C-N-CA	7.20	129.80	120.44
7	I	106	LYS	CA-C-N	7.20	129.92	120.28
7	I	106	LYS	C-N-CA	7.20	129.92	120.28
11	R	33	ALA	O-C-N	7.20	129.78	122.08
4	D	477	SER	CA-C-O	-7.19	112.69	120.17
10	O	388	TYR	CA-CB-CG	-7.19	100.95	113.90
11	W	107	ALA	CA-C-N	7.19	131.83	120.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	W	107	ALA	C-N-CA	7.19	131.83	120.47
3	C	231	TYR	CA-C-N	7.19	128.82	119.84
3	C	231	TYR	C-N-CA	7.19	128.82	119.84
3	A	609	GLU	O-C-N	-7.19	114.33	122.09
4	F	273	HIS	ND1-CE1-NE2	7.18	115.58	108.40
5	Q	173	ASP	CA-CB-CG	7.18	119.78	112.60
4	B	430	LYS	CA-C-N	7.17	130.48	120.29
4	B	430	LYS	C-N-CA	7.17	130.48	120.29
3	A	516	ASP	CA-CB-CG	-7.17	105.43	112.60
3	E	87	ARG	NE-CZ-NH1	-7.17	114.33	121.50
7	K	76	THR	CA-C-N	7.17	129.88	120.28
7	K	76	THR	C-N-CA	7.17	129.88	120.28
8	P	25	VAL	N-CA-C	-7.17	98.07	108.11
7	G	41	GLN	CA-C-O	7.17	128.02	120.42
8	P	210	PHE	CA-CB-CG	7.17	120.97	113.80
10	O	30	THR	CA-C-N	7.17	129.76	120.44
10	O	30	THR	C-N-CA	7.17	129.76	120.44
11	U	14	ALA	N-CA-C	7.17	119.09	111.28
5	Q	344	VAL	CA-C-O	7.16	126.79	119.20
3	E	61	ILE	N-CA-C	-7.16	103.19	111.00
6	L	17	ALA	N-CA-C	7.15	119.08	111.28
8	P	9	ASP	N-CA-C	-7.15	102.86	112.94
11	R	146	VAL	CA-C-O	-7.15	113.52	120.95
11	W	57	VAL	N-CA-C	7.15	118.77	110.62
7	I	126	VAL	O-C-N	7.14	128.80	121.87
11	T	15	ILE	CA-C-N	7.14	127.87	119.94
11	T	15	ILE	C-N-CA	7.14	127.87	119.94
4	D	286	ASP	CA-C-N	7.14	129.84	120.28
4	D	286	ASP	C-N-CA	7.14	129.84	120.28
11	Z	11	PHE	CA-CB-CG	7.14	120.94	113.80
3	A	268	SER	N-CA-C	-7.13	103.50	111.28
7	G	126	VAL	N-CA-C	7.13	117.90	110.62
11	S	113	ASP	CA-C-N	7.13	131.15	120.31
11	S	113	ASP	C-N-CA	7.13	131.15	120.31
3	C	87	ARG	NE-CZ-NH2	7.13	125.62	119.20
1	M	20	THR	N-CA-CB	-7.13	99.32	110.30
6	L	87	ALA	O-C-N	-7.12	112.97	122.23
11	S	148	LEU	O-C-N	7.12	129.50	122.09
10	O	131	ILE	N-CA-C	-7.12	103.36	110.62
11	X	135	PHE	N-CA-CB	7.12	121.32	110.28
1	M	212	ASN	CA-C-N	7.12	130.40	120.29
1	M	212	ASN	C-N-CA	7.12	130.40	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	23	PHE	CA-CB-CG	7.12	120.92	113.80
11	R	93	ALA	CA-C-N	7.11	128.00	120.03
11	R	93	ALA	C-N-CA	7.11	128.00	120.03
11	Z	32	THR	O-C-N	7.11	129.77	122.09
3	C	279	ILE	N-CA-C	-7.11	97.37	107.75
4	D	339	ASN	OD1-CG-ND2	7.11	129.71	122.60
11	S	143	GLY	CA-C-O	-7.11	113.12	120.66
3	A	468	ASN	CB-CG-ND2	-7.11	105.74	116.40
1	M	27	GLN	CA-C-N	7.10	127.87	119.98
1	M	27	GLN	C-N-CA	7.10	127.87	119.98
4	F	80	PHE	CA-CB-CG	7.10	120.90	113.80
6	L	50	LYS	N-CA-CB	7.10	120.67	110.16
7	I	29	GLU	CA-C-N	7.10	129.80	120.28
7	I	29	GLU	C-N-CA	7.10	129.80	120.28
11	U	19	SER	CA-C-N	7.10	130.13	120.54
11	U	19	SER	C-N-CA	7.10	130.13	120.54
1	M	60	VAL	N-CA-C	-7.10	103.55	110.72
4	F	139	ILE	N-CA-C	-7.10	99.04	107.70
8	P	12	HIS	ND1-CE1-NE2	7.09	115.50	108.40
1	M	207	GLN	CA-C-N	7.09	129.78	120.28
1	M	207	GLN	C-N-CA	7.09	129.78	120.28
2	N	28	ILE	N-CA-C	-7.09	96.87	107.37
3	C	470	PHE	CA-CB-CG	-7.09	106.71	113.80
5	Q	242	LEU	O-C-N	-7.09	116.02	121.55
4	D	142	TYR	CA-C-N	7.09	135.08	121.54
4	D	142	TYR	C-N-CA	7.09	135.08	121.54
7	G	55	THR	O-C-N	-7.09	114.07	122.15
4	D	480	ILE	O-C-N	7.08	128.85	121.91
11	Y	119	SER	CA-C-N	7.08	130.10	120.54
11	Y	119	SER	C-N-CA	7.08	130.10	120.54
10	O	129	ASP	CA-CB-CG	7.08	119.68	112.60
10	O	119	ARG	N-CA-C	-7.08	103.88	114.64
10	O	160	ALA	CB-CA-C	-7.08	98.82	110.85
11	Z	138	VAL	CA-C-N	7.08	129.76	120.28
11	Z	138	VAL	C-N-CA	7.08	129.76	120.28
7	K	146	VAL	N-CA-CB	7.07	121.19	110.58
11	X	111	VAL	CA-C-N	7.07	127.98	119.99
11	X	111	VAL	C-N-CA	7.07	127.98	119.99
4	B	201	HIS	ND1-CE1-NE2	7.07	115.47	108.40
11	Y	75	CYS	N-CA-C	7.07	122.97	111.37
3	E	84	PRO	CA-C-O	-7.07	113.24	121.86
3	C	467	LEU	N-CA-C	7.07	118.98	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	396	GLY	N-CA-C	-7.07	100.95	110.56
7	K	34	GLU	N-CA-CB	7.07	120.62	110.16
11	Y	151	ASN	CA-C-N	7.07	129.75	120.28
11	Y	151	ASN	C-N-CA	7.07	129.75	120.28
11	T	139	LEU	O-C-N	-7.07	114.63	122.12
7	K	87	LYS	CA-C-N	7.06	129.46	120.56
7	K	87	LYS	C-N-CA	7.06	129.46	120.56
7	I	41	GLN	CA-C-N	7.06	130.31	120.29
7	I	41	GLN	C-N-CA	7.06	130.31	120.29
8	P	341	ASN	N-CA-C	-7.06	103.52	111.14
6	H	17	ALA	CA-C-N	7.06	129.74	120.28
6	H	17	ALA	C-N-CA	7.06	129.74	120.28
4	D	222	ALA	O-C-N	7.06	129.71	122.09
3	A	386	ALA	N-CA-CB	7.05	120.60	110.16
11	Y	108	ILE	N-CA-C	7.05	117.81	110.62
4	D	179	PRO	CA-C-N	7.04	129.72	120.28
4	D	179	PRO	C-N-CA	7.04	129.72	120.28
11	Y	70	VAL	N-CA-C	7.04	117.18	110.42
3	C	112	LEU	N-CA-C	-7.04	103.69	111.36
10	O	336	ASN	OD1-CG-ND2	-7.04	115.56	122.60
11	U	35	SER	CA-C-N	7.04	127.94	119.99
11	U	35	SER	C-N-CA	7.04	127.94	119.99
3	C	561	VAL	CA-C-N	7.03	130.28	120.29
3	C	561	VAL	C-N-CA	7.03	130.28	120.29
11	a	100	SER	N-CA-CB	7.03	120.21	110.01
11	Y	117	ARG	N-CA-C	-7.03	103.67	111.82
11	a	156	GLN	OE1-CD-NE2	7.02	129.62	122.60
4	F	322	VAL	CA-C-N	7.02	130.68	120.71
4	F	322	VAL	C-N-CA	7.02	130.68	120.71
8	P	176	ASN	CA-C-N	7.02	130.50	122.36
8	P	176	ASN	C-N-CA	7.02	130.50	122.36
3	C	176	PRO	N-CA-CB	7.02	109.45	103.35
11	Y	84	LEU	N-CA-C	-7.01	103.64	111.28
11	a	19	SER	N-CA-CB	7.01	120.39	109.94
1	M	206	VAL	CA-C-N	7.01	129.67	120.28
1	M	206	VAL	C-N-CA	7.01	129.67	120.28
3	C	567	TRP	CE2-CD2-CE3	7.01	125.81	118.80
3	A	528	GLN	N-CA-C	-7.00	102.82	113.89
9	b	208	ARG	N-CA-C	-7.00	102.58	113.02
11	T	145	ILE	N-CA-C	7.00	117.51	110.23
4	F	246	ASN	OD1-CG-ND2	-7.00	115.60	122.60
11	R	56	PRO	CB-CA-C	-7.00	101.93	113.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	129	MET	CA-C-N	7.00	129.63	120.60
11	T	129	MET	C-N-CA	7.00	129.63	120.60
4	B	124	PRO	CA-C-N	6.99	131.31	120.75
4	B	124	PRO	C-N-CA	6.99	131.31	120.75
4	D	93	VAL	O-C-N	-6.99	115.52	123.00
8	P	98	ASN	OD1-CG-ND2	6.99	129.59	122.60
11	X	23	PHE	CA-CB-CG	6.99	120.79	113.80
1	M	145	THR	N-CA-C	-6.99	103.66	111.28
5	Q	128	HIS	CE1-NE2-CD2	-6.98	102.02	109.00
11	S	73	LEU	CA-C-N	6.98	129.36	120.56
11	S	73	LEU	C-N-CA	6.98	129.36	120.56
4	F	320	GLY	N-CA-C	-6.98	103.60	111.63
10	O	250	ALA	CA-C-N	6.98	129.63	120.28
10	O	250	ALA	C-N-CA	6.98	129.63	120.28
11	U	104	ALA	CA-C-N	6.98	127.73	119.98
11	U	104	ALA	C-N-CA	6.98	127.73	119.98
6	H	26	LYS	CA-C-N	6.98	129.51	120.44
6	H	26	LYS	C-N-CA	6.98	129.51	120.44
6	J	29	GLN	CA-C-N	6.98	129.63	120.28
6	J	29	GLN	C-N-CA	6.98	129.63	120.28
8	P	225	GLN	OE1-CD-NE2	-6.98	115.62	122.60
10	O	244	GLN	N-CA-C	6.97	118.88	111.28
11	X	88	PHE	CA-CB-CG	-6.97	106.83	113.80
11	S	51	PHE	N-CA-C	6.97	118.88	111.28
6	L	90	LYS	CA-C-N	6.97	129.92	120.44
6	L	90	LYS	C-N-CA	6.97	129.92	120.44
7	K	120	ILE	CA-C-N	6.97	129.62	120.28
7	K	120	ILE	C-N-CA	6.97	129.62	120.28
4	D	182	GLU	CA-C-N	6.97	130.31	120.42
4	D	182	GLU	C-N-CA	6.97	130.31	120.42
5	Q	327	ALA	CA-C-N	6.97	129.62	120.28
5	Q	327	ALA	C-N-CA	6.97	129.62	120.28
4	F	386	ALA	O-C-N	6.96	129.61	122.09
6	H	92	ASP	CA-CB-CG	-6.96	105.64	112.60
3	E	213	HIS	N-CA-C	-6.96	98.73	109.52
11	Y	80	GLN	CA-C-O	6.96	127.97	119.97
11	W	153	ARG	CD-NE-CZ	-6.95	114.67	124.40
4	B	282	SER	CA-C-O	-6.95	112.25	120.10
11	Z	84	LEU	CA-C-N	6.95	129.59	120.28
11	Z	84	LEU	C-N-CA	6.95	129.59	120.28
4	D	40	ILE	CB-CA-C	6.95	121.10	110.96
4	F	367	LYS	O-C-N	6.95	130.07	122.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	151	HIS	CE1-NE2-CD2	-6.95	102.06	109.00
3	E	450	HIS	CB-CG-CD2	-6.94	122.18	131.20
4	B	374	ASN	N-CA-CB	6.94	121.74	110.43
8	P	19	ILE	O-C-N	6.94	128.71	121.91
3	E	478	PHE	CA-C-N	6.94	127.23	119.32
3	E	478	PHE	C-N-CA	6.94	127.23	119.32
7	G	26	LYS	CA-C-N	6.93	130.85	120.31
7	G	26	LYS	C-N-CA	6.93	130.85	120.31
6	H	91	LYS	O-C-N	6.93	129.21	122.07
11	R	143	GLY	CA-C-N	6.93	129.89	120.54
11	R	143	GLY	C-N-CA	6.93	129.89	120.54
3	C	120	GLN	N-CA-C	-6.93	101.66	111.56
11	Y	57	VAL	N-CA-C	6.93	118.52	110.62
3	C	492	ALA	CA-C-O	-6.92	113.22	120.55
9	b	245	ILE	CA-C-N	6.92	129.94	120.46
9	b	245	ILE	C-N-CA	6.92	129.94	120.46
11	Z	59	MET	CG-SD-CE	-6.92	85.68	100.90
3	E	486	LYS	CA-C-N	6.91	129.43	120.44
3	E	486	LYS	C-N-CA	6.91	129.43	120.44
11	U	18	ALA	N-CA-CB	6.91	120.33	109.82
11	a	108	ILE	O-C-N	-6.91	114.89	121.87
11	Z	116	VAL	N-CA-C	6.91	119.73	111.09
1	M	131	GLN	CA-C-O	-6.91	113.23	120.55
7	G	37	LEU	CA-C-N	6.91	130.23	120.28
7	G	37	LEU	C-N-CA	6.91	130.23	120.28
5	Q	65	THR	CA-C-N	6.91	129.83	120.44
5	Q	65	THR	C-N-CA	6.91	129.83	120.44
9	b	196	VAL	O-C-N	6.90	129.60	121.80
11	W	68	LEU	O-C-N	6.90	129.43	122.12
3	C	174	LEU	CA-C-N	6.90	127.48	120.38
3	C	174	LEU	C-N-CA	6.90	127.48	120.38
3	A	123	TYR	N-CA-C	-6.90	100.00	110.14
3	E	48	LEU	N-CA-C	-6.89	99.31	110.20
11	U	113	ASP	CA-C-O	6.89	128.66	121.07
3	E	218	ARG	N-CA-C	-6.89	104.84	113.18
1	M	70	GLU	CA-C-N	6.89	129.90	120.46
1	M	70	GLU	C-N-CA	6.89	129.90	120.46
3	C	340	ALA	CA-C-N	6.89	129.51	120.28
3	C	340	ALA	C-N-CA	6.89	129.51	120.28
3	A	296	GLU	CA-C-O	-6.89	112.05	119.97
11	a	33	ALA	N-CA-CB	6.89	120.29	109.82
4	B	255	THR	O-C-N	-6.88	114.35	120.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	V	94	GLY	CA-C-N	6.88	129.83	120.54
11	V	94	GLY	C-N-CA	6.88	129.83	120.54
8	P	371	SER	CB-CA-C	-6.88	102.37	110.76
3	E	339	LEU	CA-C-N	6.88	129.50	120.28
3	E	339	LEU	C-N-CA	6.88	129.50	120.28
11	S	51	PHE	CA-CB-CG	-6.88	106.92	113.80
4	B	220	GLU	CA-C-O	6.88	127.84	120.55
4	F	190	GLN	OE1-CD-NE2	6.87	129.47	122.60
4	B	159	ASP	CB-CA-C	-6.87	100.05	110.90
3	E	83	ASP	CA-C-O	6.87	126.78	120.60
3	E	288	ASN	CA-CB-CG	-6.87	105.73	112.60
7	I	49	ASN	CB-CA-C	-6.86	100.10	110.88
8	P	364	ASP	N-CA-C	6.86	118.41	111.07
1	M	54	LYS	CA-C-N	6.86	130.03	120.29
1	M	54	LYS	C-N-CA	6.86	130.03	120.29
4	B	85	GLY	N-CA-C	-6.86	105.41	115.63
11	V	107	ALA	N-CA-C	6.86	118.41	111.07
4	F	301	ARG	CA-C-N	6.86	132.34	122.40
4	F	301	ARG	C-N-CA	6.86	132.34	122.40
3	C	90	LYS	CA-C-O	-6.86	113.11	119.76
7	I	16	GLU	N-CA-CB	6.86	120.86	110.30
5	Q	47	SER	N-CA-C	6.86	120.53	111.75
9	b	28	ASP	CA-C-N	6.86	129.70	120.65
9	b	28	ASP	C-N-CA	6.86	129.70	120.65
11	Z	49	LEU	CA-C-N	6.85	131.10	120.82
11	Z	49	LEU	C-N-CA	6.85	131.10	120.82
8	P	269	SER	O-C-N	6.85	129.22	122.09
3	E	417	SER	O-C-N	-6.85	117.06	121.85
3	E	425	ASP	CA-CB-CG	6.85	119.45	112.60
11	T	53	ASN	N-CA-C	6.85	119.33	111.11
3	E	174	LEU	N-CA-C	-6.85	101.02	109.65
10	O	340	CYS	N-CA-C	6.85	118.40	111.07
11	T	12	PHE	CA-C-N	6.85	127.41	119.94
11	T	12	PHE	C-N-CA	6.85	127.41	119.94
3	E	587	PHE	CA-CB-CG	-6.85	106.95	113.80
3	A	106	ASP	CA-CB-CG	-6.84	105.75	112.60
3	A	612	ALA	CA-C-N	6.84	129.45	120.28
3	A	612	ALA	C-N-CA	6.84	129.45	120.28
5	Q	254	PHE	N-CA-CB	6.84	120.29	110.16
11	S	85	TYR	N-CA-CB	-6.84	100.06	110.12
8	P	390	ASP	N-CA-C	-6.84	96.23	110.80
8	P	206	HIS	CG-CD2-NE2	6.84	114.04	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	230	ILE	N-CA-C	-6.84	99.25	108.96
11	R	23	PHE	CA-CB-CG	-6.84	106.96	113.80
3	A	185	ILE	N-CA-CB	6.83	120.07	111.46
9	b	276	LYS	N-CA-C	6.83	118.73	111.28
11	X	48	ASP	CA-CB-CG	6.83	119.43	112.60
3	C	174	LEU	N-CA-C	-6.83	101.04	109.65
1	M	67	SER	N-CA-CB	6.83	120.16	110.12
3	C	435	THR	N-CA-C	-6.83	101.07	110.35
11	U	76	TYR	N-CA-C	6.82	119.56	111.71
7	K	148	LEU	CA-C-N	6.82	129.15	120.56
7	K	148	LEU	C-N-CA	6.82	129.15	120.56
4	F	71	ARG	NE-CZ-NH2	-6.82	113.06	119.20
10	O	372	HIS	CE1-NE2-CD2	-6.82	102.18	109.00
3	A	175	PRO	CA-C-N	6.82	126.58	119.76
3	A	175	PRO	C-N-CA	6.82	126.58	119.76
6	L	35	ALA	CA-C-N	6.82	130.67	120.31
6	L	35	ALA	C-N-CA	6.82	130.67	120.31
7	I	210	LEU	CA-C-N	6.81	129.71	120.38
7	I	210	LEU	C-N-CA	6.81	129.71	120.38
11	U	129	MET	CA-C-N	6.81	129.39	120.60
11	U	129	MET	C-N-CA	6.81	129.39	120.60
3	C	474	ASN	CA-CB-CG	6.81	119.41	112.60
3	A	381	PRO	CA-C-N	6.80	133.04	121.14
3	A	381	PRO	C-N-CA	6.80	133.04	121.14
7	I	53	ASN	CB-CA-C	-6.80	99.50	110.79
11	U	28	ALA	CA-C-O	-6.80	113.21	120.42
3	A	374	MET	O-C-N	6.80	128.63	121.42
3	A	516	ASP	CB-CA-C	-6.80	100.16	110.90
7	I	211	SER	N-CA-CB	6.80	120.25	110.06
11	U	89	ILE	CB-CA-C	-6.79	103.14	112.24
11	a	57	VAL	N-CA-CB	6.79	118.50	110.55
4	F	400	SER	N-CA-CB	-6.79	99.88	110.06
3	A	292	GLU	N-CA-C	6.79	118.47	111.14
3	C	60	VAL	CB-CA-C	6.79	119.87	111.25
4	B	144	ARG	N-CA-CB	6.79	120.91	110.80
3	A	168	SER	N-CA-CB	6.78	120.47	109.95
11	V	28	ALA	CA-C-N	6.78	129.26	120.44
11	V	28	ALA	C-N-CA	6.78	129.26	120.44
1	M	93	LYS	N-CA-C	-6.78	99.55	109.18
3	A	517	VAL	N-CA-C	-6.78	103.87	110.72
4	B	229	PHE	CA-C-N	6.78	129.25	120.44
4	B	229	PHE	C-N-CA	6.78	129.25	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	198	LYS	N-CA-C	6.78	119.68	111.82
3	E	164	ASN	OD1-CG-ND2	-6.78	115.82	122.60
8	P	332	ASP	CA-C-N	6.77	129.35	120.28
8	P	332	ASP	C-N-CA	6.77	129.35	120.28
10	O	23	VAL	CA-C-N	6.77	129.91	120.29
10	O	23	VAL	C-N-CA	6.77	129.91	120.29
4	B	310	THR	CA-C-N	6.77	129.24	120.44
4	B	310	THR	C-N-CA	6.77	129.24	120.44
9	b	241	HIS	ND1-CE1-NE2	6.77	115.17	108.40
7	G	24	ILE	CA-C-O	-6.77	114.00	121.17
8	P	125	GLU	N-CA-C	-6.77	103.90	111.28
6	H	39	ALA	N-CA-C	-6.77	104.03	112.90
3	A	213	HIS	CE1-NE2-CD2	-6.77	102.23	109.00
3	A	374	MET	CA-C-O	-6.76	113.74	119.76
4	D	249	THR	CA-C-N	6.76	129.72	120.46
4	D	249	THR	C-N-CA	6.76	129.72	120.46
11	Z	93	ALA	N-CA-C	-6.76	103.38	111.69
10	O	236	VAL	O-C-N	-6.76	115.55	123.05
10	O	249	ALA	O-C-N	-6.75	114.96	122.12
8	P	180	MET	N-CA-C	-6.75	103.85	111.07
3	E	579	HIS	CE1-NE2-CD2	-6.75	102.25	109.00
1	M	34	ARG	NE-CZ-NH1	6.75	128.25	121.50
10	O	219	PRO	CA-C-N	6.75	131.70	122.19
10	O	219	PRO	C-N-CA	6.75	131.70	122.19
6	H	61	ASN	CA-C-N	6.74	131.97	120.71
6	H	61	ASN	C-N-CA	6.74	131.97	120.71
4	F	248	PRO	CA-C-N	6.74	129.31	120.28
4	F	248	PRO	C-N-CA	6.74	129.31	120.28
4	D	181	ASN	OD1-CG-ND2	6.74	129.34	122.60
8	P	158	VAL	CA-C-N	6.74	129.31	120.28
8	P	158	VAL	C-N-CA	6.74	129.31	120.28
11	V	103	ALA	CA-C-N	6.74	129.20	120.44
11	V	103	ALA	C-N-CA	6.74	129.20	120.44
5	Q	144	ASP	CA-C-N	6.74	129.85	120.29
5	Q	144	ASP	C-N-CA	6.74	129.85	120.29
5	Q	345	TYR	N-CA-CB	6.74	121.95	110.50
4	B	158	ILE	O-C-N	6.73	129.14	121.94
6	L	99	ILE	N-CA-C	-6.73	104.20	110.53
3	E	552	SER	CA-C-O	-6.73	113.29	120.42
3	E	145	LYS	CA-C-O	6.73	126.54	119.14
6	J	8	ALA	CA-C-N	6.72	129.84	120.29
6	J	8	ALA	C-N-CA	6.72	129.84	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	153	ARG	CA-C-N	6.72	129.18	120.44
11	a	153	ARG	C-N-CA	6.72	129.18	120.44
11	V	96	SER	CB-CA-C	-6.72	100.06	110.81
3	C	479	PRO	CA-C-N	6.72	129.96	120.42
3	C	479	PRO	C-N-CA	6.72	129.96	120.42
4	D	329	ILE	N-CA-C	-6.72	97.94	107.75
4	B	304	TYR	CA-C-N	6.72	128.24	119.84
4	B	304	TYR	C-N-CA	6.72	128.24	119.84
10	O	76	GLY	CA-C-N	6.71	129.17	120.44
10	O	76	GLY	C-N-CA	6.71	129.17	120.44
10	O	365	ASN	N-CA-CB	6.71	122.09	110.81
3	C	388	LEU	N-CA-C	6.71	118.60	111.28
11	V	86	THR	N-CA-C	-6.71	104.04	111.36
8	P	456	HIS	CE1-NE2-CD2	-6.71	102.29	109.00
10	O	35	ASN	CA-C-O	-6.71	113.79	120.70
10	O	236	VAL	N-CA-C	-6.71	98.52	108.45
6	J	2	SER	CA-C-N	6.71	129.56	120.44
6	J	2	SER	C-N-CA	6.71	129.56	120.44
11	R	141	LEU	N-CA-C	6.70	119.16	111.11
11	V	128	GLY	CA-C-N	6.70	129.56	120.44
11	V	128	GLY	C-N-CA	6.70	129.56	120.44
3	E	62	ARG	CA-C-N	6.70	132.47	122.75
3	E	62	ARG	C-N-CA	6.70	132.47	122.75
9	b	239	PHE	O-C-N	-6.70	114.48	123.19
3	C	438	PHE	CA-CB-CG	6.70	120.50	113.80
4	F	159	ASP	N-CA-CB	6.70	119.72	110.01
4	F	207	ASN	OD1-CG-ND2	6.70	129.29	122.60
3	C	601	GLU	CB-CA-C	-6.69	99.47	110.85
3	E	586	PHE	N-CA-C	-6.69	103.42	112.26
3	E	110	ARG	CA-C-O	-6.69	112.80	120.03
7	I	190	VAL	N-CA-C	-6.69	98.79	108.36
7	K	38	LYS	CA-C-N	6.69	129.79	120.29
7	K	38	LYS	C-N-CA	6.69	129.79	120.29
5	Q	50	ASP	CA-CB-CG	6.69	119.29	112.60
8	P	450	ILE	CA-C-N	6.69	129.24	120.28
8	P	450	ILE	C-N-CA	6.69	129.24	120.28
3	E	324	MET	O-C-N	6.69	128.92	121.43
3	A	429	THR	N-CA-CB	6.68	119.95	110.12
6	L	51	ASP	CA-C-N	6.68	129.13	120.44
6	L	51	ASP	C-N-CA	6.68	129.13	120.44
5	Q	52	GLY	CA-C-N	6.68	129.23	120.28
5	Q	52	GLY	C-N-CA	6.68	129.23	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	82	ASP	CA-C-O	6.68	127.63	120.55
3	A	286	ARG	CB-CA-C	-6.68	99.49	110.85
1	M	65	ALA	N-CA-CB	6.68	120.04	110.16
7	K	127	GLU	CA-C-N	6.68	129.77	120.29
7	K	127	GLU	C-N-CA	6.68	129.77	120.29
8	P	121	PRO	CA-C-N	6.68	129.77	120.29
8	P	121	PRO	C-N-CA	6.68	129.77	120.29
11	X	34	LYS	O-C-N	6.67	129.03	122.09
11	V	55	VAL	CA-C-N	6.67	128.18	119.84
11	V	55	VAL	C-N-CA	6.67	128.18	119.84
10	O	224	VAL	CA-C-O	6.67	128.85	121.04
3	A	142	THR	CA-CB-OG1	6.67	119.61	109.60
5	Q	157	PRO	N-CA-CB	6.67	109.94	102.60
11	Z	117	ARG	CA-C-O	6.67	127.64	119.97
3	E	545	ASP	CB-CA-C	-6.67	99.73	110.79
8	P	85	SER	CA-C-N	6.67	129.50	120.44
8	P	85	SER	C-N-CA	6.67	129.50	120.44
11	Z	35	SER	N-CA-CB	6.67	119.92	110.12
4	F	361	ASP	CA-C-N	6.66	129.75	120.29
4	F	361	ASP	C-N-CA	6.66	129.75	120.29
10	O	30	THR	N-CA-C	-6.66	104.10	111.36
4	D	344	HIS	CA-C-N	6.66	127.19	119.47
4	D	344	HIS	C-N-CA	6.66	127.19	119.47
4	F	204	HIS	CB-CG-CD2	-6.66	122.55	131.20
11	Z	94	GLY	CA-C-N	6.66	129.20	120.28
11	Z	94	GLY	C-N-CA	6.66	129.20	120.28
8	P	301	ARG	N-CA-C	6.66	118.54	111.28
6	H	43	ILE	N-CA-CB	6.66	120.11	110.52
11	X	18	ALA	O-C-N	-6.65	114.96	122.08
11	a	32	THR	O-C-N	-6.65	115.22	122.07
3	C	397	LYS	CB-CG-CD	6.65	126.60	111.30
4	D	243	ASN	N-CA-C	-6.65	98.06	108.90
8	P	51	LEU	CA-C-O	6.65	127.47	120.42
3	C	597	HIS	CE1-NE2-CD2	-6.65	102.35	109.00
10	O	101	PRO	N-CA-CB	6.65	109.25	103.27
3	E	83	ASP	N-CA-CB	6.65	118.07	110.03
10	O	219	PRO	N-CA-CB	6.65	109.52	103.34
8	P	294	ILE	CA-C-N	6.64	129.18	120.28
8	P	294	ILE	C-N-CA	6.64	129.18	120.28
3	A	224	THR	N-CA-CB	6.64	119.83	110.07
8	P	147	VAL	CA-C-O	-6.64	113.81	120.85
11	V	91	LEU	CA-C-O	-6.64	113.77	121.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	157	ASN	CB-CA-C	-6.63	100.55	110.24
8	P	377	ASN	CA-C-N	6.63	128.43	120.14
8	P	377	ASN	C-N-CA	6.63	128.43	120.14
10	O	190	HIS	ND1-CE1-NE2	6.63	115.03	108.40
3	E	525	PHE	CA-CB-CG	-6.63	107.17	113.80
11	Y	143	GLY	O-C-N	-6.63	115.83	122.19
3	A	384	LEU	CA-C-N	6.63	127.34	119.98
3	A	384	LEU	C-N-CA	6.63	127.34	119.98
3	C	448	ARG	N-CA-CB	6.62	121.15	110.42
4	B	450	GLU	CB-CG-CD	-6.62	101.34	112.60
2	N	31	GLU	N-CA-C	-6.62	105.11	113.72
4	B	94	GLU	N-CA-C	-6.62	97.80	109.06
3	E	230	ASP	CA-CB-CG	6.62	119.22	112.60
4	F	137	SER	CA-C-O	-6.62	111.92	118.34
3	A	608	GLN	CA-C-N	6.62	129.44	120.44
3	A	608	GLN	C-N-CA	6.62	129.44	120.44
8	P	382	ASP	CA-C-O	-6.62	113.40	120.42
3	C	442	ASP	CA-CB-CG	6.62	119.22	112.60
6	L	25	ARG	N-CA-C	-6.62	104.15	111.36
3	A	213	HIS	CB-CG-ND1	-6.62	112.78	122.70
9	b	47	LYS	CA-C-N	6.62	128.90	120.56
9	b	47	LYS	C-N-CA	6.62	128.90	120.56
9	b	199	LEU	CA-C-N	6.62	129.04	120.44
9	b	199	LEU	C-N-CA	6.62	129.04	120.44
3	A	320	ASN	CA-CB-CG	-6.61	105.99	112.60
4	B	196	PRO	N-CA-CB	6.61	110.53	103.52
7	K	216	PRO	CA-C-N	6.61	129.14	120.28
7	K	216	PRO	C-N-CA	6.61	129.14	120.28
2	N	38	PHE	CA-C-N	6.61	130.63	122.37
2	N	38	PHE	C-N-CA	6.61	130.63	122.37
4	B	204	HIS	CG-CD2-NE2	6.61	113.81	107.20
3	A	135	ARG	NE-CZ-NH2	6.61	125.15	119.20
7	I	208	LYS	N-CA-CB	6.61	119.94	110.16
2	N	85	THR	N-CA-C	-6.61	103.45	113.89
3	C	442	ASP	CA-C-O	-6.61	113.18	120.38
3	A	599	GLU	N-CA-C	6.60	118.48	111.28
4	D	241	PHE	CA-CB-CG	-6.60	107.20	113.80
3	A	486	LYS	CA-C-N	6.60	129.12	120.28
3	A	486	LYS	C-N-CA	6.60	129.12	120.28
3	A	493	GLU	CA-C-N	6.60	129.12	120.28
3	A	493	GLU	C-N-CA	6.60	129.12	120.28
8	P	333	GLU	CA-C-O	6.60	127.55	120.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	b	304	LYS	CA-C-N	6.60	129.12	120.28
9	b	304	LYS	C-N-CA	6.60	129.12	120.28
11	V	46	ARG	NE-CZ-NH1	-6.60	114.90	121.50
10	O	85	ILE	CA-C-O	-6.60	114.09	120.95
11	U	66	TYR	CA-C-N	6.59	127.42	120.03
11	U	66	TYR	C-N-CA	6.59	127.42	120.03
9	b	322	ILE	N-CA-CB	6.59	117.54	110.62
11	U	93	ALA	CA-C-N	6.59	127.44	119.99
11	U	93	ALA	C-N-CA	6.59	127.44	119.99
11	T	60	ALA	CA-C-N	6.59	128.59	120.22
11	T	60	ALA	C-N-CA	6.59	128.59	120.22
10	O	79	ILE	N-CA-CB	6.59	119.50	110.54
10	O	107	VAL	N-CA-CB	-6.59	106.35	110.50
11	Z	88	PHE	CA-CB-CG	-6.59	107.21	113.80
8	P	237	HIS	ND1-CE1-NE2	6.59	114.99	108.40
10	O	183	ASP	CA-CB-CG	-6.58	106.02	112.60
8	P	338	ASP	CA-CB-CG	-6.58	106.02	112.60
3	C	55	ASN	CA-CB-CG	6.58	119.18	112.60
4	F	79	VAL	CA-C-N	6.58	131.87	120.68
4	F	79	VAL	C-N-CA	6.58	131.87	120.68
4	F	463	SER	N-CA-CB	6.58	119.80	110.12
3	A	538	CYS	CA-C-O	-6.58	113.43	119.62
11	T	94	GLY	CA-C-N	6.58	129.43	120.54
11	T	94	GLY	C-N-CA	6.58	129.43	120.54
1	M	64	ALA	CA-C-N	6.58	129.63	120.29
1	M	64	ALA	C-N-CA	6.58	129.63	120.29
2	N	72	HIS	CE1-NE2-CD2	-6.58	102.42	109.00
4	B	427	ILE	CA-C-N	6.58	129.09	120.28
4	B	427	ILE	C-N-CA	6.58	129.09	120.28
6	L	18	HIS	CG-CD2-NE2	6.58	113.78	107.20
10	O	281	GLU	CA-C-N	6.58	129.09	120.28
10	O	281	GLU	C-N-CA	6.58	129.09	120.28
3	C	53	HIS	CE1-NE2-CD2	-6.57	102.43	109.00
11	W	12	PHE	CB-CA-C	-6.57	97.33	109.29
4	F	112	ILE	CA-C-N	6.57	133.85	122.82
4	F	112	ILE	C-N-CA	6.57	133.85	122.82
11	V	51	PHE	N-CA-C	6.57	119.28	111.33
11	W	111	VAL	CA-C-O	-6.57	114.44	121.27
4	F	111	ARG	NE-CZ-NH1	-6.57	114.94	121.50
3	A	365	ARG	NE-CZ-NH2	6.56	125.11	119.20
4	D	247	ASP	N-CA-C	-6.56	101.86	110.39
11	X	138	VAL	O-C-N	6.56	128.32	121.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	100	GLU	N-CA-C	6.56	118.43	111.28
4	B	326	ASN	CA-CB-CG	-6.56	106.04	112.60
4	F	224	PHE	CA-CB-CG	6.56	120.36	113.80
1	M	213	GLU	N-CA-C	-6.55	104.22	111.36
4	F	273	HIS	CE1-NE2-CD2	-6.55	102.44	109.00
11	Z	122	GLN	CA-C-N	6.55	126.06	119.24
11	Z	122	GLN	C-N-CA	6.55	126.06	119.24
1	M	110	GLU	CA-C-O	-6.55	113.05	120.32
11	X	153	ARG	CA-C-N	6.55	129.36	120.38
11	X	153	ARG	C-N-CA	6.55	129.36	120.38
3	C	360	TRP	CA-C-N	6.55	129.06	120.28
3	C	360	TRP	C-N-CA	6.55	129.06	120.28
9	b	142	ARG	CA-C-N	6.55	129.06	120.28
9	b	142	ARG	C-N-CA	6.55	129.06	120.28
11	S	139	LEU	N-CA-C	-6.55	104.06	111.07
9	b	137	ASP	CA-CB-CG	-6.55	106.05	112.60
5	Q	49	THR	CA-C-N	6.55	129.05	120.28
5	Q	49	THR	C-N-CA	6.55	129.05	120.28
5	Q	180	ILE	CA-C-O	-6.55	114.23	121.17
11	U	118	GLY	CA-C-N	6.55	131.60	121.19
11	U	118	GLY	C-N-CA	6.55	131.60	121.19
11	Y	35	SER	CA-C-N	6.54	134.24	121.41
11	Y	35	SER	C-N-CA	6.54	134.24	121.41
7	K	153	LYS	CA-C-N	6.54	128.94	120.44
7	K	153	LYS	C-N-CA	6.54	128.94	120.44
11	W	145	ILE	N-CA-C	6.54	117.03	110.23
3	A	483	ASP	CA-CB-CG	-6.54	106.06	112.60
11	X	146	VAL	CA-C-N	6.54	129.36	120.54
11	X	146	VAL	C-N-CA	6.54	129.36	120.54
4	B	199	ASP	O-C-N	6.54	129.05	122.12
8	P	22	SER	N-CA-CB	6.54	119.73	110.12
3	C	328	ALA	CA-C-O	-6.53	112.46	119.97
1	M	162	VAL	CA-C-O	-6.53	113.93	120.85
5	Q	18	ARG	CA-C-N	6.53	127.18	120.00
5	Q	18	ARG	C-N-CA	6.53	127.18	120.00
11	Y	90	GLN	O-C-N	6.53	129.14	122.09
5	Q	89	GLY	CA-C-N	6.53	130.23	120.31
5	Q	89	GLY	C-N-CA	6.53	130.23	120.31
7	G	76	THR	CA-C-N	6.53	129.68	120.28
7	G	76	THR	C-N-CA	6.53	129.68	120.28
11	V	150	LEU	CA-C-N	6.52	129.35	120.54
11	V	150	LEU	C-N-CA	6.52	129.35	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	218	ILE	CA-C-N	6.52	129.02	120.28
7	G	218	ILE	C-N-CA	6.52	129.02	120.28
11	S	104	ALA	CA-C-N	6.52	128.50	120.22
11	S	104	ALA	C-N-CA	6.52	128.50	120.22
5	Q	116	HIS	CB-CG-CD2	-6.52	122.73	131.20
3	C	576	ASP	CA-CB-CG	-6.51	106.09	112.60
4	F	130	ASP	CA-CB-CG	-6.51	106.09	112.60
9	b	76	LEU	CA-C-N	6.51	129.33	120.54
9	b	76	LEU	C-N-CA	6.51	129.33	120.54
11	R	86	THR	CA-C-N	6.51	127.35	119.99
11	R	86	THR	C-N-CA	6.51	127.35	119.99
3	A	337	ILE	O-C-N	6.51	128.54	121.83
3	A	179	ARG	CA-C-O	-6.51	114.48	121.38
11	X	142	TYR	CA-CB-CG	6.51	125.61	113.90
11	a	22	ILE	CA-C-N	6.51	129.00	120.28
11	a	22	ILE	C-N-CA	6.51	129.00	120.28
1	M	210	LYS	O-C-N	6.50	128.77	122.07
8	P	310	LYS	CA-C-N	6.50	128.89	120.44
8	P	310	LYS	C-N-CA	6.50	128.89	120.44
8	P	425	ASN	CA-C-N	6.50	128.99	120.28
8	P	425	ASN	C-N-CA	6.50	128.99	120.28
11	R	153	ARG	CA-C-N	6.50	129.29	120.38
11	R	153	ARG	C-N-CA	6.50	129.29	120.38
11	S	89	ILE	CA-C-N	6.50	128.89	120.44
11	S	89	ILE	C-N-CA	6.50	128.89	120.44
11	Y	114	ALA	N-CA-C	6.50	119.36	111.82
11	R	49	LEU	CA-C-N	6.50	131.53	121.19
11	R	49	LEU	C-N-CA	6.50	131.53	121.19
3	E	475	TYR	O-C-N	-6.50	113.85	121.32
11	a	71	SER	CA-C-N	6.50	128.75	120.56
11	a	71	SER	C-N-CA	6.50	128.75	120.56
11	T	48	ASP	CA-CB-CG	-6.50	106.10	112.60
3	A	213	HIS	ND1-CE1-NE2	6.50	114.89	108.40
4	F	107	ASP	CA-C-N	6.49	129.28	120.38
4	F	107	ASP	C-N-CA	6.49	129.28	120.38
4	B	277	ILE	N-CA-CB	6.49	120.08	111.64
3	E	542	LYS	CA-C-N	6.49	128.97	120.28
3	E	542	LYS	C-N-CA	6.49	128.97	120.28
4	B	181	ASN	CA-CB-CG	-6.49	106.11	112.60
8	P	242	LEU	N-CA-CB	6.49	119.42	110.01
9	b	143	PHE	CA-CB-CG	-6.49	107.31	113.80
3	E	591	ARG	N-CA-C	-6.49	103.88	113.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	145	ASP	O-C-N	-6.49	114.37	122.35
10	O	3	THR	N-CA-C	-6.49	104.78	114.64
3	C	539	PRO	CA-C-N	6.48	130.72	120.47
3	C	539	PRO	C-N-CA	6.48	130.72	120.47
4	D	210	ILE	CB-CA-C	-6.48	100.86	110.33
7	K	83	LYS	CB-CA-C	-6.48	98.22	110.67
8	P	117	PHE	CA-C-N	6.48	128.97	120.28
8	P	117	PHE	C-N-CA	6.48	128.97	120.28
11	Z	100	SER	CA-C-N	6.48	127.31	119.99
11	Z	100	SER	C-N-CA	6.48	127.31	119.99
1	M	181	THR	CA-C-O	-6.48	113.55	120.42
3	E	66	ASP	CA-CB-CG	-6.48	106.12	112.60
11	Z	33	ALA	N-CA-C	6.48	118.03	110.97
7	K	11	ASN	CA-CB-CG	-6.48	106.12	112.60
9	b	21	ILE	CA-C-N	6.48	127.01	120.14
9	b	21	ILE	C-N-CA	6.48	127.01	120.14
4	D	77	VAL	N-CA-C	-6.47	99.16	108.48
4	F	356	GLY	N-CA-C	-6.47	102.50	111.76
6	J	56	GLU	N-CA-C	6.47	118.42	111.36
11	V	105	GLY	CA-C-N	6.47	129.25	120.44
11	V	105	GLY	C-N-CA	6.47	129.25	120.44
4	F	357	GLN	N-CA-CB	6.47	121.40	111.56
3	C	100	LEU	CB-CA-C	-6.47	99.92	110.79
1	M	45	ASP	CA-CB-CG	6.47	119.07	112.60
6	H	46	TYR	CA-C-O	6.47	127.42	119.79
11	W	107	ALA	N-CA-C	6.47	118.87	111.11
11	R	148	LEU	CA-C-N	6.47	128.85	120.44
11	R	148	LEU	C-N-CA	6.47	128.85	120.44
11	Z	34	LYS	CA-C-N	6.47	128.94	120.28
11	Z	34	LYS	C-N-CA	6.47	128.94	120.28
11	S	154	ALA	N-CA-C	6.47	118.87	111.11
11	X	40	CYS	CA-C-N	6.46	129.23	120.44
11	X	40	CYS	C-N-CA	6.46	129.23	120.44
3	A	353	ILE	CB-CA-C	6.46	120.39	110.96
3	A	108	ILE	CA-C-N	6.46	132.17	122.68
3	A	108	ILE	C-N-CA	6.46	132.17	122.68
10	O	42	ARG	CA-C-N	6.46	129.92	120.82
10	O	42	ARG	C-N-CA	6.46	129.92	120.82
8	P	419	ILE	CA-C-N	6.45	128.69	120.56
8	P	419	ILE	C-N-CA	6.45	128.69	120.56
7	G	118	LYS	CA-C-N	6.45	126.03	119.19
7	G	118	LYS	C-N-CA	6.45	126.03	119.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	S	127	VAL	CA-C-N	6.45	128.41	120.22
11	S	127	VAL	C-N-CA	6.45	128.41	120.22
4	D	304	TYR	CA-C-N	6.45	127.90	119.84
4	D	304	TYR	C-N-CA	6.45	127.90	119.84
7	K	92	ARG	NE-CZ-NH2	-6.45	113.39	119.20
1	M	57	MET	CA-C-N	6.45	127.28	119.99
1	M	57	MET	C-N-CA	6.45	127.28	119.99
4	D	339	ASN	N-CA-CB	6.45	121.39	110.49
5	Q	35	GLN	N-CA-C	6.45	119.13	111.33
11	R	80	GLN	N-CA-C	-6.45	104.46	112.90
1	M	90	ALA	CA-C-N	6.44	129.20	120.44
1	M	90	ALA	C-N-CA	6.44	129.20	120.44
11	X	34	LYS	N-CA-C	6.44	118.84	111.11
11	X	123	PRO	N-CA-CB	6.44	110.02	103.25
4	D	223	ARG	CA-C-N	6.44	128.91	120.28
4	D	223	ARG	C-N-CA	6.44	128.91	120.28
3	A	491	ASN	CA-C-O	-6.44	113.59	120.42
9	b	150	GLU	N-CA-C	6.44	118.38	111.36
11	a	32	THR	CA-C-N	6.44	129.74	120.79
11	a	32	THR	C-N-CA	6.44	129.74	120.79
10	O	127	ILE	N-CA-C	6.44	117.19	110.62
8	P	108	LYS	N-CA-C	-6.44	105.96	113.88
8	P	339	ILE	N-CA-CB	6.43	118.08	110.55
10	O	71	VAL	N-CA-CB	6.43	119.29	110.54
3	E	273	SER	N-CA-CB	6.43	119.18	109.34
3	C	466	VAL	O-C-N	6.43	128.45	121.83
4	D	343	THR	CA-C-N	6.43	129.28	120.67
4	D	343	THR	C-N-CA	6.43	129.28	120.67
4	B	396	HIS	CA-C-N	6.43	128.38	120.22
4	B	396	HIS	C-N-CA	6.43	128.38	120.22
8	P	425	ASN	CA-CB-CG	6.43	119.03	112.60
11	U	30	TYR	CA-C-N	6.43	127.25	119.99
11	U	30	TYR	C-N-CA	6.43	127.25	119.99
11	a	84	LEU	CA-C-O	6.43	127.32	120.70
3	C	569	LYS	CA-C-N	6.43	128.89	120.28
3	C	569	LYS	C-N-CA	6.43	128.89	120.28
10	O	266	LEU	CA-C-N	6.43	128.66	120.56
10	O	266	LEU	C-N-CA	6.43	128.66	120.56
8	P	263	LEU	N-CA-CB	6.43	119.33	110.01
7	G	43	TYR	CA-C-N	6.43	128.79	120.44
7	G	43	TYR	C-N-CA	6.43	128.79	120.44
4	D	300	GLY	CA-C-O	-6.42	115.12	121.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	7	LEU	CA-C-O	-6.42	113.75	121.40
11	X	54	ILE	CA-C-O	-6.42	113.64	120.64
2	N	9	ALA	CA-C-N	-6.42	114.06	122.99
2	N	9	ALA	C-N-CA	-6.42	114.06	122.99
4	B	459	ASP	N-CA-CB	6.42	119.66	110.16
7	I	105	GLU	CA-C-N	6.42	128.88	120.28
7	I	105	GLU	C-N-CA	6.42	128.88	120.28
11	Z	66	TYR	CA-C-N	6.42	127.25	119.99
11	Z	66	TYR	C-N-CA	6.42	127.25	119.99
10	O	168	GLY	CA-C-N	6.42	129.83	120.71
10	O	168	GLY	C-N-CA	6.42	129.83	120.71
3	C	575	GLY	CA-C-N	6.42	129.40	120.29
3	C	575	GLY	C-N-CA	6.42	129.40	120.29
11	a	158	VAL	N-CA-CB	6.42	120.14	110.13
11	a	95	LEU	CB-CA-C	-6.42	100.55	110.81
11	W	27	GLY	N-CA-C	6.41	120.40	112.64
4	B	404	TYR	CB-CG-CD2	-6.41	111.19	120.80
11	a	131	LEU	CA-C-O	-6.41	113.71	120.63
11	V	65	ILE	CA-C-N	6.41	129.16	120.44
11	V	65	ILE	C-N-CA	6.41	129.16	120.44
4	D	267	ALA	O-C-N	6.41	128.67	122.07
6	J	95	VAL	CB-CA-C	-6.41	103.64	112.04
3	C	588	GLU	CA-C-N	6.41	126.09	119.56
3	C	588	GLU	C-N-CA	6.41	126.09	119.56
8	P	11	THR	N-CA-C	6.41	118.34	111.36
8	P	120	ASP	CA-C-N	6.41	126.09	119.56
8	P	120	ASP	C-N-CA	6.41	126.09	119.56
5	Q	290	GLN	CA-C-O	6.40	127.21	120.42
5	Q	234	ASP	CA-CB-CG	-6.40	106.20	112.60
2	N	25	ILE	N-CA-CB	6.40	121.79	111.23
11	X	101	GLY	CA-C-O	-6.40	114.09	121.00
11	T	126	PHE	CA-C-N	6.40	130.58	120.47
11	T	126	PHE	C-N-CA	6.40	130.58	120.47
11	S	106	PHE	CA-C-N	6.39	128.75	120.44
11	S	106	PHE	C-N-CA	6.39	128.75	120.44
9	b	186	TYR	N-CA-C	-6.39	99.49	109.72
7	G	28	ALA	O-C-N	6.39	129.44	122.15
1	M	207	GLN	O-C-N	-6.39	115.35	122.12
5	Q	130	LEU	N-CA-CB	6.39	120.61	110.65
11	a	35	SER	CB-CA-C	-6.39	100.85	110.88
3	C	414	ALA	N-CA-CB	6.38	121.40	110.68
4	D	293	ALA	CA-C-N	6.38	129.12	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	293	ALA	C-N-CA	6.38	129.12	120.44
5	Q	96	ASP	O-C-N	6.38	128.64	122.07
11	X	73	LEU	N-CA-C	6.38	118.81	111.02
11	S	60	ALA	N-CA-C	-6.38	104.98	112.89
4	D	267	ALA	CA-C-O	-6.38	114.12	120.82
4	F	184	ALA	CA-C-N	6.38	128.73	120.44
4	F	184	ALA	C-N-CA	6.38	128.73	120.44
3	C	468	ASN	N-CA-CB	6.38	119.50	110.12
3	A	243	LEU	N-CA-C	6.38	121.22	112.04
8	P	19	ILE	CA-C-O	-6.38	114.41	121.17
7	G	15	ASP	CA-CB-CG	-6.38	106.22	112.60
6	J	17	ALA	N-CA-C	6.38	118.23	111.28
3	E	131	PRO	CA-C-O	-6.37	114.12	121.96
8	P	206	HIS	ND1-CE1-NE2	6.37	114.77	108.40
3	A	534	TYR	N-CA-CB	6.37	119.45	109.83
8	P	449	ASP	CA-CB-CG	-6.37	106.23	112.60
10	O	256	ILE	CA-C-N	6.37	126.29	119.85
10	O	256	ILE	C-N-CA	6.37	126.29	119.85
11	U	87	GLY	CA-C-N	6.37	129.45	120.28
11	U	87	GLY	C-N-CA	6.37	129.45	120.28
5	Q	249	TYR	CA-C-N	6.37	126.58	119.32
5	Q	249	TYR	C-N-CA	6.37	126.58	119.32
3	A	174	LEU	N-CA-C	-6.37	101.74	109.83
4	B	301	ARG	CA-C-N	6.37	131.18	122.07
4	B	301	ARG	C-N-CA	6.37	131.18	122.07
11	T	24	THR	N-CA-C	6.37	119.20	111.82
8	P	82	HIS	CA-C-N	6.37	128.81	120.28
8	P	82	HIS	C-N-CA	6.37	128.81	120.28
10	O	278	ALA	CA-C-N	6.37	128.81	120.28
10	O	278	ALA	C-N-CA	6.37	128.81	120.28
3	C	508	SER	CA-C-N	6.36	129.98	120.31
3	C	508	SER	C-N-CA	6.36	129.98	120.31
3	E	207	SER	N-CA-CB	6.36	121.25	110.49
7	I	14	ASN	CA-CB-CG	-6.36	106.24	112.60
11	X	132	ILE	CA-C-N	6.36	128.71	120.44
11	X	132	ILE	C-N-CA	6.36	128.71	120.44
4	F	364	LEU	CA-C-N	6.36	128.80	120.28
4	F	364	LEU	C-N-CA	6.36	128.80	120.28
10	O	355	ALA	CA-C-O	6.36	126.14	119.14
7	G	14	ASN	CA-C-N	6.36	128.80	120.28
7	G	14	ASN	C-N-CA	6.36	128.80	120.28
11	Y	140	GLY	O-C-N	6.36	128.29	122.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	314	THR	CA-C-O	-6.36	113.81	120.55
4	D	446	GLN	CB-CG-CD	-6.36	101.79	112.60
3	E	267	GLN	OE1-CD-NE2	6.36	128.96	122.60
4	B	276	THR	N-CA-CB	6.36	120.55	110.57
6	L	97	ILE	CB-CA-C	-6.36	103.45	112.22
10	O	316	VAL	CA-C-O	6.36	127.56	120.95
7	I	78	SER	N-CA-C	6.36	118.29	111.36
7	I	132	LEU	CA-C-N	6.36	131.63	122.35
7	I	132	LEU	C-N-CA	6.36	131.63	122.35
4	D	294	ALA	N-CA-C	-6.36	104.28	111.14
4	F	235	LEU	CA-C-N	6.36	128.80	120.28
4	F	235	LEU	C-N-CA	6.36	128.80	120.28
3	A	272	TYR	CB-CG-CD2	-6.36	111.27	120.80
11	a	148	LEU	CA-C-N	6.35	129.04	120.65
11	a	148	LEU	C-N-CA	6.35	129.04	120.65
4	B	201	HIS	CE1-NE2-CD2	-6.35	102.65	109.00
4	B	460	GLN	OE1-CD-NE2	-6.35	116.25	122.60
3	C	110	ARG	NE-CZ-NH2	6.35	124.92	119.20
3	C	591	ARG	CD-NE-CZ	-6.35	115.51	124.40
4	D	309	TYR	CA-C-N	6.35	128.79	120.28
4	D	309	TYR	C-N-CA	6.35	128.79	120.28
10	O	64	GLU	CA-C-N	6.35	128.79	120.28
10	O	64	GLU	C-N-CA	6.35	128.79	120.28
11	R	131	LEU	CA-C-N	6.35	128.56	120.56
11	R	131	LEU	C-N-CA	6.35	128.56	120.56
3	A	324	MET	CA-C-N	6.35	127.78	119.84
3	A	324	MET	C-N-CA	6.35	127.78	119.84
9	b	133	VAL	CA-CB-CG1	6.35	121.19	110.40
8	P	225	GLN	N-CA-CB	6.35	119.41	109.83
1	M	212	ASN	N-CA-C	-6.34	104.29	111.14
10	O	190	HIS	CB-CG-CD2	-6.34	122.95	131.20
3	A	420	GLY	N-CA-C	-6.34	104.68	115.08
5	Q	239	SER	CA-C-N	6.34	133.65	121.54
5	Q	239	SER	C-N-CA	6.34	133.65	121.54
11	W	55	VAL	CA-C-O	-6.34	111.45	119.95
3	E	468	ASN	N-CA-CB	6.34	120.11	110.28
4	F	406	LYS	CA-C-N	6.34	128.78	120.28
4	F	406	LYS	C-N-CA	6.34	128.78	120.28
3	C	102	GLU	CB-CA-C	-6.34	103.71	111.82
11	a	155	THR	CA-CB-CG2	-6.34	99.72	110.50
7	I	9	THR	N-CA-CB	6.33	119.59	110.03
11	W	27	GLY	CA-C-O	6.33	127.57	121.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	98	ASP	N-CA-CB	6.33	121.19	110.49
3	C	122	ILE	N-CA-C	-6.33	104.68	110.82
9	b	150	GLU	O-C-N	6.33	129.36	122.15
3	C	526	LEU	CA-C-O	-6.33	113.72	120.42
8	P	308	VAL	CA-C-N	6.33	129.13	120.46
8	P	308	VAL	C-N-CA	6.33	129.13	120.46
8	P	381	SER	N-CA-C	6.33	118.17	111.28
10	O	351	LEU	CB-CA-C	-6.33	100.29	110.79
11	R	146	VAL	CB-CA-C	-6.33	103.60	112.14
3	E	417	SER	CA-C-N	6.32	127.74	119.84
3	E	417	SER	C-N-CA	6.32	127.74	119.84
7	G	62	PHE	CA-CB-CG	6.32	120.12	113.80
11	a	156	GLN	N-CA-C	-6.32	102.71	110.61
11	Z	75	CYS	CA-C-N	6.32	128.75	120.28
11	Z	75	CYS	C-N-CA	6.32	128.75	120.28
7	K	119	PRO	CA-C-N	6.32	128.65	120.56
7	K	119	PRO	C-N-CA	6.32	128.65	120.56
8	P	429	HIS	CA-C-N	6.32	128.52	120.56
8	P	429	HIS	C-N-CA	6.32	128.52	120.56
11	Z	113	ASP	CA-C-N	6.32	129.38	120.28
11	Z	113	ASP	C-N-CA	6.32	129.38	120.28
10	O	246	PHE	CA-CB-CG	-6.32	107.48	113.80
11	X	75	CYS	CA-C-N	6.32	128.74	120.28
11	X	75	CYS	C-N-CA	6.32	128.74	120.28
11	Z	69	VAL	CA-C-N	6.32	128.52	120.56
11	Z	69	VAL	C-N-CA	6.32	128.52	120.56
3	C	613	GLU	O-C-N	6.31	129.34	122.15
3	E	112	LEU	O-C-N	6.31	128.81	122.12
11	Y	101	GLY	CA-C-N	6.31	129.06	120.54
11	Y	101	GLY	C-N-CA	6.31	129.06	120.54
3	C	331	ALA	CA-C-N	6.31	129.06	120.54
3	C	331	ALA	C-N-CA	6.31	129.06	120.54
9	b	32	THR	CA-C-N	6.31	128.64	120.44
9	b	32	THR	C-N-CA	6.31	128.64	120.44
4	B	309	TYR	N-CA-CB	6.31	119.16	110.01
10	O	375	ALA	N-CA-CB	6.31	121.15	110.49
2	N	88	PHE	CB-CA-C	-6.31	101.68	110.13
7	G	111	ALA	N-CA-C	6.30	118.96	111.71
11	Z	151	ASN	CB-CA-C	-6.30	100.73	110.81
11	Z	101	GLY	CA-C-N	6.30	128.63	120.44
11	Z	101	GLY	C-N-CA	6.30	128.63	120.44
4	D	475	ARG	CA-C-N	6.30	131.22	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	475	ARG	C-N-CA	6.30	131.22	123.10
3	A	186	ALA	CA-C-O	-6.30	113.83	120.70
8	P	275	LEU	CA-C-N	6.30	128.72	120.28
8	P	275	LEU	C-N-CA	6.30	128.72	120.28
3	C	288	ASN	CA-CB-CG	-6.30	106.30	112.60
3	E	550	PHE	CA-CB-CG	-6.30	107.50	113.80
10	O	144	ASP	CA-C-O	-6.30	114.21	120.70
6	H	51	ASP	N-CA-CB	6.30	120.04	110.28
11	V	91	LEU	O-C-N	6.29	128.82	122.08
3	E	598	GLY	CA-C-N	6.29	128.71	120.28
3	E	598	GLY	C-N-CA	6.29	128.71	120.28
10	O	329	ILE	N-CA-C	-6.29	98.45	107.77
11	Z	68	LEU	CA-C-N	6.29	128.49	120.56
11	Z	68	LEU	C-N-CA	6.29	128.49	120.56
4	F	121	ASP	N-CA-C	-6.29	104.07	112.94
5	Q	128	HIS	CG-CD2-NE2	6.29	113.49	107.20
8	P	370	TRP	CD2-CE2-CZ2	-6.29	116.11	122.40
10	O	383	GLU	CA-C-O	-6.29	113.51	119.80
11	S	12	PHE	N-CA-C	-6.29	105.64	113.38
3	C	558	GLN	CA-C-N	6.29	128.62	120.44
3	C	558	GLN	C-N-CA	6.29	128.62	120.44
9	b	198	THR	N-CA-C	6.29	117.93	111.14
11	Z	141	LEU	N-CA-C	6.29	118.66	111.11
7	K	150	GLU	N-CA-C	6.29	118.13	111.28
10	O	4	ALA	CA-C-N	6.29	133.00	121.94
10	O	4	ALA	C-N-CA	6.29	133.00	121.94
4	F	463	SER	CA-C-N	6.28	128.70	120.28
4	F	463	SER	C-N-CA	6.28	128.70	120.28
3	A	282	GLY	O-C-N	6.28	127.31	123.35
4	B	153	THR	N-CA-C	-6.28	105.25	113.17
4	B	364	LEU	CA-C-N	6.28	128.70	120.28
4	B	364	LEU	C-N-CA	6.28	128.70	120.28
9	b	127	ALA	O-C-N	6.28	129.31	122.15
11	W	131	LEU	N-CA-C	6.28	118.93	111.33
3	E	493	GLU	CA-C-N	6.28	129.21	120.29
3	E	493	GLU	C-N-CA	6.28	129.21	120.29
8	P	458	ASP	CA-C-N	6.28	128.61	120.44
8	P	458	ASP	C-N-CA	6.28	128.61	120.44
4	D	281	MET	N-CA-CB	6.28	120.01	110.28
3	A	334	TYR	CA-C-N	6.28	128.70	120.28
3	A	334	TYR	C-N-CA	6.28	128.70	120.28
10	O	249	ALA	CA-C-O	6.28	127.21	120.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Z	62	ILE	N-CA-C	-6.27	104.48	113.07
3	E	606	THR	CA-C-N	6.27	128.68	120.28
3	E	606	THR	C-N-CA	6.27	128.68	120.28
3	A	413	VAL	N-CA-CB	6.27	119.79	111.64
4	B	402	GLN	CA-C-N	6.27	128.68	120.28
4	B	402	GLN	C-N-CA	6.27	128.68	120.28
7	I	72	SER	CA-C-O	6.27	127.09	119.38
4	B	456	GLU	CA-C-N	6.27	128.97	120.38
4	B	456	GLU	C-N-CA	6.27	128.97	120.38
8	P	433	LEU	O-C-N	-6.26	115.62	122.07
11	T	145	ILE	CA-C-N	6.26	129.36	120.53
11	T	145	ILE	C-N-CA	6.26	129.36	120.53
1	M	193	ASP	CA-CB-CG	6.26	118.86	112.60
9	b	78	LYS	N-CA-C	6.26	118.11	111.28
3	C	224	THR	CB-CA-C	-6.26	101.05	110.88
7	I	127	GLU	N-CA-C	6.26	118.10	111.28
4	D	395	ASP	CA-C-N	6.26	128.58	120.44
4	D	395	ASP	C-N-CA	6.26	128.58	120.44
8	P	345	ILE	CB-CA-C	-6.26	103.96	111.97
3	C	451	PHE	CB-CA-C	-6.26	101.84	110.16
4	D	84	SER	CA-C-O	-6.26	114.01	120.89
3	A	511	ASP	CA-C-N	6.26	129.18	120.29
3	A	511	ASP	C-N-CA	6.26	129.18	120.29
11	V	55	VAL	N-CA-CB	6.26	119.97	111.21
2	N	70	ASN	CA-CB-CG	-6.25	106.34	112.60
4	F	478	PRO	N-CA-CB	6.25	109.73	103.48
3	A	536	ALA	O-C-N	6.25	130.07	123.06
1	M	16	GLY	CA-C-N	6.25	128.94	120.44
1	M	16	GLY	C-N-CA	6.25	128.94	120.44
9	b	17	VAL	CA-CB-CG2	-6.25	99.77	110.40
11	Z	111	VAL	CA-C-N	6.25	127.05	119.99
11	Z	111	VAL	C-N-CA	6.25	127.05	119.99
11	W	29	ALA	CA-C-N	6.25	128.57	120.44
11	W	29	ALA	C-N-CA	6.25	128.57	120.44
10	O	273	GLU	CA-C-N	6.25	128.94	120.44
10	O	273	GLU	C-N-CA	6.25	128.94	120.44
3	C	292	GLU	CB-CG-CD	-6.25	101.98	112.60
10	O	301	ILE	CA-C-N	6.24	129.16	120.29
10	O	301	ILE	C-N-CA	6.24	129.16	120.29
11	W	135	PHE	N-CA-CB	6.24	119.96	110.28
1	M	118	ASN	N-CA-CB	6.24	120.33	110.84
11	U	106	PHE	CA-C-O	-6.24	114.27	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	444	LYS	O-C-N	6.24	129.26	122.15
4	B	382	LEU	CA-C-N	6.24	129.27	120.28
4	B	382	LEU	C-N-CA	6.24	129.27	120.28
3	E	529	ASN	N-CA-C	-6.24	98.11	108.34
6	J	91	LYS	O-C-N	6.24	128.77	122.03
9	b	324	ASN	OD1-CG-ND2	6.24	128.84	122.60
8	P	446	GLY	CA-C-O	-6.24	113.67	120.40
11	Z	58	ILE	CA-C-N	6.24	128.64	120.28
11	Z	58	ILE	C-N-CA	6.24	128.64	120.28
11	S	66	TYR	CA-C-N	6.24	126.90	119.98
11	S	66	TYR	C-N-CA	6.24	126.90	119.98
11	Z	117	ARG	CB-CG-CD	6.23	125.64	111.30
2	N	41	GLN	O-C-N	6.23	130.91	123.24
5	Q	222	ASN	CB-CA-C	-6.23	100.26	110.85
3	C	494	GLU	CB-CA-C	-6.23	100.26	110.85
4	B	430	LYS	N-CA-CB	6.23	119.38	110.16
8	P	275	LEU	N-CA-CB	6.23	119.28	110.12
11	V	155	THR	N-CA-C	6.23	118.75	110.53
3	C	287	GLY	N-CA-C	-6.23	107.07	114.48
2	N	56	HIS	O-C-N	6.23	128.72	122.12
11	U	156	GLN	CA-C-N	6.23	133.43	121.54
11	U	156	GLN	C-N-CA	6.23	133.43	121.54
8	P	443	LYS	CA-C-N	6.23	129.13	120.29
8	P	443	LYS	C-N-CA	6.23	129.13	120.29
10	O	303	TRP	CE2-CD2-CE3	6.22	125.02	118.80
11	S	28	ALA	CA-C-N	6.22	128.53	120.44
11	S	28	ALA	C-N-CA	6.22	128.53	120.44
2	N	115	LEU	CA-C-O	6.22	129.41	120.51
8	P	261	ASN	CA-C-N	6.22	128.62	120.28
8	P	261	ASN	C-N-CA	6.22	128.62	120.28
3	E	430	ALA	O-C-N	6.22	129.24	122.15
8	P	299	SER	N-CA-C	6.22	118.81	110.35
8	P	386	GLU	CA-C-N	6.22	128.61	120.28
8	P	386	GLU	C-N-CA	6.22	128.61	120.28
6	H	33	LYS	CA-C-N	6.22	128.61	120.28
6	H	33	LYS	C-N-CA	6.22	128.61	120.28
4	D	172	ILE	N-CA-C	-6.21	98.79	107.80
4	F	81	GLU	CA-C-N	6.21	132.38	120.07
4	F	81	GLU	C-N-CA	6.21	132.38	120.07
4	F	424	ALA	N-CA-C	-6.21	105.28	112.92
11	X	89	ILE	CA-C-N	6.21	128.89	120.44
11	X	89	ILE	C-N-CA	6.21	128.89	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	454	LEU	CA-C-N	6.21	132.01	121.14
8	P	454	LEU	C-N-CA	6.21	132.01	121.14
11	W	104	ALA	CA-C-N	6.21	127.90	120.14
11	W	104	ALA	C-N-CA	6.21	127.90	120.14
11	W	45	LEU	N-CA-CB	6.21	119.16	110.90
7	K	200	ASN	CA-CB-CG	-6.21	106.39	112.60
8	P	235	SER	N-CA-C	-6.21	105.28	112.92
4	D	162	ASN	OD1-CG-ND2	-6.21	116.39	122.60
8	P	322	VAL	O-C-N	6.21	128.22	121.83
9	b	51	PHE	N-CA-C	6.21	119.02	111.82
9	b	58	GLU	N-CA-C	6.21	119.02	111.82
11	a	133	LEU	CA-C-N	6.21	130.27	120.47
11	a	133	LEU	C-N-CA	6.21	130.27	120.47
11	W	105	GLY	CA-C-N	6.21	130.93	120.88
11	W	105	GLY	C-N-CA	6.21	130.93	120.88
1	M	126	GLY	CA-C-N	6.20	128.59	120.28
1	M	126	GLY	C-N-CA	6.20	128.59	120.28
3	C	332	SER	O-C-N	6.20	128.54	122.09
4	B	381	ARG	N-CA-C	-6.20	105.75	113.38
7	I	15	ASP	CB-CA-C	-6.20	100.50	110.79
7	G	168	PRO	CA-C-O	-6.20	114.20	121.95
7	I	202	THR	CA-C-N	6.20	128.58	120.28
7	I	202	THR	C-N-CA	6.20	128.58	120.28
11	Y	153	ARG	CA-C-N	6.20	131.04	121.19
11	Y	153	ARG	C-N-CA	6.20	131.04	121.19
11	V	33	ALA	N-CA-C	6.20	118.58	111.02
11	S	42	THR	N-CA-C	-6.19	104.64	111.82
5	Q	54	PHE	CA-CB-CG	-6.19	107.61	113.80
11	V	125	LEU	N-CA-C	-6.19	105.58	112.57
3	C	52	GLY	CA-C-N	6.19	131.97	121.14
3	C	52	GLY	C-N-CA	6.19	131.97	121.14
11	Z	46	ARG	CB-CA-C	-6.19	102.47	111.01
8	P	429	HIS	CA-CB-CG	6.18	119.98	113.80
6	H	20	ILE	CA-C-O	-6.18	114.52	120.95
11	T	63	ILE	CA-C-N	6.18	129.41	120.38
11	T	63	ILE	C-N-CA	6.18	129.41	120.38
4	B	39	VAL	CA-C-O	-6.18	113.90	120.39
9	b	129	ASP	CA-C-O	6.18	126.97	120.42
7	K	156	ILE	CB-CA-C	-6.18	103.92	112.02
7	K	37	LEU	N-CA-C	-6.18	104.62	111.36
9	b	21	ILE	O-C-N	-6.18	114.06	121.10
11	W	66	TYR	CA-C-N	6.18	126.80	119.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	W	66	TYR	C-N-CA	6.18	126.80	119.94
11	S	90	GLN	CA-C-N	6.18	128.88	120.54
11	S	90	GLN	C-N-CA	6.18	128.88	120.54
3	E	413	VAL	N-CA-CB	6.17	119.24	111.46
3	A	210	THR	N-CA-C	-6.17	100.41	109.18
7	K	157	MET	CA-C-N	6.17	128.84	120.44
7	K	157	MET	C-N-CA	6.17	128.84	120.44
3	C	415	ALA	CA-C-O	6.17	128.77	121.36
8	P	7	LEU	N-CA-CB	6.17	122.12	112.25
9	b	320	PHE	CA-CB-CG	-6.17	107.63	113.80
3	E	176	PRO	CA-C-N	6.17	131.62	122.74
3	E	176	PRO	C-N-CA	6.17	131.62	122.74
4	F	273	HIS	N-CA-C	-6.17	99.15	108.96
11	V	12	PHE	N-CA-C	-6.17	105.91	113.50
7	K	16	GLU	CB-CA-C	-6.17	98.83	110.67
9	b	345	GLU	CA-C-N	6.17	129.38	120.38
9	b	345	GLU	C-N-CA	6.17	129.38	120.38
4	D	466	ARG	CA-C-N	6.16	128.91	120.46
4	D	466	ARG	C-N-CA	6.16	128.91	120.46
7	G	11	ASN	CA-C-O	-6.16	114.35	120.70
1	M	54	LYS	CA-C-O	-6.16	114.02	120.55
3	A	208	ASP	CA-CB-CG	6.16	118.76	112.60
4	B	46	PHE	CA-C-N	6.16	127.54	119.84
4	B	46	PHE	C-N-CA	6.16	127.54	119.84
7	G	35	ILE	CB-CA-C	-6.16	104.08	111.97
11	W	100	SER	CA-C-N	6.16	126.78	119.94
11	W	100	SER	C-N-CA	6.16	126.78	119.94
11	T	19	SER	N-CA-CB	6.16	119.82	109.78
11	T	55	VAL	CA-C-O	-6.16	111.69	119.95
11	R	72	VAL	CA-C-N	6.16	128.85	120.54
11	R	72	VAL	C-N-CA	6.16	128.85	120.54
4	D	246	ASN	N-CA-CB	6.16	120.89	110.49
3	A	465	ASN	CA-CB-CG	-6.16	106.44	112.60
4	B	282	SER	N-CA-C	-6.16	104.63	111.71
7	G	174	ILE	CB-CA-C	6.16	119.07	111.25
11	V	124	ARG	NE-CZ-NH2	6.15	124.74	119.20
4	F	401	ASN	CA-CB-CG	-6.15	106.45	112.60
11	a	35	SER	CA-C-N	6.15	126.94	119.99
11	a	35	SER	C-N-CA	6.15	126.94	119.99
11	W	154	ALA	CA-C-N	6.15	133.29	121.54
11	W	154	ALA	C-N-CA	6.15	133.29	121.54
11	a	80	GLN	O-C-N	-6.15	115.45	122.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	542	LYS	CA-C-N	6.15	129.02	120.29
3	C	542	LYS	C-N-CA	6.15	129.02	120.29
9	b	31	TYR	O-C-N	6.15	128.40	122.07
9	b	123	GLN	N-CA-CB	6.15	118.92	110.01
10	O	321	LEU	O-C-N	-6.15	114.54	121.43
7	G	82	ASN	CA-CB-CG	6.15	118.75	112.60
3	A	485	MET	CG-SD-CE	-6.15	87.38	100.90
11	T	147	ALA	CA-C-N	6.15	128.84	120.54
11	T	147	ALA	C-N-CA	6.15	128.84	120.54
5	Q	212	LEU	CA-C-N	6.14	126.76	119.94
5	Q	212	LEU	C-N-CA	6.14	126.76	119.94
11	U	105	GLY	CA-C-N	6.14	128.79	120.44
11	U	105	GLY	C-N-CA	6.14	128.79	120.44
3	C	116	LYS	CA-C-N	6.14	128.79	120.44
3	C	116	LYS	C-N-CA	6.14	128.79	120.44
11	V	151	ASN	CA-CB-CG	6.14	118.74	112.60
8	P	256	ASN	OD1-CG-ND2	6.14	128.74	122.60
10	O	116	TRP	CA-C-N	6.14	130.58	120.94
10	O	116	TRP	C-N-CA	6.14	130.58	120.94
7	I	56	ASN	N-CA-CB	6.14	119.14	110.12
4	F	254	ILE	CA-C-O	-6.14	113.84	120.47
11	W	50	LEU	CA-C-N	6.14	128.50	120.28
11	W	50	LEU	C-N-CA	6.14	128.50	120.28
11	V	18	ALA	CA-C-O	-6.14	114.32	121.07
3	C	102	GLU	N-CA-CB	6.13	122.06	112.25
3	A	473	SER	CA-C-N	6.13	129.63	120.31
3	A	473	SER	C-N-CA	6.13	129.63	120.31
11	U	64	ALA	CA-C-O	-6.13	113.33	120.20
4	D	181	ASN	N-CA-C	6.13	117.97	111.28
11	R	141	LEU	CB-CA-C	-6.13	101.00	110.81
11	V	124	ARG	N-CA-C	6.13	118.76	111.71
4	B	236	GLU	N-CA-CB	6.13	119.23	110.16
11	V	54	ILE	CA-C-O	-6.13	114.01	120.57
3	A	508	SER	CB-CA-C	-6.13	99.45	110.36
11	a	117	ARG	NE-CZ-NH1	-6.13	115.37	121.50
9	b	181	GLY	O-C-N	6.13	129.31	122.82
4	D	71	ARG	N-CA-C	-6.12	100.22	108.86
7	G	79	THR	N-CA-C	-6.12	104.69	111.36
7	I	9	THR	CA-C-O	-6.12	113.77	120.69
11	V	137	GLU	CA-C-N	6.12	128.85	120.46
11	V	137	GLU	C-N-CA	6.12	128.85	120.46
11	W	123	PRO	CA-C-N	6.12	128.48	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	W	123	PRO	C-N-CA	6.12	128.48	120.28
3	C	556	GLU	CA-C-N	6.12	128.76	120.44
3	C	556	GLU	C-N-CA	6.12	128.76	120.44
3	C	579	HIS	CG-CD2-NE2	6.12	113.32	107.20
3	A	213	HIS	CA-CB-CG	6.12	119.92	113.80
4	B	217	VAL	O-C-N	6.12	127.81	122.12
9	b	247	LYS	N-CA-CB	6.12	119.12	110.12
3	A	422	ASP	CA-CB-CG	-6.12	106.48	112.60
3	C	491	ASN	OD1-CG-ND2	6.12	128.72	122.60
11	U	130	ILE	CA-C-O	-6.12	114.91	121.27
3	E	125	PRO	CA-C-N	6.12	130.54	120.94
3	E	125	PRO	C-N-CA	6.12	130.54	120.94
11	S	57	VAL	N-CA-C	6.12	116.78	110.36
3	E	600	PHE	CA-CB-CG	-6.12	107.69	113.80
3	A	203	ASP	CA-CB-CG	-6.12	106.48	112.60
4	B	208	PHE	N-CA-C	-6.12	99.43	109.40
8	P	30	LEU	CA-C-N	6.12	128.76	120.44
8	P	30	LEU	C-N-CA	6.12	128.76	120.44
7	G	55	THR	N-CA-CB	6.12	119.21	110.16
11	S	70	VAL	N-CA-CB	6.12	117.04	110.62
3	E	60	VAL	N-CA-C	-6.11	98.19	107.73
4	B	255	THR	CA-C-N	6.11	126.00	119.28
4	B	255	THR	C-N-CA	6.11	126.00	119.28
5	Q	7	ASN	CA-C-N	6.11	129.10	120.42
5	Q	7	ASN	C-N-CA	6.11	129.10	120.42
9	b	124	MET	N-CA-C	6.11	118.44	111.11
11	T	144	LEU	N-CA-C	6.11	118.45	111.11
4	F	404	TYR	CB-CA-C	-6.11	100.65	110.79
10	O	79	ILE	O-C-N	-6.11	115.94	121.87
11	Z	145	ILE	CA-C-N	6.11	128.26	120.56
11	Z	145	ILE	C-N-CA	6.11	128.26	120.56
4	F	435	PHE	CA-C-N	6.11	128.47	120.28
4	F	435	PHE	C-N-CA	6.11	128.47	120.28
9	b	186	TYR	CB-CG-CD1	6.11	129.96	120.80
11	V	116	VAL	N-CA-CB	6.11	121.83	110.77
11	W	113	ASP	CA-CB-CG	6.11	118.70	112.60
3	C	399	VAL	O-C-N	6.10	130.38	122.94
8	P	31	ALA	CA-C-N	6.10	128.37	120.44
8	P	31	ALA	C-N-CA	6.10	128.37	120.44
2	N	10	VAL	N-CA-C	-6.10	99.33	108.12
11	R	145	ILE	N-CA-CB	6.10	117.03	110.62
4	B	157	ALA	CA-C-N	6.10	128.16	120.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	157	ALA	C-N-CA	6.10	128.16	120.72
8	P	395	PHE	CA-CB-CG	-6.10	107.70	113.80
11	T	150	LEU	CA-C-O	-6.10	114.42	120.82
3	A	414	ALA	CA-C-N	6.09	131.11	122.09
3	A	414	ALA	C-N-CA	6.09	131.11	122.09
3	A	60	VAL	N-CA-CB	6.09	118.80	111.31
5	Q	192	PHE	CA-C-N	6.09	128.94	120.29
5	Q	192	PHE	C-N-CA	6.09	128.94	120.29
7	K	34	GLU	CB-CA-C	-6.09	100.50	110.85
9	b	263	VAL	N-CA-CB	6.09	121.00	111.99
3	E	364	LEU	O-C-N	6.09	129.09	122.15
9	b	325	LYS	O-C-N	-6.09	114.44	122.42
11	U	19	SER	N-CA-CB	6.09	119.01	109.94
8	P	287	SER	CA-C-O	-6.09	114.43	120.82
8	P	433	LEU	N-CA-C	6.09	117.58	111.07
4	B	285	ALA	N-CA-C	6.08	117.99	111.36
1	M	179	PRO	CB-CA-C	-6.08	101.52	111.31
11	W	132	ILE	CA-C-N	6.08	128.75	120.54
11	W	132	ILE	C-N-CA	6.08	128.75	120.54
3	C	312	MET	O-C-N	6.08	128.56	122.12
1	M	27	GLN	N-CA-CB	6.08	119.16	110.16
7	G	28	ALA	CA-C-N	6.08	128.71	120.44
7	G	28	ALA	C-N-CA	6.08	128.71	120.44
5	Q	340	ASN	CA-CB-CG	-6.08	106.52	112.60
8	P	468	ALA	N-CA-C	-6.08	104.74	111.36
1	M	62	GLN	N-CA-C	6.07	117.90	111.28
3	C	141	PHE	CA-C-O	-6.07	113.68	120.54
5	Q	165	CYS	CA-C-O	-6.07	112.99	119.97
3	C	249	GLY	N-CA-C	-6.07	106.02	115.67
3	E	135	ARG	NE-CZ-NH1	-6.07	115.43	121.50
10	O	25	ALA	CA-C-N	6.07	127.43	119.84
10	O	25	ALA	C-N-CA	6.07	127.43	119.84
3	E	448	ARG	N-CA-C	-6.07	105.84	113.18
5	Q	233	ILE	CA-C-N	6.07	127.67	120.09
5	Q	233	ILE	C-N-CA	6.07	127.67	120.09
5	Q	311	ALA	O-C-N	6.07	129.73	122.27
11	U	146	VAL	CB-CA-C	-6.07	104.11	111.88
11	X	78	LEU	CA-C-N	6.06	129.34	122.67
11	X	78	LEU	C-N-CA	6.06	129.34	122.67
4	F	33	GLY	O-C-N	-6.06	116.41	123.44
9	b	272	GLN	CB-CG-CD	-6.06	102.30	112.60
11	Z	117	ARG	NE-CZ-NH1	-6.06	115.44	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	121	PRO	N-CA-CB	6.06	109.54	103.48
10	O	335	LYS	CA-C-N	6.06	131.70	122.37
10	O	335	LYS	C-N-CA	6.06	131.70	122.37
11	R	126	PHE	CA-C-N	6.06	130.98	120.86
11	R	126	PHE	C-N-CA	6.06	130.98	120.86
4	F	298	VAL	CA-C-N	6.06	127.41	119.84
4	F	298	VAL	C-N-CA	6.06	127.41	119.84
5	Q	281	THR	CA-C-O	-6.06	114.46	120.82
5	Q	295	LEU	CB-CA-C	6.06	115.83	109.83
11	R	124	ARG	NE-CZ-NH1	6.06	127.56	121.50
11	T	133	LEU	CA-C-N	6.06	130.98	120.86
11	T	133	LEU	C-N-CA	6.06	130.98	120.86
10	O	75	ILE	CA-CB-CG1	-6.06	100.11	110.40
11	R	63	ILE	CA-CB-CG1	6.06	120.70	110.40
3	C	528	GLN	OE1-CD-NE2	6.05	128.66	122.60
4	F	243	ASN	CA-CB-CG	-6.05	106.55	112.60
4	F	365	HIS	CE1-NE2-CD2	-6.05	102.94	109.00
8	P	212	PRO	CA-C-N	6.05	128.31	120.44
8	P	212	PRO	C-N-CA	6.05	128.31	120.44
11	U	67	GLY	CA-C-N	6.05	128.39	120.28
11	U	67	GLY	C-N-CA	6.05	128.39	120.28
11	W	83	ALA	CA-C-O	-6.05	114.20	121.89
5	Q	321	ARG	N-CA-C	6.05	117.88	111.28
8	P	219	GLN	CB-CG-CD	-6.05	102.31	112.60
8	P	237	HIS	CE1-NE2-CD2	-6.05	102.95	109.00
8	P	256	ASN	CA-C-N	6.05	125.77	119.05
8	P	256	ASN	C-N-CA	6.05	125.77	119.05
1	M	118	ASN	O-C-N	-6.05	115.14	123.12
11	Z	91	LEU	CA-C-O	-6.05	114.42	121.07
4	F	34	VAL	N-CA-C	-6.05	99.34	108.17
4	B	428	GLU	CB-CG-CD	-6.05	102.32	112.60
4	B	474	ASN	CA-C-O	6.05	125.79	119.14
4	D	87	ASP	CA-CB-CG	-6.04	106.56	112.60
8	P	180	MET	CA-C-N	6.04	128.30	120.44
8	P	180	MET	C-N-CA	6.04	128.30	120.44
3	E	510	SER	CB-CA-C	-6.04	100.76	110.79
7	K	142	LEU	CA-C-O	-6.04	114.97	121.56
10	O	87	GLN	CA-C-N	6.04	126.65	120.00
10	O	87	GLN	C-N-CA	6.04	126.65	120.00
11	V	19	SER	O-C-N	6.04	128.37	122.09
8	P	317	ASN	N-CA-C	-6.04	105.21	112.58
4	D	420	VAL	CA-CB-CG2	6.04	120.67	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	107	ASP	N-CA-C	-6.04	105.78	113.02
10	O	346	ASP	N-CA-CB	6.04	118.99	110.12
3	A	545	ASP	CA-C-O	6.04	126.95	120.55
4	B	195	ARG	CA-C-N	6.04	125.59	119.19
4	B	195	ARG	C-N-CA	6.04	125.59	119.19
9	b	89	ASP	CA-C-N	6.04	130.42	120.94
9	b	89	ASP	C-N-CA	6.04	130.42	120.94
10	O	100	LEU	O-C-N	6.04	128.26	121.32
4	B	392	THR	N-CA-C	-6.03	99.90	109.07
6	L	26	LYS	CA-C-N	6.03	128.37	120.28
6	L	26	LYS	C-N-CA	6.03	128.37	120.28
7	I	158	ARG	CA-C-N	6.03	128.36	120.28
7	I	158	ARG	C-N-CA	6.03	128.36	120.28
11	X	136	ALA	CA-C-O	-6.03	111.98	119.28
11	R	51	PHE	CA-CB-CG	6.03	119.83	113.80
4	D	150	MET	CA-C-N	6.03	131.04	123.14
4	D	150	MET	C-N-CA	6.03	131.04	123.14
11	a	126	PHE	N-CA-CB	6.03	118.99	110.12
8	P	142	SER	N-CA-CB	6.03	118.75	110.01
8	P	157	ASN	CA-CB-CG	-6.03	106.57	112.60
11	T	16	GLY	CA-C-O	6.03	127.51	121.00
11	V	132	ILE	N-CA-C	6.03	116.21	110.42
2	N	110	LYS	N-CA-CB	6.03	118.75	110.01
4	D	468	TYR	CA-C-N	6.03	126.00	120.21
4	D	468	TYR	C-N-CA	6.03	126.00	120.21
7	K	25	ARG	NE-CZ-NH2	6.03	124.62	119.20
11	U	153	ARG	NH1-CZ-NH2	-6.03	111.46	119.30
3	E	237	GLN	CG-CD-NE2	6.03	125.44	116.40
3	A	108	ILE	N-CA-C	-6.03	105.49	111.88
8	P	469	THR	N-CA-CB	6.03	119.08	110.16
4	B	113	PHE	CA-C-O	6.02	128.26	121.51
5	Q	43	LYS	N-CA-CB	6.02	118.97	110.12
11	a	82	GLN	O-C-N	6.02	131.02	123.19
11	W	12	PHE	N-CA-CB	6.02	119.38	110.53
3	E	490	SER	CB-CA-C	-6.02	101.39	110.90
5	Q	138	THR	CA-CB-OG1	6.02	118.63	109.60
11	R	150	LEU	O-C-N	6.02	128.35	122.09
4	D	151	ILE	N-CA-C	-6.02	99.68	108.11
6	J	38	ASP	CA-CB-CG	-6.02	106.58	112.60
3	A	492	ALA	CA-C-N	6.02	128.62	120.44
3	A	492	ALA	C-N-CA	6.02	128.62	120.44
3	A	170	HIS	CB-CG-ND1	6.01	131.72	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	460	GLN	N-CA-C	6.01	117.92	111.36
7	G	113	ASN	N-CA-C	-6.01	97.91	108.20
9	b	239	PHE	N-CA-C	-6.01	100.10	109.72
11	Z	108	ILE	CA-C-O	-6.01	114.14	120.57
11	W	91	LEU	CA-C-N	6.01	127.65	120.14
11	W	91	LEU	C-N-CA	6.01	127.65	120.14
3	C	25	GLY	N-CA-C	-6.01	103.39	112.89
3	E	475	TYR	N-CA-CB	6.01	121.07	110.37
7	I	64	SER	CA-C-O	-6.01	113.57	120.24
3	A	140	GLN	CA-C-O	6.01	126.79	120.54
3	E	249	GLY	N-CA-C	-6.01	106.80	115.27
6	H	30	ASP	N-CA-CB	6.01	118.72	110.01
7	G	13	VAL	N-CA-C	6.01	116.79	110.72
3	C	33	PRO	N-CA-C	-6.00	106.27	114.80
8	P	206	HIS	CE1-NE2-CD2	-6.00	103.00	109.00
8	P	276	LYS	N-CA-C	6.00	117.82	111.28
10	O	45	VAL	N-CA-C	-6.00	99.84	108.48
4	B	186	GLN	OE1-CD-NE2	-6.00	116.60	122.60
8	P	303	LYS	CA-C-N	6.00	130.68	122.34
8	P	303	LYS	C-N-CA	6.00	130.68	122.34
4	D	346	ILE	N-CA-CB	6.00	115.13	110.45
8	P	309	ILE	CA-C-O	6.00	127.19	120.95
7	G	181	LYS	N-CA-C	-6.00	105.54	112.92
4	F	201	HIS	N-CA-CB	6.00	119.58	110.28
7	K	101	GLU	CB-CG-CD	-6.00	102.41	112.60
11	a	56	PRO	CA-N-CD	-6.00	103.60	112.00
4	D	81	GLU	CA-C-O	5.99	126.87	120.46
3	A	592	GLY	N-CA-C	-5.99	98.97	113.18
7	K	212	GLU	CA-C-O	-5.99	114.16	120.63
9	b	53	ARG	N-CA-C	-5.99	100.52	110.17
11	X	63	ILE	N-CA-CB	5.99	118.24	110.57
2	N	95	PRO	CA-C-O	-5.99	114.79	121.32
4	D	411	LYS	N-CA-CB	5.99	118.93	110.12
3	A	591	ARG	N-CA-C	-5.99	104.82	113.21
9	b	202	ILE	O-C-N	5.99	127.78	121.91
3	C	470	PHE	O-C-N	-5.99	115.90	122.07
10	O	375	ALA	N-CA-C	-5.99	98.05	110.80
3	C	606	THR	CA-C-N	5.99	128.30	120.28
3	C	606	THR	C-N-CA	5.99	128.30	120.28
4	D	157	ALA	O-C-N	5.99	128.97	122.15
3	E	281	VAL	O-C-N	5.99	129.55	123.20
9	b	96	GLY	CA-C-O	5.99	127.00	120.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	223	TYR	CA-C-N	-5.98	110.93	121.70
7	G	223	TYR	C-N-CA	-5.98	110.93	121.70
7	I	129	LEU	N-CA-CB	5.98	119.55	110.28
11	U	43	CYS	N-CA-C	5.98	118.59	111.71
11	X	118	GLY	CA-C-N	5.98	128.62	120.54
11	X	118	GLY	C-N-CA	5.98	128.62	120.54
11	a	90	GLN	CA-C-N	5.98	129.11	120.79
11	a	90	GLN	C-N-CA	5.98	129.11	120.79
3	C	383	TYR	N-CA-C	-5.98	105.24	112.54
7	K	52	ARG	CA-C-N	5.98	128.61	120.54
7	K	52	ARG	C-N-CA	5.98	128.61	120.54
7	K	141	ALA	O-C-N	5.98	129.98	123.10
8	P	400	GLU	N-CA-CB	5.98	118.91	110.12
4	F	175	ALA	O-C-N	5.98	129.97	123.10
5	Q	216	ALA	N-CA-C	5.98	117.47	111.07
8	P	351	GLN	N-CA-C	-5.98	104.85	111.36
10	O	332	VAL	CA-C-O	5.98	123.07	119.19
3	E	408	GLY	CA-C-O	-5.97	114.62	121.49
4	F	122	ASN	O-C-N	-5.97	116.04	123.33
4	B	280	ASP	CA-C-N	5.97	128.77	120.29
4	B	280	ASP	C-N-CA	5.97	128.77	120.29
5	Q	325	TRP	O-C-N	-5.97	115.34	122.15
5	Q	317	GLU	N-CA-CB	5.97	119.00	110.16
11	T	91	LEU	CA-C-N	5.97	127.61	120.14
11	T	91	LEU	C-N-CA	5.97	127.61	120.14
1	M	208	GLU	CB-CG-CD	-5.97	102.45	112.60
7	G	167	ALA	N-CA-CB	5.97	121.00	110.37
11	T	90	GLN	OE1-CD-NE2	5.97	128.57	122.60
4	F	310	THR	CA-C-N	5.97	128.27	120.28
4	F	310	THR	C-N-CA	5.97	128.27	120.28
11	T	39	ILE	N-CA-C	5.97	116.15	110.42
3	E	450	HIS	CE1-NE2-CD2	-5.96	103.03	109.00
1	M	66	PHE	CA-C-N	5.96	128.27	120.28
1	M	66	PHE	C-N-CA	5.96	128.27	120.28
4	D	420	VAL	CA-C-N	5.96	133.09	121.41
4	D	420	VAL	C-N-CA	5.96	133.09	121.41
7	I	152	MET	CA-C-O	-5.96	111.98	120.51
3	E	501	LEU	CA-C-O	-5.96	114.76	120.90
8	P	129	ASP	CA-CB-CG	-5.96	106.64	112.60
11	S	41	ALA	O-C-N	5.96	128.53	122.09
3	E	445	LEU	CA-C-N	5.96	128.86	120.28
3	E	445	LEU	C-N-CA	5.96	128.86	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	164	ASN	OD1-CG-ND2	5.96	128.56	122.60
11	a	150	LEU	CA-C-N	5.96	128.58	120.54
11	a	150	LEU	C-N-CA	5.96	128.58	120.54
11	Y	86	THR	CA-CB-OG1	-5.96	100.67	109.60
2	N	71	GLN	N-CA-C	5.96	118.54	111.33
8	P	33	SER	N-CA-CB	5.96	120.07	110.42
3	A	309	GLU	O-C-N	5.95	128.17	121.32
11	U	136	ALA	CB-CA-C	-5.95	98.10	109.95
11	X	55	VAL	CA-C-N	5.95	125.16	118.97
11	X	55	VAL	C-N-CA	5.95	125.16	118.97
3	C	186	ALA	N-CA-CB	5.95	119.32	109.98
5	Q	72	ALA	CA-C-N	5.95	128.74	120.29
5	Q	72	ALA	C-N-CA	5.95	128.74	120.29
11	Z	90	GLN	CA-C-N	5.95	129.06	120.79
11	Z	90	GLN	C-N-CA	5.95	129.06	120.79
3	C	334	TYR	O-C-N	5.95	128.43	122.12
5	Q	37	ASP	CA-CB-CG	5.95	118.55	112.60
7	K	146	VAL	CB-CA-C	-5.95	104.01	112.22
3	E	340	ALA	CA-C-O	5.95	126.85	120.55
4	F	347	PRO	N-CA-CB	5.95	110.10	103.44
3	A	219	VAL	CA-C-O	-5.95	114.86	119.20
1	M	80	GLY	CA-C-N	5.95	128.17	120.44
1	M	80	GLY	C-N-CA	5.95	128.17	120.44
3	E	564	GLY	CA-C-N	5.95	132.90	121.54
3	E	564	GLY	C-N-CA	5.95	132.90	121.54
4	F	428	GLU	CB-CG-CD	-5.95	102.49	112.60
6	H	34	GLN	CA-C-N	5.95	128.25	120.28
6	H	34	GLN	C-N-CA	5.95	128.25	120.28
11	Y	151	ASN	N-CA-C	5.95	118.24	111.11
9	b	247	LYS	O-C-N	5.94	128.42	122.12
10	O	303	TRP	CG-CD2-CE3	-5.94	127.96	133.90
4	B	144	ARG	N-CA-C	-5.94	104.70	113.61
11	X	143	GLY	O-C-N	5.94	127.89	122.19
11	T	100	SER	CA-C-N	5.94	126.54	119.94
11	T	100	SER	C-N-CA	5.94	126.54	119.94
3	A	450	HIS	CB-CG-CD2	-5.94	123.48	131.20
5	Q	128	HIS	CA-CB-CG	5.94	119.74	113.80
6	J	9	THR	CA-C-N	5.94	128.72	120.29
6	J	9	THR	C-N-CA	5.94	128.72	120.29
4	F	341	ASP	CA-CB-CG	5.94	118.54	112.60
4	B	172	ILE	N-CA-C	-5.94	99.32	107.99
4	B	406	LYS	CB-CG-CD	5.94	124.95	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	15	ASP	O-C-N	5.94	128.41	122.12
7	I	131	LYS	N-CA-C	-5.94	106.20	113.50
11	S	147	ALA	CA-C-N	5.94	128.55	120.54
11	S	147	ALA	C-N-CA	5.94	128.55	120.54
3	A	492	ALA	O-C-N	-5.93	115.83	122.12
4	D	193	LEU	N-CA-C	-5.93	106.08	113.38
4	D	201	HIS	CG-CD2-NE2	5.93	113.13	107.20
8	P	345	ILE	N-CA-CB	5.93	117.49	110.55
11	U	29	ALA	N-CA-CB	5.93	118.78	109.94
1	M	29	TYR	CA-C-N	5.93	128.15	120.44
1	M	29	TYR	C-N-CA	5.93	128.15	120.44
7	I	87	LYS	N-CA-CB	5.93	118.61	110.01
9	b	142	ARG	NE-CZ-NH2	-5.93	113.86	119.20
3	E	383	TYR	CB-CG-CD1	-5.93	111.91	120.80
3	A	306	GLY	CA-C-N	5.92	131.52	123.11
3	A	306	GLY	C-N-CA	5.92	131.52	123.11
4	B	476	ILE	CA-C-O	-5.92	115.66	121.58
8	P	210	PHE	CA-C-N	5.92	127.49	120.09
8	P	210	PHE	C-N-CA	5.92	127.49	120.09
4	D	98	GLU	CA-C-N	5.92	130.24	120.94
4	D	98	GLU	C-N-CA	5.92	130.24	120.94
4	F	45	LYS	N-CA-C	5.92	118.92	110.10
10	O	366	LYS	CA-C-O	-5.92	114.18	121.11
11	T	61	GLY	CA-C-O	-5.92	113.78	120.30
4	F	189	ARG	CD-NE-CZ	-5.92	116.11	124.40
4	B	121	ASP	CA-CB-CG	-5.92	106.68	112.60
6	J	99	ILE	CA-C-N	5.92	128.21	120.28
6	J	99	ILE	C-N-CA	5.92	128.21	120.28
11	T	116	VAL	N-CA-C	-5.92	103.51	111.44
2	N	46	THR	CA-C-N	5.92	128.48	120.38
2	N	46	THR	C-N-CA	5.92	128.48	120.38
7	K	161	GLY	CA-C-O	-5.92	113.79	120.30
9	b	325	LYS	CA-C-O	5.92	125.89	119.15
10	O	256	ILE	N-CA-CB	5.92	119.49	111.21
10	O	317	LEU	N-CA-C	5.92	117.73	111.28
10	O	338	SER	CA-C-N	5.92	128.69	120.29
10	O	338	SER	C-N-CA	5.92	128.69	120.29
11	V	31	GLY	CA-C-N	5.92	128.13	120.44
11	V	31	GLY	C-N-CA	5.92	128.13	120.44
4	B	146	TYR	CA-C-N	5.92	125.93	119.90
4	B	146	TYR	C-N-CA	5.92	125.93	119.90
8	P	331	SER	CA-C-O	-5.92	114.61	120.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	200	ASN	N-CA-CB	5.92	118.82	110.24
7	I	218	ILE	N-CA-C	-5.92	104.75	110.72
4	D	381	ARG	N-CA-C	-5.91	99.56	108.96
6	H	74	ALA	CA-C-N	5.91	126.39	119.94
6	H	74	ALA	C-N-CA	5.91	126.39	119.94
4	D	60	GLY	N-CA-C	-5.91	107.10	115.43
3	A	316	THR	CA-C-O	-5.91	114.32	120.70
8	P	439	ASP	CA-CB-CG	-5.91	106.69	112.60
8	P	50	ILE	CA-C-N	5.91	128.68	120.29
8	P	50	ILE	C-N-CA	5.91	128.68	120.29
11	T	151	ASN	CA-C-N	5.91	128.48	120.38
11	T	151	ASN	C-N-CA	5.91	128.48	120.38
9	b	105	SER	CA-C-N	5.91	131.13	123.10
9	b	105	SER	C-N-CA	5.91	131.13	123.10
3	A	545	ASP	O-C-N	-5.91	115.86	122.12
11	T	123	PRO	CB-CA-C	5.91	117.89	110.27
2	N	100	PRO	CA-C-N	5.90	129.76	121.02
2	N	100	PRO	C-N-CA	5.90	129.76	121.02
7	K	148	LEU	CA-C-O	5.90	126.67	120.42
11	T	82	GLN	OE1-CD-NE2	5.90	128.50	122.60
1	M	211	GLN	CA-C-O	5.90	126.80	120.55
5	Q	80	PHE	CA-C-N	5.90	128.18	120.28
5	Q	80	PHE	C-N-CA	5.90	128.18	120.28
9	b	33	LEU	CA-C-O	-5.90	114.63	120.82
3	C	446	ALA	CA-C-N	5.90	129.27	120.31
3	C	446	ALA	C-N-CA	5.90	129.27	120.31
7	I	63	LYS	CB-CG-CD	5.90	124.86	111.30
11	S	129	MET	CA-C-N	5.90	128.21	120.60
11	S	129	MET	C-N-CA	5.90	128.21	120.60
5	Q	58	VAL	N-CA-C	-5.89	99.56	108.17
8	P	21	ARG	CA-C-N	5.89	128.18	120.28
8	P	21	ARG	C-N-CA	5.89	128.18	120.28
4	D	422	GLU	N-CA-C	-5.89	106.71	114.31
9	b	263	VAL	N-CA-C	-5.89	99.00	107.78
7	G	85	ARG	NE-CZ-NH2	-5.89	113.90	119.20
4	D	184	ALA	CA-C-O	-5.89	114.18	120.42
10	O	218	VAL	CA-C-N	5.89	125.65	119.76
10	O	218	VAL	C-N-CA	5.89	125.65	119.76
11	U	24	THR	N-CA-C	5.89	118.65	111.82
11	U	138	VAL	N-CA-CB	5.89	121.43	110.77
11	W	77	SER	N-CA-C	5.89	120.20	113.19
1	M	144	GLU	CA-C-N	5.89	128.17	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	144	GLU	C-N-CA	5.89	128.17	120.28
4	B	384	LYS	CA-C-N	5.89	128.65	120.29
4	B	384	LYS	C-N-CA	5.89	128.65	120.29
5	Q	94	PHE	CA-CB-CG	-5.89	107.91	113.80
11	X	32	THR	O-C-N	5.89	128.13	122.07
3	C	81	VAL	N-CA-CB	-5.89	104.11	110.53
11	U	81	LYS	N-CA-C	-5.89	100.11	109.23
11	W	54	ILE	CA-C-O	-5.89	114.22	120.64
3	E	227	LEU	O-C-N	-5.88	115.50	123.15
11	V	119	SER	CA-C-N	5.88	128.44	120.38
11	V	119	SER	C-N-CA	5.88	128.44	120.38
1	M	36	SER	CA-C-N	5.88	128.16	120.28
1	M	36	SER	C-N-CA	5.88	128.16	120.28
5	Q	73	SER	CA-C-N	5.88	128.16	120.28
5	Q	73	SER	C-N-CA	5.88	128.16	120.28
9	b	106	VAL	N-CA-C	-5.88	97.37	106.72
1	M	198	GLU	CA-C-N	5.88	128.16	120.28
1	M	198	GLU	C-N-CA	5.88	128.16	120.28
4	F	171	PRO	CA-C-N	5.88	130.43	122.90
4	F	171	PRO	C-N-CA	5.88	130.43	122.90
2	N	62	ASP	CA-CB-CG	-5.88	106.72	112.60
3	A	238	ARG	O-C-N	5.88	128.35	122.12
4	D	239	SER	N-CA-C	-5.88	99.82	109.40
3	A	313	LYS	CB-CA-C	-5.88	99.75	110.63
5	Q	247	LYS	CA-C-N	5.88	132.38	121.62
5	Q	247	LYS	C-N-CA	5.88	132.38	121.62
3	E	312	MET	CA-C-N	5.88	128.15	120.28
3	E	312	MET	C-N-CA	5.88	128.15	120.28
4	F	201	HIS	ND1-CE1-NE2	5.88	114.28	108.40
3	A	130	THR	CA-C-N	5.88	127.19	119.84
3	A	130	THR	C-N-CA	5.88	127.19	119.84
7	K	106	LYS	CA-C-N	5.88	128.63	120.29
7	K	106	LYS	C-N-CA	5.88	128.63	120.29
3	A	439	TRP	CB-CG-CD2	-5.88	118.58	126.80
10	O	4	ALA	CA-C-O	5.88	126.77	119.78
7	G	86	LEU	CA-C-O	5.88	126.65	120.42
11	X	122	GLN	CA-C-N	5.87	127.18	119.84
11	X	122	GLN	C-N-CA	5.87	127.18	119.84
3	C	405	ASP	CA-CB-CG	-5.87	106.73	112.60
4	B	395	ASP	CA-CB-CG	-5.87	106.73	112.60
8	P	2	GLY	O-C-N	5.87	129.20	122.33
11	R	12	PHE	N-CA-C	-5.87	106.12	113.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	263	ALA	CA-C-N	5.87	128.62	120.29
4	D	263	ALA	C-N-CA	5.87	128.62	120.29
7	G	95	SER	CA-C-N	5.87	128.15	120.28
7	G	95	SER	C-N-CA	5.87	128.15	120.28
11	X	100	SER	N-CA-CB	5.87	118.85	110.16
11	Y	118	GLY	CA-C-O	-5.87	114.33	120.90
1	M	15	LEU	CA-C-N	5.87	126.45	119.94
1	M	15	LEU	C-N-CA	5.87	126.45	119.94
3	E	228	SER	CB-CA-C	-5.87	99.62	109.65
7	G	46	GLU	O-C-N	-5.87	115.46	122.15
7	G	85	ARG	CA-CB-CG	5.87	125.83	114.10
7	I	128	ALA	CA-C-O	-5.87	114.20	120.42
11	Z	124	ARG	O-C-N	-5.87	115.90	122.12
3	E	579	HIS	CG-CD2-NE2	5.87	113.07	107.20
3	A	610	ARG	NE-CZ-NH2	5.87	124.48	119.20
4	B	219	LEU	N-CA-C	-5.87	104.97	111.36
5	Q	80	PHE	CB-CA-C	-5.87	101.52	111.26
8	P	27	TRP	CA-C-N	5.87	128.07	120.44
8	P	27	TRP	C-N-CA	5.87	128.07	120.44
11	R	132	ILE	CA-C-O	-5.87	114.95	121.17
4	D	143	ALA	N-CA-C	5.87	123.30	110.80
4	F	205	GLU	CB-CG-CD	-5.87	102.63	112.60
9	b	180	ILE	CA-C-N	5.87	129.93	122.83
9	b	180	ILE	C-N-CA	5.87	129.93	122.83
7	I	15	ASP	N-CA-CB	5.87	118.74	110.12
7	I	110	ILE	CA-C-N	5.87	129.23	120.31
7	I	110	ILE	C-N-CA	5.87	129.23	120.31
11	T	75	CYS	CA-C-N	5.87	128.94	120.38
11	T	75	CYS	C-N-CA	5.87	128.94	120.38
11	W	113	ASP	N-CA-C	5.87	118.18	111.02
4	D	277	ILE	O-C-N	-5.86	116.98	123.20
8	P	115	LYS	CA-C-N	5.86	128.14	120.28
8	P	115	LYS	C-N-CA	5.86	128.14	120.28
9	b	69	TYR	N-CA-CB	5.86	118.51	110.01
3	A	524	ASP	CA-C-O	-5.86	112.87	119.79
10	O	311	VAL	CA-C-O	-5.86	114.64	120.85
1	M	208	GLU	N-CA-CB	5.86	118.73	110.12
3	A	83	ASP	O-C-N	-5.86	113.72	121.34
3	A	164	ASN	CA-CB-CG	5.86	118.46	112.60
5	Q	317	GLU	CB-CA-C	-5.86	100.89	110.85
7	K	165	GLN	CB-CG-CD	-5.86	102.64	112.60
10	O	21	GLN	CB-CA-C	-5.86	100.89	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	136	LYS	CA-C-N	5.86	128.13	120.28
1	M	136	LYS	C-N-CA	5.86	128.13	120.28
3	C	266	SER	CA-C-N	5.86	128.60	120.29
3	C	266	SER	C-N-CA	5.86	128.60	120.29
3	A	304	MET	N-CA-C	-5.86	104.80	112.41
11	Y	32	THR	O-C-N	-5.86	115.91	122.12
3	E	523	GLU	CB-CG-CD	-5.85	102.65	112.60
5	Q	145	LEU	CA-C-N	5.85	128.12	120.28
5	Q	145	LEU	C-N-CA	5.85	128.12	120.28
4	D	478	PRO	N-CD-CG	5.85	111.98	103.20
3	E	548	ARG	CA-C-N	5.85	128.60	120.29
3	E	548	ARG	C-N-CA	5.85	128.60	120.29
8	P	191	GLN	CA-C-N	5.85	128.12	120.28
8	P	191	GLN	C-N-CA	5.85	128.12	120.28
8	P	334	GLU	CA-C-N	5.85	128.12	120.28
8	P	334	GLU	C-N-CA	5.85	128.12	120.28
8	P	168	ASN	CA-CB-CG	-5.85	106.75	112.60
7	G	192	ASN	O-C-N	-5.85	115.83	122.68
3	A	91	PRO	N-CA-C	5.85	119.69	111.33
8	P	205	LEU	N-CA-C	5.85	117.65	111.28
10	O	257	PRO	CA-C-N	5.85	131.61	123.07
10	O	257	PRO	C-N-CA	5.85	131.61	123.07
3	E	439	TRP	N-CA-C	-5.85	99.48	109.24
4	B	260	LEU	CA-C-O	5.85	126.75	120.55
4	F	231	GLU	CB-CA-C	-5.84	101.70	110.88
4	F	339	ASN	CA-CB-CG	-5.84	106.76	112.60
4	B	113	PHE	CA-CB-CG	-5.84	107.96	113.80
11	S	38	GLY	CA-C-N	5.84	128.14	120.60
11	S	38	GLY	C-N-CA	5.84	128.14	120.60
11	W	76	TYR	N-CA-CB	5.84	118.71	110.12
3	E	552	SER	CA-C-N	5.84	128.11	120.28
3	E	552	SER	C-N-CA	5.84	128.11	120.28
4	F	42	GLU	N-CA-C	-5.84	99.72	109.24
11	X	64	ALA	N-CA-C	5.84	119.23	111.75
4	D	391	MET	CA-C-N	5.84	133.41	123.01
4	D	391	MET	C-N-CA	5.84	133.41	123.01
3	E	234	LEU	CA-C-N	5.84	128.58	120.29
3	E	234	LEU	C-N-CA	5.84	128.58	120.29
8	P	219	GLN	O-C-N	5.84	128.31	122.12
11	U	82	GLN	N-CA-C	-5.84	100.47	109.52
11	S	71	SER	CA-C-N	5.84	127.92	120.56
11	S	71	SER	C-N-CA	5.84	127.92	120.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	321	ARG	CA-C-O	5.84	126.74	120.55
4	B	445	THR	N-CA-C	-5.84	99.00	108.52
11	Z	130	ILE	N-CA-CB	5.84	117.38	110.55
11	Z	131	LEU	N-CA-CB	5.83	118.63	109.94
3	E	99	GLY	CA-C-N	5.83	128.57	120.29
3	E	99	GLY	C-N-CA	5.83	128.57	120.29
3	E	108	ILE	CA-C-O	5.83	124.45	119.38
4	F	297	GLU	O-C-N	-5.83	116.06	123.06
3	C	486	LYS	O-C-N	5.83	128.38	122.09
3	E	451	PHE	N-CA-CB	5.83	118.36	110.14
9	b	294	THR	N-CA-CB	5.83	118.79	110.16
3	C	163	GLU	N-CA-C	-5.83	103.89	113.50
4	B	324	GLY	CA-C-N	5.83	130.86	122.35
4	B	324	GLY	C-N-CA	5.83	130.86	122.35
3	A	75	GLU	N-CA-CB	5.82	118.25	109.34
6	J	31	LYS	CA-C-N	5.82	128.56	120.29
6	J	31	LYS	C-N-CA	5.82	128.56	120.29
11	U	131	LEU	CA-C-N	5.82	127.90	120.56
11	U	131	LEU	C-N-CA	5.82	127.90	120.56
7	K	126	VAL	N-CA-CB	5.82	119.31	110.58
4	B	188	CYS	N-CA-C	5.82	117.70	111.36
5	Q	200	ILE	N-CA-C	5.82	121.45	108.88
11	V	126	PHE	N-CA-CB	5.82	118.77	110.16
4	B	377	PRO	O-C-N	5.82	130.50	122.64
7	G	72	SER	CA-C-O	-5.82	113.28	119.97
2	N	31	GLU	CA-C-O	-5.82	112.65	119.05
4	D	169	LYS	CA-C-O	-5.82	115.07	121.58
5	Q	32	ASN	O-C-N	-5.82	115.52	122.15
6	L	74	ALA	N-CA-C	5.82	118.40	111.71
7	K	66	LEU	CA-C-N	5.82	128.07	120.28
7	K	66	LEU	C-N-CA	5.82	128.07	120.28
3	A	613	GLU	N-CA-C	-5.81	104.94	111.28
11	X	27	GLY	CA-C-N	5.81	128.00	120.44
11	X	27	GLY	C-N-CA	5.81	128.00	120.44
3	A	361	ALA	CA-C-N	5.81	129.15	120.31
3	A	361	ALA	C-N-CA	5.81	129.15	120.31
4	B	184	ALA	N-CA-C	5.81	117.29	111.07
7	I	116	GLU	N-CA-C	-5.81	105.29	112.90
11	R	19	SER	CA-C-O	5.81	126.92	120.82
4	D	350	THR	CA-C-N	5.81	127.40	120.14
4	D	350	THR	C-N-CA	5.81	127.40	120.14
1	M	92	PHE	CB-CG-CD2	-5.80	110.83	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	110	ARG	N-CA-CB	5.80	120.70	110.37
3	C	399	VAL	N-CA-CB	5.80	117.62	111.00
3	A	148	VAL	N-CA-CB	5.80	117.45	110.31
5	Q	214	PHE	CA-C-N	5.80	128.06	120.28
5	Q	214	PHE	C-N-CA	5.80	128.06	120.28
3	C	600	PHE	CA-CB-CG	-5.80	108.00	113.80
4	D	240	LEU	CB-CA-C	-5.80	99.09	109.71
9	b	97	GLU	N-CA-CB	5.80	118.75	110.16
3	C	403	SER	O-C-N	-5.80	115.24	120.92
4	D	319	ALA	N-CA-CB	5.80	120.29	110.49
4	F	326	ASN	CB-CA-C	-5.80	101.44	111.30
4	B	460	GLN	CA-C-O	5.80	126.57	120.42
10	O	18	GLN	N-CA-C	-5.80	105.97	113.16
4	D	308	MET	O-C-N	5.80	128.76	122.15
3	A	106	ASP	CA-C-O	-5.80	114.53	121.89
8	P	262	GLU	CA-C-N	5.80	127.98	120.44
8	P	262	GLU	C-N-CA	5.80	127.98	120.44
11	Z	72	VAL	CA-C-O	-5.80	115.24	121.27
11	V	13	GLY	CA-C-N	5.80	128.84	120.38
11	V	13	GLY	C-N-CA	5.80	128.84	120.38
4	F	98	GLU	CA-C-O	5.79	126.75	120.32
5	Q	149	TYR	CA-C-N	5.79	128.52	120.29
5	Q	149	TYR	C-N-CA	5.79	128.52	120.29
9	b	68	GLN	O-C-N	5.79	128.04	122.07
3	A	325	PRO	N-CA-C	5.79	124.40	112.47
9	b	343	ARG	N-CA-C	5.79	117.59	111.28
6	J	72	ALA	N-CA-C	-5.79	105.31	112.90
11	V	130	ILE	O-C-N	-5.79	116.15	121.94
1	M	163	ILE	N-CA-CB	5.79	118.41	110.54
4	D	319	ALA	N-CA-C	-5.79	98.47	110.80
3	A	475	TYR	CA-C-N	5.79	127.08	119.84
3	A	475	TYR	C-N-CA	5.79	127.08	119.84
3	C	66	ASP	CA-C-N	5.79	130.35	122.19
3	C	66	ASP	C-N-CA	5.79	130.35	122.19
8	P	432	GLU	CA-C-O	5.79	126.69	120.55
11	W	55	VAL	CA-C-N	5.79	124.99	118.97
11	W	55	VAL	C-N-CA	5.79	124.99	118.97
3	A	577	VAL	CB-CA-C	-5.79	104.33	112.14
7	K	40	ASP	CB-CA-C	-5.79	101.19	110.79
11	U	92	GLY	N-CA-C	5.79	121.40	113.99
3	A	337	ILE	CA-C-O	-5.78	114.72	120.85
5	Q	207	CYS	CA-C-N	5.78	128.03	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	207	CYS	C-N-CA	5.78	128.03	120.28
5	Q	287	HIS	CA-C-O	-5.78	114.29	120.42
6	L	15	LYS	N-CA-CB	5.78	118.46	110.07
2	N	74	ALA	CB-CA-C	-5.78	101.19	110.79
3	C	495	LEU	CA-C-N	5.78	128.03	120.28
3	C	495	LEU	C-N-CA	5.78	128.03	120.28
3	A	370	ARG	O-C-N	5.78	128.33	122.09
3	A	484	ARG	NE-CZ-NH2	5.78	124.40	119.20
7	K	127	GLU	N-CA-C	5.78	117.58	111.28
8	P	188	ARG	N-CA-C	5.78	117.58	111.28
11	S	123	PRO	N-CA-CB	5.78	109.32	103.25
4	F	358	ILE	N-CA-C	-5.78	98.09	107.28
8	P	274	LEU	N-CA-CB	5.78	118.61	110.12
9	b	340	TRP	CA-C-N	5.78	127.88	122.85
9	b	340	TRP	C-N-CA	5.78	127.88	122.85
11	U	69	VAL	CA-C-N	5.78	127.92	120.70
11	U	69	VAL	C-N-CA	5.78	127.92	120.70
8	P	364	ASP	CA-CB-CG	5.78	118.38	112.60
3	A	146	PHE	CA-CB-CG	-5.77	108.03	113.80
4	B	279	THR	O-C-N	-5.77	116.56	123.31
6	L	62	ALA	N-CA-C	-5.77	103.59	111.56
9	b	99	TYR	N-CA-C	-5.77	105.57	113.30
7	K	43	TYR	CA-C-O	-5.77	114.73	120.90
11	X	12	PHE	N-CA-C	-5.77	106.40	113.50
3	A	590	SER	CA-C-N	5.77	129.04	119.35
3	A	590	SER	C-N-CA	5.77	129.04	119.35
8	P	173	ILE	CA-C-N	5.77	128.01	120.28
8	P	173	ILE	C-N-CA	5.77	128.01	120.28
9	b	30	ALA	CA-C-N	5.77	127.94	120.44
9	b	30	ALA	C-N-CA	5.77	127.94	120.44
11	R	23	PHE	CA-C-N	5.77	128.48	120.29
11	R	23	PHE	C-N-CA	5.77	128.48	120.29
4	D	119	PRO	N-CD-CG	5.76	111.85	103.20
4	B	468	TYR	CB-CG-CD1	5.76	129.45	120.80
10	O	145	VAL	N-CA-CB	5.76	119.23	110.58
3	E	143	PRO	CA-C-O	-5.76	114.70	122.08
11	X	41	ALA	N-CA-C	5.76	117.36	111.14
11	T	25	SER	CA-C-O	-5.76	114.76	120.70
7	G	194	SER	CA-C-N	5.76	132.54	121.54
7	G	194	SER	C-N-CA	5.76	132.54	121.54
11	Z	140	GLY	N-CA-C	-5.76	105.82	112.50
3	E	519	THR	CA-C-N	5.76	128.00	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	519	THR	C-N-CA	5.76	128.00	120.28
4	F	449	TYR	N-CA-C	-5.76	104.44	113.02
4	F	347	PRO	O-C-N	-5.76	115.03	122.23
10	O	116	TRP	N-CA-CB	5.76	120.22	110.49
3	C	191	TYR	N-CA-C	-5.76	100.55	109.24
4	F	202	ASP	N-CA-CB	5.76	120.22	110.49
5	Q	188	TYR	CA-C-N	5.76	129.06	120.31
5	Q	188	TYR	C-N-CA	5.76	129.06	120.31
8	P	417	LYS	O-C-N	-5.76	115.19	122.27
7	I	115	ASP	N-CA-C	-5.76	106.09	113.23
11	U	133	LEU	N-CA-C	5.76	118.30	111.33
4	D	102	ILE	CA-C-O	-5.75	114.09	119.62
11	R	88	PHE	N-CA-C	5.75	118.33	111.71
11	Z	29	ALA	CA-C-O	5.75	127.06	120.90
1	M	176	VAL	N-CA-C	5.75	116.80	111.45
4	D	120	ILE	N-CA-C	-5.75	106.70	112.17
3	A	444	LYS	O-C-N	5.75	128.22	122.12
11	T	50	LEU	CA-C-N	5.75	127.99	120.28
11	T	50	LEU	C-N-CA	5.75	127.99	120.28
11	W	38	GLY	CA-C-N	5.75	128.34	120.46
11	W	38	GLY	C-N-CA	5.75	128.34	120.46
3	C	32	GLY	O-C-N	-5.75	116.02	121.77
4	D	38	LEU	N-CA-CB	5.75	118.86	109.95
8	P	189	LEU	N-CA-C	-5.75	104.92	111.07
7	G	49	ASN	O-C-N	5.75	128.01	122.03
7	G	105	GLU	CA-C-N	5.75	127.99	120.28
7	G	105	GLU	C-N-CA	5.75	127.99	120.28
7	I	45	ILE	N-CA-C	-5.75	104.90	110.42
11	T	143	GLY	CA-C-N	5.75	128.31	120.54
11	T	143	GLY	C-N-CA	5.75	128.31	120.54
4	D	475	ARG	NE-CZ-NH2	-5.75	114.03	119.20
3	E	570	LEU	N-CA-C	5.75	117.63	111.36
4	F	143	ALA	N-CA-C	5.75	119.50	111.74
8	P	421	GLN	CA-C-N	5.75	127.80	120.56
8	P	421	GLN	C-N-CA	5.75	127.80	120.56
10	O	243	VAL	CA-C-O	-5.75	115.08	121.17
3	C	294	LEU	CB-CA-C	-5.75	101.82	110.90
8	P	146	VAL	CA-C-N	5.75	128.58	120.42
8	P	146	VAL	C-N-CA	5.75	128.58	120.42
8	P	461	VAL	CA-C-O	-5.75	115.08	121.17
9	b	150	GLU	CA-C-O	-5.75	114.33	120.42
9	b	324	ASN	CB-CG-OD1	-5.75	109.31	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	O	81	LYS	CG-CD-CE	5.75	124.52	111.30
4	D	194	VAL	CA-C-N	5.75	127.27	120.09
4	D	194	VAL	C-N-CA	5.75	127.27	120.09
11	U	126	PHE	CA-CB-CG	5.75	119.55	113.80
11	W	132	ILE	O-C-N	-5.75	116.28	121.91
3	C	175	PRO	N-CA-CB	5.74	108.65	103.08
3	C	386	ALA	CA-C-O	-5.74	114.46	120.55
4	D	79	VAL	N-CA-CB	5.74	118.48	110.56
4	F	190	GLN	CG-CD-NE2	-5.74	107.79	116.40
3	C	488	ILE	N-CA-C	5.74	116.48	110.62
3	A	511	ASP	CA-C-O	5.74	126.57	119.97
11	V	90	GLN	CA-C-N	5.74	128.77	120.79
11	V	90	GLN	C-N-CA	5.74	128.77	120.79
8	P	77	LEU	N-CA-CB	5.74	118.33	110.01
11	U	36	GLY	CA-C-N	5.74	128.32	120.46
11	U	36	GLY	C-N-CA	5.74	128.32	120.46
2	N	52	ASP	CA-C-N	5.74	127.90	120.44
2	N	52	ASP	C-N-CA	5.74	127.90	120.44
10	O	285	ARG	N-CA-C	5.74	117.53	111.28
7	G	71	LEU	CA-C-N	5.74	129.03	120.31
7	G	71	LEU	C-N-CA	5.74	129.03	120.31
11	a	89	ILE	N-CA-C	-5.74	104.93	110.72
3	C	352	MET	N-CA-C	-5.73	99.38	108.73
4	F	408	ALA	CA-C-N	5.73	128.31	120.46
4	F	408	ALA	C-N-CA	5.73	128.31	120.46
3	A	172	ILE	N-CA-CB	5.73	117.53	111.00
6	H	21	VAL	CA-C-N	5.73	127.96	120.28
6	H	21	VAL	C-N-CA	5.73	127.96	120.28
11	a	155	THR	N-CA-C	5.73	118.50	109.96
3	C	269	LEU	CA-C-N	5.73	127.96	120.28
3	C	269	LEU	C-N-CA	5.73	127.96	120.28
9	b	64	ASN	CA-C-N	5.73	128.56	120.42
9	b	64	ASN	C-N-CA	5.73	128.56	120.42
10	O	30	THR	N-CA-CB	5.73	118.64	110.16
3	C	341	GLU	O-C-N	-5.73	116.05	122.12
4	F	256	PRO	CB-CA-C	-5.73	103.28	112.21
3	A	609	GLU	N-CA-C	-5.73	104.95	111.14
10	O	372	HIS	CA-CB-CG	-5.73	108.07	113.80
1	M	69	ALA	N-CA-C	5.73	117.52	111.28
4	D	90	LYS	N-CA-C	-5.73	105.63	113.30
10	O	361	LYS	N-CA-C	-5.73	98.75	108.26
11	X	151	ASN	CA-CB-CG	5.73	118.33	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	V	148	LEU	CA-C-N	5.73	128.27	120.54
11	V	148	LEU	C-N-CA	5.73	128.27	120.54
3	A	611	PHE	CA-C-N	5.72	128.42	120.29
3	A	611	PHE	C-N-CA	5.72	128.42	120.29
4	B	336	THR	CB-CA-C	5.72	119.58	110.19
11	S	71	SER	O-C-N	-5.72	116.14	122.09
3	A	500	GLN	N-CA-C	5.72	117.19	111.07
4	B	429	ASP	CA-C-N	5.72	128.42	120.29
4	B	429	ASP	C-N-CA	5.72	128.42	120.29
9	b	329	ASP	O-C-N	-5.72	116.06	122.12
6	H	7	ILE	N-CA-C	-5.72	105.15	110.53
7	G	59	ASP	CA-C-N	5.72	126.29	119.94
7	G	59	ASP	C-N-CA	5.72	126.29	119.94
7	I	175	SER	N-CA-C	-5.72	101.99	110.46
3	E	139	TRP	CB-CG-CD1	5.72	135.48	126.90
4	B	349	LEU	O-C-N	5.72	128.67	122.15
9	b	282	SER	O-C-N	5.72	130.48	122.36
7	G	24	ILE	O-C-N	5.72	127.52	121.91
6	J	27	TYR	CB-CA-C	-5.72	101.90	110.88
11	U	134	ILE	O-C-N	-5.72	116.09	121.87
4	D	484	PHE	CA-C-N	5.72	131.99	121.70
4	D	484	PHE	C-N-CA	5.72	131.99	121.70
2	N	99	HIS	CB-CA-C	-5.72	102.22	109.65
3	C	50	LYS	O-C-N	-5.72	116.64	123.27
3	C	222	PRO	CB-CA-C	5.72	118.49	110.60
3	C	349	ASN	OD1-CG-ND2	5.72	128.32	122.60
3	E	450	HIS	CB-CG-ND1	5.72	131.27	122.70
3	E	510	SER	N-CA-C	5.72	117.51	111.28
11	V	57	VAL	N-CA-C	5.72	116.36	110.36
4	D	180	HIS	CE1-NE2-CD2	-5.71	103.29	109.00
8	P	305	HIS	ND1-CE1-NE2	5.71	114.11	108.40
9	b	101	PRO	CA-C-N	5.71	126.21	120.04
9	b	101	PRO	C-N-CA	5.71	126.21	120.04
3	C	524	ASP	CA-CB-CG	-5.71	106.89	112.60
4	B	260	LEU	CB-CA-C	-5.71	101.31	110.79
11	R	15	ILE	N-CA-C	-5.71	104.04	112.04
3	C	340	ALA	CA-C-O	5.71	126.60	120.55
4	F	324	GLY	CA-C-N	5.71	130.24	122.07
4	F	324	GLY	C-N-CA	5.71	130.24	122.07
4	F	429	ASP	CA-C-N	5.71	128.99	120.31
4	F	429	ASP	C-N-CA	5.71	128.99	120.31
8	P	287	SER	N-CA-C	5.71	117.18	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	79	THR	N-CA-C	-5.71	105.14	111.36
9	b	147	SER	CA-C-N	5.71	127.47	120.22
9	b	147	SER	C-N-CA	5.71	127.47	120.22
7	K	132	LEU	CA-C-N	5.71	130.69	122.35
7	K	132	LEU	C-N-CA	5.71	130.69	122.35
9	b	31	TYR	CA-C-O	-5.71	114.83	120.82
10	O	213	LEU	O-C-N	-5.71	115.64	122.15
10	O	333	PRO	N-CA-C	-5.71	103.73	110.70
11	T	92	GLY	CA-C-O	-5.71	114.23	120.40
4	D	208	PHE	N-CA-C	-5.71	100.10	109.40
4	D	247	ASP	CA-C-N	5.71	125.71	119.89
4	D	247	ASP	C-N-CA	5.71	125.71	119.89
4	F	416	MET	N-CA-C	-5.71	105.20	111.82
3	A	251	THR	N-CA-C	-5.71	99.36	109.06
8	P	172	ASN	CA-C-N	5.71	128.52	120.42
8	P	172	ASN	C-N-CA	5.71	128.52	120.42
6	H	91	LYS	N-CA-C	5.71	117.18	111.07
3	A	372	GLY	O-C-N	-5.71	115.28	122.41
3	A	379	GLY	CA-C-O	5.71	126.55	119.25
4	D	417	LYS	CA-C-N	5.70	127.86	120.44
4	D	417	LYS	C-N-CA	5.70	127.86	120.44
4	B	232	ASN	OD1-CG-ND2	5.70	128.30	122.60
8	P	199	TYR	CA-C-N	5.70	128.19	120.38
8	P	199	TYR	C-N-CA	5.70	128.19	120.38
3	C	254	ILE	N-CA-CB	5.70	119.19	111.21
3	E	411	SER	CA-C-O	-5.70	114.21	120.43
3	E	576	ASP	N-CA-CB	5.70	118.34	110.07
7	K	99	ILE	N-CA-C	-5.70	104.96	110.72
7	G	107	LEU	CA-C-N	5.70	128.97	120.31
7	G	107	LEU	C-N-CA	5.70	128.97	120.31
4	D	326	ASN	N-CA-CB	5.70	120.55	111.66
3	A	129	ASP	CB-CA-C	5.70	119.32	111.23
4	B	129	GLU	CA-C-O	-5.70	112.36	120.51
11	V	72	VAL	N-CA-C	5.70	116.34	110.36
3	C	332	SER	CA-C-O	-5.70	114.81	120.90
3	C	232	PRO	N-CA-C	-5.70	100.74	112.47
2	N	81	VAL	N-CA-CB	5.69	117.86	110.57
8	P	47	LEU	CA-C-O	5.69	126.58	120.55
6	J	84	LYS	CA-C-O	5.69	126.37	119.31
3	C	442	ASP	N-CA-CB	5.69	119.50	110.57
3	E	175	PRO	CB-CA-C	5.69	117.86	110.92
3	E	441	LEU	N-CA-C	-5.69	98.68	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	76	ILE	O-C-N	5.69	129.41	123.26
9	b	49	ARG	CD-NE-CZ	-5.69	116.43	124.40
11	a	127	VAL	CA-C-N	5.69	127.51	120.34
11	a	127	VAL	C-N-CA	5.69	127.51	120.34
11	Z	32	THR	CA-C-N	5.69	128.16	120.65
11	Z	32	THR	C-N-CA	5.69	128.16	120.65
11	S	76	TYR	CA-CB-CG	-5.69	103.66	113.90
11	V	75	CYS	N-CA-C	5.69	117.96	111.02
10	O	208	LYS	CA-C-O	-5.69	114.39	120.42
11	S	63	ILE	CA-C-N	5.69	127.90	120.28
11	S	63	ILE	C-N-CA	5.69	127.90	120.28
11	T	109	GLY	CA-C-N	5.69	127.73	120.56
11	T	109	GLY	C-N-CA	5.69	127.73	120.56
1	M	175	HIS	CB-CG-ND1	5.69	131.23	122.70
4	D	92	THR	N-CA-C	-5.69	100.70	109.52
4	D	209	SER	CA-C-O	5.69	127.83	121.40
3	A	364	LEU	N-CA-C	5.69	117.56	111.36
9	b	25	ILE	CA-C-O	5.69	126.09	119.89
11	W	101	GLY	CA-C-N	5.69	128.22	120.54
11	W	101	GLY	C-N-CA	5.69	128.22	120.54
4	D	48	ARG	N-CA-CB	5.69	118.57	110.44
3	A	349	ASN	N-CA-C	-5.69	100.02	109.46
10	O	182	GLU	N-CA-C	-5.69	103.84	112.99
11	R	22	ILE	CA-C-N	5.69	127.90	120.28
11	R	22	ILE	C-N-CA	5.69	127.90	120.28
4	D	331	GLN	OE1-CD-NE2	5.68	128.28	122.60
11	Z	151	ASN	N-CA-CB	5.68	118.41	109.94
11	W	50	LEU	CB-CA-C	-5.68	101.30	110.74
6	L	43	ILE	CA-C-O	-5.68	114.20	120.96
7	G	183	LEU	N-CA-C	-5.68	107.34	114.56
11	U	61	GLY	N-CA-C	5.68	121.04	114.16
11	Y	82	GLN	N-CA-CB	5.68	120.21	111.46
8	P	317	ASN	OD1-CG-ND2	-5.68	116.92	122.60
11	R	116	VAL	CB-CA-C	5.68	121.42	112.16
3	C	451	PHE	CA-CB-CG	-5.68	108.12	113.80
4	F	252	ARG	CA-C-O	-5.68	114.86	120.82
5	Q	299	ALA	N-CA-C	5.68	118.24	111.71
8	P	314	LEU	CA-C-O	5.68	126.75	120.90
9	b	40	GLN	CA-C-N	5.68	130.52	121.66
9	b	40	GLN	C-N-CA	5.68	130.52	121.66
10	O	334	PRO	N-CA-C	5.68	120.51	111.26
3	C	522	LYS	N-CA-CB	5.68	118.24	110.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	466	ARG	CA-C-O	5.68	126.51	120.10
5	Q	105	ASP	CA-C-N	5.68	128.16	120.44
5	Q	105	ASP	C-N-CA	5.68	128.16	120.44
3	A	318	VAL	N-CA-C	-5.67	99.57	107.80
4	B	344	HIS	CE1-NE2-CD2	-5.67	103.33	109.00
9	b	291	THR	CB-CA-C	-5.67	101.37	110.79
10	O	190	HIS	CE1-NE2-CD2	-5.67	103.33	109.00
11	U	115	GLY	CA-C-O	5.67	126.20	119.50
11	R	51	PHE	N-CA-CB	-5.67	101.78	110.12
10	O	288	LEU	N-CA-C	5.67	117.27	111.14
4	D	55	LEU	O-C-N	-5.67	116.75	123.22
3	E	318	VAL	N-CA-C	-5.67	99.58	107.80
3	E	602	LYS	N-CA-C	5.67	118.23	111.71
8	P	267	TYR	CA-CB-CG	-5.67	103.69	113.90
11	a	106	PHE	CA-CB-CG	-5.67	108.13	113.80
3	E	588	GLU	N-CA-C	-5.67	103.12	108.22
11	T	38	GLY	CA-C-N	5.67	127.70	120.56
11	T	38	GLY	C-N-CA	5.67	127.70	120.56
11	a	93	ALA	N-CA-CB	5.67	118.29	110.07
4	F	188	CYS	N-CA-CB	5.67	118.45	110.12
3	E	51	VAL	N-CA-C	-5.66	100.24	108.17
5	Q	138	THR	CA-C-N	5.66	128.14	120.44
5	Q	138	THR	C-N-CA	5.66	128.14	120.44
7	K	120	ILE	N-CA-C	-5.66	105.21	110.53
8	P	444	THR	CB-CA-C	-5.66	101.22	110.85
10	O	196	VAL	CA-CB-CG2	-5.66	100.77	110.40
1	M	82	GLN	OE1-CD-NE2	5.66	128.26	122.60
1	M	153	GLN	CA-C-N	5.66	127.87	120.28
1	M	153	GLN	C-N-CA	5.66	127.87	120.28
4	D	80	PHE	CA-CB-CG	-5.66	108.14	113.80
3	A	359	ARG	O-C-N	5.66	129.92	122.33
4	F	246	ASN	CA-C-O	5.66	125.13	118.90
11	T	19	SER	CA-C-N	5.66	128.12	120.65
11	T	19	SER	C-N-CA	5.66	128.12	120.65
4	F	88	VAL	N-CA-C	-5.66	106.69	111.56
4	F	106	GLU	CB-CA-C	-5.66	101.00	110.56
3	A	213	HIS	CB-CG-CD2	5.66	138.56	131.20
3	A	557	ALA	CB-CA-C	-5.66	101.23	110.85
5	Q	66	SER	N-CA-CB	5.66	118.28	110.07
5	Q	180	ILE	CA-C-N	5.66	128.32	120.29
5	Q	180	ILE	C-N-CA	5.66	128.32	120.29
7	K	149	ILE	N-CA-C	-5.66	104.99	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	S	28	ALA	N-CA-C	5.66	117.53	111.36
7	G	171	GLU	N-CA-CB	-5.66	101.00	111.52
4	D	425	LEU	O-C-N	-5.66	116.57	122.96
3	A	392	TYR	O-C-N	-5.66	115.70	122.15
6	L	102	VAL	O-C-N	-5.66	115.41	121.80
10	O	351	LEU	CA-C-N	5.66	126.22	120.00
10	O	351	LEU	C-N-CA	5.66	126.22	120.00
3	C	161	VAL	N-CA-C	-5.65	100.03	108.46
4	D	404	TYR	N-CA-CB	5.65	118.27	110.07
8	P	294	ILE	N-CA-C	5.65	116.39	110.62
11	U	15	ILE	O-C-N	-5.65	115.41	121.80
4	D	122	ASN	CA-CB-CG	5.65	118.25	112.60
8	P	227	ALA	CA-C-O	5.65	126.40	119.05
11	a	84	LEU	N-CA-CB	5.65	118.27	110.07
11	R	42	THR	CA-CB-CG2	5.65	120.11	110.50
1	M	164	LYS	N-CA-C	5.65	117.44	111.28
11	R	33	ALA	CA-C-N	5.65	127.79	120.44
11	R	33	ALA	C-N-CA	5.65	127.79	120.44
11	S	58	ILE	CA-C-N	5.65	127.85	120.28
11	S	58	ILE	C-N-CA	5.65	127.85	120.28
4	B	320	GLY	N-CA-C	-5.65	104.12	111.52
11	Y	138	VAL	O-C-N	5.65	127.35	121.87
3	C	497	GLN	CA-C-N	5.65	128.44	120.42
3	C	497	GLN	C-N-CA	5.65	128.44	120.42
5	Q	144	ASP	CA-C-O	-5.65	114.61	121.05
11	Z	71	SER	CA-C-O	-5.65	114.86	121.07
4	B	326	ASN	N-CA-C	-5.65	106.06	114.64
9	b	63	ASP	N-CA-CB	5.65	118.42	110.12
11	Z	119	SER	CA-C-N	5.65	127.78	120.44
11	Z	119	SER	C-N-CA	5.65	127.78	120.44
11	S	93	ALA	CA-C-N	5.65	126.21	119.94
11	S	93	ALA	C-N-CA	5.65	126.21	119.94
1	M	14	THR	N-CA-C	-5.64	105.89	112.89
3	C	139	TRP	CE2-CD2-CE3	5.64	124.44	118.80
3	A	265	ILE	O-C-N	-5.64	115.42	121.80
11	X	54	ILE	CA-CB-CG2	5.64	120.10	110.50
3	E	344	ARG	CA-C-N	5.64	130.14	120.72
3	E	344	ARG	C-N-CA	5.64	130.14	120.72
4	F	101	ARG	N-CA-C	-5.64	100.72	109.24
4	F	146	TYR	CB-CG-CD1	-5.64	112.33	120.80
8	P	111	ASP	CA-C-N	5.64	127.84	120.28
8	P	111	ASP	C-N-CA	5.64	127.84	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Z	56	PRO	N-CA-C	5.64	122.92	113.78
3	E	110	ARG	N-CA-CB	5.64	123.64	110.95
3	A	235	THR	CA-C-N	5.64	131.17	121.07
3	A	235	THR	C-N-CA	5.64	131.17	121.07
3	A	597	HIS	O-C-N	-5.64	116.74	123.06
3	A	598	GLY	CA-C-N	5.64	127.84	120.28
3	A	598	GLY	C-N-CA	5.64	127.84	120.28
1	M	113	ILE	O-C-N	5.64	129.10	123.18
2	N	72	HIS	ND1-CE1-NE2	5.64	114.04	108.40
7	K	65	LYS	CA-C-O	-5.64	114.58	120.55
8	P	342	LEU	CA-C-O	5.64	126.47	120.10
4	D	50	ASN	N-CA-CB	5.63	120.01	110.49
11	a	71	SER	CB-CA-C	-5.63	102.03	110.88
3	C	407	THR	CA-CB-OG1	5.63	118.05	109.60
11	W	80	GLN	CB-CG-CD	-5.63	103.02	112.60
3	C	326	VAL	N-CA-C	5.63	118.13	111.09
4	D	282	SER	CA-C-N	5.63	127.83	120.28
4	D	282	SER	C-N-CA	5.63	127.83	120.28
3	A	498	VAL	CA-C-O	-5.63	115.09	120.95
7	K	22	ALA	CA-C-N	5.63	127.76	120.44
7	K	22	ALA	C-N-CA	5.63	127.76	120.44
7	I	47	LYS	O-C-N	-5.63	116.27	122.07
7	I	115	ASP	CA-CB-CG	-5.63	106.97	112.60
4	D	199	ASP	N-CA-C	-5.63	105.14	111.28
3	E	596	VAL	N-CA-C	-5.63	99.44	107.77
6	J	87	ALA	CA-C-O	-5.63	114.45	120.42
3	C	217	VAL	CA-C-N	5.63	131.79	122.73
3	C	217	VAL	C-N-CA	5.63	131.79	122.73
5	Q	25	LEU	N-CA-C	5.63	118.64	110.42
11	T	96	SER	CA-C-N	5.63	128.41	120.42
11	T	96	SER	C-N-CA	5.63	128.41	120.42
11	V	56	PRO	N-CA-CB	5.63	109.16	103.25
11	W	33	ALA	CA-C-N	5.63	127.75	120.44
11	W	33	ALA	C-N-CA	5.63	127.75	120.44
6	L	12	GLN	CA-C-N	5.62	127.82	120.28
6	L	12	GLN	C-N-CA	5.62	127.82	120.28
11	X	40	CYS	O-C-N	-5.62	116.16	122.12
4	F	247	ASP	CA-C-O	-5.62	115.05	119.66
10	O	303	TRP	CA-C-O	5.62	126.49	120.70
6	H	101	THR	CA-CB-CG2	-5.62	100.94	110.50
11	R	23	PHE	N-CA-C	5.62	117.41	111.28
3	A	602	LYS	N-CA-C	5.62	118.34	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	319	ALA	CB-CA-C	-5.62	99.87	110.16
5	Q	203	PRO	CB-CA-C	-5.62	102.28	111.56
10	O	287	GLN	CA-C-N	5.62	128.09	120.44
10	O	287	GLN	C-N-CA	5.62	128.09	120.44
4	B	409	ILE	CA-C-N	5.62	127.17	120.14
4	B	409	ILE	C-N-CA	5.62	127.17	120.14
4	D	358	ILE	CA-C-O	-5.62	114.55	120.39
7	K	156	ILE	N-CA-C	-5.62	105.25	110.53
8	P	369	CYS	O-C-N	-5.62	117.19	123.48
8	P	378	GLY	CA-C-N	5.62	127.74	120.44
8	P	378	GLY	C-N-CA	5.62	127.74	120.44
11	U	106	PHE	CA-C-N	5.62	127.74	120.44
11	U	106	PHE	C-N-CA	5.62	127.74	120.44
11	Z	84	LEU	N-CA-C	-5.62	105.16	111.28
3	A	450	HIS	CB-CG-ND1	5.62	131.12	122.70
5	Q	295	LEU	CA-C-N	5.62	130.09	120.71
5	Q	295	LEU	C-N-CA	5.62	130.09	120.71
9	b	195	LYS	CA-C-N	5.62	129.51	120.30
9	b	195	LYS	C-N-CA	5.62	129.51	120.30
11	Z	19	SER	CA-C-O	-5.62	114.89	121.07
4	F	67	VAL	CA-C-O	5.61	127.66	120.76
5	Q	302	GLN	O-C-N	-5.61	116.65	123.16
6	L	87	ALA	CA-C-N	5.61	128.84	120.31
6	L	87	ALA	C-N-CA	5.61	128.84	120.31
7	I	85	ARG	N-CA-CB	5.61	119.71	110.39
11	U	41	ALA	O-C-N	5.61	127.85	122.07
11	X	62	ILE	CA-CB-CG1	5.61	119.94	110.40
11	a	153	ARG	CA-C-O	5.61	126.56	120.55
11	V	14	ALA	N-CA-C	5.61	118.94	111.75
4	F	148	GLU	O-C-N	-5.61	115.13	122.59
6	L	14	GLU	CA-C-O	-5.61	114.47	120.42
6	L	53	GLU	O-C-N	-5.61	114.24	122.43
4	D	384	LYS	N-CA-C	-5.61	106.20	113.16
11	V	95	LEU	CA-C-N	5.61	128.11	120.54
11	V	95	LEU	C-N-CA	5.61	128.11	120.54
3	E	202	PHE	N-CA-C	-5.61	98.86	110.80
4	F	112	ILE	N-CA-CB	5.61	118.88	111.25
3	A	601	GLU	CA-C-N	5.61	128.83	120.31
3	A	601	GLU	C-N-CA	5.61	128.83	120.31
11	U	153	ARG	NE-CZ-NH2	5.61	124.25	119.20
11	X	64	ALA	CB-CA-C	-5.61	99.58	110.46
11	V	52	LYS	CB-CA-C	-5.61	102.04	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	100	LEU	CA-C-O	5.61	126.36	120.42
3	A	610	ARG	NE-CZ-NH1	-5.61	115.89	121.50
6	L	58	GLU	CB-CG-CD	-5.61	103.07	112.60
11	R	141	LEU	N-CA-CB	5.61	118.29	109.94
3	E	304	MET	CG-SD-CE	-5.60	88.57	100.90
5	Q	114	THR	CA-C-O	5.60	126.43	120.10
11	W	76	TYR	CA-CB-CG	-5.60	103.81	113.90
4	D	49	TYR	CB-CA-C	5.60	118.66	110.26
7	I	51	VAL	CB-CA-C	5.60	119.14	111.97
11	X	156	GLN	OE1-CD-NE2	-5.60	117.00	122.60
4	D	64	GLN	N-CA-C	-5.60	100.76	109.72
4	B	318	ARG	N-CA-C	-5.60	101.22	109.62
8	P	336	ARG	N-CA-CB	5.60	118.35	110.12
11	T	52	LYS	CA-C-N	5.60	128.10	120.54
11	T	52	LYS	C-N-CA	5.60	128.10	120.54
1	M	133	GLN	CB-CG-CD	-5.60	103.08	112.60
11	X	94	GLY	N-CA-C	5.60	118.99	112.50
3	E	279	ILE	O-C-N	5.60	129.13	123.20
3	A	541	TRP	CZ3-CH2-CZ2	-5.60	114.22	121.50
8	P	238	LEU	CB-CA-C	-5.60	102.09	110.88
9	b	344	ASP	CA-C-N	5.60	128.34	120.28
9	b	344	ASP	C-N-CA	5.60	128.34	120.28
11	V	33	ALA	CA-C-N	5.60	128.09	120.54
11	V	33	ALA	C-N-CA	5.60	128.09	120.54
3	C	354	ALA	N-CA-C	-5.59	100.28	109.40
4	D	368	GLY	N-CA-C	-5.59	106.83	116.01
3	E	123	TYR	CA-C-N	5.59	132.48	122.13
3	E	123	TYR	C-N-CA	5.59	132.48	122.13
3	E	247	VAL	CA-C-N	5.59	130.72	123.00
3	E	247	VAL	C-N-CA	5.59	130.72	123.00
4	B	286	ASP	CA-C-N	5.59	127.78	120.28
4	B	286	ASP	C-N-CA	5.59	127.78	120.28
4	D	127	PHE	CA-CB-CG	-5.59	108.21	113.80
3	A	472	ASP	CA-C-N	5.59	127.71	120.44
3	A	472	ASP	C-N-CA	5.59	127.71	120.44
4	B	416	MET	N-CA-CB	5.59	118.44	110.16
1	M	110	GLU	N-CA-C	-5.59	99.31	108.76
4	B	465	LEU	N-CA-C	5.59	118.31	111.82
10	O	136	ASN	CB-CA-C	-5.59	101.51	110.79
11	X	22	ILE	CA-C-N	5.59	127.71	120.44
11	X	22	ILE	C-N-CA	5.59	127.71	120.44
11	X	80	GLN	CA-C-N	5.59	128.23	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	X	80	GLN	C-N-CA	5.59	128.23	120.29
11	X	132	ILE	N-CA-CB	-5.59	103.41	110.57
11	Z	85	TYR	CB-CG-CD1	-5.59	112.41	120.80
3	C	406	ARG	N-CA-C	-5.59	100.98	108.86
6	H	39	ALA	CA-C-N	5.59	128.81	120.31
6	H	39	ALA	C-N-CA	5.59	128.81	120.31
10	O	25	ALA	CB-CA-C	-5.59	103.71	110.81
3	E	534	TYR	N-CA-C	-5.59	106.46	113.28
3	A	52	GLY	O-C-N	-5.59	117.46	122.77
9	b	82	LYS	CA-C-N	5.59	132.21	121.54
9	b	82	LYS	C-N-CA	5.59	132.21	121.54
9	b	236	PHE	N-CA-C	-5.59	100.08	108.96
3	C	241	ASP	CA-CB-CG	-5.58	107.02	112.60
11	Z	73	LEU	CA-C-N	5.58	128.11	120.46
11	Z	73	LEU	C-N-CA	5.58	128.11	120.46
11	W	25	SER	CA-C-O	-5.58	114.95	120.70
4	D	462	TRP	CG-CD2-CE3	-5.58	128.32	133.90
4	B	398	ASP	CA-CB-CG	5.58	118.18	112.60
8	P	354	THR	CA-C-N	5.58	128.22	120.29
8	P	354	THR	C-N-CA	5.58	128.22	120.29
11	X	27	GLY	CA-C-O	5.58	126.80	121.05
11	T	105	GLY	O-C-N	-5.58	116.44	122.19
1	M	35	LYS	CB-CA-C	-5.58	101.52	110.79
8	P	390	ASP	N-CA-CB	5.58	119.92	110.49
6	L	98	LEU	N-CA-CB	5.58	118.32	110.12
7	I	75	ILE	N-CA-C	-5.58	105.08	110.72
3	C	579	HIS	CE1-NE2-CD2	-5.58	103.42	109.00
4	D	180	HIS	CA-C-O	5.58	126.46	120.55
4	D	355	GLU	CB-CA-C	-5.58	103.56	111.76
5	Q	276	ARG	N-CA-C	-5.58	99.83	108.42
10	O	50	ILE	CA-CB-CG1	5.58	119.88	110.40
11	R	143	GLY	N-CA-C	-5.58	105.74	112.49
4	F	138	PRO	O-C-N	5.58	128.47	122.17
4	F	228	ASP	N-CA-C	5.58	117.36	111.28
4	F	426	SER	N-CA-C	-5.58	100.85	108.38
11	R	16	GLY	O-C-N	5.58	127.53	122.18
3	C	554	HIS	CE1-NE2-CD2	-5.58	103.42	109.00
4	F	200	VAL	CB-CA-C	-5.58	104.53	112.22
4	F	347	PRO	N-CA-C	-5.58	105.93	113.40
7	I	112	ASN	OD1-CG-ND2	5.58	128.18	122.60
7	I	183	LEU	O-C-N	-5.58	115.17	122.59
1	M	181	THR	O-C-N	5.57	128.50	122.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	102	GLU	CB-CA-C	-5.57	103.81	111.73
5	Q	176	ASN	CA-C-N	5.57	127.58	120.56
5	Q	176	ASN	C-N-CA	5.57	127.58	120.56
11	T	142	TYR	CA-C-N	5.57	126.01	119.94
11	T	142	TYR	C-N-CA	5.57	126.01	119.94
3	E	362	GLU	CA-C-N	5.57	127.75	120.28
3	E	362	GLU	C-N-CA	5.57	127.75	120.28
11	Y	117	ARG	CA-CB-CG	-5.57	102.96	114.10
3	C	425	ASP	CA-C-O	-5.57	114.74	120.87
4	F	170	ILE	CB-CA-C	-5.57	104.53	110.16
10	O	160	ALA	CA-C-O	5.57	126.32	120.42
4	F	344	HIS	CA-C-N	5.57	125.03	119.24
4	F	344	HIS	C-N-CA	5.57	125.03	119.24
9	b	121	LEU	N-CA-C	5.57	117.43	111.36
9	b	200	GLU	N-CA-C	-5.57	105.11	111.07
1	M	147	VAL	N-CA-CB	5.57	117.69	110.57
3	C	164	ASN	CA-CB-CG	5.57	118.17	112.60
3	E	250	GLY	O-C-N	5.57	128.89	122.60
4	F	311	ASP	CA-C-N	5.57	127.67	120.44
4	F	311	ASP	C-N-CA	5.57	127.67	120.44
8	P	38	GLU	CB-CG-CD	-5.57	103.14	112.60
11	U	152	SER	O-C-N	5.57	128.02	122.12
11	a	71	SER	O-C-N	5.57	127.80	122.07
4	F	404	TYR	CA-C-O	-5.56	114.65	120.55
10	O	286	VAL	CB-CA-C	5.56	119.31	112.02
10	O	368	ASP	CA-C-N	5.56	132.17	121.54
10	O	368	ASP	C-N-CA	5.56	132.17	121.54
4	F	275	LEU	N-CA-C	-5.56	99.34	108.41
5	Q	300	PHE	CB-CG-CD1	5.56	130.16	120.70
7	G	204	GLU	CA-C-N	5.56	128.01	120.44
7	G	204	GLU	C-N-CA	5.56	128.01	120.44
4	D	53	VAL	N-CA-C	-5.56	99.77	108.95
4	F	116	SER	N-CA-C	-5.56	106.62	113.41
8	P	237	HIS	N-CA-CB	5.56	118.40	110.06
7	G	114	ARG	O-C-N	5.56	128.49	122.15
11	a	56	PRO	N-CD-CG	5.56	111.54	103.20
3	E	223	VAL	N-CA-C	-5.56	99.68	108.90
4	D	287	ALA	CA-C-N	5.55	127.72	120.28
4	D	287	ALA	C-N-CA	5.55	127.72	120.28
10	O	155	ALA	CA-C-N	5.55	128.18	120.29
10	O	155	ALA	C-N-CA	5.55	128.18	120.29
11	W	142	TYR	CA-C-O	5.55	126.44	120.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	233	LEU	N-CA-C	-5.55	99.97	109.24
7	G	77	LYS	CA-C-O	-5.55	113.83	120.10
3	C	115	ILE	CA-C-N	5.55	127.72	120.28
3	C	115	ILE	C-N-CA	5.55	127.72	120.28
3	E	73	TYR	N-CA-C	-5.55	106.09	112.92
10	O	73	ASN	CA-C-N	5.55	127.72	120.28
10	O	73	ASN	C-N-CA	5.55	127.72	120.28
5	Q	30	TYR	N-CA-CB	5.55	118.28	110.12
7	K	145	ASP	CA-C-N	5.55	128.30	120.42
7	K	145	ASP	C-N-CA	5.55	128.30	120.42
10	O	260	PHE	CA-CB-CG	-5.55	108.25	113.80
5	Q	288	PHE	CA-C-O	-5.55	114.67	120.55
6	J	81	ALA	N-CA-C	-5.55	104.74	112.45
4	D	180	HIS	CG-CD2-NE2	5.55	112.75	107.20
4	F	86	ILE	CA-CB-CG1	-5.55	100.97	110.40
3	A	50	LYS	N-CA-C	-5.55	99.37	108.41
6	H	53	GLU	N-CA-C	5.55	119.67	113.01
6	H	89	LYS	CA-C-O	5.55	126.61	120.90
4	F	322	VAL	O-C-N	-5.54	117.48	123.14
4	F	334	ILE	CA-C-N	5.54	130.81	122.99
4	F	334	ILE	C-N-CA	5.54	130.81	122.99
8	P	473	ILE	CA-C-N	5.54	126.10	120.00
8	P	473	ILE	C-N-CA	5.54	126.10	120.00
5	Q	19	GLY	CA-C-N	5.54	128.16	120.29
5	Q	19	GLY	C-N-CA	5.54	128.16	120.29
8	P	7	LEU	O-C-N	5.54	128.93	122.67
11	a	135	PHE	O-C-N	5.54	129.09	122.27
3	C	478	PHE	N-CA-C	5.54	121.08	113.77
4	F	173	PHE	N-CA-C	-5.54	100.21	109.24
6	L	104	LYS	N-CA-CB	5.54	120.31	110.39
7	I	212	GLU	CA-C-O	-5.54	114.65	120.63
4	D	204	HIS	CE1-NE2-CD2	-5.54	103.46	109.00
4	F	201	HIS	CA-C-N	5.54	132.12	121.54
4	F	201	HIS	C-N-CA	5.54	132.12	121.54
3	A	587	PHE	O-C-N	-5.54	116.32	122.86
5	Q	254	PHE	CB-CA-C	-5.54	101.44	110.85
5	Q	300	PHE	CA-CB-CG	-5.54	108.26	113.80
10	O	330	ILE	N-CA-C	-5.54	100.36	108.11
11	T	15	ILE	CB-CG1-CD1	5.54	125.43	113.80
10	O	358	LYS	N-CA-C	-5.54	101.10	109.85
3	E	113	LYS	N-CA-CB	5.54	118.26	110.12
4	B	337	MET	CA-C-O	-5.54	115.12	119.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	163	LYS	N-CA-CB	5.54	118.67	110.53
8	P	448	ALA	CA-C-N	5.54	127.70	120.28
8	P	448	ALA	C-N-CA	5.54	127.70	120.28
11	R	97	VAL	CA-C-O	5.54	126.45	120.47
3	C	543	THR	CA-C-N	5.53	128.15	120.29
3	C	543	THR	C-N-CA	5.53	128.15	120.29
4	B	304	TYR	CA-CB-CG	-5.53	103.94	113.90
10	O	63	VAL	N-CA-CB	5.53	118.06	110.54
8	P	377	ASN	CA-CB-CG	-5.53	107.07	112.60
11	R	88	PHE	CB-CA-C	-5.53	100.40	110.63
3	A	613	GLU	O-C-N	5.53	127.98	122.12
8	P	82	HIS	CB-CA-C	5.53	119.56	110.88
11	a	95	LEU	N-CA-CB	5.53	118.17	109.94
4	F	50	ASN	CA-C-N	5.53	129.40	121.50
4	F	50	ASN	C-N-CA	5.53	129.40	121.50
11	S	85	TYR	CA-C-O	-5.53	114.69	120.55
6	L	15	LYS	CA-C-N	5.52	127.68	120.28
6	L	15	LYS	C-N-CA	5.52	127.68	120.28
9	b	245	ILE	CB-CA-C	-5.52	104.80	112.36
9	b	303	ALA	CA-C-N	5.52	127.95	120.44
9	b	303	ALA	C-N-CA	5.52	127.95	120.44
3	C	384	LEU	CA-C-O	-5.52	115.03	120.82
3	A	615	THR	N-CA-CB	5.52	118.01	110.01
4	B	251	GLU	CA-C-N	5.52	128.13	120.29
4	B	251	GLU	C-N-CA	5.52	128.13	120.29
7	I	98	GLY	CA-C-N	5.52	127.63	120.56
7	I	98	GLY	C-N-CA	5.52	127.63	120.56
11	T	65	ILE	CB-CA-C	-5.52	103.16	112.16
3	E	580	ALA	N-CA-C	5.52	117.29	111.28
4	F	426	SER	CA-C-O	5.52	127.21	121.31
4	F	445	THR	CA-C-N	5.52	130.88	122.11
4	F	445	THR	C-N-CA	5.52	130.88	122.11
4	B	286	ASP	N-CA-CB	5.52	118.72	110.22
7	K	88	VAL	CA-C-O	-5.52	115.32	121.17
3	A	390	SER	CB-CA-C	-5.52	101.63	110.79
6	L	61	ASN	N-CA-C	-5.52	106.45	114.12
9	b	91	TYR	CB-CA-C	-5.52	100.28	109.55
1	M	168	ARG	NE-CZ-NH2	5.51	124.16	119.20
3	C	34	VAL	N-CA-C	-5.51	100.64	108.58
3	C	499	VAL	N-CA-C	5.51	116.24	110.62
4	F	265	TYR	N-CA-C	5.51	116.97	111.07
9	b	63	ASP	CA-C-N	5.51	128.22	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	b	63	ASP	C-N-CA	5.51	128.22	120.28
3	C	571	ALA	CA-C-N	5.51	128.69	120.31
3	C	571	ALA	C-N-CA	5.51	128.69	120.31
5	Q	321	ARG	CA-C-N	5.51	127.94	120.44
5	Q	321	ARG	C-N-CA	5.51	127.94	120.44
4	D	446	GLN	OE1-CD-NE2	5.51	128.11	122.60
4	B	297	GLU	CA-C-N	5.51	128.84	121.23
4	B	297	GLU	C-N-CA	5.51	128.84	121.23
8	P	465	ALA	CA-C-N	5.51	127.94	120.44
8	P	465	ALA	C-N-CA	5.51	127.94	120.44
11	X	145	ILE	N-CA-CB	5.51	116.41	110.62
3	C	298	PRO	CB-CA-C	-5.51	103.64	111.68
5	Q	149	TYR	CB-CA-C	-5.51	101.64	110.79
11	V	142	TYR	N-CA-C	5.51	117.29	111.28
11	W	53	ASN	CA-C-N	5.51	129.66	120.62
11	W	53	ASN	C-N-CA	5.51	129.66	120.62
4	D	147	PRO	N-CA-C	5.51	119.51	111.03
3	E	231	TYR	CG-CD1-CE1	-5.51	112.94	121.20
4	F	230	GLU	CA-C-N	5.51	127.60	120.44
4	F	230	GLU	C-N-CA	5.51	127.60	120.44
4	D	159	ASP	N-CA-C	5.51	116.96	111.07
3	E	484	ARG	CA-C-O	-5.51	113.64	119.97
3	C	165	SER	N-CA-C	-5.50	106.27	114.64
11	X	134	ILE	CA-C-O	5.50	126.69	120.03
4	F	159	ASP	O-C-N	-5.50	116.40	122.07
9	b	27	ARG	NE-CZ-NH2	-5.50	114.25	119.20
7	G	51	VAL	CA-C-O	-5.50	115.34	121.17
11	R	29	ALA	CA-C-N	5.50	127.65	120.28
11	R	29	ALA	C-N-CA	5.50	127.65	120.28
4	D	394	LYS	N-CA-C	-5.50	106.57	113.28
4	B	144	ARG	NE-CZ-NH2	5.50	124.15	119.20
4	B	195	ARG	O-C-N	-5.50	115.54	120.71
7	K	16	GLU	CA-C-N	5.50	127.59	120.44
7	K	16	GLU	C-N-CA	5.50	127.59	120.44
11	U	47	PRO	CB-CA-C	-5.50	102.48	111.56
11	R	31	GLY	CA-C-N	5.50	127.92	120.44
11	R	31	GLY	C-N-CA	5.50	127.92	120.44
4	D	45	LYS	N-CA-C	-5.50	99.08	110.80
1	M	84	GLN	CA-C-N	5.50	128.10	120.29
1	M	84	GLN	C-N-CA	5.50	128.10	120.29
4	D	258	LEU	CB-CA-C	-5.50	101.50	110.85
8	P	269	SER	CA-C-O	-5.50	115.02	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	O	19	ASN	CA-CB-CG	5.50	118.10	112.60
9	b	39	VAL	N-CA-CB	5.50	121.67	112.44
11	a	119	SER	CA-C-N	5.50	127.96	120.54
11	a	119	SER	C-N-CA	5.50	127.96	120.54
3	E	40	MET	CA-C-N	5.50	128.26	122.11
3	E	40	MET	C-N-CA	5.50	128.26	122.11
11	Y	147	ALA	N-CA-CB	5.50	117.98	110.01
3	C	579	HIS	CA-C-N	5.49	128.09	120.29
3	C	579	HIS	C-N-CA	5.49	128.09	120.29
4	D	90	LYS	N-CA-CB	5.49	118.91	110.61
3	E	188	ALA	CA-C-N	5.49	128.59	121.23
3	E	188	ALA	C-N-CA	5.49	128.59	121.23
4	B	399	VAL	CA-C-N	5.49	127.64	120.28
4	B	399	VAL	C-N-CA	5.49	127.64	120.28
6	H	47	LYS	N-CA-C	-5.49	104.93	111.03
11	X	133	LEU	CA-C-N	5.49	130.03	120.86
11	X	133	LEU	C-N-CA	5.49	130.03	120.86
3	C	221	ARG	CA-C-O	-5.49	114.63	120.23
7	I	159	GLU	CA-C-N	5.49	127.64	120.28
7	I	159	GLU	C-N-CA	5.49	127.64	120.28
11	Z	157	ASP	CA-C-N	5.49	131.85	121.97
11	Z	157	ASP	C-N-CA	5.49	131.85	121.97
3	A	578	LYS	N-CA-CB	5.49	118.28	110.16
11	S	39	ILE	N-CA-CB	5.49	116.60	110.51
8	P	40	ASP	CA-CB-CG	-5.49	107.11	112.60
11	T	153	ARG	CA-C-N	5.49	127.90	120.38
11	T	153	ARG	C-N-CA	5.49	127.90	120.38
8	P	133	LYS	CA-C-N	5.49	132.16	121.41
8	P	133	LYS	C-N-CA	5.49	132.16	121.41
8	P	256	ASN	CA-C-O	-5.49	114.31	119.80
10	O	344	LEU	N-CA-C	5.49	117.26	111.28
11	U	108	ILE	CA-C-N	5.49	127.19	120.22
11	U	108	ILE	C-N-CA	5.49	127.19	120.22
11	Y	19	SER	N-CA-CB	5.49	118.11	109.94
4	D	337	MET	N-CA-C	-5.48	103.22	110.40
11	X	71	SER	CB-CA-C	-5.48	102.27	110.88
11	a	126	PHE	CA-C-N	5.48	129.29	120.30
11	a	126	PHE	C-N-CA	5.48	129.29	120.30
4	F	56	THR	CA-C-O	5.48	126.35	120.32
7	K	212	GLU	O-C-N	5.48	127.93	122.12
6	H	48	ILE	CA-C-N	5.48	128.08	120.29
6	H	48	ILE	C-N-CA	5.48	128.08	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	12	ARG	CA-C-O	5.48	126.05	120.24
4	B	480	ILE	CA-C-N	5.48	128.07	120.29
4	B	480	ILE	C-N-CA	5.48	128.07	120.29
8	P	379	PHE	CA-C-N	5.48	128.07	120.29
8	P	379	PHE	C-N-CA	5.48	128.07	120.29
3	E	129	ASP	N-CA-C	-5.48	100.74	109.07
4	F	289	ARG	CD-NE-CZ	-5.48	116.73	124.40
5	Q	77	TYR	N-CA-CB	5.48	118.17	110.12
7	G	52	ARG	N-CA-CB	-5.48	102.05	110.16
11	W	15	ILE	CB-CA-C	-5.48	103.38	112.26
11	W	106	PHE	O-C-N	5.48	128.47	122.11
4	D	218	ASN	N-CA-C	-5.48	102.41	110.52
3	E	358	SER	N-CA-C	-5.48	105.47	111.82
6	J	99	ILE	N-CA-C	-5.48	105.16	110.42
3	C	429	THR	CA-CB-OG1	5.48	117.81	109.60
1	M	48	LYS	N-CA-C	5.47	117.33	111.36
6	J	82	GLU	CA-C-O	-5.47	112.52	119.31
11	U	34	LYS	N-CA-CB	5.47	117.95	110.01
11	S	117	ARG	NE-CZ-NH2	-5.47	114.27	119.20
11	T	49	LEU	CA-C-N	5.47	127.93	120.54
11	T	49	LEU	C-N-CA	5.47	127.93	120.54
3	A	416	VAL	N-CA-C	-5.47	100.72	108.65
7	K	189	VAL	N-CA-C	-5.47	98.58	107.28
11	Y	111	VAL	CA-C-N	5.47	126.17	119.99
11	Y	111	VAL	C-N-CA	5.47	126.17	119.99
7	G	202	THR	CA-C-N	5.47	128.06	120.29
7	G	202	THR	C-N-CA	5.47	128.06	120.29
3	E	579	HIS	ND1-CE1-NE2	5.47	113.87	108.40
8	P	358	GLU	CA-C-N	5.47	127.55	120.44
8	P	358	GLU	C-N-CA	5.47	127.55	120.44
6	L	21	VAL	CA-C-N	5.47	127.61	120.28
6	L	21	VAL	C-N-CA	5.47	127.61	120.28
4	B	254	ILE	O-C-N	-5.47	115.62	121.80
7	K	49	ASN	CB-CA-C	-5.47	102.30	110.88
11	X	131	LEU	CA-C-N	5.47	127.56	120.56
11	X	131	LEU	C-N-CA	5.47	127.56	120.56
4	D	301	ARG	N-CA-CB	5.46	118.38	109.69
4	F	96	THR	N-CA-C	-5.46	104.97	111.69
5	Q	66	SER	O-C-N	5.46	127.99	122.09
10	O	11	PHE	CA-CB-CG	-5.46	108.34	113.80
4	F	275	LEU	N-CA-CB	5.46	119.17	110.65
9	b	195	LYS	CA-C-O	5.46	126.34	120.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	365	ARG	NE-CZ-NH2	-5.46	114.28	119.20
3	E	585	LYS	N-CA-CB	5.46	118.57	110.49
3	C	595	GLU	N-CA-C	-5.46	107.27	114.04
4	F	56	THR	N-CA-C	-5.46	99.63	108.52
4	F	213	ALA	N-CA-C	-5.46	99.39	108.34
5	Q	35	GLN	CB-CA-C	-5.46	101.41	110.68
8	P	45	LYS	N-CA-C	5.46	117.23	111.28
11	X	98	GLY	CA-C-O	-5.46	115.11	121.00
11	T	72	VAL	CA-CB-CG1	5.46	119.68	110.40
11	W	132	ILE	N-CA-CB	5.46	116.93	110.55
5	Q	93	LYS	CA-C-N	5.46	127.59	120.28
5	Q	93	LYS	C-N-CA	5.46	127.59	120.28
8	P	301	ARG	CA-C-N	5.46	128.40	120.98
8	P	301	ARG	C-N-CA	5.46	128.40	120.98
11	S	148	LEU	CA-C-O	-5.46	115.06	120.90
11	U	15	ILE	CA-C-O	5.45	126.36	120.47
3	C	616	ASP	N-CA-CB	5.45	119.77	110.50
10	O	53	PHE	CA-C-O	-5.45	114.95	121.11
11	V	67	GLY	CA-C-N	5.45	127.59	120.28
11	V	67	GLY	C-N-CA	5.45	127.59	120.28
3	A	228	SER	N-CA-CB	5.45	118.05	110.04
5	Q	117	ASP	N-CA-CB	5.45	119.70	110.49
5	Q	148	LEU	N-CA-C	5.45	117.22	111.28
8	P	416	GLU	CA-C-N	5.45	128.60	120.31
8	P	416	GLU	C-N-CA	5.45	128.60	120.31
10	O	59	ASP	CA-C-N	5.45	128.59	120.31
10	O	59	ASP	C-N-CA	5.45	128.59	120.31
11	V	80	GLN	CG-CD-NE2	-5.45	108.22	116.40
3	C	108	ILE	CA-C-N	5.45	131.95	121.54
3	C	108	ILE	C-N-CA	5.45	131.95	121.54
8	P	402	LEU	CA-C-O	5.45	126.19	120.42
7	I	45	ILE	CB-CA-C	5.45	118.94	111.97
11	R	11	PHE	CA-CB-CG	5.45	119.25	113.80
11	Y	32	THR	N-CA-C	-5.45	105.34	111.28
3	E	528	GLN	CA-C-N	5.45	130.45	122.77
3	E	528	GLN	C-N-CA	5.45	130.45	122.77
10	O	237	HIS	CG-CD2-NE2	5.45	112.65	107.20
11	Y	129	MET	N-CA-CB	5.45	117.91	110.01
4	D	172	ILE	CA-C-O	5.44	126.36	120.53
4	D	272	ARG	NE-CZ-NH1	5.44	126.94	121.50
4	B	214	ALA	CA-C-O	5.44	126.31	120.38
4	B	232	ASN	N-CA-C	-5.44	105.43	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	O	136	ASN	N-CA-CB	5.44	118.12	110.12
3	C	288	ASN	OD1-CG-ND2	-5.44	117.16	122.60
4	D	397	GLY	CA-C-O	5.44	126.43	120.66
4	F	87	ASP	CA-C-N	-5.44	117.58	123.08
4	F	87	ASP	C-N-CA	-5.44	117.58	123.08
4	B	289	ARG	N-CA-C	-5.44	105.43	111.36
5	Q	254	PHE	CA-C-N	5.44	127.57	120.28
5	Q	254	PHE	C-N-CA	5.44	127.57	120.28
11	a	66	TYR	CA-C-N	5.44	125.98	119.94
11	a	66	TYR	C-N-CA	5.44	125.98	119.94
4	F	323	GLU	O-C-N	-5.44	116.18	122.87
11	W	46	ARG	CB-CA-C	-5.44	99.45	110.17
4	B	155	VAL	CA-C-N	5.44	127.57	120.28
4	B	155	VAL	C-N-CA	5.44	127.57	120.28
6	L	18	HIS	N-CA-CB	5.44	118.20	110.16
3	C	568	SER	CA-C-N	5.43	128.01	120.29
3	C	568	SER	C-N-CA	5.43	128.01	120.29
4	F	76	ILE	N-CA-CB	5.43	118.91	111.41
3	A	482	ARG	CB-CG-CD	5.43	123.80	111.30
5	Q	156	THR	O-C-N	-5.43	115.09	121.23
7	G	157	MET	O-C-N	5.43	128.95	122.27
11	U	34	LYS	N-CA-C	5.43	116.89	111.07
3	C	324	MET	CA-C-N	5.43	125.44	119.90
3	C	324	MET	C-N-CA	5.43	125.44	119.90
4	D	408	ALA	CA-C-N	5.43	128.13	120.42
4	D	408	ALA	C-N-CA	5.43	128.13	120.42
5	Q	73	SER	CB-CA-C	-5.43	101.61	110.85
4	D	159	ASP	CA-CB-CG	-5.43	107.17	112.60
4	F	326	ASN	CA-C-O	5.43	126.57	120.92
4	B	254	ILE	CA-C-N	5.43	127.54	120.26
4	B	254	ILE	C-N-CA	5.43	127.54	120.26
9	b	218	ILE	CB-CA-C	5.43	119.42	111.33
11	Z	58	ILE	CA-CB-CG1	5.43	119.63	110.40
11	W	106	PHE	N-CA-C	-5.43	104.24	111.24
4	D	371	PRO	N-CA-CB	5.43	108.57	102.60
4	F	278	LEU	N-CA-C	-5.43	98.36	108.02
5	Q	257	ALA	CA-C-N	5.43	128.95	120.75
5	Q	257	ALA	C-N-CA	5.43	128.95	120.75
1	M	164	LYS	CA-C-N	5.43	127.89	120.46
1	M	164	LYS	C-N-CA	5.43	127.89	120.46
1	M	209	LYS	CA-C-N	5.43	127.50	120.44
1	M	209	LYS	C-N-CA	5.43	127.50	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	42	THR	N-CA-CB	-5.43	101.87	110.28
11	a	76	TYR	CB-CA-C	-5.43	101.78	110.79
11	S	29	ALA	CA-C-N	5.43	127.49	120.44
11	S	29	ALA	C-N-CA	5.43	127.49	120.44
4	F	131	TYR	N-CA-C	-5.42	100.34	109.07
3	A	426	PRO	N-CA-CB	5.42	109.44	103.26
8	P	142	SER	CA-C-N	5.42	126.00	119.98
8	P	142	SER	C-N-CA	5.42	126.00	119.98
6	J	43	ILE	CA-CB-CG1	5.42	119.62	110.40
11	a	140	GLY	O-C-N	5.42	127.40	122.19
3	C	343	PHE	N-CA-CB	5.42	118.69	110.28
3	E	32	GLY	CA-C-N	5.42	126.47	120.45
3	E	32	GLY	C-N-CA	5.42	126.47	120.45
6	H	36	LYS	CA-C-N	5.42	127.81	120.44
6	H	36	LYS	C-N-CA	5.42	127.81	120.44
3	A	447	GLN	O-C-N	-5.42	116.37	122.12
3	A	588	GLU	CA-C-N	5.42	125.40	120.03
3	A	588	GLU	C-N-CA	5.42	125.40	120.03
4	B	313	SER	CB-CA-C	-5.42	101.46	110.68
7	G	18	ASN	CA-CB-CG	-5.42	107.18	112.60
7	G	22	ALA	CA-C-N	5.42	127.55	120.28
7	G	22	ALA	C-N-CA	5.42	127.55	120.28
11	Z	128	GLY	CA-C-N	5.42	127.81	120.44
11	Z	128	GLY	C-N-CA	5.42	127.81	120.44
11	Y	86	THR	O-C-N	-5.42	116.37	122.12
11	S	23	PHE	N-CA-CB	5.42	118.09	110.12
3	C	214	THR	N-CA-C	-5.42	101.44	110.17
3	E	487	GLU	N-CA-CB	5.42	117.87	110.01
4	F	323	GLU	CB-CA-C	-5.42	100.72	109.72
3	A	332	SER	CB-CA-C	5.42	119.39	110.88
4	B	344	HIS	CB-CG-CD2	-5.42	124.16	131.20
8	P	451	MET	N-CA-C	-5.42	105.37	111.28
11	T	84	LEU	N-CA-C	5.42	117.19	111.28
3	C	110	ARG	N-CA-C	-5.42	97.84	109.81
4	B	395	ASP	CA-C-N	5.42	127.48	120.44
4	B	395	ASP	C-N-CA	5.42	127.48	120.44
5	Q	114	THR	CA-CB-OG1	5.42	117.72	109.60
7	G	148	LEU	O-C-N	5.42	128.33	122.15
11	a	133	LEU	N-CA-C	5.42	117.18	111.28
11	Z	51	PHE	CA-C-N	5.42	127.81	120.44
11	Z	51	PHE	C-N-CA	5.42	127.81	120.44
4	D	312	LEU	CA-C-N	5.42	128.08	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	312	LEU	C-N-CA	5.42	128.08	120.28
7	G	139	VAL	CA-C-O	5.42	126.08	120.39
11	Z	29	ALA	CB-CA-C	-5.42	102.15	110.81
1	M	122	LEU	CA-C-N	-5.41	114.58	122.65
1	M	122	LEU	C-N-CA	-5.41	114.58	122.65
3	C	370	ARG	CA-C-N	5.41	127.98	120.29
3	C	370	ARG	C-N-CA	5.41	127.98	120.29
4	B	263	ALA	N-CA-C	5.41	117.26	111.36
7	I	128	ALA	CA-C-N	5.41	128.54	120.31
7	I	128	ALA	C-N-CA	5.41	128.54	120.31
11	a	67	GLY	CA-C-N	5.41	127.53	120.28
11	a	67	GLY	C-N-CA	5.41	127.53	120.28
11	V	48	ASP	CA-CB-CG	-5.41	107.19	112.60
3	A	567	TRP	CG-CD2-CE3	-5.41	128.49	133.90
10	O	39	ILE	N-CA-C	5.41	120.60	109.34
5	Q	119	ASP	CA-C-N	5.41	128.53	120.31
5	Q	119	ASP	C-N-CA	5.41	128.53	120.31
7	G	38	LYS	N-CA-CB	5.41	118.55	110.22
7	G	117	TYR	N-CA-CB	5.41	118.63	110.30
7	K	149	ILE	CA-C-N	5.41	127.53	120.28
7	K	149	ILE	C-N-CA	5.41	127.53	120.28
7	I	67	LYS	CA-C-N	5.41	127.53	120.28
7	I	67	LYS	C-N-CA	5.41	127.53	120.28
7	I	91	ALA	CA-C-O	5.41	126.60	120.00
11	Y	76	TYR	CA-C-O	5.41	126.28	120.55
11	T	105	GLY	CA-C-N	5.41	127.80	120.44
11	T	105	GLY	C-N-CA	5.41	127.80	120.44
11	W	98	GLY	CA-C-O	-5.41	114.84	120.90
3	E	425	ASP	CA-C-N	5.41	125.23	119.28
3	E	425	ASP	C-N-CA	5.41	125.23	119.28
3	A	272	TYR	N-CA-C	5.41	119.04	112.23
3	E	393	GLU	CA-C-N	5.40	128.52	120.31
3	E	393	GLU	C-N-CA	5.40	128.52	120.31
4	F	180	HIS	CG-CD2-NE2	5.40	112.60	107.20
4	F	480	ILE	CA-C-N	5.40	128.06	120.28
4	F	480	ILE	C-N-CA	5.40	128.06	120.28
4	B	241	PHE	CA-C-O	-5.40	114.52	120.30
4	F	144	ARG	N-CA-CB	5.40	118.73	110.95
11	R	91	LEU	N-CA-C	5.40	116.85	111.07
8	P	259	PHE	CA-C-N	5.40	127.96	120.29
8	P	259	PHE	C-N-CA	5.40	127.96	120.29
9	b	50	ALA	CA-C-N	5.40	128.51	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	b	50	ALA	C-N-CA	5.40	128.51	120.31
10	O	79	ILE	CB-CA-C	-5.40	104.85	112.14
3	C	364	LEU	N-CA-CB	5.40	118.05	110.12
1	M	97	ARG	NE-CZ-NH1	5.39	126.89	121.50
3	A	448	ARG	N-CA-C	-5.39	106.65	113.18
9	b	318	ALA	CA-C-N	5.39	127.85	120.46
9	b	318	ALA	C-N-CA	5.39	127.85	120.46
10	O	79	ILE	CA-C-N	5.39	125.97	119.98
10	O	79	ILE	C-N-CA	5.39	125.97	119.98
7	G	157	MET	CA-C-N	5.39	127.78	120.44
7	G	157	MET	C-N-CA	5.39	127.78	120.44
11	X	41	ALA	CA-C-N	5.39	128.05	120.28
11	X	41	ALA	C-N-CA	5.39	128.05	120.28
11	S	141	LEU	CA-C-O	-5.39	115.13	120.90
3	C	64	ASP	CA-C-O	-5.39	114.74	120.40
4	D	237	ARG	NE-CZ-NH2	5.39	124.05	119.20
4	B	446	GLN	CA-C-O	5.39	127.03	120.99
8	P	463	TYR	CB-CG-CD2	-5.39	112.71	120.80
10	O	299	VAL	CA-CB-CG2	-5.39	101.23	110.40
6	H	8	ALA	CB-CA-C	-5.39	101.84	110.79
3	E	105	TYR	CA-C-O	-5.39	115.32	121.68
3	E	550	PHE	O-C-N	5.39	127.62	122.07
3	A	43	CYS	N-CA-CB	5.39	119.60	110.49
5	Q	64	THR	N-CA-C	-5.39	101.56	109.81
6	H	86	ILE	CA-CB-CG2	-5.39	101.34	110.50
11	Z	148	LEU	N-CA-C	5.39	117.58	111.11
11	V	37	VAL	CB-CA-C	-5.39	104.98	112.04
3	A	594	LYS	CA-C-O	5.39	126.13	120.42
6	L	97	ILE	CA-C-N	5.39	127.50	120.28
6	L	97	ILE	C-N-CA	5.39	127.50	120.28
11	a	156	GLN	CB-CA-C	5.39	120.61	111.35
7	K	125	ILE	CA-C-N	5.38	128.06	120.42
7	K	125	ILE	C-N-CA	5.38	128.06	120.42
10	O	181	PRO	O-C-N	-5.38	115.37	122.64
11	S	90	GLN	N-CA-C	5.38	116.83	111.07
1	M	113	ILE	N-CA-C	-5.38	100.63	108.17
3	C	124	ILE	O-C-N	-5.38	117.26	121.46
3	A	543	THR	CA-C-N	5.38	127.49	120.28
3	A	543	THR	C-N-CA	5.38	127.49	120.28
11	S	13	GLY	CA-C-N	5.38	127.49	120.28
11	S	13	GLY	C-N-CA	5.38	127.49	120.28
11	V	11	PHE	CA-CB-CG	5.38	119.18	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	V	154	ALA	N-CA-CB	5.38	117.81	110.01
2	N	113	ARG	NE-CZ-NH2	-5.38	114.36	119.20
3	C	130	THR	CA-C-O	-5.38	116.03	120.71
4	F	138	PRO	CA-C-N	-5.38	116.59	121.97
4	F	138	PRO	C-N-CA	-5.38	116.59	121.97
8	P	317	ASN	N-CA-CB	5.38	120.65	112.47
4	D	39	VAL	N-CA-C	-5.38	100.58	108.11
4	D	300	GLY	O-C-N	5.38	128.06	122.79
4	F	396	HIS	CA-CB-CG	5.38	119.18	113.80
8	P	50	ILE	CA-C-O	-5.38	114.96	120.71
8	P	272	LEU	CA-C-N	5.38	129.70	120.72
8	P	272	LEU	C-N-CA	5.38	129.70	120.72
9	b	330	THR	CA-CB-OG1	-5.38	101.54	109.60
11	W	126	PHE	CA-C-N	5.38	128.96	120.47
11	W	126	PHE	C-N-CA	5.38	128.96	120.47
8	P	185	VAL	N-CA-CB	5.38	116.84	110.55
6	H	44	ASP	CA-CB-CG	5.37	117.97	112.60
11	Z	143	GLY	CA-C-N	5.37	127.80	120.54
11	Z	143	GLY	C-N-CA	5.37	127.80	120.54
4	D	334	ILE	N-CA-CB	5.37	118.82	111.41
7	G	36	GLN	N-CA-CB	5.37	119.16	110.40
3	C	148	VAL	CA-CB-CG1	-5.37	101.27	110.40
7	I	100	PHE	CA-CB-CG	5.37	119.17	113.80
11	R	156	GLN	OE1-CD-NE2	5.37	127.97	122.60
11	Z	131	LEU	CB-CA-C	-5.37	102.22	110.81
3	E	586	PHE	CA-C-O	-5.37	114.05	120.55
4	F	430	LYS	CA-C-N	5.37	127.47	120.28
4	F	430	LYS	C-N-CA	5.37	127.47	120.28
11	T	81	LYS	CA-CB-CG	-5.37	103.36	114.10
11	S	101	GLY	CA-C-N	5.37	127.78	120.54
11	S	101	GLY	C-N-CA	5.37	127.78	120.54
8	P	200	ARG	CA-C-N	5.37	127.74	120.44
8	P	200	ARG	C-N-CA	5.37	127.74	120.44
9	b	185	ASN	CA-C-O	5.37	126.40	120.71
4	F	286	ASP	CA-CB-CG	5.36	117.96	112.60
4	B	236	GLU	CA-C-N	5.36	128.21	120.38
4	B	236	GLU	C-N-CA	5.36	128.21	120.38
5	Q	98	ILE	N-CA-C	-5.36	105.30	110.72
7	G	11	ASN	CA-C-N	5.36	127.47	120.28
7	G	11	ASN	C-N-CA	5.36	127.47	120.28
11	V	80	GLN	OE1-CD-NE2	5.36	127.96	122.60
11	V	116	VAL	N-CA-C	-5.36	104.39	111.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	303	GLY	CA-C-O	5.36	124.97	119.02
4	B	283	SER	CA-C-N	5.36	127.91	120.29
4	B	283	SER	C-N-CA	5.36	127.91	120.29
1	M	141	ARG	N-CA-C	5.36	117.20	111.36
11	W	68	LEU	N-CA-C	5.36	117.12	111.28
5	Q	250	PRO	CA-C-N	5.36	127.41	120.44
5	Q	250	PRO	C-N-CA	5.36	127.41	120.44
8	P	91	ASP	CA-C-O	-5.36	114.74	120.42
8	P	195	VAL	CA-C-O	5.36	126.48	120.64
8	P	422	VAL	N-CA-C	5.36	115.56	110.42
4	B	49	TYR	CB-CG-CD2	5.36	128.84	120.80
5	Q	302	GLN	N-CA-C	-5.36	100.96	109.96
4	D	376	LEU	CA-C-O	-5.36	112.82	120.16
11	U	148	LEU	O-C-N	-5.36	116.35	122.08
11	X	84	LEU	CA-C-N	5.36	127.46	120.28
11	X	84	LEU	C-N-CA	5.36	127.46	120.28
11	a	20	ALA	CA-C-N	5.36	129.42	120.64
11	a	20	ALA	C-N-CA	5.36	129.42	120.64
3	C	305	SER	N-CA-CB	5.35	119.54	110.49
10	O	87	GLN	N-CA-CB	5.35	118.08	110.16
11	U	106	PHE	N-CA-C	-5.35	105.36	111.14
1	M	87	VAL	N-CA-CB	5.35	117.41	110.99
3	E	555	ASP	CA-C-N	5.35	127.89	120.29
3	E	555	ASP	C-N-CA	5.35	127.89	120.29
5	Q	128	HIS	CB-CA-C	5.35	117.29	110.76
8	P	21	ARG	NE-CZ-NH2	5.35	124.02	119.20
11	V	13	GLY	O-C-N	5.35	127.33	122.19
11	Z	38	GLY	CA-C-N	5.35	127.30	120.56
11	Z	38	GLY	C-N-CA	5.35	127.30	120.56
4	D	201	HIS	ND1-CE1-NE2	5.35	113.75	108.40
7	I	138	ILE	N-CA-C	-5.35	100.71	108.36
1	M	78	ASN	CA-C-N	5.35	127.79	120.46
1	M	78	ASN	C-N-CA	5.35	127.79	120.46
3	E	467	LEU	CA-C-O	-5.35	114.88	120.55
3	A	170	HIS	CB-CG-CD2	-5.35	124.25	131.20
6	L	57	PHE	CA-C-O	5.35	126.09	120.42
8	P	236	ASN	OD1-CG-ND2	-5.35	117.25	122.60
8	P	285	LYS	CA-CB-CG	-5.35	103.41	114.10
11	V	106	PHE	CA-C-O	-5.35	115.19	120.70
11	V	153	ARG	NE-CZ-NH2	-5.35	114.39	119.20
1	M	13	MET	CG-SD-CE	-5.34	89.14	100.90
3	E	352	MET	N-CA-C	-5.34	99.81	108.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	342	ILE	CA-CB-CG1	5.34	119.49	110.40
5	Q	236	ASP	O-C-N	-5.34	116.92	122.96
11	X	16	GLY	CA-C-N	5.34	128.22	120.79
11	X	16	GLY	C-N-CA	5.34	128.22	120.79
11	X	51	PHE	CB-CG-CD2	-5.34	111.61	120.70
11	X	81	LYS	O-C-N	5.34	128.24	122.15
11	X	81	LYS	CA-CB-CG	5.34	124.79	114.10
11	W	49	LEU	N-CA-CB	5.34	118.36	110.56
2	N	63	ASP	N-CA-C	-5.34	106.14	113.30
4	F	311	ASP	CA-CB-CG	-5.34	107.26	112.60
3	A	177	ARG	CD-NE-CZ	-5.34	116.92	124.40
3	A	242	ALA	N-CA-CB	5.34	117.82	110.07
10	O	310	ARG	O-C-N	-5.34	116.06	122.15
11	U	120	SER	CB-CA-C	-5.34	102.26	110.81
11	Z	20	ALA	CB-CA-C	-5.34	102.49	110.88
11	W	65	ILE	CA-C-O	-5.34	114.70	120.47
3	E	83	ASP	CB-CA-C	-5.34	101.17	108.86
9	b	79	HIS	CA-C-N	5.34	131.74	121.54
9	b	79	HIS	C-N-CA	5.34	131.74	121.54
1	M	84	GLN	OE1-CD-NE2	5.34	127.94	122.60
2	N	109	LEU	CA-C-N	5.34	127.38	120.44
2	N	109	LEU	C-N-CA	5.34	127.38	120.44
6	L	64	GLY	O-C-N	5.34	129.59	122.27
8	P	403	GLN	O-C-N	5.34	128.24	122.15
7	G	53	ASN	CA-C-O	-5.34	115.21	120.82
11	U	131	LEU	O-C-N	-5.34	116.46	122.12
3	C	268	SER	CB-CA-C	-5.34	101.78	110.85
5	Q	9	ASP	N-CA-CB	5.34	118.06	110.16
8	P	353	LEU	CA-C-N	5.34	128.29	120.71
8	P	353	LEU	C-N-CA	5.34	128.29	120.71
9	b	25	ILE	N-CA-CB	5.34	120.00	112.15
11	Y	145	ILE	O-C-N	5.34	127.72	121.96
9	b	36	LEU	N-CA-CB	5.33	118.76	110.44
3	C	417	SER	CA-C-N	5.33	125.34	119.90
3	C	417	SER	C-N-CA	5.33	125.34	119.90
4	D	468	TYR	CA-CB-CG	-5.33	104.30	113.90
3	A	139	TRP	CD2-CE2-CZ2	-5.33	117.07	122.40
8	P	239	GLY	N-CA-C	5.33	119.13	112.73
7	I	83	LYS	CB-CG-CD	5.33	123.57	111.30
11	U	143	GLY	CA-C-O	5.33	126.87	120.90
3	C	55	ASN	OD1-CG-ND2	5.33	127.93	122.60
3	C	133	LEU	N-CA-C	-5.33	101.08	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	258	VAL	CA-C-N	5.33	127.42	120.28
8	P	258	VAL	C-N-CA	5.33	127.42	120.28
8	P	202	VAL	N-CA-CB	5.33	119.46	110.56
6	J	62	ALA	N-CA-C	-5.33	106.84	113.55
5	Q	304	PHE	CB-CA-C	5.33	118.64	111.82
1	M	101	VAL	N-CA-C	-5.33	99.97	107.75
4	D	52	ILE	CA-CB-CG1	5.33	119.45	110.40
7	G	176	ASN	N-CA-C	-5.33	106.65	112.72
2	N	64	ILE	N-CA-CB	5.32	116.52	110.72
4	D	201	HIS	CB-CG-CD2	-5.32	124.28	131.20
3	E	288	ASN	CA-C-N	5.32	127.85	120.29
3	E	288	ASN	C-N-CA	5.32	127.85	120.29
3	E	544	PHE	CB-CG-CD1	5.32	129.75	120.70
6	L	96	LYS	CA-C-N	5.32	127.98	120.42
6	L	96	LYS	C-N-CA	5.32	127.98	120.42
6	J	18	HIS	CB-CG-CD2	-5.32	124.28	131.20
11	S	144	LEU	CA-C-N	5.32	127.74	120.77
11	S	144	LEU	C-N-CA	5.32	127.74	120.77
7	I	81	ALA	N-CA-C	5.32	118.87	112.38
3	E	343	PHE	CA-C-N	5.32	127.84	120.29
3	E	343	PHE	C-N-CA	5.32	127.84	120.29
3	A	217	VAL	CA-C-O	-5.32	114.13	120.78
3	A	497	GLN	CA-C-O	-5.32	114.78	120.42
5	Q	105	ASP	CA-CB-CG	-5.32	107.28	112.60
11	Y	147	ALA	N-CA-C	5.32	116.76	111.07
2	N	17	THR	CB-CA-C	-5.32	101.96	110.79
7	I	95	SER	CA-C-O	-5.32	114.33	120.24
1	M	100	ASN	CA-C-N	5.32	130.17	123.10
1	M	100	ASN	C-N-CA	5.32	130.17	123.10
3	E	295	MET	O-C-N	-5.32	116.09	122.15
3	E	328	ALA	CB-CA-C	-5.32	101.81	110.85
4	B	358	ILE	CA-C-N	5.32	130.34	123.00
4	B	358	ILE	C-N-CA	5.32	130.34	123.00
8	P	90	GLU	N-CA-CB	5.32	118.41	110.22
8	P	429	HIS	ND1-CE1-NE2	5.32	113.72	108.40
11	W	128	GLY	O-C-N	5.32	128.07	122.28
1	M	103	GLY	CA-C-N	5.32	132.05	122.43
1	M	103	GLY	C-N-CA	5.32	132.05	122.43
2	N	39	VAL	N-CA-CB	5.32	117.06	111.00
11	R	109	GLY	CA-C-O	-5.32	114.40	120.09
7	G	67	LYS	CA-C-N	5.31	127.40	120.28
7	G	67	LYS	C-N-CA	5.31	127.40	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	W	32	THR	CA-C-N	5.31	128.18	120.79
11	W	32	THR	C-N-CA	5.31	128.18	120.79
4	D	262	THR	CA-C-N	5.31	127.40	120.28
4	D	262	THR	C-N-CA	5.31	127.40	120.28
11	X	34	LYS	CA-C-N	5.31	127.35	120.44
11	X	34	LYS	C-N-CA	5.31	127.35	120.44
11	Z	53	ASN	CA-C-N	5.31	129.33	120.62
11	Z	53	ASN	C-N-CA	5.31	129.33	120.62
11	T	89	ILE	N-CA-CB	5.31	120.39	110.77
2	N	78	ARG	N-CA-C	5.31	117.76	111.33
4	D	178	LEU	N-CA-C	-5.31	99.84	108.82
3	E	268	SER	N-CA-C	-5.31	105.57	111.36
4	F	177	GLY	N-CA-C	-5.31	107.92	115.30
5	Q	287	HIS	ND1-CE1-NE2	5.31	113.71	108.40
8	P	202	VAL	CA-C-N	5.31	127.74	120.46
8	P	202	VAL	C-N-CA	5.31	127.74	120.46
11	W	16	GLY	CA-C-N	5.31	127.71	120.54
11	W	16	GLY	C-N-CA	5.31	127.71	120.54
1	M	123	THR	N-CA-C	-5.31	101.05	109.76
3	E	412	ILE	N-CA-CB	5.31	117.42	111.21
3	A	413	VAL	N-CA-C	-5.31	100.00	107.75
3	A	465	ASN	CB-CA-C	-5.31	102.78	110.96
11	R	70	VAL	N-CA-CB	5.31	116.40	110.51
1	M	168	ARG	NE-CZ-NH1	-5.31	116.19	121.50
3	C	410	VAL	CB-CA-C	-5.31	104.41	110.73
4	F	160	THR	CA-C-N	5.31	127.83	120.29
4	F	160	THR	C-N-CA	5.31	127.83	120.29
4	F	332	ILE	CA-C-N	5.31	125.77	120.14
4	F	332	ILE	C-N-CA	5.31	125.77	120.14
4	B	80	PHE	CA-C-N	5.31	129.68	122.19
4	B	80	PHE	C-N-CA	5.31	129.68	122.19
4	B	127	PHE	CA-CB-CG	5.31	119.11	113.80
3	C	476	PRO	N-CA-CB	-5.31	98.40	103.39
4	D	438	LYS	N-CA-C	5.31	117.14	111.36
3	A	475	TYR	CA-C-O	-5.31	112.89	120.16
3	A	496	GLU	N-CA-C	5.31	117.81	111.71
1	M	200	PHE	N-CA-C	-5.30	105.58	111.36
3	C	78	GLY	CA-C-O	-5.30	113.12	119.06
4	D	343	THR	N-CA-C	-5.30	105.55	112.23
5	Q	191	ASP	O-C-N	5.30	128.79	122.27
7	G	159	GLU	O-C-N	5.30	127.74	122.12
11	U	40	CYS	CA-C-N	5.30	127.34	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	U	40	CYS	C-N-CA	5.30	127.34	120.44
3	A	468	ASN	CB-CG-OD1	5.30	131.41	120.80
8	P	456	HIS	ND1-CE1-NE2	5.30	113.70	108.40
10	O	108	PRO	CB-CA-C	-5.30	104.59	112.55
10	O	348	PHE	N-CA-C	5.30	120.02	113.50
7	I	205	GLU	CA-C-N	5.30	127.39	120.28
7	I	205	GLU	C-N-CA	5.30	127.39	120.28
3	E	372	GLY	CA-C-N	5.30	130.51	121.29
3	E	372	GLY	C-N-CA	5.30	130.51	121.29
3	A	305	SER	N-CA-CB	5.30	119.45	110.49
8	P	141	ILE	CB-CA-C	-5.30	105.08	112.02
4	F	220	GLU	CA-C-N	5.30	128.37	120.31
4	F	220	GLU	C-N-CA	5.30	128.37	120.31
5	Q	247	LYS	N-CA-C	-5.30	104.93	111.40
7	K	208	LYS	N-CA-C	5.30	117.06	111.28
6	J	55	LYS	N-CA-C	-5.30	105.67	111.82
11	a	15	ILE	N-CA-C	-5.30	104.34	111.44
3	A	163	GLU	N-CA-CB	-5.30	101.51	110.51
5	Q	97	TYR	CB-CG-CD2	-5.30	112.86	120.80
11	U	33	ALA	CA-C-N	5.30	127.33	120.44
11	U	33	ALA	C-N-CA	5.30	127.33	120.44
3	E	98	PRO	N-CA-CB	5.29	108.27	103.34
1	M	207	GLN	OE1-CD-NE2	5.29	127.89	122.60
4	B	295	ARG	N-CA-CB	5.29	118.99	111.05
5	Q	134	ASP	CA-CB-CG	5.29	117.89	112.60
5	Q	144	ASP	O-C-N	5.29	129.26	123.01
10	O	379	ASP	CA-CB-CG	5.29	117.89	112.60
4	B	187	ILE	CB-CA-C	5.29	119.28	112.14
7	G	48	THR	CA-C-N	5.29	127.64	120.65
7	G	48	THR	C-N-CA	5.29	127.64	120.65
11	Z	125	LEU	CA-C-N	5.29	127.90	120.28
11	Z	125	LEU	C-N-CA	5.29	127.90	120.28
3	C	449	LYS	O-C-N	-5.29	116.69	122.67
7	G	138	ILE	N-CA-CB	-5.29	105.02	111.21
11	X	21	ILE	N-CA-C	5.29	120.27	113.07
11	S	145	ILE	N-CA-C	5.29	115.73	110.23
11	W	143	GLY	CA-C-N	5.29	127.68	120.54
11	W	143	GLY	C-N-CA	5.29	127.68	120.54
3	C	246	CYS	CA-C-O	5.29	126.32	120.71
3	A	121	SER	N-CA-C	-5.29	98.40	107.23
9	b	262	ASP	CA-CB-CG	-5.29	107.31	112.60
10	O	239	PHE	CA-C-O	5.29	127.08	121.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	U	138	VAL	CA-C-N	5.29	127.80	120.29
11	U	138	VAL	C-N-CA	5.29	127.80	120.29
11	a	151	ASN	OD1-CG-ND2	-5.29	117.31	122.60
11	R	63	ILE	N-CA-C	5.29	115.50	110.42
11	Z	35	SER	CB-CA-C	-5.29	102.01	110.79
11	S	14	ALA	CA-C-O	5.29	126.16	120.55
10	O	162	ALA	CA-C-O	-5.29	114.82	120.42
11	S	132	ILE	N-CA-CB	5.29	116.74	110.55
3	C	94	VAL	CA-CB-CG2	-5.29	101.42	110.40
4	D	308	MET	CA-C-N	5.29	127.31	120.44
4	D	308	MET	C-N-CA	5.29	127.31	120.44
4	D	446	GLN	O-C-N	-5.29	117.77	123.42
9	b	288	LEU	CA-C-O	5.29	126.02	120.42
7	I	154	ASP	N-CA-C	5.29	117.04	111.28
11	X	65	ILE	CB-CA-C	-5.29	103.54	112.16
4	D	299	PRO	CA-C-N	5.28	129.24	122.85
4	D	299	PRO	C-N-CA	5.28	129.24	122.85
11	W	120	SER	N-CA-CB	5.28	117.99	110.06
4	D	170	ILE	CA-C-O	-5.28	115.44	119.98
11	X	50	LEU	CA-C-N	5.28	127.62	120.38
11	X	50	LEU	C-N-CA	5.28	127.62	120.38
3	C	584	SER	N-CA-C	5.28	117.04	111.28
4	D	140	ASN	N-CA-C	5.28	121.48	109.81
4	D	416	MET	CA-C-N	5.28	127.31	120.44
4	D	416	MET	C-N-CA	5.28	127.31	120.44
8	P	454	LEU	N-CA-C	-5.28	105.53	111.28
10	O	65	SER	CA-C-N	5.28	127.31	120.44
10	O	65	SER	C-N-CA	5.28	127.31	120.44
4	B	251	GLU	N-CA-C	5.28	117.03	111.28
3	C	538	CYS	CA-C-N	5.28	126.44	119.84
3	C	538	CYS	C-N-CA	5.28	126.44	119.84
3	A	53	HIS	CA-C-N	5.28	127.78	120.29
3	A	53	HIS	C-N-CA	5.28	127.78	120.29
7	I	65	LYS	CA-C-O	5.28	126.04	119.97
11	W	126	PHE	N-CA-C	-5.28	105.53	111.28
4	F	170	ILE	CA-C-N	5.28	126.41	120.66
4	F	170	ILE	C-N-CA	5.28	126.41	120.66
10	O	123	LEU	O-C-N	5.28	129.20	122.39
11	U	23	PHE	N-CA-C	5.28	117.03	111.28
11	R	80	GLN	CB-CG-CD	5.28	121.57	112.60
11	S	19	SER	O-C-N	5.28	127.58	122.09
11	V	145	ILE	CA-C-N	5.28	127.41	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	V	145	ILE	C-N-CA	5.28	127.41	120.60
3	E	548	ARG	CA-CB-CG	5.27	124.65	114.10
5	Q	156	THR	CA-CB-OG1	5.27	117.51	109.60
5	Q	307	SER	CA-C-N	5.27	127.30	120.44
5	Q	307	SER	C-N-CA	5.27	127.30	120.44
9	b	26	SER	CA-C-N	5.27	127.61	120.44
9	b	26	SER	C-N-CA	5.27	127.61	120.44
10	O	201	SER	CA-C-N	5.27	131.86	121.58
10	O	201	SER	C-N-CA	5.27	131.86	121.58
2	N	94	ILE	CA-C-N	5.27	125.57	119.93
2	N	94	ILE	C-N-CA	5.27	125.57	119.93
4	D	171	PRO	CA-C-N	5.27	129.97	123.12
4	D	171	PRO	C-N-CA	5.27	129.97	123.12
11	U	65	ILE	O-C-N	-5.27	115.84	121.80
11	a	33	ALA	O-C-N	5.27	127.72	122.08
11	V	139	LEU	CA-C-O	5.27	126.01	120.42
3	E	386	ALA	CA-C-O	-5.27	114.83	120.42
3	E	478	PHE	N-CA-C	5.27	121.46	109.81
3	A	35	VAL	CA-CB-CG1	5.27	119.36	110.40
5	Q	318	GLN	CA-C-O	-5.27	114.83	120.42
7	G	156	ILE	N-CA-C	-5.27	105.40	110.72
11	a	95	LEU	CA-C-O	5.27	126.54	120.90
2	N	78	ARG	CA-C-N	5.27	127.29	120.44
2	N	78	ARG	C-N-CA	5.27	127.29	120.44
3	C	568	SER	N-CA-C	5.27	117.11	111.36
3	E	360	TRP	O-C-N	-5.27	116.14	122.15
4	F	441	LYS	CB-CA-C	-5.27	101.29	110.09
3	A	365	ARG	N-CA-C	5.27	117.02	111.28
3	A	566	ASN	CA-C-N	5.27	127.77	120.29
3	A	566	ASN	C-N-CA	5.27	127.77	120.29
3	A	580	ALA	CA-C-N	5.27	127.90	120.42
3	A	580	ALA	C-N-CA	5.27	127.90	120.42
4	B	62	VAL	N-CA-CB	5.27	120.96	111.21
5	Q	280	GLU	CA-C-N	5.27	127.29	120.44
5	Q	280	GLU	C-N-CA	5.27	127.29	120.44
11	Z	79	GLY	CA-C-N	5.27	130.49	122.37
11	Z	79	GLY	C-N-CA	5.27	130.49	122.37
3	A	578	LYS	CB-CA-C	-5.27	101.90	110.85
9	b	103	SER	N-CA-CB	5.27	117.89	110.36
9	b	201	GLN	CG-CD-NE2	5.27	124.30	116.40
11	V	86	THR	O-C-N	5.27	128.15	122.15
4	D	160	THR	N-CA-C	-5.26	104.98	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	348	ASP	CB-CA-C	-5.26	102.58	110.90
10	O	237	HIS	CA-C-O	-5.26	115.13	120.71
7	G	86	LEU	CA-C-N	5.26	127.33	120.28
7	G	86	LEU	C-N-CA	5.26	127.33	120.28
11	X	97	VAL	CA-C-N	5.26	125.78	119.94
11	X	97	VAL	C-N-CA	5.26	125.78	119.94
11	Y	144	LEU	CA-C-N	5.26	127.67	120.77
11	Y	144	LEU	C-N-CA	5.26	127.67	120.77
3	E	531	TYR	CB-CA-C	-5.26	101.28	110.17
3	E	558	GLN	OE1-CD-NE2	-5.26	117.34	122.60
4	B	64	GLN	O-C-N	5.26	129.15	123.10
4	B	248	PRO	O-C-N	5.26	129.03	122.71
4	D	182	GLU	N-CA-C	5.26	117.09	111.36
4	F	189	ARG	O-C-N	5.26	128.15	122.15
3	A	289	GLU	CA-C-N	5.26	129.63	120.68
3	A	289	GLU	C-N-CA	5.26	129.63	120.68
4	B	296	GLU	N-CA-C	-5.26	106.54	113.17
4	B	406	LYS	CA-C-O	-5.26	113.92	119.97
8	P	456	HIS	CG-CD2-NE2	5.26	112.46	107.20
3	E	349	ASN	OD1-CG-ND2	-5.26	117.34	122.60
3	A	481	LEU	CA-C-N	5.26	127.33	120.28
3	A	481	LEU	C-N-CA	5.26	127.33	120.28
5	Q	258	GLN	O-C-N	5.26	129.28	122.81
7	K	57	ASN	CB-CA-C	-5.26	101.91	110.85
7	K	140	LYS	CG-CD-CE	5.26	123.40	111.30
11	S	124	ARG	CB-CG-CD	5.26	123.40	111.30
9	b	80	ASP	CB-CA-C	5.26	120.88	110.42
7	G	47	LYS	CA-C-N	5.26	127.28	120.44
7	G	47	LYS	C-N-CA	5.26	127.28	120.44
7	I	82	ASN	OD1-CG-ND2	5.26	127.86	122.60
4	B	106	GLU	N-CA-C	-5.26	106.10	112.88
8	P	456	HIS	CA-CB-CG	-5.26	108.54	113.80
11	a	20	ALA	CA-C-O	-5.26	115.29	121.07
5	Q	248	LEU	N-CA-C	-5.25	100.75	108.79
11	V	123	PRO	CA-C-N	5.25	127.85	120.28
11	V	123	PRO	C-N-CA	5.25	127.85	120.28
4	B	50	ASN	OD1-CG-ND2	5.25	127.85	122.60
4	B	99	SER	N-CA-C	-5.25	103.09	110.50
4	B	201	HIS	CG-CD2-NE2	5.25	112.45	107.20
7	G	188	VAL	CA-CB-CG1	-5.25	101.47	110.40
7	I	191	SER	O-C-N	5.25	129.53	123.17
11	Z	40	CYS	N-CA-C	5.25	117.01	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	V	96	SER	N-CA-CB	5.25	117.77	109.94
11	W	68	LEU	CA-C-N	5.25	127.18	120.56
11	W	68	LEU	C-N-CA	5.25	127.18	120.56
4	D	58	PRO	N-CA-C	-5.25	101.65	112.47
3	E	327	ALA	N-CA-C	-5.25	105.56	111.28
4	B	88	VAL	CA-C-O	-5.25	114.22	120.78
7	I	121	LEU	N-CA-C	5.25	117.00	111.28
11	T	68	LEU	CA-C-N	5.25	127.28	120.56
11	T	68	LEU	C-N-CA	5.25	127.28	120.56
4	D	182	GLU	N-CA-CB	5.25	117.93	110.16
3	E	606	THR	CA-CB-OG1	5.25	117.47	109.60
3	A	195	GLU	CB-CG-CD	-5.25	103.67	112.60
7	K	108	SER	CB-CA-C	-5.25	101.92	110.85
4	F	469	PRO	N-CA-CB	5.25	108.76	103.25
7	K	99	ILE	CA-C-O	-5.25	115.29	120.85
8	P	217	ILE	O-C-N	-5.25	116.78	121.87
11	U	46	ARG	CB-CA-C	-5.25	103.18	110.16
11	R	71	SER	CA-C-N	5.25	127.37	120.60
11	R	71	SER	C-N-CA	5.25	127.37	120.60
11	S	92	GLY	CA-C-N	5.25	127.74	120.29
11	S	92	GLY	C-N-CA	5.25	127.74	120.29
11	T	83	ALA	CA-C-N	5.25	127.31	120.28
11	T	83	ALA	C-N-CA	5.25	127.31	120.28
8	P	446	GLY	O-C-N	5.25	127.80	122.24
9	b	343	ARG	NE-CZ-NH1	5.25	126.75	121.50
11	U	110	ILE	CA-C-N	5.25	127.37	120.60
11	U	110	ILE	C-N-CA	5.25	127.37	120.60
4	D	112	ILE	N-CA-C	-5.24	100.86	108.36
4	D	211	VAL	N-CA-CB	5.24	118.38	111.25
3	E	394	ARG	CD-NE-CZ	-5.24	117.06	124.40
3	A	184	TRP	N-CA-CB	5.24	119.62	110.81
3	A	277	ALA	N-CA-C	-5.24	101.10	109.23
3	A	413	VAL	CA-C-N	-5.24	114.67	122.74
3	A	413	VAL	C-N-CA	-5.24	114.67	122.74
10	O	296	TYR	CA-C-N	5.24	127.87	120.42
10	O	296	TYR	C-N-CA	5.24	127.87	120.42
3	C	355	ASP	CA-C-N	5.24	131.14	121.70
3	C	355	ASP	C-N-CA	5.24	131.14	121.70
5	Q	341	TYR	CA-CB-CG	-5.24	104.47	113.90
7	G	12	GLN	CG-CD-OE1	-5.24	110.32	120.80
1	M	197	ARG	N-CA-CB	5.24	117.91	110.16
3	A	184	TRP	CA-C-N	5.24	129.93	123.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	184	TRP	C-N-CA	5.24	129.93	123.12
10	O	305	HIS	CB-CG-ND1	5.24	130.56	122.70
7	I	128	ALA	O-C-N	5.24	128.12	122.15
4	B	173	PHE	N-CA-C	-5.24	100.19	108.73
11	V	56	PRO	N-CD-CG	5.24	111.06	103.20
9	b	33	LEU	N-CA-CB	5.24	117.60	110.01
9	b	100	VAL	O-C-N	-5.24	115.13	121.10
10	O	173	ARG	NE-CZ-NH2	-5.24	114.49	119.20
7	G	206	ARG	N-CA-CB	5.24	117.81	110.12
11	Z	50	LEU	CA-C-N	5.24	127.30	120.28
11	Z	50	LEU	C-N-CA	5.24	127.30	120.28
11	Y	86	THR	CA-C-O	5.24	126.10	120.55
11	T	70	VAL	CA-C-N	5.24	127.61	120.54
11	T	70	VAL	C-N-CA	5.24	127.61	120.54
3	C	213	HIS	ND1-CE1-NE2	5.23	113.63	108.40
3	E	111	PRO	CA-C-N	5.23	127.29	120.28
3	E	111	PRO	C-N-CA	5.23	127.29	120.28
4	D	238	THR	CA-C-N	5.23	130.79	122.94
4	D	238	THR	C-N-CA	5.23	130.79	122.94
5	Q	218	ARG	CA-C-N	5.23	127.72	120.29
5	Q	218	ARG	C-N-CA	5.23	127.72	120.29
7	K	149	ILE	N-CA-CB	5.23	116.67	110.55
10	O	236	VAL	CA-C-O	5.23	126.52	120.76
11	X	138	VAL	CA-C-O	-5.23	115.61	121.05
2	N	114	LYS	CA-C-N	5.23	131.53	121.54
2	N	114	LYS	C-N-CA	5.23	131.53	121.54
3	C	254	ILE	CA-CB-CG2	-5.23	101.61	110.50
11	T	80	GLN	CA-C-N	5.23	130.16	122.63
11	T	80	GLN	C-N-CA	5.23	130.16	122.63
3	C	358	SER	CA-C-N	5.23	129.57	120.68
3	C	358	SER	C-N-CA	5.23	129.57	120.68
8	P	294	ILE	CB-CG1-CD1	-5.23	102.82	113.80
11	X	62	ILE	CA-C-N	5.23	127.25	120.56
11	X	62	ILE	C-N-CA	5.23	127.25	120.56
11	R	69	VAL	CA-C-O	5.23	126.39	120.95
3	C	139	TRP	CG-CD2-CE3	-5.23	128.67	133.90
11	T	106	PHE	CA-C-N	5.23	127.24	120.44
11	T	106	PHE	C-N-CA	5.23	127.24	120.44
3	E	82	GLY	N-CA-C	-5.23	108.01	115.64
10	O	383	GLU	CB-CG-CD	-5.23	103.72	112.60
6	H	48	ILE	CA-C-O	-5.23	113.37	119.85
11	W	93	ALA	N-CA-CB	5.23	117.59	110.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	465	ASN	CA-C-O	-5.22	115.33	120.82
4	F	77	VAL	N-CA-C	-5.22	100.80	108.85
8	P	218	LEU	CA-C-N	5.22	127.28	120.28
8	P	218	LEU	C-N-CA	5.22	127.28	120.28
11	a	61	GLY	CA-C-O	5.22	124.77	118.97
11	R	110	ILE	CA-C-N	5.22	127.34	120.60
11	R	110	ILE	C-N-CA	5.22	127.34	120.60
1	M	139	TYR	CA-C-O	-5.22	114.89	120.42
11	T	69	VAL	CB-CA-C	-5.22	105.18	112.02
5	Q	164	ASN	CA-C-N	5.22	128.25	120.31
5	Q	164	ASN	C-N-CA	5.22	128.25	120.31
6	J	95	VAL	CA-CB-CG1	5.22	119.28	110.40
7	I	38	LYS	N-CA-CB	5.22	118.37	110.28
11	X	75	CYS	N-CA-C	5.22	119.93	111.37
1	M	79	ILE	N-CA-C	5.22	115.94	110.62
3	C	104	ILE	CB-CA-C	5.22	118.61	110.83
4	F	100	LEU	N-CA-CB	5.22	117.63	109.85
4	F	454	VAL	N-CA-CB	5.22	120.22	110.77
5	Q	326	ILE	N-CA-CB	5.22	117.25	110.57
6	L	104	LYS	O-C-N	-5.22	116.91	121.35
8	P	253	LEU	CA-C-O	5.22	126.08	120.55
6	H	94	VAL	N-CA-C	-5.22	105.31	111.00
7	G	139	VAL	O-C-N	-5.22	117.62	123.26
7	I	148	LEU	CA-C-N	5.22	127.61	120.46
7	I	148	LEU	C-N-CA	5.22	127.61	120.46
4	F	311	ASP	N-CA-C	5.22	116.97	111.28
3	A	614	SER	CA-C-N	5.22	127.22	120.44
3	A	614	SER	C-N-CA	5.22	127.22	120.44
3	C	520	LEU	CA-C-N	5.22	127.13	120.56
3	C	520	LEU	C-N-CA	5.22	127.13	120.56
10	O	332	VAL	CB-CA-C	5.22	116.06	110.53
6	H	46	TYR	N-CA-CB	-5.22	102.27	110.30
7	I	173	VAL	CB-CA-C	5.22	118.13	110.98
3	C	292	GLU	CB-CA-C	-5.21	101.99	110.85
3	C	580	ALA	CA-C-N	5.21	127.82	120.42
3	C	580	ALA	C-N-CA	5.21	127.82	120.42
3	E	426	PRO	CA-C-N	5.21	127.13	120.56
3	E	426	PRO	C-N-CA	5.21	127.13	120.56
4	B	137	SER	CA-C-O	-5.21	113.02	120.16
8	P	233	THR	N-CA-C	-5.21	99.69	110.80
10	O	193	THR	N-CA-C	-5.21	100.53	109.24
3	C	244	PHE	CA-C-N	5.21	126.36	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	244	PHE	C-N-CA	5.21	126.36	119.84
3	E	447	GLN	CB-CG-CD	5.21	121.46	112.60
5	Q	96	ASP	N-CA-CB	5.21	117.57	110.01
8	P	131	SER	N-CA-CB	5.21	118.21	110.29
1	M	127	ARG	CA-C-N	5.21	126.66	120.14
1	M	127	ARG	C-N-CA	5.21	126.66	120.14
1	M	133	GLN	CA-C-N	5.21	127.26	120.28
1	M	133	GLN	C-N-CA	5.21	127.26	120.28
3	C	291	ALA	CA-C-N	5.21	127.69	120.29
3	C	291	ALA	C-N-CA	5.21	127.69	120.29
4	D	330	THR	N-CA-C	-5.21	101.20	109.59
3	E	87	ARG	NH1-CZ-NH2	5.21	126.07	119.30
3	E	173	LEU	CA-C-N	5.21	130.84	120.94
3	E	173	LEU	C-N-CA	5.21	130.84	120.94
3	E	274	ASN	OD1-CG-ND2	-5.21	117.39	122.60
6	L	69	GLU	CB-CA-C	-5.21	100.12	109.24
11	Z	53	ASN	N-CA-CB	5.21	117.70	109.94
11	S	138	VAL	CA-C-O	-5.21	115.00	120.57
3	C	435	THR	OG1-CB-CG2	5.21	119.72	109.30
4	D	418	ALA	CB-CA-C	-5.21	102.70	110.88
11	U	146	VAL	CA-C-O	-5.21	115.85	121.27
4	F	149	GLU	CA-C-N	5.21	129.12	120.94
4	F	149	GLU	C-N-CA	5.21	129.12	120.94
3	A	571	ALA	CA-C-N	5.21	128.23	120.31
3	A	571	ALA	C-N-CA	5.21	128.23	120.31
4	B	401	ASN	OD1-CG-ND2	5.21	127.81	122.60
7	K	154	ASP	CB-CA-C	-5.21	102.70	110.88
8	P	399	ILE	CA-C-N	5.21	127.26	120.28
8	P	399	ILE	C-N-CA	5.21	127.26	120.28
9	b	26	SER	CB-CA-C	-5.21	102.14	110.79
7	I	64	SER	CA-C-N	5.21	128.23	120.31
7	I	64	SER	C-N-CA	5.21	128.23	120.31
11	X	55	VAL	N-CA-CB	5.21	118.50	111.21
4	D	314	THR	N-CA-C	-5.21	105.61	111.28
3	E	370	ARG	CA-C-O	-5.21	115.34	120.70
8	P	424	LEU	N-CA-C	5.21	117.86	111.82
3	C	126	ARG	O-C-N	-5.20	116.41	122.81
4	D	201	HIS	CB-CG-ND1	5.20	130.50	122.70
4	F	42	GLU	CB-CG-CD	5.20	121.44	112.60
3	A	484	ARG	NE-CZ-NH1	-5.20	116.30	121.50
11	Y	157	ASP	CA-C-N	5.20	131.34	121.97
11	Y	157	ASP	C-N-CA	5.20	131.34	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	41	ILE	N-CA-CB	5.20	121.55	111.93
3	C	604	LEU	N-CA-C	5.20	116.95	111.28
3	E	436	GLN	OE1-CD-NE2	-5.20	117.40	122.60
3	A	264	VAL	CA-C-N	5.20	128.83	120.30
3	A	264	VAL	C-N-CA	5.20	128.83	120.30
10	O	382	TYR	CA-C-O	5.20	125.61	120.56
11	X	28	ALA	CA-C-N	5.20	127.56	120.54
11	X	28	ALA	C-N-CA	5.20	127.56	120.54
1	M	34	ARG	NE-CZ-NH2	-5.20	114.52	119.20
3	E	202	PHE	CB-CG-CD2	-5.20	111.86	120.70
10	O	83	ILE	CA-C-N	5.20	127.25	120.28
10	O	83	ILE	C-N-CA	5.20	127.25	120.28
10	O	329	ILE	CB-CA-C	5.20	117.44	110.42
11	Z	85	TYR	CB-CA-C	-5.20	102.16	110.79
11	W	22	ILE	CA-C-N	5.20	127.25	120.28
11	W	22	ILE	C-N-CA	5.20	127.25	120.28
5	Q	322	ASN	CA-CB-CG	5.20	117.80	112.60
6	L	33	LYS	CA-C-N	5.20	127.24	120.28
6	L	33	LYS	C-N-CA	5.20	127.24	120.28
4	F	266	LEU	CA-C-O	-5.20	115.35	120.70
10	O	51	PRO	O-C-N	5.20	129.30	122.86
7	G	213	GLU	CB-CG-CD	-5.20	103.77	112.60
11	V	138	VAL	O-C-N	5.20	126.91	121.87
11	V	142	TYR	CA-C-N	5.20	125.75	119.98
11	V	142	TYR	C-N-CA	5.20	125.75	119.98
3	A	465	ASN	O-C-N	-5.19	116.63	122.03
9	b	320	PHE	CB-CG-CD1	5.19	129.53	120.70
11	U	78	LEU	N-CA-CB	5.19	117.61	109.97
11	a	160	CYS	CA-CB-SG	-5.19	102.45	114.40
11	Z	42	THR	CA-C-N	5.19	128.20	120.31
11	Z	42	THR	C-N-CA	5.19	128.20	120.31
11	S	32	THR	CA-C-O	-5.19	115.35	120.70
4	D	99	SER	CA-C-N	5.19	128.70	121.02
4	D	99	SER	C-N-CA	5.19	128.70	121.02
4	D	200	VAL	CB-CA-C	-5.19	105.13	112.14
3	E	432	LEU	N-CA-C	-5.19	105.80	111.82
4	B	443	PHE	CA-C-O	5.19	125.92	120.42
11	Y	128	GLY	CA-C-N	5.19	127.19	120.44
11	Y	128	GLY	C-N-CA	5.19	127.19	120.44
11	T	90	GLN	CB-CA-C	-5.19	102.70	110.90
4	F	286	ASP	CA-C-N	5.19	127.23	120.28
4	F	286	ASP	C-N-CA	5.19	127.23	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	93	VAL	CA-C-N	5.19	130.85	122.29
4	D	93	VAL	C-N-CA	5.19	130.85	122.29
3	E	145	LYS	CA-C-N	5.19	130.94	122.07
3	E	145	LYS	C-N-CA	5.19	130.94	122.07
3	E	450	HIS	CG-CD2-NE2	5.19	112.39	107.20
4	F	396	HIS	N-CA-C	5.19	116.62	111.07
4	F	398	ASP	CA-CB-CG	-5.19	107.41	112.60
7	K	46	GLU	CB-CG-CD	-5.19	103.78	112.60
8	P	201	ASP	CA-CB-CG	-5.19	107.41	112.60
11	X	136	ALA	O-C-N	5.19	129.53	122.37
4	D	225	PHE	CB-CA-C	-5.19	102.03	110.85
3	E	76	THR	CA-CB-CG2	-5.18	101.69	110.50
9	b	259	ASN	N-CA-C	-5.18	106.71	112.57
1	M	194	GLU	CB-CA-C	-5.18	102.04	110.85
2	N	86	ASN	O-C-N	5.18	128.74	122.68
3	C	481	LEU	O-C-N	-5.18	115.49	122.23
4	B	63	ARG	O-C-N	5.18	129.62	123.24
4	B	344	HIS	N-CA-CB	-5.18	102.83	110.14
9	b	359	ARG	CA-C-N	5.18	128.46	121.05
9	b	359	ARG	C-N-CA	5.18	128.46	121.05
10	O	9	ASN	N-CA-CB	5.18	119.86	111.21
3	C	360	TRP	N-CA-C	-5.18	105.71	111.36
3	A	562	ALA	N-CA-C	-5.18	105.63	111.28
5	Q	136	LEU	CA-C-N	5.18	124.80	119.05
5	Q	136	LEU	C-N-CA	5.18	124.80	119.05
10	O	247	THR	CA-C-N	5.18	127.17	120.44
10	O	247	THR	C-N-CA	5.18	127.17	120.44
4	D	324	GLY	N-CA-C	-5.18	100.90	113.18
7	G	194	SER	N-CA-C	-5.18	105.32	111.69
4	D	465	LEU	CA-C-N	5.18	127.73	120.28
4	D	465	LEU	C-N-CA	5.18	127.73	120.28
3	E	175	PRO	CA-C-N	5.18	125.18	119.90
3	E	175	PRO	C-N-CA	5.18	125.18	119.90
8	P	54	LYS	CA-C-N	5.18	131.02	121.70
8	P	54	LYS	C-N-CA	5.18	131.02	121.70
11	R	12	PHE	N-CA-CB	5.18	118.59	110.46
3	C	240	LEU	CA-C-N	5.17	127.48	120.44
3	C	240	LEU	C-N-CA	5.17	127.48	120.44
3	C	292	GLU	N-CA-C	5.17	117.00	111.36
7	G	114	ARG	CA-C-N	5.17	127.64	120.29
7	G	114	ARG	C-N-CA	5.17	127.64	120.29
11	Y	19	SER	CA-C-N	5.17	127.53	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	19	SER	C-N-CA	5.17	127.53	120.54
10	O	80	GLY	N-CA-C	-5.17	106.52	112.73
6	H	3	GLN	N-CA-C	5.17	116.61	111.07
3	E	349	ASN	N-CA-C	-5.17	100.81	109.24
8	P	268	LEU	CA-C-O	-5.17	115.37	120.90
6	H	29	GLN	CB-CA-C	-5.17	102.20	110.79
7	G	160	TYR	CA-C-N	5.17	126.79	120.22
7	G	160	TYR	C-N-CA	5.17	126.79	120.22
7	I	27	GLU	N-CA-C	-5.17	105.82	111.82
11	V	37	VAL	N-CA-C	5.17	116.51	110.62
11	V	95	LEU	N-CA-C	5.17	117.31	111.11
4	F	345	PRO	N-CA-C	5.17	122.15	113.78
3	A	415	ALA	N-CA-C	-5.17	101.28	109.96
5	Q	281	THR	O-C-N	5.17	127.39	122.07
8	P	304	GLN	CB-CG-CD	-5.17	103.81	112.60
8	P	412	ASN	OD1-CG-ND2	5.17	127.77	122.60
9	b	301	ALA	N-CA-C	5.17	117.82	111.82
11	U	144	LEU	N-CA-C	5.17	117.33	111.02
2	N	99	HIS	CE1-NE2-CD2	-5.17	103.83	109.00
4	D	385	SER	N-CA-C	-5.17	104.67	112.99
5	Q	267	ALA	N-CA-CB	5.17	117.81	110.16
9	b	115	SER	CA-C-N	5.17	127.20	120.28
9	b	115	SER	C-N-CA	5.17	127.20	120.28
4	D	255	THR	CA-C-N	5.17	124.67	119.19
4	D	255	THR	C-N-CA	5.17	124.67	119.19
1	M	62	GLN	O-C-N	5.16	127.59	122.12
3	C	316	THR	N-CA-C	-5.16	100.03	108.76
1	M	30	SER	CA-C-N	5.16	127.20	120.28
1	M	30	SER	C-N-CA	5.16	127.20	120.28
3	C	156	ASP	CA-CB-CG	5.16	117.76	112.60
3	E	90	LYS	CA-C-N	5.16	126.29	119.84
3	E	90	LYS	C-N-CA	5.16	126.29	119.84
3	A	233	LEU	N-CA-C	-5.16	100.00	108.41
4	B	178	LEU	N-CA-C	-5.16	103.44	110.36
6	L	76	VAL	CB-CA-C	-5.16	102.83	111.29
6	L	93	ASP	CA-CB-CG	-5.16	107.44	112.60
11	Z	30	TYR	O-C-N	5.16	127.40	122.03
11	Y	100	SER	CA-C-N	5.16	125.67	119.94
11	Y	100	SER	C-N-CA	5.16	125.67	119.94
3	C	223	VAL	CA-C-O	-5.16	116.28	121.49
5	Q	250	PRO	O-C-N	5.16	128.17	122.24
8	P	257	PRO	O-C-N	-5.16	116.04	122.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	O	344	LEU	CA-C-N	5.16	127.06	120.56
10	O	344	LEU	C-N-CA	5.16	127.06	120.56
10	O	360	LYS	CB-CG-CD	5.16	123.16	111.30
3	E	554	HIS	CA-C-O	-5.16	115.09	120.55
5	Q	209	GLN	CA-C-N	5.16	127.19	120.28
5	Q	209	GLN	C-N-CA	5.16	127.19	120.28
7	K	154	ASP	N-CA-C	-5.16	105.56	111.07
9	b	253	ALA	O-C-N	5.16	127.38	122.07
11	U	90	GLN	CA-CB-CG	-5.16	103.79	114.10
11	T	116	VAL	CA-C-O	-5.16	114.68	120.25
3	C	33	PRO	N-CD-CG	5.15	110.93	103.20
8	P	269	SER	N-CA-C	5.15	117.29	111.11
8	P	450	ILE	O-C-N	5.15	126.87	121.87
9	b	201	GLN	CB-CG-CD	-5.15	103.84	112.60
3	A	547	MET	CA-C-O	-5.15	115.09	120.55
8	P	176	ASN	OD1-CG-ND2	5.15	127.75	122.60
9	b	295	LEU	N-CA-C	5.15	116.58	111.07
6	H	26	LYS	N-CA-C	5.15	116.90	111.28
11	R	60	ALA	CB-CA-C	-5.15	99.70	109.95
3	E	311	ILE	CA-C-N	5.15	127.60	120.29
3	E	311	ILE	C-N-CA	5.15	127.60	120.29
4	F	107	ASP	N-CA-C	-5.15	106.40	113.30
5	Q	329	CYS	CA-C-N	5.15	128.61	120.47
5	Q	329	CYS	C-N-CA	5.15	128.61	120.47
7	K	197	ILE	N-CA-C	-5.15	101.06	108.53
9	b	343	ARG	CA-C-O	5.15	126.01	120.55
7	I	16	GLU	CB-CG-CD	-5.15	103.84	112.60
11	X	141	LEU	N-CA-C	5.15	117.29	111.11
3	E	389	ALA	CA-C-O	-5.15	114.96	120.42
3	A	149	GLY	CA-C-O	5.15	124.84	119.07
4	B	302	ARG	CA-CB-CG	-5.15	103.80	114.10
10	O	198	VAL	CB-CA-C	-5.15	101.99	111.36
10	O	324	HIS	N-CA-C	-5.15	101.76	109.95
1	M	9	PHE	CA-C-N	5.15	126.27	119.84
1	M	9	PHE	C-N-CA	5.15	126.27	119.84
1	M	13	MET	CB-CA-C	5.15	119.04	111.73
3	A	339	LEU	CA-C-N	5.15	127.18	120.28
3	A	339	LEU	C-N-CA	5.15	127.18	120.28
8	P	371	SER	O-C-N	-5.15	116.47	121.56
11	R	111	VAL	CA-C-N	5.15	125.81	119.99
11	R	111	VAL	C-N-CA	5.15	125.81	119.99
4	B	114	ASP	N-CA-C	-5.15	101.49	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	201	ASN	O-C-N	5.15	129.43	122.59
3	A	611	PHE	O-C-N	5.14	128.02	122.15
4	B	158	ILE	CA-C-N	5.14	127.44	120.44
4	B	158	ILE	C-N-CA	5.14	127.44	120.44
11	U	18	ALA	CA-C-N	5.14	127.48	120.54
11	U	18	ALA	C-N-CA	5.14	127.48	120.54
1	M	144	GLU	CA-CB-CG	5.14	124.39	114.10
3	E	342	TYR	N-CA-C	-5.14	105.57	111.07
4	F	169	LYS	CA-C-N	5.14	127.32	122.85
4	F	169	LYS	C-N-CA	5.14	127.32	122.85
8	P	156	HIS	CE1-NE2-CD2	-5.14	103.86	109.00
11	T	20	ALA	CA-C-N	5.14	129.18	120.64
11	T	20	ALA	C-N-CA	5.14	129.18	120.64
4	D	331	GLN	CB-CG-CD	-5.14	103.86	112.60
4	F	258	LEU	CA-C-N	5.14	127.59	120.29
4	F	258	LEU	C-N-CA	5.14	127.59	120.29
9	b	76	LEU	CB-CA-C	-5.14	102.26	110.79
5	Q	97	TYR	CB-CA-C	-5.14	102.81	110.88
5	Q	132	TRP	CD2-CE2-CZ2	-5.14	117.26	122.40
8	P	396	ARG	CA-C-N	5.14	127.17	120.28
8	P	396	ARG	C-N-CA	5.14	127.17	120.28
9	b	240	SER	O-C-N	5.14	129.55	123.33
10	O	326	ASN	CA-CB-CG	5.14	117.74	112.60
6	J	28	ARG	CA-C-N	5.14	127.48	120.54
6	J	28	ARG	C-N-CA	5.14	127.48	120.54
11	V	149	LEU	CA-C-N	5.14	127.93	120.79
11	V	149	LEU	C-N-CA	5.14	127.93	120.79
3	E	444	LYS	CA-C-N	5.14	127.58	120.29
3	E	444	LYS	C-N-CA	5.14	127.58	120.29
3	C	398	ALA	CA-C-O	-5.14	115.78	121.33
4	D	208	PHE	CA-C-O	5.14	126.25	120.70
4	B	284	TYR	CA-C-N	5.14	127.58	120.29
4	B	284	TYR	C-N-CA	5.14	127.58	120.29
4	F	446	GLN	CA-C-N	5.13	129.01	121.67
4	F	446	GLN	C-N-CA	5.13	129.01	121.67
4	B	330	THR	CA-C-O	-5.13	115.27	120.71
8	P	138	THR	CB-CA-C	-5.13	102.82	110.88
9	b	45	ASN	O-C-N	-5.13	116.96	123.17
7	I	26	LYS	N-CA-C	5.13	116.88	111.28
11	X	156	GLN	CA-C-N	5.13	131.35	121.54
11	X	156	GLN	C-N-CA	5.13	131.35	121.54
11	R	56	PRO	N-CA-C	5.13	120.81	113.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	70	VAL	CA-C-N	5.13	127.93	120.79
11	Y	70	VAL	C-N-CA	5.13	127.93	120.79
11	Y	76	TYR	CB-CA-C	-5.13	102.27	110.79
11	T	55	VAL	CA-C-N	5.13	124.31	118.97
11	T	55	VAL	C-N-CA	5.13	124.31	118.97
11	V	74	VAL	O-C-N	5.13	126.94	121.91
5	Q	18	ARG	CA-C-O	5.13	125.87	119.97
11	a	91	LEU	N-CA-CB	5.13	117.62	109.82
3	C	557	ALA	CA-C-O	-5.13	115.42	120.70
3	C	608	GLN	CA-C-N	5.13	127.58	120.29
3	C	608	GLN	C-N-CA	5.13	127.58	120.29
8	P	158	VAL	N-CA-C	5.13	115.86	110.62
2	N	23	ALA	N-CA-C	5.13	117.61	111.71
4	D	311	ASP	CA-C-N	5.13	127.15	120.28
4	D	311	ASP	C-N-CA	5.13	127.15	120.28
4	F	135	ASN	CA-CB-CG	-5.13	107.47	112.60
4	F	304	TYR	CA-C-N	5.13	126.25	119.84
4	F	304	TYR	C-N-CA	5.13	126.25	119.84
3	A	125	PRO	N-CA-C	-5.13	101.91	112.47
11	X	141	LEU	CA-C-N	5.13	127.41	120.38
11	X	141	LEU	C-N-CA	5.13	127.41	120.38
11	Z	28	ALA	CA-C-N	5.13	127.46	120.54
11	Z	28	ALA	C-N-CA	5.13	127.46	120.54
3	C	242	ALA	N-CA-C	5.13	116.68	111.14
3	A	417	SER	CA-C-O	-5.13	115.05	119.72
4	B	253	ILE	N-CA-C	5.13	115.90	110.72
10	O	12	ILE	N-CA-C	-5.13	100.93	108.11
10	O	261	ASN	OD1-CG-ND2	5.13	127.73	122.60
11	Y	83	ALA	N-CA-C	5.13	117.15	110.43
11	Y	132	ILE	CA-C-N	5.13	127.41	120.44
11	Y	132	ILE	C-N-CA	5.13	127.41	120.44
6	L	9	THR	O-C-N	5.12	127.99	122.15
9	b	128	THR	CA-C-N	5.12	127.57	120.29
9	b	128	THR	C-N-CA	5.12	127.57	120.29
3	C	387	LYS	N-CA-CB	5.12	117.74	110.16
10	O	324	HIS	CE1-NE2-CD2	-5.12	103.88	109.00
1	M	110	GLU	O-C-N	5.12	129.30	123.31
3	E	540	ILE	CA-C-O	-5.12	115.62	120.95
8	P	86	THR	CA-C-N	5.12	128.98	120.94
8	P	86	THR	C-N-CA	5.12	128.98	120.94
10	O	285	ARG	CA-C-N	5.12	127.11	120.56
10	O	285	ARG	C-N-CA	5.12	127.11	120.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	O	372	HIS	CG-CD2-NE2	5.12	112.32	107.20
11	U	25	SER	CA-C-N	5.12	127.45	120.54
11	U	25	SER	C-N-CA	5.12	127.45	120.54
11	R	142	TYR	CA-C-N	5.12	125.52	119.94
11	R	142	TYR	C-N-CA	5.12	125.52	119.94
3	C	392	TYR	CA-C-O	-5.12	115.12	120.55
7	K	112	ASN	N-CA-CB	5.12	118.71	110.42
10	O	377	LEU	O-C-N	5.12	127.56	122.03
7	G	202	THR	N-CA-CB	5.12	118.65	110.46
3	C	265	ILE	CA-C-N	5.12	127.14	120.28
3	C	265	ILE	C-N-CA	5.12	127.14	120.28
3	A	449	LYS	N-CA-CB	5.12	119.14	110.49
4	B	307	TYR	N-CA-C	-5.12	106.35	112.59
8	P	89	ASN	CA-CB-CG	5.12	117.72	112.60
8	P	412	ASN	CA-CB-CG	-5.12	107.48	112.60
10	O	243	VAL	CB-CA-C	-5.12	105.42	111.97
11	X	112	GLY	CA-C-N	5.12	127.09	120.44
11	X	112	GLY	C-N-CA	5.12	127.09	120.44
3	A	158	TYR	N-CA-C	-5.11	106.55	112.89
8	P	269	SER	CB-CA-C	-5.11	102.63	110.81
8	P	401	LEU	N-CA-CB	5.11	117.64	110.12
7	G	107	LEU	N-CA-CB	5.11	117.73	110.16
7	I	206	ARG	CA-C-N	5.11	127.13	120.28
7	I	206	ARG	C-N-CA	5.11	127.13	120.28
11	X	145	ILE	CA-C-O	-5.11	116.09	121.41
8	P	32	ARG	CD-NE-CZ	-5.11	117.24	124.40
11	a	27	GLY	CA-C-N	5.11	127.55	120.29
11	a	27	GLY	C-N-CA	5.11	127.55	120.29
1	M	90	ALA	N-CA-C	-5.11	100.08	108.41
4	D	275	LEU	N-CA-CB	5.11	118.57	110.55
4	F	68	LEU	CA-C-N	5.11	131.16	122.37
4	F	68	LEU	C-N-CA	5.11	131.16	122.37
3	A	482	ARG	N-CA-C	-5.11	105.71	111.28
7	K	207	LEU	CB-CA-C	-5.11	102.31	110.79
11	Y	130	ILE	CB-CA-C	5.11	118.42	111.88
3	C	471	TYR	CB-CA-C	-5.11	100.86	110.67
4	F	169	LYS	CA-C-O	5.11	125.94	120.32
11	Y	30	TYR	CA-C-O	-5.11	115.45	120.82
1	M	21	LYS	N-CA-C	5.11	116.93	111.36
3	E	57	VAL	CA-CB-CG2	5.11	119.08	110.40
4	B	304	TYR	N-CA-CB	5.11	118.54	110.11
7	K	176	ASN	N-CA-C	-5.11	106.89	113.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	b	185	ASN	CA-C-N	5.11	130.83	122.81
9	b	185	ASN	C-N-CA	5.11	130.83	122.81
7	G	131	LYS	CB-CG-CD	5.11	123.05	111.30
6	J	74	ALA	N-CA-CB	5.11	118.19	110.28
11	V	23	PHE	CA-CB-CG	-5.11	108.69	113.80
2	N	25	ILE	CB-CA-C	-5.11	102.92	111.29
4	F	162	ASN	OD1-CG-ND2	5.11	127.71	122.60
3	A	368	SER	CA-C-N	-5.11	114.38	120.00
3	A	368	SER	C-N-CA	-5.11	114.38	120.00
4	B	448	ALA	CB-CA-C	-5.11	99.32	109.99
5	Q	114	THR	O-C-N	-5.11	116.25	122.22
9	b	296	GLU	CA-C-O	-5.11	115.44	120.90
11	R	127	VAL	CB-CA-C	-5.11	102.04	111.79
4	D	448	ALA	CB-CA-C	5.10	119.52	109.72
3	A	54	ASP	CB-CA-C	-5.10	102.18	110.85
8	P	223	ASP	N-CA-CB	5.10	118.19	110.28
6	H	77	GLN	N-CA-CB	5.10	119.11	110.49
11	U	119	SER	CA-C-O	5.10	126.99	121.02
11	W	56	PRO	CA-C-O	-5.10	112.63	120.03
3	C	319	ALA	CA-C-N	-5.10	115.29	122.94
3	C	319	ALA	C-N-CA	-5.10	115.29	122.94
3	C	429	THR	O-C-N	5.10	127.97	122.15
3	E	47	GLU	N-CA-CB	5.10	117.53	109.83
3	E	553	TYR	CA-C-O	-5.10	115.14	120.55
3	C	265	ILE	CA-CB-CG2	-5.10	101.83	110.50
6	J	98	LEU	N-CA-C	5.10	116.84	111.28
11	a	59	MET	O-C-N	5.10	127.53	122.12
4	B	228	ASP	CA-C-N	5.10	127.11	120.28
4	B	228	ASP	C-N-CA	5.10	127.11	120.28
11	S	53	ASN	N-CA-C	5.10	116.53	111.07
7	G	83	LYS	CA-C-N	5.10	127.53	120.29
7	G	83	LYS	C-N-CA	5.10	127.53	120.29
7	I	149	ILE	CB-CA-C	-5.10	105.26	112.14
11	T	157	ASP	N-CA-CB	5.10	119.10	110.49
7	K	218	ILE	CB-CA-C	-5.09	105.19	112.22
8	P	176	ASN	CA-CB-CG	-5.09	107.50	112.60
9	b	116	TYR	CB-CA-C	-5.09	102.33	110.79
1	M	67	SER	CA-C-N	5.09	127.52	120.29
1	M	67	SER	C-N-CA	5.09	127.52	120.29
4	F	281	MET	N-CA-CB	5.09	118.17	110.28
11	U	22	ILE	CA-C-O	-5.09	114.62	120.83
3	E	84	PRO	N-CA-CB	5.09	108.09	103.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	192	PHE	CA-C-O	5.09	125.94	120.55
7	I	95	SER	CA-C-N	5.09	127.52	120.29
7	I	95	SER	C-N-CA	5.09	127.52	120.29
11	Z	50	LEU	O-C-N	5.09	127.96	122.11
11	W	148	LEU	CA-C-O	5.09	126.34	120.90
10	O	279	SER	CA-C-N	5.09	127.05	120.44
10	O	279	SER	C-N-CA	5.09	127.05	120.44
11	U	114	ALA	CA-C-O	-5.09	114.35	120.10
11	R	75	CYS	CB-CA-C	-5.09	102.29	110.74
1	M	196	ASP	N-CA-CB	5.09	117.69	110.16
4	D	413	ALA	CA-C-N	5.09	127.05	120.44
4	D	413	ALA	C-N-CA	5.09	127.05	120.44
4	F	263	ALA	CA-C-N	5.09	127.51	120.29
4	F	263	ALA	C-N-CA	5.09	127.51	120.29
3	A	324	MET	CA-C-O	-5.09	114.94	120.69
4	B	46	PHE	O-C-N	-5.09	115.47	121.32
7	K	183	LEU	N-CA-C	-5.09	105.92	112.68
8	P	385	ASP	N-CA-CB	-5.09	102.63	110.16
9	b	202	ILE	N-CA-C	5.09	115.30	110.42
7	I	168	PRO	N-CA-CB	5.09	108.72	103.38
3	C	221	ARG	CA-C-N	5.08	125.29	120.31
3	C	221	ARG	C-N-CA	5.08	125.29	120.31
4	D	358	ILE	CA-C-N	5.08	129.74	122.72
4	D	358	ILE	C-N-CA	5.08	129.74	122.72
3	E	108	ILE	N-CA-C	-5.08	108.17	113.10
11	R	142	TYR	N-CA-CB	5.08	118.05	110.22
3	C	29	SER	CA-C-N	5.08	130.13	123.11
3	C	29	SER	C-N-CA	5.08	130.13	123.11
3	E	254	ILE	CA-CB-CG1	5.08	119.04	110.40
4	B	484	PHE	N-CA-CB	5.08	119.35	110.81
9	b	17	VAL	CA-CB-CG1	5.08	119.04	110.40
10	O	240	LYS	CA-C-N	5.08	127.09	120.28
10	O	240	LYS	C-N-CA	5.08	127.09	120.28
11	X	65	ILE	CA-C-N	5.08	127.35	120.44
11	X	65	ILE	C-N-CA	5.08	127.35	120.44
11	Y	15	ILE	N-CA-C	-5.08	105.43	112.50
11	T	51	PHE	N-CA-CB	-5.08	102.65	110.12
1	M	16	GLY	N-CA-C	5.08	118.39	112.50
4	D	171	PRO	CB-CA-C	-5.08	103.18	111.56
10	O	69	SER	CB-CA-C	-5.08	102.87	110.90
10	O	107	VAL	CA-C-O	-5.08	114.53	118.85
4	D	105	SER	N-CA-C	-5.08	101.73	108.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	202	PHE	CB-CG-CD1	5.08	129.34	120.70
1	M	125	LEU	CA-C-N	5.08	127.65	119.98
1	M	125	LEU	C-N-CA	5.08	127.65	119.98
10	O	176	HIS	ND1-CE1-NE2	5.08	113.48	108.40
7	I	146	VAL	CA-C-N	5.08	127.50	120.29
7	I	146	VAL	C-N-CA	5.08	127.50	120.29
4	D	444	ILE	CA-C-N	5.08	128.53	121.02
4	D	444	ILE	C-N-CA	5.08	128.53	121.02
5	Q	238	LYS	CB-CA-C	-5.08	100.32	110.42
3	C	430	ALA	O-C-N	5.08	127.50	122.12
4	D	269	GLN	N-CA-CB	5.08	118.11	110.30
4	B	241	PHE	CB-CA-C	-5.08	101.73	110.16
7	K	126	VAL	CA-CB-CG1	5.08	119.03	110.40
8	P	319	LEU	N-CA-CB	5.08	117.42	110.11
3	C	339	LEU	O-C-N	5.07	127.93	122.15
4	D	485	TYR	CA-CB-CG	5.07	123.03	113.90
4	F	163	SER	N-CA-CB	5.07	118.69	110.42
3	E	296	GLU	CA-C-N	5.07	126.43	120.09
3	E	296	GLU	C-N-CA	5.07	126.43	120.09
3	E	365	ARG	CA-C-N	5.07	127.08	120.28
3	E	365	ARG	C-N-CA	5.07	127.08	120.28
6	J	104	LYS	CA-C-O	-5.07	115.50	119.66
11	W	156	GLN	CA-C-N	5.07	131.23	121.54
11	W	156	GLN	C-N-CA	5.07	131.23	121.54
7	K	23	PHE	CA-C-N	5.07	126.95	120.56
7	K	23	PHE	C-N-CA	5.07	126.95	120.56
11	S	140	GLY	N-CA-C	-5.07	106.62	112.50
1	M	50	ILE	CA-C-N	5.07	127.07	120.28
1	M	50	ILE	C-N-CA	5.07	127.07	120.28
1	M	60	VAL	O-C-N	-5.07	116.61	121.83
10	O	273	GLU	N-CA-C	5.07	116.89	111.36
11	V	89	ILE	CA-C-N	5.07	127.33	120.44
11	V	89	ILE	C-N-CA	5.07	127.33	120.44
4	D	86	ILE	O-C-N	-5.07	117.97	123.14
4	D	180	HIS	CB-CG-CD2	5.07	137.79	131.20
3	E	169	SER	N-CA-CB	5.07	117.72	110.67
6	H	88	GLU	N-CA-CB	5.07	118.13	110.28
11	R	120	SER	N-CA-C	5.07	117.46	111.33
4	F	132	LEU	N-CA-C	-5.07	101.61	109.72
4	F	217	VAL	N-CA-C	-5.07	104.48	110.21
3	A	398	ALA	O-C-N	5.07	128.93	123.10
3	A	606	THR	CA-C-N	5.07	127.07	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	606	THR	C-N-CA	5.07	127.07	120.28
4	B	43	LYS	N-CA-CB	5.07	119.05	110.49
7	I	162	GLU	N-CA-C	-5.07	106.61	112.89
6	H	19	GLU	N-CA-CB	5.06	117.65	110.16
11	X	145	ILE	CA-C-N	5.06	126.94	120.56
11	X	145	ILE	C-N-CA	5.06	126.94	120.56
11	Y	100	SER	O-C-N	5.06	127.92	122.15
4	B	391	MET	CA-C-N	5.06	130.51	121.75
4	B	391	MET	C-N-CA	5.06	130.51	121.75
5	Q	162	PHE	CA-C-N	5.06	127.48	120.29
5	Q	162	PHE	C-N-CA	5.06	127.48	120.29
10	O	279	SER	O-C-N	5.06	127.48	122.12
11	Y	23	PHE	N-CA-C	5.06	116.48	111.07
9	b	315	ARG	N-CA-C	5.06	117.53	111.71
6	J	72	ALA	N-CA-CB	5.06	117.92	110.33
11	T	131	LEU	N-CA-C	5.06	116.80	111.28
11	V	122	GLN	O-C-N	-5.06	116.82	121.37
1	M	175	HIS	CE1-NE2-CD2	-5.06	103.94	109.00
3	E	320	ASN	N-CA-C	-5.06	100.79	109.24
5	Q	111	ILE	N-CA-C	-5.06	105.78	110.53
9	b	45	ASN	CB-CA-C	-5.06	98.94	110.07
6	H	56	GLU	CB-CA-C	-5.06	102.25	110.85
11	Z	156	GLN	N-CA-C	5.06	117.23	110.35
11	T	151	ASN	N-CA-CB	5.06	117.51	109.82
3	C	187	PRO	N-CA-CB	5.06	108.56	103.25
5	Q	166	PHE	CA-C-N	5.06	127.01	120.44
5	Q	166	PHE	C-N-CA	5.06	127.01	120.44
8	P	175	GLN	N-CA-CB	5.06	117.34	110.01
4	D	313	SER	CB-CA-C	-5.05	101.28	110.63
6	L	28	ARG	NE-CZ-NH2	-5.05	114.65	119.20
6	J	73	GLU	CA-C-N	5.05	127.99	120.31
6	J	73	GLU	C-N-CA	5.05	127.99	120.31
10	O	100	LEU	CA-C-N	5.05	125.29	119.83
10	O	100	LEU	C-N-CA	5.05	125.29	119.83
6	H	34	GLN	CB-CG-CD	-5.05	104.01	112.60
11	S	144	LEU	CA-C-O	-5.05	115.49	120.90
11	W	158	VAL	N-CA-CB	5.05	119.57	111.23
3	E	151	HIS	ND1-CE1-NE2	5.05	113.45	108.40
4	B	39	VAL	CA-C-N	5.05	129.37	122.90
4	B	39	VAL	C-N-CA	5.05	129.37	122.90
11	Y	72	VAL	CA-C-N	5.05	129.22	121.19
11	Y	72	VAL	C-N-CA	5.05	129.22	121.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	270	ALA	N-CA-CB	5.05	118.24	110.21
6	L	17	ALA	O-C-N	5.05	127.47	122.12
9	b	70	ARG	O-C-N	-5.05	116.77	122.12
9	b	238	VAL	N-CA-C	-5.05	100.80	108.17
10	O	190	HIS	N-CA-CB	5.05	117.69	110.67
7	G	139	VAL	CA-C-N	5.05	129.97	123.00
7	G	139	VAL	C-N-CA	5.05	129.97	123.00
3	C	428	THR	N-CA-CB	5.05	117.39	110.07
9	b	330	THR	N-CA-CB	5.05	117.39	110.07
1	M	87	VAL	CA-C-O	5.05	125.97	120.57
3	C	580	ALA	N-CA-CB	5.05	117.63	110.16
3	A	364	LEU	CA-C-N	5.05	127.04	120.28
3	A	364	LEU	C-N-CA	5.05	127.04	120.28
5	Q	12	PHE	N-CA-C	-5.05	105.69	111.14
9	b	325	LYS	CA-C-N	5.05	130.48	121.75
9	b	325	LYS	C-N-CA	5.05	130.48	121.75
11	U	26	LEU	CA-C-N	5.05	125.54	119.94
11	U	26	LEU	C-N-CA	5.05	125.54	119.94
11	R	145	ILE	CA-C-N	5.05	127.37	120.46
11	R	145	ILE	C-N-CA	5.05	127.37	120.46
7	K	86	LEU	CA-C-N	5.04	127.00	120.44
7	K	86	LEU	C-N-CA	5.04	127.00	120.44
11	a	133	LEU	CB-CA-C	-5.04	102.42	110.79
11	Y	109	GLY	CA-C-N	5.04	126.88	120.72
11	Y	109	GLY	C-N-CA	5.04	126.88	120.72
4	D	272	ARG	NH1-CZ-NH2	-5.04	112.74	119.30
3	E	508	SER	N-CA-C	-5.04	103.49	110.35
4	B	479	LYS	CA-CB-CG	5.04	124.19	114.10
10	O	235	ASN	CA-C-O	-5.04	115.25	120.70
3	E	53	HIS	CG-CD2-NE2	5.04	112.24	107.20
3	E	297	PHE	CD1-CG-CD2	-5.04	111.04	118.60
3	A	266	SER	N-CA-C	5.04	116.86	111.36
8	P	172	ASN	CB-CA-C	-5.04	102.42	110.79
10	O	380	THR	CA-C-O	5.04	124.75	119.51
11	a	31	GLY	CA-C-N	5.04	126.99	120.44
11	a	31	GLY	C-N-CA	5.04	126.99	120.44
3	E	276	ASP	O-C-N	-5.04	116.07	122.27
3	A	596	VAL	N-CA-C	-5.04	100.81	108.17
5	Q	128	HIS	ND1-CE1-NE2	5.04	113.44	108.40
8	P	243	GLN	O-C-N	5.04	127.46	122.12
8	P	267	TYR	O-C-N	-5.04	116.15	122.35
11	R	68	LEU	CB-CA-C	-5.04	102.42	110.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	S	63	ILE	CA-C-O	5.04	126.19	120.95
4	D	166	ARG	CA-C-N	5.04	130.72	121.85
4	D	166	ARG	C-N-CA	5.04	130.72	121.85
10	O	57	SER	CB-CA-C	-5.04	99.96	111.95
10	O	86	LEU	CA-C-N	5.04	127.44	120.29
10	O	86	LEU	C-N-CA	5.04	127.44	120.29
1	M	112	TYR	N-CA-CB	5.04	120.54	111.37
4	D	182	GLU	O-C-N	5.04	127.89	122.15
3	E	60	VAL	CA-C-O	-5.04	114.61	120.75
8	P	332	ASP	CA-CB-CG	5.04	117.64	112.60
10	O	364	ILE	N-CA-CB	5.04	116.02	110.53
11	R	52	LYS	CA-C-N	5.04	127.34	120.54
11	R	52	LYS	C-N-CA	5.04	127.34	120.54
3	E	387	LYS	CA-C-O	-5.04	115.08	120.42
4	B	144	ARG	CB-CG-CD	5.03	122.88	111.30
11	X	101	GLY	N-CA-C	5.03	118.34	112.50
11	a	138	VAL	CA-C-N	5.03	126.98	120.44
11	a	138	VAL	C-N-CA	5.03	126.98	120.44
4	D	373	ILE	CA-C-N	5.03	129.94	123.00
4	D	373	ILE	C-N-CA	5.03	129.94	123.00
4	B	89	LYS	CA-C-N	5.03	130.52	121.66
4	B	89	LYS	C-N-CA	5.03	130.52	121.66
11	U	63	ILE	CA-C-O	-5.03	115.46	121.05
4	D	166	ARG	O-C-N	5.03	129.28	122.59
3	A	481	LEU	O-C-N	-5.03	116.41	122.15
8	P	333	GLU	N-CA-CB	5.03	117.51	110.12
11	Z	41	ALA	CA-C-N	5.03	127.02	120.28
11	Z	41	ALA	C-N-CA	5.03	127.02	120.28
11	V	19	SER	N-CA-C	5.03	117.15	111.11
3	E	320	ASN	CA-CB-CG	-5.03	107.57	112.60
3	A	543	THR	N-CA-C	-5.03	105.80	111.28
6	H	25	ARG	CA-C-N	5.03	127.02	120.28
6	H	25	ARG	C-N-CA	5.03	127.02	120.28
3	E	53	HIS	N-CA-C	-5.03	106.83	113.17
7	K	71	LEU	N-CA-CB	5.03	117.75	110.26
7	G	13	VAL	N-CA-CB	5.03	118.12	110.58
3	C	88	THR	N-CA-C	-5.03	106.66	112.89
4	F	478	PRO	O-C-N	5.03	128.97	122.24
4	B	468	TYR	CB-CG-CD2	-5.03	113.26	120.80
8	P	152	GLN	O-C-N	-5.03	116.76	122.89
9	b	188	THR	N-CA-C	-5.03	102.33	110.32
6	H	75	GLY	CA-C-O	-5.03	115.27	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	164	ALA	CA-C-N	5.03	129.93	121.14
7	G	164	ALA	C-N-CA	5.03	129.93	121.14
11	a	112	GLY	CA-C-N	5.03	126.97	120.44
11	a	112	GLY	C-N-CA	5.03	126.97	120.44
11	T	103	ALA	N-CA-C	-5.03	105.51	111.69
8	P	253	LEU	CA-C-N	5.02	129.11	120.72
8	P	253	LEU	C-N-CA	5.02	129.11	120.72
4	D	471	GLU	N-CA-C	-5.02	106.93	113.16
3	A	614	SER	N-CA-CB	5.02	117.35	110.07
4	B	464	LEU	CA-C-N	5.02	127.94	120.31
4	B	464	LEU	C-N-CA	5.02	127.94	120.31
10	O	91	GLU	N-CA-C	-5.02	99.23	108.02
10	O	296	TYR	CB-CG-CD2	-5.02	113.27	120.80
7	G	131	LYS	CB-CA-C	-5.02	101.51	110.70
11	S	107	ALA	N-CA-CB	5.02	117.29	110.01
3	A	76	THR	CA-CB-OG1	5.02	117.13	109.60
7	K	199	ILE	N-CA-C	-5.02	100.42	107.75
8	P	372	PRO	CA-C-O	-5.02	113.28	120.56
11	Y	91	LEU	O-C-N	5.02	127.45	122.08
3	E	27	ILE	CA-C-O	5.02	126.66	120.74
4	F	125	LYS	N-CA-CB	5.02	118.97	110.49
4	F	223	ARG	NE-CZ-NH2	5.02	123.72	119.20
3	A	539	PRO	CA-C-N	5.02	127.34	120.46
3	A	539	PRO	C-N-CA	5.02	127.34	120.46
6	J	11	LEU	CA-C-N	5.02	127.42	120.29
6	J	11	LEU	C-N-CA	5.02	127.42	120.29
11	S	153	ARG	CD-NE-CZ	-5.02	117.37	124.40
11	V	130	ILE	CA-C-N	5.02	127.71	120.38
11	V	130	ILE	C-N-CA	5.02	127.71	120.38
3	A	487	GLU	CB-CA-C	-5.02	102.46	110.79
4	B	259	ALA	O-C-N	5.02	127.44	122.12
5	Q	306	ILE	CA-C-N	5.02	127.00	120.28
5	Q	306	ILE	C-N-CA	5.02	127.00	120.28
10	O	231	TYR	N-CA-C	-5.02	101.66	109.24
11	U	152	SER	CA-C-O	-5.02	115.23	120.55
11	Y	93	ALA	N-CA-CB	5.02	117.59	110.16
11	W	138	VAL	CA-C-N	5.02	127.41	120.29
11	W	138	VAL	C-N-CA	5.02	127.41	120.29
4	B	434	GLU	CA-C-N	5.02	126.96	120.44
4	B	434	GLU	C-N-CA	5.02	126.96	120.44
4	B	445	THR	CA-CB-CG2	-5.02	101.97	110.50
10	O	18	GLN	CA-C-N	5.02	130.94	122.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	O	18	GLN	C-N-CA	5.02	130.94	122.26
11	R	33	ALA	CA-C-O	-5.02	115.55	121.07
4	B	30	THR	N-CA-C	-5.01	101.45	109.07
8	P	215	PHE	CA-CB-CG	-5.01	108.79	113.80
11	Y	155	THR	CA-C-N	5.01	131.12	121.54
11	Y	155	THR	C-N-CA	5.01	131.12	121.54
6	L	65	VAL	CB-CA-C	-5.01	105.48	111.85
3	C	69	THR	N-CA-C	-5.01	100.35	108.52
3	A	215	TRP	CA-C-N	5.01	124.77	119.76
3	A	215	TRP	C-N-CA	5.01	124.77	119.76
7	K	128	ALA	CA-C-N	5.01	127.93	120.31
7	K	128	ALA	C-N-CA	5.01	127.93	120.31
11	U	22	ILE	N-CA-C	-5.01	106.79	111.45
2	N	95	PRO	O-C-N	5.01	128.96	122.85
4	D	197	THR	CA-C-N	5.01	126.99	120.28
4	D	197	THR	C-N-CA	5.01	126.99	120.28
3	A	367	ILE	O-C-N	-5.01	117.00	121.91
10	O	38	LEU	CA-C-O	-5.01	114.94	120.70
6	J	95	VAL	CA-CB-CG2	-5.01	101.89	110.40
10	O	1	MET	CG-SD-CE	-5.01	89.88	100.90
7	G	57	ASN	CA-C-N	5.01	127.32	120.46
7	G	57	ASN	C-N-CA	5.01	127.32	120.46
2	N	81	VAL	CB-CA-C	-5.01	105.46	112.02
3	C	238	ARG	CA-C-N	5.01	128.38	120.47
3	C	238	ARG	C-N-CA	5.01	128.38	120.47
3	C	290	MET	CG-SD-CE	5.01	111.91	100.90
4	F	124	PRO	N-CD-CG	5.01	110.71	103.20
3	A	218	ARG	CA-C-N	5.01	128.23	123.02
3	A	218	ARG	C-N-CA	5.01	128.23	123.02
3	A	573	SER	CA-C-N	5.01	126.95	120.44
3	A	573	SER	C-N-CA	5.01	126.95	120.44
11	V	126	PHE	CA-C-N	5.01	128.38	120.47
11	V	126	PHE	C-N-CA	5.01	128.38	120.47
4	D	192	GLY	N-CA-C	-5.00	108.70	115.36
11	U	25	SER	CA-C-O	-5.00	115.56	120.82
11	R	151	ASN	CA-C-N	5.00	127.40	120.29
11	R	151	ASN	C-N-CA	5.00	127.40	120.29
11	S	83	ALA	O-C-N	-5.00	115.78	122.94
11	T	123	PRO	CA-C-N	5.00	130.97	122.36
11	T	123	PRO	C-N-CA	5.00	130.97	122.36
4	F	29	ASN	N-CA-C	-5.00	96.99	111.00
4	B	435	PHE	N-CA-C	-5.00	105.72	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Z	18	ALA	N-CA-C	5.00	117.11	111.11
11	T	103	ALA	O-C-N	-5.00	115.73	122.23
4	F	397	GLY	N-CA-C	-5.00	106.37	112.77
3	A	85	VAL	O-C-N	-5.00	117.90	123.20
3	A	555	ASP	CA-C-N	5.00	127.39	120.29
3	A	555	ASP	C-N-CA	5.00	127.39	120.29
5	Q	160	PRO	CA-C-N	5.00	128.60	120.60
5	Q	160	PRO	C-N-CA	5.00	128.60	120.60
11	X	25	SER	N-CA-CB	5.00	117.32	110.07

There are no chirality outliers.

All (163) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	126	ARG	Sidechain
3	A	177	ARG	Sidechain
3	A	179	ARG	Sidechain
3	A	28	TYR	Sidechain
3	A	280	TYR	Sidechain
3	A	359	ARG	Sidechain
3	A	460	TYR	Sidechain
3	A	478	PHE	Sidechain
3	A	531	TYR	Sidechain
3	A	553	TYR	Sidechain
3	A	610	ARG	Sidechain
3	A	73	TYR	Sidechain
4	B	224	PHE	Sidechain
4	B	229	PHE	Sidechain
4	B	237	ARG	Sidechain
4	B	265	TYR	Sidechain
4	B	284	TYR	Sidechain
4	B	307	TYR	Sidechain
4	B	316	TYR	Sidechain
4	B	318	ARG	Sidechain
4	B	321	ARG	Sidechain
4	B	352	TYR	Sidechain
4	B	381	ARG	Sidechain
4	B	393	ARG	Sidechain
4	B	404	TYR	Sidechain
4	B	44	VAL	Peptide
4	B	466	ARG	Sidechain
4	B	468	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
4	B	475	ARG	Sidechain
3	C	105	TYR	Sidechain
3	C	123	TYR	Sidechain
3	C	135	ARG	Sidechain
3	C	231	TYR	Sidechain
3	C	24	TYR	Sidechain
3	C	343	PHE	Sidechain
3	C	370	ARG	Sidechain
3	C	383	TYR	Sidechain
3	C	46	TYR	Sidechain
3	C	460	TYR	Sidechain
3	C	478	PHE	Sidechain
3	C	600	PHE	Sidechain
3	C	87	ARG	Sidechain
4	D	127	PHE	Sidechain
4	D	131	TYR	Sidechain
4	D	146	TYR	Sidechain
4	D	237	ARG	Sidechain
4	D	307	TYR	Sidechain
4	D	309	TYR	Sidechain
4	D	325	ARG	Sidechain
4	D	352	TYR	Sidechain
4	D	370	TYR	Sidechain
4	D	404	TYR	Sidechain
4	D	443	PHE	Sidechain
4	D	468	TYR	Sidechain
4	D	71	ARG	Sidechain
3	E	158	TYR	Sidechain
3	E	170	HIS	Sidechain
3	E	177	ARG	Sidechain
3	E	213	HIS	Sidechain
3	E	218	ARG	Sidechain
3	E	272	TYR	Sidechain
3	E	28	TYR	Sidechain
3	E	365	ARG	Sidechain
3	E	383	TYR	Sidechain
3	E	463	TYR	Sidechain
3	E	475	TYR	Sidechain
3	E	482	ARG	Sidechain
3	E	484	ARG	Sidechain
3	E	591	ARG	Sidechain
3	E	611	PHE	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
4	F	146	TYR	Sidechain
4	F	166	ARG	Sidechain
4	F	208	PHE	Sidechain
4	F	225	PHE	Sidechain
4	F	241	PHE	Sidechain
4	F	265	TYR	Sidechain
4	F	272	ARG	Sidechain
4	F	289	ARG	Sidechain
4	F	316	TYR	Sidechain
4	F	362	ARG	Sidechain
4	F	393	ARG	Sidechain
4	F	449	TYR	Sidechain
4	F	452	ARG	Sidechain
4	F	48	ARG	Sidechain
7	G	62	PHE	Sidechain
7	I	114	ARG	Sidechain
7	I	166	ARG	Sidechain
7	I	43	TYR	Sidechain
6	J	25	ARG	Sidechain
6	J	27	TYR	Sidechain
6	J	46	TYR	Sidechain
7	K	100	PHE	Sidechain
7	K	117	TYR	Sidechain
7	K	158	ARG	Sidechain
7	K	160	TYR	Sidechain
7	K	166	ARG	Sidechain
7	K	178	TYR	Sidechain
6	L	46	TYR	Sidechain
1	M	105	TYR	Sidechain
1	M	112	TYR	Sidechain
1	M	127	ARG	Sidechain
1	M	134	ARG	Sidechain
1	M	180	ARG	Sidechain
1	M	187	TYR	Sidechain
1	M	197	ARG	Sidechain
1	M	34	ARG	Sidechain
1	M	81	TYR	Sidechain
2	N	111	ARG	Sidechain
2	N	40	TYR	Sidechain
2	N	5	ARG	Sidechain
2	N	88	PHE	Sidechain
10	O	110	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
10	O	152	TYR	Sidechain
10	O	312	TYR	Sidechain
10	O	325	PHE	Sidechain
10	O	356	PHE	Sidechain
10	O	388	TYR	Sidechain
10	O	6	TYR	Sidechain
10	O	98	ARG	Sidechain
8	P	23	ARG	Sidechain
8	P	32	ARG	Sidechain
8	P	396	ARG	Sidechain
8	P	460	ARG	Sidechain
8	P	477	PHE	Sidechain
5	Q	100	TYR	Sidechain
5	Q	116	HIS	Sidechain
5	Q	12	PHE	Sidechain
5	Q	162	PHE	Sidechain
5	Q	18	ARG	Sidechain
5	Q	193	TYR	Sidechain
5	Q	297	ARG	Sidechain
5	Q	77	TYR	Sidechain
11	R	46	ARG	Sidechain
11	S	142	TYR	Sidechain
11	S	76	TYR	Sidechain
11	T	117	ARG	Sidechain
11	T	142	TYR	Sidechain
11	T	46	ARG	Sidechain
11	T	85	TYR	Sidechain
11	U	11	PHE	Sidechain
11	U	126	PHE	Sidechain
11	U	153	ARG	Sidechain
11	U	46	ARG	Sidechain
11	V	12	PHE	Sidechain
11	V	46	ARG	Sidechain
11	V	76	TYR	Sidechain
11	W	11	PHE	Sidechain
11	W	30	TYR	Sidechain
11	X	142	TYR	Sidechain
11	X	76	TYR	Sidechain
11	Y	76	TYR	Sidechain
11	Y	85	TYR	Sidechain
11	Z	142	TYR	Sidechain
11	Z	46	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
11	Z	85	TYR	Sidechain
11	a	135	PHE	Sidechain
11	a	23	PHE	Sidechain
9	b	268	GLU	Peptide
9	b	300	TYR	Sidechain
9	b	84	TYR	Sidechain
9	b	86	GLY	Peptide
9	b	91	TYR	Sidechain
9	b	99	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1691	0	1740	5	0
2	N	928	0	926	2	0
3	A	4578	0	4519	18	0
3	C	4578	0	4519	4	0
3	E	4578	0	4519	19	0
4	B	3585	0	3567	11	0
4	D	3585	0	3567	12	0
4	F	3585	0	3567	11	0
5	Q	2802	0	2689	5	0
6	H	824	0	877	0	0
6	J	824	0	877	4	0
6	L	824	0	877	3	0
7	G	1731	0	1797	2	0
7	I	1731	0	1797	5	0
7	K	1731	0	1797	6	0
8	P	3712	0	3829	18	0
9	b	2540	0	2537	18	0
10	O	3122	0	3155	7	0
11	R	1071	0	1141	19	0
11	S	1071	0	1141	8	0
11	T	1071	0	1141	2	0
11	U	1071	0	1141	4	0
11	V	1071	0	1141	9	0
11	W	1071	0	1141	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	X	1071	0	1141	5	0
11	Y	1071	0	1141	7	0
11	Z	1071	0	1141	6	0
11	a	1071	0	1141	7	0
All	All	57659	0	58566	208	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 2.

All (208) 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)
11:R:97:VAL:CG1	11:R:144:LEU:CD2	1.93	1.47
11:R:97:VAL:HG11	11:R:144:LEU:CD2	1.54	1.31
11:R:97:VAL:CG1	11:R:144:LEU:HD23	1.53	1.27
9:b:200:GLU:O	9:b:204:TRP:HD1	1.26	1.18
11:R:97:VAL:HG13	11:R:144:LEU:HD23	1.17	1.16
11:R:97:VAL:CG1	11:R:144:LEU:HD21	1.64	1.13
11:R:97:VAL:HG13	11:R:144:LEU:CD2	1.64	1.10
9:b:200:GLU:O	9:b:204:TRP:CD1	2.04	1.09
11:V:66:TYR:HB3	11:V:144:LEU:HD22	1.45	0.98
9:b:200:GLU:C	9:b:204:TRP:HD1	1.80	0.88
11:V:66:TYR:CB	11:V:144:LEU:HD22	2.06	0.85
11:V:66:TYR:HB3	11:V:144:LEU:CD2	2.09	0.83
11:a:66:TYR:HB3	11:a:144:LEU:HD22	1.62	0.82
11:S:66:TYR:HB3	11:S:144:LEU:HD22	1.60	0.82
11:R:97:VAL:HG11	11:R:144:LEU:HD21	1.36	0.81
11:V:66:TYR:CG	11:V:144:LEU:HD22	2.17	0.79
11:W:66:TYR:HB3	11:W:144:LEU:HD22	1.65	0.78
11:U:66:TYR:HB3	11:U:144:LEU:HD22	1.68	0.74
9:b:204:TRP:CZ3	9:b:249:ILE:HG22	2.25	0.71
9:b:204:TRP:HZ3	9:b:249:ILE:HG22	1.53	0.71
9:b:204:TRP:HH2	9:b:249:ILE:HB	1.56	0.70
11:Y:62:ILE:HD12	11:Y:66:TYR:OH	1.92	0.70
4:D:263:ALA:HB3	4:D:329:ILE:HD12	1.77	0.66
9:b:246:ILE:O	9:b:249:ILE:HG12	1.95	0.66
9:b:204:TRP:CZ3	9:b:241:HIS:NE2	2.65	0.65
3:E:124:ILE:HD12	3:E:124:ILE:H	1.61	0.64
11:a:66:TYR:CG	11:a:144:LEU:HD22	2.33	0.63
11:R:66:TYR:HB3	11:R:144:LEU:HD13	1.82	0.61
11:a:66:TYR:CB	11:a:144:LEU:HD22	2.29	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:6:ILE:HG22	8:P:7:LEU:HD22	1.84	0.60
11:Z:74:VAL:HG13	11:Z:90:GLN:HE21	1.67	0.59
9:b:200:GLU:C	9:b:204:TRP:CD1	2.69	0.59
3:E:286:ARG:HE	4:F:381:ARG:HH21	1.50	0.59
3:A:77:ALA:H	3:A:126:ARG:HE	1.51	0.58
11:Z:80:GLN:HE21	11:Y:85:TYR:HA	1.68	0.58
4:B:71:ARG:HH22	4:B:76:ILE:HD11	1.67	0.58
8:P:12:HIS:NE2	8:P:238:LEU:HD22	2.18	0.58
4:D:308:MET:HE1	4:D:346:ILE:HA	1.87	0.57
3:E:192:THR:HG22	3:E:193:LEU:HD23	1.85	0.57
3:C:233:LEU:HD13	3:C:234:LEU:H	1.69	0.57
11:S:96:SER:HB3	11:T:21:ILE:HD11	1.86	0.57
11:R:66:TYR:CB	11:R:144:LEU:HD13	2.34	0.57
8:P:161:VAL:HG21	8:P:199:TYR:CE1	2.41	0.56
4:D:402:GLN:HA	4:D:475:ARG:HE	1.71	0.55
11:V:66:TYR:CG	11:V:144:LEU:CD2	2.87	0.55
3:E:503:GLY:HA2	4:F:424:ALA:HB2	1.87	0.55
11:R:140:GLY:O	11:R:144:LEU:HG	2.07	0.55
11:U:66:TYR:HB3	11:U:144:LEU:CD2	2.37	0.54
3:E:193:LEU:HD23	3:E:193:LEU:H	1.73	0.54
11:Y:118:GLY:HA3	11:Y:129:MET:HE3	1.90	0.54
11:R:97:VAL:HG11	11:R:144:LEU:HD23	1.38	0.54
11:S:73:LEU:HD23	11:S:151:ASN:HD22	1.73	0.54
11:W:66:TYR:CB	11:W:144:LEU:HD22	2.36	0.54
3:A:290:MET:HE2	3:A:290:MET:HA	1.90	0.53
4:F:236:GLU:CD	4:F:236:GLU:H	2.15	0.53
4:D:462:TRP:CD2	4:D:484:PHE:HB3	2.44	0.53
3:A:406:ARG:HE	3:A:406:ARG:N	2.07	0.52
4:D:407:TYR:CE1	4:D:436:LEU:HD12	2.45	0.52
3:A:27:ILE:HD12	3:A:83:ASP:HB2	1.92	0.52
4:F:46:PHE:H	4:F:47:PRO:HD2	1.75	0.52
9:b:204:TRP:HH2	9:b:249:ILE:CB	2.22	0.52
4:B:114:ASP:HB2	4:B:120:ILE:H	1.75	0.51
6:L:103:ILE:HG22	7:K:120:ILE:HG23	1.91	0.51
11:W:63:ILE:HA	11:W:66:TYR:CD2	2.46	0.51
11:W:66:TYR:CG	11:W:144:LEU:HD22	2.45	0.51
8:P:81:ILE:HG13	8:P:123:GLN:HE21	1.76	0.51
3:E:192:THR:HG22	3:E:193:LEU:H	1.74	0.51
11:S:62:ILE:HD12	11:S:66:TYR:OH	2.11	0.51
11:Y:31:GLY:HA2	11:Y:109:GLY:HA3	1.92	0.51
11:R:46:ARG:HE	11:R:49:LEU:HD11	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:158:TYR:CE1	3:A:198:LEU:HD13	2.46	0.51
3:A:27:ILE:HB	3:A:82:GLY:H	1.76	0.50
8:P:6:ILE:HG21	8:P:188:ARG:HE	1.77	0.50
11:a:78:LEU:HD13	11:Z:89:ILE:HD13	1.94	0.49
10:O:179:VAL:HG11	10:O:267:ILE:HD13	1.95	0.49
9:b:210:ASN:HD22	7:I:19:LYS:HD2	1.77	0.49
4:D:102:ILE:HD12	4:D:103:PRO:HD2	1.94	0.49
1:M:111:SER:HB2	1:M:147:VAL:HG11	1.95	0.49
6:L:3:GLN:HE22	9:b:42:ARG:HA	1.77	0.49
7:K:211:SER:O	7:K:215:LEU:HD13	2.13	0.48
11:R:84:LEU:HD12	11:R:84:LEU:H	1.78	0.48
11:X:50:LEU:HD12	11:X:50:LEU:H	1.78	0.48
3:A:213:HIS:HE1	3:A:221:ARG:HH12	1.60	0.48
10:O:200:LYS:HG2	10:O:232:VAL:HG13	1.95	0.48
11:U:66:TYR:CB	11:U:144:LEU:HD22	2.39	0.48
3:A:47:GLU:HA	3:A:91:PRO:HA	1.95	0.48
8:P:391:ASN:HB3	8:P:396:ARG:HH22	1.79	0.48
4:B:462:TRP:CZ2	4:B:484:PHE:HB2	2.49	0.48
3:C:202:PHE:HB3	3:C:206:LYS:HD2	1.95	0.48
3:A:262:LYS:HA	3:A:265:ILE:HG12	1.95	0.48
11:V:13:GLY:H	11:V:82:GLN:HE22	1.61	0.48
11:W:97:VAL:HG22	11:W:144:LEU:HA	1.96	0.48
3:E:306:GLY:H	3:E:310:PRO:HB3	1.78	0.47
3:C:574:THR:HG23	3:C:578:LYS:HB2	1.96	0.47
5:Q:293:MET:HG2	5:Q:345:TYR:CD2	2.49	0.47
5:Q:25:LEU:H	5:Q:25:LEU:HD12	1.78	0.47
3:C:249:GLY:H	3:C:411:SER:HB2	1.78	0.47
4:D:175:ALA:HB1	4:D:362:ARG:HH21	1.79	0.47
3:E:104:ILE:HG12	3:E:112:LEU:HD12	1.97	0.47
9:b:269:GLY:H	9:b:276:LYS:HD3	1.79	0.47
10:O:30:THR:HG22	10:O:34:PHE:CE2	2.50	0.47
11:V:99:LEU:HB2	11:W:22:ILE:HG12	1.95	0.47
7:G:166:ARG:H	7:G:166:ARG:HD3	1.80	0.47
3:E:143:PRO:HD3	3:E:188:ALA:HB2	1.97	0.47
4:D:440:GLU:HA	4:D:444:ILE:HD12	1.96	0.46
3:A:265:ILE:HG22	3:A:528:GLN:HE22	1.79	0.46
4:B:296:GLU:CD	4:B:296:GLU:H	2.23	0.46
11:S:66:TYR:HB3	11:S:144:LEU:CD2	2.37	0.46
1:M:106:LEU:HD13	1:M:155:ALA:HB1	1.98	0.46
8:P:305:HIS:HA	8:P:308:VAL:HG22	1.96	0.46
11:R:97:VAL:HG12	11:R:144:LEU:HD21	1.82	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:467:ILE:HG23	4:F:468:TYR:CD2	2.51	0.46
11:a:66:TYR:CE2	11:a:141:LEU:CD2	2.98	0.46
8:P:301:ARG:HG3	8:P:301:ARG:HH11	1.79	0.46
11:X:54:ILE:HG23	11:W:135:PHE:CZ	2.50	0.45
11:X:24:THR:HG23	11:X:101:GLY:HA3	1.99	0.45
4:B:260:LEU:HD13	4:B:318:ARG:HD3	1.98	0.45
4:B:453:THR:HG23	4:B:456:GLU:H	1.80	0.45
11:Z:84:LEU:HD12	11:Z:84:LEU:H	1.82	0.45
3:A:192:THR:HG22	3:A:193:LEU:H	1.82	0.45
11:V:24:THR:HG21	11:V:63:ILE:HG22	1.98	0.45
11:V:143:GLY:HA2	11:W:21:ILE:HD11	1.99	0.45
4:B:51:GLU:HA	4:B:99:SER:HA	1.99	0.45
1:M:139:TYR:CE2	2:N:19:GLY:HA3	2.52	0.44
11:X:54:ILE:HG23	11:W:135:PHE:HZ	1.83	0.44
11:S:66:TYR:CB	11:S:144:LEU:HD22	2.39	0.44
4:B:344:HIS:HA	4:B:345:PRO:HD3	1.88	0.44
10:O:12:ILE:HG22	10:O:14:ILE:HG23	1.99	0.44
10:O:268:ASP:O	10:O:272:LYS:HG3	2.17	0.44
3:E:124:ILE:H	3:E:124:ILE:CD1	2.30	0.44
4:D:245:ALA:HB1	3:E:389:ALA:HB1	1.99	0.44
3:E:93:SER:HA	3:E:216:PRO:HA	1.99	0.44
3:A:290:MET:HE2	3:A:290:MET:CA	2.48	0.44
11:R:39:ILE:HG23	11:R:53:ASN:HB3	1.99	0.44
6:J:7:ILE:HD13	6:J:7:ILE:O	2.18	0.43
3:E:79:LEU:HD12	3:E:126:ARG:HH22	1.83	0.43
9:b:204:TRP:CZ3	9:b:241:HIS:CE1	3.07	0.43
10:O:296:TYR:CE1	10:O:300:PHE:CE2	3.07	0.43
3:E:223:VAL:HG21	3:E:398:ALA:HB1	1.99	0.43
5:Q:21:ARG:HH12	5:Q:308:THR:CG2	2.32	0.43
6:J:65:VAL:HA	6:J:68:LEU:HB2	2.00	0.43
11:Z:66:TYR:CG	11:Z:144:LEU:HD22	2.53	0.43
3:E:158:TYR:CZ	3:E:198:LEU:HB2	2.54	0.43
8:P:131:SER:O	8:P:132:LEU:HB2	2.19	0.43
7:I:149:ILE:HG21	7:I:174:ILE:HD11	1.99	0.43
4:D:369:ILE:HG23	4:D:445:THR:OG1	2.18	0.43
8:P:319:LEU:HB3	8:P:320:PRO:HD3	2.00	0.43
9:b:79:HIS:HE1	9:b:302:ILE:HD11	1.84	0.43
8:P:424:LEU:HA	8:P:427:ILE:HG12	1.99	0.43
4:F:154:GLY:HA2	4:F:452:ARG:H	1.83	0.43
6:J:103:ILE:HG22	7:I:120:ILE:HD13	2.01	0.43
3:A:240:LEU:HD13	3:A:439:TRP:CH2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:138:ILE:HG21	7:I:195:ASP:OD2	2.19	0.43
7:G:142:LEU:HG	7:G:179:LEU:HB2	1.99	0.43
11:Y:122:GLN:HA	11:Y:122:GLN:OE1	2.19	0.43
4:B:304:TYR:HB3	4:B:308:MET:SD	2.59	0.42
8:P:165:LEU:HD21	8:P:190:LEU:HD22	2.00	0.42
8:P:476:THR:HG21	9:b:280:ASN:HD21	1.84	0.42
9:b:249:ILE:HG13	9:b:250:ARG:N	2.34	0.42
4:B:371:PRO:HA	4:B:372:PRO:HD3	1.83	0.42
8:P:12:HIS:HB3	8:P:181:ASP:HA	2.01	0.42
2:N:21:LEU:HD23	2:N:21:LEU:HA	1.92	0.42
5:Q:42:LEU:HD23	5:Q:63:LEU:HD22	2.01	0.42
6:L:103:ILE:CG2	7:K:120:ILE:HG23	2.49	0.42
9:b:325:LYS:H	9:b:325:LYS:HD3	1.84	0.42
4:F:360:VAL:HA	4:F:373:ILE:HA	2.01	0.42
11:W:112:GLY:O	11:W:116:VAL:HG23	2.19	0.42
1:M:11:THR:HA	1:M:188:ILE:HG23	2.01	0.42
11:Z:54:ILE:O	11:Z:57:VAL:HG12	2.19	0.42
11:R:38:GLY:C	11:R:116:VAL:HG21	2.44	0.42
3:A:53:HIS:CE1	3:A:84:PRO:CD	3.03	0.42
3:A:73:TYR:HB3	3:A:327:ALA:H	1.85	0.42
7:K:34:GLU:HG2	8:P:289:LEU:HD21	2.02	0.42
7:K:128:ALA:HB2	7:K:201:ASN:OD1	2.20	0.42
8:P:424:LEU:HD21	8:P:453:LEU:HD13	2.01	0.42
3:E:148:VAL:HG13	3:E:183:THR:O	2.20	0.41
7:I:155:ASP:O	7:I:159:GLU:HB2	2.19	0.41
4:F:46:PHE:H	4:F:47:PRO:CD	2.32	0.41
3:A:256:GLY:H	3:A:418:PRO:HD3	1.86	0.41
3:A:526:LEU:N	3:A:526:LEU:HD12	2.35	0.41
4:B:161:MET:HG3	4:B:375:VAL:HG11	2.02	0.41
8:P:194:ALA:HB3	8:P:252:LEU:HD13	2.02	0.41
11:a:150:LEU:HA	11:a:153:ARG:HH12	1.85	0.41
11:Y:46:ARG:HB2	11:Y:49:LEU:CD1	2.51	0.41
4:F:413:ALA:HB3	4:F:433:LEU:HG	2.03	0.41
11:X:79:GLY:H	11:X:158:VAL:HG22	1.84	0.41
4:F:138:PRO:O	4:F:139:ILE:HG23	2.20	0.41
7:K:187:GLY:HA3	7:K:202:THR:HA	2.03	0.41
5:Q:208:MET:HG2	5:Q:310:TRP:CE3	2.55	0.41
3:A:100:LEU:H	3:A:170:HIS:CE1	2.39	0.41
11:U:59:MET:O	11:U:62:ILE:HG12	2.20	0.41
11:a:66:TYR:CE2	11:a:141:LEU:HD23	2.56	0.41
11:Y:66:TYR:HB3	11:Y:144:LEU:HD22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:318:VAL:HG21	3:E:335:THR:HG22	2.03	0.41
11:S:85:TYR:CE2	11:T:11:PHE:HB2	2.56	0.41
11:S:114:ALA:HB1	11:S:117:ARG:HH21	1.85	0.41
1:M:83:VAL:HG22	1:M:122:LEU:HD21	2.01	0.41
4:D:111:ARG:HH11	4:D:111:ARG:HD2	1.74	0.41
3:E:182:ILE:HG22	3:E:198:LEU:HD11	2.03	0.41
3:E:173:LEU:HD12	3:E:342:TYR:CE1	2.56	0.41
4:F:210:ILE:HA	4:F:275:LEU:O	2.21	0.41
6:J:91:LYS:O	6:J:95:VAL:HG23	2.21	0.41
11:R:97:VAL:HG13	11:R:144:LEU:CG	2.44	0.41
8:P:77:LEU:HD11	8:P:117:PHE:CZ	2.56	0.40
10:O:198:VAL:HG11	10:O:206:PHE:HB2	2.02	0.40
11:R:128:GLY:HA2	11:R:131:LEU:HD12	2.03	0.40
11:R:46:ARG:HH22	11:R:123:PRO:HD3	1.86	0.40
4:D:164:ILE:HG12	4:D:170:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	208/256 (81%)	202 (97%)	5 (2%)	1 (0%)	24	63
2	N	113/118 (96%)	102 (90%)	7 (6%)	4 (4%)	3	20
3	A	591/616 (96%)	551 (93%)	23 (4%)	17 (3%)	3	23
3	C	591/616 (96%)	545 (92%)	31 (5%)	15 (2%)	4	26
3	E	591/616 (96%)	544 (92%)	31 (5%)	16 (3%)	4	25
4	B	455/517 (88%)	415 (91%)	26 (6%)	14 (3%)	3	22
4	D	455/517 (88%)	410 (90%)	32 (7%)	13 (3%)	3	23
4	F	455/517 (88%)	425 (93%)	20 (4%)	10 (2%)	5	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Q	343/345 (99%)	317 (92%)	18 (5%)	8 (2%)	5	28
6	H	103/114 (90%)	102 (99%)	0	1 (1%)	12	48
6	J	103/114 (90%)	100 (97%)	3 (3%)	0	100	100
6	L	103/114 (90%)	98 (95%)	4 (4%)	1 (1%)	12	48
7	G	215/233 (92%)	206 (96%)	7 (3%)	2 (1%)	14	51
7	I	215/233 (92%)	207 (96%)	6 (3%)	2 (1%)	14	51
7	K	215/233 (92%)	206 (96%)	8 (4%)	1 (0%)	24	63
8	P	457/478 (96%)	434 (95%)	18 (4%)	5 (1%)	11	46
9	b	306/840 (36%)	289 (94%)	11 (4%)	6 (2%)	6	31
10	O	390/392 (100%)	350 (90%)	26 (7%)	14 (4%)	2	20
11	R	148/160 (92%)	137 (93%)	7 (5%)	4 (3%)	4	25
11	S	148/160 (92%)	136 (92%)	9 (6%)	3 (2%)	6	31
11	T	148/160 (92%)	138 (93%)	7 (5%)	3 (2%)	6	31
11	U	148/160 (92%)	138 (93%)	7 (5%)	3 (2%)	6	31
11	V	148/160 (92%)	141 (95%)	6 (4%)	1 (1%)	18	56
11	W	148/160 (92%)	137 (93%)	9 (6%)	2 (1%)	9	40
11	X	148/160 (92%)	138 (93%)	5 (3%)	5 (3%)	3	21
11	Y	148/160 (92%)	139 (94%)	6 (4%)	3 (2%)	6	31
11	Z	148/160 (92%)	145 (98%)	2 (1%)	1 (1%)	18	56
11	a	148/160 (92%)	138 (93%)	7 (5%)	3 (2%)	6	31
All	All	7389/8469 (87%)	6890 (93%)	341 (5%)	158 (2%)	8	30

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	475	TYR
4	D	45	LYS
4	D	59	ASP
4	D	143	ALA
3	E	475	TYR
3	E	565	ALA
3	E	575	GLY
4	F	46	PHE
3	A	202	PHE
3	A	475	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	141	PRO
4	B	372	PRO
10	O	120	LYS
10	O	186	LEU
6	H	77	GLN
7	I	167	ALA
7	I	192	ASN
11	U	157	ASP
11	X	47	PRO
11	Y	158	VAL
11	T	158	VAL
2	N	115	LEU
3	C	575	GLY
4	D	319	ALA
4	D	372	PRO
3	E	164	ASN
4	F	467	ILE
3	A	230	ASP
3	A	258	PHE
3	A	532	SER
3	A	575	GLY
4	B	139	ILE
4	B	377	PRO
5	Q	133	PHE
5	Q	240	ASP
8	P	3	ALA
9	b	24	GLU
9	b	87	ASP
9	b	356	MET
10	O	39	ILE
10	O	172	VAL
10	O	375	ALA
11	X	82	GLN
11	X	157	ASP
11	a	47	PRO
11	R	123	PRO
11	R	158	VAL
11	Y	156	GLN
11	T	157	ASP
11	T	159	VAL
11	W	156	GLN
1	M	124	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	98	ASP
3	C	230	ASP
3	C	261	GLY
3	C	310	PRO
4	D	58	PRO
4	D	141	PRO
4	D	149	GLU
3	E	405	ASP
3	E	449	LYS
3	E	536	ALA
4	F	299	PRO
3	A	39	ASN
3	A	203	ASP
3	A	284	GLY
3	A	441	LEU
3	A	565	ALA
6	L	63	GLY
8	P	35	GLU
9	b	83	LEU
9	b	86	GLY
9	b	257	ASP
10	O	90	ASN
10	O	167	THR
10	O	176	HIS
11	X	156	GLN
11	a	123	PRO
11	R	156	GLN
11	R	159	VAL
11	S	47	PRO
11	W	159	VAL
3	C	257	ALA
3	C	305	SER
3	C	591	ARG
4	D	136	GLY
4	D	424	ALA
3	E	207	SER
3	E	257	ALA
4	F	83	THR
4	F	202	ASP
4	F	372	PRO
4	F	391	MET
3	A	325	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	405	ASP
3	A	531	TYR
3	A	590	SER
4	B	83	THR
4	B	116	SER
4	B	127	PHE
4	B	163	SER
4	B	167	GLY
4	B	292	SER
5	Q	134	ASP
5	Q	230	SER
10	O	171	SER
7	G	195	ASP
11	Y	159	VAL
3	C	207	SER
3	C	420	GLY
4	D	83	THR
3	E	230	ASP
3	E	305	SER
3	E	590	SER
4	F	123	GLY
4	F	125	LYS
4	F	360	VAL
4	B	143	ALA
4	B	202	ASP
5	Q	117	ASP
5	Q	174	ASP
7	K	152	MET
8	P	458	ASP
10	O	7	THR
10	O	95	ASN
10	O	100	LEU
10	O	116	TRP
7	G	135	PRO
11	U	158	VAL
11	X	48	ASP
11	Z	159	VAL
11	S	159	VAL
11	V	159	VAL
2	N	4	LYS
3	C	109	GLN
3	C	405	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	50	ASN
4	D	137	SER
3	E	259	GLY
3	A	456	THR
5	Q	129	PRO
8	P	390	ASP
8	P	412	ASN
11	a	159	VAL
3	E	310	PRO
3	A	78	GLY
4	B	88	VAL
3	E	284	GLY
2	N	25	ILE
3	C	284	GLY
5	Q	203	PRO
11	S	79	GLY
10	O	106	PRO
3	C	381	PRO
3	C	539	PRO
3	E	197	ILE
4	B	179	PRO
11	U	47	PRO

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	M	183/221 (83%)	175 (96%)	8 (4%)	25	47
2	N	102/104 (98%)	101 (99%)	1 (1%)	68	78
3	A	497/515 (96%)	476 (96%)	21 (4%)	26	48
3	C	497/515 (96%)	476 (96%)	21 (4%)	26	48
3	E	497/515 (96%)	476 (96%)	21 (4%)	26	48
4	B	391/444 (88%)	374 (96%)	17 (4%)	26	47
4	D	391/444 (88%)	377 (96%)	14 (4%)	31	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	391/444 (88%)	375 (96%)	16 (4%)	27	48
5	Q	309/309 (100%)	303 (98%)	6 (2%)	50	67
6	H	87/94 (93%)	85 (98%)	2 (2%)	44	64
6	J	87/94 (93%)	84 (97%)	3 (3%)	32	54
6	L	87/94 (93%)	85 (98%)	2 (2%)	44	64
7	G	194/208 (93%)	187 (96%)	7 (4%)	31	52
7	I	194/208 (93%)	190 (98%)	4 (2%)	47	65
7	K	194/208 (93%)	188 (97%)	6 (3%)	35	56
8	P	426/439 (97%)	416 (98%)	10 (2%)	44	64
9	b	275/728 (38%)	264 (96%)	11 (4%)	28	49
10	O	348/348 (100%)	341 (98%)	7 (2%)	48	66
11	R	110/119 (92%)	105 (96%)	5 (4%)	24	46
11	S	110/119 (92%)	108 (98%)	2 (2%)	51	68
11	T	110/119 (92%)	109 (99%)	1 (1%)	70	79
11	U	110/119 (92%)	102 (93%)	8 (7%)	13	34
11	V	110/119 (92%)	109 (99%)	1 (1%)	70	79
11	W	110/119 (92%)	107 (97%)	3 (3%)	39	61
11	X	110/119 (92%)	103 (94%)	7 (6%)	16	37
11	Y	110/119 (92%)	101 (92%)	9 (8%)	10	30
11	Z	110/119 (92%)	104 (94%)	6 (6%)	19	41
11	a	110/119 (92%)	107 (97%)	3 (3%)	39	61
All	All	6250/7122 (88%)	6028 (96%)	222 (4%)	32	52

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	68	LEU
1	M	102	SER
1	M	117	ILE
1	M	122	LEU
1	M	139	TYR
1	M	176	VAL
1	M	189	ASN
1	M	216	LYS
2	N	81	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	60	VAL
3	C	126	ARG
3	C	131	PRO
3	C	143	PRO
3	C	179	ARG
3	C	196	LYS
3	C	233	LEU
3	C	264	VAL
3	C	278	ILE
3	C	279	ILE
3	C	286	ARG
3	C	325	PRO
3	C	353	ILE
3	C	364	LEU
3	C	406	ARG
3	C	422	ASP
3	C	476	PRO
3	C	505	SER
3	C	532	SER
3	C	544	PHE
3	C	588	GLU
4	D	42	GLU
4	D	43	LYS
4	D	62	VAL
4	D	79	VAL
4	D	86	ILE
4	D	92	THR
4	D	112	ILE
4	D	139	ILE
4	D	250	ILE
4	D	346	ILE
4	D	392	THR
4	D	454	VAL
4	D	467	ILE
4	D	474	ASN
3	E	60	VAL
3	E	91	PRO
3	E	167	ILE
3	E	182	ILE
3	E	192	THR
3	E	197	ILE
3	E	254	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	263	THR
3	E	274	ASN
3	E	279	ILE
3	E	304	MET
3	E	317	LEU
3	E	335	THR
3	E	359	ARG
3	E	406	ARG
3	E	441	LEU
3	E	466	VAL
3	E	478	PHE
3	E	504	LYS
3	E	524	ASP
3	E	603	LEU
4	F	53	VAL
4	F	64	GLN
4	F	91	THR
4	F	95	PHE
4	F	169	LYS
4	F	198	LYS
4	F	219	LEU
4	F	250	ILE
4	F	254	ILE
4	F	297	GLU
4	F	299	PRO
4	F	305	PRO
4	F	329	ILE
4	F	337	MET
4	F	357	GLN
4	F	472	MET
3	A	61	ILE
3	A	80	THR
3	A	96	LEU
3	A	179	ARG
3	A	192	THR
3	A	205	LYS
3	A	238	ARG
3	A	260	CYS
3	A	271	LYS
3	A	286	ARG
3	A	300	LEU
3	A	302	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	313	LYS
3	A	317	LEU
3	A	324	MET
3	A	406	ARG
3	A	416	VAL
3	A	482	ARG
3	A	526	LEU
3	A	599	GLU
3	A	605	SER
4	B	32	SER
4	B	34	VAL
4	B	68	LEU
4	B	70	ILE
4	B	91	THR
4	B	126	VAL
4	B	164	ILE
4	B	170	ILE
4	B	248	PRO
4	B	329	ILE
4	B	340	ASP
4	B	346	ILE
4	B	389	GLU
4	B	394	LYS
4	B	427	ILE
4	B	444	ILE
4	B	458	LEU
5	Q	114	THR
5	Q	176	ASN
5	Q	196	VAL
5	Q	301	THR
5	Q	307	SER
5	Q	323	ILE
6	L	7	ILE
6	L	102	VAL
7	K	49	ASN
7	K	85	ARG
7	K	93	GLU
7	K	168	PRO
7	K	182	ASP
7	K	213	GLU
8	P	53	LYS
8	P	90	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	P	93	LYS
8	P	149	LEU
8	P	198	GLU
8	P	224	SER
8	P	325	LEU
8	P	327	GLU
8	P	456	HIS
8	P	466	LEU
9	b	20	TYR
9	b	21	ILE
9	b	56	VAL
9	b	65	VAL
9	b	144	ILE
9	b	186	TYR
9	b	187	VAL
9	b	203	LEU
9	b	250	ARG
9	b	325	LYS
9	b	342	PRO
10	O	26	PRO
10	O	35	ASN
10	O	79	ILE
10	O	106	PRO
10	O	121	PHE
10	O	212	THR
10	O	311	VAL
6	H	55	LYS
6	H	59	GLN
7	G	9	THR
7	G	23	PHE
7	G	43	TYR
7	G	61	ASN
7	G	143	GLU
7	G	166	ARG
7	G	184	VAL
6	J	4	LYS
6	J	7	ILE
6	J	9	THR
7	I	63	LYS
7	I	89	LEU
7	I	166	ARG
7	I	192	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	U	44	VAL
11	U	54	ILE
11	U	97	VAL
11	U	108	ILE
11	U	124	ARG
11	U	125	LEU
11	U	139	LEU
11	U	159	VAL
11	X	75	CYS
11	X	81	LYS
11	X	91	LEU
11	X	97	VAL
11	X	116	VAL
11	X	138	VAL
11	X	139	LEU
11	a	56	PRO
11	a	116	VAL
11	a	126	PHE
11	R	37	VAL
11	R	58	ILE
11	R	62	ILE
11	R	97	VAL
11	R	119	SER
11	Z	11	PHE
11	Z	21	ILE
11	Z	99	LEU
11	Z	117	ARG
11	Z	123	PRO
11	Z	160	CYS
11	S	116	VAL
11	S	152	SER
11	Y	17	CYS
11	Y	34	LYS
11	Y	57	VAL
11	Y	63	ILE
11	Y	81	LYS
11	Y	97	VAL
11	Y	120	SER
11	Y	132	ILE
11	Y	159	VAL
11	T	127	VAL
11	V	97	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	W	73	LEU
11	W	97	VAL
11	W	139	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (141) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	26	ASN
1	M	98	GLN
1	M	100	ASN
1	M	130	GLN
1	M	175	HIS
1	M	212	ASN
2	N	71	GLN
3	C	53	HIS
3	C	120	GLN
3	C	151	HIS
3	C	164	ASN
3	C	267	GLN
3	C	320	ASN
3	C	491	ASN
4	D	50	ASN
4	D	66	GLN
4	D	78	GLN
4	D	181	ASN
4	D	227	GLN
4	D	246	ASN
4	D	339	ASN
4	D	402	GLN
4	D	446	GLN
4	D	474	ASN
3	E	147	GLN
3	E	151	HIS
3	E	164	ASN
3	E	213	HIS
3	E	267	GLN
3	E	274	ASN
3	E	320	ASN
3	E	447	GLN
3	E	465	ASN
3	E	528	GLN
4	F	50	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	64	GLN
4	F	135	ASN
4	F	190	GLN
4	F	204	HIS
4	F	246	ASN
4	F	269	GLN
4	F	366	ASN
4	F	396	HIS
4	F	474	ASN
3	A	53	HIS
3	A	71	GLN
3	A	140	GLN
3	A	213	HIS
3	A	267	GLN
3	A	288	ASN
3	A	436	GLN
3	A	450	HIS
3	A	465	ASN
3	A	500	GLN
3	A	528	GLN
3	A	554	HIS
3	A	558	GLN
3	A	597	HIS
4	B	54	ASN
4	B	64	GLN
4	B	140	ASN
4	B	181	ASN
4	B	207	ASN
4	B	331	GLN
4	B	344	HIS
4	B	374	ASN
4	B	396	HIS
5	Q	53	ASN
5	Q	86	GLN
5	Q	106	ASN
5	Q	116	HIS
5	Q	128	HIS
5	Q	194	ASN
5	Q	209	GLN
5	Q	229	GLN
5	Q	283	ASN
5	Q	287	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	Q	322	ASN
5	Q	333	ASN
6	L	3	GLN
6	L	29	GLN
7	K	73	GLN
7	K	113	ASN
7	K	122	GLN
7	K	200	ASN
8	P	14	ASN
8	P	97	GLN
8	P	118	GLN
8	P	123	GLN
8	P	126	GLN
8	P	172	ASN
8	P	191	GLN
8	P	219	GLN
8	P	241	GLN
8	P	261	ASN
8	P	265	GLN
8	P	304	GLN
8	P	348	ASN
8	P	408	ASN
8	P	415	GLN
8	P	455	ASN
8	P	456	HIS
9	b	52	GLN
9	b	79	HIS
9	b	146	GLN
9	b	185	ASN
9	b	210	ASN
9	b	220	GLN
9	b	267	ASN
9	b	273	GLN
9	b	280	ASN
10	O	74	GLN
10	O	187	ASN
10	O	216	ASN
10	O	302	ASN
10	O	336	ASN
6	H	12	GLN
6	H	61	ASN
7	G	14	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	36	GLN
7	G	49	ASN
7	G	73	GLN
7	G	201	ASN
7	I	18	ASN
7	I	73	GLN
7	I	74	GLN
7	I	201	ASN
11	X	53	ASN
11	X	80	GLN
11	R	80	GLN
11	R	121	GLN
11	R	151	ASN
11	Z	80	GLN
11	Z	90	GLN
11	S	151	ASN
11	T	82	GLN
11	T	122	GLN
11	T	156	GLN
11	V	82	GLN
11	W	53	ASN
11	W	156	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

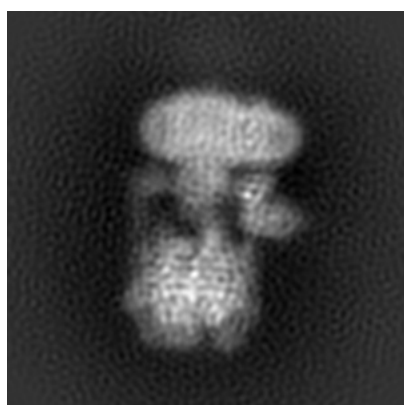
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6285. These allow visual inspection of the internal detail of the map and identification of artifacts.

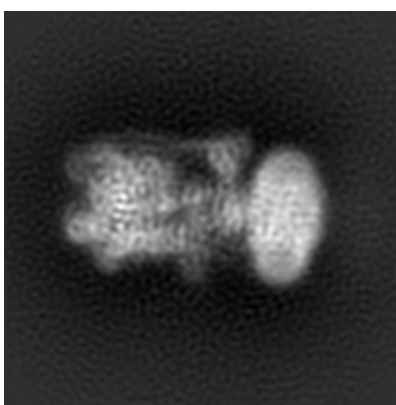
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

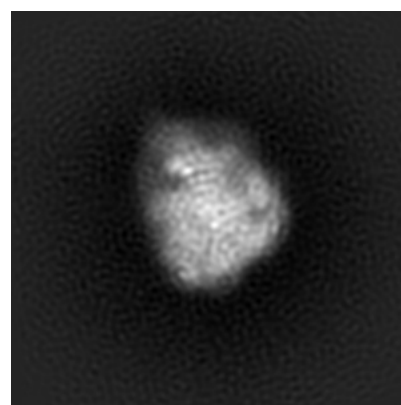
6.1.1 Primary map



X



Y

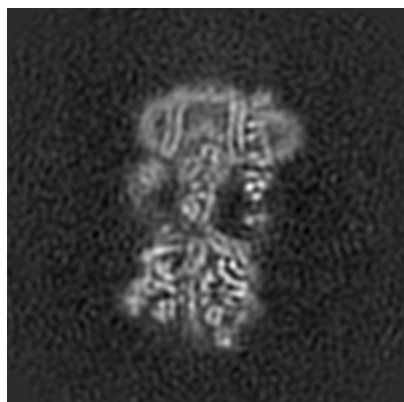


Z

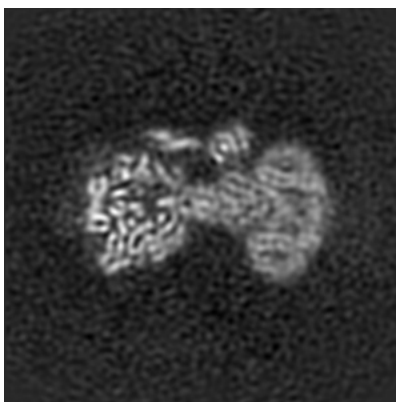
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

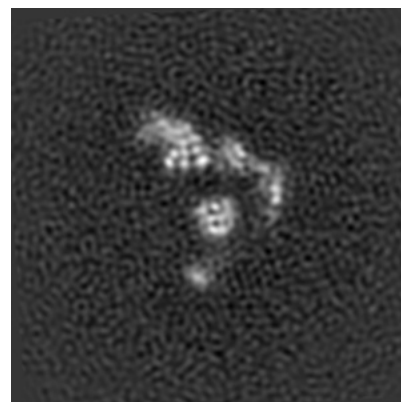
6.2.1 Primary map



X Index: 128



Y Index: 128

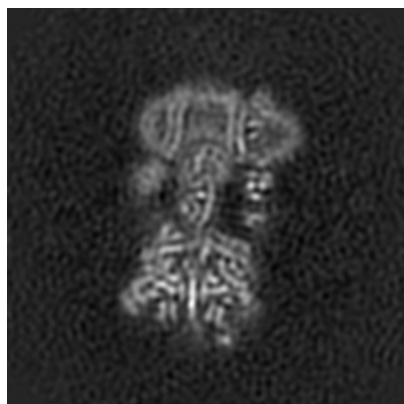


Z Index: 128

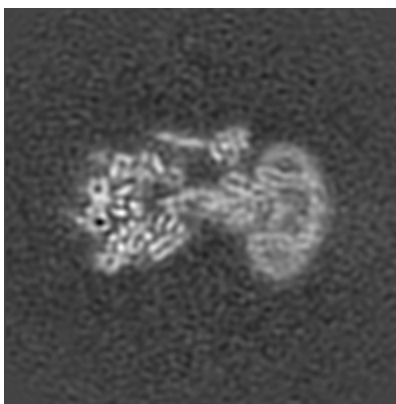
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

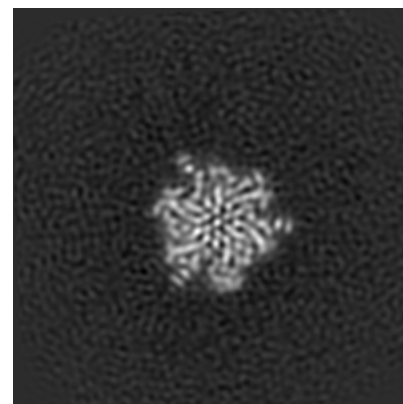
6.3.1 Primary map



X Index: 130



Y Index: 130

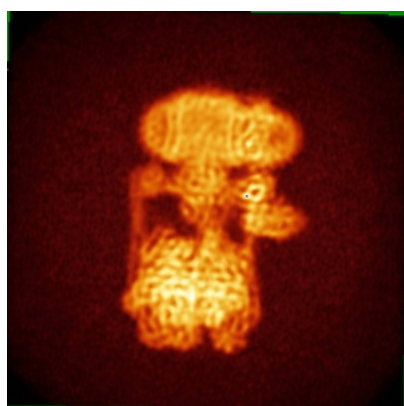


Z Index: 75

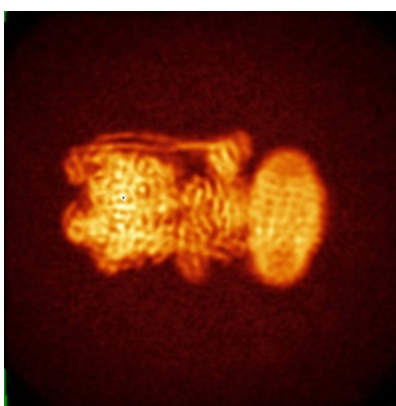
The images above show the largest variance slices of the map in three orthogonal directions.

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

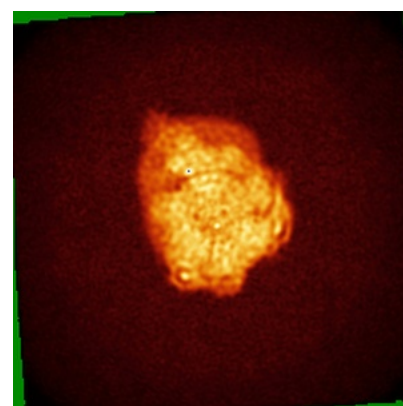
6.4.1 Primary map



X



Y

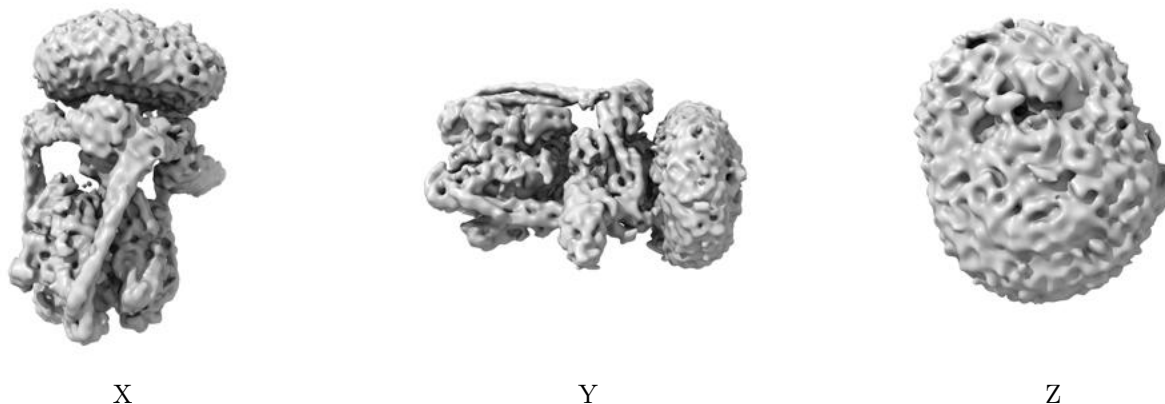


Z

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

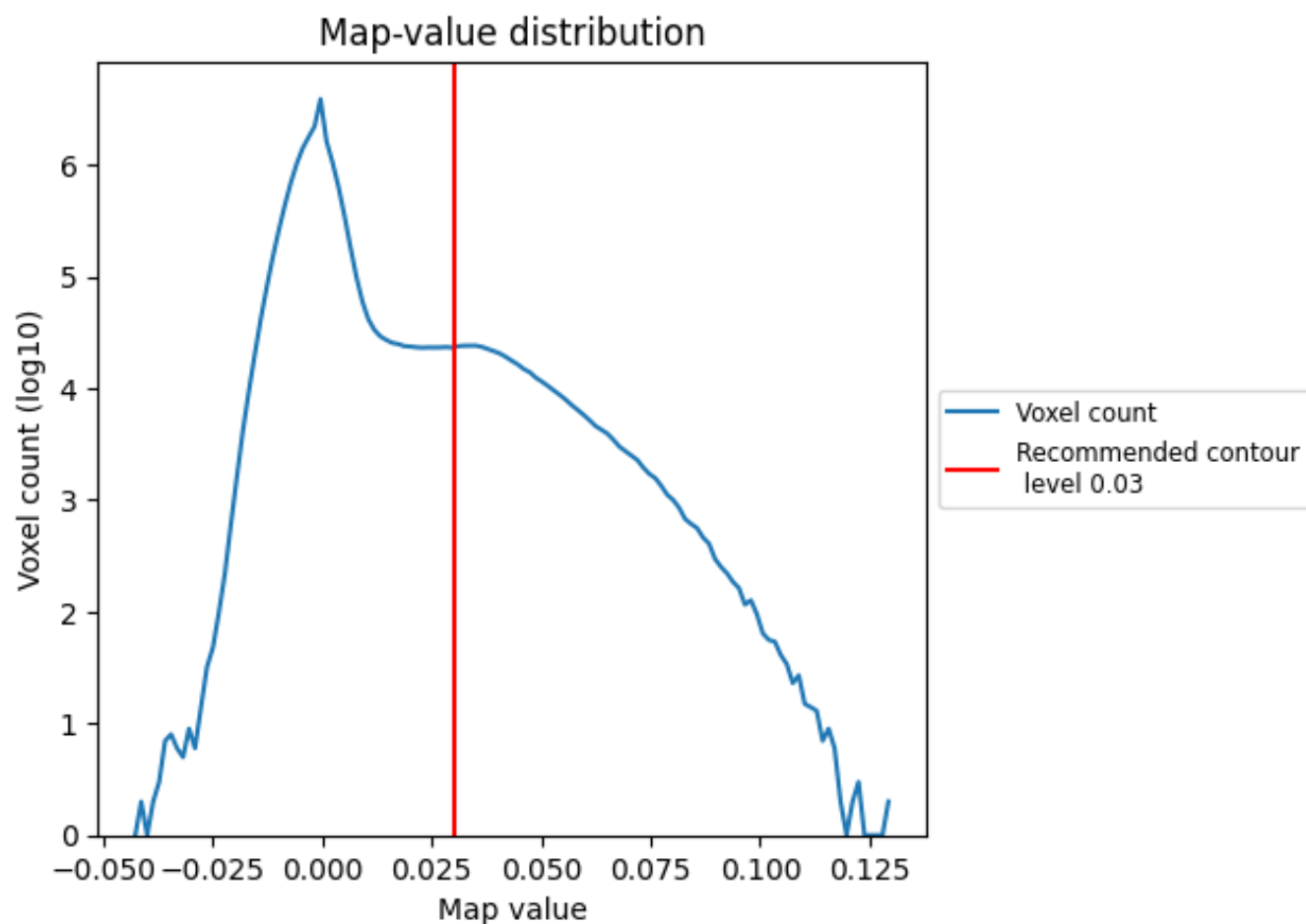
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

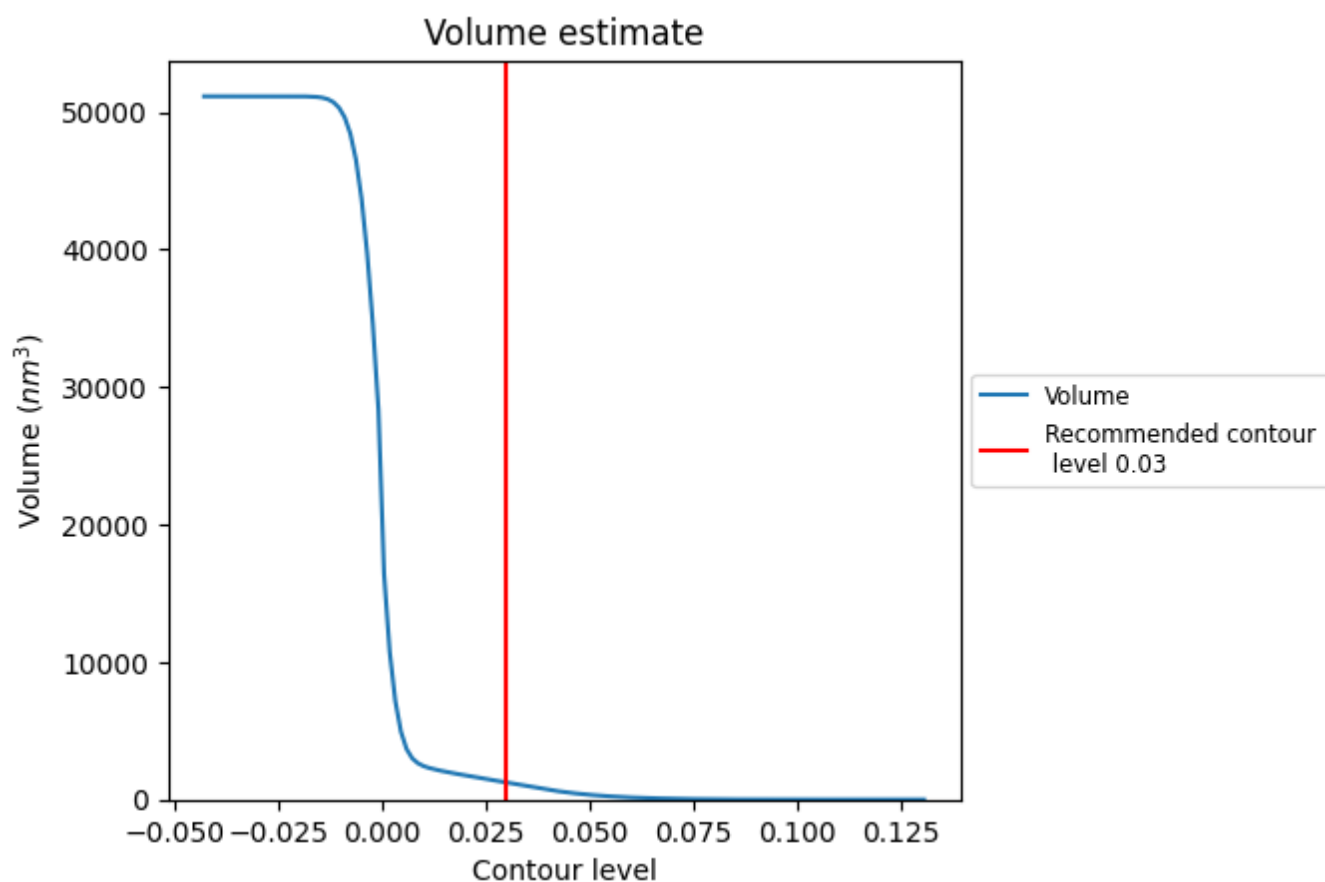
This section contains the results of statistical analysis of the map.

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.

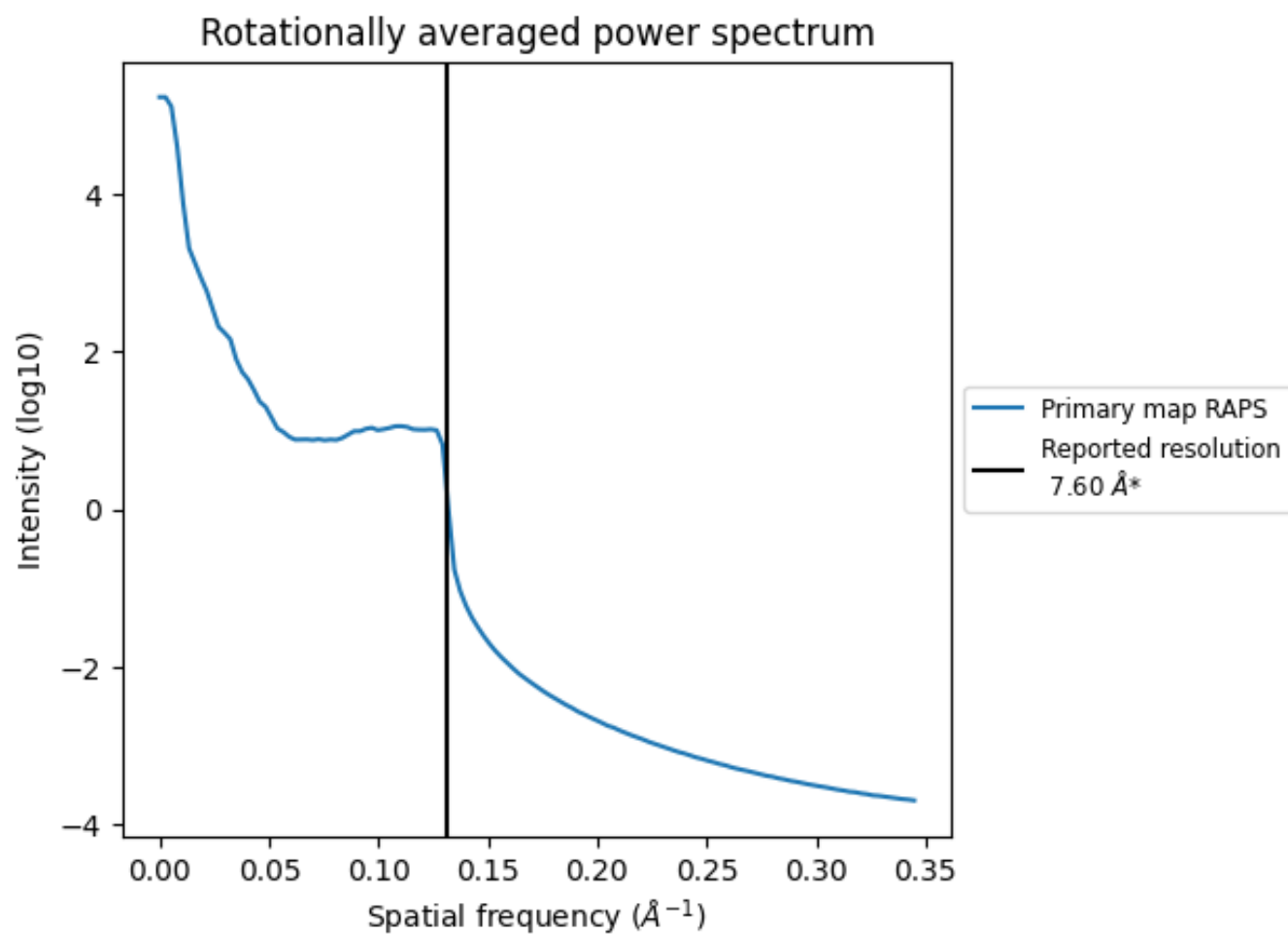
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1247 nm³; this corresponds to an approximate mass of 1126 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 ⓘ

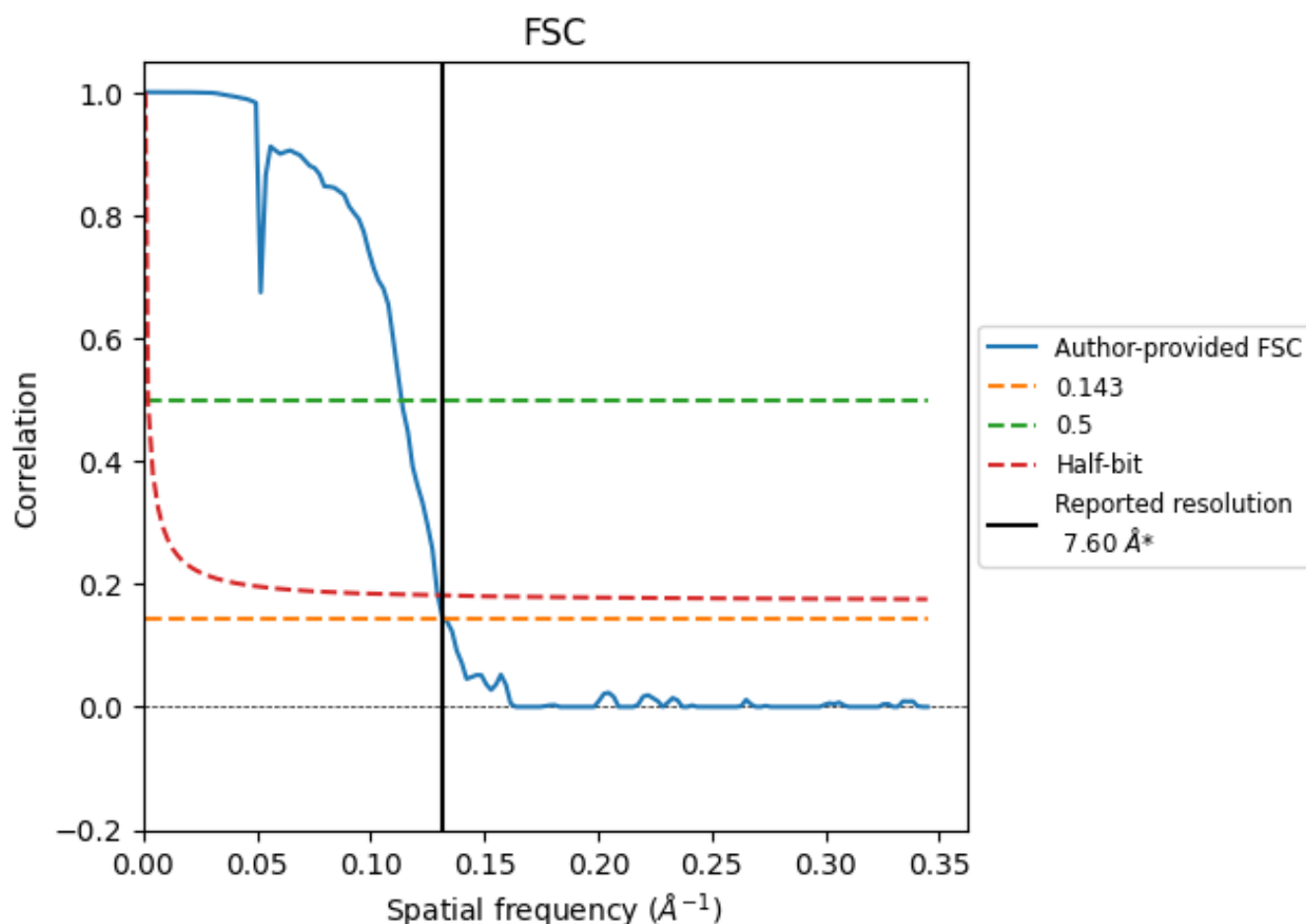


*Reported resolution corresponds to spatial frequency of 0.132 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.132 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

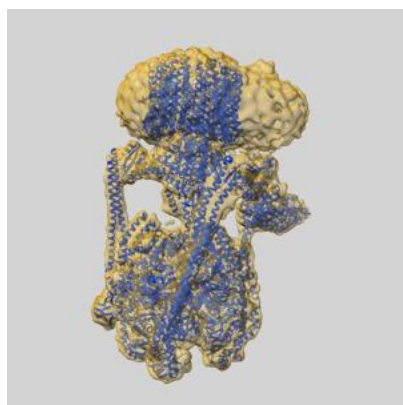
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.60	-	-
Author-provided FSC curve	7.54	8.80	7.72
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

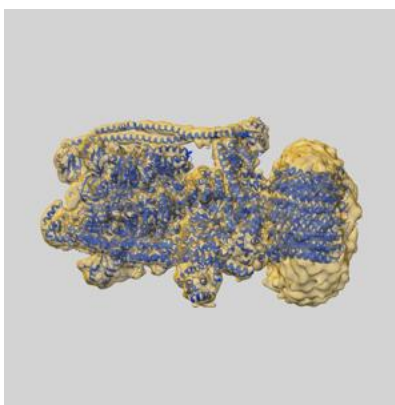
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6285 and PDB model 3J9U. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

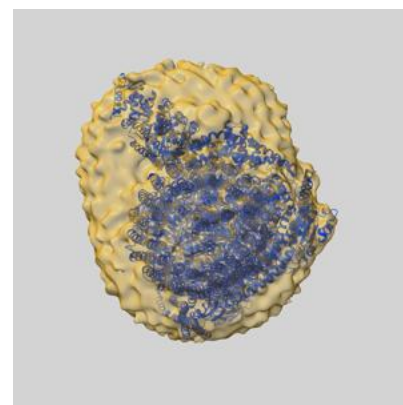
9.1 Map-model overlay [i](#)



X



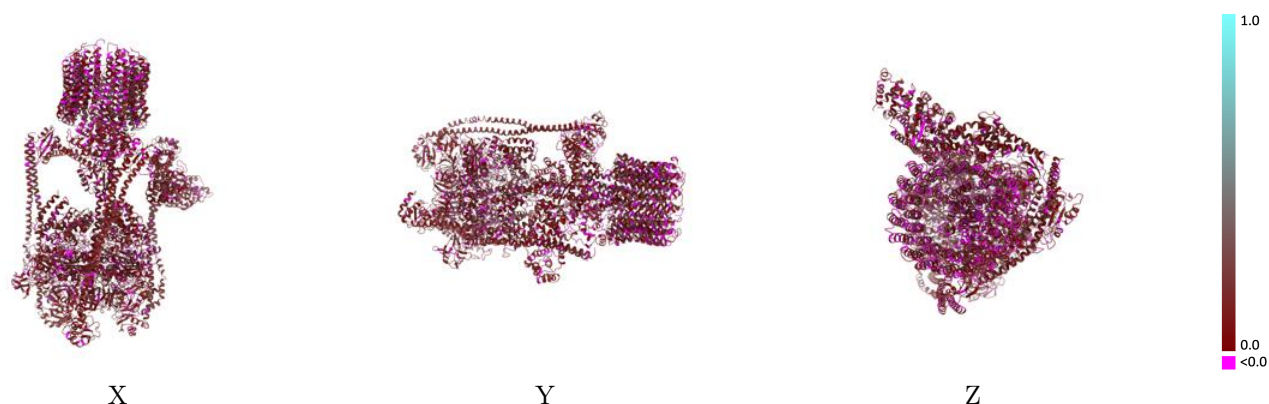
Y



Z

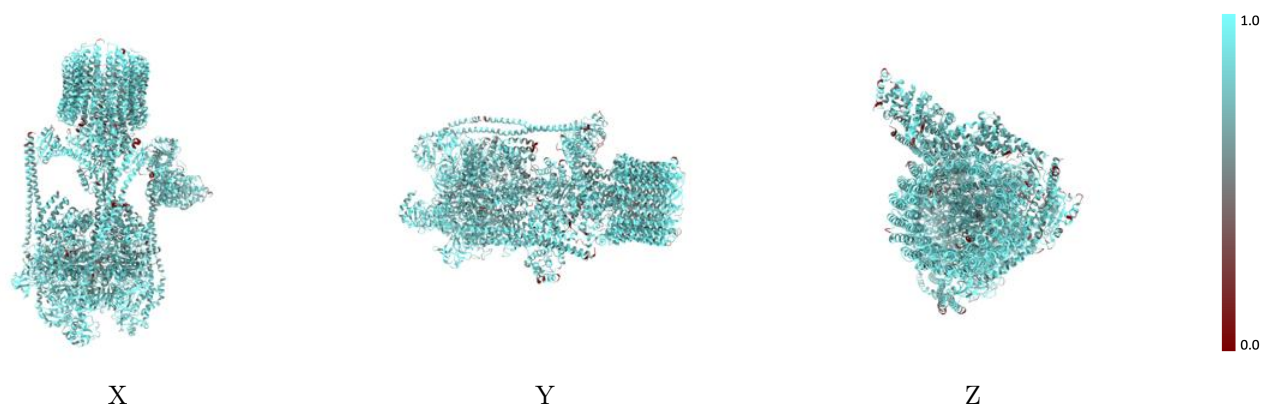
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



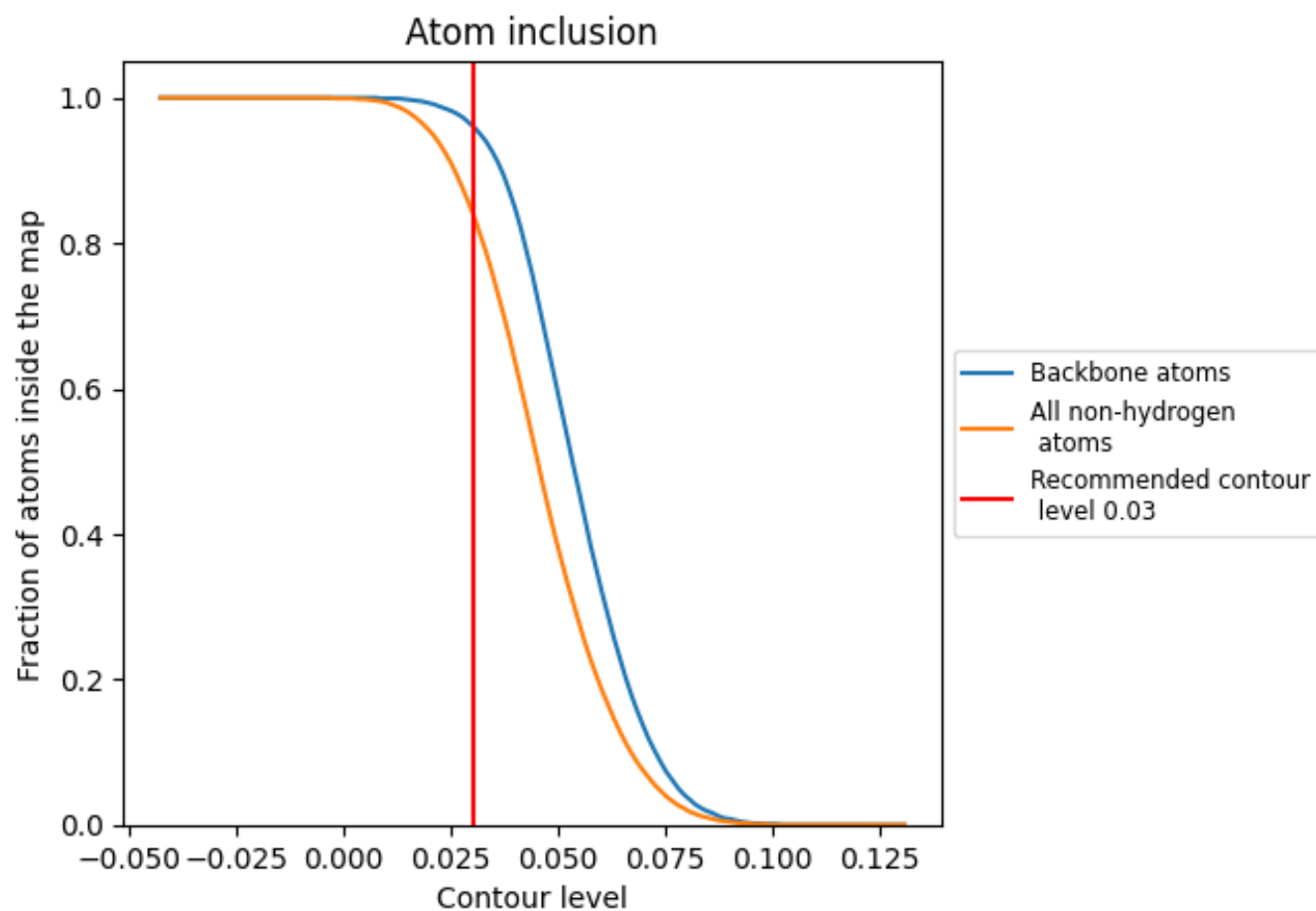
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 84% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.1210
A	 0.8720	 0.1340
B	 0.8360	 0.1250
C	 0.8250	 0.1320
D	 0.8360	 0.1220
E	 0.8650	 0.1260
F	 0.8450	 0.1220
G	 0.8280	 0.1440
H	 0.7870	 0.1460
I	 0.8420	 0.1480
J	 0.7920	 0.1550
K	 0.8350	 0.1450
L	 0.7900	 0.1580
M	 0.8110	 0.1110
N	 0.8000	 0.1260
O	 0.8210	 0.1210
P	 0.7990	 0.1300
Q	 0.7870	 0.0840
R	 0.8510	 0.1240
S	 0.8720	 0.1180
T	 0.9280	 0.1010
U	 0.9040	 0.0840
V	 0.9270	 0.0980
W	 0.9090	 0.1000
X	 0.9150	 0.0860
Y	 0.9100	 0.0800
Z	 0.9070	 0.0810
a	 0.8940	 0.1120
b	 0.7980	 0.1090

