



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 09:53 PM UTC

PDB ID : 6FVU / pdb_00006fvu
EMDB ID : EMD-3535
Title : 26S proteasome, s2 state
Authors : Eisele, M.R.; Reed, R.G.; Rudack, T.; Schweitzer, A.; Beck, F.; Nagy, I.; Pfeifer, G.; Plitzko, J.M.; Baumeister, W.; Tomko, R.J.; Sakata, E.
Deposited on : 2018-03-05
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

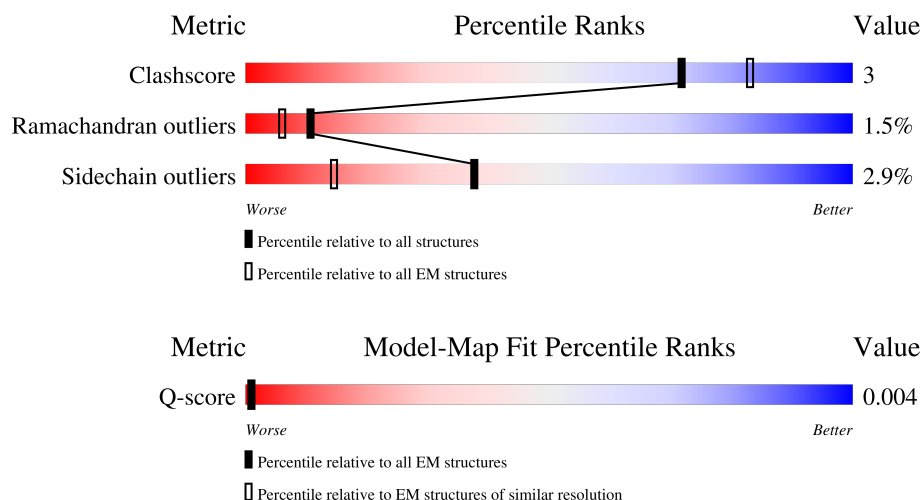
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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

Mol	Chain	Length	Quality of chain
1	A	242	29% 43% 49% 8%
1	a	242	67% 52% 45% .
2	B	249	42% 52% 47% .
2	b	249	67% 50% 47% .

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Mol	Chain	Length	Quality of chain
3	C	244	
3	c	244	
4	D	251	
4	d	251	
5	E	249	
5	e	249	
6	F	231	
6	f	231	
7	G	242	
7	g	242	
8	1	196	
8	h	196	
9	2	226	
9	i	226	
10	3	204	
10	j	204	
11	4	195	
11	k	195	
12	5	212	
12	l	212	
13	6	222	
13	m	222	
14	7	232	
14	n	232	
15	W	197	

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Mol	Chain	Length	Quality of chain
16	V	289	
17	T	266	
18	X	127	
19	Y	89	
20	Z	970	
21	N	922	
22	S	475	
23	P	440	
24	Q	434	
25	R	405	
26	U	304	
27	O	388	
28	H	426	
29	I	384	
30	K	394	
31	L	388	
32	M	421	
33	J	405	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	ATP	H	501	-	-	X	-
34	ATP	I	501	-	-	X	-
34	ATP	K	501	-	-	X	-
34	ATP	M	501	-	-	X	-
36	ADP	J	501	-	-	X	-

2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 110592 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	242	Total	C	N	O	S	0	0
			1913	1217	321	367	8		
1	A	242	Total	C	N	O	S	0	0
			1913	1217	321	367	8		

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	249	Total	C	N	O	S	0	0
			1907	1214	314	376	3		
2	B	249	Total	C	N	O	S	0	0
			1907	1214	314	376	3		

- Molecule 3 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	244	Total	C	N	O	S	0	0
			1905	1201	321	380	3		
3	C	244	Total	C	N	O	S	0	0
			1905	1201	321	380	3		

- Molecule 4 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	251	Total	C	N	O	S	0	0
			1982	1235	350	393	4		
4	D	237	Total	C	N	O	S	0	0
			1859	1164	325	366	4		

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	249	Total	C	N	O	S	0	0
			1926	1204	324	391	7		
5	E	249	Total	C	N	O	S	0	0
			1926	1204	324	391	7		

- Molecule 6 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		
6	F	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		

- Molecule 7 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	242	Total	C	N	O	S	0	0
			1886	1199	328	355	4		
7	G	242	Total	C	N	O	S	0	0
			1886	1199	328	355	4		

- Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		
8	1	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	226	Total	C	N	O	S	0	0
			1720	1082	298	333	7		
9	2	226	Total	C	N	O	S	0	0
			1720	1082	298	333	7		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	195	Total	C	N	O	S	0	0
			1562	992	264	300	6		
11	4	195	Total	C	N	O	S	0	0
			1562	992	264	300	6		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
12	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
13	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	232	Total	C	N	O	S	0	0
			1816	1148	311	350	7		
14	7	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		

- Molecule 15 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	197	Total	C	N	O	S	0	0
			1535	962	269	301	3		

- Molecule 16 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

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

- Molecule 17 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	266	Total	C	N	O	S	0	0
			2193	1405	349	433	6		

- Molecule 18 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	127	Total	C	N	O	S	0	0
			1033	664	169	196	4		

- Molecule 19 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y	89	Total	C	N	O	S	0	0
			731	447	119	164	1		

- Molecule 20 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	906	Total	C	N	O	S	0	0
			7006	4416	1150	1410	30		

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	922	Total	C	N	O	S	0	0
			7158	4536	1205	1389	28		

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	475	Total	C	N	O	S	0	0
			3895	2488	653	739	15		

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	440	Total	C	N	O	S	0	0
			3609	2297	604	698	10		

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN6.

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

- Molecule 25 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	405	Total	C	N	O	S	0	0
			3259	2077	535	637	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	304	Total	C	N	O	S	0	0
			2427	1529	414	477	7		

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN9.

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

- Molecule 28 is a protein called 26S proteasome regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	H	426	Total	C	N	O	S	0	0
			3313	2056	592	648	17		

- Molecule 29 is a protein called 26S proteasome regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	I	384	Total	C	N	O	S	0	0
			3015	1895	507	596	17		

- Molecule 30 is a protein called 26S proteasome regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	K	394	Total	C	N	O	S	0	0
			3113	1951	548	604	10		

- Molecule 31 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L	388	Total	C	N	O	S	0	0
			3083	1942	548	581	12		

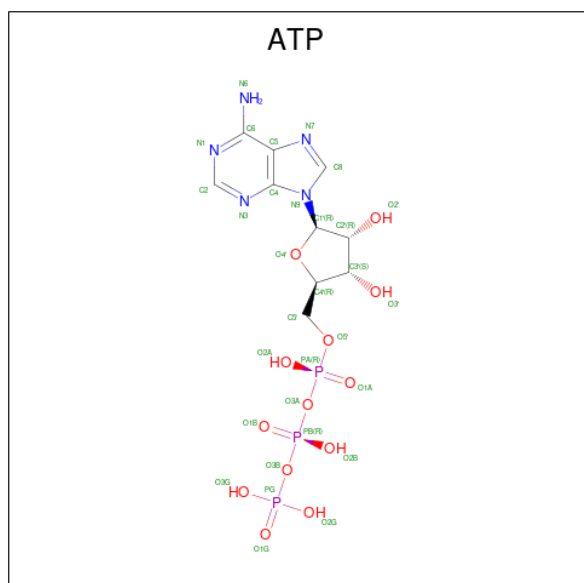
- Molecule 32 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	421	Total	C	N	O	S	0	0
			3285	2043	573	656	13		

- Molecule 33 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	405	Total	C	N	O	S	0	0
			3171	1995	565	593	18		

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



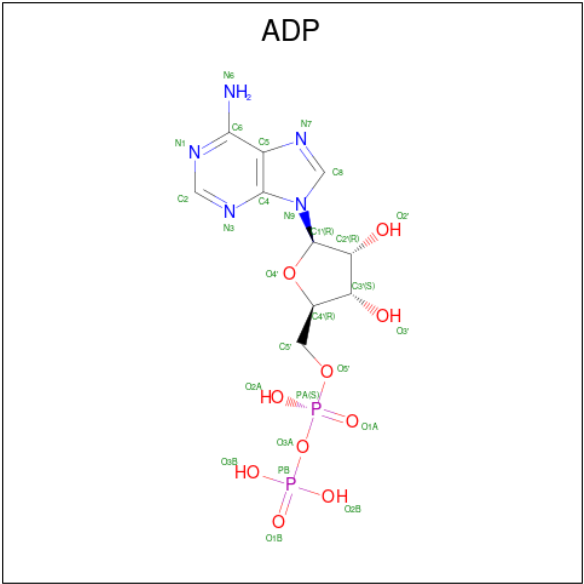
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Mol	Chain	Residues	Atoms					AltConf
34	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	H	1	Total	Mg	0
			1	1	
35	I	1	Total	Mg	0
			1	1	
35	K	1	Total	Mg	0
			1	1	
35	L	1	Total	Mg	0
			1	1	
35	M	1	Total	Mg	0
			1	1	
35	J	1	Total	Mg	0
			1	1	

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

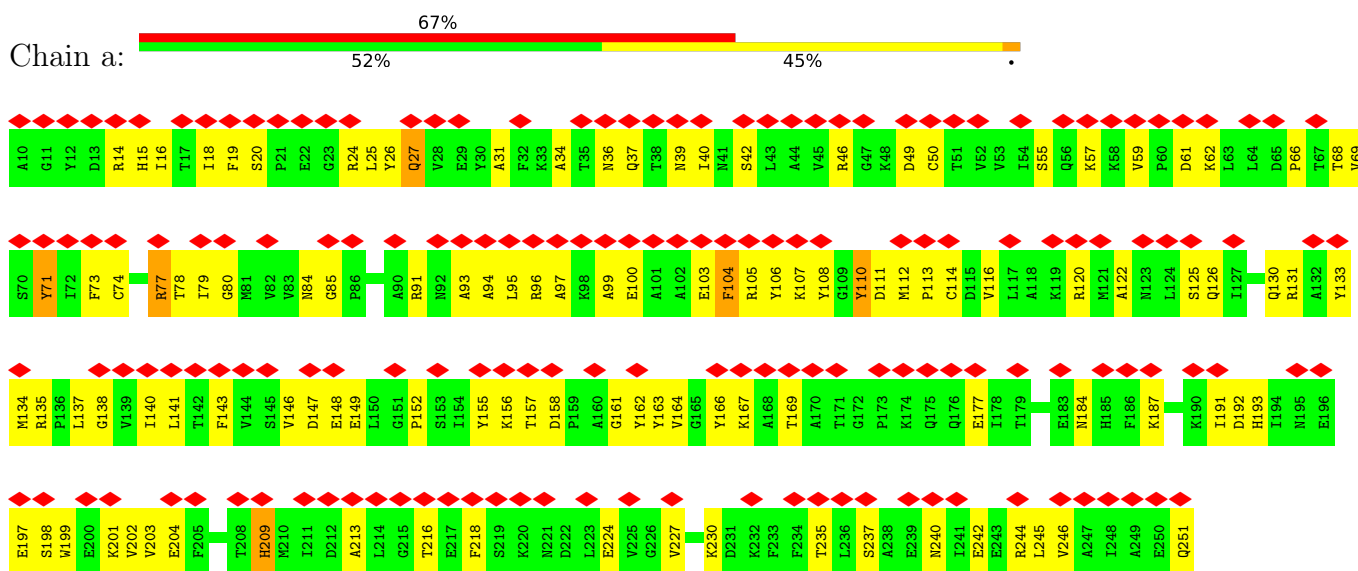


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
36	J	1	27	10	5	10	2	0

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.

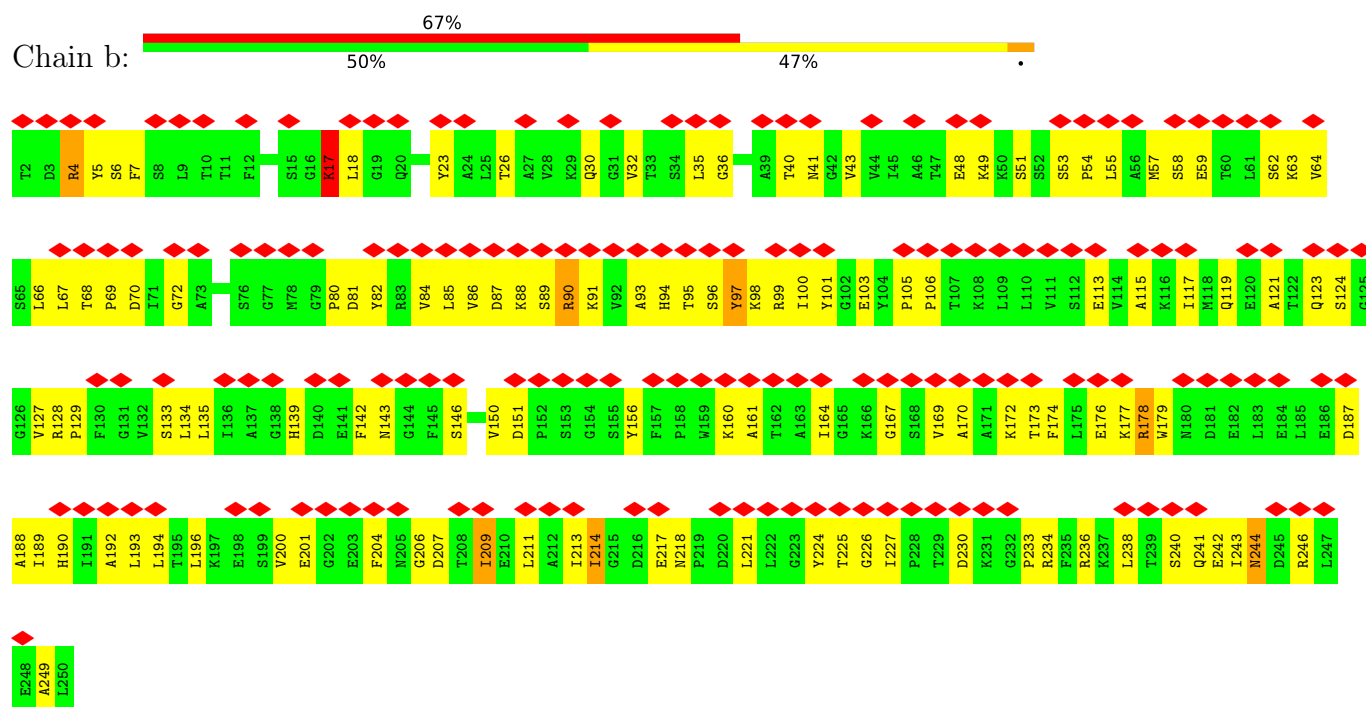
• Molecule 1: Proteasome subunit alpha type-1



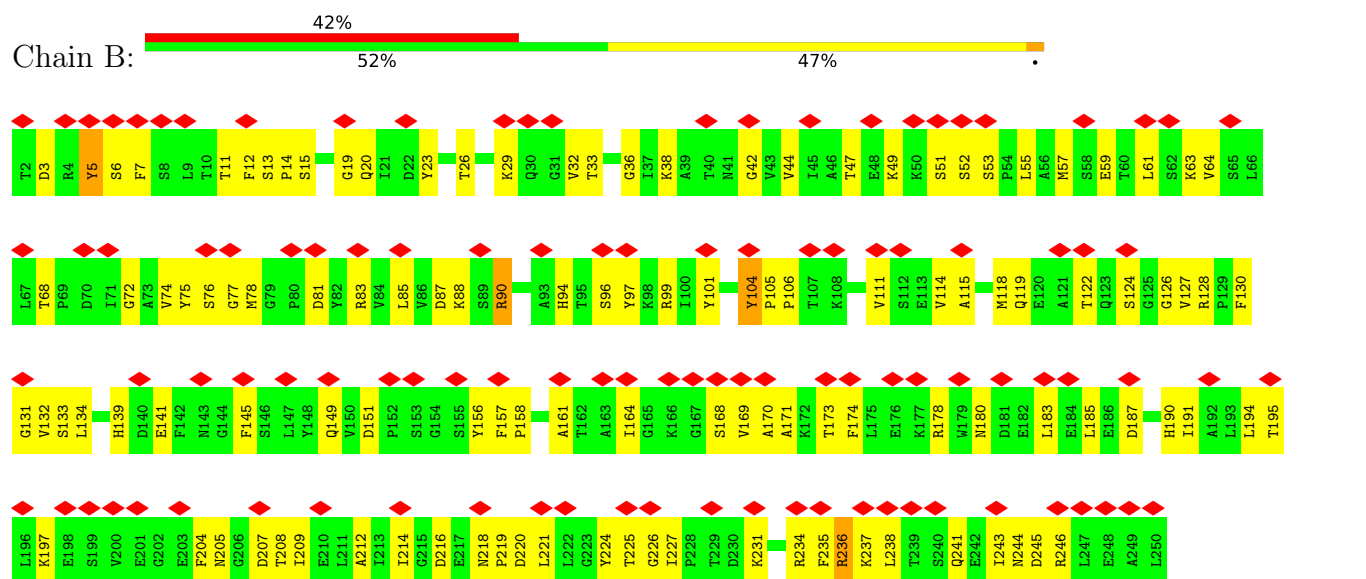
• Molecule 1: Proteasome subunit alpha type-1



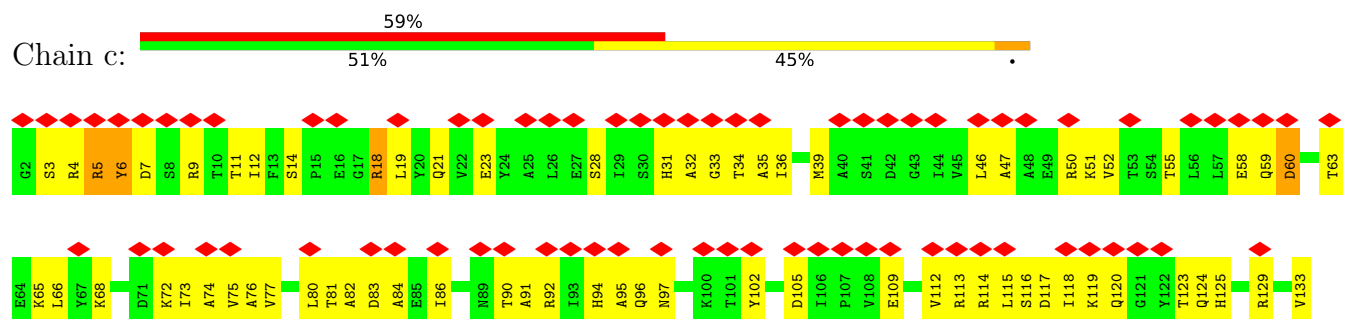
• Molecule 2: Proteasome subunit alpha type-2

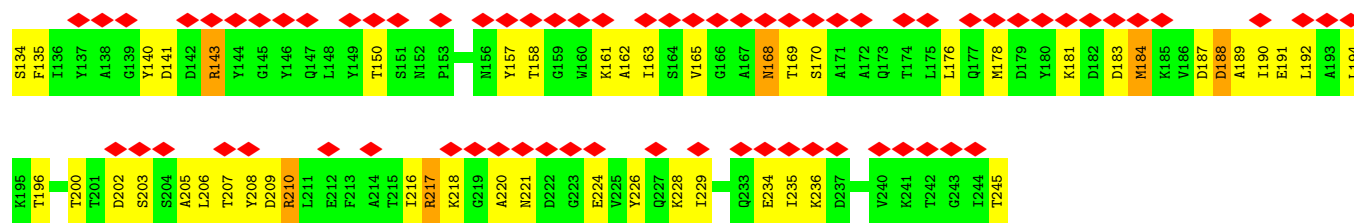


• Molecule 2: Proteasome subunit alpha type-2

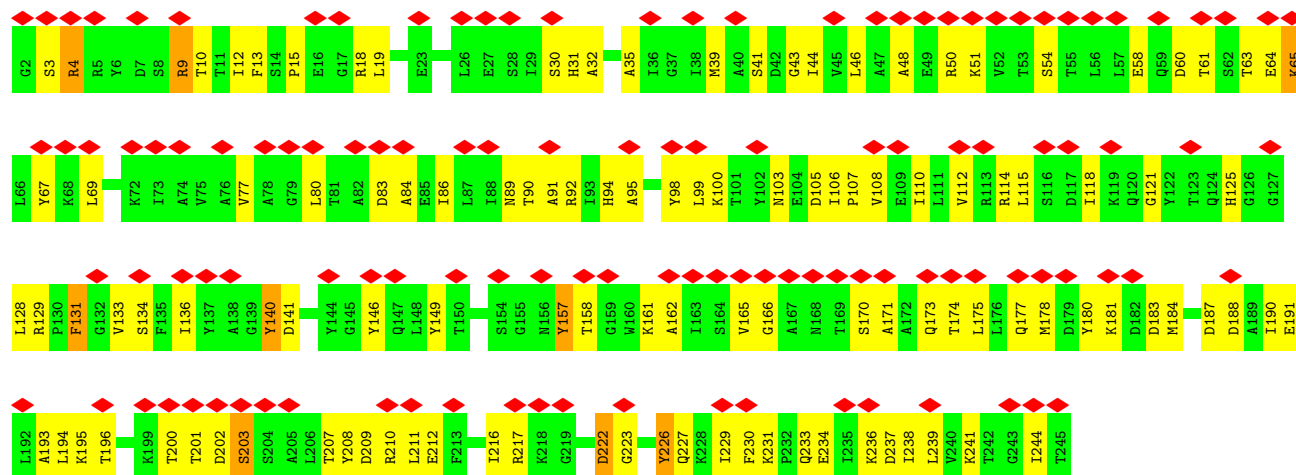


• Molecule 3: Proteasome subunit alpha type-3

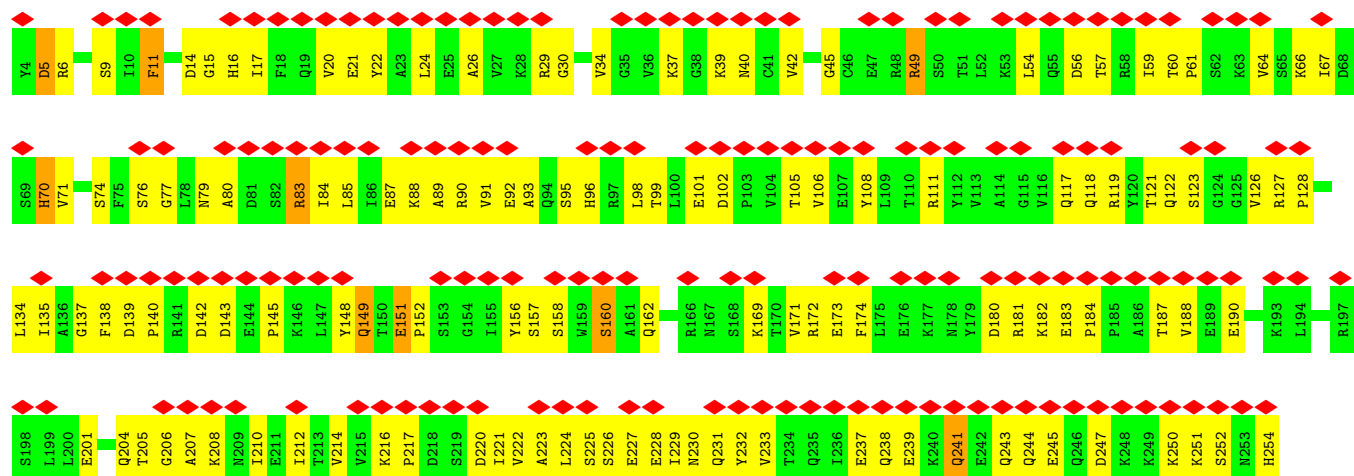




• Molecule 3: Proteasome subunit alpha type-3

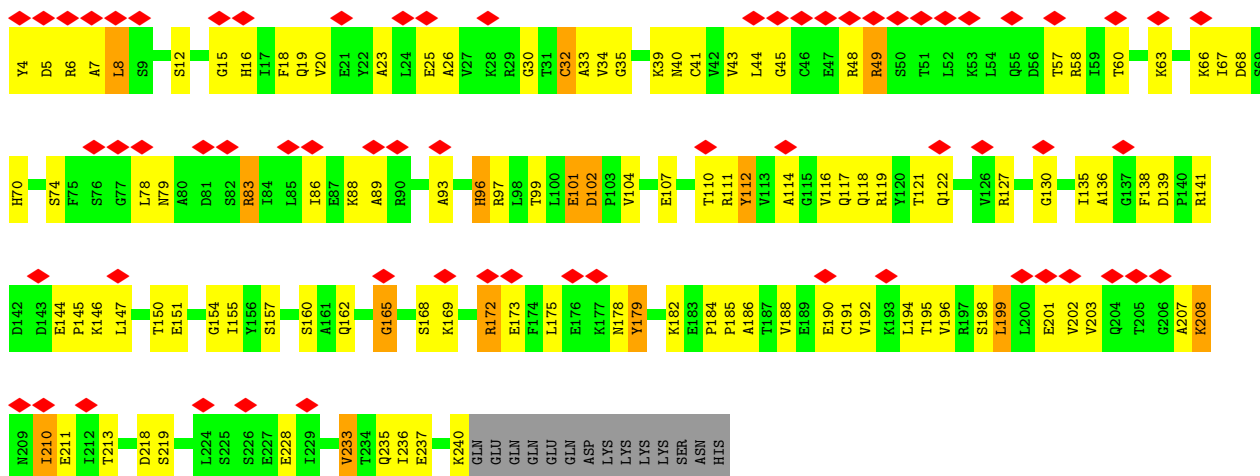


• Molecule 4: Proteasome subunit alpha type-4

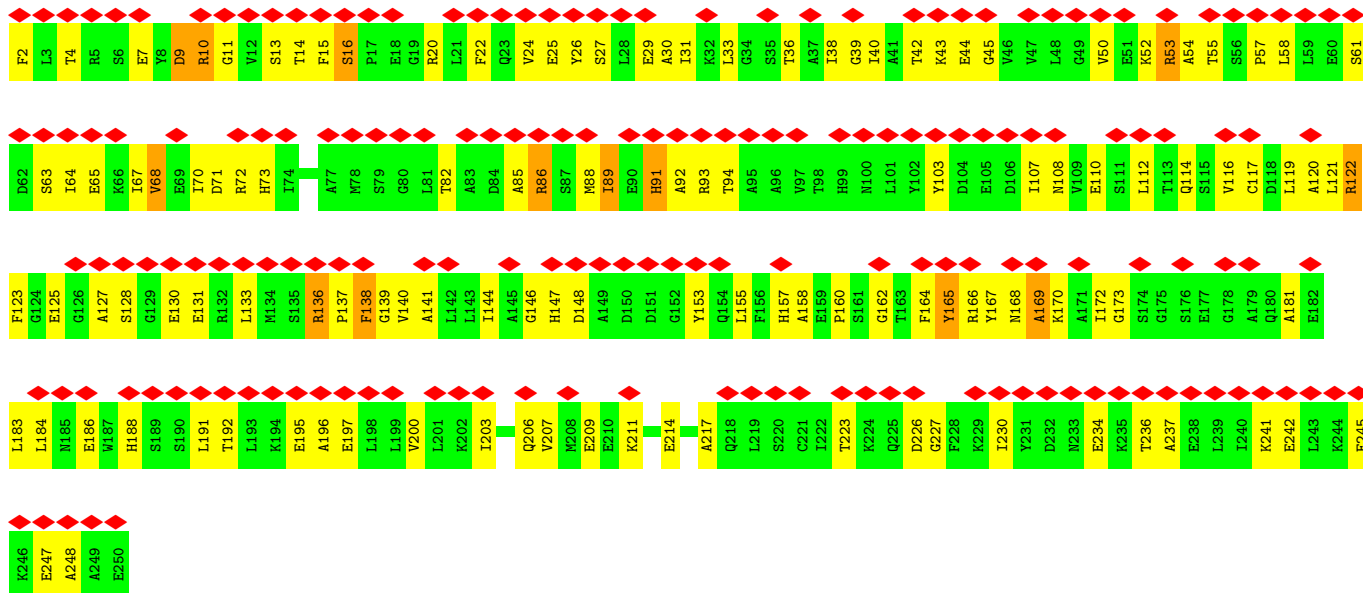


• Molecule 4: Proteasome subunit alpha type-4

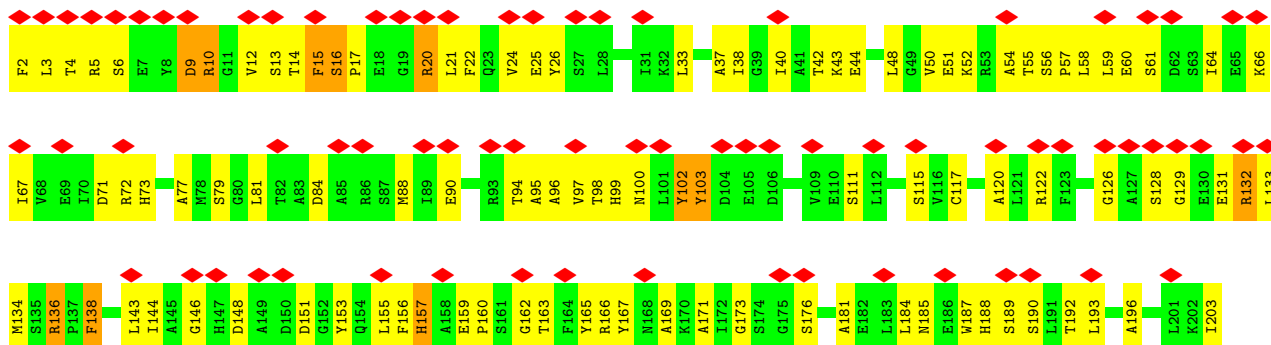


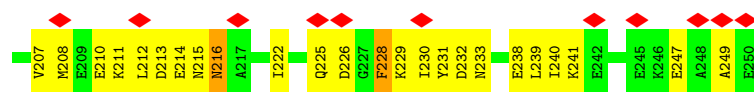


• Molecule 5: Proteasome subunit alpha type-5

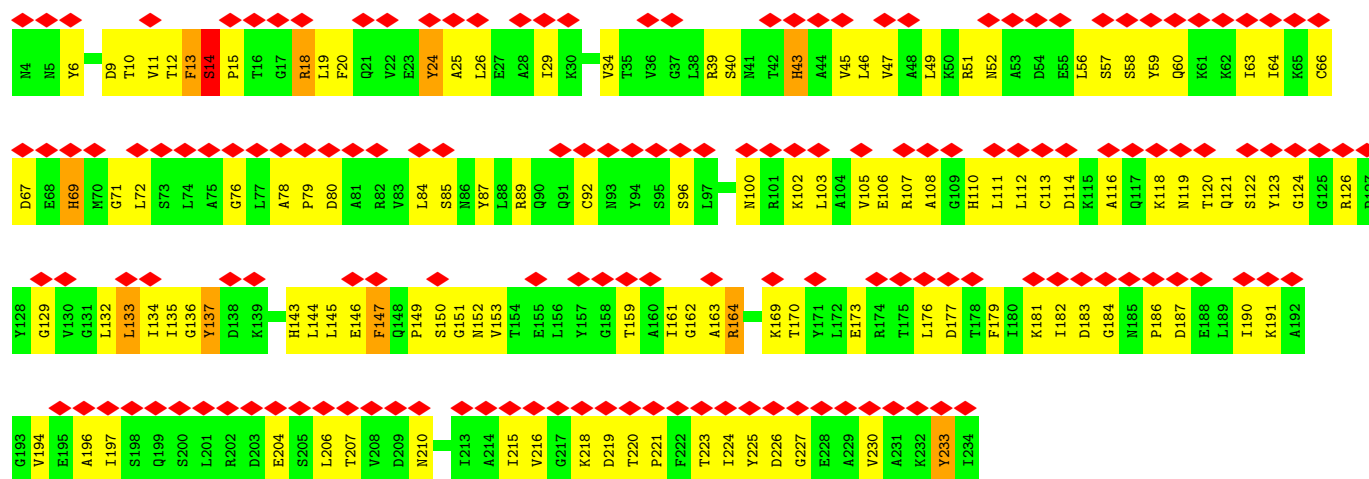


• Molecule 5: Proteasome subunit alpha type-5

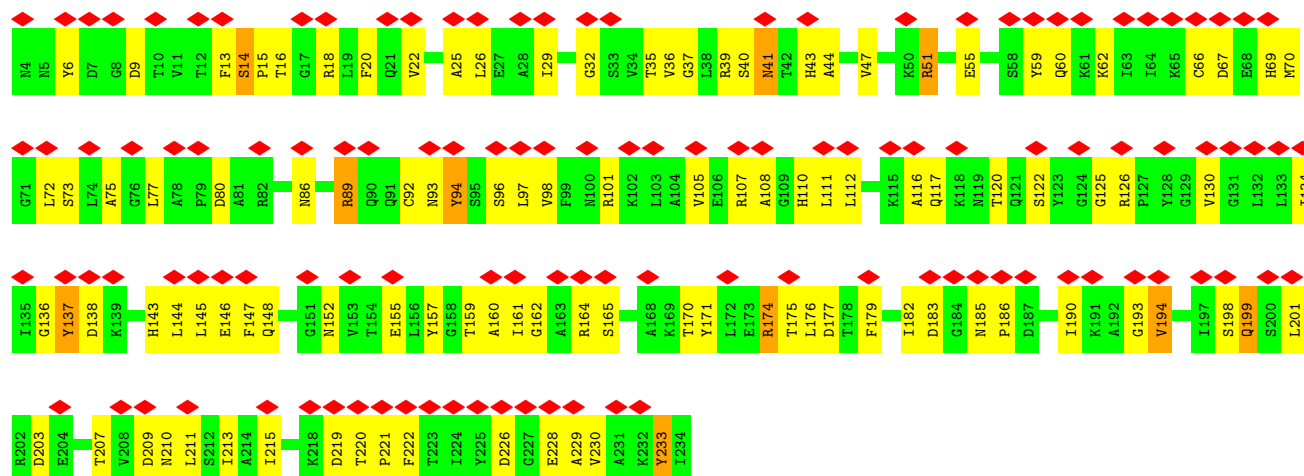




• Molecule 6: Proteasome subunit alpha type-6

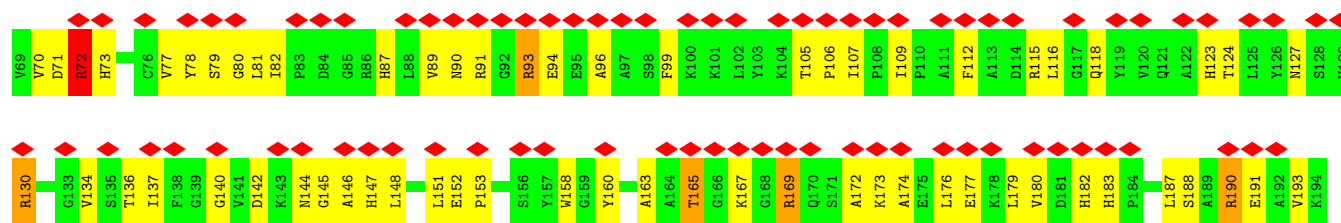


• Molecule 6: Proteasome subunit alpha type-6

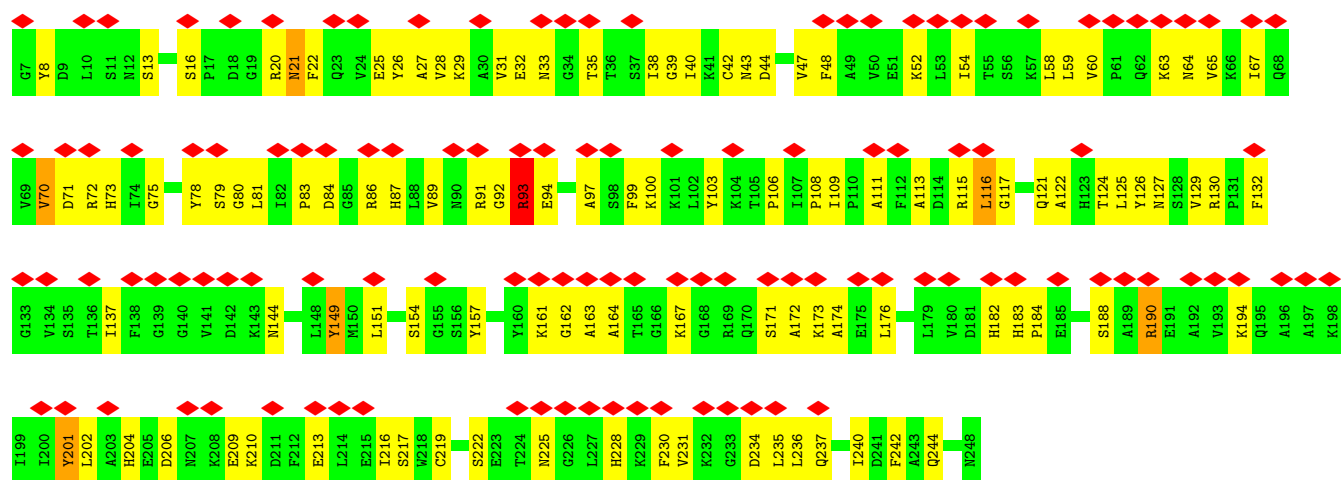


• Molecule 7: Probable proteasome subunit alpha type-7

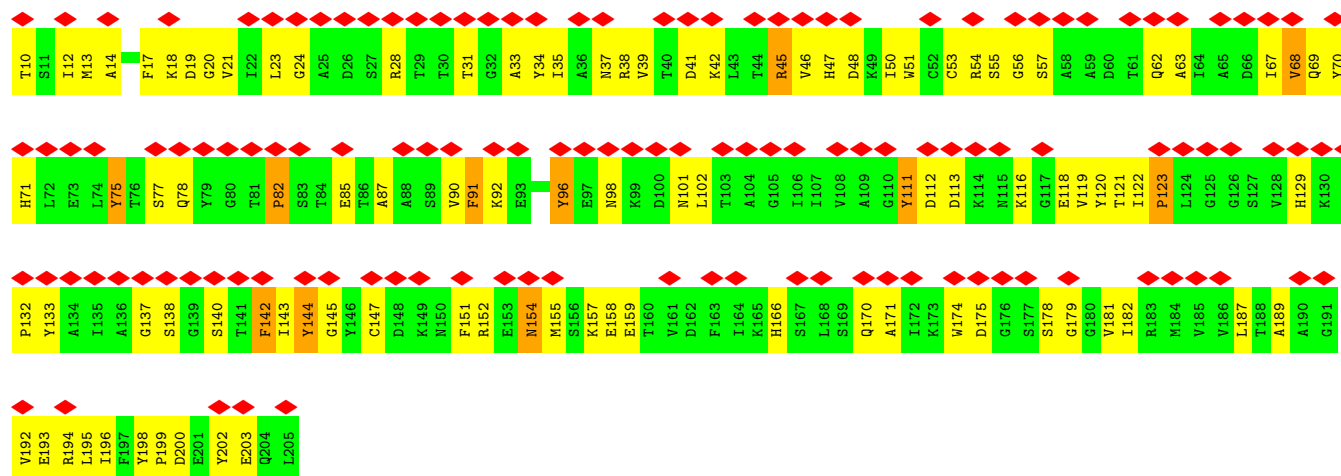




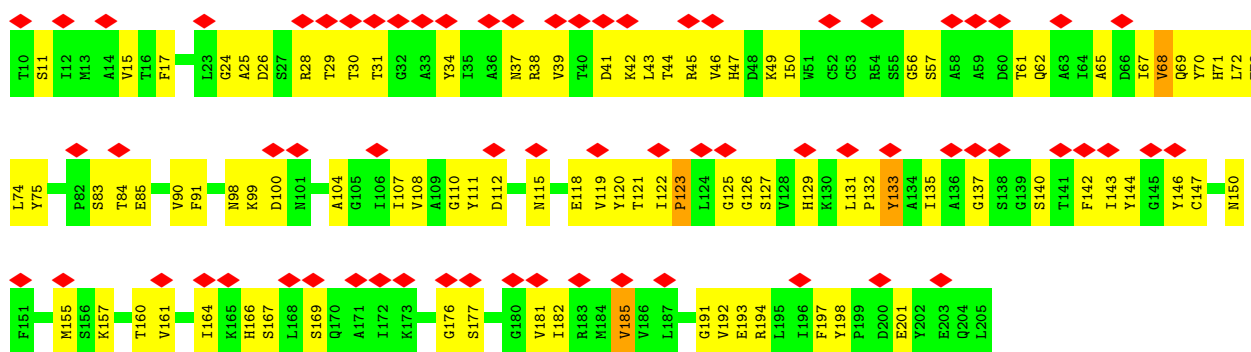
• Molecule 7: Probable proteasome subunit alpha type-7



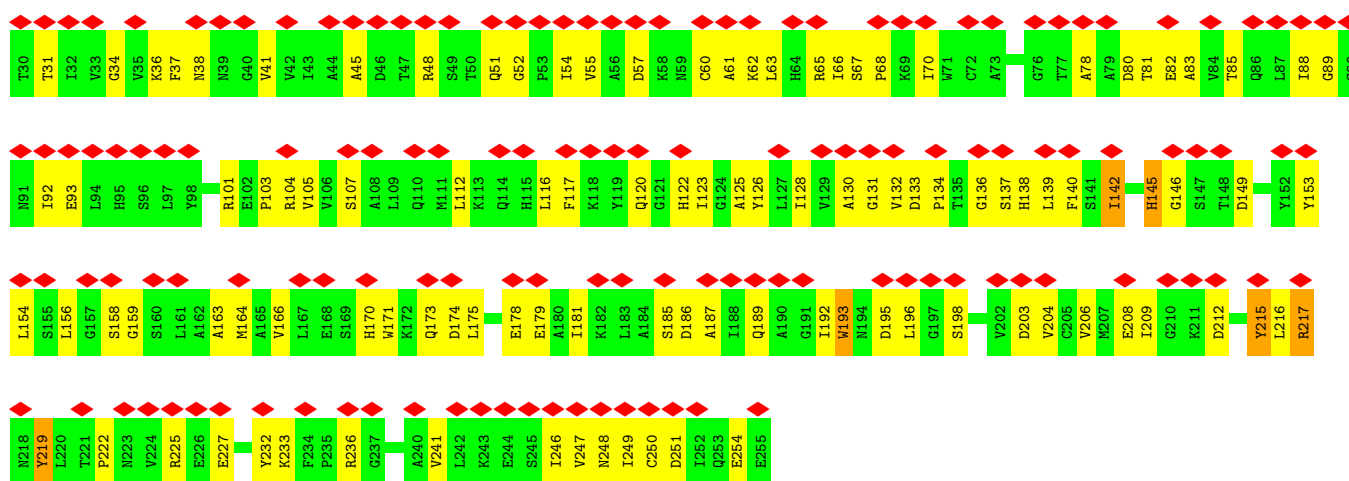
• Molecule 8: Proteasome subunit beta type-1



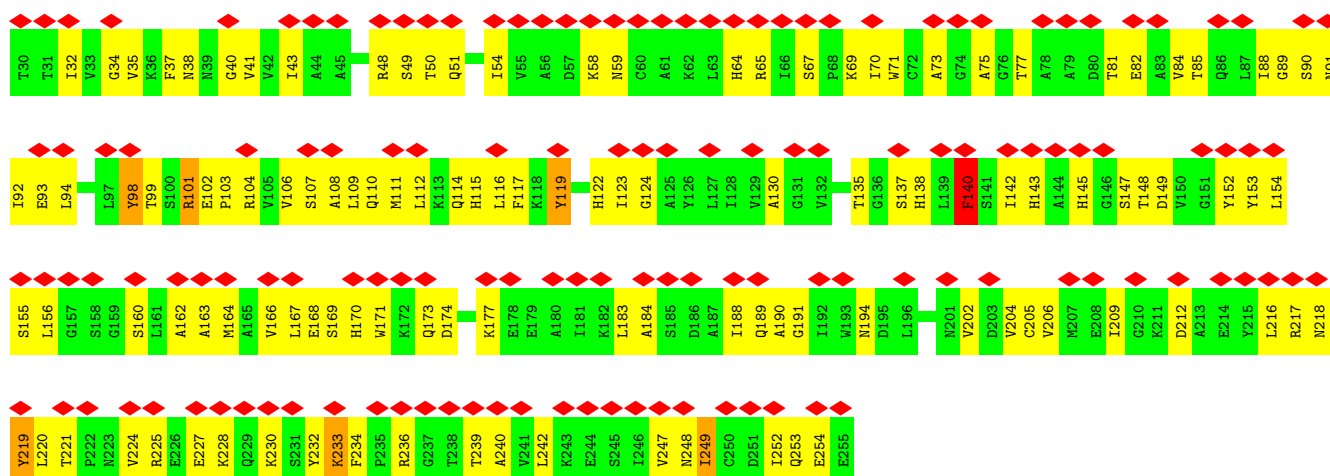
• Molecule 8: Proteasome subunit beta type-1



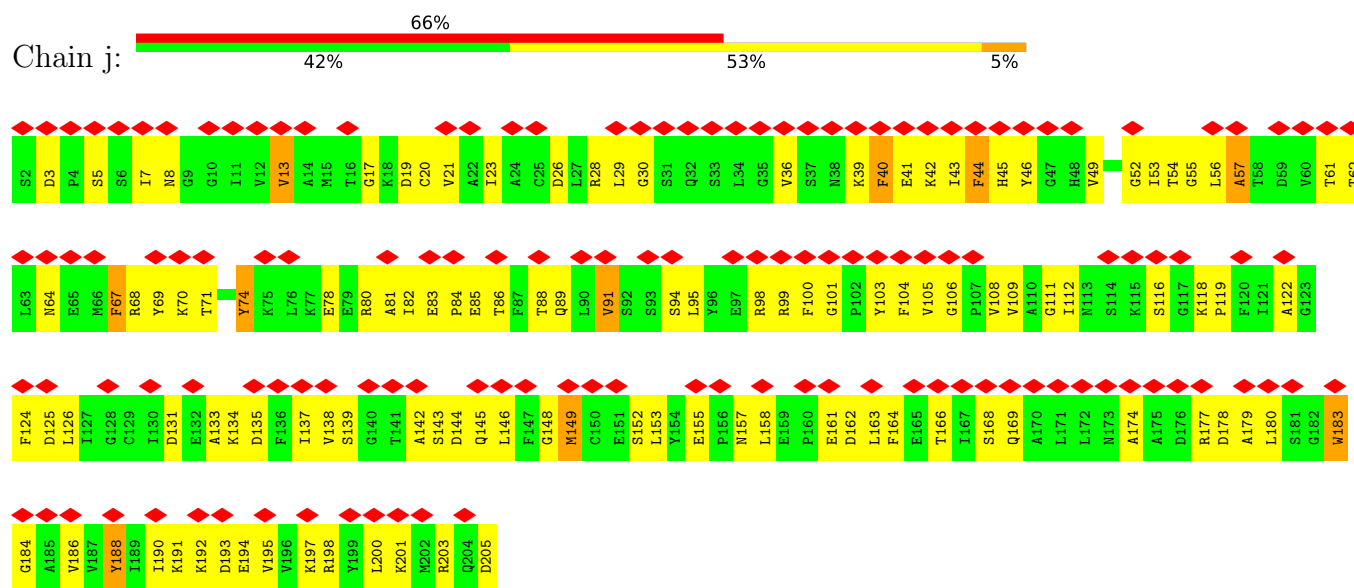
• Molecule 9: Proteasome subunit beta type-2



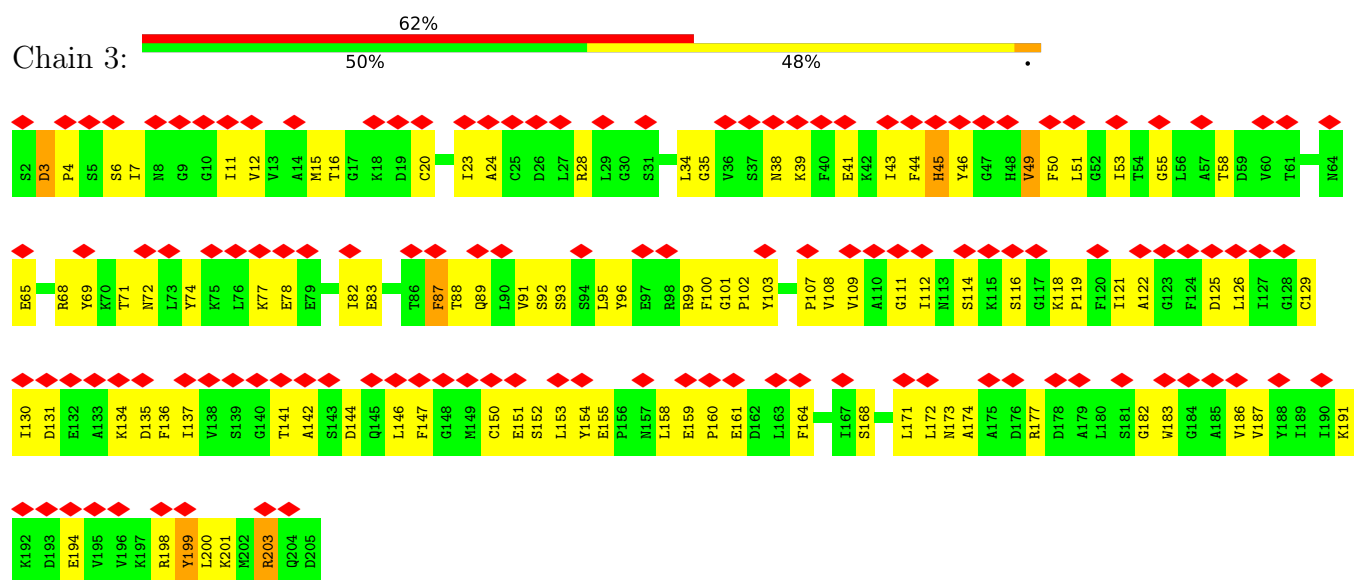
• Molecule 9: Proteasome subunit beta type-2



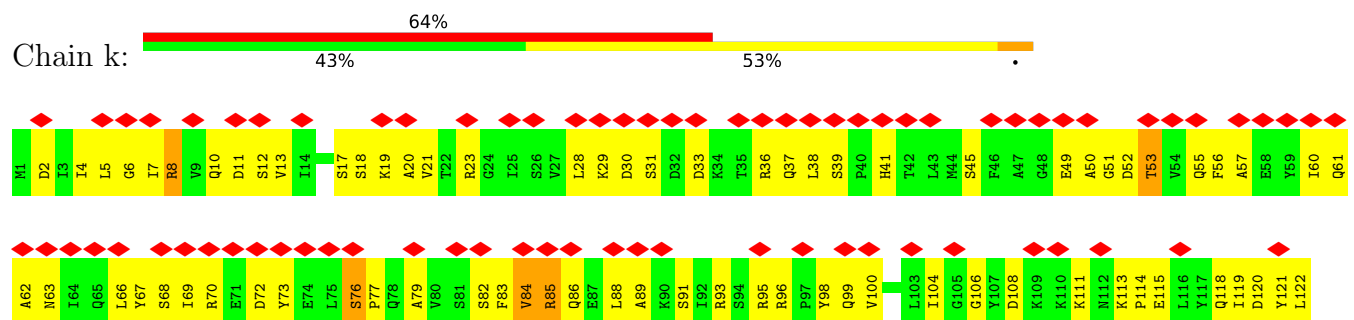
- Molecule 10: Proteasome subunit beta type-3

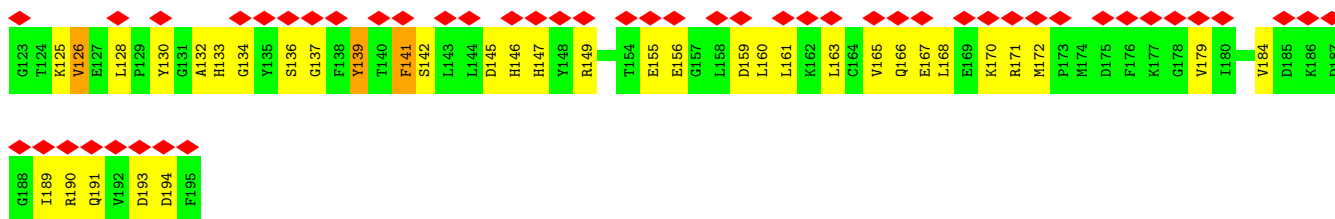


- Molecule 10: Proteasome subunit beta type-3

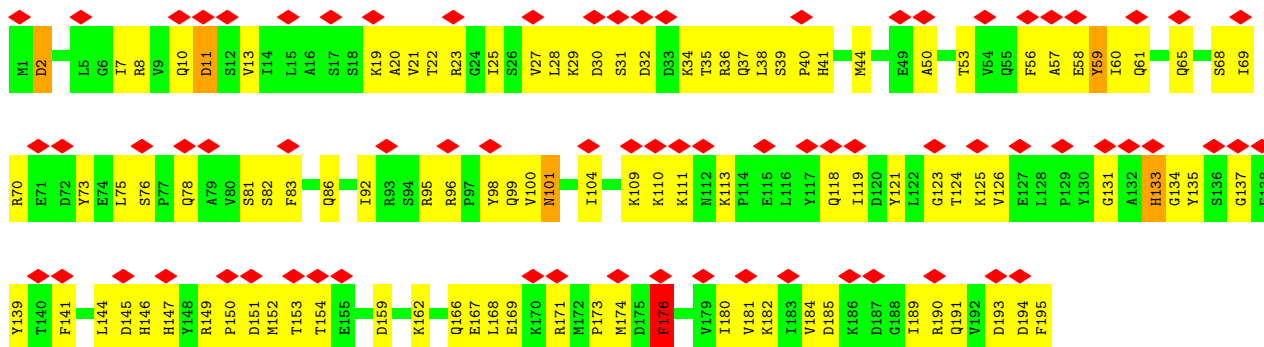


- Molecule 11: Proteasome subunit beta type-4

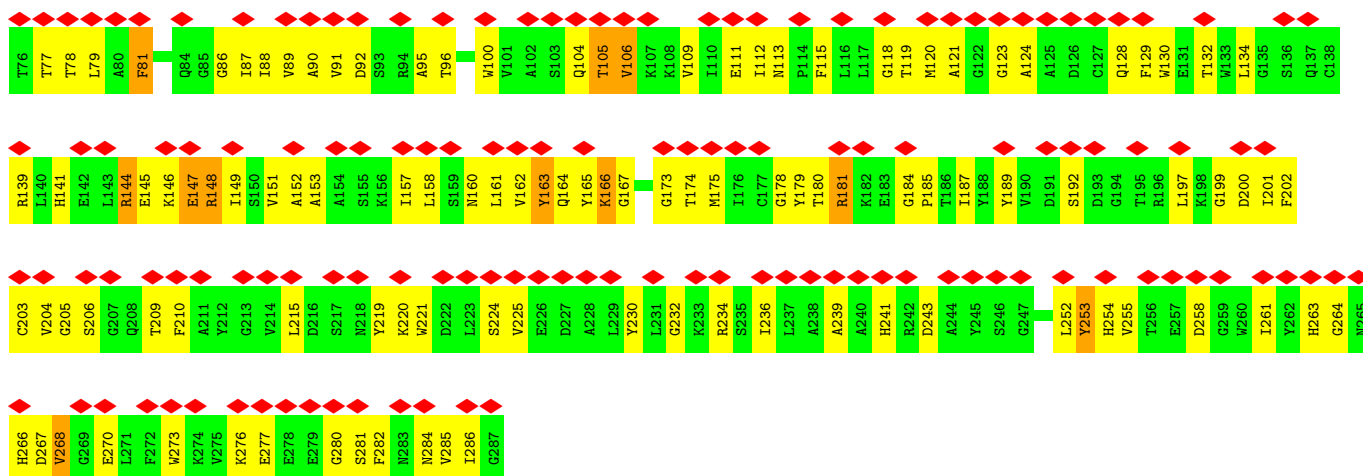




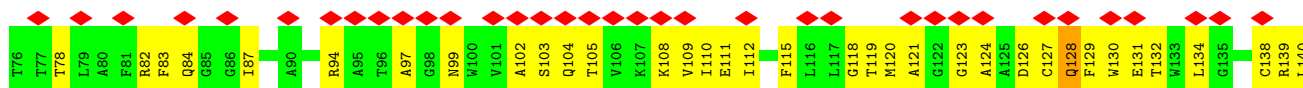
• Molecule 11: Proteasome subunit beta type-4

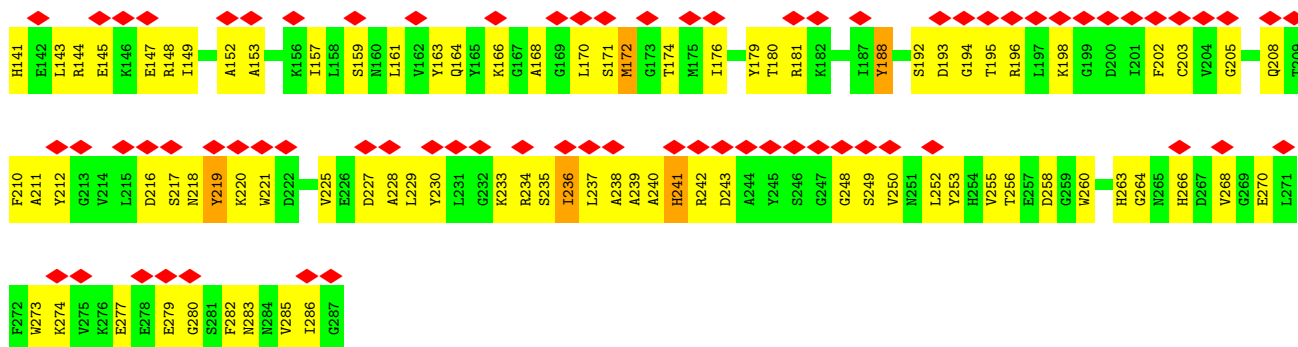


• Molecule 12: Proteasome subunit beta type-5

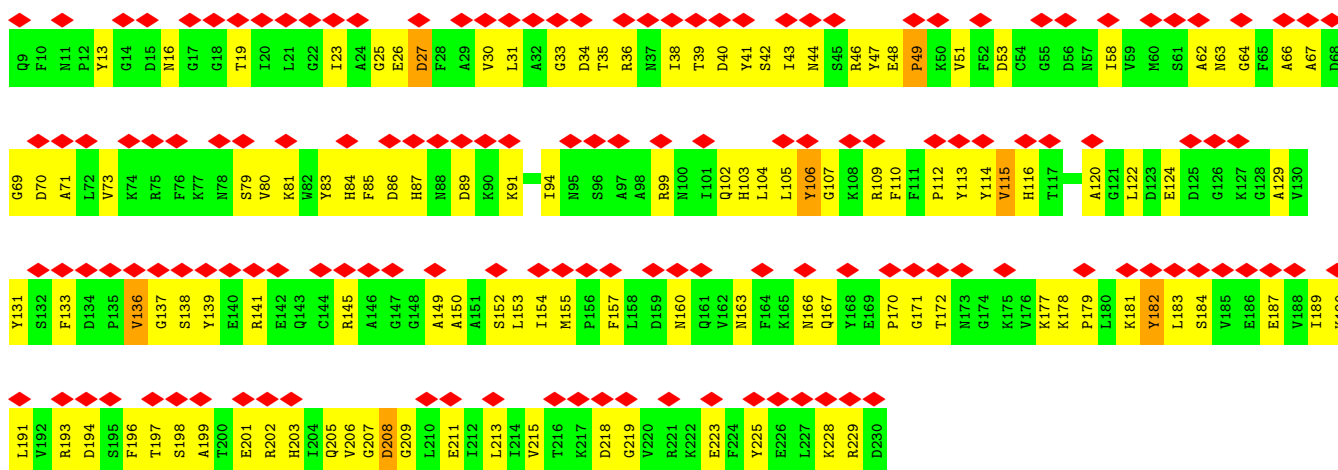


• Molecule 12: Proteasome subunit beta type-5

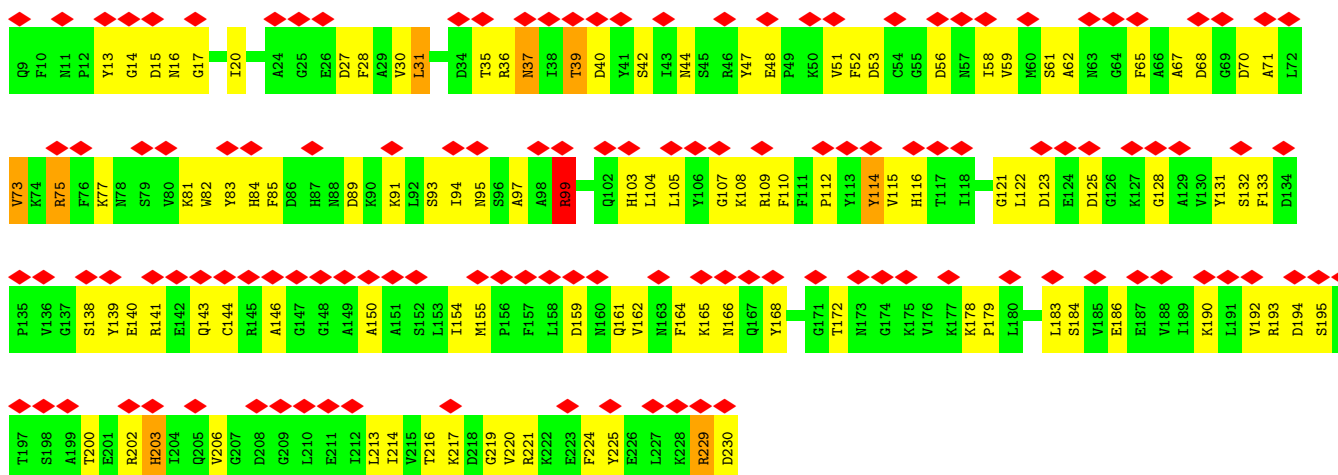




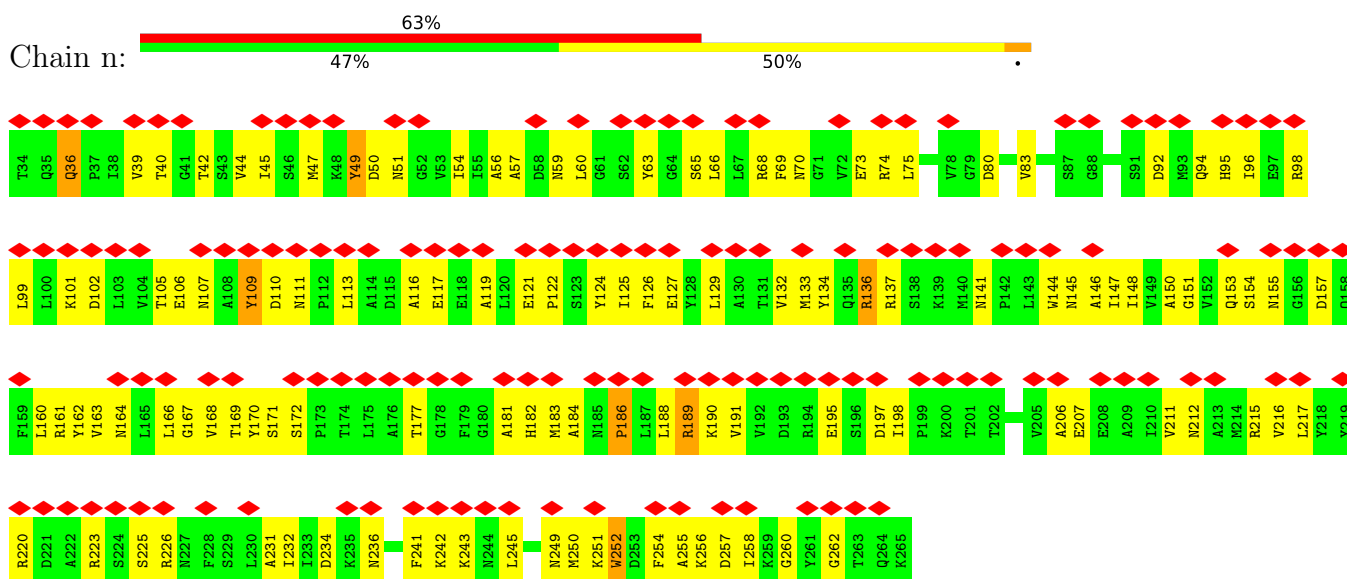
• Molecule 13: Proteasome subunit beta type-6



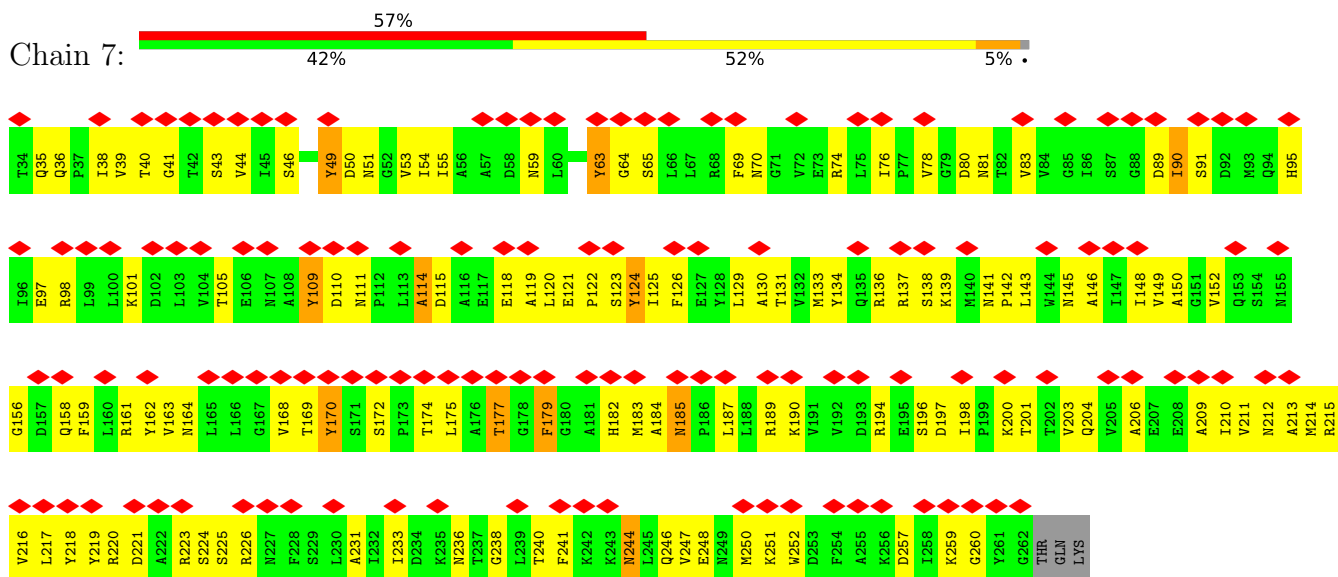
• Molecule 13: Proteasome subunit beta type-6



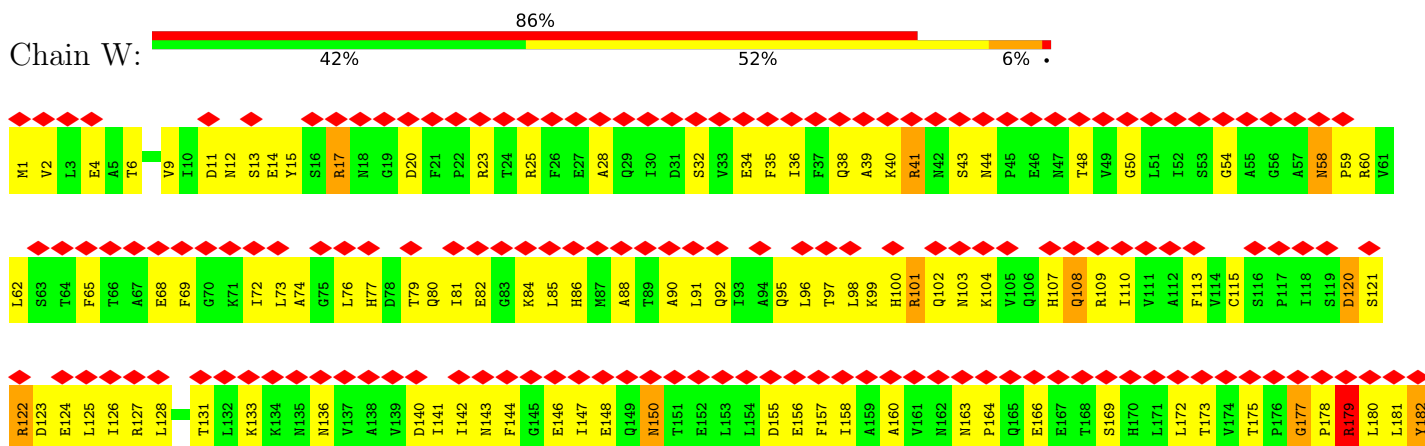
• Molecule 14: Proteasome subunit beta type-7



• Molecule 14: Proteasome subunit beta type-7

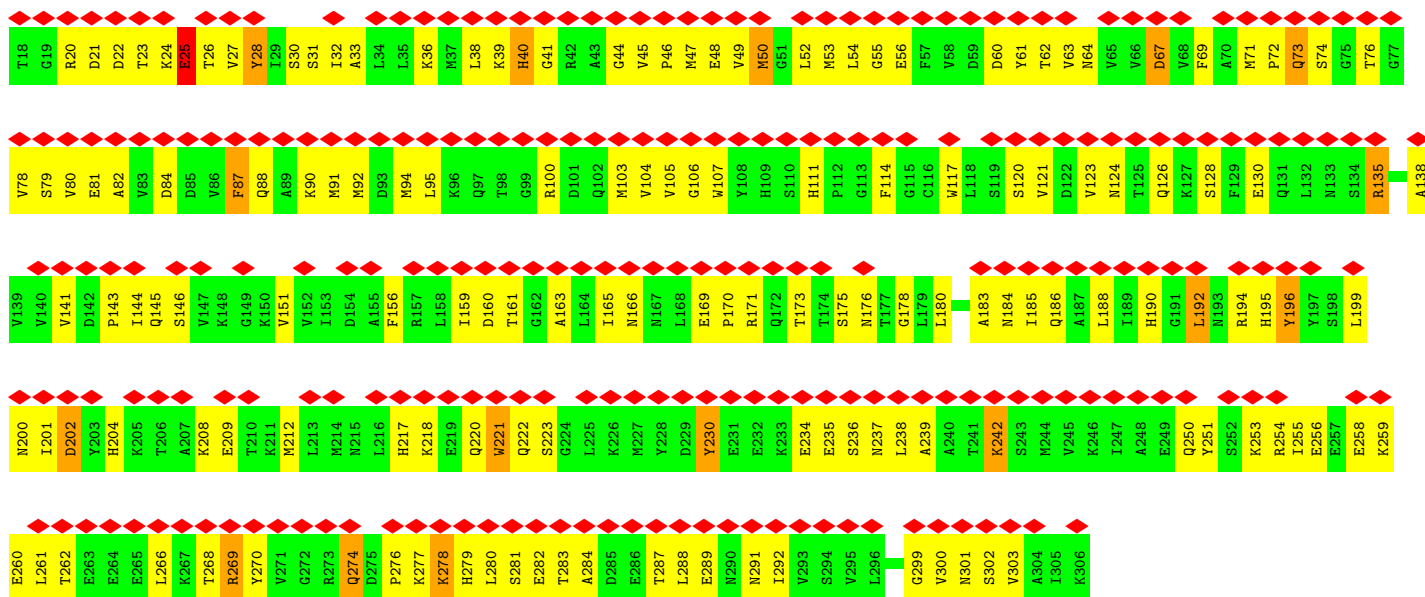
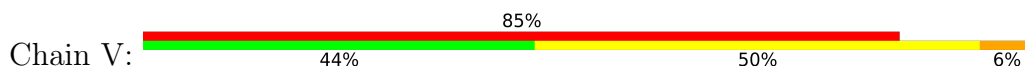


• Molecule 15: 26S proteasome regulatory subunit RPN10

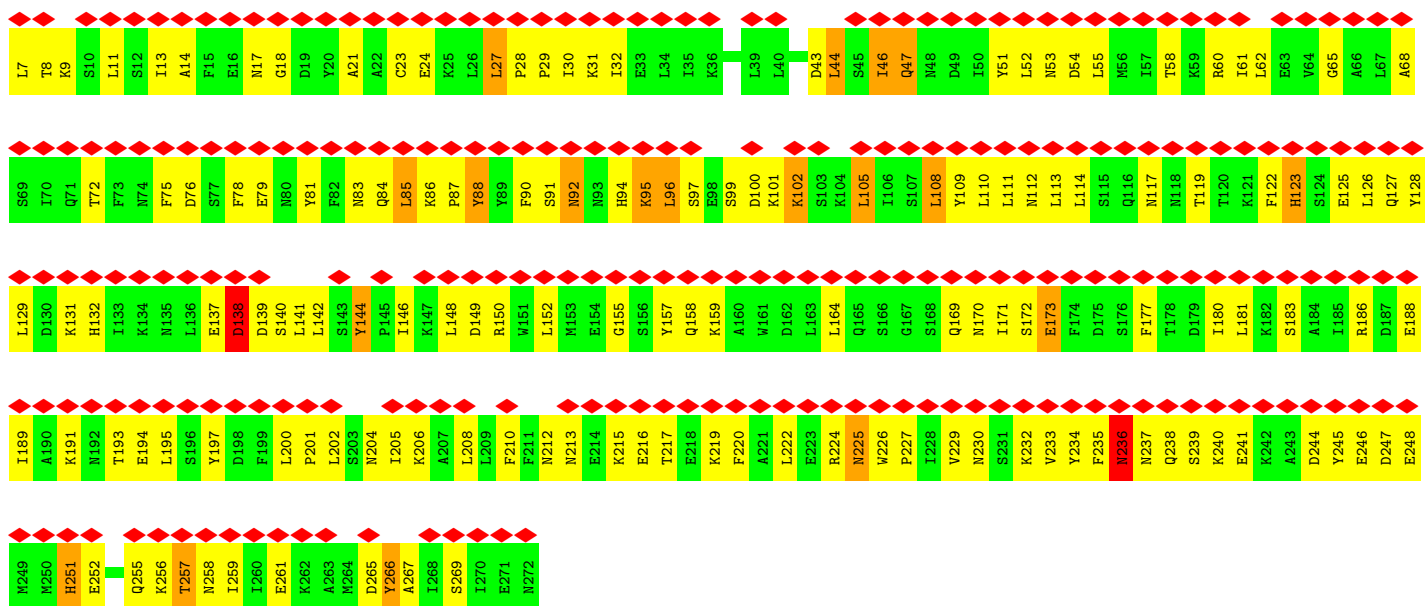
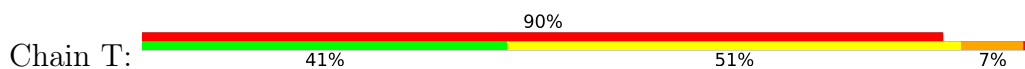




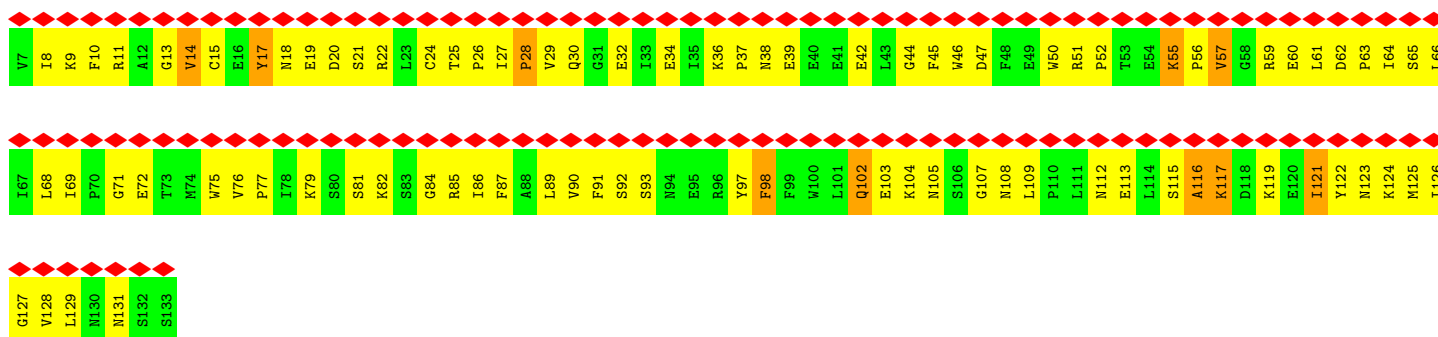
• Molecule 16: Ubiquitin carboxyl-terminal hydrolase RPN11



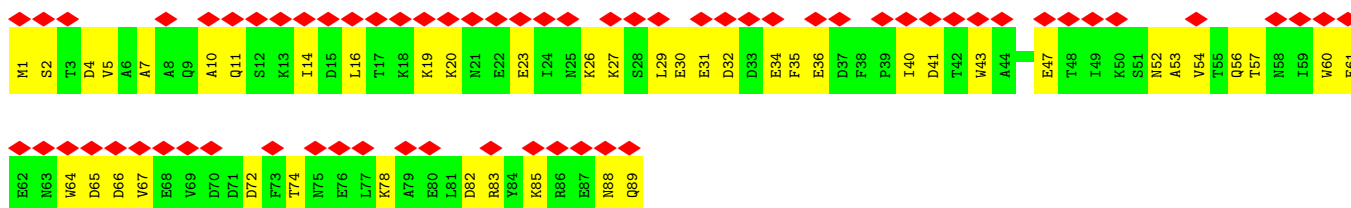
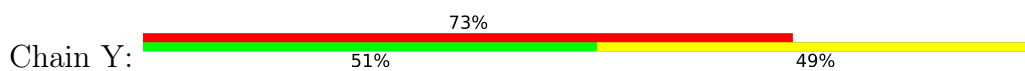
• Molecule 17: 26S proteasome regulatory subunit RPN12



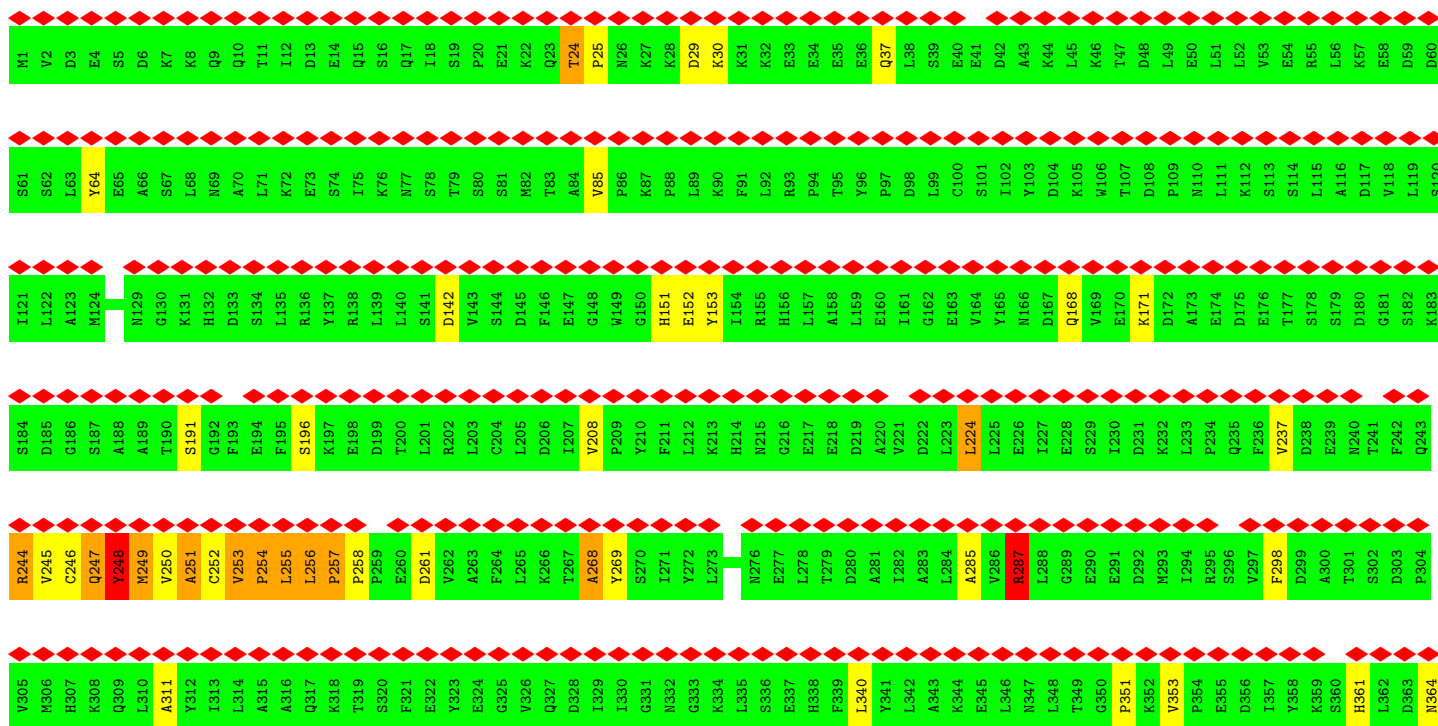
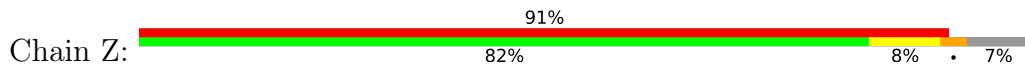
• Molecule 18: 26S proteasome regulatory subunit RPN13

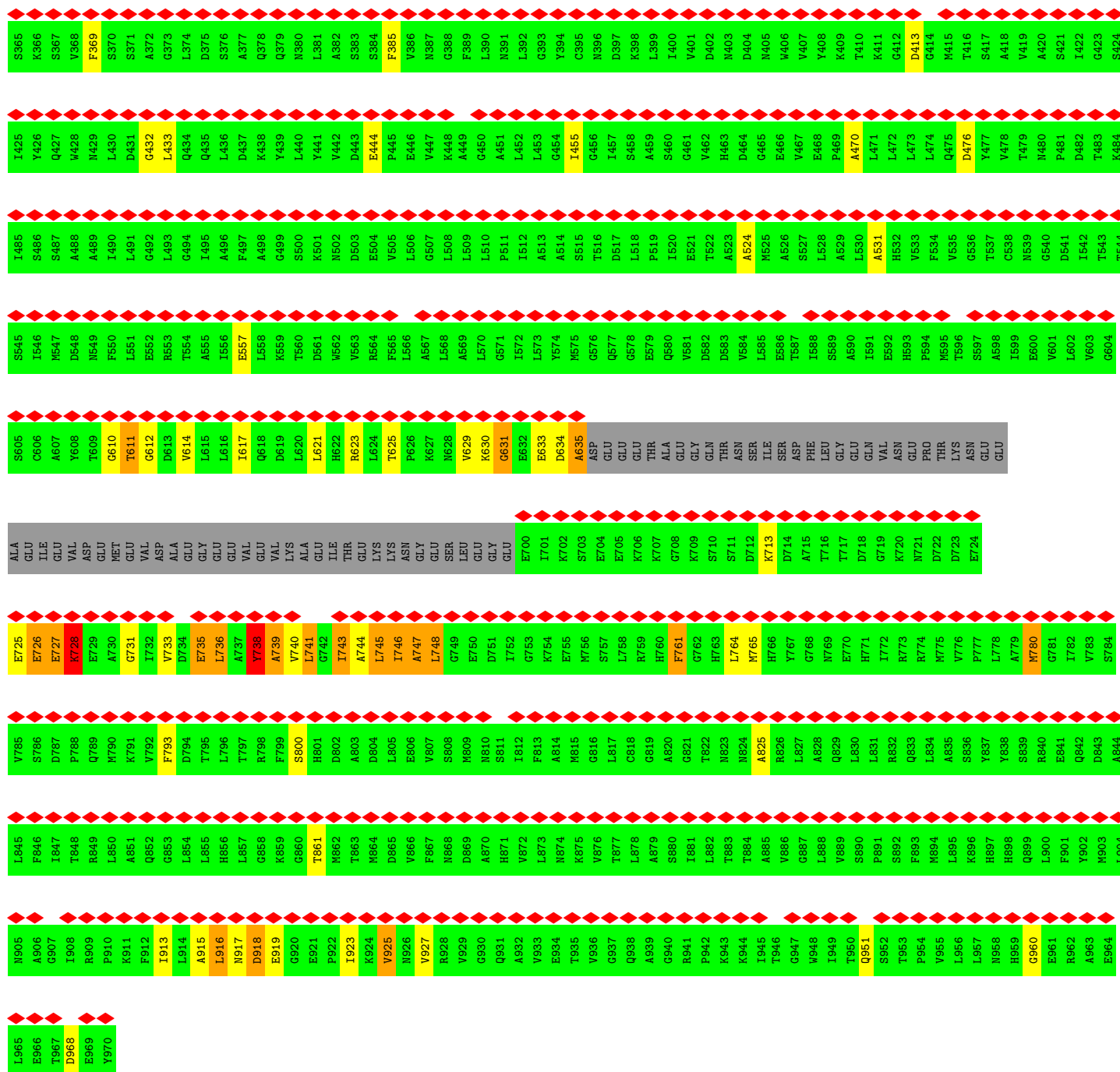


• Molecule 19: 26S proteasome complex subunit SEM1

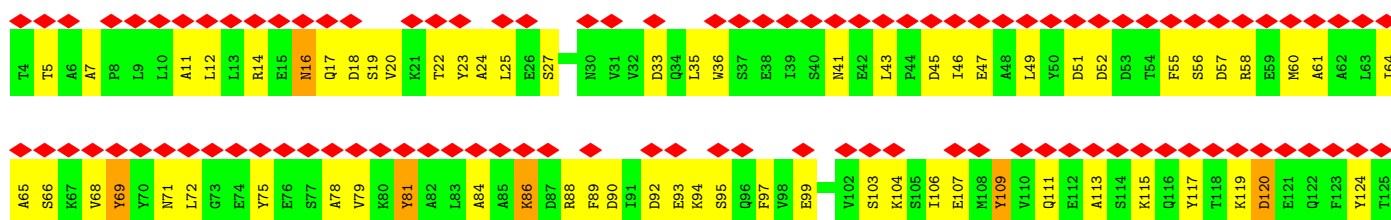
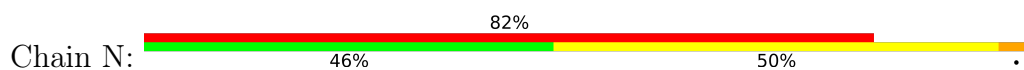


• Molecule 20: 26S proteasome regulatory subunit RPN1



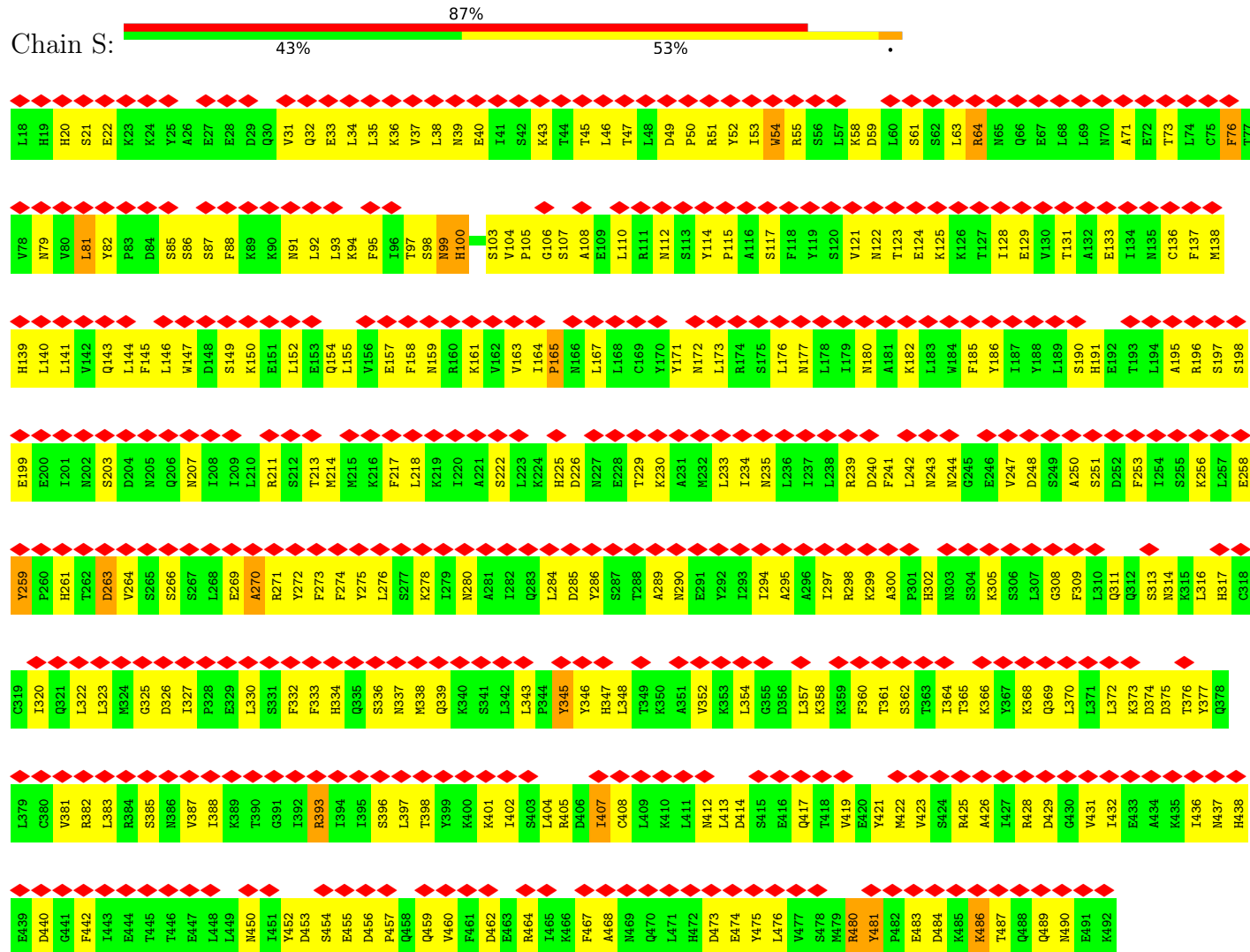


• Molecule 21: 26S proteasome regulatory subunit RPN2

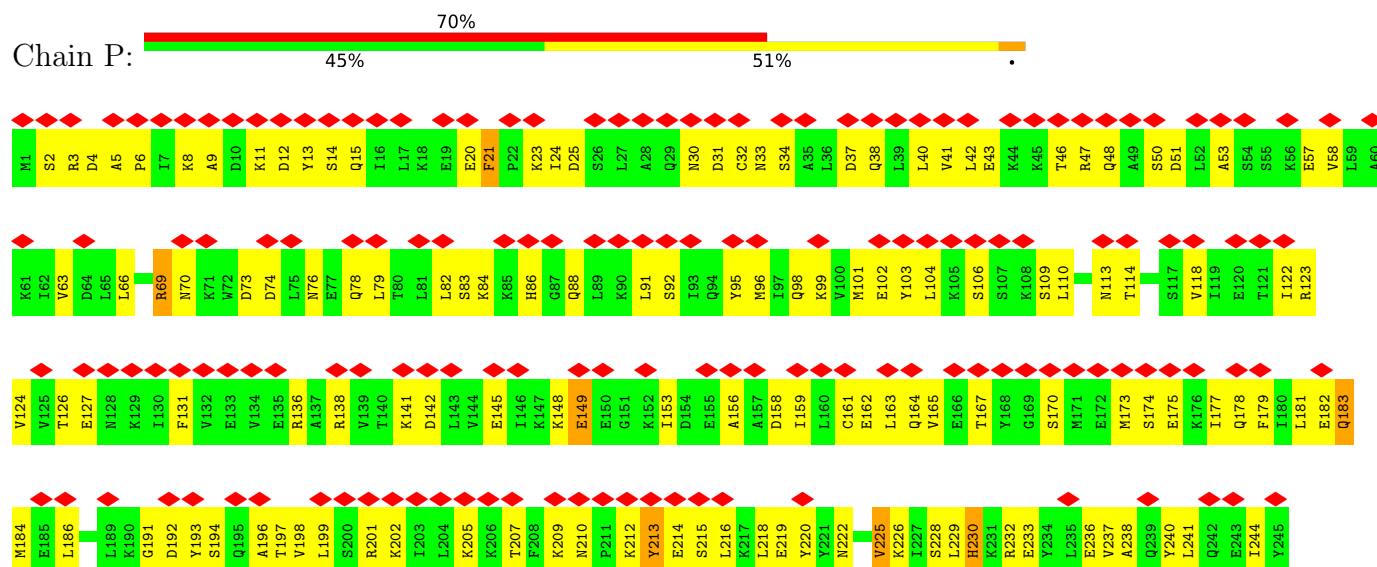




• Molecule 22: 26S proteasome regulatory subunit RPN3

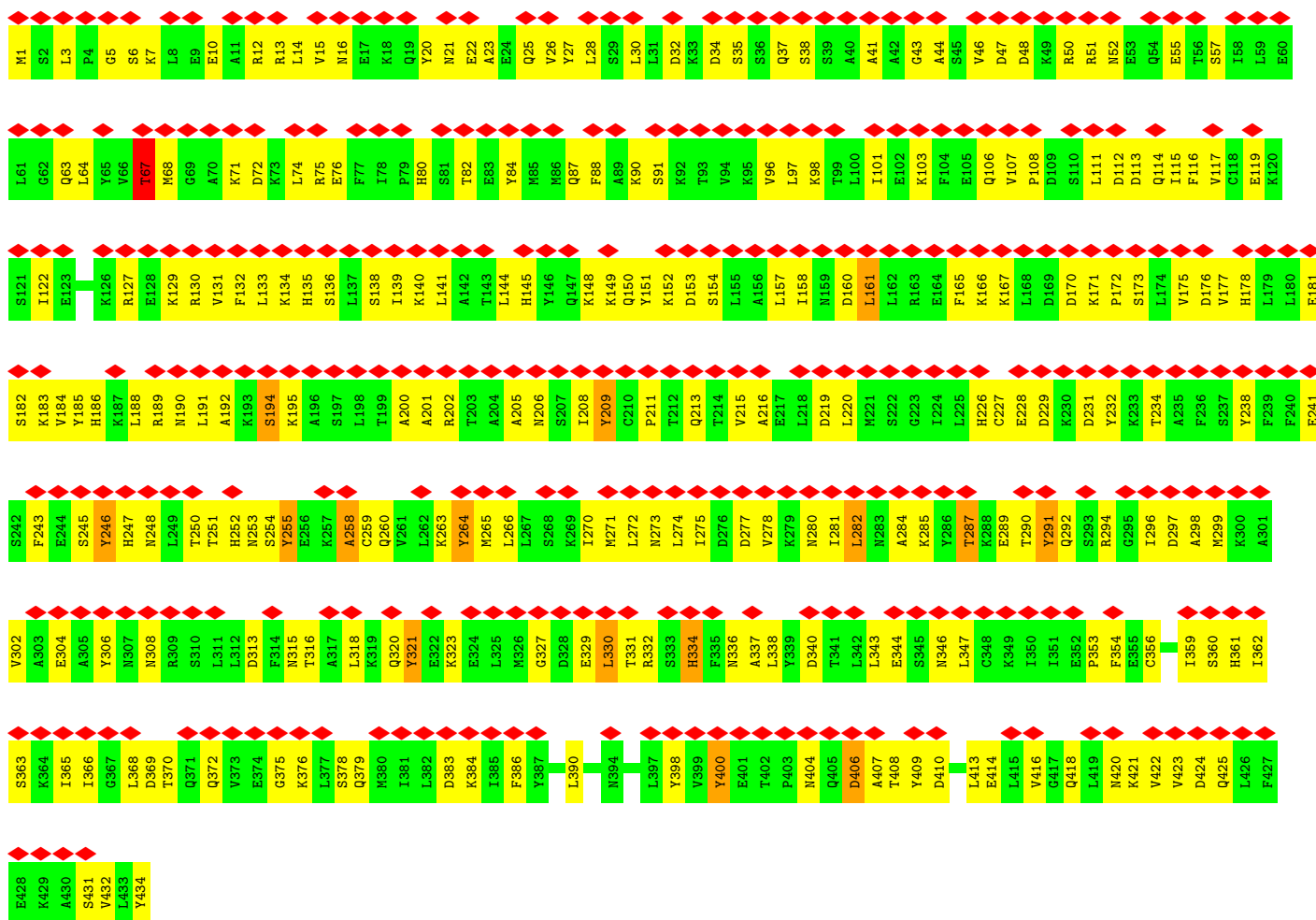
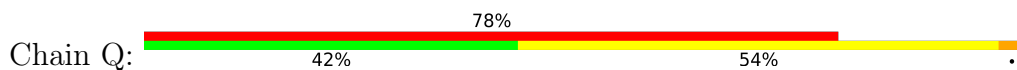


• Molecule 23: 26S proteasome regulatory subunit RPN5

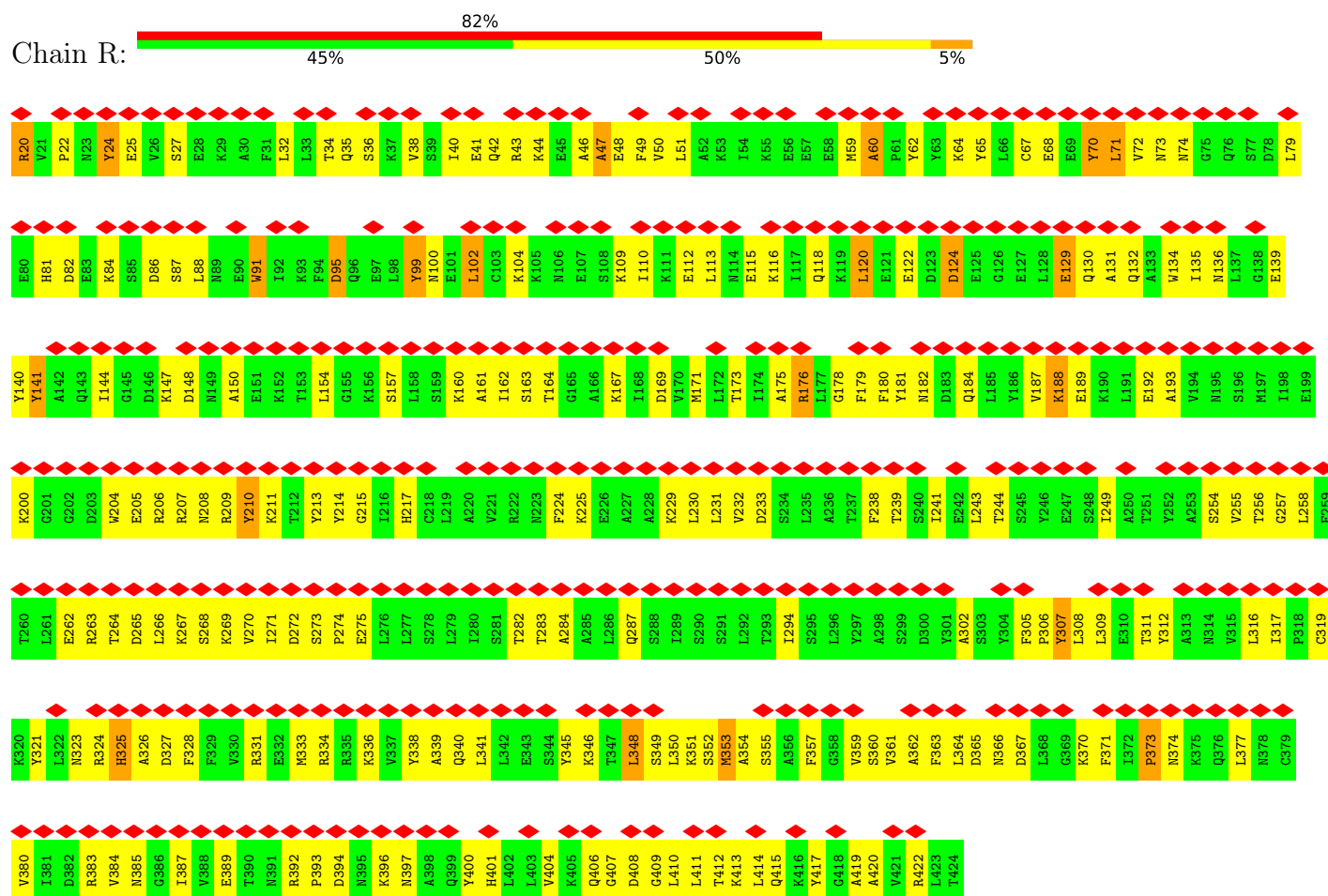




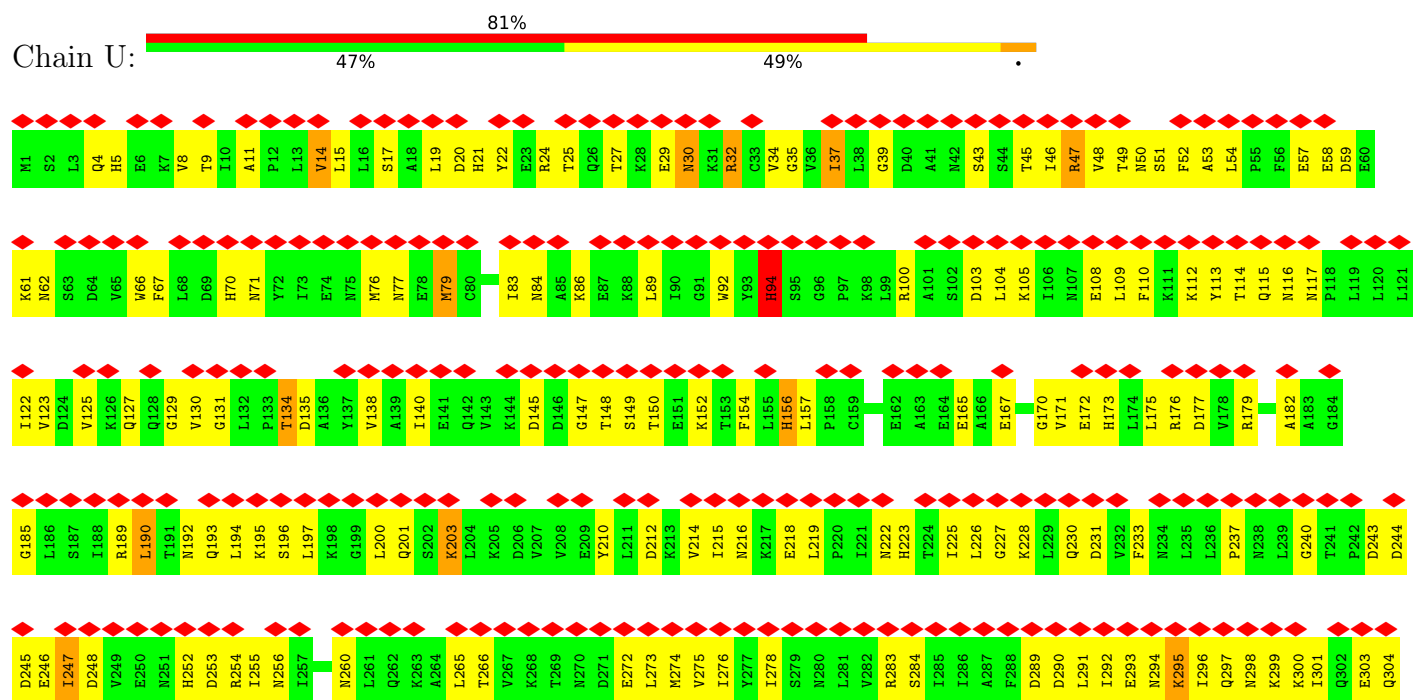
• Molecule 24: 26S proteasome regulatory subunit RPN6



• Molecule 25: 26S proteasome regulatory subunit RPN7

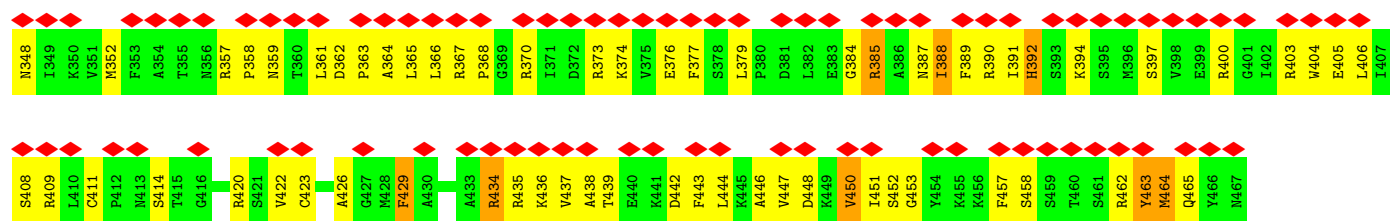


• Molecule 26: 26S proteasome regulatory subunit RPN8

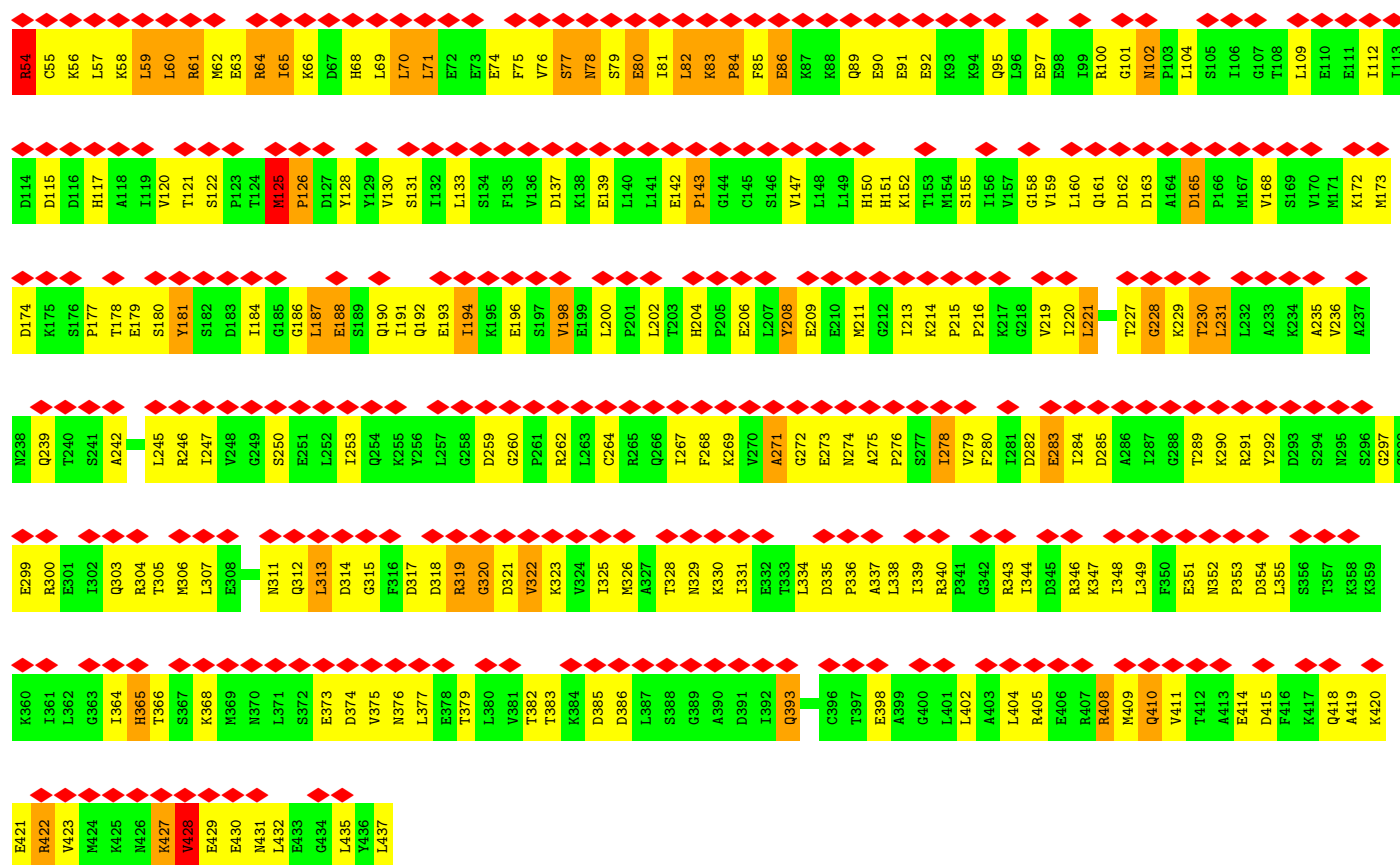
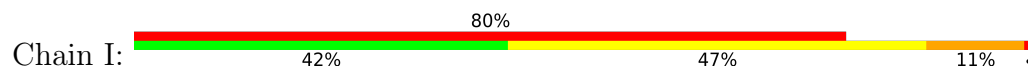


• Molecule 27: 26S proteasome regulatory subunit RPN9

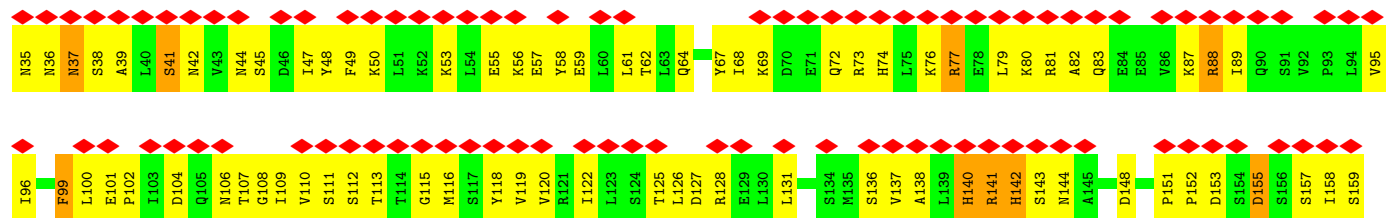
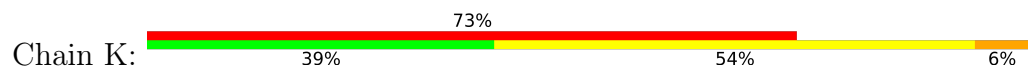


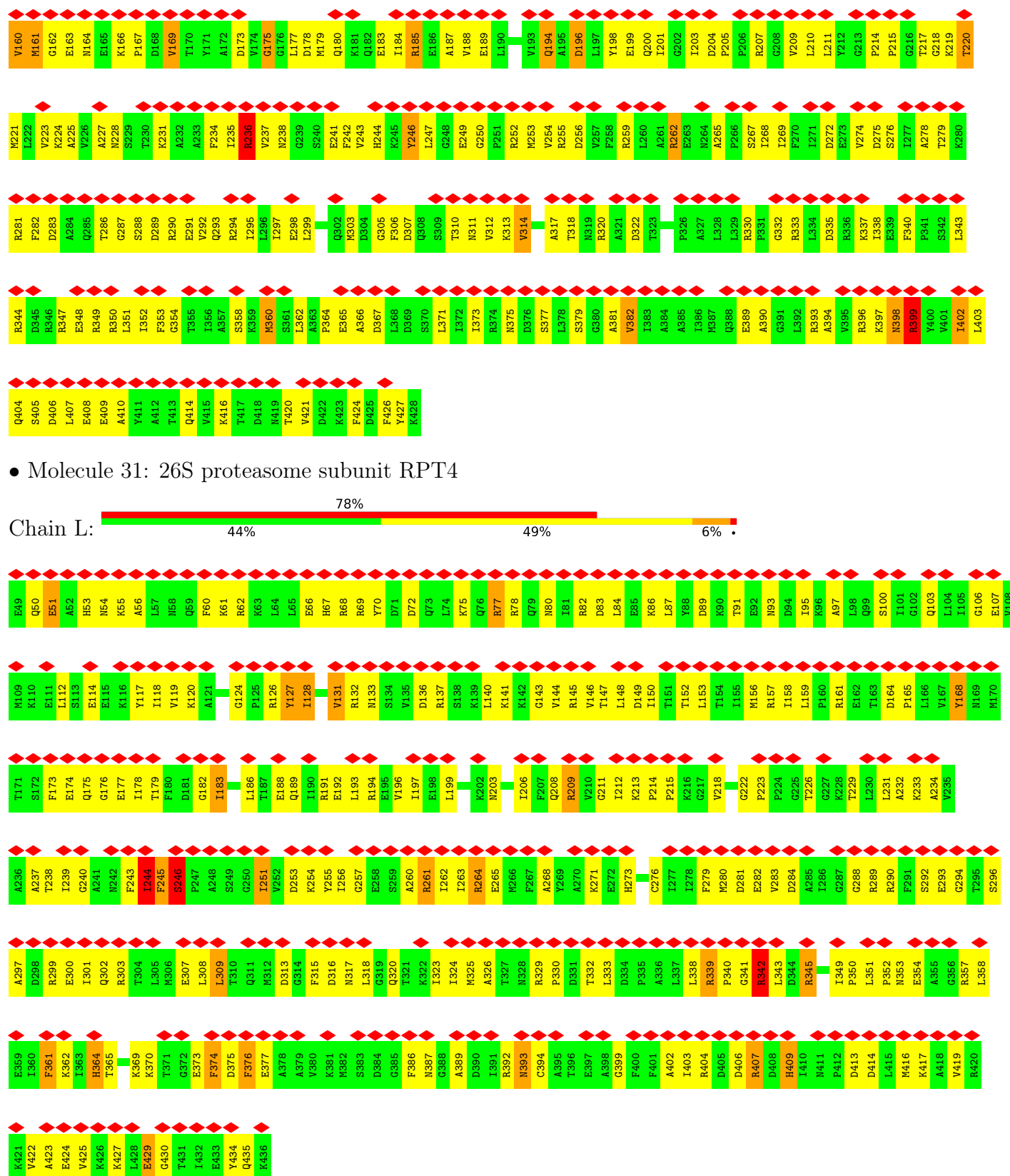


• Molecule 29: 26S proteasome regulatory subunit 4 homolog

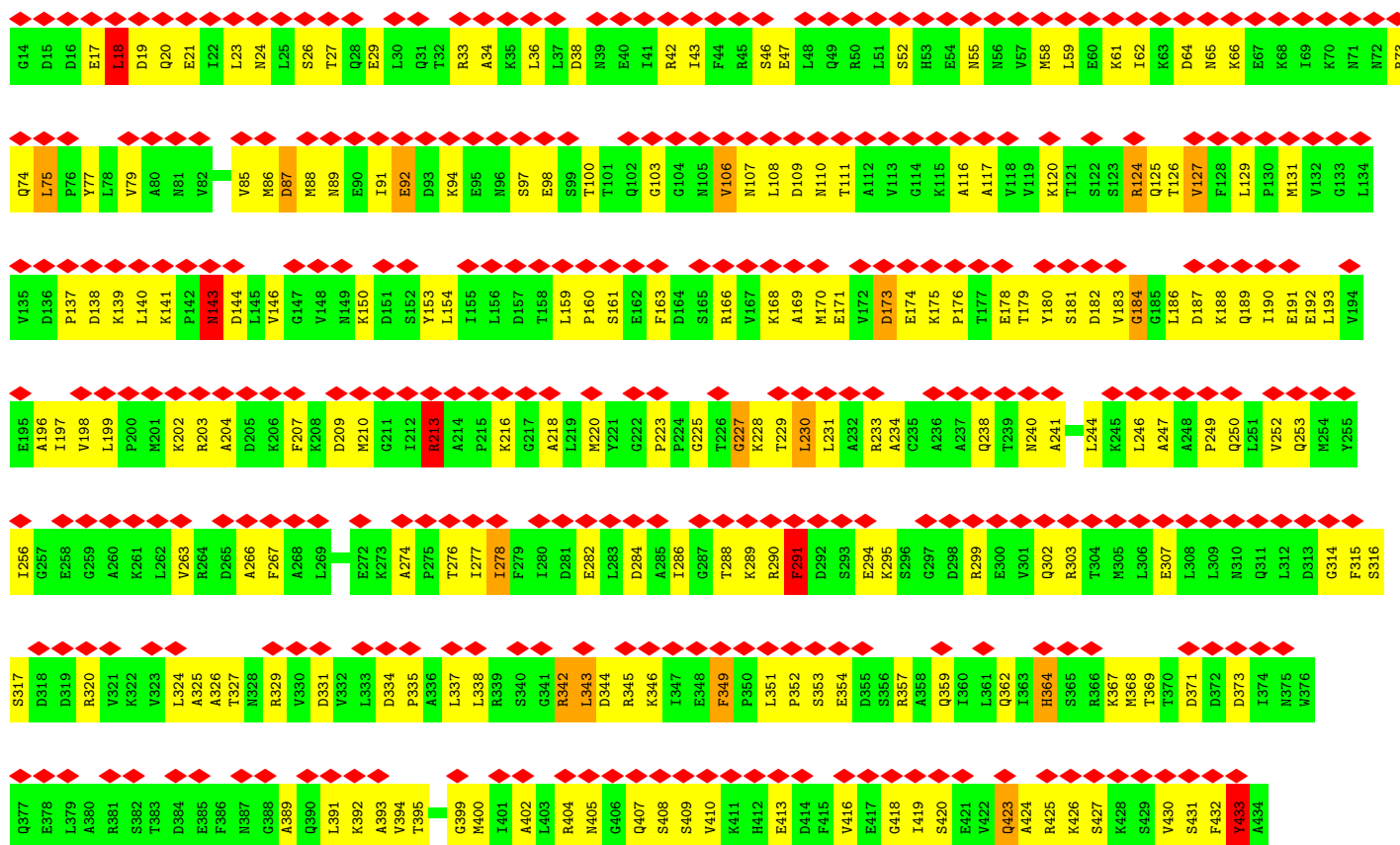
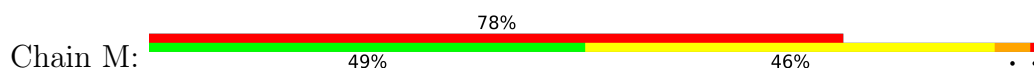


• Molecule 30: 26S proteasome regulatory subunit 6B homolog

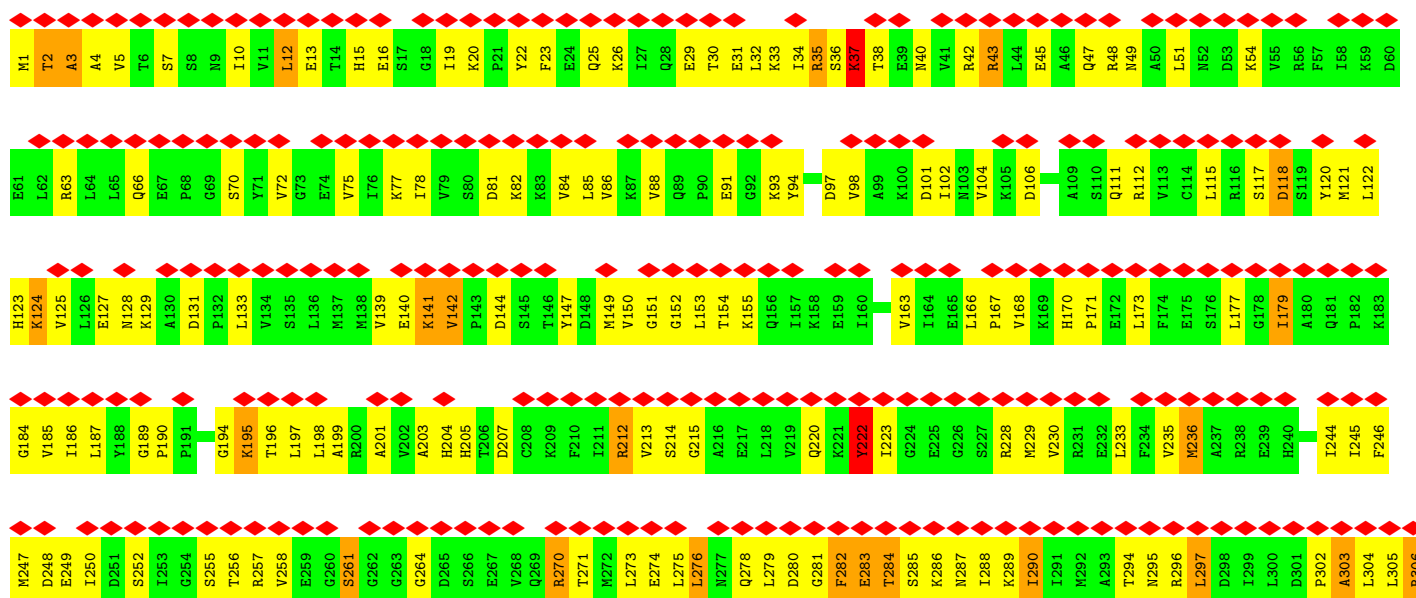
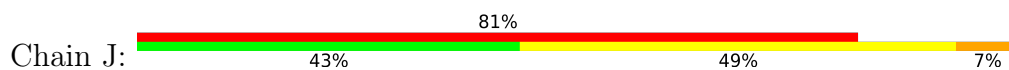




- Molecule 32: 26S proteasome regulatory subunit 6A



• Molecule 33: 26S proteasome regulatory subunit 8 homolog



Y368	A369	L370	R371	E372	R373	R374	L375	H376	V377	T378	Q379	E380	D381	F382	E383	L384	A385	V386	G387	K388	V389	M390	N391	K392	N393	Q394	E395	T396	A397	L398	S399	V400	A401	K402	L403	F404	K405
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	193337	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.131	Depositor
Minimum map value	-0.092	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	2.33	81/1951 (4.2%)	2.44	138/2641 (5.2%)
1	a	2.18	56/1951 (2.9%)	2.41	110/2641 (4.2%)
2	B	2.26	81/1944 (4.2%)	2.34	102/2632 (3.9%)
2	b	2.30	78/1944 (4.0%)	2.38	117/2632 (4.4%)
3	C	2.29	65/1935 (3.4%)	2.44	121/2618 (4.6%)
3	c	2.23	64/1935 (3.3%)	2.47	123/2618 (4.7%)
4	D	2.28	66/1888 (3.5%)	2.41	107/2557 (4.2%)
4	d	2.29	76/2012 (3.8%)	2.43	128/2718 (4.7%)
5	E	2.33	85/1953 (4.4%)	2.38	113/2630 (4.3%)
5	e	2.25	75/1953 (3.8%)	2.36	125/2630 (4.8%)
6	F	2.18	51/1800 (2.8%)	2.42	119/2433 (4.9%)
6	f	2.31	68/1800 (3.8%)	2.37	119/2433 (4.9%)
7	G	2.53	57/1926 (3.0%)	2.38	105/2599 (4.0%)
7	g	2.67	77/1926 (4.0%)	2.44	124/2599 (4.8%)
8	1	2.24	50/1541 (3.2%)	2.40	95/2087 (4.6%)
8	h	2.30	58/1541 (3.8%)	2.36	88/2087 (4.2%)
9	2	2.29	70/1751 (4.0%)	2.42	117/2373 (4.9%)
9	i	2.34	67/1751 (3.8%)	2.42	96/2373 (4.0%)
10	3	2.32	72/1611 (4.5%)	2.38	88/2174 (4.0%)
10	j	2.34	65/1611 (4.0%)	2.38	99/2174 (4.6%)
11	4	2.34	70/1590 (4.4%)	2.39	97/2142 (4.5%)
11	k	2.27	61/1590 (3.8%)	2.43	114/2142 (5.3%)
12	5	2.39	77/1681 (4.6%)	2.38	112/2274 (4.9%)
12	l	2.22	51/1681 (3.0%)	2.36	95/2274 (4.2%)
13	6	2.26	70/1795 (3.9%)	2.38	101/2420 (4.2%)
13	m	2.30	68/1795 (3.8%)	2.32	108/2420 (4.5%)
14	7	2.83	79/1821 (4.3%)	2.46	131/2470 (5.3%)
14	n	2.79	74/1847 (4.0%)	2.37	107/2503 (4.3%)
15	W	2.29	60/1558 (3.9%)	2.50	111/2111 (5.3%)
16	V	2.31	82/2309 (3.6%)	2.48	167/3115 (5.4%)
17	T	2.22	71/2236 (3.2%)	2.58	190/3017 (6.3%)
18	X	2.23	51/1059 (4.8%)	2.45	84/1432 (5.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	Y	2.06	14/741 (1.9%)	2.50	49/1000 (4.9%)
20	Z	2.06	30/7123 (0.4%)	1.92	178/9645 (1.8%)
21	N	2.28	267/7273 (3.7%)	2.49	541/9822 (5.5%)
22	S	2.26	129/3967 (3.3%)	2.54	304/5355 (5.7%)
23	P	2.21	110/3664 (3.0%)	2.55	301/4940 (6.1%)
24	Q	2.29	132/3556 (3.7%)	2.59	297/4787 (6.2%)
25	R	2.19	105/3314 (3.2%)	2.54	272/4469 (6.1%)
26	U	2.24	82/2461 (3.3%)	2.43	157/3327 (4.7%)
27	O	2.24	117/3247 (3.6%)	2.56	271/4380 (6.2%)
28	H	2.51	132/3363 (3.9%)	2.44	224/4532 (4.9%)
29	I	2.37	118/3054 (3.9%)	2.65	188/4111 (4.6%)
30	K	2.32	122/3156 (3.9%)	2.49	241/4261 (5.7%)
31	L	2.26	114/3129 (3.6%)	2.41	187/4204 (4.4%)
32	M	2.21	99/3323 (3.0%)	2.38	183/4478 (4.1%)
33	J	2.26	116/3212 (3.6%)	2.44	202/4316 (4.7%)
All	All	2.30	3863/112269 (3.4%)	2.42	7246/151596 (4.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	a	0	6
2	B	0	8
2	b	0	3
3	C	0	6
3	c	0	8
4	D	0	8
4	d	0	5
5	E	0	10
5	e	0	7
6	F	0	10
6	f	0	8
7	G	0	7
7	g	0	7
8	1	0	4
8	h	0	7
9	2	0	5
9	i	0	3
10	3	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	j	0	7
11	4	0	3
11	k	0	4
12	5	0	5
12	l	0	5
13	6	0	7
13	m	0	8
14	7	0	7
14	n	0	6
15	W	0	4
16	V	0	6
17	T	0	5
18	X	0	3
20	Z	1	5
21	N	0	24
22	S	0	12
23	P	0	8
24	Q	0	14
25	R	0	17
26	U	0	4
27	O	0	5
28	H	0	8
29	I	0	8
30	K	0	10
31	L	0	23
32	M	0	9
33	J	0	10
All	All	1	350

All (3863) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	728	LYS	CG-CD	82.01	3.98	1.52
20	Z	748	LEU	CG-CD2	75.36	4.01	1.52
7	g	93	ARG	CZ-NH2	60.78	2.12	1.33
7	G	93	ARG	CZ-NH2	57.06	2.07	1.33
20	Z	635	ALA	CA-CB	44.18	2.98	1.52
28	H	307	PHE	C-N	41.32	1.91	1.33
14	7	109	TYR	CG-CD2	35.66	2.14	1.39
29	I	322	VAL	C-N	35.05	1.82	1.33
14	n	109	TYR	CG-CD1	34.28	2.11	1.39
20	Z	738	TYR	CZ-OH	34.00	2.09	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	308	PHE	C-N	33.94	1.81	1.33
14	n	109	TYR	CG-CD2	32.57	2.07	1.39
14	7	109	TYR	CG-CD1	32.17	2.06	1.39
20	Z	748	LEU	CG-CD1	31.69	2.57	1.52
14	7	109	TYR	CE1-CZ	29.87	2.10	1.38
14	n	109	TYR	CE2-CZ	29.80	2.09	1.38
20	Z	748	LEU	CB-CG	28.27	2.10	1.53
14	7	109	TYR	CE2-CZ	26.82	2.02	1.38
14	n	109	TYR	CE1-CZ	26.57	2.02	1.38
14	7	109	TYR	CD2-CE2	21.77	2.04	1.38
14	n	109	TYR	CD2-CE2	21.19	2.02	1.38
14	7	109	TYR	CD1-CE1	20.80	2.01	1.38
14	n	109	TYR	CD1-CE1	20.28	1.99	1.38
20	Z	728	LYS	CD-CE	19.86	2.12	1.52
20	Z	728	LYS	CA-CB	18.82	1.85	1.53
20	Z	748	LEU	CA-CB	17.83	1.81	1.53
20	Z	748	LEU	CA-C	15.47	1.72	1.52
20	Z	728	LYS	N-CA	15.42	1.66	1.46
31	L	182	GLY	CA-C	-14.15	1.43	1.51
30	K	379	SER	CA-C	-13.46	1.36	1.52
29	I	313	LEU	C-N	13.07	1.51	1.33
14	7	41	GLY	CA-C	-12.98	1.41	1.52
21	N	602	VAL	CA-C	12.93	1.63	1.52
20	Z	728	LYS	CB-CG	11.74	1.87	1.52
14	7	183	MET	CA-C	-11.68	1.44	1.52
20	Z	745	LEU	CA-C	-11.48	1.38	1.52
11	4	44	MET	CA-C	-11.28	1.39	1.52
20	Z	727	GLU	C-N	11.07	1.49	1.33
3	C	35	ALA	CA-C	-11.07	1.39	1.52
4	D	138	PHE	CA-C	-10.64	1.40	1.52
20	Z	727	GLU	CA-C	10.63	1.67	1.53
28	H	385	ARG	CD-NE	10.56	1.61	1.46
13	m	229	ARG	NE-CZ	10.54	1.44	1.33
32	M	196	ALA	CA-C	-10.38	1.39	1.52
28	H	70	LYS	CA-C	-10.37	1.39	1.52
4	d	183	GLU	C-O	-10.35	1.14	1.24
17	T	8	THR	CA-C	-10.34	1.38	1.52
2	B	42	GLY	N-CA	-10.30	1.33	1.45
9	i	132	VAL	N-CA	-10.26	1.33	1.46
11	k	12	SER	CA-C	-10.09	1.40	1.52
4	D	70	HIS	N-CA	-10.04	1.38	1.47
1	A	49	ASP	N-CA	-10.03	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	35	GLY	CA-C	-10.01	1.43	1.52
24	Q	171	LYS	C-N	9.88	1.41	1.33
6	f	230	VAL	CA-CB	-9.81	1.44	1.54
19	Y	27	LYS	CA-C	-9.80	1.40	1.52
21	N	361	ASN	CA-C	-9.76	1.44	1.53
21	N	839	ARG	CD-NE	9.72	1.59	1.46
29	I	131	SER	CA-C	-9.69	1.40	1.52
11	k	95	ARG	CD-NE	9.68	1.59	1.46
4	D	45	GLY	CA-C	-9.67	1.45	1.52
24	Q	398	TYR	CA-C	-9.65	1.40	1.52
16	V	217	HIS	ND1-CE1	9.65	1.42	1.32
4	D	118	GLN	CA-C	-9.60	1.40	1.52
21	N	115	LYS	CA-C	-9.60	1.40	1.52
28	H	159	LEU	CA-C	-9.60	1.41	1.52
10	3	77	LYS	CA-C	-9.57	1.40	1.52
17	T	210	PHE	CA-C	-9.57	1.44	1.53
28	H	231	SER	CA-CB	9.54	1.61	1.53
31	L	407	ARG	CD-NE	9.54	1.59	1.46
25	R	112	GLU	CA-CB	9.53	1.68	1.53
3	C	158	THR	N-CA	-9.51	1.34	1.46
10	j	30	GLY	CA-C	-9.50	1.40	1.52
10	j	174	ALA	CA-C	-9.50	1.40	1.52
11	4	81	SER	CA-C	-9.49	1.40	1.52
22	S	64	ARG	NE-CZ	9.49	1.43	1.33
17	T	227	PRO	C-N	9.48	1.44	1.33
28	H	374	LYS	CA-C	-9.48	1.41	1.52
30	K	265	ALA	CA-C	-9.48	1.43	1.53
24	Q	299	MET	N-CA	-9.48	1.34	1.46
4	D	151	GLU	CA-C	-9.47	1.43	1.52
26	U	32	ARG	NE-CZ	9.47	1.43	1.33
16	V	255	ILE	CA-C	-9.46	1.42	1.53
15	W	48	THR	CA-C	-9.42	1.41	1.52
14	n	234	ASP	CA-C	-9.42	1.41	1.52
20	Z	635	ALA	CA-C	9.41	1.72	1.52
28	H	249	TYR	CA-C	-9.38	1.41	1.52
11	4	190	ARG	CA-C	-9.36	1.41	1.52
16	V	50	MET	C-N	9.34	1.43	1.32
15	W	131	THR	C-N	9.30	1.46	1.33
14	7	240	THR	CA-C	-9.29	1.41	1.52
5	E	228	PHE	CA-C	-9.28	1.41	1.52
7	G	184	PRO	N-CA	-9.27	1.39	1.47
14	n	141	ASN	N-CA	-9.26	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	120	GLN	C-N	9.25	1.44	1.33
18	X	64	ILE	N-CA	-9.24	1.36	1.46
11	4	96	ARG	N-CA	-9.24	1.35	1.46
1	A	31	ALA	CA-CB	9.24	1.67	1.53
10	j	52	GLY	CA-C	-9.21	1.45	1.52
12	l	241	HIS	ND1-CE1	9.15	1.41	1.32
22	S	464	ARG	NE-CZ	9.15	1.43	1.33
2	B	94	HIS	CE1-NE2	9.13	1.41	1.32
33	J	257	ARG	CD-NE	9.11	1.59	1.46
7	G	63	LYS	N-CA	-9.08	1.39	1.47
23	P	409	SER	N-CA	-9.08	1.35	1.46
22	S	195	ALA	CA-C	9.06	1.64	1.52
31	L	82	ARG	CZ-NH2	9.05	1.45	1.33
30	K	207	ARG	CD-NE	9.05	1.58	1.46
31	L	325	MET	CA-CB	9.04	1.67	1.53
1	a	155	TYR	CA-C	-9.00	1.41	1.52
1	a	166	TYR	CA-C	-9.00	1.41	1.52
21	N	362	TRP	NE1-CE2	9.00	1.47	1.37
22	S	47	THR	CA-C	-8.98	1.40	1.52
6	F	138	ASP	CA-C	-8.98	1.40	1.52
20	Z	255	LEU	N-CA	-8.97	1.35	1.46
10	3	23	ILE	C-N	8.97	1.44	1.33
24	Q	135	HIS	ND1-CE1	8.96	1.41	1.32
8	h	196	ILE	CA-CB	-8.95	1.45	1.55
7	g	47	VAL	CA-C	-8.94	1.41	1.52
17	T	194	GLU	CA-C	-8.94	1.41	1.52
1	a	42	SER	CA-C	-8.93	1.41	1.52
2	b	139	HIS	ND1-CE1	8.92	1.41	1.32
3	C	195	LYS	CA-C	-8.92	1.41	1.52
13	m	31	LEU	CA-C	-8.92	1.42	1.52
3	c	95	ALA	CA-C	-8.91	1.41	1.52
24	Q	270	ILE	C-N	8.90	1.46	1.33
6	f	69	HIS	CB-CG	-8.88	1.37	1.50
7	G	176	LEU	CA-C	-8.88	1.40	1.52
26	U	214	VAL	CA-CB	-8.88	1.43	1.54
33	J	305	LEU	CA-C	-8.87	1.41	1.52
2	B	99	ARG	CD-NE	8.86	1.58	1.46
10	3	45	HIS	ND1-CE1	8.85	1.41	1.32
2	b	35	LEU	CA-C	-8.83	1.41	1.52
1	A	193	HIS	CA-CB	8.83	1.68	1.53
1	a	84	ASN	N-CA	-8.82	1.35	1.46
14	7	76	ILE	CA-C	-8.82	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	124	SER	CA-CB	8.79	1.68	1.53
32	M	146	VAL	CA-C	-8.78	1.42	1.52
6	f	71	GLY	N-CA	-8.78	1.36	1.45
7	G	13	SER	N-CA	-8.77	1.34	1.46
32	M	431	SER	CA-CB	8.74	1.66	1.53
7	G	242	PHE	N-CA	-8.73	1.35	1.46
6	f	134	ILE	C-N	8.72	1.42	1.33
9	i	217	ARG	NE-CZ	8.70	1.42	1.33
11	k	179	VAL	CA-C	-8.71	1.45	1.52
12	l	157	ILE	C-N	8.70	1.45	1.33
12	l	132	THR	CA-C	-8.70	1.41	1.52
1	A	131	ARG	CA-C	-8.69	1.41	1.52
2	b	139	HIS	CA-C	-8.68	1.42	1.52
32	M	325	ALA	CA-C	-8.65	1.42	1.52
12	5	180	THR	CA-C	-8.65	1.42	1.52
24	Q	195	LYS	N-CA	-8.64	1.35	1.46
10	3	99	ARG	NE-CZ	8.63	1.42	1.33
31	L	144	VAL	CA-CB	-8.63	1.43	1.54
9	i	138	HIS	ND1-CE1	8.62	1.41	1.32
21	N	228	VAL	N-CA	8.62	1.56	1.46
21	N	789	GLU	N-CA	-8.61	1.35	1.46
29	I	284	ILE	N-CA	-8.59	1.35	1.46
1	A	18	ILE	N-CA	-8.59	1.36	1.46
21	N	413	ALA	CA-C	8.58	1.63	1.52
3	c	217	ARG	N-CA	-8.56	1.35	1.46
25	R	409	GLY	CA-C	-8.56	1.42	1.52
31	L	299	ARG	NE-CZ	8.56	1.42	1.33
24	Q	130	ARG	CA-CB	8.54	1.65	1.53
15	W	6	THR	CA-C	-8.54	1.42	1.52
10	3	201	LYS	CA-C	-8.53	1.41	1.52
14	7	257	ASP	N-CA	-8.53	1.34	1.46
10	j	131	ASP	CA-C	-8.50	1.42	1.53
5	e	43	LYS	N-CA	-8.50	1.35	1.46
11	4	184	VAL	CA-CB	-8.49	1.44	1.53
15	W	85	LEU	N-CA	-8.49	1.35	1.46
7	g	11	SER	N-CA	-8.48	1.35	1.45
3	C	107	PRO	CA-C	-8.47	1.42	1.52
28	H	306	ILE	CA-CB	-8.46	1.44	1.53
30	K	310	THR	C-N	8.45	1.45	1.33
16	V	117	TRP	CA-C	-8.45	1.41	1.52
11	4	191	GLN	CA-C	-8.44	1.42	1.52
28	H	194	SER	C-N	8.43	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	299	MET	CA-C	-8.43	1.41	1.52
29	I	150	HIS	ND1-CE1	8.41	1.41	1.32
30	K	199	GLU	N-CA	-8.41	1.36	1.46
7	g	151	LEU	CA-C	-8.40	1.42	1.52
32	M	110	ASN	N-CA	-8.40	1.36	1.46
33	J	229	MET	N-CA	-8.40	1.35	1.46
22	S	131	THR	CA-C	8.40	1.64	1.52
28	H	72	SER	CA-C	-8.39	1.42	1.52
12	5	260	TRP	CA-C	-8.39	1.42	1.52
9	i	101	ARG	CA-C	-8.39	1.42	1.52
7	G	163	ALA	N-CA	-8.39	1.35	1.45
30	K	218	GLY	C-N	8.38	1.44	1.33
13	6	108	LYS	CA-C	-8.38	1.42	1.52
32	M	58	MET	CA-C	-8.37	1.42	1.52
9	2	216	LEU	CA-CB	-8.36	1.41	1.52
13	6	94	ILE	CA-CB	-8.36	1.45	1.54
4	d	76	SER	CA-C	-8.35	1.42	1.52
6	f	63	ILE	N-CA	-8.33	1.36	1.46
5	E	43	LYS	CA-C	-8.33	1.41	1.52
28	H	259	CYS	CA-C	-8.32	1.41	1.52
3	c	228	LYS	CA-C	-8.31	1.42	1.52
18	X	129	LEU	C-N	8.29	1.44	1.33
4	d	229	ILE	CA-C	-8.28	1.42	1.52
15	W	60	ARG	CD-NE	8.27	1.57	1.46
2	B	49	LYS	C-N	8.27	1.44	1.33
22	S	58	LYS	CA-CB	8.27	1.66	1.53
4	d	149	GLN	CA-C	-8.27	1.42	1.52
1	a	16	ILE	CA-C	-8.26	1.42	1.52
4	d	172	ARG	NE-CZ	8.26	1.42	1.33
28	H	361	LEU	CA-CB	8.25	1.67	1.53
1	a	50	CYS	CA-C	-8.25	1.42	1.52
21	N	219	ASN	CA-C	-8.25	1.42	1.52
3	c	181	LYS	CA-C	-8.25	1.43	1.52
9	2	75	ALA	CA-C	-8.24	1.42	1.52
1	A	75	ILE	CA-C	-8.24	1.42	1.52
5	E	99	HIS	ND1-CE1	8.23	1.40	1.32
16	V	279	HIS	CE1-NE2	-8.23	1.24	1.32
25	R	267	LYS	C-N	8.23	1.44	1.33
30	K	282	PHE	CA-C	-8.23	1.42	1.52
3	C	9	ARG	NE-CZ	8.23	1.42	1.33
10	j	161	GLU	C-N	8.22	1.44	1.33
9	2	236	ARG	NE-CZ	8.22	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	218	TYR	CA-C	-8.21	1.41	1.52
5	E	143	LEU	C-N	8.21	1.41	1.33
16	V	256	GLU	CA-C	-8.21	1.42	1.52
3	c	129	ARG	CZ-NH2	8.20	1.44	1.33
8	h	38	ARG	CD-NE	8.20	1.57	1.46
26	U	252	HIS	C-N	8.20	1.44	1.33
1	A	155	TYR	CA-C	-8.19	1.42	1.52
3	C	50	ARG	CD-NE	8.19	1.57	1.46
8	1	50	ILE	CA-C	-8.19	1.42	1.52
32	M	256	ILE	CA-C	-8.19	1.42	1.52
8	1	104	ALA	N-CA	-8.17	1.35	1.45
23	P	321	VAL	CA-C	8.17	1.63	1.52
10	3	41	GLU	CA-C	-8.16	1.42	1.52
8	h	28	ARG	CD-NE	8.15	1.57	1.46
16	V	268	THR	N-CA	-8.14	1.36	1.46
30	K	136	SER	C-N	8.13	1.38	1.33
8	h	158	GLU	C-N	8.12	1.44	1.33
3	c	114	ARG	CD-NE	8.11	1.57	1.46
28	H	339	GLN	C-N	8.11	1.44	1.33
7	g	145	GLY	CA-C	-8.10	1.43	1.52
14	n	215	ARG	NE-CZ	8.10	1.42	1.33
19	Y	83	ARG	NE-CZ	8.08	1.42	1.33
20	Z	635	ALA	N-CA	8.08	1.61	1.46
33	J	341	ILE	CA-CB	-8.08	1.44	1.54
5	e	25	GLU	C-N	8.07	1.44	1.33
1	A	185	HIS	CA-CB	8.07	1.66	1.53
10	3	126	LEU	CA-C	-8.07	1.46	1.53
3	c	4	ARG	CD-NE	8.07	1.57	1.46
6	f	107	ARG	CD-NE	8.07	1.57	1.46
33	J	255	SER	CA-C	8.07	1.63	1.52
17	T	94	HIS	N-CA	-8.07	1.36	1.46
22	S	124	GLU	CA-CB	8.07	1.66	1.53
3	C	46	LEU	CA-C	-8.05	1.43	1.52
4	D	49	ARG	CD-NE	8.05	1.57	1.46
23	P	9	ALA	N-CA	-8.03	1.36	1.46
31	L	67	HIS	ND1-CE1	8.03	1.40	1.32
4	D	114	ALA	CA-C	-8.03	1.42	1.52
2	b	67	LEU	CA-C	-8.02	1.42	1.53
6	f	49	LEU	C-N	8.01	1.44	1.33
27	O	342	ASP	CA-C	-8.01	1.43	1.52
21	N	438	ASP	CA-C	-8.01	1.42	1.52
33	J	70	SER	CA-C	-8.01	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	873	ARG	CD-NE	8.00	1.57	1.46
31	L	357	ARG	CD-NE	7.99	1.57	1.46
5	e	170	LYS	N-CA	-7.99	1.36	1.46
8	h	187	LEU	CA-CB	7.98	1.64	1.53
16	V	44	GLY	C-N	7.98	1.42	1.33
11	k	133	HIS	CA-C	-7.98	1.42	1.52
17	T	244	ASP	N-CA	7.96	1.55	1.46
27	O	283	HIS	CB-CG	7.96	1.61	1.50
8	l	72	LEU	CA-C	-7.95	1.42	1.52
21	N	814	ALA	N-CA	-7.95	1.36	1.46
27	O	147	ARG	CA-C	-7.95	1.42	1.52
4	d	224	LEU	C-N	7.95	1.44	1.33
22	S	480	ARG	CD-NE	7.94	1.57	1.46
30	K	200	GLN	C-N	7.94	1.43	1.33
12	5	141	HIS	ND1-CE1	7.94	1.40	1.32
9	2	138	HIS	ND1-CE1	7.93	1.40	1.32
17	T	24	GLU	CA-CB	7.92	1.65	1.53
1	a	227	VAL	CA-C	-7.92	1.43	1.52
4	d	9	SER	CA-C	-7.92	1.43	1.52
13	6	112	PRO	CA-C	-7.92	1.44	1.52
29	I	220	ILE	CA-C	7.92	1.62	1.52
28	H	231	SER	N-CA	-7.92	1.39	1.46
1	A	136	PRO	C-N	7.91	1.44	1.33
24	Q	361	HIS	ND1-CE1	7.90	1.40	1.32
21	N	859	ASN	C-N	7.90	1.42	1.33
8	l	194	ARG	NE-CZ	7.90	1.41	1.33
12	5	94	ARG	CD-NE	7.88	1.57	1.46
3	c	124	GLN	CA-C	-7.88	1.42	1.52
1	a	97	ALA	CA-C	-7.88	1.42	1.52
28	H	232	PRO	N-CA	-7.88	1.42	1.47
6	F	89	ARG	NE-CZ	7.87	1.41	1.33
17	T	126	LEU	C-N	7.86	1.43	1.33
21	N	208	ARG	NE-CZ	7.86	1.41	1.33
25	R	272	ASP	N-CA	-7.86	1.37	1.46
11	4	101	ASN	C-N	7.85	1.44	1.33
5	E	24	VAL	C-N	7.84	1.44	1.33
15	W	107	HIS	CG-CD2	7.84	1.44	1.35
10	j	28	ARG	NE-CZ	7.84	1.41	1.33
22	S	320	ILE	C-N	7.83	1.44	1.33
7	g	227	LEU	CA-C	-7.83	1.43	1.52
9	i	198	SER	CA-CB	7.83	1.65	1.53
16	V	259	LYS	CA-C	-7.83	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1	107	ILE	C-N	7.82	1.43	1.33
10	3	151	GLU	C-N	7.82	1.45	1.33
1	A	152	PRO	C-N	7.82	1.43	1.33
5	E	165	TYR	CA-C	-7.81	1.43	1.52
25	R	238	PHE	N-CA	-7.81	1.36	1.46
14	n	161	ARG	CD-NE	7.81	1.57	1.46
7	G	100	LYS	CA-C	-7.81	1.42	1.52
31	L	146	VAL	CA-C	-7.80	1.43	1.52
1	A	120	ARG	CD-NE	7.80	1.57	1.46
26	U	127	GLN	CA-CB	7.80	1.66	1.53
27	O	347	LEU	CA-C	-7.80	1.43	1.52
31	L	357	ARG	CZ-NH1	7.80	1.43	1.32
6	F	146	GLU	CA-C	-7.79	1.43	1.52
33	J	307	PRO	CA-C	-7.78	1.43	1.52
5	e	65	GLU	CA-CB	7.77	1.66	1.53
1	A	38	THR	C-N	7.77	1.44	1.33
33	J	170	HIS	CG-CD2	7.77	1.44	1.35
13	m	141	ARG	CA-C	-7.77	1.42	1.52
29	I	423	VAL	CA-CB	-7.76	1.44	1.54
11	4	134	GLY	N-CA	-7.76	1.36	1.45
12	5	159	SER	N-CA	7.75	1.55	1.46
10	j	28	ARG	CD-NE	7.75	1.57	1.46
13	m	105	LEU	N-CA	-7.75	1.37	1.46
4	D	211	GLU	C-N	7.75	1.43	1.33
12	5	82	ARG	C-N	7.75	1.40	1.33
13	m	141	ARG	CD-NE	7.74	1.57	1.46
15	W	23	ARG	CD-NE	7.74	1.57	1.46
10	3	28	ARG	CZ-NH2	7.74	1.43	1.33
6	F	69	HIS	ND1-CE1	7.73	1.40	1.32
16	V	195	HIS	ND1-CE1	7.73	1.40	1.32
14	7	38	ILE	N-CA	7.72	1.53	1.46
10	j	29	LEU	C-N	7.72	1.42	1.33
30	K	278	ALA	N-CA	-7.72	1.36	1.46
28	H	317	ALA	CA-C	-7.71	1.42	1.52
30	K	393	ARG	NE-CZ	7.71	1.41	1.33
8	1	15	VAL	C-N	7.71	1.43	1.33
32	M	349	PHE	C-N	-7.70	1.24	1.33
12	5	149	ILE	CA-CB	-7.70	1.46	1.54
6	F	162	GLY	CA-C	-7.70	1.42	1.51
3	c	143	ARG	NE-CZ	7.70	1.41	1.33
25	R	167	LYS	C-O	-7.70	1.15	1.24
32	M	399	GLY	C-N	7.69	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I	352	ASN	N-CA	-7.69	1.36	1.45
21	N	391	PRO	CA-C	-7.69	1.43	1.52
23	P	425	HIS	C-O	-7.69	1.15	1.24
5	E	239	LEU	N-CA	-7.69	1.37	1.46
6	f	71	GLY	CA-C	-7.68	1.43	1.51
3	C	92	ARG	CA-C	-7.68	1.42	1.52
13	6	13	TYR	CA-C	-7.68	1.43	1.52
18	X	62	ASP	N-CA	-7.68	1.39	1.46
25	R	387	ILE	CA-C	-7.68	1.43	1.52
33	J	396	THR	CA-C	-7.68	1.43	1.52
33	J	397	ALA	N-CA	-7.67	1.38	1.46
24	Q	41	ALA	CA-C	-7.67	1.43	1.52
27	O	366	MET	CA-C	-7.67	1.42	1.52
22	S	426	ALA	CA-C	-7.67	1.42	1.52
17	T	219	LYS	CA-C	-7.66	1.43	1.52
23	P	344	ARG	CA-C	-7.66	1.43	1.52
3	c	102	TYR	CA-C	7.66	1.62	1.52
14	7	182	HIS	CE1-NE2	-7.66	1.24	1.32
24	Q	246	TYR	N-CA	-7.66	1.36	1.46
27	O	207	LEU	CA-C	-7.66	1.43	1.52
3	c	34	THR	C-N	7.65	1.44	1.33
28	H	190	ARG	NE-CZ	7.65	1.41	1.33
30	K	61	LEU	CA-C	-7.65	1.42	1.52
6	f	43	HIS	N-CA	-7.64	1.36	1.46
14	n	182	HIS	ND1-CE1	7.64	1.40	1.32
21	N	450	ILE	CA-CB	-7.63	1.44	1.54
18	X	37	PRO	CA-C	-7.63	1.44	1.52
2	b	62	SER	CA-C	-7.63	1.43	1.52
12	l	141	HIS	CB-CG	7.61	1.60	1.50
31	L	323	ILE	N-CA	7.61	1.55	1.46
13	m	178	LYS	CA-C	7.61	1.60	1.53
27	O	25	LEU	C-N	7.60	1.44	1.33
5	e	40	ILE	CA-C	-7.60	1.43	1.52
2	b	236	ARG	NE-CZ	7.60	1.41	1.33
21	N	394	ARG	NE-CZ	7.60	1.41	1.33
13	6	225	TYR	CA-C	-7.59	1.43	1.52
14	7	168	VAL	CA-CB	-7.59	1.46	1.54
14	7	194	ARG	CD-NE	7.58	1.56	1.46
22	S	397	LEU	CA-CB	7.58	1.65	1.53
3	c	168	ASN	N-CA	-7.58	1.36	1.46
30	K	142	HIS	ND1-CE1	7.57	1.40	1.32
29	I	151	HIS	ND1-CE1	7.57	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	X	60	GLU	C-N	7.56	1.43	1.33
2	B	231	LYS	N-CA	-7.56	1.35	1.45
3	c	178	MET	CA-C	-7.56	1.42	1.52
11	4	104	ILE	N-CA	-7.56	1.36	1.46
10	j	135	ASP	CA-C	-7.56	1.42	1.52
18	X	82	LYS	CA-C	-7.56	1.43	1.52
5	E	240	ILE	CA-CB	-7.55	1.44	1.54
14	7	168	VAL	C-N	7.55	1.43	1.33
31	L	158	ILE	CA-C	-7.55	1.43	1.52
5	E	148	ASP	CA-C	-7.55	1.43	1.52
9	i	45	ALA	CA-C	-7.55	1.43	1.52
22	S	100	HIS	CE1-NE2	-7.55	1.25	1.32
9	2	65	ARG	C-N	-7.54	1.24	1.33
2	b	4	ARG	CD-NE	7.54	1.56	1.46
2	B	212	ALA	CA-C	-7.54	1.43	1.52
15	W	90	ALA	CA-C	7.53	1.62	1.52
24	Q	106	GLN	CA-CB	7.53	1.65	1.53
30	K	350	ARG	NE-CZ	7.53	1.41	1.33
2	b	96	SER	CA-C	-7.53	1.43	1.52
7	G	75	GLY	CA-C	7.53	1.59	1.52
13	6	192	VAL	CA-CB	-7.52	1.45	1.54
23	P	392	LYS	CA-C	-7.51	1.43	1.52
24	Q	424	ASP	C-N	7.51	1.44	1.33
11	4	95	ARG	CZ-NH1	7.50	1.43	1.32
21	N	482	ALA	C-N	7.50	1.44	1.33
8	h	182	ILE	CA-CB	-7.49	1.45	1.54
4	d	145	PRO	N-CA	-7.49	1.38	1.47
24	Q	291	TYR	CA-C	-7.49	1.43	1.52
5	E	228	PHE	CA-CB	7.49	1.63	1.53
11	4	70	ARG	CD-NE	7.49	1.56	1.46
21	N	597	ARG	N-CA	-7.48	1.37	1.46
4	D	185	PRO	CA-C	-7.48	1.45	1.52
32	M	188	LYS	CA-C	-7.48	1.43	1.52
9	i	241	VAL	CA-C	-7.48	1.43	1.52
10	j	109	VAL	N-CA	-7.47	1.37	1.46
13	m	40	ASP	CA-CB	7.47	1.66	1.53
9	2	228	LYS	CA-C	-7.47	1.43	1.52
25	R	27	SER	C-N	7.47	1.43	1.33
30	K	409	GLU	CA-CB	7.47	1.65	1.53
5	e	237	ALA	N-CA	7.47	1.55	1.46
20	Z	251	ALA	CA-C	-7.47	1.43	1.52
22	S	385	SER	CA-C	-7.47	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	188	TYR	CA-C	-7.46	1.43	1.52
12	5	286	ILE	N-CA	-7.46	1.37	1.46
5	e	20	ARG	NE-CZ	7.46	1.41	1.33
6	f	105	VAL	CA-CB	-7.46	1.45	1.54
7	g	38	ILE	CA-C	-7.46	1.43	1.52
13	6	59	VAL	CA-C	-7.45	1.43	1.52
9	i	233	LYS	N-CA	-7.45	1.36	1.46
4	d	214	VAL	N-CA	7.45	1.54	1.46
30	K	109	ILE	CA-C	-7.45	1.43	1.52
32	M	47	GLU	N-CA	-7.45	1.36	1.46
12	5	266	HIS	CB-CG	-7.45	1.39	1.50
21	N	604	ARG	NE-CZ	7.45	1.41	1.33
31	L	157	ARG	CA-C	-7.45	1.43	1.52
27	O	185	PHE	N-CA	-7.44	1.37	1.46
32	M	286	ILE	N-CA	7.44	1.53	1.46
24	Q	16	ASN	C-N	7.44	1.44	1.33
22	S	35	LEU	CA-C	-7.43	1.43	1.52
24	Q	362	ILE	CA-C	-7.43	1.43	1.52
27	O	27	GLU	CA-C	-7.42	1.43	1.52
33	J	312	ARG	CZ-NH1	7.42	1.43	1.32
28	H	318	ARG	CA-C	-7.42	1.43	1.52
12	l	175	MET	N-CA	-7.41	1.36	1.46
19	Y	14	ILE	C-N	7.41	1.43	1.33
8	h	166	HIS	ND1-CE1	7.41	1.40	1.32
13	m	179	PRO	CA-CB	7.40	1.63	1.53
14	n	124	TYR	N-CA	7.40	1.55	1.46
24	Q	96	VAL	C-N	7.40	1.43	1.33
8	l	191	GLY	CA-C	-7.40	1.43	1.52
24	Q	160	ASP	C-N	7.40	1.43	1.33
5	E	6	SER	CA-C	-7.39	1.44	1.52
4	d	95	SER	CA-C	-7.39	1.43	1.52
27	O	128	LEU	CA-CB	7.39	1.64	1.53
28	H	400	ARG	NE-CZ	7.38	1.41	1.33
28	H	453	GLY	CA-C	-7.38	1.43	1.52
24	Q	353	PRO	C-N	7.38	1.44	1.33
10	j	74	TYR	C-N	7.38	1.44	1.33
21	N	770	LYS	CA-CB	7.38	1.63	1.53
6	f	51	ARG	NE-CZ	7.37	1.41	1.33
16	V	171	ARG	NE-CZ	7.37	1.41	1.33
33	J	97	ASP	C-N	7.37	1.43	1.33
7	G	72	ARG	NE-CZ	7.37	1.41	1.33
30	K	185	ARG	CA-C	-7.36	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	273	HIS	CD2-NE2	-7.36	1.29	1.37
24	Q	51	ARG	CZ-NH1	7.36	1.43	1.32
16	V	258	GLU	CA-CB	7.35	1.65	1.53
21	N	528	ARG	CA-C	-7.35	1.42	1.52
25	R	348	LEU	CA-C	-7.35	1.43	1.52
30	K	303	MET	CA-C	7.35	1.62	1.52
11	k	120	ASP	CA-C	-7.34	1.43	1.53
2	B	246	ARG	CZ-NH2	7.34	1.43	1.33
9	i	206	VAL	CA-C	-7.33	1.44	1.52
12	5	145	GLU	N-CA	-7.33	1.36	1.46
8	1	31	THR	C-N	7.32	1.43	1.33
14	n	144	TRP	CA-CB	7.32	1.62	1.52
11	4	126	VAL	CA-C	-7.32	1.43	1.52
29	I	61	ARG	NE-CZ	7.32	1.41	1.33
2	b	32	VAL	C-N	7.31	1.44	1.33
30	K	367	ASP	CA-C	-7.31	1.43	1.52
6	f	71	GLY	C-O	-7.30	1.16	1.24
2	B	227	ILE	N-CA	-7.30	1.39	1.46
2	B	158	PRO	N-CD	-7.29	1.37	1.47
1	A	20	SER	N-CA	-7.29	1.35	1.46
14	7	179	PHE	C-N	7.29	1.43	1.33
27	O	289	GLN	N-CA	7.29	1.55	1.46
31	L	161	ARG	NE-CZ	7.29	1.41	1.33
4	D	40	ASN	N-CA	-7.29	1.39	1.46
28	H	90	ARG	NE-CZ	7.29	1.41	1.33
16	V	100	ARG	NE-CZ	7.28	1.41	1.33
23	P	359	ARG	CD-NE	7.28	1.56	1.46
7	g	59	LEU	C-N	7.28	1.40	1.33
5	e	148	ASP	CA-C	-7.28	1.44	1.52
28	H	414	SER	C-N	7.28	1.43	1.33
22	S	286	TYR	CA-CB	7.28	1.64	1.54
24	Q	347	LEU	C-N	7.27	1.43	1.33
7	g	82	ILE	CA-C	7.27	1.58	1.52
10	3	28	ARG	CD-NE	7.27	1.56	1.46
14	7	248	GLU	CA-C	-7.27	1.43	1.52
16	V	184	ASN	CA-CB	7.27	1.65	1.53
24	Q	370	THR	CA-C	-7.27	1.43	1.52
11	k	33	ASP	N-CA	-7.26	1.37	1.45
3	C	200	THR	C-N	7.26	1.43	1.33
8	1	25	ALA	CA-CB	-7.26	1.42	1.53
4	D	165	GLY	CA-C	-7.26	1.44	1.52
13	6	48	GLU	CA-C	-7.25	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	180	ASP	CA-CB	7.25	1.64	1.53
14	n	146	ALA	CA-C	-7.24	1.43	1.52
11	4	109	LYS	C-N	7.24	1.43	1.33
14	n	50	ASP	C-O	-7.24	1.15	1.24
13	6	141	ARG	NE-CZ	7.24	1.41	1.33
18	X	113	GLU	N-CA	-7.24	1.38	1.46
21	N	752	SER	C-N	7.24	1.43	1.33
12	5	115	PHE	N-CA	7.24	1.54	1.46
17	T	227	PRO	CA-C	7.23	1.62	1.52
5	e	107	ILE	CA-C	-7.23	1.43	1.52
12	5	83	PHE	CA-C	-7.23	1.44	1.53
5	e	139	GLY	CA-C	-7.23	1.41	1.51
24	Q	201	ALA	C-N	7.23	1.43	1.33
27	O	372	GLU	CA-CB	7.22	1.64	1.53
6	F	75	ALA	CA-C	-7.22	1.44	1.52
17	T	99	SER	N-CA	-7.22	1.37	1.46
13	m	219	GLY	CA-C	-7.22	1.44	1.52
21	N	873	ARG	NE-CZ	7.21	1.41	1.33
13	m	209	GLY	CA-C	-7.21	1.45	1.51
25	R	397	ASN	CA-C	-7.21	1.43	1.52
6	f	136	GLY	CA-C	-7.21	1.43	1.51
9	i	126	TYR	CA-C	-7.21	1.44	1.53
7	g	115	ARG	CA-C	-7.20	1.43	1.52
30	K	161	MET	N-CA	-7.20	1.36	1.46
23	P	356	TYR	CA-CB	7.20	1.65	1.53
13	m	223	GLU	N-CA	-7.20	1.37	1.46
1	a	197	GLU	CA-C	-7.19	1.43	1.52
2	B	57	MET	CA-C	-7.19	1.43	1.52
15	W	142	ILE	N-CA	-7.19	1.37	1.46
16	V	74	SER	N-CA	-7.18	1.36	1.45
12	5	109	VAL	CA-CB	-7.17	1.45	1.54
12	l	267	ASP	CA-C	-7.17	1.43	1.52
24	Q	368	LEU	N-CA	7.17	1.54	1.45
8	1	161	VAL	N-CA	-7.17	1.38	1.46
21	N	14	ARG	N-CA	-7.17	1.36	1.46
4	D	175	LEU	C-N	7.17	1.43	1.34
31	L	127	TYR	CA-C	-7.17	1.43	1.52
33	J	66	GLN	C-N	7.16	1.41	1.32
7	g	37	SER	CA-C	-7.16	1.43	1.52
22	S	129	GLU	N-CA	-7.15	1.37	1.46
12	5	108	LYS	CA-CB	7.15	1.63	1.53
24	Q	334	HIS	ND1-CE1	7.15	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	125	ALA	CA-C	-7.14	1.44	1.52
21	N	256	GLN	CA-CB	7.14	1.64	1.53
28	H	77	ALA	N-CA	-7.14	1.40	1.46
21	N	231	ASN	CA-CB	7.14	1.64	1.53
26	U	57	GLU	CA-C	-7.14	1.43	1.52
12	l	96	THR	CA-C	-7.13	1.43	1.52
11	4	153	THR	C-N	7.13	1.43	1.33
22	S	459	GLN	CA-C	-7.13	1.43	1.52
17	T	17	ASN	CA-C	-7.13	1.43	1.52
6	f	221	PRO	C-N	7.13	1.43	1.33
10	j	112	ILE	CA-C	-7.13	1.43	1.52
7	g	244	GLN	C-N	7.13	1.43	1.33
5	e	188	HIS	ND1-CE1	7.12	1.39	1.32
21	N	614	ASN	N-CA	-7.12	1.37	1.46
5	E	37	ALA	CA-C	-7.12	1.44	1.52
26	U	116	ASN	CA-CB	7.12	1.64	1.53
29	I	351	GLU	CA-C	-7.12	1.43	1.53
6	F	117	GLN	N-CA	-7.12	1.37	1.46
3	C	18	ARG	NE-CZ	7.12	1.40	1.33
7	G	58	LEU	CA-C	-7.12	1.43	1.52
27	O	235	HIS	ND1-CE1	7.11	1.39	1.32
21	N	918	GLU	CA-C	-7.11	1.44	1.52
15	W	17	ARG	NE-CZ	7.11	1.40	1.33
2	b	64	VAL	C-N	7.10	1.43	1.33
14	n	125	ILE	CA-CB	7.10	1.62	1.54
29	I	253	ILE	CA-C	-7.10	1.44	1.52
28	H	296	GLU	CA-CB	7.10	1.65	1.53
2	b	204	PHE	C-N	7.09	1.42	1.33
6	F	144	LEU	CA-C	-7.09	1.44	1.52
22	S	233	LEU	CA-C	-7.09	1.43	1.52
12	l	263	HIS	ND1-CE1	7.09	1.39	1.32
32	M	433	TYR	C-N	7.09	1.43	1.33
1	A	233	PHE	C-N	7.08	1.43	1.33
26	U	47	ARG	CA-C	-7.08	1.44	1.52
8	h	51	TRP	NE1-CE2	7.08	1.45	1.37
16	V	41	GLY	C-N	7.08	1.43	1.33
11	k	70	ARG	CD-NE	7.08	1.56	1.46
31	L	83	ASP	C-N	7.08	1.43	1.33
2	b	117	ILE	C-N	7.07	1.43	1.33
14	n	107	ASN	CA-C	-7.07	1.43	1.52
12	5	174	THR	CB-OG1	-7.07	1.32	1.43
21	N	214	LEU	N-CA	-7.07	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	51	LEU	C-N	7.07	1.43	1.33
12	5	203	CYS	CA-C	-7.07	1.44	1.52
16	V	278	LYS	CA-CB	7.07	1.64	1.53
1	a	230	LYS	N-CA	-7.06	1.37	1.46
3	c	50	ARG	CD-NE	7.06	1.56	1.46
16	V	24	LYS	CA-C	-7.06	1.43	1.52
24	Q	13	ARG	CD-NE	7.06	1.56	1.46
13	6	103	HIS	CG-ND1	-7.06	1.30	1.38
13	6	116	HIS	ND1-CE1	7.05	1.39	1.32
25	R	371	PHE	C-N	7.05	1.41	1.33
21	N	880	ARG	NE-CZ	7.05	1.40	1.33
3	c	208	TYR	N-CA	-7.05	1.37	1.46
2	B	26	THR	CA-C	-7.05	1.43	1.52
21	N	739	PHE	CA-CB	7.05	1.65	1.53
13	m	219	GLY	N-CA	-7.04	1.38	1.45
9	i	103	PRO	C-N	7.04	1.43	1.33
1	A	98	LYS	CA-C	-7.04	1.43	1.52
17	T	105	LEU	CA-CB	7.04	1.64	1.53
4	D	78	LEU	N-CA	-7.04	1.37	1.46
3	c	169	THR	C-N	7.03	1.43	1.33
21	N	480	ALA	CA-C	-7.03	1.43	1.52
22	S	63	LEU	CA-CB	7.03	1.64	1.53
25	R	389	GLU	CA-C	-7.03	1.44	1.52
4	d	67	ILE	CA-C	-7.03	1.43	1.52
13	m	124	GLU	CA-C	-7.03	1.42	1.52
5	E	79	SER	CA-C	-7.03	1.44	1.52
17	T	88	TYR	CA-CB	7.02	1.64	1.53
28	H	447	VAL	C-N	7.02	1.43	1.33
9	i	248	ASN	N-CA	-7.02	1.38	1.46
21	N	408	LEU	CA-C	-7.02	1.43	1.52
28	H	51	GLN	N-CA	-7.02	1.37	1.46
6	F	182	ILE	CA-CB	-7.01	1.46	1.54
24	Q	278	VAL	CA-CB	-7.01	1.46	1.54
26	U	127	GLN	C-N	7.01	1.42	1.33
16	V	279	HIS	ND1-CE1	7.01	1.39	1.32
25	R	206	ARG	NE-CZ	7.01	1.40	1.33
25	R	217	HIS	ND1-CE1	7.00	1.39	1.32
29	I	330	LYS	C-N	7.00	1.42	1.34
7	g	35	THR	C-N	7.00	1.43	1.33
1	A	55	SER	CA-C	-6.99	1.44	1.52
26	U	45	THR	CA-C	-6.99	1.44	1.52
31	L	425	VAL	C-N	6.99	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	73	ALA	CA-C	-6.99	1.44	1.52
12	5	212	TYR	C-N	6.99	1.42	1.33
6	f	105	VAL	C-O	-6.99	1.16	1.24
25	R	32	LEU	CA-CB	6.99	1.64	1.53
12	5	210	PHE	CA-C	-6.99	1.43	1.52
10	j	64	ASN	CA-C	-6.98	1.43	1.52
28	H	357	ARG	NE-CZ	6.98	1.40	1.33
29	I	305	THR	CA-C	-6.98	1.44	1.52
6	F	194	VAL	CA-CB	-6.98	1.46	1.54
10	3	108	VAL	N-CA	-6.98	1.37	1.46
10	j	52	GLY	N-CA	-6.98	1.36	1.45
21	N	584	ARG	N-CA	-6.97	1.37	1.46
8	h	20	GLY	C-N	6.97	1.40	1.33
13	m	145	ARG	CD-NE	6.97	1.56	1.46
10	j	138	VAL	N-CA	-6.96	1.38	1.46
28	H	281	GLN	CA-CB	6.96	1.65	1.53
30	K	424	PHE	C-N	6.96	1.42	1.33
2	b	105	PRO	CA-C	6.96	1.58	1.52
2	B	226	GLY	C-N	6.96	1.39	1.33
22	S	314	ASN	CA-C	-6.96	1.43	1.52
12	l	144	ARG	CZ-NH2	6.96	1.42	1.33
21	N	520	GLY	CA-C	6.96	1.60	1.51
14	n	250	MET	N-CA	-6.95	1.37	1.45
5	E	6	SER	N-CA	-6.95	1.38	1.46
22	S	425	ARG	CD-NE	6.95	1.55	1.46
17	T	150	ARG	CD-NE	6.95	1.55	1.46
29	I	410	GLN	N-CA	-6.95	1.37	1.45
14	n	223	ARG	CD-NE	6.95	1.55	1.46
9	i	204	VAL	CA-C	-6.94	1.44	1.52
10	j	191	LYS	CA-CB	6.94	1.65	1.53
2	b	80	PRO	CA-C	-6.94	1.42	1.52
7	g	21	ASN	CA-C	-6.94	1.46	1.53
18	X	37	PRO	C-N	6.94	1.43	1.33
20	Z	743	ILE	CA-CB	-6.94	1.46	1.54
24	Q	188	LEU	C-N	6.94	1.43	1.33
23	P	395	ARG	CZ-NH1	6.94	1.42	1.32
25	R	110	ILE	CA-CB	-6.94	1.47	1.54
27	O	150	LEU	CA-C	-6.94	1.43	1.52
10	j	80	ARG	NE-CZ	6.94	1.40	1.33
10	j	186	VAL	C-N	6.94	1.42	1.33
11	k	86	GLN	CA-C	-6.94	1.44	1.52
13	m	103	HIS	ND1-CE1	6.94	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	160	LEU	C-N	6.94	1.42	1.33
26	U	79	MET	C-N	6.94	1.43	1.33
27	O	281	ALA	C-N	6.93	1.44	1.33
5	e	45	GLY	CA-C	-6.93	1.44	1.52
2	B	68	THR	CA-C	-6.93	1.44	1.52
9	2	204	VAL	CA-C	-6.93	1.44	1.52
3	C	31	HIS	ND1-CE1	6.93	1.39	1.32
15	W	86	HIS	CE1-NE2	-6.93	1.25	1.32
4	D	93	ALA	C-O	-6.92	1.15	1.24
21	N	79	VAL	N-CA	-6.92	1.38	1.46
32	M	106	VAL	C-N	6.92	1.42	1.33
14	n	157	ASP	N-CA	-6.92	1.37	1.46
23	P	136	ARG	NE-CZ	6.92	1.40	1.33
6	f	92	CYS	CA-C	-6.92	1.43	1.52
10	3	121	ILE	N-CA	-6.92	1.38	1.46
21	N	375	HIS	CB-CG	-6.92	1.40	1.50
28	H	390	ARG	CD-NE	6.91	1.55	1.46
4	D	188	VAL	CA-CB	-6.91	1.45	1.54
4	D	173	GLU	CA-C	-6.91	1.43	1.52
15	W	160	ALA	CA-C	-6.91	1.44	1.52
24	Q	202	ARG	CD-NE	6.91	1.55	1.46
29	I	196	GLU	CA-C	-6.91	1.44	1.53
5	e	227	GLY	CA-C	-6.90	1.44	1.52
21	N	683	LEU	N-CA	6.90	1.54	1.46
25	R	411	LEU	C-N	6.90	1.43	1.33
25	R	249	ILE	C-N	6.90	1.43	1.33
22	S	428	ARG	CD-NE	6.90	1.55	1.46
32	M	395	THR	N-CA	-6.90	1.37	1.46
21	N	115	LYS	CA-CB	6.89	1.64	1.53
24	Q	284	ALA	CA-CB	6.89	1.61	1.52
33	J	205	HIS	ND1-CE1	6.89	1.39	1.32
12	l	119	THR	N-CA	-6.89	1.38	1.46
21	N	628	ALA	C-N	-6.89	1.24	1.33
29	I	57	LEU	CA-C	-6.89	1.43	1.52
33	J	129	LYS	CA-C	-6.89	1.44	1.52
2	B	38	LYS	CA-CB	6.88	1.62	1.53
29	I	235	ALA	N-CA	-6.88	1.37	1.46
32	M	159	LEU	CA-C	-6.88	1.45	1.52
12	5	239	ALA	CA-C	-6.88	1.43	1.52
21	N	422	TYR	C-O	-6.87	1.16	1.24
23	P	84	LYS	C-N	6.87	1.42	1.33
33	J	170	HIS	CA-CB	-6.87	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	309	ASP	CA-C	-6.87	1.43	1.52
6	F	134	ILE	C-N	6.87	1.40	1.33
32	M	213	ARG	NE-CZ	6.87	1.40	1.33
24	Q	170	ASP	CA-C	-6.86	1.43	1.52
24	Q	13	ARG	NE-CZ	6.86	1.40	1.33
1	A	88	PRO	CA-CB	6.86	1.64	1.53
16	V	185	ILE	C-N	6.85	1.43	1.33
19	Y	61	GLU	C-N	6.85	1.42	1.33
22	S	393	ARG	CD-NE	6.85	1.55	1.46
24	Q	266	LEU	CA-C	-6.85	1.44	1.52
27	O	272	VAL	CA-C	-6.85	1.44	1.52
27	O	227	ILE	CB-CG1	6.85	1.67	1.53
26	U	15	LEU	N-CA	-6.85	1.38	1.46
4	D	136	ALA	CA-C	-6.84	1.44	1.52
7	g	190	ARG	CD-NE	6.84	1.55	1.46
6	f	183	ASP	C-N	6.84	1.42	1.33
12	l	255	VAL	CA-C	-6.84	1.45	1.52
27	O	104	ALA	CA-C	-6.84	1.43	1.52
2	b	40	THR	CA-C	6.84	1.61	1.52
9	2	93	GLU	C-N	6.84	1.42	1.33
21	N	814	ALA	C-N	6.84	1.42	1.33
1	a	156	LYS	CA-C	-6.83	1.44	1.52
6	f	15	PRO	CA-C	-6.83	1.45	1.52
23	P	183	GLN	CA-C	-6.83	1.44	1.52
2	b	200	VAL	CA-CB	-6.83	1.46	1.54
21	N	636	SER	C-O	-6.83	1.16	1.24
9	2	183	LEU	CA-C	-6.83	1.44	1.52
28	H	300	THR	CA-C	-6.83	1.44	1.52
9	2	143	HIS	ND1-CE1	6.83	1.39	1.32
13	6	35	THR	CA-C	6.83	1.61	1.52
16	V	36	LYS	N-CA	-6.82	1.38	1.46
21	N	439	VAL	N-CA	-6.82	1.38	1.46
3	C	69	LEU	N-CA	-6.82	1.37	1.46
14	7	252	TRP	N-CA	-6.82	1.40	1.46
21	N	731	VAL	CA-C	-6.82	1.44	1.52
6	F	137	TYR	CA-C	-6.81	1.44	1.52
26	U	254	ARG	CD-NE	6.81	1.55	1.46
28	H	88	ARG	CZ-NH1	6.81	1.42	1.32
9	i	134	PRO	CA-CB	6.81	1.63	1.53
7	g	183	HIS	C-O	-6.81	1.19	1.25
22	S	361	THR	C-N	6.81	1.43	1.33
5	e	166	ARG	CZ-NH2	6.80	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	85	VAL	CA-C	-6.80	1.44	1.52
31	L	294	GLY	CA-C	-6.80	1.42	1.51
16	V	48	GLU	C-N	6.80	1.40	1.33
21	N	609	LEU	CA-C	-6.80	1.43	1.52
3	C	86	ILE	N-CA	-6.80	1.38	1.46
30	K	138	ALA	CA-C	-6.80	1.44	1.52
23	P	38	GLN	CA-CB	6.80	1.64	1.53
2	b	190	HIS	C-N	6.80	1.42	1.33
9	2	191	GLY	C-N	6.80	1.42	1.33
21	N	376	LYS	CA-C	6.80	1.61	1.52
33	J	294	THR	CA-C	-6.80	1.44	1.52
1	A	43	LEU	CA-C	-6.79	1.44	1.52
24	Q	408	THR	CA-C	-6.79	1.44	1.52
31	L	93	ASN	CA-C	-6.79	1.43	1.52
12	5	171	SER	CA-CB	6.79	1.63	1.53
11	k	121	TYR	CA-CB	6.79	1.64	1.53
28	H	358	PRO	N-CD	-6.79	1.38	1.47
24	Q	80	HIS	ND1-CE1	6.78	1.39	1.32
1	A	110	TYR	CA-C	-6.78	1.44	1.52
26	U	182	ALA	CA-C	-6.78	1.43	1.52
14	n	136	ARG	NE-CZ	6.77	1.40	1.33
29	I	97	GLU	CA-C	-6.77	1.44	1.52
11	4	95	ARG	NE-CZ	6.77	1.40	1.33
10	3	45	HIS	CE1-NE2	-6.77	1.25	1.32
28	H	107	LYS	CA-C	6.77	1.61	1.52
3	C	136	ILE	CA-C	-6.76	1.44	1.52
22	S	280	ASN	CA-CB	6.76	1.63	1.53
3	C	244	ILE	CA-C	-6.76	1.44	1.52
9	2	123	ILE	CA-CB	6.76	1.62	1.54
25	R	102	LEU	CA-C	-6.76	1.43	1.52
26	U	17	SER	CA-C	-6.76	1.44	1.52
3	C	94	HIS	CB-CG	6.76	1.59	1.50
29	I	276	PRO	C-N	6.76	1.42	1.33
5	e	54	ALA	N-CA	-6.75	1.36	1.45
4	D	141	ARG	CD-NE	6.75	1.55	1.46
15	W	173	THR	N-CA	-6.75	1.38	1.46
31	L	78	ARG	CZ-NH2	6.75	1.42	1.33
9	2	32	ILE	CA-CB	-6.75	1.45	1.54
5	e	26	TYR	N-CA	-6.75	1.38	1.46
27	O	114	GLN	CA-CB	6.75	1.64	1.53
2	B	114	VAL	CA-CB	-6.75	1.45	1.54
17	T	51	TYR	C-O	-6.75	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	765	ASP	C-N	6.75	1.43	1.33
6	f	39	ARG	NE-CZ	6.75	1.40	1.33
4	D	112	TYR	C-N	6.74	1.42	1.33
29	I	137	ASP	CA-C	-6.74	1.44	1.52
26	U	223	HIS	ND1-CE1	6.74	1.39	1.32
28	H	408	SER	C-N	6.74	1.43	1.33
30	K	185	ARG	NE-CZ	6.74	1.40	1.33
21	N	573	HIS	CA-C	-6.74	1.44	1.52
27	O	142	ASP	CA-C	-6.74	1.44	1.53
3	C	32	ALA	N-CA	-6.74	1.38	1.45
12	5	105	THR	CA-C	6.74	1.61	1.52
7	G	201	TYR	N-CA	6.73	1.54	1.46
24	Q	103	LYS	C-N	6.73	1.42	1.33
17	T	113	LEU	CA-C	-6.73	1.44	1.52
4	d	127	ARG	NE-CZ	6.73	1.40	1.33
9	2	162	ALA	C-N	6.73	1.43	1.33
13	6	115	VAL	N-CA	-6.73	1.38	1.46
9	2	230	LYS	C-N	6.72	1.42	1.33
25	R	302	ALA	CA-C	-6.72	1.44	1.52
2	B	75	TYR	CA-C	-6.72	1.44	1.52
14	7	126	PHE	CA-CB	6.72	1.64	1.53
21	N	654	GLN	CA-CB	6.72	1.63	1.53
9	i	153	TYR	CA-CB	6.72	1.65	1.53
2	b	66	LEU	CA-C	-6.72	1.44	1.52
14	n	127	GLU	CA-C	-6.72	1.44	1.52
22	S	239	ARG	CD-NE	6.72	1.55	1.46
14	7	168	VAL	C-O	-6.71	1.16	1.24
13	6	62	ALA	N-CA	-6.71	1.38	1.46
33	J	270	ARG	CZ-NH1	6.71	1.42	1.32
21	N	760	GLY	CA-C	-6.70	1.45	1.52
14	n	95	HIS	ND1-CE1	6.70	1.39	1.32
21	N	205	SER	CA-C	-6.70	1.44	1.52
33	J	308	GLY	CA-C	-6.70	1.42	1.51
30	K	371	LEU	C-N	6.70	1.42	1.33
33	J	374	ARG	NE-CZ	6.70	1.40	1.33
3	C	94	HIS	ND1-CE1	6.70	1.39	1.32
6	F	69	HIS	CG-ND1	-6.70	1.30	1.38
5	E	20	ARG	CZ-NH1	6.69	1.42	1.32
9	i	70	ILE	CA-C	-6.69	1.47	1.53
18	X	21	SER	C-N	6.69	1.43	1.33
21	N	911	LYS	CA-C	-6.69	1.43	1.52
28	H	404	TRP	N-CA	-6.69	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I	173	MET	CA-C	-6.69	1.44	1.52
14	n	94	GLN	CA-C	-6.68	1.44	1.52
21	N	576	VAL	N-CA	-6.68	1.38	1.46
29	I	59	LEU	C-N	6.68	1.42	1.33
8	h	152	ARG	CD-NE	6.68	1.55	1.46
20	Z	634	ASP	C-N	6.68	1.42	1.33
33	J	86	VAL	CA-C	-6.68	1.44	1.52
4	d	148	TYR	CA-C	-6.68	1.44	1.52
24	Q	271	MET	CA-C	-6.68	1.44	1.52
4	d	205	THR	CA-C	6.68	1.61	1.53
13	m	181	LYS	CA-CB	6.68	1.62	1.53
1	A	83	VAL	CA-CB	-6.68	1.45	1.54
17	T	246	GLU	CA-CB	6.68	1.63	1.53
33	J	324	ARG	CD-NE	6.68	1.55	1.46
2	b	227	ILE	CA-C	-6.67	1.46	1.52
33	J	349	LYS	CA-C	-6.67	1.44	1.52
9	2	64	HIS	ND1-CE1	6.67	1.39	1.32
31	L	80	ASN	C-N	6.67	1.42	1.33
31	L	144	VAL	CA-C	-6.67	1.44	1.52
13	m	170	PRO	N-CD	-6.67	1.38	1.47
11	4	10	GLN	N-CA	6.67	1.54	1.46
8	1	112	ASP	N-CA	-6.66	1.37	1.45
13	6	75	ARG	CD-NE	6.66	1.55	1.46
13	6	144	CYS	C-N	6.66	1.41	1.33
21	N	428	VAL	CA-CB	-6.66	1.45	1.54
24	Q	172	PRO	N-CA	-6.66	1.40	1.47
28	H	436	LYS	C-N	6.66	1.39	1.33
22	S	285	ASP	CA-C	-6.66	1.44	1.52
26	U	66	TRP	CA-C	-6.66	1.44	1.52
18	X	39	GLU	C-N	6.66	1.43	1.33
13	6	128	GLY	CA-C	-6.66	1.46	1.52
29	I	339	ILE	CA-CB	-6.66	1.45	1.54
13	m	48	GLU	CA-C	-6.65	1.44	1.52
6	F	143	HIS	CE1-NE2	6.65	1.39	1.32
14	n	245	LEU	N-CA	-6.65	1.37	1.45
11	4	139	TYR	N-CA	-6.65	1.38	1.46
11	4	147	HIS	ND1-CE1	6.65	1.39	1.32
23	P	401	ASN	CA-C	-6.65	1.44	1.52
7	g	91	ARG	C-O	-6.65	1.15	1.24
13	m	184	SER	C-N	6.65	1.41	1.34
13	m	58	ILE	CA-CB	-6.65	1.46	1.54
24	Q	202	ARG	CZ-NH1	6.65	1.42	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	308	ASN	CA-CB	6.65	1.63	1.53
33	J	13	GLU	CA-CB	6.65	1.58	1.53
29	I	161	GLN	C-N	6.65	1.41	1.33
1	A	104	PHE	CA-C	-6.64	1.44	1.52
10	j	105	VAL	CA-CB	-6.64	1.45	1.54
21	N	172	SER	C-N	6.64	1.42	1.33
1	A	190	LYS	CA-CB	6.64	1.63	1.53
5	E	176	SER	CA-C	-6.64	1.44	1.52
8	1	185	VAL	CA-C	-6.64	1.44	1.52
31	L	107	GLU	CA-C	-6.64	1.44	1.52
27	O	171	PHE	CA-C	-6.63	1.44	1.52
11	4	118	GLN	CA-C	-6.63	1.44	1.52
16	V	106	GLY	C-N	6.63	1.41	1.33
18	X	22	ARG	NE-CZ	6.63	1.40	1.33
5	e	234	GLU	C-N	6.63	1.43	1.34
11	k	68	SER	N-CA	-6.63	1.37	1.46
27	O	163	ILE	N-CA	-6.63	1.40	1.46
27	O	387	ARG	NE-CZ	6.63	1.40	1.33
27	O	391	ILE	C-N	6.63	1.41	1.33
28	H	187	LEU	CA-C	6.63	1.58	1.52
30	K	318	THR	CA-C	6.62	1.60	1.52
21	N	127	ASP	C-N	6.62	1.42	1.33
18	X	104	LYS	CA-C	-6.62	1.44	1.52
32	M	17	GLU	CA-CB	6.62	1.63	1.53
21	N	392	GLY	CA-C	-6.61	1.42	1.51
32	M	176	PRO	CA-C	-6.61	1.45	1.52
10	3	20	CYS	CA-C	-6.61	1.44	1.52
15	W	163	ASN	CA-C	6.61	1.59	1.52
33	J	25	GLN	CA-CB	6.61	1.63	1.53
22	S	360	PHE	CA-CB	6.61	1.63	1.53
1	a	131	ARG	NE-CZ	6.61	1.40	1.33
4	d	121	THR	CA-C	-6.61	1.46	1.53
10	j	197	LYS	CA-C	-6.61	1.44	1.52
32	M	46	SER	C-N	6.61	1.43	1.34
29	I	275	ALA	N-CA	6.61	1.54	1.45
23	P	86	HIS	ND1-CE1	6.60	1.39	1.32
17	T	220	PHE	CA-CB	6.60	1.63	1.53
9	2	138	HIS	CG-ND1	-6.60	1.30	1.38
11	4	8	ARG	CD-NE	6.60	1.55	1.46
17	T	29	PRO	N-CD	-6.60	1.38	1.47
21	N	328	PHE	C-N	6.60	1.43	1.33
24	Q	241	GLU	N-CA	-6.60	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	168	LEU	CA-C	-6.59	1.43	1.52
14	7	44	VAL	CA-CB	-6.59	1.45	1.54
14	7	122	PRO	CA-C	-6.59	1.42	1.52
26	U	195	LYS	CA-CB	6.59	1.63	1.53
27	O	202	SER	CA-CB	6.59	1.61	1.53
29	I	184	ILE	C-N	6.59	1.41	1.33
4	d	227	GLU	C-N	6.59	1.42	1.33
7	g	78	TYR	CA-C	-6.59	1.44	1.52
26	U	21	HIS	C-N	6.59	1.42	1.33
28	H	346	ARG	NE-CZ	6.59	1.40	1.33
7	G	35	THR	CA-C	-6.59	1.44	1.52
2	b	101	TYR	CA-C	-6.59	1.44	1.52
10	j	190	ILE	CA-C	-6.58	1.44	1.52
11	4	27	VAL	C-N	6.58	1.43	1.33
13	6	203	HIS	N-CA	-6.58	1.38	1.46
30	K	73	ARG	N-CA	-6.58	1.38	1.46
16	V	103	MET	C-N	6.58	1.41	1.33
18	X	11	ARG	CD-NE	6.58	1.55	1.46
32	M	359	GLN	CA-CB	6.58	1.63	1.53
5	e	30	ALA	N-CA	-6.58	1.37	1.46
15	W	11	ASP	CA-C	-6.58	1.44	1.52
20	Z	728	LYS	CE-NZ	6.58	1.69	1.49
9	2	71	TRP	NE1-CE2	-6.58	1.30	1.37
14	7	197	ASP	CA-C	-6.58	1.43	1.52
3	C	173	GLN	C-N	6.58	1.42	1.33
27	O	12	SER	CA-C	-6.58	1.44	1.52
21	N	104	LYS	C-N	6.57	1.42	1.33
12	l	81	PHE	CA-C	-6.57	1.44	1.52
13	m	94	ILE	CA-CB	-6.57	1.46	1.54
26	U	189	ARG	NE-CZ	6.57	1.40	1.33
12	5	153	ALA	CA-C	-6.57	1.44	1.52
11	k	191	GLN	C-N	6.57	1.41	1.33
4	D	236	ILE	CA-CB	-6.57	1.46	1.54
9	i	123	ILE	CA-C	-6.56	1.45	1.52
15	W	88	ALA	CA-CB	6.56	1.63	1.53
21	N	623	PHE	C-N	6.56	1.42	1.33
25	R	204	TRP	CA-C	-6.56	1.43	1.52
30	K	106	ASN	CA-C	-6.56	1.44	1.52
4	d	181	ARG	N-CA	6.56	1.54	1.46
11	4	58	GLU	CA-C	-6.56	1.43	1.52
27	O	12	SER	N-CA	6.56	1.54	1.46
27	O	249	ASP	N-CA	-6.56	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	440	HIS	ND1-CE1	6.56	1.39	1.32
33	J	32	LEU	CA-CB	6.56	1.63	1.53
11	k	156	GLU	C-N	6.55	1.41	1.33
21	N	769	PRO	CA-CB	6.55	1.62	1.53
10	j	144	ASP	CA-C	-6.55	1.44	1.52
4	D	35	GLY	CA-C	-6.55	1.42	1.51
5	e	226	ASP	CA-CB	-6.55	1.44	1.54
5	E	208	MET	C-N	6.55	1.43	1.33
12	5	128	GLN	C-N	6.55	1.41	1.33
13	6	220	VAL	CA-C	-6.55	1.44	1.52
2	B	218	ASN	C-N	-6.55	1.27	1.34
25	R	325	HIS	ND1-CE1	6.55	1.39	1.32
2	b	4	ARG	C-N	6.54	1.42	1.33
3	C	105	ASP	C-N	6.54	1.41	1.33
24	Q	231	ASP	CA-C	-6.54	1.44	1.52
3	c	188	ASP	CA-CB	6.54	1.63	1.53
10	j	99	ARG	NE-CZ	6.54	1.40	1.33
28	H	299	ARG	CD-NE	6.54	1.55	1.46
7	g	196	ALA	N-CA	6.54	1.54	1.46
30	K	59	GLU	N-CA	-6.54	1.37	1.46
16	V	79	SER	N-CA	-6.54	1.37	1.45
2	B	88	LYS	CA-C	-6.54	1.44	1.52
12	5	127	CYS	CA-C	-6.54	1.44	1.53
11	4	56	PHE	CA-C	-6.53	1.43	1.52
21	N	826	GLU	CA-C	-6.53	1.44	1.52
7	g	16	SER	N-CA	-6.53	1.40	1.45
27	O	111	SER	CA-C	-6.53	1.44	1.52
30	K	333	ARG	CD-NE	6.53	1.55	1.46
13	m	187	GLU	C-N	6.53	1.42	1.33
5	E	3	LEU	CA-CB	6.52	1.62	1.53
7	G	174	ALA	CA-CB	6.52	1.64	1.53
21	N	238	ALA	C-O	6.52	1.31	1.24
6	F	194	VAL	N-CA	-6.52	1.39	1.46
11	4	70	ARG	NE-CZ	6.52	1.40	1.33
29	I	355	LEU	CA-C	-6.52	1.44	1.52
13	m	91	LYS	C-N	6.52	1.43	1.33
9	i	112	LEU	C-O	-6.51	1.16	1.24
21	N	272	ILE	C-N	6.51	1.42	1.33
24	Q	151	TYR	N-CA	6.51	1.54	1.46
2	B	11	THR	C-N	6.51	1.42	1.33
21	N	208	ARG	CZ-NH2	6.51	1.42	1.33
24	Q	6	SER	N-CA	-6.51	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	156	LEU	C-N	6.51	1.41	1.33
5	E	146	GLY	C-N	6.51	1.42	1.33
8	1	24	GLY	CA-C	-6.51	1.44	1.51
33	J	403	LEU	C-N	6.51	1.41	1.33
10	3	28	ARG	NE-CZ	6.50	1.40	1.33
11	4	190	ARG	C-N	6.50	1.42	1.33
11	k	161	LEU	N-CA	-6.50	1.38	1.46
13	6	213	LEU	N-CA	-6.50	1.38	1.46
21	N	918	GLU	CA-CB	6.50	1.62	1.53
22	S	251	SER	C-N	6.50	1.42	1.33
3	c	60	ASP	N-CA	-6.50	1.37	1.46
25	R	400	TYR	CA-C	-6.50	1.44	1.52
27	O	42	SER	CA-C	-6.50	1.44	1.52
8	1	42	LYS	CA-CB	6.50	1.63	1.54
24	Q	144	LEU	N-CA	6.50	1.54	1.46
28	H	162	ARG	CA-C	-6.50	1.44	1.52
4	d	143	ASP	CA-C	-6.49	1.44	1.52
16	V	55	GLY	N-CA	-6.49	1.37	1.45
7	G	188	SER	CA-C	-6.49	1.44	1.52
21	N	427	ILE	CA-C	-6.49	1.44	1.52
12	5	129	PHE	C-N	6.49	1.42	1.33
27	O	71	ASP	N-CA	6.49	1.52	1.46
31	L	175	GLN	C-N	6.49	1.41	1.33
31	L	194	ARG	CD-NE	6.49	1.55	1.46
2	B	141	GLU	CA-CB	6.48	1.64	1.53
2	B	94	HIS	CA-C	-6.48	1.44	1.52
7	g	207	ASN	CA-CB	6.48	1.61	1.53
21	N	338	PHE	CA-CB	6.48	1.63	1.53
8	h	193	GLU	CA-CB	6.48	1.63	1.53
9	i	217	ARG	N-CA	-6.48	1.37	1.46
7	G	122	ALA	N-CA	-6.48	1.38	1.46
13	6	31	LEU	C-N	6.48	1.42	1.33
1	a	100	GLU	CA-C	-6.47	1.44	1.52
5	E	132	ARG	CA-C	-6.47	1.44	1.52
27	O	333	SER	CA-CB	6.47	1.63	1.53
31	L	265	GLU	C-N	6.47	1.43	1.33
21	N	880	ARG	CA-CB	6.47	1.64	1.53
18	X	55	LYS	CA-CB	6.47	1.62	1.53
24	Q	189	ARG	NE-CZ	6.47	1.40	1.33
8	1	126	GLY	CA-C	-6.47	1.42	1.51
25	R	175	ALA	CA-C	-6.47	1.44	1.52
24	Q	115	ILE	CA-CB	-6.46	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	189	PRO	C-N	6.46	1.42	1.33
28	H	336	LEU	CA-C	-6.46	1.43	1.52
9	i	219	TYR	CA-C	-6.46	1.44	1.52
30	K	253	MET	N-CA	-6.46	1.38	1.46
1	a	131	ARG	CZ-NH1	6.46	1.41	1.32
3	c	75	VAL	C-N	6.46	1.42	1.33
30	K	235	ILE	CA-C	-6.46	1.44	1.52
12	l	90	ALA	CA-C	-6.46	1.44	1.52
24	Q	320	GLN	CA-C	-6.46	1.43	1.52
2	B	237	LYS	N-CA	-6.46	1.38	1.46
5	E	77	ALA	C-N	6.46	1.42	1.33
18	X	93	SER	C-N	6.46	1.41	1.33
29	I	206	GLU	CA-C	-6.46	1.44	1.52
25	R	309	LEU	CA-C	-6.45	1.44	1.52
27	O	218	SER	C-N	6.45	1.42	1.33
28	H	198	MET	CA-C	-6.45	1.44	1.52
29	I	54	ARG	NE-CZ	6.45	1.40	1.33
31	L	251	ILE	CB-CG1	6.45	1.66	1.53
33	J	54	LYS	CA-CB	6.45	1.63	1.53
10	3	111	GLY	C-O	-6.45	1.17	1.23
33	J	81	ASP	N-CA	-6.45	1.37	1.46
23	P	31	ASP	CA-CB	6.45	1.64	1.53
16	V	64	ASN	C-N	6.44	1.41	1.33
2	b	99	ARG	CA-C	-6.44	1.44	1.52
11	k	119	ILE	CA-C	-6.44	1.44	1.52
4	D	147	LEU	CA-C	-6.44	1.45	1.52
30	K	295	ILE	C-N	6.44	1.42	1.33
21	N	637	ALA	N-CA	-6.44	1.38	1.46
1	A	91	ARG	CD-NE	6.44	1.55	1.46
4	D	127	ARG	C-O	-6.43	1.16	1.24
30	K	406	ASP	CA-CB	6.43	1.63	1.53
31	L	409	HIS	CD2-NE2	6.43	1.45	1.37
31	L	419	VAL	CA-C	-6.43	1.44	1.52
14	7	251	LYS	CA-CB	6.43	1.63	1.53
23	P	184	MET	C-N	6.43	1.42	1.33
3	C	217	ARG	CA-C	-6.43	1.45	1.52
5	E	188	HIS	ND1-CE1	6.43	1.39	1.32
2	b	135	LEU	CA-C	-6.43	1.44	1.52
22	S	171	TYR	C-N	6.43	1.42	1.33
31	L	237	ALA	C-N	6.43	1.42	1.33
10	j	143	SER	CA-CB	6.42	1.63	1.53
10	3	103	TYR	C-N	6.42	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	180	LYS	CA-C	-6.42	1.44	1.52
29	I	158	GLY	C-N	6.42	1.41	1.33
26	U	51	SER	CA-C	-6.42	1.44	1.52
26	U	295	LYS	CA-CB	6.42	1.63	1.53
26	U	148	THR	CA-C	-6.42	1.45	1.52
21	N	884	PHE	N-CA	-6.42	1.38	1.46
27	O	312	ASP	C-N	6.42	1.42	1.33
27	O	336	LEU	C-N	6.42	1.42	1.33
29	I	239	GLN	C-N	6.42	1.42	1.33
9	i	57	ASP	CA-C	-6.42	1.44	1.52
5	E	60	GLU	N-CA	-6.42	1.38	1.46
12	5	166	LYS	C-N	6.41	1.40	1.33
21	N	599	TYR	CA-C	-6.41	1.44	1.52
32	M	33	ARG	CD-NE	6.41	1.55	1.46
9	2	145	HIS	ND1-CE1	6.41	1.39	1.32
7	G	64	ASN	CA-C	-6.41	1.44	1.52
15	W	172	LEU	N-CA	-6.41	1.38	1.46
22	S	115	PRO	CA-C	6.41	1.61	1.52
14	n	59	ASN	N-CA	-6.41	1.37	1.46
32	M	407	GLN	CA-C	6.41	1.61	1.52
16	V	104	VAL	C-N	6.41	1.41	1.33
22	S	203	SER	CA-C	-6.41	1.44	1.52
32	M	433	TYR	CA-C	-6.41	1.44	1.52
5	e	82	THR	N-CA	-6.40	1.37	1.46
6	F	51	ARG	NE-CZ	6.40	1.40	1.33
16	V	299	GLY	N-CA	-6.40	1.37	1.45
17	T	266	TYR	CA-C	-6.40	1.44	1.52
26	U	50	ASN	N-CA	6.40	1.54	1.45
33	J	128	ASN	N-CA	-6.40	1.38	1.45
1	A	224	GLU	CA-C	-6.40	1.44	1.52
14	7	214	MET	C-N	6.40	1.41	1.33
2	b	196	LEU	C-N	6.40	1.43	1.33
5	e	136	ARG	NE-CZ	6.40	1.40	1.33
10	j	5	SER	C-N	6.40	1.41	1.33
5	E	134	MET	C-N	6.40	1.42	1.33
8	1	85	GLU	CA-CB	6.40	1.63	1.53
30	K	225	ALA	C-N	6.40	1.41	1.33
30	K	255	ARG	NE-CZ	6.40	1.40	1.33
33	J	324	ARG	NE-CZ	6.40	1.40	1.33
7	g	91	ARG	CD-NE	6.39	1.55	1.46
10	3	15	MET	CA-C	-6.39	1.44	1.52
28	H	290	MET	C-N	6.39	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	279	THR	CA-C	-6.39	1.44	1.52
21	N	470	LEU	CA-CB	6.39	1.63	1.53
3	c	228	LYS	C-N	-6.39	1.25	1.33
3	C	136	ILE	C-O	-6.39	1.17	1.24
17	T	125	GLU	N-CA	-6.39	1.38	1.46
30	K	289	ASP	CA-CB	6.39	1.63	1.53
13	6	93	SER	CA-C	-6.39	1.44	1.53
17	T	149	ASP	CA-CB	6.39	1.63	1.53
2	b	226	GLY	C-N	6.39	1.40	1.33
2	b	244	ASN	C-N	6.39	1.42	1.33
6	F	183	ASP	N-CA	-6.39	1.38	1.46
33	J	273	LEU	CA-C	-6.39	1.44	1.52
26	U	39	GLY	C-N	6.38	1.42	1.33
14	n	171	SER	N-CA	6.38	1.53	1.45
11	4	69	ILE	CA-CB	-6.38	1.46	1.54
28	H	154	LYS	C-N	6.38	1.41	1.33
16	V	111	HIS	CG-ND1	-6.38	1.31	1.38
23	P	14	SER	N-CA	6.38	1.53	1.46
7	g	46	VAL	C-N	6.38	1.41	1.33
13	m	201	GLU	CA-C	-6.38	1.44	1.52
32	M	432	PHE	CA-CB	6.38	1.63	1.53
6	f	120	THR	C-N	6.38	1.42	1.33
5	e	197	GLU	CA-C	-6.37	1.44	1.52
14	7	189	ARG	NE-CZ	6.37	1.40	1.33
16	V	107	TRP	N-CA	-6.37	1.38	1.46
29	I	120	VAL	CA-C	-6.37	1.44	1.52
2	B	234	ARG	C-N	6.37	1.41	1.33
3	C	44	ILE	C-N	6.37	1.41	1.33
16	V	79	SER	C-N	6.37	1.41	1.33
28	H	224	VAL	C-N	6.37	1.42	1.33
1	A	46	ARG	CZ-NH1	6.37	1.41	1.32
5	E	81	LEU	N-CA	-6.37	1.38	1.46
6	F	32	GLY	CA-C	-6.37	1.45	1.52
2	b	169	VAL	CA-C	-6.36	1.44	1.52
3	C	210	ARG	CD-NE	6.36	1.55	1.46
5	E	25	GLU	C-N	6.36	1.42	1.33
5	E	163	THR	CA-C	-6.36	1.45	1.52
8	h	181	VAL	C-N	6.36	1.42	1.33
24	Q	138	SER	CA-C	-6.36	1.44	1.52
8	h	71	HIS	ND1-CE1	6.36	1.39	1.32
29	I	405	ARG	CZ-NH1	6.36	1.41	1.32
32	M	404	ARG	CZ-NH1	6.36	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	285	SER	CA-C	-6.36	1.44	1.52
28	H	219	GLU	N-CA	-6.36	1.38	1.46
32	M	75	LEU	N-CA	-6.35	1.37	1.46
12	l	197	LEU	N-CA	-6.35	1.38	1.46
21	N	597	ARG	C-N	6.35	1.42	1.33
7	g	118	GLN	N-CA	-6.35	1.38	1.46
14	n	96	ILE	CA-C	-6.35	1.44	1.53
10	j	39	LYS	N-CA	-6.35	1.38	1.46
3	c	194	LEU	CA-C	-6.34	1.44	1.52
3	c	206	LEU	CA-C	-6.34	1.45	1.52
22	S	36	LYS	CA-C	6.34	1.61	1.52
32	M	223	PRO	CA-C	-6.34	1.46	1.52
6	f	143	HIS	CA-C	-6.34	1.44	1.52
9	2	218	ASN	CA-C	-6.34	1.45	1.53
11	4	166	GLN	CA-C	-6.34	1.44	1.52
33	J	205	HIS	CA-C	-6.34	1.44	1.52
3	C	166	GLY	N-CA	-6.34	1.39	1.45
8	1	28	ARG	CZ-NH1	6.34	1.41	1.32
29	I	246	ARG	CZ-NH2	6.34	1.41	1.33
1	a	104	PHE	N-CA	-6.33	1.38	1.46
13	m	215	VAL	N-CA	-6.33	1.38	1.46
28	H	403	ARG	CA-C	-6.33	1.45	1.52
8	1	38	ARG	CA-CB	6.33	1.63	1.53
10	3	24	ALA	C-N	6.33	1.41	1.33
13	6	39	THR	N-CA	-6.33	1.38	1.46
1	A	135	ARG	CA-C	-6.33	1.44	1.52
4	D	58	ARG	CZ-NH1	6.33	1.41	1.32
24	Q	12	ARG	CZ-NH1	6.33	1.41	1.32
30	K	128	ARG	NE-CZ	6.33	1.40	1.33
28	H	84	ILE	N-CA	-6.33	1.39	1.46
6	f	19	LEU	N-CA	-6.33	1.38	1.46
15	W	25	ARG	CZ-NH1	6.33	1.41	1.32
21	N	892	PRO	C-N	6.33	1.41	1.33
13	m	163	ASN	CA-C	-6.33	1.43	1.52
9	2	50	THR	N-CA	-6.32	1.38	1.45
10	3	82	ILE	CA-CB	-6.32	1.46	1.54
16	V	239	ALA	CA-C	-6.32	1.44	1.52
10	3	88	THR	N-CA	-6.32	1.38	1.46
16	V	180	LEU	N-CA	-6.32	1.37	1.45
4	D	4	TYR	C-N	6.32	1.42	1.33
22	S	55	ARG	CZ-NH2	6.32	1.41	1.33
7	g	106	PRO	CA-CB	6.32	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	98	ARG	CD-NE	6.32	1.55	1.46
21	N	423	LEU	CA-C	-6.32	1.44	1.52
24	Q	421	LYS	CA-CB	6.32	1.63	1.53
21	N	697	PHE	CA-CB	6.32	1.63	1.53
27	O	143	LEU	N-CA	-6.32	1.37	1.46
6	f	34	VAL	CA-C	-6.31	1.45	1.52
12	l	129	PHE	CA-C	-6.31	1.44	1.52
7	G	157	TYR	CA-CB	6.31	1.64	1.53
14	7	63	TYR	CA-CB	6.31	1.57	1.53
10	3	168	SER	N-CA	-6.31	1.38	1.46
5	E	166	ARG	CA-C	-6.31	1.44	1.52
10	j	89	GLN	CA-C	-6.31	1.44	1.52
6	F	86	ASN	CA-CB	6.31	1.63	1.53
21	N	409	GLY	CA-C	-6.31	1.45	1.52
1	A	133	TYR	N-CA	-6.30	1.38	1.46
6	F	164	ARG	CD-NE	6.30	1.55	1.46
3	C	13	PHE	CA-C	-6.30	1.44	1.52
4	D	63	LYS	N-CA	-6.30	1.38	1.46
17	T	52	LEU	N-CA	-6.30	1.38	1.46
4	d	61	PRO	CA-CB	-6.30	1.44	1.53
6	f	107	ARG	NE-CZ	6.30	1.40	1.33
1	A	62	LYS	N-CA	-6.30	1.37	1.46
21	N	176	GLN	CA-C	-6.29	1.47	1.53
1	a	135	ARG	NE-CZ	6.29	1.40	1.33
7	g	123	HIS	ND1-CE1	6.29	1.38	1.32
9	2	220	LEU	CA-C	-6.29	1.45	1.52
26	U	114	THR	CA-C	-6.29	1.44	1.53
26	U	246	GLU	C-N	6.29	1.41	1.33
16	V	100	ARG	CD-NE	6.29	1.55	1.46
23	P	310	ARG	CD-NE	6.29	1.55	1.46
31	L	238	THR	CA-C	-6.29	1.45	1.52
14	n	137	ARG	NE-CZ	6.29	1.40	1.33
2	B	185	LEU	N-CA	-6.29	1.38	1.46
1	a	138	GLY	N-CA	6.29	1.54	1.45
29	I	100	ARG	CD-NE	6.29	1.55	1.46
31	L	373	GLU	C-N	6.29	1.42	1.33
11	4	110	LYS	C-N	6.28	1.43	1.33
24	Q	346	ASN	C-N	6.28	1.42	1.33
24	Q	409	TYR	CA-CB	6.28	1.63	1.53
32	M	166	ARG	CZ-NH2	6.28	1.41	1.33
1	A	228	ALA	CA-C	-6.28	1.45	1.52
12	5	229	LEU	C-N	6.28	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	301	ASN	CA-C	-6.28	1.44	1.52
21	N	497	ALA	C-N	6.28	1.41	1.33
4	D	172	ARG	CD-NE	6.28	1.55	1.46
15	W	2	VAL	CA-C	-6.28	1.47	1.52
21	N	415	PHE	CA-C	-6.28	1.45	1.53
26	U	231	ASP	CA-C	-6.28	1.44	1.52
28	H	261	ARG	CD-NE	6.28	1.55	1.46
10	j	30	GLY	C-N	6.27	1.41	1.33
28	H	408	SER	CA-C	-6.27	1.44	1.52
7	G	113	ALA	C-N	6.27	1.42	1.33
21	N	813	ARG	CA-CB	6.27	1.63	1.53
29	I	159	VAL	N-CA	-6.27	1.38	1.46
28	H	327	ASN	CA-C	-6.27	1.44	1.52
13	m	193	ARG	C-N	6.27	1.42	1.33
1	a	14	ARG	N-CA	-6.27	1.40	1.46
12	l	264	GLY	N-CA	-6.27	1.38	1.45
13	m	137	GLY	CA-C	-6.27	1.43	1.51
7	G	173	LYS	C-O	-6.26	1.16	1.24
23	P	194	SER	CA-CB	6.26	1.63	1.53
25	R	324	ARG	CD-NE	6.26	1.55	1.46
25	R	357	PHE	N-CA	6.26	1.53	1.46
5	e	112	LEU	CA-C	-6.26	1.44	1.52
12	5	264	GLY	CA-C	-6.26	1.43	1.51
15	W	92	GLN	N-CA	-6.26	1.38	1.46
8	h	10	THR	N-CA	6.26	1.58	1.46
9	2	92	ILE	CA-CB	-6.26	1.46	1.54
22	S	322	LEU	N-CA	-6.26	1.38	1.46
23	P	438	ILE	CA-CB	-6.26	1.45	1.54
2	b	119	GLN	CA-C	-6.26	1.44	1.52
13	m	23	ILE	N-CA	-6.26	1.38	1.46
5	E	60	GLU	CA-C	-6.26	1.45	1.52
30	K	366	ALA	CA-CB	-6.26	1.42	1.53
2	B	134	LEU	CA-C	-6.25	1.45	1.52
28	H	405	GLU	CA-C	-6.25	1.44	1.52
2	b	90	ARG	CA-CB	6.25	1.63	1.53
24	Q	238	TYR	C-N	6.25	1.43	1.33
5	e	108	ASN	CA-C	-6.25	1.44	1.52
8	h	174	TRP	NE1-CE2	6.25	1.44	1.37
11	k	7	ILE	CA-CB	-6.25	1.46	1.54
21	N	94	LYS	CA-C	-6.25	1.44	1.52
24	Q	247	HIS	ND1-CE1	6.25	1.38	1.32
15	W	84	LYS	C-N	6.25	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	117	TRP	NE1-CE2	6.25	1.44	1.37
11	k	37	GLN	CA-CB	6.24	1.62	1.53
30	K	292	VAL	CA-CB	-6.24	1.47	1.54
29	I	155	SER	C-N	6.24	1.39	1.33
17	T	61	ILE	CA-CB	6.24	1.62	1.54
33	J	249	GLU	N-CA	-6.23	1.38	1.46
14	n	161	ARG	CZ-NH1	6.23	1.41	1.32
27	O	157	LEU	C-N	6.23	1.43	1.33
31	L	153	LEU	CA-C	-6.23	1.47	1.53
31	L	423	ALA	CA-C	-6.23	1.44	1.52
11	4	37	GLN	N-CA	-6.23	1.38	1.46
12	5	188	TYR	CA-C	-6.23	1.45	1.52
25	R	217	HIS	C-N	6.23	1.42	1.34
15	W	98	LEU	CA-C	6.23	1.61	1.52
21	N	130	ASP	CA-C	6.23	1.59	1.53
32	M	137	PRO	N-CA	-6.23	1.39	1.47
9	i	215	TYR	CA-CB	6.23	1.61	1.53
19	Y	41	ASP	CA-C	-6.23	1.44	1.52
21	N	684	SER	C-N	6.23	1.42	1.33
24	Q	340	ASP	CA-C	-6.22	1.44	1.52
30	K	399	ARG	NE-CZ	6.22	1.39	1.33
31	L	133	ASN	CA-C	-6.22	1.44	1.52
14	7	250	MET	C-N	6.22	1.41	1.33
21	N	839	ARG	CZ-NH2	6.22	1.41	1.33
4	d	173	GLU	CA-CB	6.22	1.62	1.53
15	W	194	GLU	C-N	6.22	1.44	1.33
2	b	160	LYS	CA-CB	6.21	1.62	1.54
12	5	102	ALA	CA-CB	6.21	1.63	1.53
18	X	85	ARG	CZ-NH1	6.21	1.41	1.32
23	P	106	SER	C-N	6.21	1.42	1.33
13	6	140	GLU	C-N	6.21	1.41	1.33
28	H	52	THR	CA-CB	6.21	1.63	1.53
7	g	72	ARG	NE-CZ	6.21	1.39	1.33
27	O	218	SER	CA-CB	6.21	1.63	1.53
30	K	115	GLY	CA-C	-6.21	1.43	1.51
2	b	106	PRO	CA-C	-6.21	1.45	1.52
24	Q	220	LEU	CA-CB	6.21	1.62	1.53
1	A	160	ALA	CA-C	-6.21	1.44	1.52
5	e	131	GLU	N-CA	-6.21	1.37	1.45
13	6	195	SER	CA-CB	6.21	1.62	1.53
22	S	103	SER	N-CA	-6.21	1.38	1.46
30	K	83	GLN	CA-CB	6.21	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	144	ILE	CA-C	-6.21	1.46	1.53
5	e	209	GLU	N-CA	-6.20	1.37	1.46
23	P	248	ASP	CA-CB	6.20	1.62	1.53
25	R	393	PRO	N-CA	-6.20	1.43	1.47
24	Q	152	LYS	CA-CB	6.20	1.63	1.53
3	c	161	LYS	CA-C	-6.20	1.44	1.52
28	H	292	ARG	CZ-NH1	6.20	1.41	1.32
4	D	49	ARG	CZ-NH1	6.20	1.41	1.32
9	2	171	TRP	CA-C	-6.19	1.44	1.53
21	N	137	PHE	CA-C	6.19	1.60	1.52
25	R	365	ASP	CA-C	-6.19	1.44	1.52
27	O	203	THR	CA-C	-6.19	1.45	1.52
31	L	56	ALA	CA-C	-6.19	1.44	1.52
3	c	32	ALA	CA-C	-6.19	1.44	1.53
2	b	243	ILE	CA-CB	-6.19	1.45	1.54
32	M	192	GLU	CA-CB	6.19	1.63	1.53
19	Y	64	TRP	CA-C	-6.19	1.45	1.53
22	S	39	ASN	CA-CB	6.19	1.62	1.53
6	f	103	LEU	CB-CG	6.18	1.65	1.53
21	N	513	ILE	C-N	6.18	1.42	1.33
10	j	98	ARG	CD-NE	6.18	1.54	1.46
14	n	47	MET	CA-C	-6.18	1.45	1.52
16	V	234	GLU	CA-C	-6.18	1.44	1.52
7	G	210	LYS	CA-C	-6.18	1.45	1.52
19	Y	23	GLU	C-N	6.18	1.41	1.33
21	N	306	ASN	C-N	6.18	1.42	1.33
21	N	528	ARG	CD-NE	6.18	1.54	1.46
4	D	83	ARG	CD-NE	6.18	1.54	1.46
9	2	82	GLU	CA-C	-6.18	1.44	1.52
13	6	103	HIS	ND1-CE1	6.18	1.38	1.32
23	P	422	LEU	C-N	6.17	1.42	1.34
29	I	92	GLU	CA-C	-6.17	1.44	1.52
7	g	214	LEU	CA-C	-6.17	1.45	1.52
14	7	220	ARG	NE-CZ	6.17	1.39	1.33
3	C	140	TYR	C-N	6.17	1.41	1.33
17	T	171	ILE	CA-C	-6.17	1.45	1.52
3	c	72	LYS	CA-CB	6.17	1.63	1.53
9	2	217	ARG	CZ-NH1	6.17	1.41	1.32
23	P	417	HIS	CG-ND1	6.17	1.45	1.38
24	Q	90	LYS	C-O	6.17	1.30	1.23
12	5	144	ARG	CZ-NH1	6.17	1.41	1.32
4	d	225	SER	N-CA	6.17	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I	190	GLN	N-CA	-6.17	1.39	1.46
14	n	68	ARG	CD-NE	6.16	1.54	1.46
5	E	230	ILE	CA-C	-6.16	1.45	1.52
30	K	351	LEU	CA-CB	-6.16	1.43	1.53
10	3	82	ILE	CA-C	-6.16	1.45	1.52
2	b	234	ARG	CD-NE	6.16	1.54	1.46
21	N	483	LEU	C-N	6.16	1.41	1.33
7	g	87	HIS	ND1-CE1	6.16	1.38	1.32
14	7	201	THR	CA-C	-6.16	1.45	1.52
21	N	208	ARG	C-N	6.15	1.42	1.33
17	T	55	LEU	N-CA	-6.15	1.38	1.46
24	Q	88	PHE	CA-C	-6.15	1.45	1.52
11	k	93	ARG	NE-CZ	6.15	1.39	1.33
5	E	181	ALA	CA-CB	-6.15	1.43	1.53
11	4	185	ASP	C-N	6.15	1.42	1.33
7	g	20	ARG	CD-NE	6.15	1.54	1.46
11	k	159	ASP	C-N	6.15	1.42	1.33
21	N	152	LEU	CA-CB	6.15	1.62	1.53
24	Q	130	ARG	CD-NE	6.15	1.54	1.46
24	Q	353	PRO	CA-CB	6.15	1.60	1.53
27	O	29	PHE	CA-CB	6.15	1.62	1.53
29	I	150	HIS	N-CA	-6.15	1.38	1.46
8	h	143	ILE	CA-CB	-6.15	1.48	1.54
12	l	95	ALA	N-CA	-6.15	1.37	1.45
9	i	196	LEU	CA-C	-6.14	1.44	1.52
4	D	30	GLY	C-N	6.14	1.41	1.33
31	L	215	PRO	CA-C	-6.14	1.45	1.52
5	e	42	THR	N-CA	-6.14	1.37	1.46
9	i	136	GLY	N-CA	-6.14	1.38	1.45
10	3	65	GLU	C-N	6.14	1.41	1.33
21	N	795	GLU	CA-C	-6.14	1.44	1.52
23	P	167	THR	CA-C	-6.14	1.44	1.52
26	U	30	ASN	C-N	6.14	1.42	1.33
2	b	51	SER	N-CA	-6.14	1.38	1.45
2	b	7	PHE	CA-C	-6.14	1.45	1.52
14	n	54	ILE	C-N	6.14	1.40	1.33
12	5	260	TRP	CA-CB	6.14	1.62	1.53
24	Q	263	LYS	C-N	6.14	1.42	1.33
13	m	177	LYS	CA-C	-6.14	1.44	1.52
9	2	51	GLN	N-CA	-6.13	1.37	1.47
14	7	194	ARG	NE-CZ	6.13	1.39	1.33
1	A	12	TYR	CA-C	-6.13	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	141	ARG	CZ-NH1	6.13	1.41	1.32
22	S	313	SER	CA-C	-6.13	1.44	1.52
30	K	45	SER	N-CA	-6.13	1.37	1.46
1	a	106	TYR	CA-C	6.13	1.60	1.52
4	d	254	HIS	ND1-CE1	6.13	1.38	1.32
25	R	307	TYR	CA-C	-6.13	1.44	1.52
27	O	339	GLY	N-CA	-6.13	1.38	1.45
6	f	206	LEU	N-CA	-6.12	1.37	1.46
23	P	244	ILE	CA-C	-6.12	1.45	1.52
20	Z	248	TYR	CA-C	-6.12	1.44	1.52
24	Q	106	GLN	C-N	6.12	1.38	1.33
25	R	353	MET	C-N	6.12	1.42	1.33
8	1	45	ARG	CD-NE	6.12	1.54	1.46
29	I	431	ASN	CA-C	-6.12	1.44	1.52
9	i	55	VAL	CA-CB	-6.12	1.46	1.53
14	n	190	LYS	C-N	6.12	1.41	1.33
1	a	224	GLU	C-O	-6.12	1.16	1.23
4	d	26	ALA	C-N	6.12	1.41	1.33
21	N	162	ARG	CD-NE	6.12	1.54	1.46
32	M	161	SER	C-N	6.12	1.41	1.33
4	d	39	LYS	C-O	-6.12	1.15	1.24
21	N	231	ASN	CA-C	6.12	1.60	1.52
12	l	266	HIS	ND1-CE1	6.12	1.38	1.32
13	6	99	ARG	NE-CZ	6.12	1.39	1.33
26	U	94	HIS	CA-C	-6.12	1.45	1.52
32	M	43	ILE	CA-C	-6.12	1.44	1.52
8	h	102	LEU	C-N	6.11	1.42	1.33
10	3	125	ASP	C-N	6.11	1.41	1.33
18	X	129	LEU	CA-C	-6.11	1.45	1.52
29	I	260	GLY	CA-C	-6.11	1.43	1.51
2	b	94	HIS	CE1-NE2	-6.11	1.26	1.32
8	h	182	ILE	CA-C	-6.11	1.45	1.52
22	S	317	HIS	ND1-CE1	6.11	1.38	1.32
24	Q	346	ASN	CA-CB	6.11	1.62	1.53
31	L	282	GLU	C-N	6.11	1.40	1.33
4	d	231	GLN	N-CA	-6.11	1.39	1.46
7	G	73	HIS	C-N	6.11	1.41	1.33
8	1	62	GLN	N-CA	-6.11	1.39	1.46
8	1	198	TYR	CA-CB	6.11	1.62	1.53
27	O	10	ILE	CA-C	-6.11	1.44	1.52
5	E	21	LEU	CB-CG	6.10	1.65	1.53
11	4	92	ILE	CA-C	6.10	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	199	GLU	C-N	6.10	1.41	1.33
9	i	225	ARG	CD-NE	6.10	1.54	1.46
2	B	96	SER	CA-C	-6.10	1.45	1.52
3	C	67	TYR	CA-C	-6.10	1.45	1.52
24	Q	361	HIS	CA-CB	6.10	1.62	1.53
5	e	223	THR	CA-C	-6.10	1.45	1.52
2	B	127	VAL	N-CA	6.10	1.53	1.46
17	T	157	TYR	CA-C	6.10	1.60	1.52
22	S	196	ARG	NE-CZ	6.10	1.39	1.33
30	K	377	SER	CA-C	-6.10	1.47	1.53
22	S	382	ARG	N-CA	-6.10	1.38	1.46
31	L	120	LYS	N-CA	-6.10	1.38	1.46
10	3	203	ARG	NE-CZ	6.10	1.39	1.33
14	n	144	TRP	C-O	6.09	1.31	1.23
5	E	133	LEU	CA-C	-6.09	1.44	1.52
7	G	190	ARG	NE-CZ	6.09	1.39	1.33
13	6	168	TYR	C-N	6.09	1.41	1.33
28	H	234	ARG	NE-CZ	6.09	1.39	1.33
8	h	20	GLY	CA-C	-6.09	1.43	1.51
16	V	81	GLU	C-N	6.09	1.42	1.33
12	l	252	LEU	N-CA	-6.09	1.38	1.46
2	B	87	ASP	CA-C	-6.09	1.45	1.52
6	F	36	VAL	CA-CB	6.09	1.62	1.54
6	F	215	ILE	CB-CG1	6.09	1.65	1.53
22	S	173	LEU	C-N	6.09	1.41	1.33
23	P	299	LEU	C-N	6.09	1.41	1.33
13	6	77	LYS	C-N	6.09	1.42	1.33
33	J	370	LEU	CA-C	-6.09	1.45	1.52
21	N	308	ASN	N-CA	-6.09	1.39	1.46
21	N	535	LEU	N-CA	-6.09	1.38	1.46
30	K	343	LEU	C-N	6.09	1.42	1.33
8	h	147	CYS	CA-C	-6.08	1.45	1.52
21	N	147	ALA	C-N	6.08	1.42	1.33
30	K	88	ARG	CZ-NH1	6.08	1.41	1.32
14	n	164	ASN	C-N	6.08	1.41	1.33
21	N	606	VAL	CA-C	-6.08	1.43	1.52
31	L	362	LYS	N-CA	-6.08	1.38	1.46
1	A	36	ASN	CA-C	-6.08	1.46	1.53
3	C	234	GLU	CA-CB	6.08	1.63	1.53
6	F	89	ARG	CD-NE	6.08	1.54	1.46
13	m	79	SER	CA-CB	6.08	1.63	1.53
2	b	103	GLU	CA-C	-6.08	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	362	ILE	C-O	-6.08	1.17	1.24
6	f	163	ALA	CA-C	-6.07	1.45	1.52
9	2	69	LYS	CA-C	-6.07	1.44	1.52
26	U	274	MET	C-N	6.07	1.41	1.33
11	4	78	GLN	C-N	6.07	1.41	1.33
12	5	221	TRP	CA-CB	6.07	1.62	1.53
4	d	49	ARG	CZ-NH2	6.07	1.41	1.33
11	4	41	HIS	N-CA	-6.07	1.40	1.46
21	N	616	HIS	ND1-CE1	6.07	1.38	1.32
2	b	123	GLN	N-CA	-6.07	1.38	1.45
5	e	4	THR	C-N	6.07	1.42	1.33
4	D	228	GLU	CA-C	-6.07	1.45	1.52
21	N	427	ILE	CA-CB	-6.07	1.47	1.54
18	X	15	CYS	N-CA	-6.07	1.37	1.45
30	K	389	GLU	CA-C	-6.07	1.44	1.52
4	d	111	ARG	CZ-NH2	6.06	1.41	1.33
13	m	202	ARG	NE-CZ	6.06	1.39	1.33
14	7	131	THR	N-CA	-6.06	1.38	1.46
26	U	298	ASN	CA-C	-6.06	1.44	1.52
9	2	217	ARG	CZ-NH2	6.06	1.41	1.33
21	N	36	TRP	NE1-CE2	6.06	1.44	1.37
27	O	81	TYR	CA-C	-6.06	1.45	1.52
33	J	195	LYS	N-CA	-6.06	1.39	1.46
8	h	23	LEU	N-CA	-6.06	1.38	1.45
5	E	247	GLU	C-N	6.06	1.41	1.33
11	4	171	ARG	CD-NE	6.06	1.54	1.46
9	2	110	GLN	N-CA	-6.06	1.39	1.46
11	k	190	ARG	N-CA	6.05	1.53	1.45
6	F	40	SER	CA-C	-6.05	1.48	1.52
32	M	204	ALA	CA-C	-6.05	1.44	1.52
22	S	428	ARG	NE-CZ	6.05	1.39	1.33
23	P	232	ARG	CD-NE	6.05	1.54	1.46
29	I	174	ASP	CA-C	-6.05	1.44	1.52
28	H	364	ALA	N-CA	-6.05	1.38	1.46
17	T	188	GLU	C-N	6.05	1.41	1.33
27	O	74	ASN	C-N	6.05	1.41	1.33
31	L	326	ALA	CA-C	-6.05	1.45	1.52
17	T	122	PHE	CA-C	6.04	1.60	1.52
13	m	112	PRO	N-CA	-6.04	1.40	1.47
6	F	220	THR	CA-C	-6.04	1.48	1.52
10	3	199	TYR	CA-C	-6.04	1.45	1.52
22	S	483	GLU	CA-C	-6.04	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	86	HIS	CA-C	-6.04	1.44	1.52
28	H	329	VAL	CA-CB	-6.04	1.46	1.54
11	k	23	ARG	NE-CZ	6.04	1.39	1.33
10	3	53	ILE	N-CA	-6.04	1.38	1.46
32	M	181	SER	C-N	6.04	1.41	1.33
7	G	21	ASN	CA-C	-6.04	1.47	1.53
13	6	131	TYR	CA-C	-6.04	1.45	1.52
12	l	254	HIS	C-N	6.04	1.40	1.33
24	Q	297	ASP	C-N	6.04	1.41	1.33
26	U	70	HIS	ND1-CE1	6.04	1.38	1.32
28	H	420	ARG	CD-NE	6.04	1.54	1.46
24	Q	112	ASP	N-CA	-6.04	1.39	1.46
24	Q	114	GLN	CA-CB	6.04	1.62	1.53
29	I	101	GLY	C-N	6.04	1.40	1.33
3	c	221	ASN	C-N	6.03	1.42	1.33
18	X	66	LEU	C-N	6.03	1.42	1.33
21	N	309	ILE	CA-C	-6.03	1.45	1.52
23	P	263	HIS	CA-C	-6.03	1.45	1.52
25	R	38	VAL	CA-C	-6.03	1.45	1.52
28	H	318	ARG	CD-NE	6.03	1.54	1.46
12	5	111	GLU	CA-C	-6.03	1.45	1.52
23	P	24	ILE	N-CA	6.03	1.53	1.46
24	Q	26	VAL	C-N	6.03	1.41	1.33
28	H	162	ARG	NE-CZ	6.03	1.39	1.33
2	b	91	LYS	CA-CB	6.03	1.62	1.53
13	6	166	ASN	CA-C	-6.03	1.44	1.52
22	S	270	ALA	C-N	6.03	1.41	1.33
12	5	196	ARG	CZ-NH2	6.03	1.41	1.33
5	e	147	HIS	CB-CG	6.02	1.58	1.50
14	n	189	ARG	CD-NE	6.02	1.54	1.46
5	E	79	SER	C-O	6.02	1.30	1.23
25	R	263	ARG	CZ-NH2	6.02	1.41	1.33
27	O	125	GLY	CA-C	-6.02	1.45	1.52
21	N	208	ARG	CD-NE	6.02	1.54	1.46
31	L	112	LEU	C-N	6.02	1.42	1.33
33	J	118	ASP	C-N	6.02	1.42	1.33
12	5	230	TYR	N-CA	-6.02	1.38	1.46
14	7	91	SER	CA-C	-6.02	1.45	1.52
4	d	122	GLN	CA-C	-6.02	1.44	1.52
21	N	898	GLY	C-N	6.02	1.41	1.33
10	j	139	SER	CA-C	-6.01	1.45	1.52
5	E	249	ALA	N-CA	-6.01	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	505	SER	N-CA	-6.01	1.38	1.46
14	7	137	ARG	CD-NE	6.01	1.54	1.46
7	G	43	ASN	C-N	6.01	1.42	1.33
9	2	169	SER	CA-CB	6.01	1.63	1.53
12	5	274	LYS	CA-C	-6.01	1.45	1.52
21	N	444	HIS	CB-CG	-6.01	1.41	1.50
21	N	843	LYS	N-CA	-6.01	1.39	1.46
21	N	868	VAL	CA-C	-6.01	1.45	1.52
3	c	96	GLN	N-CA	-6.01	1.39	1.46
4	D	88	LYS	CA-C	-6.01	1.45	1.52
22	S	358	LYS	CA-C	-6.01	1.45	1.52
28	H	408	SER	CA-CB	6.01	1.62	1.53
32	M	91	ILE	CA-C	-6.01	1.46	1.53
3	C	134	SER	CA-C	-6.01	1.45	1.52
30	K	338	ILE	CA-CB	-6.00	1.47	1.53
8	h	132	PRO	C-O	-6.00	1.17	1.24
16	V	280	LEU	C-N	6.00	1.41	1.33
32	M	276	THR	C-N	6.00	1.41	1.33
32	M	394	VAL	CA-C	6.00	1.59	1.52
7	g	123	HIS	CB-CG	6.00	1.58	1.50
16	V	80	VAL	N-CA	-6.00	1.38	1.46
29	I	250	SER	CA-C	-6.00	1.44	1.52
10	j	201	LYS	CA-CB	6.00	1.60	1.53
14	n	150	ALA	CA-CB	-6.00	1.42	1.53
2	B	104	TYR	C-N	6.00	1.40	1.33
3	C	208	TYR	CA-CB	6.00	1.62	1.53
21	N	509	GLN	CA-C	-6.00	1.45	1.53
6	f	129	GLY	C-N	5.99	1.40	1.33
5	E	247	GLU	CA-C	-5.99	1.44	1.52
21	N	88	ARG	NE-CZ	5.99	1.39	1.33
25	R	410	LEU	CA-C	-5.99	1.45	1.52
30	K	39	ALA	CA-C	-5.99	1.45	1.53
8	h	90	VAL	N-CA	-5.99	1.39	1.46
11	4	59	TYR	C-N	5.99	1.41	1.33
21	N	549	TYR	C-N	5.99	1.41	1.33
31	L	376	PHE	C-N	5.99	1.41	1.33
5	e	72	ARG	NE-CZ	5.99	1.39	1.33
10	j	95	LEU	CA-CB	5.99	1.62	1.53
5	E	88	MET	CA-C	-5.99	1.44	1.52
14	7	159	PHE	CA-C	-5.99	1.45	1.52
16	V	202	ASP	C-N	5.99	1.41	1.33
1	a	177	GLU	N-CA	-5.99	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	94	ALA	CA-C	-5.99	1.45	1.52
4	d	77	GLY	C-O	-5.99	1.15	1.23
31	L	345	ARG	CA-C	-5.99	1.45	1.52
7	g	22	PHE	CA-CB	5.98	1.62	1.53
4	d	127	ARG	C-N	5.98	1.41	1.33
6	f	29	ILE	N-CA	-5.98	1.39	1.46
29	I	343	ARG	C-N	5.98	1.41	1.33
12	5	208	GLN	N-CA	-5.98	1.38	1.46
16	V	62	THR	C-O	-5.98	1.17	1.24
22	S	54	TRP	CA-CB	5.98	1.62	1.53
22	S	436	ILE	CA-C	-5.98	1.45	1.52
9	i	122	HIS	CD2-NE2	5.98	1.44	1.37
11	k	29	LYS	N-CA	-5.98	1.38	1.46
13	6	42	SER	CA-C	5.98	1.60	1.52
25	R	231	LEU	N-CA	-5.98	1.38	1.46
14	7	170	TYR	CA-CB	5.98	1.63	1.53
21	N	910	PRO	N-CA	-5.98	1.40	1.47
25	R	205	GLU	C-N	5.98	1.42	1.33
13	6	84	HIS	CG-ND1	-5.97	1.31	1.38
21	N	427	ILE	C-N	5.97	1.41	1.33
3	C	64	GLU	CA-C	-5.97	1.44	1.52
7	G	204	HIS	CB-CG	5.97	1.58	1.50
17	T	114	LEU	CA-C	-5.97	1.45	1.52
28	H	234	ARG	CD-NE	5.97	1.54	1.46
31	L	313	ASP	CA-C	-5.97	1.45	1.52
7	g	70	VAL	N-CA	-5.96	1.39	1.46
11	4	190	ARG	CZ-NH1	5.96	1.41	1.32
29	I	422	ARG	NE-CZ	5.96	1.39	1.33
27	O	334	LEU	C-N	5.96	1.41	1.33
4	d	96	HIS	CG-CD2	5.96	1.42	1.35
8	h	111	TYR	CA-C	-5.96	1.45	1.52
14	7	46	SER	CA-C	-5.96	1.44	1.52
15	W	190	ILE	C-N	5.96	1.41	1.33
23	P	58	VAL	C-N	5.96	1.41	1.33
8	h	19	ASP	C-N	5.96	1.42	1.33
25	R	407	GLY	C-N	5.96	1.42	1.34
27	O	327	LEU	CA-C	-5.96	1.45	1.52
28	H	80	HIS	CD2-NE2	5.96	1.44	1.37
14	n	183	MET	CA-CB	5.96	1.60	1.53
10	3	182	GLY	C-N	5.96	1.42	1.33
23	P	263	HIS	ND1-CE1	5.96	1.38	1.32
6	f	150	SER	N-CA	-5.95	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	87	HIS	C-N	5.95	1.42	1.33
23	P	170	SER	CA-CB	-5.95	1.45	1.53
23	P	197	THR	CA-C	-5.95	1.45	1.52
11	k	147	HIS	CA-C	-5.95	1.45	1.52
17	T	236	ASN	C-N	5.95	1.41	1.33
5	e	122	ARG	NE-CZ	5.95	1.39	1.33
3	C	208	TYR	N-CA	5.95	1.53	1.46
6	F	219	ASP	CA-C	-5.95	1.45	1.52
4	D	169	LYS	N-CA	-5.95	1.39	1.46
16	V	55	GLY	CA-C	-5.95	1.44	1.51
30	K	283	ASP	CA-C	-5.95	1.46	1.53
9	2	49	SER	CA-C	-5.95	1.45	1.52
8	h	112	ASP	CA-CB	5.95	1.63	1.53
29	I	411	VAL	CA-C	-5.95	1.45	1.52
32	M	430	VAL	C-N	5.95	1.41	1.33
1	A	176	GLN	CA-C	-5.94	1.45	1.52
28	H	54	ASN	CA-C	5.94	1.60	1.52
30	K	294	ARG	CA-C	5.94	1.60	1.52
33	J	171	PRO	N-CA	-5.94	1.40	1.47
5	e	85	ALA	N-CA	-5.94	1.38	1.46
5	E	48	LEU	CA-C	-5.94	1.45	1.52
13	6	107	GLY	N-CA	-5.94	1.37	1.45
22	S	348	LEU	C-N	5.94	1.42	1.33
24	Q	116	PHE	C-N	5.94	1.41	1.33
2	B	81	ASP	CA-CB	5.94	1.63	1.53
2	b	217	GLU	CA-C	-5.94	1.45	1.52
8	1	194	ARG	CD-NE	5.94	1.54	1.46
13	6	179	PRO	N-CA	-5.94	1.40	1.46
13	6	224	PHE	C-N	5.94	1.42	1.33
3	c	5	ARG	NE-CZ	5.94	1.39	1.33
2	B	132	VAL	CA-C	-5.93	1.45	1.52
10	3	135	ASP	N-CA	-5.93	1.39	1.46
21	N	178	SER	C-N	5.93	1.41	1.33
29	I	181	TYR	C-N	5.93	1.42	1.33
15	W	102	GLN	C-N	5.93	1.40	1.33
27	O	40	GLN	CA-CB	5.93	1.63	1.53
23	P	312	PRO	CA-C	-5.93	1.41	1.52
12	5	234	ARG	NE-CZ	5.93	1.39	1.33
24	Q	127	ARG	NE-CZ	5.93	1.39	1.33
33	J	249	GLU	CA-C	-5.93	1.45	1.52
31	L	406	ASP	CA-C	-5.93	1.48	1.53
31	L	424	GLU	C-N	5.92	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	205	GLY	C-N	5.92	1.42	1.34
24	Q	7	LYS	CA-C	-5.92	1.45	1.52
7	g	35	THR	CA-C	-5.92	1.45	1.52
21	N	274	VAL	C-N	5.92	1.41	1.33
21	N	707	ASN	CA-C	-5.92	1.44	1.52
26	U	197	LEU	CA-C	-5.92	1.45	1.52
29	I	409	MET	N-CA	5.92	1.53	1.46
30	K	77	ARG	CD-NE	5.92	1.54	1.46
23	P	251	LYS	C-N	5.92	1.42	1.34
30	K	373	ILE	N-CA	5.92	1.54	1.46
3	C	241	LYS	CA-CB	5.92	1.62	1.53
29	I	112	ILE	C-N	5.92	1.42	1.33
29	I	421	GLU	C-N	5.92	1.42	1.33
32	M	393	ALA	N-CA	-5.92	1.38	1.46
7	g	140	GLY	C-N	5.92	1.41	1.33
9	i	236	ARG	N-CA	-5.91	1.38	1.46
10	j	62	THR	CA-C	-5.91	1.45	1.52
10	3	131	ASP	CA-CB	5.91	1.60	1.52
24	Q	296	ILE	N-CA	5.91	1.53	1.46
29	I	337	ALA	N-CA	-5.91	1.38	1.46
10	j	68	ARG	CA-CB	5.91	1.62	1.53
12	l	234	ARG	CZ-NH2	5.91	1.41	1.33
3	c	36	ILE	CB-CG1	5.91	1.65	1.53
4	d	212	ILE	C-N	5.91	1.41	1.33
14	n	73	GLU	CA-CB	5.91	1.61	1.53
13	6	183	LEU	N-CA	-5.91	1.39	1.46
31	L	316	ASP	CA-CB	5.91	1.61	1.53
33	J	214	SER	N-CA	-5.91	1.42	1.47
23	P	306	ASN	CA-CB	5.91	1.62	1.53
5	E	14	THR	CA-CB	5.91	1.63	1.53
24	Q	344	GLU	C-N	5.91	1.41	1.33
31	L	152	THR	C-N	5.90	1.40	1.33
27	O	215	TYR	CA-C	-5.90	1.45	1.52
29	I	422	ARG	CD-NE	5.90	1.54	1.46
32	M	107	ASN	CA-C	-5.90	1.45	1.52
9	i	131	GLY	C-N	5.90	1.40	1.33
7	G	91	ARG	NE-CZ	5.90	1.39	1.33
26	U	275	VAL	C-N	5.90	1.41	1.33
28	H	128	ASN	N-CA	-5.90	1.38	1.46
20	Z	743	ILE	CA-C	-5.90	1.45	1.52
33	J	247	MET	CA-C	-5.90	1.45	1.52
28	H	434	ARG	CZ-NH1	5.90	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	115	PHE	CA-C	-5.90	1.45	1.52
9	2	122	HIS	CB-CG	-5.89	1.41	1.50
22	S	51	ARG	CD-NE	5.89	1.54	1.46
24	Q	133	LEU	CA-C	-5.89	1.45	1.52
14	n	74	ARG	NE-CZ	5.89	1.39	1.33
16	V	192	LEU	CA-C	-5.89	1.45	1.52
1	a	69	VAL	CA-C	-5.89	1.46	1.52
3	c	114	ARG	NE-CZ	5.89	1.39	1.33
12	l	224	SER	CA-CB	5.89	1.62	1.53
7	g	167	LYS	CA-CB	5.88	1.62	1.53
16	V	63	VAL	CA-C	-5.88	1.45	1.52
18	X	119	LYS	N-CA	5.88	1.54	1.46
21	N	895	LYS	CA-CB	5.88	1.62	1.53
6	f	187	ASP	CA-C	-5.88	1.44	1.52
10	j	122	ALA	CA-C	-5.88	1.45	1.52
9	2	37	PHE	CA-CB	5.88	1.62	1.53
26	U	300	LYS	N-CA	-5.88	1.39	1.46
4	D	160	SER	C-N	5.88	1.40	1.33
18	X	108	ASN	CA-C	-5.88	1.44	1.52
30	K	214	PRO	CA-C	5.88	1.57	1.52
31	L	157	ARG	CA-CB	5.88	1.63	1.53
33	J	312	ARG	CD-NE	5.88	1.54	1.46
25	R	169	ASP	CA-CB	5.88	1.62	1.53
6	F	174	ARG	NE-CZ	5.88	1.39	1.33
11	k	91	SER	C-N	5.87	1.40	1.33
3	C	211	LEU	N-CA	-5.87	1.38	1.46
13	6	28	PHE	CA-CB	5.87	1.64	1.54
15	W	193	GLU	CA-CB	5.87	1.62	1.53
18	X	103	GLU	CA-C	-5.87	1.45	1.52
25	R	351	LYS	CA-CB	5.87	1.62	1.53
27	O	93	ASP	CA-CB	5.87	1.62	1.53
12	5	82	ARG	CZ-NH2	5.87	1.41	1.33
22	S	464	ARG	CZ-NH2	5.87	1.41	1.33
24	Q	145	HIS	ND1-CE1	5.87	1.38	1.32
30	K	144	ASN	CA-C	-5.87	1.45	1.52
6	f	190	ILE	CA-C	-5.87	1.45	1.52
13	m	105	LEU	CA-CB	5.87	1.62	1.53
15	W	4	GLU	N-CA	-5.87	1.38	1.46
17	T	200	LEU	CA-C	-5.87	1.46	1.53
2	B	44	VAL	CA-CB	-5.87	1.47	1.54
21	N	19	SER	N-CA	-5.87	1.39	1.46
31	L	393	ASN	CA-CB	5.87	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	W	163	ASN	N-CA	-5.87	1.40	1.45
16	V	156	PHE	CA-C	-5.87	1.45	1.52
27	O	58	ARG	NE-CZ	5.87	1.39	1.33
31	L	264	ARG	CZ-NH2	5.87	1.41	1.33
7	G	109	ILE	CA-C	-5.86	1.46	1.52
19	Y	30	GLU	CA-C	-5.86	1.44	1.52
22	S	164	ILE	N-CA	-5.86	1.39	1.46
24	Q	365	ILE	C-N	5.86	1.40	1.34
25	R	173	THR	C-O	-5.86	1.17	1.24
31	L	302	GLN	C-N	5.86	1.41	1.33
8	h	175	ASP	CA-CB	5.86	1.62	1.53
24	Q	275	ILE	CA-CB	-5.86	1.47	1.54
7	g	79	SER	CA-C	-5.86	1.45	1.52
7	g	202	LEU	N-CA	5.86	1.53	1.46
2	B	133	SER	CA-C	-5.86	1.45	1.52
31	L	350	PRO	CA-CB	5.86	1.62	1.53
1	a	106	TYR	N-CA	-5.86	1.39	1.46
9	2	152	TYR	CA-C	-5.86	1.44	1.52
13	6	68	ASP	CA-C	-5.86	1.45	1.52
22	S	117	SER	CA-CB	5.86	1.61	1.53
1	a	78	THR	C-N	5.86	1.40	1.33
6	f	40	SER	CA-C	-5.86	1.45	1.52
26	U	77	ASN	CA-CB	5.86	1.62	1.53
28	H	254	THR	C-N	5.86	1.42	1.33
14	n	190	LYS	CA-C	-5.85	1.44	1.52
6	f	76	GLY	CA-C	-5.85	1.45	1.52
33	J	124	LYS	N-CA	-5.85	1.38	1.45
14	n	216	VAL	CA-CB	5.85	1.61	1.54
2	b	234	ARG	NE-CZ	5.85	1.39	1.33
2	B	6	SER	C-O	-5.85	1.17	1.23
17	T	11	LEU	CA-C	-5.85	1.45	1.52
11	k	149	ARG	CD-NE	5.85	1.54	1.46
3	C	98	TYR	CZ-OH	5.85	1.50	1.38
5	E	229	LYS	N-CA	-5.85	1.38	1.46
11	4	11	ASP	CA-CB	5.85	1.63	1.53
12	5	180	THR	N-CA	5.85	1.53	1.45
33	J	270	ARG	N-CA	-5.85	1.39	1.46
13	m	99	ARG	NE-CZ	5.84	1.39	1.33
24	Q	353	PRO	CA-C	-5.84	1.46	1.52
26	U	193	GLN	CA-C	-5.84	1.45	1.52
27	O	303	LYS	N-CA	-5.84	1.38	1.45
7	g	9	ASP	CA-CB	5.84	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	58	ARG	NE-CZ	5.84	1.39	1.33
3	C	227	GLN	CA-CB	5.84	1.61	1.53
16	V	105	VAL	CA-CB	-5.84	1.47	1.54
2	b	89	SER	N-CA	5.84	1.53	1.46
21	N	470	LEU	N-CA	-5.84	1.39	1.46
23	P	344	ARG	NE-CZ	5.84	1.39	1.33
24	Q	270	ILE	N-CA	-5.84	1.39	1.46
27	O	155	LYS	CA-C	-5.84	1.45	1.52
8	h	140	SER	CA-C	5.84	1.60	1.52
27	O	308	LEU	CB-CG	5.84	1.65	1.53
29	I	376	ASN	CA-CB	5.84	1.62	1.53
4	d	230	ASN	C-N	5.84	1.41	1.33
5	e	11	GLY	CA-C	-5.84	1.46	1.52
25	R	263	ARG	NE-CZ	5.84	1.39	1.33
21	N	770	LYS	C-O	-5.83	1.17	1.24
27	O	121	ASP	CA-C	-5.83	1.45	1.52
30	K	88	ARG	CD-NE	5.83	1.54	1.46
33	J	186	ILE	N-CA	-5.83	1.39	1.46
4	d	99	THR	CA-C	-5.83	1.44	1.52
6	f	207	THR	CA-C	-5.83	1.45	1.52
13	m	194	ASP	C-N	5.83	1.41	1.33
13	6	110	PHE	CA-CB	5.83	1.62	1.53
22	S	275	TYR	C-N	5.83	1.41	1.33
4	D	34	VAL	N-CA	5.83	1.52	1.46
31	L	237	ALA	C-O	-5.83	1.17	1.24
33	J	289	LYS	C-N	5.83	1.42	1.33
4	d	45	GLY	CA-C	-5.83	1.48	1.52
19	Y	20	LYS	CA-C	-5.83	1.45	1.52
27	O	303	LYS	C-N	5.83	1.42	1.33
30	K	112	SER	CA-C	-5.83	1.45	1.53
14	n	80	ASP	C-O	-5.83	1.16	1.24
5	E	73	HIS	ND1-CE1	5.83	1.38	1.32
9	2	32	ILE	CA-C	-5.83	1.45	1.52
22	S	401	LYS	N-CA	-5.83	1.39	1.46
24	Q	274	LEU	CA-C	-5.83	1.45	1.52
33	J	356	ALA	N-CA	-5.82	1.38	1.46
31	L	126	ARG	C-N	5.82	1.41	1.33
25	R	84	LYS	CA-C	-5.82	1.45	1.52
31	L	53	HIS	ND1-CE1	5.82	1.38	1.32
13	m	69	GLY	CA-C	5.82	1.60	1.51
12	5	192	SER	CA-CB	5.82	1.63	1.53
16	V	92	MET	C-N	5.82	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	73	HIS	CA-C	-5.82	1.45	1.52
24	Q	376	LYS	N-CA	-5.82	1.39	1.46
31	L	352	PRO	CA-CB	-5.82	1.45	1.53
1	a	15	HIS	ND1-CE1	5.82	1.38	1.32
9	2	242	LEU	CA-CB	5.82	1.62	1.53
21	N	43	LEU	CA-CB	5.82	1.62	1.53
21	N	582	ASP	CA-CB	5.82	1.62	1.53
23	P	425	HIS	ND1-CE1	5.82	1.38	1.32
27	O	325	GLU	C-N	5.82	1.41	1.33
2	B	114	VAL	CA-C	-5.81	1.44	1.52
18	X	26	PRO	N-CA	-5.81	1.40	1.46
1	a	46	ARG	CZ-NH1	5.81	1.40	1.32
9	i	181	ILE	N-CA	5.81	1.53	1.46
28	H	88	ARG	NE-CZ	5.81	1.39	1.33
29	I	89	GLN	CA-CB	5.81	1.63	1.53
6	f	69	HIS	C-N	5.81	1.41	1.33
10	3	49	VAL	CA-C	-5.81	1.45	1.52
26	U	152	LYS	CA-C	-5.81	1.45	1.52
5	e	92	ALA	C-N	5.81	1.41	1.33
33	J	389	VAL	CA-C	-5.81	1.45	1.52
6	F	37	GLY	C-N	5.81	1.41	1.33
13	6	28	PHE	CA-C	-5.81	1.45	1.52
2	B	236	ARG	NE-CZ	5.80	1.39	1.33
3	C	4	ARG	C-N	5.80	1.41	1.33
14	7	220	ARG	CA-C	-5.80	1.44	1.52
28	H	48	LYS	CA-C	-5.80	1.44	1.52
28	H	406	LEU	C-N	5.80	1.41	1.33
12	l	221	TRP	N-CA	-5.80	1.39	1.46
15	W	84	LYS	N-CA	-5.80	1.39	1.46
30	K	44	ASN	CA-CB	5.80	1.62	1.53
13	6	67	ALA	CA-C	-5.80	1.45	1.52
22	S	234	ILE	N-CA	-5.80	1.39	1.46
23	P	30	ASN	CA-CB	5.80	1.62	1.53
25	R	334	ARG	CZ-NH1	5.80	1.40	1.32
21	N	741	TYR	CA-C	-5.80	1.44	1.52
21	N	789	GLU	CA-C	-5.80	1.45	1.52
33	J	246	PHE	CA-C	-5.80	1.46	1.53
3	c	113	ARG	CD-NE	5.79	1.54	1.46
13	6	184	SER	C-N	5.79	1.41	1.33
8	1	110	GLY	N-CA	-5.79	1.39	1.45
33	J	304	LEU	N-CA	-5.79	1.38	1.46
23	P	131	PHE	N-CA	-5.79	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	397	ASN	N-CA	5.79	1.53	1.46
26	U	293	GLU	CA-C	5.79	1.60	1.52
5	E	37	ALA	CA-CB	5.79	1.64	1.53
15	W	100	HIS	CE1-NE2	-5.79	1.26	1.32
21	N	780	ASP	C-N	5.79	1.40	1.33
25	R	44	LYS	CA-CB	5.79	1.62	1.53
14	n	168	VAL	CA-CB	-5.78	1.47	1.54
28	H	145	TYR	CA-C	-5.78	1.45	1.52
2	b	128	ARG	CA-C	-5.78	1.46	1.52
32	M	357	ARG	C-O	-5.78	1.17	1.24
7	G	86	ARG	CZ-NH1	5.78	1.40	1.32
14	7	175	LEU	N-CA	-5.78	1.39	1.46
14	7	196	SER	N-CA	-5.78	1.38	1.46
15	W	73	LEU	N-CA	-5.78	1.39	1.46
22	S	366	LYS	CA-C	-5.78	1.45	1.52
27	O	35	GLU	N-CA	-5.78	1.38	1.46
30	K	421	VAL	CA-CB	-5.78	1.45	1.54
33	J	5	VAL	CA-CB	-5.78	1.47	1.54
5	e	188	HIS	CA-C	-5.78	1.45	1.52
11	k	104	ILE	N-CA	-5.78	1.39	1.46
26	U	272	GLU	C-N	5.78	1.41	1.33
14	n	117	GLU	C-N	5.78	1.41	1.33
21	N	141	ILE	C-N	5.78	1.41	1.33
21	N	897	LYS	CA-C	-5.78	1.45	1.52
22	S	366	LYS	C-N	5.78	1.41	1.33
31	L	329	ARG	CZ-NH2	5.78	1.41	1.33
32	M	342	ARG	NE-CZ	5.78	1.39	1.33
5	e	117	CYS	C-N	5.78	1.42	1.34
23	P	69	ARG	NE-CZ	5.78	1.39	1.33
23	P	142	ASP	CA-CB	5.78	1.62	1.53
28	H	300	THR	N-CA	5.77	1.53	1.46
2	B	124	SER	N-CA	-5.77	1.38	1.46
14	7	41	GLY	N-CA	5.77	1.50	1.44
23	P	255	ALA	C-O	5.77	1.30	1.24
23	P	257	TRP	CA-CB	5.77	1.62	1.53
25	R	284	ALA	CA-C	5.77	1.60	1.52
12	l	86	GLY	C-N	5.77	1.40	1.33
30	K	194	GLN	CA-CB	5.77	1.63	1.53
1	a	80	GLY	N-CA	-5.77	1.38	1.44
15	W	40	LYS	N-CA	-5.77	1.39	1.46
15	W	101	ARG	CD-NE	5.77	1.54	1.46
27	O	134	ALA	N-CA	-5.77	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	348	ASN	N-CA	-5.77	1.38	1.46
29	I	418	GLN	CA-C	-5.77	1.45	1.52
10	3	15	MET	C-N	5.77	1.41	1.33
7	g	134	VAL	C-N	5.76	1.41	1.33
7	g	187	LEU	CA-CB	5.76	1.63	1.54
13	m	87	HIS	CD2-NE2	5.76	1.44	1.37
22	S	481	TYR	CA-C	5.76	1.59	1.52
25	R	200	LYS	C-N	5.76	1.40	1.33
5	E	188	HIS	C-N	5.76	1.41	1.33
15	W	38	GLN	N-CA	-5.76	1.39	1.46
21	N	379	LEU	C-N	5.76	1.41	1.33
10	3	164	PHE	N-CA	-5.76	1.39	1.46
14	7	210	ILE	C-O	-5.76	1.17	1.24
17	T	131	LYS	C-N	5.76	1.42	1.33
21	N	78	ALA	CA-C	-5.76	1.45	1.52
21	N	340	HIS	CE1-NE2	5.76	1.38	1.32
17	T	235	PHE	CA-C	-5.76	1.44	1.52
18	X	57	VAL	N-CA	-5.76	1.39	1.46
32	M	299	ARG	NE-CZ	5.76	1.39	1.33
9	i	136	GLY	CA-C	-5.76	1.46	1.52
9	2	142	ILE	CA-C	-5.76	1.45	1.52
16	V	208	LYS	N-CA	-5.76	1.39	1.46
26	U	11	ALA	C-N	5.76	1.41	1.33
3	c	96	GLN	C-N	5.75	1.41	1.33
4	D	146	LYS	N-CA	-5.75	1.39	1.46
6	f	92	CYS	C-N	5.75	1.42	1.34
22	S	40	GLU	N-CA	-5.75	1.39	1.46
23	P	99	LYS	CA-CB	5.75	1.62	1.53
25	R	233	ASP	CA-CB	5.75	1.62	1.53
29	I	64	ARG	CD-NE	5.75	1.54	1.46
29	I	126	PRO	N-CA	-5.75	1.40	1.47
29	I	230	THR	N-CA	5.75	1.53	1.46
29	I	262	ARG	CZ-NH2	5.75	1.41	1.33
10	j	80	ARG	C-N	5.75	1.41	1.33
9	2	188	ILE	C-N	5.75	1.41	1.33
15	W	88	ALA	N-CA	-5.75	1.39	1.46
23	P	262	SER	CA-C	-5.75	1.45	1.52
4	d	5	ASP	CA-C	-5.75	1.45	1.52
29	I	76	VAL	CA-C	-5.75	1.45	1.52
9	i	128	ILE	CA-CB	-5.75	1.47	1.54
4	d	204	GLN	C-N	5.75	1.41	1.33
13	m	42	SER	N-CA	-5.75	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	61	LEU	CA-C	-5.75	1.45	1.52
15	W	109	ARG	NE-CZ	5.75	1.39	1.33
9	i	251	ASP	N-CA	5.75	1.53	1.45
18	X	46	TRP	C-N	5.75	1.41	1.33
2	b	194	LEU	CA-C	-5.74	1.45	1.52
6	f	173	GLU	CA-C	-5.74	1.44	1.52
13	m	36	ARG	NE-CZ	5.74	1.39	1.33
13	m	145	ARG	CZ-NH2	5.74	1.41	1.33
2	B	77	GLY	CA-C	-5.74	1.43	1.51
30	K	267	SER	N-CA	-5.74	1.39	1.46
9	i	195	ASP	N-CA	-5.74	1.39	1.46
2	b	146	SER	CA-C	-5.74	1.45	1.52
21	N	303	LEU	C-O	-5.74	1.17	1.24
22	S	152	LEU	CA-CB	5.74	1.63	1.53
22	S	405	ARG	CA-CB	5.74	1.62	1.53
24	Q	160	ASP	CA-C	-5.74	1.45	1.52
27	O	343	GLN	C-N	5.74	1.38	1.33
4	d	15	GLY	N-CA	-5.74	1.37	1.45
2	B	128	ARG	CD-NE	5.74	1.54	1.46
5	E	176	SER	CA-CB	5.74	1.62	1.53
27	O	126	ILE	N-CA	-5.74	1.39	1.46
27	O	356	ARG	CZ-NH1	5.74	1.40	1.32
7	g	93	ARG	NE-CZ	5.74	1.39	1.33
9	i	192	ILE	CA-C	-5.74	1.45	1.52
4	D	116	VAL	CA-C	-5.74	1.44	1.52
14	7	158	GLN	CA-C	-5.74	1.45	1.52
33	J	12	LEU	CB-CG	5.74	1.65	1.53
21	N	787	MET	C-N	5.73	1.40	1.33
24	Q	294	ARG	NE-CZ	5.73	1.39	1.33
27	O	281	ALA	CA-C	-5.73	1.45	1.52
27	O	392	TRP	C-N	5.73	1.41	1.33
6	f	147	PHE	N-CA	-5.73	1.39	1.46
16	V	288	LEU	CA-CB	5.73	1.62	1.53
28	H	435	ARG	CA-C	-5.73	1.45	1.52
29	I	231	LEU	N-CA	-5.73	1.38	1.46
1	A	91	ARG	C-N	5.73	1.41	1.34
4	D	102	ASP	CA-CB	5.73	1.62	1.53
13	6	30	VAL	CA-C	-5.73	1.45	1.52
29	I	349	LEU	CA-C	-5.73	1.45	1.52
7	g	115	ARG	CD-NE	5.73	1.54	1.46
10	j	191	LYS	C-N	5.73	1.41	1.33
5	E	61	SER	CA-C	-5.73	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	117	SER	C-N	5.73	1.41	1.33
22	S	408	CYS	CA-CB	5.73	1.62	1.53
10	3	151	GLU	CA-C	-5.73	1.45	1.52
16	V	104	VAL	CA-C	-5.73	1.46	1.52
32	M	345	ARG	CZ-NH1	5.73	1.40	1.32
9	i	83	ALA	N-CA	-5.72	1.39	1.46
21	N	328	PHE	N-CA	-5.72	1.39	1.46
21	N	567	ALA	C-N	5.72	1.41	1.33
24	Q	372	GLN	CA-C	-5.72	1.45	1.52
2	b	218	ASN	N-CA	-5.72	1.38	1.46
13	m	131	TYR	N-CA	5.72	1.53	1.46
14	n	231	ALA	CA-C	-5.72	1.45	1.52
1	A	181	ASN	C-O	-5.72	1.17	1.24
21	N	18	ASP	N-CA	-5.72	1.39	1.46
21	N	160	GLY	C-O	-5.72	1.16	1.24
25	R	71	LEU	CA-CB	5.72	1.62	1.53
11	k	57	ALA	N-CA	-5.72	1.39	1.46
6	F	111	LEU	CA-CB	5.72	1.62	1.53
7	G	65	VAL	C-N	5.72	1.41	1.33
21	N	373	VAL	CA-CB	-5.72	1.47	1.54
24	Q	47	ASP	C-N	5.72	1.41	1.33
1	a	96	ARG	CZ-NH1	5.72	1.40	1.32
3	c	183	ASP	N-CA	-5.72	1.39	1.46
5	e	10	ARG	CZ-NH1	5.72	1.40	1.32
8	h	138	SER	CA-C	-5.72	1.45	1.52
9	2	219	TYR	C-N	5.72	1.41	1.33
14	7	215	ARG	CA-CB	5.72	1.62	1.53
26	U	243	ASP	CA-CB	5.72	1.62	1.53
32	M	359	GLN	C-N	5.72	1.41	1.33
17	T	236	ASN	CA-CB	5.72	1.62	1.53
22	S	432	ILE	CA-CB	-5.72	1.46	1.54
23	P	66	LEU	C-N	5.72	1.41	1.33
29	I	91	GLU	CA-CB	5.72	1.62	1.53
4	d	237	GLU	C-N	5.72	1.41	1.33
10	j	78	GLU	CA-C	-5.72	1.44	1.52
1	A	183	GLU	CA-C	5.72	1.60	1.52
7	G	20	ARG	CZ-NH1	5.72	1.40	1.32
12	5	202	PHE	CA-C	-5.72	1.45	1.52
12	5	205	GLY	CA-C	-5.72	1.43	1.51
18	X	51	ARG	NE-CZ	5.72	1.39	1.33
22	S	369	GLN	CA-C	5.72	1.60	1.52
25	R	325	HIS	CD2-NE2	-5.72	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	21	GLN	CA-C	5.71	1.60	1.52
5	e	88	MET	CA-C	-5.71	1.45	1.52
7	g	64	ASN	C-O	-5.71	1.17	1.23
9	i	138	HIS	CE1-NE2	-5.71	1.26	1.32
5	E	94	THR	CA-C	-5.71	1.45	1.52
21	N	496	GLU	N-CA	-5.71	1.39	1.46
27	O	255	LEU	CA-CB	5.71	1.62	1.53
32	M	230	LEU	CA-C	-5.71	1.45	1.52
4	d	201	GLU	CA-CB	5.71	1.62	1.53
21	N	14	ARG	CD-NE	5.71	1.54	1.46
4	D	172	ARG	CZ-NH1	5.71	1.40	1.32
13	m	145	ARG	CA-CB	5.71	1.63	1.53
2	B	227	ILE	CA-CB	-5.71	1.47	1.54
11	4	99	GLN	CA-C	-5.71	1.45	1.53
6	f	226	ASP	CA-CB	5.71	1.63	1.53
12	5	266	HIS	CE1-NE2	-5.71	1.26	1.32
23	P	308	LEU	CA-CB	5.71	1.62	1.53
16	V	175	SER	CA-CB	5.70	1.61	1.53
22	S	396	SER	N-CA	-5.70	1.39	1.46
3	c	18	ARG	CA-C	-5.70	1.45	1.52
21	N	51	ASP	N-CA	-5.70	1.39	1.46
28	H	403	ARG	CZ-NH2	5.70	1.40	1.33
8	h	57	SER	CA-C	-5.70	1.45	1.52
24	Q	329	GLU	N-CA	-5.70	1.39	1.46
9	i	38	ASN	CA-CB	5.70	1.62	1.53
4	D	25	GLU	CA-C	-5.70	1.45	1.52
25	R	73	ASN	CA-C	-5.70	1.45	1.52
10	3	109	VAL	N-CA	-5.70	1.39	1.46
33	J	63	ARG	CD-NE	5.70	1.54	1.46
13	m	205	GLN	CA-CB	5.70	1.62	1.53
14	7	215	ARG	CZ-NH2	5.70	1.40	1.33
21	N	473	ASP	C-N	5.70	1.41	1.33
25	R	87	SER	CA-C	-5.70	1.45	1.52
33	J	341	ILE	C-N	5.70	1.41	1.33
11	k	6	GLY	N-CA	-5.69	1.39	1.45
8	h	45	ARG	NE-CZ	5.69	1.39	1.33
9	i	217	ARG	CA-CB	5.69	1.62	1.53
10	j	20	CYS	C-N	5.69	1.41	1.33
21	N	583	VAL	CA-C	-5.69	1.45	1.52
21	N	618	ARG	CD-NE	5.69	1.54	1.46
23	P	177	ILE	C-N	5.69	1.41	1.33
28	H	165	PRO	C-N	5.69	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	154	THR	N-CA	5.69	1.53	1.46
12	5	129	PHE	CA-C	-5.69	1.45	1.52
13	6	221	ARG	CD-NE	5.69	1.54	1.46
25	R	366	ASN	N-CA	-5.69	1.39	1.46
2	b	113	GLU	C-N	5.69	1.41	1.33
21	N	598	ASP	C-N	5.69	1.41	1.33
25	R	210	TYR	CA-CB	5.69	1.62	1.53
29	I	102	ASN	CA-C	-5.69	1.45	1.52
5	e	127	ALA	C-N	5.69	1.41	1.33
12	l	124	ALA	C-O	-5.69	1.17	1.24
33	J	115	LEU	CA-C	-5.68	1.45	1.52
2	b	207	ASP	CA-C	-5.68	1.45	1.52
3	c	163	ILE	N-CA	5.68	1.52	1.46
4	D	210	ILE	N-CA	-5.68	1.39	1.46
21	N	41	ASN	C-N	5.68	1.40	1.33
21	N	534	ASP	CA-CB	5.68	1.62	1.53
22	S	214	MET	CA-C	-5.68	1.45	1.52
29	I	282	ASP	CA-CB	5.68	1.60	1.53
14	n	215	ARG	CZ-NH1	5.68	1.40	1.32
12	5	110	ILE	C-O	-5.68	1.18	1.24
22	S	20	HIS	C-N	5.68	1.41	1.33
24	Q	343	LEU	N-CA	-5.68	1.39	1.46
4	d	225	SER	CA-C	-5.68	1.45	1.52
7	g	87	HIS	C-N	5.68	1.41	1.33
14	n	125	ILE	CB-CG1	5.68	1.64	1.53
15	W	157	PHE	CA-CB	5.68	1.62	1.53
3	c	51	LYS	CA-C	-5.68	1.44	1.52
11	k	53	THR	C-N	5.68	1.41	1.33
15	W	23	ARG	NE-CZ	5.68	1.39	1.33
26	U	225	ILE	CA-CB	5.68	1.62	1.54
4	D	111	ARG	CZ-NH1	5.67	1.40	1.32
3	c	192	LEU	CA-CB	5.67	1.62	1.53
1	A	56	GLN	CA-C	5.67	1.60	1.52
9	2	65	ARG	NE-CZ	5.67	1.39	1.33
15	W	101	ARG	NE-CZ	5.67	1.39	1.33
33	J	16	GLU	CA-CB	5.67	1.60	1.53
2	b	70	ASP	CA-C	-5.67	1.45	1.52
12	5	134	LEU	N-CA	-5.67	1.39	1.46
16	V	67	ASP	N-CA	5.67	1.52	1.46
24	Q	422	VAL	CA-CB	-5.67	1.47	1.54
28	H	320	ASP	N-CA	5.67	1.52	1.45
1	A	167	LYS	N-CA	-5.67	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	912	GLU	CA-CB	5.67	1.62	1.53
14	n	191	VAL	N-CA	-5.67	1.39	1.46
4	D	162	GLN	CA-C	-5.67	1.45	1.52
32	M	373	ASP	CA-CB	5.67	1.61	1.53
8	h	198	TYR	CZ-OH	5.67	1.50	1.38
11	k	99	GLN	C-N	5.67	1.40	1.33
13	m	190	LYS	C-N	5.67	1.41	1.33
9	2	117	PHE	N-CA	-5.67	1.39	1.46
10	3	58	THR	C-N	5.67	1.42	1.33
21	N	835	LYS	N-CA	-5.67	1.38	1.46
23	P	79	LEU	C-O	-5.67	1.17	1.24
30	K	48	TYR	N-CA	-5.67	1.39	1.46
5	e	91	HIS	ND1-CE1	5.67	1.38	1.32
18	X	13	GLY	CA-C	-5.66	1.46	1.52
26	U	248	ASP	CA-C	-5.66	1.45	1.52
31	L	365	THR	N-CA	-5.66	1.38	1.46
4	D	145	PRO	CA-C	-5.66	1.45	1.52
21	N	894	ARG	CD-NE	5.66	1.54	1.46
30	K	252	ARG	C-N	5.66	1.41	1.34
18	X	105	ASN	C-N	5.66	1.40	1.33
14	n	147	ILE	N-CA	-5.66	1.39	1.46
33	J	42	ARG	CA-CB	-5.66	1.44	1.53
12	l	200	ASP	CA-CB	5.66	1.61	1.54
5	E	203	ILE	CA-CB	-5.66	1.46	1.54
17	T	169	GLN	CA-C	-5.66	1.45	1.52
21	N	839	ARG	N-CA	-5.66	1.38	1.45
24	Q	10	GLU	CA-CB	5.66	1.62	1.53
33	J	309	ARG	NE-CZ	5.66	1.39	1.33
27	O	33	TYR	N-CA	-5.65	1.39	1.46
11	4	22	THR	CA-C	-5.65	1.45	1.52
21	N	482	ALA	CA-CB	5.65	1.62	1.53
28	H	384	GLY	CA-C	-5.65	1.44	1.51
5	e	165	TYR	CA-C	-5.65	1.45	1.52
12	l	139	ARG	NE-CZ	5.65	1.39	1.33
12	l	152	ALA	CA-C	-5.65	1.45	1.52
1	A	182	LEU	C-N	5.65	1.41	1.33
10	3	34	LEU	C-N	5.65	1.37	1.33
26	U	49	THR	CA-C	-5.65	1.45	1.52
28	H	278	GLU	CA-C	-5.65	1.45	1.52
4	d	226	SER	CA-CB	5.65	1.62	1.53
8	h	68	VAL	C-N	5.65	1.41	1.33
29	I	204	HIS	ND1-CE1	5.65	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	175	LYS	C-N	-5.65	1.26	1.33
10	j	174	ALA	N-CA	-5.65	1.39	1.46
12	l	112	ILE	N-CA	-5.65	1.39	1.46
21	N	282	TYR	CA-C	-5.65	1.45	1.52
27	O	148	ASP	C-O	-5.65	1.17	1.24
21	N	159	GLU	CA-CB	5.65	1.62	1.53
1	a	25	LEU	CA-C	-5.64	1.46	1.53
25	R	141	TYR	N-CA	-5.64	1.39	1.46
13	m	34	ASP	CA-CB	5.64	1.62	1.53
21	N	381	GLU	C-N	5.64	1.40	1.33
23	P	348	HIS	N-CA	-5.64	1.39	1.46
2	b	174	PHE	CA-C	-5.64	1.45	1.52
5	e	123	PHE	C-N	5.64	1.39	1.32
13	m	145	ARG	N-CA	-5.64	1.39	1.46
4	D	194	LEU	C-O	-5.64	1.16	1.24
13	6	51	VAL	CA-C	-5.64	1.48	1.53
16	V	48	GLU	CA-CB	5.64	1.62	1.53
21	N	825	GLU	CA-C	-5.64	1.45	1.52
22	S	450	ASN	CA-C	-5.64	1.46	1.53
24	Q	28	LEU	C-N	5.64	1.41	1.33
31	L	374	PHE	N-CA	-5.64	1.39	1.46
33	J	35	ARG	NE-CZ	5.64	1.39	1.33
4	d	57	THR	CA-C	-5.64	1.45	1.52
10	j	178	ASP	CA-CB	5.64	1.64	1.54
14	n	186	PRO	C-N	5.64	1.41	1.33
3	C	136	ILE	C-N	5.64	1.41	1.33
23	P	123	ARG	CZ-NH2	5.64	1.40	1.33
26	U	172	GLU	C-N	5.64	1.41	1.33
26	U	203	LYS	CA-C	5.64	1.60	1.52
33	J	342	ASN	C-N	5.64	1.41	1.33
14	n	49	TYR	C-N	5.63	1.41	1.33
9	2	147	SER	CA-C	-5.63	1.45	1.52
26	U	83	ILE	CA-C	-5.63	1.46	1.52
3	c	97	ASN	C-N	-5.63	1.26	1.33
5	e	137	PRO	CA-C	5.63	1.59	1.52
27	O	215	TYR	N-CA	-5.63	1.39	1.46
3	c	217	ARG	NE-CZ	5.63	1.39	1.33
13	6	193	ARG	NE-CZ	5.63	1.39	1.33
23	P	42	LEU	CA-CB	5.63	1.62	1.53
27	O	210	ARG	CD-NE	5.63	1.54	1.46
6	F	221	PRO	N-CA	-5.63	1.40	1.47
21	N	867	LYS	CA-C	5.63	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	149	TYR	C-N	5.62	1.41	1.33
12	5	243	ASP	CA-CB	5.62	1.62	1.53
6	f	149	PRO	N-CD	-5.62	1.39	1.47
7	g	216	ILE	C-N	5.62	1.40	1.33
8	h	24	GLY	N-CA	-5.62	1.37	1.45
8	h	118	GLU	CA-CB	5.62	1.64	1.54
5	E	10	ARG	CZ-NH2	5.62	1.40	1.33
10	3	16	THR	CA-C	-5.62	1.45	1.52
13	6	121	GLY	CA-C	-5.62	1.46	1.52
23	P	101	MET	CA-C	-5.62	1.45	1.52
29	I	120	VAL	N-CA	-5.62	1.39	1.46
33	J	112	ARG	NE-CZ	5.62	1.39	1.33
11	4	11	ASP	C-N	5.62	1.40	1.33
15	W	183	GLU	CA-CB	5.62	1.62	1.53
21	N	339	MET	C-N	5.62	1.41	1.33
21	N	357	GLY	C-N	5.62	1.41	1.33
29	I	97	GLU	N-CA	-5.62	1.39	1.46
31	L	358	LEU	CA-CB	5.62	1.62	1.53
7	g	203	ALA	N-CA	-5.62	1.38	1.46
6	F	185	ASN	N-CA	-5.62	1.40	1.46
27	O	382	LYS	N-CA	-5.62	1.39	1.46
32	M	238	GLN	N-CA	-5.61	1.39	1.46
16	V	163	ALA	CA-CB	5.61	1.62	1.53
13	m	199	ALA	N-CA	5.61	1.53	1.46
9	2	117	PHE	C-N	5.61	1.42	1.33
17	T	110	LEU	C-N	5.61	1.41	1.33
29	I	377	LEU	CB-CG	5.61	1.64	1.53
32	M	277	ILE	C-N	5.61	1.39	1.33
12	5	255	VAL	CA-C	-5.61	1.46	1.52
17	T	102	LYS	CA-C	-5.61	1.45	1.52
9	2	54	ILE	CA-CB	-5.61	1.47	1.54
10	3	101	GLY	CA-C	-5.61	1.43	1.51
24	Q	386	PHE	C-N	5.61	1.40	1.33
7	g	130	ARG	NE-CZ	5.61	1.39	1.33
1	A	91	ARG	CA-C	-5.61	1.45	1.52
5	E	42	THR	CA-CB	-5.61	1.45	1.53
18	X	52	PRO	CA-CB	5.61	1.61	1.53
21	N	204	SER	CA-CB	5.61	1.62	1.53
1	A	194	ILE	CB-CG1	5.60	1.64	1.53
28	H	168	ILE	CA-CB	-5.60	1.47	1.54
7	g	33	ASN	N-CA	5.60	1.52	1.46
25	R	154	LEU	N-CA	-5.60	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	272	ASP	CA-CB	5.60	1.62	1.53
22	S	274	PHE	C-N	5.60	1.41	1.33
26	U	54	LEU	CA-C	-5.60	1.46	1.52
30	K	179	MET	CA-CB	5.60	1.62	1.53
22	S	138	MET	C-O	-5.60	1.17	1.24
23	P	226	LYS	CA-CB	5.60	1.62	1.53
24	Q	165	PHE	N-CA	-5.60	1.39	1.46
3	c	81	THR	C-N	5.60	1.41	1.33
3	c	115	LEU	CA-C	-5.60	1.45	1.52
25	R	161	ALA	CA-C	-5.60	1.46	1.52
4	d	207	ALA	CA-C	-5.59	1.44	1.52
10	j	112	ILE	N-CA	-5.59	1.39	1.46
1	A	184	ASN	CA-CB	5.59	1.62	1.53
22	S	59	ASP	C-N	5.59	1.41	1.33
27	O	222	LEU	CA-CB	5.59	1.62	1.53
28	H	269	ALA	N-CA	-5.59	1.39	1.45
3	c	18	ARG	NE-CZ	5.59	1.39	1.33
6	f	84	LEU	CB-CG	5.59	1.64	1.53
4	d	83	ARG	CZ-NH2	5.59	1.40	1.33
1	A	206	ALA	C-N	5.59	1.41	1.33
8	1	176	GLY	C-N	5.59	1.42	1.33
27	O	34	GLU	CA-CB	5.59	1.62	1.53
2	B	53	SER	CA-C	-5.59	1.46	1.52
2	B	219	PRO	C-O	-5.59	1.17	1.24
13	6	216	THR	CA-C	5.59	1.60	1.53
23	P	298	SER	C-O	-5.59	1.17	1.24
23	P	392	LYS	CA-CB	5.59	1.63	1.53
31	L	137	ARG	NE-CZ	5.59	1.39	1.33
31	L	292	SER	CA-C	-5.59	1.45	1.53
32	M	127	VAL	CA-C	-5.59	1.45	1.52
7	g	64	ASN	N-CA	-5.58	1.39	1.46
1	A	247	ALA	N-CA	-5.58	1.38	1.46
21	N	761	ILE	C-N	5.58	1.41	1.33
1	A	198	SER	N-CA	-5.58	1.39	1.46
5	E	171	ALA	CA-C	-5.58	1.46	1.52
28	H	48	LYS	CA-CB	5.58	1.62	1.53
30	K	318	THR	C-N	5.58	1.41	1.33
9	i	63	LEU	CA-CB	5.58	1.61	1.53
13	m	136	VAL	C-N	5.58	1.41	1.33
18	X	76	VAL	CA-C	-5.58	1.47	1.52
22	S	163	VAL	CA-C	-5.58	1.45	1.52
29	I	100	ARG	N-CA	-5.58	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	23	LYS	CA-C	5.58	1.59	1.52
28	H	79	SER	N-CA	5.58	1.53	1.46
11	k	68	SER	CA-CB	5.58	1.62	1.53
12	l	145	GLU	N-CA	-5.58	1.38	1.46
10	3	83	GLU	CA-C	5.58	1.59	1.53
21	N	477	SER	C-N	5.58	1.41	1.33
23	P	23	LYS	CA-CB	-5.58	1.44	1.53
24	Q	366	ILE	N-CA	5.58	1.54	1.46
30	K	218	GLY	CA-C	5.58	1.58	1.51
30	K	305	GLY	CA-C	-5.58	1.45	1.52
7	g	151	LEU	N-CA	-5.57	1.39	1.46
12	l	253	TYR	CA-C	-5.57	1.45	1.52
8	1	155	MET	CA-C	-5.57	1.45	1.52
18	X	34	GLU	CA-CB	5.57	1.62	1.53
21	N	906	ARG	CZ-NH2	5.57	1.40	1.33
24	Q	122	ILE	C-N	5.57	1.41	1.33
31	L	325	MET	N-CA	-5.57	1.39	1.46
32	M	277	ILE	CA-C	-5.57	1.45	1.52
24	Q	343	LEU	CA-CB	5.57	1.61	1.53
5	e	188	HIS	CB-CG	-5.57	1.42	1.50
7	g	40	ILE	CA-C	-5.57	1.45	1.52
27	O	23	HIS	CD2-NE2	5.57	1.44	1.37
13	m	133	PHE	CA-C	-5.57	1.45	1.52
21	N	323	GLY	C-N	5.57	1.41	1.33
21	N	828	LYS	CA-C	-5.57	1.45	1.52
27	O	37	LEU	CA-CB	5.57	1.60	1.53
31	L	422	VAL	C-O	-5.57	1.17	1.24
5	e	136	ARG	CD-NE	-5.57	1.38	1.46
24	Q	246	TYR	CA-C	-5.57	1.45	1.52
9	i	65	ARG	N-CA	-5.56	1.40	1.46
3	C	129	ARG	CD-NE	5.56	1.54	1.46
30	K	396	ARG	C-N	5.56	1.41	1.33
17	T	144	TYR	CA-CB	5.56	1.60	1.53
32	M	220	MET	N-CA	-5.56	1.39	1.46
33	J	362	CYS	CA-CB	5.56	1.62	1.53
3	c	235	ILE	C-N	5.56	1.41	1.33
14	n	141	ASN	CA-CB	5.56	1.59	1.53
10	3	43	ILE	CA-CB	-5.56	1.47	1.54
22	S	289	ALA	C-N	5.56	1.41	1.33
26	U	14	VAL	CA-CB	5.56	1.61	1.54
29	I	379	THR	CA-C	-5.56	1.45	1.52
33	J	297	LEU	C-N	5.56	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	42	VAL	N-CA	-5.56	1.39	1.46
6	f	218	LYS	N-CA	-5.56	1.39	1.46
1	A	54	ILE	CA-C	5.56	1.59	1.52
2	B	218	ASN	N-CA	-5.56	1.40	1.46
5	E	167	TYR	CA-C	-5.56	1.46	1.52
9	2	163	ALA	CA-C	-5.56	1.45	1.52
13	6	40	ASP	C-O	5.56	1.29	1.24
14	7	143	LEU	N-CA	-5.56	1.39	1.46
27	O	75	GLN	CA-C	-5.56	1.45	1.52
31	L	223	PRO	CA-C	5.56	1.55	1.52
32	M	120	LYS	C-N	5.56	1.41	1.33
14	7	182	HIS	CA-CB	5.56	1.62	1.53
13	m	48	GLU	CA-CB	5.55	1.62	1.53
8	1	129	HIS	ND1-CE1	5.55	1.38	1.32
33	J	144	ASP	N-CA	-5.55	1.38	1.45
2	b	243	ILE	C-N	5.55	1.41	1.34
10	j	145	GLN	CA-CB	5.55	1.62	1.53
22	S	354	LEU	CA-C	5.55	1.60	1.52
1	A	105	ARG	NE-CZ	5.55	1.39	1.33
25	R	283	THR	C-N	5.55	1.41	1.33
29	I	289	THR	CA-C	-5.55	1.45	1.52
30	K	141	ARG	CZ-NH2	5.55	1.40	1.33
6	f	69	HIS	ND1-CE1	5.55	1.38	1.32
1	A	84	ASN	C-N	5.55	1.41	1.33
7	G	230	PHE	CA-C	5.55	1.59	1.52
9	2	49	SER	N-CA	-5.55	1.39	1.46
12	5	260	TRP	N-CA	-5.55	1.38	1.46
16	V	20	ARG	CA-C	-5.55	1.45	1.52
1	A	81	MET	C-N	5.55	1.40	1.33
4	D	127	ARG	CD-NE	5.55	1.54	1.46
12	5	198	LYS	N-CA	5.55	1.52	1.45
28	H	193	PRO	C-O	-5.55	1.17	1.23
12	l	174	THR	C-N	5.55	1.41	1.33
2	B	57	MET	CA-CB	5.55	1.62	1.53
13	6	132	SER	N-CA	-5.55	1.39	1.46
26	U	21	HIS	CA-C	-5.55	1.45	1.52
32	M	290	ARG	N-CA	-5.55	1.39	1.46
8	h	155	MET	CA-C	-5.54	1.45	1.52
11	k	95	ARG	NE-CZ	5.54	1.39	1.33
7	G	130	ARG	C-O	5.54	1.30	1.24
4	d	243	GLN	C-O	-5.54	1.17	1.24
11	k	37	GLN	N-CA	-5.54	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	157	PHE	C-N	5.54	1.41	1.33
14	n	47	MET	CA-CB	5.54	1.62	1.53
5	E	144	ILE	CA-CB	-5.54	1.47	1.53
11	4	168	LEU	N-CA	-5.54	1.39	1.46
8	1	47	HIS	CG-CD2	5.54	1.42	1.35
18	X	17	TYR	CA-CB	5.54	1.63	1.53
18	X	84	GLY	N-CA	5.54	1.50	1.44
1	A	225	VAL	N-CA	-5.54	1.39	1.46
18	X	65	SER	C-N	5.54	1.40	1.33
4	d	228	GLU	CA-CB	5.54	1.61	1.53
23	P	351	ARG	CA-C	-5.54	1.45	1.52
28	H	389	PHE	C-N	5.54	1.42	1.33
33	J	353	CYS	N-CA	-5.54	1.39	1.46
2	b	48	GLU	C-N	5.53	1.41	1.33
5	e	86	ARG	NE-CZ	5.53	1.39	1.33
14	n	119	ALA	C-N	5.53	1.40	1.33
3	C	136	ILE	CA-CB	-5.53	1.47	1.54
18	X	14	VAL	CA-C	-5.53	1.46	1.52
32	M	140	LEU	N-CA	-5.53	1.39	1.46
11	k	167	GLU	CA-C	-5.53	1.45	1.52
1	A	79	ILE	N-CA	-5.53	1.39	1.46
1	A	158	ASP	C-N	5.53	1.40	1.34
8	1	57	SER	C-N	5.53	1.41	1.33
15	W	25	ARG	N-CA	-5.53	1.39	1.46
28	H	81	LEU	CA-C	-5.53	1.45	1.52
32	M	166	ARG	CD-NE	5.53	1.53	1.46
22	S	345	TYR	CA-C	-5.53	1.45	1.52
22	S	476	LEU	CA-C	5.53	1.59	1.52
14	n	153	GLN	CA-C	-5.53	1.45	1.53
2	B	74	VAL	CA-C	-5.53	1.46	1.52
4	D	19	GLN	C-N	5.53	1.40	1.33
12	l	106	VAL	C-N	5.53	1.41	1.33
13	6	37	ASN	CA-C	-5.53	1.45	1.52
33	J	167	PRO	N-CD	-5.53	1.40	1.47
6	f	223	THR	C-N	5.52	1.40	1.33
13	m	211	GLU	CA-CB	-5.52	1.45	1.53
9	2	89	GLY	CA-C	-5.52	1.46	1.52
15	W	15	TYR	C-N	5.52	1.41	1.33
23	P	249	ALA	CA-C	-5.52	1.45	1.52
23	P	299	LEU	CA-CB	5.52	1.62	1.53
30	K	87	LYS	N-CA	5.52	1.53	1.46
2	B	51	SER	C-N	5.52	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	276	PRO	CA-C	5.52	1.60	1.52
4	d	29	ARG	NE-CZ	5.52	1.39	1.33
4	d	123	SER	C-N	5.52	1.41	1.33
1	A	139	VAL	N-CA	-5.52	1.39	1.46
17	T	60	ARG	CD-NE	5.52	1.53	1.46
21	N	636	SER	C-N	5.52	1.41	1.33
25	R	327	ASP	C-O	-5.52	1.17	1.24
28	H	248	LEU	CA-C	-5.52	1.46	1.52
29	I	385	ASP	N-CA	-5.52	1.40	1.46
4	d	56	ASP	CA-C	-5.52	1.46	1.52
10	j	166	THR	CA-C	-5.52	1.45	1.52
21	N	877	GLN	N-CA	-5.52	1.39	1.46
1	A	58	LYS	C-O	-5.52	1.17	1.23
8	1	166	HIS	C-N	5.51	1.41	1.33
14	7	49	TYR	C-N	5.51	1.41	1.33
18	X	51	ARG	CZ-NH2	5.51	1.40	1.33
32	M	203	ARG	CA-CB	5.51	1.60	1.52
7	g	152	GLU	CA-CB	5.51	1.61	1.53
7	G	237	GLN	C-N	5.51	1.41	1.33
16	V	268	THR	C-N	5.51	1.40	1.33
21	N	68	VAL	N-CA	-5.51	1.40	1.46
1	a	77	ARG	NE-CZ	5.51	1.39	1.33
1	A	208	THR	N-CA	5.51	1.53	1.46
5	E	5	ARG	CD-NE	5.51	1.53	1.46
7	G	204	HIS	CG-ND1	5.51	1.44	1.38
24	Q	188	LEU	N-CA	5.51	1.53	1.46
6	f	105	VAL	N-CA	-5.51	1.40	1.46
7	g	228	HIS	CA-CB	-5.51	1.46	1.53
8	h	138	SER	N-CA	-5.51	1.39	1.46
17	T	95	LYS	N-CA	-5.51	1.39	1.46
21	N	545	SER	CA-CB	5.51	1.62	1.53
22	S	480	ARG	CZ-NH1	5.51	1.40	1.32
23	P	179	PHE	CG-CD2	5.51	1.50	1.38
33	J	54	LYS	CA-C	-5.51	1.45	1.52
10	j	3	ASP	C-N	5.50	1.41	1.34
9	2	225	ARG	C-N	5.50	1.41	1.33
10	3	51	LEU	N-CA	-5.50	1.39	1.46
16	V	38	LEU	C-O	-5.50	1.17	1.24
21	N	505	SER	C-O	-5.50	1.17	1.24
27	O	284	GLU	CA-C	-5.50	1.45	1.52
32	M	18	LEU	CA-CB	5.50	1.61	1.54
14	n	99	LEU	CA-C	-5.50	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	72	ARG	N-CA	-5.50	1.39	1.46
17	T	117	ASN	CA-CB	5.50	1.62	1.53
21	N	479	GLU	C-N	5.50	1.41	1.34
21	N	544	GLU	N-CA	-5.50	1.39	1.46
7	g	112	PHE	CA-C	-5.50	1.45	1.52
4	D	68	ASP	CA-CB	5.50	1.61	1.53
10	3	200	LEU	CA-C	-5.50	1.45	1.53
12	5	152	ALA	C-N	5.50	1.41	1.33
21	N	221	ASP	CA-C	-5.50	1.45	1.52
22	S	393	ARG	NE-CZ	5.50	1.39	1.33
23	P	286	ASN	CA-CB	5.50	1.62	1.53
28	H	273	ARG	NE-CZ	5.50	1.39	1.33
30	K	122	ILE	N-CA	-5.50	1.40	1.46
21	N	863	SER	CA-C	-5.50	1.45	1.52
7	g	29	LYS	CA-C	-5.49	1.45	1.52
8	h	199	PRO	C-N	5.49	1.41	1.34
10	3	44	PHE	C-N	5.49	1.40	1.33
30	K	262	ARG	CD-NE	5.49	1.53	1.46
7	G	93	ARG	CA-C	-5.49	1.45	1.52
5	E	189	SER	CA-C	-5.49	1.45	1.52
8	1	39	VAL	CA-CB	-5.49	1.48	1.54
18	X	24	CYS	N-CA	-5.49	1.39	1.45
18	X	90	VAL	CA-CB	-5.49	1.47	1.53
29	I	393	GLN	CA-C	-5.49	1.45	1.52
25	R	351	LYS	CA-C	-5.49	1.45	1.52
31	L	68	ARG	CZ-NH1	5.49	1.40	1.32
31	L	75	LYS	C-N	5.49	1.41	1.33
32	M	357	ARG	NE-CZ	5.49	1.39	1.33
33	J	42	ARG	CZ-NH2	5.49	1.40	1.33
33	J	43	ARG	CZ-NH1	5.49	1.40	1.32
33	J	348	GLU	C-N	5.49	1.41	1.33
6	f	153	VAL	CA-CB	5.49	1.62	1.54
25	R	71	LEU	CA-C	-5.49	1.45	1.52
28	H	437	VAL	C-N	5.49	1.40	1.33
10	3	141	THR	CA-C	-5.48	1.45	1.52
15	W	177	GLY	CA-C	-5.48	1.44	1.51
23	P	218	LEU	N-CA	-5.48	1.39	1.46
1	A	185	HIS	C-N	5.48	1.42	1.33
11	4	98	TYR	C-O	5.48	1.30	1.24
30	K	354	GLY	C-N	5.48	1.41	1.33
33	J	309	ARG	CD-NE	5.48	1.53	1.46
1	a	46	ARG	CD-NE	5.48	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	198	SER	C-O	5.48	1.30	1.24
4	d	90	ARG	CZ-NH1	5.48	1.40	1.32
1	A	84	ASN	CA-C	-5.48	1.46	1.52
21	N	859	ASN	N-CA	-5.48	1.39	1.46
27	O	115	ARG	NE-CZ	5.48	1.39	1.33
27	O	297	ILE	C-N	5.48	1.41	1.33
28	H	400	ARG	C-N	5.48	1.40	1.32
4	d	49	ARG	CA-CB	5.48	1.59	1.53
9	i	212	ASP	N-CA	-5.48	1.39	1.46
8	1	68	VAL	N-CA	-5.48	1.39	1.46
10	3	87	PHE	CA-CB	5.48	1.62	1.53
25	R	414	LEU	C-O	-5.48	1.17	1.24
11	4	28	LEU	CA-C	5.48	1.59	1.52
11	4	167	GLU	C-N	5.48	1.41	1.34
22	S	63	LEU	N-CA	-5.48	1.39	1.46
2	b	224	TYR	N-CA	-5.47	1.39	1.46
6	f	233	TYR	N-CA	5.47	1.53	1.46
9	i	130	ALA	C-N	5.47	1.39	1.32
7	G	222	SER	N-CA	-5.47	1.38	1.46
21	N	548	ARG	CA-C	5.47	1.59	1.52
24	Q	170	ASP	CA-CB	5.47	1.62	1.53
27	O	346	GLU	N-CA	-5.47	1.39	1.46
6	f	96	SER	CA-CB	5.47	1.62	1.53
11	4	118	GLN	C-N	5.47	1.40	1.33
21	N	306	ASN	N-CA	-5.47	1.39	1.46
28	H	438	ALA	CA-C	-5.47	1.46	1.52
32	M	266	ALA	CA-C	-5.47	1.45	1.52
6	f	227	GLY	N-CA	-5.47	1.37	1.45
22	S	140	LEU	CA-C	-5.47	1.45	1.52
28	H	154	LYS	CA-C	-5.47	1.46	1.52
31	L	340	PRO	CA-C	-5.47	1.46	1.52
8	h	90	VAL	CA-CB	-5.47	1.47	1.54
13	6	82	TRP	C-N	5.47	1.41	1.33
7	g	238	GLU	C-N	5.47	1.41	1.33
3	C	191	GLU	N-CA	-5.47	1.39	1.46
21	N	578	ASP	CA-CB	5.47	1.61	1.53
25	R	122	GLU	N-CA	5.47	1.52	1.46
32	M	229	THR	C-N	5.47	1.41	1.33
7	g	77	VAL	CA-C	-5.46	1.45	1.52
9	i	193	TRP	CA-C	-5.46	1.45	1.52
14	n	36	GLN	CA-CB	5.46	1.61	1.53
14	n	215	ARG	CA-C	-5.46	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	114	ARG	NE-CZ	5.46	1.39	1.33
5	E	143	LEU	N-CA	-5.46	1.39	1.46
30	K	58	TYR	C-N	5.46	1.42	1.33
2	b	63	LYS	CA-C	5.46	1.59	1.52
6	f	123	TYR	C-N	5.46	1.40	1.33
11	k	149	ARG	CA-C	-5.46	1.47	1.52
8	l	49	LYS	CA-C	-5.46	1.45	1.52
21	N	86	LYS	N-CA	-5.46	1.39	1.46
28	H	403	ARG	CD-NE	5.46	1.53	1.46
29	I	306	MET	CA-CB	5.46	1.61	1.53
10	j	152	SER	C-O	-5.46	1.17	1.24
16	V	166	ASN	CA-C	-5.46	1.45	1.52
3	c	73	ILE	C-N	5.46	1.41	1.33
3	C	19	LEU	N-CA	-5.46	1.39	1.46
5	E	162	GLY	CA-C	-5.46	1.44	1.51
25	R	74	ASN	C-N	5.46	1.41	1.33
11	k	93	ARG	CZ-NH2	5.46	1.40	1.33
21	N	747	HIS	ND1-CE1	5.46	1.38	1.32
23	P	314	VAL	C-O	5.46	1.30	1.24
7	g	33	ASN	CA-CB	5.45	1.61	1.53
2	B	245	ASP	N-CA	-5.45	1.39	1.46
5	E	120	ALA	C-N	-5.45	1.25	1.33
10	3	72	ASN	CA-C	-5.45	1.46	1.52
11	4	149	ARG	NE-CZ	5.45	1.39	1.33
16	V	143	PRO	CA-C	-5.45	1.45	1.52
22	S	381	VAL	CA-CB	5.45	1.61	1.54
3	c	196	THR	C-N	5.45	1.41	1.33
13	6	91	LYS	C-O	-5.45	1.17	1.24
21	N	523	LEU	N-CA	-5.45	1.39	1.46
22	S	489	GLN	CA-C	-5.45	1.46	1.52
27	O	23	HIS	CA-CB	5.45	1.62	1.53
27	O	132	GLU	C-N	5.45	1.40	1.33
6	f	24	TYR	CA-CB	5.45	1.61	1.53
13	m	207	GLY	N-CA	-5.45	1.38	1.45
2	B	234	ARG	CZ-NH1	5.45	1.40	1.32
4	D	43	VAL	C-N	5.45	1.40	1.33
14	7	101	LYS	N-CA	-5.45	1.39	1.46
29	I	56	LYS	CA-C	-5.45	1.45	1.52
3	C	227	GLN	N-CA	-5.45	1.39	1.46
12	5	228	ALA	N-CA	-5.45	1.39	1.46
24	Q	418	GLN	C-N	5.45	1.41	1.33
25	R	257	GLY	CA-C	-5.45	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	99	ARG	CD-NE	5.45	1.53	1.46
13	6	213	LEU	CA-CB	-5.45	1.45	1.53
5	e	141	ALA	CA-C	-5.44	1.46	1.52
24	Q	213	GLN	CA-CB	5.44	1.61	1.53
9	i	51	GLN	C-O	5.44	1.30	1.24
5	E	56	SER	N-CA	-5.44	1.40	1.45
9	2	34	GLY	CA-C	-5.44	1.44	1.51
9	2	227	GLU	C-N	5.44	1.40	1.33
21	N	251	GLU	C-N	5.44	1.40	1.33
30	K	290	ARG	NE-CZ	5.44	1.39	1.33
11	4	28	LEU	C-N	5.44	1.41	1.33
29	I	336	PRO	C-N	5.44	1.40	1.33
5	e	107	ILE	C-N	5.44	1.40	1.33
3	C	90	THR	CA-C	-5.44	1.45	1.52
14	7	136	ARG	NE-CZ	5.44	1.39	1.33
24	Q	150	GLN	CA-CB	5.44	1.62	1.53
32	M	120	LYS	CA-CB	5.44	1.60	1.53
1	a	79	ILE	CA-CB	-5.43	1.47	1.54
2	b	156	TYR	N-CA	-5.43	1.39	1.45
10	3	78	GLU	C-N	5.43	1.41	1.33
12	5	120	MET	SD-CE	5.43	1.93	1.79
15	W	133	LYS	CA-C	-5.43	1.45	1.52
21	N	889	ARG	N-CA	5.43	1.53	1.46
28	H	100	ALA	CA-C	-5.43	1.45	1.52
4	d	21	GLU	C-N	5.43	1.41	1.33
11	4	35	THR	C-N	5.43	1.41	1.33
15	W	41	ARG	NE-CZ	5.43	1.39	1.33
21	N	830	LYS	CA-C	-5.43	1.46	1.52
7	G	80	GLY	CA-C	-5.43	1.44	1.51
27	O	62	TYR	N-CA	-5.43	1.39	1.46
27	O	92	PHE	CA-C	-5.43	1.45	1.52
28	H	463	TYR	CA-CB	5.43	1.62	1.54
29	I	319	ARG	NE-CZ	5.43	1.39	1.33
10	j	98	ARG	CA-C	-5.43	1.46	1.52
5	E	96	ALA	CA-C	-5.43	1.45	1.52
10	3	39	LYS	CA-CB	5.43	1.60	1.53
22	S	299	LYS	CA-C	-5.43	1.45	1.52
24	Q	294	ARG	CD-NE	5.43	1.53	1.46
29	I	60	LEU	N-CA	-5.43	1.39	1.46
31	L	239	ILE	CA-C	-5.43	1.45	1.52
33	J	49	ASN	N-CA	-5.43	1.39	1.46
33	J	75	VAL	CA-CB	-5.43	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	2	ASP	C-N	5.43	1.40	1.33
28	H	357	ARG	C-N	-5.43	1.29	1.33
7	g	146	ALA	N-CA	-5.43	1.38	1.45
28	H	228	PRO	N-CD	-5.43	1.40	1.47
28	H	450	VAL	N-CA	-5.43	1.39	1.46
32	M	131	MET	C-N	5.43	1.40	1.33
22	S	139	HIS	CE1-NE2	-5.42	1.27	1.32
24	Q	369	ASP	CA-C	-5.42	1.45	1.52
25	R	225	LYS	N-CA	-5.42	1.39	1.46
28	H	120	ASN	N-CA	-5.42	1.40	1.46
1	A	210	MET	CA-C	-5.42	1.45	1.52
25	R	40	ILE	C-N	5.42	1.40	1.33
12	l	165	TYR	CA-C	-5.42	1.44	1.52
1	A	99	ALA	CA-C	-5.42	1.46	1.52
1	A	210	MET	C-N	5.42	1.40	1.33
4	D	141	ARG	CA-C	-5.42	1.45	1.52
27	O	357	ILE	CA-CB	-5.42	1.47	1.54
3	c	133	VAL	CA-C	5.42	1.59	1.52
3	c	184	MET	CA-C	-5.42	1.45	1.52
7	g	196	ALA	CA-C	-5.42	1.45	1.52
31	L	140	LEU	CA-C	-5.42	1.46	1.52
4	d	14	ASP	N-CA	-5.42	1.39	1.46
5	e	183	LEU	CA-CB	5.42	1.61	1.53
10	3	7	ILE	CA-CB	-5.42	1.47	1.54
21	N	580	ASN	N-CA	-5.42	1.39	1.46
27	O	96	LEU	C-N	5.42	1.40	1.33
31	L	233	LYS	N-CA	-5.42	1.39	1.46
3	c	216	ILE	CA-C	-5.41	1.46	1.52
5	E	67	ILE	N-CA	-5.41	1.39	1.46
23	P	212	LYS	N-CA	-5.41	1.39	1.46
7	G	22	PHE	CG-CD2	5.41	1.50	1.38
16	V	45	VAL	CA-C	-5.41	1.47	1.52
26	U	58	GLU	CA-C	5.41	1.59	1.52
26	U	222	ASN	C-O	-5.41	1.17	1.23
4	d	223	ALA	CA-CB	5.41	1.61	1.53
16	V	54	LEU	CA-C	-5.41	1.46	1.52
23	P	307	GLU	N-CA	-5.41	1.39	1.45
28	H	186	PRO	N-CD	-5.41	1.40	1.47
32	M	288	THR	CA-CB	-5.41	1.44	1.53
30	K	231	LYS	C-N	5.41	1.40	1.33
2	b	230	ASP	C-N	5.41	1.41	1.33
26	U	130	VAL	N-CA	-5.41	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	81	LEU	CA-C	5.41	1.59	1.52
10	j	124	PHE	CA-C	-5.40	1.45	1.52
13	6	104	LEU	C-O	5.40	1.30	1.24
5	e	73	HIS	ND1-CE1	5.40	1.38	1.32
5	e	247	GLU	C-N	5.40	1.41	1.33
9	i	133	ASP	N-CA	-5.40	1.38	1.46
9	i	216	LEU	C-N	5.40	1.40	1.33
4	D	60	THR	CB-OG1	-5.40	1.35	1.43
9	2	48	ARG	CD-NE	5.40	1.53	1.46
21	N	856	PHE	C-O	-5.40	1.17	1.24
28	H	307	PHE	CA-CB	5.40	1.59	1.53
31	L	263	ILE	C-N	5.40	1.41	1.33
33	J	383	GLU	CA-CB	5.40	1.61	1.53
5	e	22	PHE	N-CA	-5.40	1.39	1.46
13	m	51	VAL	N-CA	-5.40	1.39	1.46
3	C	178	MET	CA-CB	5.40	1.62	1.53
5	E	24	VAL	N-CA	5.40	1.52	1.46
14	7	259	LYS	CA-CB	5.40	1.61	1.53
17	T	201	PRO	CA-C	-5.40	1.46	1.52
21	N	661	SER	C-N	5.40	1.41	1.33
25	R	282	THR	C-N	5.40	1.40	1.33
32	M	171	GLU	CA-C	-5.40	1.45	1.52
3	c	113	ARG	NE-CZ	5.40	1.39	1.33
7	g	99	PHE	CA-CB	5.40	1.61	1.53
10	j	82	ILE	CA-C	5.40	1.58	1.52
19	Y	2	SER	N-CA	-5.40	1.38	1.45
21	N	23	TYR	CA-CB	5.40	1.61	1.53
1	a	77	ARG	CZ-NH2	5.40	1.40	1.33
9	i	31	THR	CA-C	-5.40	1.46	1.52
10	j	57	ALA	CA-CB	5.40	1.62	1.53
12	l	160	ASN	C-N	5.40	1.40	1.33
14	n	198	ILE	N-CA	-5.40	1.40	1.46
2	B	157	PHE	C-N	-5.40	1.26	1.33
22	S	311	GLN	CA-CB	5.40	1.61	1.53
33	J	142	VAL	CA-C	5.40	1.58	1.52
21	N	317	SER	CA-C	-5.40	1.45	1.52
2	b	178	ARG	CZ-NH1	5.39	1.40	1.32
9	i	137	SER	CA-C	-5.39	1.45	1.52
24	Q	220	LEU	N-CA	-5.39	1.40	1.46
10	3	174	ALA	N-CA	-5.39	1.39	1.46
11	4	123	GLY	CA-C	-5.39	1.44	1.51
12	5	221	TRP	CZ2-CH2	5.39	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	13	ILE	C-N	-5.39	1.26	1.34
23	P	359	ARG	CZ-NH2	5.39	1.40	1.33
14	7	177	THR	CA-C	-5.39	1.46	1.52
23	P	102	GLU	N-CA	-5.39	1.39	1.46
26	U	154	PHE	CA-CB	5.39	1.63	1.53
12	l	160	ASN	CA-CB	5.39	1.61	1.53
17	T	87	PRO	C-N	5.39	1.40	1.33
21	N	695	ALA	C-O	-5.39	1.17	1.24
21	N	780	ASP	CA-C	-5.39	1.45	1.52
27	O	388	GLY	CA-C	-5.39	1.44	1.51
31	L	273	HIS	CG-ND1	-5.39	1.32	1.38
11	k	11	ASP	N-CA	-5.39	1.39	1.46
22	S	88	PHE	CA-C	-5.39	1.45	1.52
32	M	294	GLU	C-N	5.39	1.40	1.33
33	J	198	LEU	C-N	5.39	1.41	1.34
10	j	119	PRO	N-CA	-5.38	1.40	1.47
11	k	7	ILE	C-N	5.38	1.41	1.33
1	A	17	THR	CA-C	-5.38	1.47	1.53
29	I	374	ASP	CA-C	-5.38	1.46	1.52
6	f	18	ARG	NE-CZ	5.38	1.39	1.33
12	5	170	LEU	CA-C	-5.38	1.46	1.52
21	N	379	LEU	CA-C	-5.38	1.45	1.52
22	S	474	GLU	C-N	5.38	1.40	1.33
24	Q	290	THR	CA-C	5.38	1.59	1.52
33	J	23	PHE	CA-C	-5.38	1.45	1.52
5	E	72	ARG	CD-NE	5.38	1.53	1.46
9	2	123	ILE	CA-C	-5.38	1.45	1.52
24	Q	346	ASN	CA-C	-5.38	1.45	1.52
33	J	15	HIS	CD2-NE2	5.38	1.43	1.37
33	J	319	PRO	N-CA	-5.38	1.40	1.46
3	c	224	GLU	C-N	5.38	1.41	1.33
17	T	90	PHE	CA-CB	5.38	1.61	1.53
29	I	428	VAL	N-CA	-5.38	1.40	1.46
1	A	24	ARG	CZ-NH1	5.38	1.40	1.32
3	C	92	ARG	CD-NE	5.38	1.53	1.46
22	S	423	VAL	CA-C	-5.38	1.46	1.52
24	Q	149	LYS	CA-C	-5.38	1.45	1.52
28	H	294	LEU	N-CA	-5.38	1.39	1.46
7	G	213	GLU	N-CA	5.38	1.52	1.46
14	7	206	ALA	C-N	5.38	1.40	1.33
1	A	47	GLY	CA-C	-5.37	1.44	1.51
1	A	184	ASN	C-N	5.37	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	247	VAL	N-CA	-5.37	1.40	1.46
21	N	208	ARG	C-O	-5.37	1.17	1.24
31	L	262	ILE	CA-CB	-5.37	1.48	1.54
1	a	163	TYR	CA-C	-5.37	1.46	1.52
2	b	178	ARG	CD-NE	5.37	1.53	1.46
14	n	220	ARG	CZ-NH2	5.37	1.40	1.33
15	W	179	ARG	NE-CZ	5.37	1.39	1.33
29	I	280	PHE	CA-C	-5.37	1.46	1.52
30	K	424	PHE	N-CA	-5.37	1.39	1.46
23	P	70	ASN	CG-ND2	5.37	1.44	1.33
2	B	244	ASN	CA-C	-5.37	1.45	1.52
5	E	185	ASN	CA-CB	5.37	1.61	1.53
6	F	62	LYS	N-CA	-5.37	1.38	1.45
12	5	161	LEU	N-CA	-5.37	1.39	1.46
22	S	58	LYS	C-O	5.37	1.30	1.24
25	R	135	ILE	N-CA	-5.37	1.40	1.46
26	U	108	GLU	N-CA	-5.37	1.39	1.46
29	I	202	LEU	C-N	5.37	1.41	1.33
30	K	41	SER	CA-CB	5.37	1.62	1.53
1	a	122	ALA	CA-C	5.37	1.59	1.52
5	e	58	LEU	CB-CG	5.37	1.64	1.53
10	j	203	ARG	NE-CZ	5.37	1.39	1.33
21	N	832	HIS	CB-CG	5.37	1.57	1.50
4	D	68	ASP	N-CA	-5.37	1.38	1.46
8	1	121	THR	C-N	5.37	1.39	1.33
9	2	104	ARG	CD-NE	5.37	1.53	1.46
32	M	419	ILE	N-CA	-5.37	1.40	1.46
6	F	29	ILE	CA-CB	5.36	1.61	1.54
13	6	143	GLN	CA-C	-5.36	1.46	1.52
15	W	184	ASN	CA-C	-5.36	1.45	1.52
21	N	525	ASN	N-CA	-5.36	1.40	1.46
26	U	212	ASP	C-N	5.36	1.41	1.33
28	H	124	ASN	CA-C	-5.36	1.45	1.52
31	L	299	ARG	CZ-NH2	5.36	1.40	1.33
13	6	84	HIS	C-O	-5.36	1.17	1.24
4	d	134	LEU	C-N	5.36	1.40	1.33
17	T	32	ILE	CB-CG1	5.36	1.64	1.53
22	S	225	HIS	ND1-CE1	5.36	1.38	1.32
21	N	813	ARG	CZ-NH1	5.36	1.40	1.32
11	k	8	ARG	CA-C	-5.36	1.46	1.52
11	4	152	MET	N-CA	-5.36	1.39	1.45
22	S	298	ARG	NE-CZ	5.36	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	118	VAL	CA-C	-5.36	1.45	1.52
30	K	377	SER	CA-CB	5.36	1.60	1.52
32	M	168	LYS	C-O	-5.36	1.17	1.24
4	d	6	ARG	N-CA	-5.36	1.39	1.46
2	B	131	GLY	CA-C	-5.36	1.44	1.51
6	F	66	CYS	CA-C	5.36	1.59	1.52
13	6	58	ILE	CA-C	-5.36	1.46	1.52
1	A	107	LYS	C-N	5.35	1.42	1.33
10	3	147	PHE	CA-CB	5.35	1.61	1.53
11	k	139	TYR	CA-CB	5.35	1.62	1.53
11	k	145	ASP	CA-CB	5.35	1.62	1.53
12	l	178	GLY	N-CA	-5.35	1.39	1.45
9	2	183	LEU	CA-CB	5.35	1.61	1.53
21	N	913	PRO	CA-C	5.35	1.59	1.52
12	5	217	SER	CA-C	-5.35	1.45	1.52
30	K	68	ILE	C-N	5.35	1.41	1.33
33	J	256	THR	C-N	5.35	1.41	1.33
7	g	106	PRO	N-CD	-5.35	1.40	1.47
8	h	77	SER	CA-C	-5.35	1.45	1.52
11	k	172	MET	CA-C	-5.35	1.46	1.53
2	B	180	ASN	N-CA	-5.35	1.39	1.45
23	P	311	TRP	CA-CB	5.35	1.60	1.53
32	M	303	ARG	CZ-NH1	5.35	1.40	1.32
9	i	34	GLY	N-CA	5.35	1.53	1.45
1	A	211	ILE	C-N	5.35	1.40	1.33
2	B	204	PHE	CA-CB	5.35	1.59	1.53
6	F	201	LEU	C-N	5.35	1.41	1.33
30	K	155	ASP	N-CA	-5.35	1.39	1.46
32	M	103	GLY	N-CA	-5.35	1.37	1.45
15	W	43	SER	CA-CB	5.34	1.61	1.53
21	N	215	MET	CA-CB	5.34	1.61	1.53
21	N	914	VAL	C-N	5.34	1.41	1.33
22	S	112	ASN	CA-C	5.34	1.59	1.53
6	f	164	ARG	NE-CZ	5.34	1.39	1.33
30	K	119	VAL	N-CA	-5.34	1.39	1.46
21	N	361	ASN	N-CA	-5.34	1.37	1.47
25	R	207	ARG	CZ-NH1	5.34	1.40	1.32
29	I	163	ASP	CA-C	5.34	1.58	1.52
31	L	290	ARG	NE-CZ	5.34	1.39	1.33
6	F	44	ALA	CA-C	-5.34	1.46	1.52
8	1	71	HIS	C-N	5.34	1.41	1.33
22	S	87	SER	CA-C	-5.34	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	102	PRO	CA-C	-5.34	1.47	1.53
31	L	188	GLU	CA-C	5.34	1.59	1.52
1	A	70	SER	N-CA	-5.34	1.39	1.46
16	V	209	GLU	C-N	5.34	1.41	1.33
32	M	89	ASN	C-N	5.34	1.40	1.33
9	i	54	ILE	C-N	5.34	1.39	1.33
11	k	106	GLY	CA-C	-5.34	1.46	1.51
2	B	220	ASP	C-N	5.34	1.41	1.33
3	C	107	PRO	N-CD	5.34	1.55	1.47
8	1	65	ALA	C-N	5.34	1.41	1.33
12	l	139	ARG	CD-NE	5.33	1.53	1.46
14	7	76	ILE	N-CA	-5.33	1.41	1.46
28	H	409	ARG	N-CA	5.33	1.52	1.46
10	j	54	THR	CA-C	-5.33	1.48	1.53
13	m	163	ASN	C-N	5.33	1.41	1.33
5	E	238	GLU	N-CA	-5.33	1.40	1.46
16	V	277	LYS	C-N	5.33	1.41	1.33
22	S	51	ARG	CZ-NH1	5.33	1.40	1.32
22	S	346	TYR	N-CA	-5.33	1.40	1.46
24	Q	6	SER	C-N	5.33	1.40	1.33
27	O	95	SER	CA-CB	5.33	1.61	1.53
11	k	132	ALA	N-CA	-5.33	1.39	1.46
12	l	185	PRO	CA-CB	5.33	1.60	1.53
1	A	241	ILE	C-N	5.33	1.41	1.33
3	C	171	ALA	CA-C	-5.33	1.46	1.52
17	T	224	ARG	CD-NE	5.33	1.53	1.46
22	S	432	ILE	C-N	5.33	1.40	1.33
26	U	230	GLN	C-O	-5.33	1.18	1.24
3	c	150	THR	N-CA	-5.33	1.39	1.46
32	M	129	LEU	N-CA	-5.33	1.39	1.45
9	i	232	TYR	CA-C	-5.33	1.45	1.52
12	l	78	THR	C-N	5.33	1.40	1.33
2	B	194	LEU	CA-C	-5.33	1.46	1.52
21	N	634	LEU	CA-C	-5.33	1.46	1.52
26	U	233	PHE	N-CA	-5.33	1.39	1.46
11	k	191	GLN	CA-C	-5.33	1.46	1.52
21	N	136	ILE	CA-C	-5.33	1.46	1.52
5	E	59	LEU	C-N	5.33	1.41	1.33
8	1	34	TYR	CA-C	-5.33	1.45	1.52
31	L	271	LYS	CA-C	5.33	1.59	1.52
6	f	224	ILE	CA-CB	-5.32	1.48	1.54
4	D	32	CYS	CA-C	-5.32	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	589	ILE	C-O	-5.32	1.18	1.24
22	S	159	ASN	CA-CB	5.32	1.61	1.53
30	K	185	ARG	CD-NE	5.32	1.53	1.46
3	c	191	GLU	C-N	5.32	1.41	1.33
4	d	70	HIS	C-N	5.32	1.40	1.33
6	f	80	ASP	CA-C	-5.32	1.46	1.52
7	g	124	THR	C-N	5.32	1.41	1.33
2	B	76	SER	CA-C	-5.32	1.46	1.52
3	C	211	LEU	C-N	5.32	1.40	1.33
21	N	364	LYS	N-CA	-5.32	1.39	1.46
24	Q	46	VAL	N-CA	-5.32	1.39	1.46
28	H	261	ARG	CZ-NH1	5.32	1.40	1.32
32	M	61	LYS	C-N	5.32	1.40	1.33
7	g	174	ALA	N-CA	-5.32	1.40	1.46
13	m	33	GLY	CA-C	5.32	1.56	1.51
5	e	44	GLU	C-N	5.32	1.37	1.33
7	G	231	VAL	CA-CB	5.32	1.60	1.54
19	Y	72	ASP	N-CA	-5.32	1.39	1.46
30	K	416	LYS	C-N	5.32	1.40	1.33
32	M	161	SER	C-O	5.32	1.30	1.23
6	f	51	ARG	CD-NE	5.32	1.53	1.46
8	h	12	ILE	C-N	5.32	1.40	1.33
8	h	75	TYR	CA-CB	5.32	1.61	1.53
25	R	72	VAL	C-N	5.32	1.40	1.33
27	O	236	HIS	ND1-CE1	5.32	1.37	1.32
2	B	128	ARG	NE-CZ	5.31	1.38	1.33
3	C	239	LEU	C-N	5.31	1.40	1.33
10	j	157	ASN	CA-CB	5.31	1.60	1.53
16	V	38	LEU	N-CA	-5.31	1.40	1.46
18	X	50	TRP	CA-CB	-5.31	1.44	1.53
21	N	545	SER	CA-C	-5.31	1.45	1.52
23	P	205	LYS	CA-CB	5.31	1.60	1.53
11	4	144	LEU	N-CA	-5.31	1.39	1.46
18	X	68	LEU	N-CA	-5.31	1.40	1.46
1	a	55	SER	CA-C	-5.31	1.46	1.52
6	f	113	CYS	CA-C	-5.31	1.45	1.52
17	T	43	ASP	CA-CB	5.31	1.61	1.53
23	P	159	ILE	C-N	5.31	1.41	1.33
25	R	116	LYS	CA-C	-5.31	1.46	1.52
25	R	239	THR	CB-OG1	-5.31	1.35	1.43
27	O	288	ARG	CZ-NH2	5.31	1.40	1.33
29	I	375	VAL	CA-C	-5.31	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	217	ARG	CD-NE	5.31	1.53	1.46
5	e	168	ASN	CA-C	-5.31	1.46	1.52
5	E	43	LYS	C-N	5.31	1.40	1.33
16	V	20	ARG	NE-CZ	5.31	1.38	1.33
27	O	247	ASN	CG-ND2	5.31	1.44	1.33
31	L	103	GLN	C-N	5.31	1.40	1.33
33	J	296	ARG	CZ-NH2	5.31	1.40	1.33
21	N	807	THR	N-CA	-5.30	1.40	1.46
24	Q	247	HIS	CG-CD2	5.30	1.41	1.35
28	H	345	PRO	N-CA	-5.30	1.40	1.47
14	n	111	ASN	CA-C	-5.30	1.46	1.53
5	e	52	LYS	C-N	5.30	1.41	1.33
8	h	200	ASP	CA-C	-5.30	1.45	1.52
11	k	10	GLN	C-N	5.30	1.40	1.33
14	n	129	LEU	N-CA	-5.30	1.40	1.46
17	T	208	LEU	N-CA	-5.30	1.39	1.46
18	X	36	LYS	N-CA	-5.30	1.40	1.46
28	H	284	VAL	CA-C	-5.30	1.45	1.52
6	f	164	ARG	N-CA	-5.30	1.39	1.46
23	P	328	ALA	CA-C	-5.30	1.45	1.52
31	L	61	LYS	CA-C	-5.30	1.45	1.52
17	T	83	ASN	C-N	5.30	1.40	1.33
11	k	66	LEU	CA-C	-5.30	1.45	1.52
12	5	144	ARG	CD-NE	5.30	1.53	1.46
23	P	186	LEU	N-CA	-5.30	1.39	1.46
24	Q	184	VAL	N-CA	-5.30	1.40	1.46
29	I	109	LEU	CA-CB	5.30	1.59	1.53
21	N	695	ALA	CA-C	-5.29	1.46	1.52
24	Q	425	GLN	CA-C	5.29	1.59	1.52
30	K	224	LYS	C-N	5.29	1.40	1.33
7	g	169	ARG	NE-CZ	5.29	1.38	1.33
13	m	150	ALA	C-N	5.29	1.40	1.33
2	B	156	TYR	C-N	5.29	1.41	1.33
9	2	212	ASP	N-CA	-5.29	1.39	1.46
27	O	244	ASN	CA-C	-5.29	1.45	1.52
4	D	130	GLY	CA-C	-5.29	1.44	1.51
10	3	161	GLU	N-CA	5.29	1.52	1.46
13	6	146	ALA	CA-C	-5.29	1.45	1.53
31	L	386	PHE	C-N	5.29	1.41	1.33
1	A	168	ALA	CA-C	-5.29	1.46	1.52
6	f	51	ARG	CA-C	-5.29	1.46	1.52
8	h	144	TYR	C-N	5.29	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	THR	CA-C	-5.29	1.45	1.53
10	3	99	ARG	CA-C	-5.29	1.46	1.52
12	5	240	ALA	CA-C	5.29	1.59	1.52
25	R	351	LYS	N-CA	-5.29	1.39	1.46
28	H	122	SER	CA-C	-5.29	1.48	1.52
28	H	434	ARG	CA-C	-5.29	1.45	1.52
31	L	392	ARG	NE-CZ	5.29	1.38	1.33
5	e	141	ALA	C-N	5.29	1.41	1.33
21	N	5	THR	CA-CB	5.29	1.62	1.53
21	N	22	THR	C-N	5.29	1.40	1.33
24	Q	22	GLU	CA-C	5.29	1.59	1.52
5	e	203	ILE	CA-CB	5.29	1.61	1.54
9	i	60	CYS	CA-CB	5.29	1.60	1.53
4	D	144	GLU	CA-CB	5.29	1.61	1.52
14	7	51	ASN	CA-C	-5.29	1.45	1.52
11	k	45	SER	C-N	5.28	1.40	1.33
23	P	415	TRP	N-CA	-5.28	1.39	1.46
10	3	46	TYR	CA-CB	5.28	1.61	1.52
1	A	80	GLY	N-CA	-5.28	1.39	1.44
31	L	375	ASP	CA-C	5.28	1.59	1.53
1	A	139	VAL	CA-C	-5.28	1.46	1.52
24	Q	186	HIS	ND1-CE1	5.28	1.37	1.32
6	F	69	HIS	CE1-NE2	-5.28	1.27	1.32
11	4	23	ARG	NE-CZ	5.28	1.38	1.33
21	N	192	LEU	N-CA	-5.28	1.40	1.46
7	g	21	ASN	C-N	5.28	1.41	1.33
14	n	98	ARG	CD-NE	5.28	1.53	1.46
4	D	157	SER	CA-CB	5.28	1.63	1.53
12	5	103	SER	CA-C	-5.28	1.45	1.52
17	T	215	LYS	CA-C	5.28	1.59	1.52
27	O	88	ASP	N-CA	-5.28	1.39	1.46
31	L	429	GLU	CA-C	-5.28	1.46	1.52
32	M	346	LYS	CA-CB	5.28	1.62	1.53
1	a	114	CYS	CA-CB	5.27	1.61	1.53
6	f	159	THR	CA-CB	-5.27	1.44	1.53
7	g	40	ILE	N-CA	-5.27	1.40	1.46
5	E	129	GLY	CA-C	-5.27	1.45	1.51
9	2	253	GLN	CA-CB	5.27	1.62	1.53
14	7	98	ARG	CZ-NH1	5.27	1.40	1.32
1	a	24	ARG	NE-CZ	5.27	1.38	1.33
31	L	342	ARG	CZ-NH2	5.27	1.40	1.33
3	c	116	SER	N-CA	5.27	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	94	THR	CA-C	5.27	1.59	1.52
10	j	44	PHE	CG-CD1	5.27	1.50	1.38
14	n	151	GLY	CA-C	-5.27	1.45	1.51
21	N	47	GLU	C-N	5.27	1.40	1.33
21	N	129	ILE	CA-CB	-5.27	1.46	1.54
26	U	20	ASP	CA-C	-5.27	1.46	1.52
27	O	285	SER	CA-CB	5.27	1.61	1.53
30	K	349	ARG	CZ-NH2	5.27	1.40	1.33
2	b	164	ILE	CA-CB	5.27	1.63	1.55
12	5	170	LEU	C-O	-5.27	1.17	1.23
14	7	142	PRO	N-CA	-5.27	1.40	1.47
22	S	250	ALA	C-N	5.27	1.41	1.33
30	K	120	VAL	N-CA	-5.27	1.40	1.46
31	L	156	MET	CA-C	-5.27	1.45	1.52
10	j	195	VAL	CA-C	-5.26	1.46	1.52
7	G	59	LEU	C-N	5.26	1.38	1.33
11	4	36	ARG	NE-CZ	5.26	1.38	1.33
15	W	108	GLN	CA-C	-5.26	1.46	1.52
5	e	93	ARG	N-CA	-5.26	1.40	1.46
12	l	141	HIS	ND1-CE1	5.26	1.37	1.32
11	4	61	GLN	CA-CB	5.26	1.61	1.53
21	N	508	THR	CB-OG1	-5.26	1.35	1.43
23	P	438	ILE	N-CA	-5.26	1.39	1.46
30	K	293	GLN	N-CA	-5.26	1.39	1.46
4	d	220	ASP	C-O	-5.26	1.16	1.23
18	X	22	ARG	CA-C	-5.26	1.45	1.52
27	O	383	LYS	CA-CB	5.26	1.61	1.53
28	H	227	LEU	CA-CB	5.26	1.61	1.53
31	L	177	GLU	N-CA	-5.26	1.39	1.45
5	E	38	ILE	CA-C	-5.26	1.46	1.52
7	G	202	LEU	N-CA	-5.26	1.39	1.46
22	S	486	LYS	C-N	5.26	1.40	1.33
9	i	173	GLN	CA-CB	5.26	1.61	1.53
17	T	144	TYR	N-CA	-5.26	1.42	1.46
18	X	86	ILE	CA-C	-5.26	1.45	1.52
23	P	226	LYS	C-N	5.26	1.40	1.33
26	U	58	GLU	N-CA	-5.26	1.39	1.46
4	D	117	GLN	N-CA	5.25	1.53	1.46
2	b	81	ASP	C-N	5.25	1.40	1.33
8	h	175	ASP	CA-C	-5.25	1.46	1.52
13	m	79	SER	C-N	5.25	1.40	1.33
15	W	107	HIS	ND1-CE1	5.25	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	38	LEU	N-CA	-5.25	1.40	1.46
22	S	298	ARG	N-CA	-5.25	1.39	1.46
25	R	233	ASP	C-O	-5.25	1.18	1.24
33	J	398	ILE	CA-C	-5.25	1.45	1.52
1	a	157	THR	CA-CB	-5.25	1.45	1.53
2	B	20	GLN	C-O	5.25	1.30	1.24
23	P	354	SER	CA-C	-5.25	1.46	1.52
23	P	427	GLU	CA-C	-5.25	1.46	1.52
31	L	100	SER	C-O	-5.25	1.17	1.23
9	2	137	SER	C-N	5.25	1.40	1.33
14	7	189	ARG	CZ-NH2	5.25	1.40	1.33
14	7	200	LYS	CA-C	-5.25	1.45	1.52
21	N	311	ILE	N-CA	-5.25	1.39	1.46
23	P	14	SER	CA-CB	5.25	1.61	1.53
14	n	189	ARG	NE-CZ	5.25	1.38	1.33
12	5	181	ARG	NE-CZ	5.25	1.38	1.33
15	W	182	TYR	CA-CB	5.25	1.61	1.53
16	V	256	GLU	C-N	5.25	1.41	1.33
16	V	284	ALA	N-CA	-5.25	1.40	1.46
22	S	165	PRO	N-CD	-5.25	1.40	1.47
23	P	277	GLN	CA-CB	5.25	1.61	1.53
25	R	120	LEU	C-N	5.25	1.41	1.33
9	i	55	VAL	C-N	5.25	1.40	1.33
2	B	243	ILE	C-N	5.25	1.41	1.34
9	2	85	THR	N-CA	5.25	1.53	1.46
4	d	96	HIS	ND1-CE1	5.24	1.37	1.32
8	h	112	ASP	CA-C	-5.24	1.45	1.53
13	m	84	HIS	ND1-CE1	5.24	1.37	1.32
23	P	8	LYS	C-N	5.24	1.40	1.33
11	4	110	LYS	N-CA	-5.24	1.39	1.46
22	S	35	LEU	C-N	5.24	1.40	1.33
3	c	31	HIS	CB-CG	-5.24	1.42	1.50
2	B	164	ILE	N-CA	-5.24	1.40	1.46
32	M	193	LEU	N-CA	-5.24	1.40	1.46
33	J	228	ARG	NE-CZ	5.24	1.38	1.33
13	m	149	ALA	CA-C	-5.24	1.46	1.52
2	B	126	GLY	N-CA	-5.24	1.38	1.45
17	T	202	LEU	N-CA	-5.24	1.40	1.46
25	R	254	SER	C-N	-5.24	1.27	1.33
27	O	52	ALA	N-CA	-5.24	1.39	1.46
5	E	51	GLU	CA-C	-5.24	1.46	1.52
33	J	371	ARG	NE-CZ	5.24	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	50	VAL	CA-C	-5.24	1.46	1.52
11	k	139	TYR	C-O	-5.24	1.17	1.24
1	A	225	VAL	CA-CB	-5.24	1.47	1.54
4	D	237	GLU	N-CA	-5.24	1.40	1.46
11	4	21	VAL	CA-CB	-5.24	1.47	1.54
18	X	127	GLY	C-N	5.24	1.40	1.33
22	S	473	ASP	C-N	5.24	1.40	1.33
24	Q	390	LEU	CA-C	-5.24	1.46	1.52
26	U	290	ASP	CA-CB	5.24	1.61	1.53
30	K	281	ARG	NE-CZ	5.24	1.38	1.33
31	L	68	ARG	NE-CZ	5.24	1.38	1.33
32	M	213	ARG	N-CA	-5.24	1.39	1.45
21	N	699	ALA	CA-C	-5.23	1.46	1.52
8	h	62	GLN	CA-C	-5.23	1.46	1.52
11	k	49	GLU	C-N	5.23	1.40	1.33
21	N	573	HIS	N-CA	-5.23	1.40	1.46
25	R	359	VAL	CA-CB	-5.23	1.47	1.54
26	U	265	LEU	C-N	5.23	1.41	1.33
30	K	217	THR	CA-C	-5.23	1.45	1.52
31	L	50	GLN	CA-CB	5.23	1.61	1.53
1	a	19	PHE	CA-C	-5.23	1.46	1.52
1	a	105	ARG	CD-NE	5.23	1.53	1.46
2	b	206	GLY	CA-C	-5.23	1.43	1.51
2	b	249	ALA	CA-C	-5.23	1.46	1.53
6	F	130	VAL	CA-C	-5.23	1.46	1.52
4	d	96	HIS	C-N	5.23	1.41	1.33
5	e	133	LEU	CA-C	-5.23	1.45	1.52
13	m	206	VAL	CA-CB	-5.23	1.47	1.54
27	O	186	ASN	CA-CB	5.23	1.61	1.53
13	m	182	TYR	CA-CB	5.23	1.59	1.53
6	F	39	ARG	CD-NE	5.23	1.53	1.46
23	P	393	VAL	N-CA	-5.23	1.40	1.46
25	R	244	THR	CA-C	-5.23	1.46	1.52
21	N	57	ASP	CA-C	-5.22	1.45	1.52
32	M	100	THR	C-N	5.22	1.40	1.33
33	J	212	ARG	CD-NE	5.22	1.53	1.46
12	l	144	ARG	NE-CZ	5.22	1.38	1.33
27	O	223	LEU	N-CA	-5.22	1.39	1.46
28	H	373	ARG	CZ-NH2	5.22	1.40	1.33
33	J	203	ALA	CA-CB	-5.22	1.44	1.53
1	a	14	ARG	CZ-NH1	5.22	1.40	1.32
8	h	12	ILE	CA-C	-5.22	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	4	ASP	C-N	5.22	1.40	1.33
29	I	398	GLU	C-N	5.22	1.41	1.33
8	1	100	ASP	CA-C	-5.22	1.45	1.52
14	7	236	ASN	C-N	5.22	1.43	1.34
24	Q	360	SER	CA-C	-5.22	1.46	1.52
3	C	165	VAL	CA-C	-5.22	1.46	1.52
7	G	132	PHE	CA-CB	5.22	1.62	1.53
10	3	199	TYR	N-CA	-5.22	1.39	1.46
30	K	72	GLN	CA-CB	5.22	1.62	1.53
4	d	137	GLY	CA-C	-5.21	1.45	1.52
10	3	103	TYR	CA-C	-5.21	1.46	1.52
18	X	10	PHE	CA-C	-5.21	1.46	1.52
33	J	151	GLY	C-N	5.21	1.39	1.34
10	3	93	SER	C-N	5.21	1.41	1.33
24	Q	76	GLU	N-CA	5.21	1.52	1.46
4	d	156	TYR	C-O	5.21	1.30	1.23
6	f	121	GLN	C-O	-5.21	1.18	1.24
12	l	134	LEU	C-N	5.21	1.40	1.33
22	S	140	LEU	CA-CB	5.21	1.61	1.53
26	U	104	LEU	C-N	5.21	1.41	1.33
11	k	50	ALA	CA-C	5.21	1.59	1.52
3	C	183	ASP	CA-CB	5.21	1.63	1.53
6	F	165	SER	CA-CB	5.21	1.61	1.53
22	S	280	ASN	C-N	5.21	1.40	1.33
2	B	7	PHE	CA-C	-5.21	1.46	1.52
9	2	91	ASN	C-N	5.21	1.40	1.33
21	N	641	LEU	N-CA	-5.21	1.39	1.46
33	J	271	THR	C-N	5.21	1.40	1.33
2	b	72	GLY	N-CA	5.20	1.49	1.44
11	k	62	ALA	N-CA	-5.20	1.40	1.46
2	B	64	VAL	CA-C	-5.20	1.45	1.52
9	2	240	ALA	C-N	5.20	1.40	1.33
29	I	307	LEU	C-N	5.20	1.40	1.33
31	L	417	LYS	CA-C	-5.20	1.45	1.52
32	M	373	ASP	C-O	-5.20	1.16	1.24
33	J	235	VAL	C-N	5.20	1.41	1.33
7	g	160	TYR	N-CA	-5.20	1.39	1.45
8	h	56	GLY	N-CA	-5.20	1.36	1.45
25	R	229	LYS	CA-C	-5.20	1.46	1.52
27	O	109	LEU	N-CA	-5.20	1.40	1.46
33	J	168	VAL	CA-CB	-5.20	1.47	1.54
3	c	33	GLY	C-N	5.20	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	46	VAL	CA-C	-5.20	1.46	1.52
12	l	285	VAL	C-N	5.20	1.40	1.33
9	2	191	GLY	N-CA	5.20	1.52	1.45
20	Z	249	MET	N-CA	-5.20	1.40	1.46
22	S	147	TRP	C-N	5.20	1.40	1.33
27	O	11	LEU	CA-C	-5.20	1.46	1.52
29	I	220	ILE	N-CA	-5.20	1.40	1.46
9	2	154	LEU	CA-C	-5.20	1.46	1.52
12	5	143	LEU	CA-C	-5.20	1.46	1.52
14	7	95	HIS	C-N	5.20	1.39	1.33
13	6	109	ARG	NE-CZ	5.20	1.38	1.33
29	I	192	GLN	CA-CB	5.20	1.60	1.53
31	L	404	ARG	CA-C	-5.20	1.46	1.52
4	d	83	ARG	CA-C	-5.20	1.45	1.52
10	3	119	PRO	C-N	5.20	1.40	1.33
21	N	541	ALA	N-CA	-5.20	1.39	1.46
26	U	266	THR	N-CA	-5.20	1.40	1.46
27	O	73	ILE	CA-C	-5.20	1.46	1.52
30	K	320	ARG	NE-CZ	5.20	1.38	1.33
11	k	38	LEU	CA-CB	5.19	1.61	1.53
9	i	68	PRO	C-N	5.19	1.41	1.33
10	3	74	TYR	CA-C	5.19	1.59	1.52
27	O	40	GLN	N-CA	-5.19	1.39	1.46
29	I	408	ARG	N-CA	-5.19	1.39	1.46
1	a	91	ARG	CD-NE	5.19	1.53	1.46
5	e	117	CYS	N-CA	-5.19	1.40	1.46
2	B	81	ASP	C-N	5.19	1.41	1.33
21	N	106	ILE	CA-C	-5.19	1.46	1.52
25	R	383	ARG	CD-NE	5.19	1.53	1.46
13	6	84	HIS	N-CA	-5.19	1.39	1.46
2	b	201	GLU	CA-C	5.19	1.59	1.52
9	i	122	HIS	CA-C	-5.19	1.45	1.52
2	B	216	ASP	CA-C	-5.19	1.46	1.52
22	S	454	SER	N-CA	-5.19	1.39	1.45
23	P	395	ARG	C-N	5.19	1.40	1.33
25	R	263	ARG	N-CA	-5.19	1.39	1.46
5	e	50	VAL	C-N	5.18	1.40	1.33
5	e	206	GLN	CA-C	-5.18	1.45	1.52
2	B	83	ARG	CD-NE	5.18	1.53	1.46
16	V	123	VAL	CA-C	-5.18	1.46	1.52
19	Y	16	LEU	CA-CB	5.18	1.62	1.53
21	N	175	ASP	CA-C	-5.18	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	89	LEU	CA-C	5.18	1.59	1.52
29	I	304	ARG	C-N	5.18	1.40	1.33
31	L	330	PRO	N-CA	-5.18	1.43	1.47
1	a	39	ASN	C-O	-5.18	1.17	1.24
5	e	91	HIS	CB-CG	5.18	1.57	1.50
6	f	132	LEU	N-CA	-5.18	1.39	1.45
4	D	33	ALA	C-O	-5.18	1.17	1.24
14	7	231	ALA	N-CA	-5.18	1.39	1.46
23	P	359	ARG	NE-CZ	5.18	1.38	1.33
25	R	99	TYR	C-O	-5.18	1.18	1.24
28	H	331	ARG	NE-CZ	5.18	1.38	1.33
30	K	234	PHE	C-N	5.18	1.40	1.33
8	h	96	TYR	C-O	-5.18	1.17	1.24
1	a	167	LYS	CA-CB	5.18	1.61	1.53
4	d	222	VAL	CA-C	-5.18	1.46	1.52
4	D	208	LYS	N-CA	-5.18	1.39	1.46
10	3	38	ASN	C-N	5.18	1.40	1.33
12	5	196	ARG	N-CA	-5.18	1.39	1.46
17	T	205	ILE	CA-CB	-5.18	1.48	1.54
21	N	337	GLY	C-N	5.18	1.40	1.33
30	K	317	ALA	CA-C	-5.18	1.46	1.52
32	M	62	ILE	C-N	5.18	1.40	1.33
5	e	247	GLU	N-CA	-5.18	1.39	1.46
3	C	114	ARG	CZ-NH1	5.18	1.40	1.32
30	K	402	ILE	N-CA	-5.18	1.40	1.46
1	A	108	TYR	C-N	5.18	1.40	1.33
2	B	83	ARG	NE-CZ	5.18	1.38	1.33
6	F	107	ARG	CZ-NH2	5.18	1.40	1.33
16	V	277	LYS	CA-C	-5.18	1.46	1.52
21	N	701	VAL	N-CA	-5.18	1.40	1.46
25	R	204	TRP	CG-CD2	5.18	1.53	1.43
33	J	381	ASP	CA-C	-5.18	1.45	1.52
2	b	236	ARG	C-N	5.17	1.40	1.33
11	4	104	ILE	CB-CG1	5.17	1.63	1.53
21	N	182	ASN	C-N	5.17	1.40	1.33
25	R	377	LEU	N-CA	-5.17	1.40	1.46
26	U	179	ARG	NE-CZ	5.17	1.38	1.33
28	H	87	ASP	CA-C	-5.17	1.45	1.52
31	L	332	THR	N-CA	5.17	1.52	1.46
5	E	55	THR	CA-C	-5.17	1.45	1.52
13	6	143	GLN	C-O	-5.17	1.18	1.24
21	N	820	GLU	C-O	5.17	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	34	THR	N-CA	5.17	1.52	1.46
12	l	111	GLU	N-CA	-5.17	1.40	1.46
10	3	129	CYS	C-N	5.17	1.39	1.33
32	M	163	PHE	CA-C	-5.17	1.46	1.52
8	h	54	ARG	CZ-NH1	5.17	1.40	1.32
12	l	120	MET	CG-SD	5.17	1.93	1.80
2	B	237	LYS	C-N	5.17	1.41	1.33
10	3	103	TYR	CA-CB	5.17	1.61	1.53
10	3	152	SER	CA-C	-5.17	1.46	1.52
33	J	141	LYS	C-N	5.17	1.39	1.33
6	f	147	PHE	CA-C	-5.17	1.46	1.52
11	k	115	GLU	CA-C	-5.17	1.46	1.52
2	B	59	GLU	CA-C	-5.17	1.45	1.52
19	Y	29	LEU	C-O	-5.17	1.18	1.24
21	N	180	SER	CA-C	-5.17	1.46	1.52
21	N	466	LEU	N-CA	5.17	1.53	1.46
22	S	143	GLN	CA-C	-5.17	1.46	1.52
5	e	10	ARG	CD-NE	5.17	1.53	1.46
7	g	16	SER	CA-C	-5.17	1.47	1.52
14	7	226	ARG	CA-CB	5.17	1.61	1.53
4	d	30	GLY	C-N	5.16	1.40	1.33
6	F	198	SER	CA-C	-5.16	1.45	1.52
11	4	38	LEU	CA-C	-5.16	1.46	1.52
24	Q	139	ILE	CA-C	-5.16	1.46	1.52
11	k	85	ARG	CZ-NH2	5.16	1.40	1.33
10	j	152	SER	CA-CB	5.16	1.61	1.53
27	O	267	ASP	CA-CB	5.16	1.61	1.53
29	I	283	GLU	N-CA	-5.16	1.39	1.46
29	I	376	ASN	N-CA	-5.16	1.40	1.46
31	L	329	ARG	C-N	5.16	1.38	1.33
2	b	190	HIS	CD2-NE2	5.16	1.43	1.37
11	4	169	GLU	N-CA	-5.16	1.40	1.46
14	7	129	LEU	CA-C	-5.16	1.46	1.52
17	T	23	CYS	N-CA	5.16	1.52	1.46
20	Z	634	ASP	N-CA	5.16	1.52	1.46
22	S	145	PHE	C-N	5.16	1.40	1.33
26	U	210	TYR	CA-CB	5.16	1.61	1.53
10	j	94	SER	CA-CB	5.16	1.61	1.53
15	W	122	ARG	CZ-NH1	5.16	1.40	1.32
20	Z	916	LEU	C-N	5.16	1.39	1.33
22	S	381	VAL	N-CA	-5.16	1.40	1.46
26	U	297	GLN	C-N	5.16	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	167	ASP	CA-C	-5.16	1.45	1.52
29	I	109	LEU	C-N	5.16	1.41	1.33
31	L	430	GLY	CA-C	-5.16	1.45	1.52
15	W	180	LEU	CA-C	-5.15	1.45	1.52
21	N	794	LYS	N-CA	-5.15	1.40	1.46
29	I	90	GLU	C-O	-5.15	1.18	1.24
31	L	402	ALA	C-N	5.15	1.40	1.33
1	A	97	ALA	CA-C	-5.15	1.46	1.52
9	2	40	GLY	C-N	5.15	1.38	1.33
12	5	274	LYS	C-N	5.15	1.39	1.33
32	M	169	ALA	N-CA	-5.15	1.39	1.46
7	g	246	GLU	CA-CB	5.15	1.61	1.53
6	F	47	VAL	C-O	-5.15	1.18	1.24
6	F	209	ASP	C-N	5.15	1.42	1.33
25	R	392	ARG	NE-CZ	5.15	1.38	1.33
33	J	75	VAL	CA-C	-5.15	1.46	1.52
12	5	139	ARG	NE-CZ	5.15	1.38	1.33
13	6	206	VAL	C-O	-5.15	1.18	1.24
21	N	810	ALA	C-N	5.15	1.40	1.33
30	K	241	GLU	N-CA	-5.15	1.38	1.45
31	L	261	ARG	NE-CZ	5.15	1.38	1.33
11	k	156	GLU	CA-CB	5.15	1.61	1.53
14	n	137	ARG	CZ-NH2	5.15	1.40	1.33
10	3	134	LYS	N-CA	-5.15	1.40	1.46
11	4	149	ARG	CZ-NH2	5.15	1.40	1.33
21	N	621	THR	CA-C	-5.15	1.46	1.52
23	P	425	HIS	CD2-NE2	5.15	1.43	1.37
32	M	218	ALA	CA-C	-5.15	1.46	1.52
33	J	48	ARG	CD-NE	5.15	1.53	1.46
17	T	44	LEU	C-O	-5.15	1.17	1.24
9	i	104	ARG	CZ-NH1	5.14	1.40	1.32
23	P	292	LYS	CA-CB	5.14	1.61	1.53
25	R	394	ASP	CA-CB	5.14	1.59	1.53
32	M	405	ASN	CA-CB	5.14	1.61	1.53
7	g	94	GLU	N-CA	-5.14	1.40	1.46
16	V	279	HIS	CA-CB	5.14	1.61	1.53
24	Q	316	THR	CA-C	-5.14	1.46	1.52
25	R	319	CYS	CA-CB	5.14	1.61	1.53
29	I	152	LYS	C-O	-5.14	1.17	1.24
29	I	297	GLY	CA-C	-5.14	1.44	1.51
5	E	40	ILE	N-CA	-5.14	1.39	1.46
28	H	443	PHE	CA-CB	5.14	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I	343	ARG	N-CA	-5.14	1.40	1.46
31	L	369	LYS	CA-CB	5.14	1.61	1.53
8	h	123	PRO	C-N	5.14	1.41	1.33
9	i	250	CYS	CA-C	5.14	1.59	1.52
2	B	101	TYR	CA-CB	5.14	1.61	1.54
3	C	175	LEU	C-N	5.14	1.41	1.33
6	F	164	ARG	CZ-NH2	5.14	1.40	1.33
12	5	78	THR	CA-CB	-5.14	1.45	1.53
21	N	570	ARG	CZ-NH1	5.14	1.40	1.32
30	K	81	ARG	CZ-NH2	5.14	1.40	1.33
32	M	402	ALA	CA-C	-5.14	1.46	1.52
33	J	177	LEU	CA-C	-5.14	1.46	1.52
5	e	166	ARG	N-CA	-5.14	1.39	1.46
6	F	70	MET	N-CA	-5.14	1.39	1.46
29	I	285	ASP	CA-C	-5.14	1.45	1.52
13	6	13	TYR	CA-CB	5.14	1.60	1.53
20	Z	247	GLN	N-CA	-5.14	1.39	1.46
21	N	165	ILE	C-N	5.14	1.40	1.33
21	N	298	TYR	CA-C	-5.14	1.46	1.52
21	N	417	ARG	CZ-NH2	5.14	1.40	1.33
21	N	437	GLU	CA-CB	5.14	1.61	1.53
22	S	452	TYR	CA-C	-5.14	1.44	1.52
30	K	47	ILE	C-O	-5.14	1.18	1.24
33	J	153	LEU	C-N	5.14	1.41	1.34
33	J	163	VAL	C-N	5.14	1.38	1.33
33	J	235	VAL	N-CA	-5.14	1.39	1.46
2	b	204	PHE	N-CA	-5.13	1.40	1.46
7	G	54	ILE	N-CA	-5.13	1.40	1.46
9	2	156	LEU	CA-CB	5.13	1.62	1.53
14	7	225	SER	N-CA	-5.13	1.40	1.46
21	N	641	LEU	CA-C	-5.13	1.45	1.52
22	S	217	PHE	C-N	5.13	1.40	1.33
22	S	258	GLU	N-CA	5.13	1.51	1.47
33	J	15	HIS	ND1-CE1	5.13	1.37	1.32
6	f	63	ILE	C-N	5.13	1.40	1.33
8	1	61	THR	N-CA	-5.13	1.40	1.46
29	I	435	LEU	N-CA	-5.13	1.39	1.46
32	M	73	ARG	CZ-NH1	5.13	1.40	1.32
2	b	87	ASP	CA-C	-5.13	1.46	1.52
13	m	208	ASP	CA-CB	5.13	1.62	1.53
8	1	90	VAL	CA-C	-5.13	1.46	1.52
8	1	166	HIS	CB-CG	5.13	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	W	100	HIS	ND1-CE1	5.13	1.37	1.32
21	N	878	GLN	CA-C	-5.13	1.45	1.52
26	U	156	HIS	N-CA	-5.13	1.39	1.46
33	J	337	LEU	C-N	5.13	1.41	1.33
2	B	127	VAL	CA-CB	-5.13	1.47	1.55
3	C	149	TYR	C-N	5.13	1.41	1.33
10	3	111	GLY	N-CA	-5.13	1.39	1.45
23	P	314	VAL	CA-CB	-5.13	1.48	1.54
27	O	314	SER	CA-CB	5.13	1.61	1.53
32	M	183	VAL	CA-C	-5.13	1.46	1.52
5	e	128	SER	CA-CB	5.13	1.62	1.53
5	E	196	ALA	CA-C	-5.13	1.46	1.52
10	3	112	ILE	CA-C	-5.13	1.46	1.52
16	V	186	GLN	CA-C	-5.13	1.48	1.52
21	N	642	ASP	CA-C	5.13	1.59	1.52
25	R	316	LEU	CA-CB	5.13	1.61	1.53
26	U	45	THR	CA-CB	5.13	1.60	1.53
32	M	227	GLY	C-N	5.13	1.40	1.33
21	N	378	ASN	CA-CB	5.13	1.61	1.53
21	N	613	HIS	ND1-CE1	5.13	1.37	1.32
22	S	154	GLN	C-N	5.13	1.41	1.33
23	P	363	LEU	N-CA	-5.13	1.40	1.46
25	R	36	SER	C-N	5.13	1.40	1.33
25	R	309	LEU	N-CA	-5.13	1.40	1.46
30	K	406	ASP	C-N	5.13	1.41	1.34
5	E	156	PHE	N-CA	-5.12	1.39	1.45
24	Q	113	ASP	N-CA	-5.12	1.40	1.46
30	K	194	GLN	CA-C	-5.12	1.46	1.52
21	N	806	THR	C-N	5.12	1.40	1.33
23	P	127	GLU	CA-CB	5.12	1.60	1.53
33	J	305	LEU	CA-CB	5.12	1.60	1.53
14	n	150	ALA	CA-C	-5.12	1.46	1.52
10	3	130	ILE	CA-C	-5.12	1.47	1.52
14	7	185	ASN	CA-CB	5.12	1.59	1.53
18	X	51	ARG	CA-C	-5.12	1.47	1.52
23	P	370	ASP	C-N	5.12	1.40	1.33
8	1	123	PRO	C-N	5.12	1.41	1.33
12	5	144	ARG	NE-CZ	5.12	1.38	1.33
29	I	276	PRO	N-CA	-5.12	1.38	1.47
2	b	26	THR	C-N	5.12	1.41	1.33
6	f	191	LYS	N-CA	-5.12	1.40	1.46
5	E	21	LEU	CA-C	-5.12	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	265	ASP	C-N	5.12	1.40	1.33
31	L	112	LEU	CA-C	-5.12	1.46	1.53
8	1	166	HIS	CE1-NE2	-5.12	1.27	1.32
11	4	57	ALA	CA-CB	5.12	1.61	1.53
15	W	9	VAL	CA-C	-5.12	1.46	1.52
28	H	286	GLU	CA-C	-5.12	1.46	1.52
3	c	229	ILE	CA-CB	-5.12	1.48	1.54
8	h	13	MET	C-N	5.12	1.40	1.33
7	G	72	ARG	CD-NE	5.12	1.53	1.46
23	P	389	ILE	CA-CB	-5.12	1.46	1.54
23	P	395	ARG	NE-CZ	5.12	1.38	1.33
29	I	70	LEU	N-CA	-5.12	1.40	1.46
4	d	128	PRO	CA-C	-5.11	1.46	1.52
4	d	182	LYS	N-CA	-5.11	1.39	1.46
7	G	25	GLU	CA-CB	5.11	1.61	1.53
23	P	310	ARG	C-O	-5.11	1.17	1.23
33	J	354	SER	N-CA	-5.11	1.39	1.45
18	X	11	ARG	CZ-NH2	5.11	1.40	1.33
2	B	90	ARG	CA-C	-5.11	1.46	1.52
14	7	224	SER	CA-C	-5.11	1.46	1.53
15	W	62	LEU	CA-C	-5.11	1.46	1.53
17	T	148	LEU	CA-CB	5.11	1.61	1.53
18	X	59	ARG	CZ-NH2	5.11	1.40	1.33
27	O	388	GLY	C-N	5.11	1.40	1.33
5	e	72	ARG	CA-C	5.11	1.59	1.52
3	C	115	LEU	CA-C	-5.11	1.46	1.52
7	G	151	LEU	C-N	5.11	1.41	1.33
11	4	50	ALA	CA-C	-5.11	1.46	1.52
20	Z	634	ASP	CA-C	5.11	1.59	1.52
7	g	193	VAL	N-CA	-5.11	1.40	1.46
21	N	531	LEU	C-O	5.11	1.30	1.24
25	R	232	VAL	C-N	5.11	1.40	1.33
25	R	420	ALA	CA-CB	-5.11	1.45	1.53
27	O	190	TYR	C-N	5.11	1.40	1.33
29	I	374	ASP	C-N	5.11	1.40	1.33
31	L	345	ARG	NE-CZ	5.11	1.38	1.33
33	J	329	ARG	CZ-NH1	5.11	1.39	1.32
16	V	92	MET	CA-CB	5.10	1.61	1.53
27	O	195	TYR	CA-CB	5.10	1.61	1.53
31	L	273	HIS	CB-CG	-5.10	1.43	1.50
3	C	238	ILE	C-N	5.10	1.41	1.33
8	1	125	GLY	C-N	5.10	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	64	ARG	CZ-NH2	5.10	1.40	1.33
23	P	50	SER	C-N	5.10	1.40	1.33
24	Q	172	PRO	CA-CB	5.10	1.60	1.53
27	O	53	LYS	C-N	5.10	1.41	1.33
29	I	344	ILE	CA-CB	-5.10	1.47	1.54
30	K	299	LEU	N-CA	5.10	1.52	1.46
32	M	107	ASN	CA-CB	5.10	1.62	1.53
1	A	103	GLU	N-CA	-5.10	1.40	1.46
28	H	102	CYS	CA-C	-5.10	1.46	1.52
32	M	410	VAL	C-O	-5.10	1.18	1.24
1	a	36	ASN	CA-CB	5.10	1.60	1.53
2	B	122	THR	C-N	5.10	1.40	1.33
6	F	73	SER	CA-C	-5.10	1.46	1.52
11	4	137	GLY	CA-C	-5.10	1.44	1.51
12	5	84	GLN	CA-CB	5.10	1.61	1.53
17	T	109	TYR	CA-C	-5.10	1.46	1.52
23	P	3	ARG	NE-CZ	5.10	1.38	1.33
25	R	43	ARG	NE-CZ	5.10	1.38	1.33
30	K	313	LYS	CA-CB	5.10	1.61	1.53
6	F	13	PHE	C-N	5.10	1.40	1.33
13	6	53	ASP	CA-CB	5.10	1.61	1.53
21	N	52	ASP	CA-C	-5.10	1.46	1.52
30	K	269	ILE	CA-C	-5.10	1.46	1.52
2	b	242	GLU	C-N	5.10	1.40	1.33
2	B	83	ARG	CZ-NH1	5.10	1.39	1.32
22	S	460	VAL	C-N	5.10	1.41	1.34
30	K	394	ALA	CA-C	5.10	1.59	1.52
3	c	245	THR	N-CA	-5.09	1.36	1.46
8	1	166	HIS	C-O	-5.09	1.18	1.24
8	1	193	GLU	C-N	5.09	1.40	1.33
9	2	168	GLU	N-CA	-5.09	1.39	1.46
14	7	44	VAL	N-CA	-5.09	1.40	1.46
25	R	167	LYS	N-CA	-5.09	1.40	1.46
33	J	391	ASN	CA-CB	5.09	1.61	1.53
17	T	152	LEU	C-N	5.09	1.40	1.33
4	d	83	ARG	CZ-NH1	5.09	1.39	1.32
5	e	191	LEU	N-CA	5.09	1.52	1.46
14	n	170	TYR	CA-C	-5.09	1.46	1.52
13	6	81	LYS	CA-CB	5.09	1.62	1.53
31	L	132	ARG	N-CA	-5.09	1.39	1.45
32	M	256	ILE	CA-CB	5.09	1.61	1.54
10	3	186	VAL	CA-C	-5.09	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	248	GLY	N-CA	-5.09	1.38	1.45
22	S	431	VAL	CA-C	5.09	1.59	1.52
28	H	61	ALA	CA-CB	5.09	1.61	1.53
6	F	174	ARG	CD-NE	5.09	1.53	1.46
30	K	289	ASP	CA-C	-5.09	1.45	1.52
30	K	344	ARG	CD-NE	5.09	1.53	1.46
31	L	193	LEU	CA-C	5.09	1.59	1.52
31	L	246	SER	CA-C	-5.09	1.46	1.52
9	i	31	THR	C-O	5.09	1.30	1.24
14	7	174	THR	C-N	5.09	1.39	1.33
15	W	127	ARG	NE-CZ	5.09	1.38	1.33
25	R	20	ARG	C-N	5.09	1.39	1.33
2	b	230	ASP	CA-C	-5.08	1.46	1.52
11	k	111	LYS	CA-C	-5.08	1.46	1.52
13	m	106	TYR	C-N	5.08	1.39	1.33
16	V	251	TYR	CZ-OH	5.08	1.48	1.38
17	T	140	SER	N-CA	-5.08	1.40	1.46
21	N	45	ASP	C-N	5.08	1.40	1.33
21	N	805	SER	C-O	-5.08	1.18	1.24
31	L	341	GLY	C-N	5.08	1.41	1.33
1	a	133	TYR	C-N	5.08	1.40	1.33
4	D	141	ARG	CZ-NH2	5.08	1.40	1.33
4	D	235	GLN	N-CA	5.08	1.52	1.46
12	5	263	HIS	CD2-NE2	5.08	1.43	1.37
21	N	566	SER	N-CA	-5.08	1.40	1.46
24	Q	291	TYR	CZ-OH	5.08	1.48	1.38
26	U	29	GLU	CA-C	-5.08	1.45	1.53
29	I	405	ARG	CZ-NH2	5.08	1.40	1.33
21	N	605	ILE	CA-CB	-5.08	1.48	1.54
23	P	408	SER	C-N	5.08	1.40	1.33
25	R	41	GLU	C-N	5.08	1.40	1.34
27	O	326	HIS	ND1-CE1	5.08	1.37	1.32
1	a	201	LYS	CA-C	-5.08	1.45	1.52
8	1	45	ARG	CA-C	-5.08	1.46	1.52
9	2	35	VAL	C-N	5.08	1.40	1.33
14	7	141	ASN	CA-CB	5.08	1.59	1.53
21	N	158	LEU	CB-CG	5.08	1.63	1.53
26	U	89	LEU	C-N	5.08	1.40	1.33
28	H	162	ARG	CZ-NH1	5.08	1.39	1.32
28	H	169	GLU	N-CA	-5.08	1.39	1.45
30	K	153	ASP	CA-C	-5.08	1.46	1.52
30	K	390	ALA	N-CA	-5.08	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	77	ARG	CD-NE	5.08	1.53	1.46
7	G	115	ARG	CZ-NH2	5.08	1.40	1.33
21	N	379	LEU	CA-CB	5.08	1.61	1.53
26	U	301	ILE	N-CA	-5.08	1.40	1.46
2	b	133	SER	CA-C	-5.08	1.46	1.52
6	f	133	LEU	C-O	-5.08	1.17	1.24
13	m	229	ARG	CZ-NH1	5.08	1.39	1.32
5	E	111	SER	N-CA	-5.08	1.40	1.46
9	2	247	VAL	N-CA	-5.08	1.40	1.46
21	N	762	ARG	CA-C	-5.08	1.46	1.52
27	O	220	SER	C-N	5.08	1.40	1.33
4	d	74	SER	CA-CB	5.07	1.61	1.53
8	h	202	TYR	CA-C	-5.07	1.45	1.52
11	k	171	ARG	CZ-NH1	5.07	1.39	1.32
2	B	128	ARG	N-CA	-5.07	1.41	1.45
7	G	230	PHE	N-CA	-5.07	1.40	1.45
8	1	182	ILE	CA-CB	-5.07	1.48	1.54
17	T	248	GLU	C-N	5.07	1.40	1.33
21	N	33	ASP	CA-CB	5.07	1.60	1.53
28	H	376	GLU	C-N	5.07	1.40	1.33
33	J	302	PRO	N-CA	5.07	1.53	1.47
9	i	48	ARG	NE-CZ	5.07	1.38	1.33
11	k	190	ARG	C-N	5.07	1.40	1.33
7	g	236	LEU	CA-CB	5.07	1.61	1.53
14	7	136	ARG	CA-C	5.07	1.59	1.52
22	S	431	VAL	N-CA	-5.07	1.40	1.46
24	Q	272	LEU	C-N	5.07	1.40	1.33
25	R	188	LYS	CA-C	-5.07	1.46	1.52
26	U	117	ASN	C-N	5.07	1.39	1.33
30	K	348	GLU	CA-C	-5.07	1.45	1.52
31	L	240	GLY	CA-C	5.07	1.58	1.51
32	M	66	LYS	CA-CB	5.07	1.61	1.53
22	S	454	SER	CA-C	-5.07	1.46	1.53
10	j	44	PHE	N-CA	-5.07	1.39	1.45
14	n	60	LEU	N-CA	-5.07	1.39	1.46
7	G	225	ASN	C-N	5.07	1.40	1.33
21	N	338	PHE	N-CA	-5.07	1.40	1.46
21	N	917	ILE	N-CA	-5.07	1.40	1.46
22	S	107	SER	N-CA	-5.07	1.39	1.46
28	H	434	ARG	CD-NE	5.07	1.53	1.46
30	K	37	ASN	CA-CB	5.07	1.61	1.53
7	g	203	ALA	CA-C	-5.07	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	146	LYS	CA-CB	5.07	1.60	1.53
13	6	53	ASP	C-O	-5.07	1.17	1.23
14	7	70	ASN	C-N	5.07	1.40	1.33
26	U	296	ILE	CA-CB	-5.07	1.48	1.54
30	K	73	ARG	CZ-NH1	5.07	1.39	1.32
30	K	207	ARG	NE-CZ	5.07	1.38	1.33
2	b	91	LYS	C-O	5.06	1.30	1.24
2	B	214	ILE	CA-C	-5.06	1.46	1.52
15	W	1	MET	C-N	5.06	1.41	1.33
29	I	130	VAL	N-CA	-5.06	1.40	1.46
3	c	134	SER	CA-C	-5.06	1.46	1.52
11	k	55	GLN	N-CA	5.06	1.52	1.46
23	P	233	GLU	CA-C	-5.06	1.47	1.53
25	R	333	MET	N-CA	-5.06	1.40	1.46
33	J	222	TYR	C-N	5.06	1.40	1.33
7	g	62	GLN	CA-C	-5.06	1.46	1.53
6	F	159	THR	N-CA	-5.06	1.39	1.46
10	3	41	GLU	C-O	-5.06	1.18	1.23
1	a	105	ARG	CZ-NH2	5.06	1.40	1.33
9	i	34	GLY	C-N	5.06	1.39	1.33
10	j	13	VAL	CA-CB	5.06	1.62	1.54
11	4	2	ASP	C-O	5.06	1.30	1.24
27	O	135	ARG	CA-C	-5.06	1.46	1.52
27	O	310	PHE	C-O	-5.06	1.17	1.24
5	e	197	GLU	N-CA	-5.06	1.40	1.46
6	f	145	LEU	CA-C	-5.06	1.46	1.52
1	A	237	SER	N-CA	5.06	1.52	1.45
3	C	184	MET	N-CA	5.06	1.52	1.45
5	E	157	HIS	CA-CB	5.06	1.61	1.53
15	W	74	ALA	CA-C	-5.06	1.46	1.52
24	Q	368	LEU	CA-C	-5.06	1.46	1.52
29	I	355	LEU	C-N	5.06	1.41	1.33
4	d	90	ARG	NE-CZ	5.06	1.38	1.33
24	Q	226	HIS	CG-ND1	5.06	1.43	1.38
27	O	358	ILE	C-N	5.06	1.40	1.33
1	a	148	GLU	CA-C	-5.05	1.45	1.52
10	j	28	ARG	C-N	5.05	1.40	1.33
1	A	40	ILE	CA-C	-5.05	1.46	1.52
4	D	146	LYS	C-N	5.05	1.40	1.33
27	O	342	ASP	C-O	-5.05	1.18	1.24
7	G	127	ASN	CA-C	-5.05	1.45	1.52
19	Y	82	ASP	C-N	5.05	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	647	ASP	CA-CB	-5.05	1.45	1.53
29	I	178	THR	CA-C	-5.05	1.45	1.52
30	K	73	ARG	CD-NE	5.05	1.53	1.46
33	J	88	VAL	N-CA	-5.05	1.39	1.46
4	D	18	PHE	CA-CB	5.05	1.61	1.53
5	E	72	ARG	CZ-NH1	5.05	1.39	1.32
16	V	194	ARG	CZ-NH1	5.05	1.39	1.32
21	N	265	ALA	N-CA	5.05	1.52	1.45
23	P	425	HIS	N-CA	5.05	1.52	1.46
28	H	453	GLY	N-CA	-5.05	1.39	1.45
32	M	92	GLU	N-CA	-5.05	1.39	1.46
30	K	207	ARG	N-CA	-5.05	1.39	1.46
1	A	200	GLU	C-O	5.05	1.29	1.24
21	N	573	HIS	C-N	5.05	1.40	1.33
29	I	70	LEU	C-N	5.05	1.40	1.33
29	I	190	GLN	C-N	5.05	1.39	1.33
29	I	219	VAL	CA-C	5.05	1.58	1.52
1	a	140	ILE	CA-C	-5.05	1.46	1.52
3	c	77	VAL	CA-CB	-5.05	1.48	1.54
13	m	30	VAL	N-CA	5.05	1.52	1.46
3	C	237	ASP	C-N	5.05	1.39	1.34
16	V	235	GLU	N-CA	-5.05	1.40	1.46
18	X	90	VAL	N-CA	-5.05	1.40	1.46
28	H	450	VAL	CA-CB	-5.05	1.47	1.54
1	a	137	LEU	N-CA	-5.04	1.39	1.46
10	j	111	GLY	N-CA	-5.04	1.40	1.45
12	l	166	LYS	N-CA	-5.04	1.40	1.46
5	E	192	THR	C-N	5.04	1.40	1.33
3	c	210	ARG	NE-CZ	5.04	1.38	1.33
26	U	34	VAL	C-N	5.04	1.42	1.34
2	B	7	PHE	C-N	5.04	1.40	1.33
7	G	21	ASN	C-O	5.04	1.29	1.23
21	N	150	LEU	CA-C	-5.04	1.45	1.52
28	H	373	ARG	CD-NE	5.04	1.53	1.46
30	K	99	PHE	CA-CB	5.04	1.60	1.53
2	b	36	GLY	N-CA	-5.04	1.38	1.45
10	j	157	ASN	N-CA	-5.04	1.39	1.46
3	C	18	ARG	C-N	5.04	1.41	1.33
9	2	48	ARG	CZ-NH1	5.04	1.39	1.32
12	5	279	GLU	N-CA	-5.04	1.40	1.46
21	N	570	ARG	NE-CZ	5.04	1.38	1.33
26	U	182	ALA	N-CA	-5.04	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	244	LEU	CA-C	-5.04	1.46	1.52
23	P	236	GLU	CA-CB	5.04	1.61	1.53
2	b	214	ILE	C-O	-5.04	1.18	1.24
11	k	98	TYR	CA-C	-5.04	1.46	1.52
8	l	57	SER	N-CA	-5.04	1.39	1.46
11	4	100	VAL	C-O	-5.04	1.18	1.23
25	R	24	TYR	N-CA	5.04	1.52	1.46
31	L	300	GLU	CA-CB	5.04	1.61	1.53
33	J	187	LEU	C-N	5.04	1.39	1.33
1	a	20	SER	C-N	5.03	1.40	1.34
2	B	33	THR	N-CA	-5.03	1.39	1.46
6	F	25	ALA	C-O	-5.03	1.17	1.24
15	W	11	ASP	C-N	-5.03	1.27	1.33
18	X	46	TRP	CA-CB	5.03	1.62	1.53
8	h	51	TRP	CA-C	-5.03	1.46	1.52
9	i	78	ALA	CA-C	-5.03	1.46	1.52
5	E	213	ASP	CA-C	-5.03	1.46	1.52
12	5	120	MET	C-O	-5.03	1.18	1.24
13	6	51	VAL	CA-CB	5.03	1.59	1.53
17	T	97	SER	N-CA	-5.03	1.41	1.46
21	N	605	ILE	CA-C	5.03	1.58	1.52
25	R	180	PHE	C-N	5.03	1.40	1.33
29	I	419	ALA	CA-C	-5.03	1.45	1.52
33	J	78	ILE	C-N	5.03	1.41	1.33
4	d	187	THR	N-CA	-5.03	1.39	1.45
8	h	14	ALA	CA-C	-5.03	1.46	1.52
21	N	694	LEU	C-N	5.03	1.40	1.33
24	Q	101	ILE	CA-C	5.03	1.59	1.52
8	h	71	HIS	CG-ND1	-5.03	1.32	1.38
2	B	244	ASN	C-N	5.03	1.40	1.33
8	l	140	SER	C-N	5.03	1.40	1.33
12	5	129	PHE	C-O	5.03	1.29	1.24
21	N	860	LYS	C-N	5.03	1.40	1.33
26	U	189	ARG	CD-NE	5.03	1.53	1.46
14	n	42	THR	CA-C	-5.03	1.46	1.52
7	G	32	GLU	C-N	5.03	1.41	1.33
29	I	365	HIS	C-N	5.03	1.40	1.33
29	I	376	ASN	CA-C	5.03	1.58	1.52
32	M	317	SER	C-N	5.03	1.40	1.33
33	J	334	LYS	CA-C	-5.03	1.45	1.52
22	S	250	ALA	CA-CB	5.02	1.61	1.53
11	4	96	ARG	CZ-NH1	5.02	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	729	SER	CA-CB	5.02	1.61	1.53
21	N	870	ASN	C-N	5.02	1.40	1.33
30	K	210	LEU	CA-CB	5.02	1.61	1.53
26	U	295	LYS	C-O	-5.02	1.18	1.24
31	L	137	ARG	N-CA	-5.02	1.40	1.46
33	J	77	LYS	CA-C	-5.02	1.46	1.52
33	J	280	ASP	N-CA	-5.02	1.39	1.46
16	V	159	ILE	C-N	5.02	1.40	1.33
23	P	25	ASP	CA-CB	5.02	1.61	1.53
30	K	290	ARG	CD-NE	5.02	1.53	1.46
3	c	6	TYR	CA-C	-5.02	1.46	1.52
4	d	151	GLU	C-N	-5.02	1.29	1.33
12	l	286	ILE	C-N	5.02	1.40	1.33
14	n	212	ASN	CG-ND2	5.02	1.43	1.33
3	C	99	LEU	CA-CB	5.02	1.61	1.53
11	4	173	PRO	C-N	5.02	1.40	1.33
14	7	217	LEU	C-N	5.02	1.40	1.34
17	T	256	LYS	C-O	-5.02	1.18	1.24
27	O	221	ALA	CA-C	-5.02	1.46	1.52
28	H	120	ASN	C-N	5.02	1.40	1.33
11	4	171	ARG	CZ-NH1	5.02	1.39	1.32
22	S	149	SER	CA-CB	5.02	1.61	1.53
1	a	95	LEU	CA-C	-5.01	1.46	1.52
10	j	61	THR	C-N	5.01	1.40	1.33
13	m	160	ASN	CA-CB	5.01	1.61	1.53
4	D	201	GLU	CA-CB	5.01	1.61	1.53
17	T	149	ASP	N-CA	-5.01	1.40	1.46
17	T	257	THR	C-N	5.01	1.40	1.33
24	Q	398	TYR	N-CA	-5.01	1.39	1.46
25	R	231	LEU	C-N	5.01	1.40	1.33
1	A	181	ASN	CA-CB	5.01	1.61	1.53
17	T	240	LYS	C-N	5.01	1.40	1.33
22	S	226	ASP	CA-CB	5.01	1.60	1.53
24	Q	15	VAL	C-O	-5.01	1.18	1.24
26	U	276	ILE	N-CA	-5.01	1.40	1.46
4	D	188	VAL	N-CA	-5.01	1.40	1.46
5	E	52	LYS	C-N	5.01	1.40	1.33
17	T	88	TYR	C-N	5.01	1.40	1.34
28	H	101	ARG	CA-C	-5.01	1.46	1.52
2	b	86	VAL	C-N	5.01	1.40	1.33
8	h	92	LYS	CA-C	-5.01	1.46	1.52
8	1	169	SER	C-N	5.01	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	161	ARG	CD-NE	5.01	1.53	1.46
16	V	254	ARG	NE-CZ	5.01	1.38	1.33
18	X	76	VAL	C-O	-5.01	1.18	1.24
23	P	53	ALA	C-N	5.01	1.41	1.33
25	R	60	ALA	N-CA	5.01	1.53	1.46
27	O	36	LYS	C-O	5.01	1.30	1.24
33	J	325	ALA	CA-C	-5.01	1.45	1.52
9	i	104	ARG	NE-CZ	5.01	1.38	1.33
5	E	102	TYR	C-N	5.01	1.40	1.33
24	Q	173	SER	C-O	-5.01	1.17	1.24
3	C	41	SER	N-CA	-5.01	1.39	1.46
16	V	20	ARG	CZ-NH1	5.01	1.39	1.32
28	H	61	ALA	CA-C	-5.01	1.46	1.52
10	3	142	ALA	C-O	5.00	1.28	1.23
12	5	147	GLU	CA-C	-5.00	1.46	1.52
22	S	32	GLN	CA-CB	5.00	1.61	1.53
33	J	399	SER	CA-C	-5.00	1.46	1.52
14	7	43	SER	C-N	5.00	1.40	1.33
16	V	33	ALA	CA-CB	5.00	1.61	1.53
27	O	170	SER	CA-CB	5.00	1.61	1.53
31	L	209	ARG	CZ-NH2	5.00	1.40	1.33
3	c	170	SER	CA-CB	5.00	1.61	1.53
4	d	134	LEU	CA-CB	5.00	1.60	1.53
1	A	36	ASN	CA-CB	5.00	1.58	1.53
3	C	110	ILE	CA-CB	5.00	1.60	1.54
5	E	67	ILE	CA-CB	-5.00	1.48	1.54
5	E	126	GLY	C-O	-5.00	1.17	1.23
20	Z	747	ALA	C-N	5.00	1.40	1.33
27	O	339	GLY	CA-C	-5.00	1.47	1.52
30	K	312	VAL	N-CA	-5.00	1.40	1.46
32	M	368	MET	CA-C	-5.00	1.46	1.53

All (7246) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I	313	LEU	CA-C-N	-46.90	31.95	121.54
29	I	313	LEU	C-N-CA	-46.90	31.95	121.54
29	I	313	LEU	O-C-N	29.73	164.58	122.36
20	Z	635	ALA	CB-CA-C	23.78	146.17	110.50
7	g	93	ARG	NE-CZ-NH1	-23.55	97.95	121.50
7	G	93	ARG	NE-CZ-NH1	-23.47	98.03	121.50
14	n	198	ILE	N-CA-CB	16.95	121.18	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	727	GLU	N-CA-CB	-16.46	84.94	110.46
20	Z	245	VAL	N-CA-C	16.30	126.07	110.42
20	Z	728	LYS	CB-CG-CD	16.07	148.26	111.30
3	C	106	ILE	CA-C-N	14.32	134.21	120.03
3	C	106	ILE	C-N-CA	14.32	134.21	120.03
7	G	93	ARG	NE-CZ-NH2	14.01	131.81	119.20
20	Z	728	LYS	N-CA-CB	13.35	133.05	110.49
10	j	99	ARG	N-CA-C	-13.18	98.15	114.75
9	i	67	SER	CA-C-N	12.93	134.06	119.32
9	i	67	SER	C-N-CA	12.93	134.06	119.32
2	B	15	SER	CA-C-N	12.59	137.46	121.85
2	B	15	SER	C-N-CA	12.59	137.46	121.85
20	Z	258	PRO	N-CA-C	12.38	125.81	110.70
20	Z	250	VAL	N-CA-C	12.32	123.16	110.72
20	Z	745	LEU	CB-CA-C	-12.29	91.58	110.88
28	H	422	VAL	N-CA-C	-12.08	99.10	110.82
20	Z	635	ALA	N-CA-CB	11.95	128.32	110.40
3	c	92	ARG	CA-C-N	11.66	135.26	120.56
3	c	92	ARG	C-N-CA	11.66	135.26	120.56
33	J	351	ASN	CA-CB-CG	-11.60	101.00	112.60
6	f	126	ARG	O-C-N	-11.46	113.83	121.85
20	Z	745	LEU	N-CA-C	11.36	123.22	111.07
20	Z	247	GLN	CB-CA-C	11.29	132.34	110.67
7	g	93	ARG	NE-CZ-NH2	11.20	129.28	119.20
11	4	110	LYS	N-CA-C	-11.09	99.58	113.55
29	I	193	GLU	N-CA-C	-11.08	98.45	113.30
24	Q	294	ARG	N-CA-CB	11.07	126.40	110.12
24	Q	3	LEU	CA-C-N	11.05	131.31	119.05
24	Q	3	LEU	C-N-CA	11.05	131.31	119.05
20	Z	634	ASP	CA-C-N	11.00	141.51	121.70
20	Z	634	ASP	C-N-CA	11.00	141.51	121.70
20	Z	728	LYS	CA-CB-CG	10.99	136.07	114.10
1	a	113	PRO	N-CA-CB	10.98	112.91	103.35
20	Z	244	ARG	CA-C-N	10.85	134.22	120.56
20	Z	244	ARG	C-N-CA	10.85	134.22	120.56
20	Z	633	GLU	N-CA-C	10.81	123.06	111.28
11	k	93	ARG	NE-CZ-NH2	-10.76	109.52	119.20
11	k	30	ASP	CA-CB-CG	10.73	123.33	112.60
15	W	123	ASP	CA-CB-CG	-10.70	101.90	112.60
17	T	46	ILE	N-CA-C	-10.67	93.15	107.88
30	K	101	GLU	CA-C-O	-10.66	110.13	120.26
24	Q	55	GLU	N-CA-C	10.64	122.88	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	X	20	ASP	CA-CB-CG	-10.64	101.96	112.60
14	7	40	THR	CA-C-N	10.63	130.72	121.58
14	7	40	THR	C-N-CA	10.63	130.72	121.58
20	Z	634	ASP	N-CA-C	10.57	122.56	111.14
21	N	674	GLN	CA-C-N	10.57	135.43	120.42
21	N	674	GLN	C-N-CA	10.57	135.43	120.42
3	C	129	ARG	CA-C-N	10.51	130.29	120.21
3	C	129	ARG	C-N-CA	10.51	130.29	120.21
14	7	38	ILE	N-CA-C	-10.51	103.32	111.62
20	Z	630	LYS	CA-C-N	10.45	131.74	120.03
20	Z	630	LYS	C-N-CA	10.45	131.74	120.03
1	A	38	THR	N-CA-C	-10.43	100.69	113.41
16	V	21	ASP	CA-CB-CG	-10.41	102.19	112.60
31	L	404	ARG	NE-CZ-NH2	-10.40	109.84	119.20
20	Z	748	LEU	N-CA-C	10.39	122.69	111.36
7	g	93	ARG	NH1-CZ-NH2	10.36	132.77	119.30
26	U	190	LEU	N-CA-C	-10.29	100.14	111.36
31	L	262	ILE	O-C-N	10.26	131.97	121.91
27	O	333	SER	N-CA-C	10.24	122.44	111.28
12	l	280	GLY	N-CA-C	-10.14	103.01	115.08
10	j	8	ASN	N-CA-C	-10.12	103.08	114.62
13	m	187	GLU	CA-C-N	10.11	133.29	120.56
13	m	187	GLU	C-N-CA	10.11	133.29	120.56
9	i	107	SER	CA-C-N	10.09	134.16	120.44
9	i	107	SER	C-N-CA	10.09	134.16	120.44
2	b	187	ASP	CA-C-N	10.06	133.77	120.28
2	b	187	ASP	C-N-CA	10.06	133.77	120.28
24	Q	206	ASN	N-CA-C	-10.06	99.55	112.23
32	M	394	VAL	N-CA-C	-10.06	103.16	111.81
4	D	67	ILE	N-CA-CB	-10.06	101.15	112.21
7	G	60	VAL	CB-CA-C	-10.05	99.95	110.71
26	U	201	GLN	OE1-CD-NE2	10.02	132.62	122.60
10	j	101	GLY	CA-C-N	9.99	129.80	120.21
10	j	101	GLY	C-N-CA	9.99	129.80	120.21
16	V	192	LEU	N-CA-C	9.96	123.17	111.02
14	7	182	HIS	ND1-CE1-NE2	9.96	118.36	108.40
25	R	74	ASN	CA-CB-CG	-9.95	102.65	112.60
22	S	104	VAL	N-CA-C	-9.95	101.03	109.19
11	4	32	ASP	CA-CB-CG	-9.94	102.66	112.60
6	F	126	ARG	O-C-N	-9.91	114.91	121.85
20	Z	918	ASP	CA-CB-CG	9.85	122.44	112.60
3	c	135	PHE	CA-CB-CG	-9.82	103.98	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	343	GLN	N-CA-C	-9.80	100.82	113.17
20	Z	251	ALA	N-CA-CB	9.78	124.49	110.12
20	Z	745	LEU	CA-C-O	-9.74	110.59	120.82
20	Z	635	ALA	N-CA-C	-9.73	83.74	111.00
23	P	316	LYS	N-CA-C	9.73	121.89	111.28
17	T	234	TYR	CA-C-N	9.72	134.58	120.38
17	T	234	TYR	C-N-CA	9.72	134.58	120.38
22	S	79	ASN	N-CA-C	9.67	121.82	111.28
11	4	2	ASP	CA-CB-CG	9.66	122.26	112.60
23	P	78	GLN	CA-C-O	-9.66	110.75	120.70
22	S	125	LYS	N-CA-C	9.65	121.40	111.07
12	5	168	ALA	N-CA-C	-9.63	99.37	112.94
25	R	49	PHE	CA-CB-CG	-9.61	104.19	113.80
21	N	7	ALA	CA-C-O	-9.60	109.03	118.34
4	d	60	THR	N-CA-C	-9.60	97.72	109.72
8	1	147	CYS	CB-CA-C	-9.60	95.81	110.88
24	Q	285	LYS	N-CA-C	-9.60	103.68	114.62
24	Q	131	VAL	CA-C-N	9.58	133.51	120.38
24	Q	131	VAL	C-N-CA	9.58	133.51	120.38
15	W	124	GLU	N-CA-C	9.58	121.72	111.28
4	D	16	HIS	ND1-CE1-NE2	9.58	117.98	108.40
2	B	207	ASP	CA-CB-CG	-9.56	103.04	112.60
15	W	2	VAL	N-CA-C	-9.55	96.88	108.53
23	P	34	SER	CA-C-N	9.54	133.06	120.28
23	P	34	SER	C-N-CA	9.54	133.06	120.28
22	S	414	ASP	CA-CB-CG	-9.52	103.08	112.60
21	N	248	GLU	N-CA-C	-9.49	98.99	111.71
24	Q	275	ILE	N-CA-C	-9.48	104.10	113.20
30	K	140	HIS	CA-C-N	9.47	133.51	120.63
30	K	140	HIS	C-N-CA	9.47	133.51	120.63
20	Z	745	LEU	O-C-N	9.43	131.78	122.07
18	X	131	ASN	O-C-N	9.43	134.15	122.65
1	a	187	LYS	N-CA-C	-9.42	101.09	111.36
21	N	602	VAL	CA-C-O	-9.42	110.84	118.85
4	D	122	GLN	N-CA-C	9.42	124.03	112.54
9	i	66	ILE	N-CA-C	-9.41	101.17	110.30
19	Y	4	ASP	CA-CB-CG	-9.41	103.19	112.60
11	k	137	GLY	CA-C-N	9.39	133.80	120.28
11	k	137	GLY	C-N-CA	9.39	133.80	120.28
4	D	18	PHE	CA-CB-CG	-9.39	104.41	113.80
27	O	113	LYS	N-CA-C	9.37	121.58	111.36
21	N	408	LEU	CA-C-N	9.37	130.31	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	408	LEU	C-N-CA	9.37	130.31	120.00
12	l	158	LEU	CA-C-N	9.35	132.60	120.44
12	l	158	LEU	C-N-CA	9.35	132.60	120.44
4	D	151	GLU	O-C-N	-9.34	115.73	121.71
13	6	70	ASP	CA-CB-CG	9.34	121.94	112.60
29	I	404	LEU	CA-C-N	9.33	132.78	120.28
29	I	404	LEU	C-N-CA	9.33	132.78	120.28
20	Z	248	TYR	N-CA-C	-9.32	101.12	111.28
7	G	67	ILE	N-CA-CB	9.31	123.63	111.90
7	G	27	ALA	N-CA-C	9.31	122.42	111.71
15	W	15	TYR	N-CA-C	-9.31	101.44	113.17
1	A	140	ILE	O-C-N	9.30	133.36	123.03
1	a	84	ASN	CA-CB-CG	-9.30	103.30	112.60
31	L	284	ASP	CA-CB-CG	-9.30	103.30	112.60
17	T	235	PHE	CA-CB-CG	9.30	123.10	113.80
4	D	218	ASP	N-CA-C	-9.29	99.74	113.40
29	I	267	ILE	CB-CA-C	-9.29	99.60	112.14
6	f	13	PHE	O-C-N	-9.29	111.42	123.21
20	Z	246	CYS	CA-C-N	9.28	134.42	120.31
20	Z	246	CYS	C-N-CA	9.28	134.42	120.31
15	W	80	GLN	N-CA-C	-9.26	93.77	109.24
14	n	257	ASP	CA-CB-CG	-9.26	103.34	112.60
14	n	198	ILE	CB-CA-C	-9.25	104.55	114.35
16	V	123	VAL	N-CA-C	-9.24	101.39	110.72
13	6	143	GLN	N-CA-C	-9.24	104.09	114.62
33	J	288	ILE	N-CA-CB	9.24	122.69	111.60
23	P	216	LEU	CA-C-O	-9.24	110.63	120.42
33	J	131	ASP	CA-CB-CG	-9.23	103.37	112.60
11	k	84	VAL	CA-C-O	-9.22	111.36	120.95
20	Z	249	MET	CA-C-O	-9.21	111.22	120.70
28	H	272	ILE	N-CA-C	-9.20	94.15	107.77
20	Z	918	ASP	CB-CA-C	-9.20	95.34	110.79
23	P	40	LEU	CA-C-N	9.16	132.28	120.56
23	P	40	LEU	C-N-CA	9.16	132.28	120.56
30	K	406	ASP	CA-CB-CG	-9.16	103.44	112.60
7	g	239	ALA	CA-C-N	9.14	132.08	120.56
7	g	239	ALA	C-N-CA	9.14	132.08	120.56
24	Q	280	ASN	CA-C-N	9.14	132.98	120.46
24	Q	280	ASN	C-N-CA	9.14	132.98	120.46
25	R	350	LEU	O-C-N	9.13	132.56	122.15
1	A	158	ASP	CA-C-O	-9.13	112.77	120.71
2	b	43	VAL	N-CA-C	-9.13	94.94	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	U	125	VAL	N-CA-C	-9.11	104.05	112.43
5	e	33	LEU	N-CA-C	-9.11	101.13	112.88
29	I	382	THR	CA-C-N	9.10	132.28	120.44
29	I	382	THR	C-N-CA	9.10	132.28	120.44
30	K	101	GLU	N-CA-C	9.10	116.41	108.22
18	X	98	PHE	N-CA-C	-9.10	95.13	109.50
21	N	289	ILE	N-CA-CB	9.09	121.18	110.55
9	i	60	CYS	N-CA-C	-9.08	96.45	108.34
20	Z	747	ALA	CA-C-N	9.07	133.18	120.29
20	Z	747	ALA	C-N-CA	9.07	133.18	120.29
21	N	601	THR	CA-C-N	9.07	125.95	120.24
21	N	601	THR	C-N-CA	9.07	125.95	120.24
20	Z	631	GLY	CA-C-N	9.06	132.42	120.28
20	Z	631	GLY	C-N-CA	9.06	132.42	120.28
33	J	127	GLU	N-CA-C	-9.04	102.41	112.72
4	d	230	ASN	CA-CB-CG	-9.01	103.59	112.60
22	S	159	ASN	CA-C-N	9.00	132.14	120.44
22	S	159	ASN	C-N-CA	9.00	132.14	120.44
26	U	25	THR	N-CA-C	-9.00	102.43	113.50
30	K	187	ALA	N-CA-C	9.00	123.57	112.23
24	Q	289	GLU	CA-C-N	8.99	132.33	120.28
24	Q	289	GLU	C-N-CA	8.99	132.33	120.28
20	Z	747	ALA	N-CA-C	-8.98	101.49	111.28
4	d	239	GLU	CA-C-N	8.97	133.02	120.29
4	d	239	GLU	C-N-CA	8.97	133.02	120.29
5	E	215	ASN	CA-CB-CG	-8.96	103.64	112.60
28	H	195	VAL	N-CA-C	-8.96	103.87	112.29
16	V	289	GLU	CA-C-O	-8.96	110.93	120.42
20	Z	918	ASP	CA-C-N	8.95	132.27	120.28
20	Z	918	ASP	C-N-CA	8.95	132.27	120.28
26	U	240	GLY	N-CA-C	-8.95	102.97	115.32
20	Z	748	LEU	O-C-N	-8.94	111.96	122.15
11	k	84	VAL	O-C-N	8.93	130.53	121.87
21	N	325	PHE	CA-CB-CG	-8.93	104.87	113.80
23	P	327	LEU	N-CA-CB	8.91	125.55	110.49
18	X	36	LYS	CA-C-O	-8.90	111.81	120.26
22	S	327	ILE	CA-C-O	-8.90	115.31	119.94
26	U	170	GLY	CA-C-N	8.89	131.94	120.56
26	U	170	GLY	C-N-CA	8.89	131.94	120.56
4	D	96	HIS	CB-CG-CD2	-8.89	119.65	131.20
14	n	126	PHE	CA-C-N	8.88	132.18	120.28
14	n	126	PHE	C-N-CA	8.88	132.18	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	20	PHE	CA-CB-CG	-8.86	104.94	113.80
6	f	108	ALA	CA-C-N	8.86	129.75	120.00
6	f	108	ALA	C-N-CA	8.86	129.75	120.00
1	a	93	ALA	CA-C-N	8.86	132.49	120.44
1	a	93	ALA	C-N-CA	8.86	132.49	120.44
7	G	117	GLY	CA-C-N	8.86	132.15	120.28
7	G	117	GLY	C-N-CA	8.86	132.15	120.28
24	Q	327	GLY	N-CA-C	8.86	124.88	114.16
21	N	97	PHE	N-CA-C	-8.86	103.06	114.04
6	F	152	ASN	CA-CB-CG	-8.85	103.75	112.60
11	k	134	GLY	CA-C-N	8.84	132.85	120.29
11	k	134	GLY	C-N-CA	8.84	132.85	120.29
24	Q	112	ASP	CA-C-N	8.84	132.13	120.28
24	Q	112	ASP	C-N-CA	8.84	132.13	120.28
2	b	156	TYR	N-CA-C	-8.84	95.90	109.24
17	T	229	VAL	CA-C-N	8.84	135.25	122.35
17	T	229	VAL	C-N-CA	8.84	135.25	122.35
24	Q	15	VAL	CB-CA-C	-8.84	100.44	112.02
21	N	870	ASN	CA-C-O	-8.83	110.54	120.43
27	O	236	HIS	CA-C-N	8.83	129.38	119.32
27	O	236	HIS	C-N-CA	8.83	129.38	119.32
19	Y	67	VAL	N-CA-C	-8.82	104.43	112.90
18	X	57	VAL	O-C-N	-8.82	113.65	123.18
22	S	429	ASP	N-CA-C	-8.82	102.54	113.38
9	2	43	ILE	N-CA-C	-8.81	95.30	108.17
23	P	96	MET	N-CA-C	8.80	120.48	111.07
30	K	398	ASN	N-CA-CB	8.79	125.34	110.49
24	Q	277	ASP	CA-C-N	8.78	131.80	120.56
24	Q	277	ASP	C-N-CA	8.78	131.80	120.56
3	c	36	ILE	CA-C-N	8.76	127.61	121.65
3	c	36	ILE	C-N-CA	8.76	127.61	121.65
25	R	361	VAL	CA-C-N	8.75	132.01	120.28
25	R	361	VAL	C-N-CA	8.75	132.01	120.28
22	S	256	LYS	CA-C-N	8.74	134.34	121.31
22	S	256	LYS	C-N-CA	8.74	134.34	121.31
1	a	218	PHE	CA-CB-CG	-8.74	105.06	113.80
10	3	83	GLU	CA-C-N	8.74	128.89	119.28
10	3	83	GLU	C-N-CA	8.74	128.89	119.28
14	7	89	ASP	CA-CB-CG	8.74	121.34	112.60
20	Z	739	ALA	N-CA-C	8.73	120.88	111.36
5	e	195	GLU	CA-C-N	8.73	132.69	120.29
5	e	195	GLU	C-N-CA	8.73	132.69	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	334	HIS	CA-CB-CG	-8.73	105.07	113.80
11	k	28	LEU	N-CA-C	-8.72	103.22	114.04
18	X	79	LYS	N-CA-C	-8.72	101.39	114.64
31	L	262	ILE	CA-C-O	-8.72	111.93	121.17
13	6	193	ARG	CA-C-N	8.72	131.77	120.44
13	6	193	ARG	C-N-CA	8.72	131.77	120.44
2	B	151	ASP	CA-C-N	8.71	130.73	119.84
2	B	151	ASP	C-N-CA	8.71	130.73	119.84
5	E	156	PHE	CA-CB-CG	-8.70	105.10	113.80
30	K	311	ASN	N-CA-C	8.69	121.53	110.24
6	f	126	ARG	CA-C-N	8.69	128.62	119.85
6	f	126	ARG	C-N-CA	8.69	128.62	119.85
30	K	113	THR	N-CA-C	-8.68	102.24	112.92
27	O	67	SER	CA-C-O	-8.67	111.36	120.55
13	m	109	ARG	N-CA-C	-8.67	102.87	113.97
19	Y	36	GLU	N-CA-C	-8.65	103.31	114.04
29	I	271	ALA	N-CA-CB	8.65	122.61	110.07
21	N	642	ASP	CA-C-N	8.65	128.79	119.28
21	N	642	ASP	C-N-CA	8.65	128.79	119.28
23	P	276	LEU	CA-C-N	8.64	132.21	120.54
23	P	276	LEU	C-N-CA	8.64	132.21	120.54
16	V	114	PHE	CA-CB-CG	-8.63	105.17	113.80
24	Q	304	GLU	CA-C-N	8.63	131.84	120.28
24	Q	304	GLU	C-N-CA	8.63	131.84	120.28
23	P	434	THR	CA-C-N	8.63	132.54	120.29
23	P	434	THR	C-N-CA	8.63	132.54	120.29
3	c	207	THR	CA-C-N	8.62	131.84	120.28
3	c	207	THR	C-N-CA	8.62	131.84	120.28
13	m	141	ARG	NE-CZ-NH1	-8.62	112.88	121.50
20	Z	727	GLU	CB-CA-C	8.62	125.37	110.45
2	B	168	SER	N-CA-C	8.62	120.30	111.07
8	h	129	HIS	CA-CB-CG	-8.62	105.18	113.80
22	S	94	LYS	CA-C-N	8.61	131.63	120.44
22	S	94	LYS	C-N-CA	8.61	131.63	120.44
28	H	240	ILE	CA-C-O	-8.61	113.53	121.97
30	K	56	LYS	N-CA-CB	8.61	123.56	110.30
3	c	4	ARG	CA-C-N	8.59	132.15	120.38
3	c	4	ARG	C-N-CA	8.59	132.15	120.38
10	j	71	THR	N-CA-CB	8.59	122.47	110.01
25	R	404	VAL	N-CA-CB	8.58	123.45	110.58
8	h	189	ALA	CA-C-N	8.58	131.77	120.28
8	h	189	ALA	C-N-CA	8.58	131.77	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	195	THR	N-CA-CB	8.57	122.50	110.07
27	O	9	THR	CA-C-N	8.56	132.58	120.42
27	O	9	THR	C-N-CA	8.56	132.58	120.42
14	7	44	VAL	N-CA-C	-8.56	95.78	108.45
10	j	134	LYS	N-CA-C	-8.55	100.82	112.03
6	F	13	PHE	CA-C-N	8.56	137.10	121.70
6	F	13	PHE	C-N-CA	8.56	137.10	121.70
30	K	219	LYS	CA-C-N	8.56	131.75	120.28
30	K	219	LYS	C-N-CA	8.56	131.75	120.28
12	5	283	ASN	CA-CB-CG	-8.55	104.05	112.60
28	H	444	LEU	CA-C-N	8.55	131.56	120.44
28	H	444	LEU	C-N-CA	8.55	131.56	120.44
5	e	10	ARG	N-CA-C	-8.55	100.28	113.02
11	k	156	GLU	CA-C-N	8.55	129.40	120.00
11	k	156	GLU	C-N-CA	8.55	129.40	120.00
1	A	205	PHE	CA-CB-CG	-8.55	105.25	113.80
23	P	313	ILE	N-CA-C	-8.55	103.55	111.67
29	I	421	GLU	CA-C-N	8.55	132.43	120.29
29	I	421	GLU	C-N-CA	8.55	132.43	120.29
23	P	142	ASP	N-CA-C	-8.55	102.05	111.36
4	d	92	GLU	CA-C-N	8.54	132.41	120.29
4	d	92	GLU	C-N-CA	8.54	132.41	120.29
4	D	102	ASP	CA-C-N	8.54	128.57	119.78
4	D	102	ASP	C-N-CA	8.54	128.57	119.78
31	L	214	PRO	CA-C-N	8.53	128.59	119.89
31	L	214	PRO	C-N-CA	8.53	128.59	119.89
25	R	241	ILE	N-CA-C	-8.53	92.42	107.18
4	D	16	HIS	CE1-NE2-CD2	-8.52	100.48	109.00
5	E	133	LEU	N-CA-C	-8.52	104.02	114.75
25	R	150	ALA	CA-C-N	8.52	131.69	120.28
25	R	150	ALA	C-N-CA	8.52	131.69	120.28
22	S	108	ALA	N-CA-C	-8.50	99.31	112.99
2	B	6	SER	N-CA-C	-8.49	101.73	114.64
27	O	66	VAL	N-CA-CB	8.49	122.09	110.54
31	L	244	ILE	N-CA-C	-8.49	91.69	109.34
26	U	219	LEU	CA-C-N	8.48	128.24	119.76
26	U	219	LEU	C-N-CA	8.48	128.24	119.76
6	F	66	CYS	N-CA-C	-8.48	102.52	113.12
21	N	633	GLY	N-CA-C	8.48	121.66	112.33
33	J	168	VAL	N-CA-CB	8.48	122.73	110.52
27	O	215	TYR	CA-C-N	8.47	131.64	120.28
27	O	215	TYR	C-N-CA	8.47	131.64	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	236	GLU	CA-C-N	8.47	131.23	120.56
23	P	236	GLU	C-N-CA	8.47	131.23	120.56
11	4	159	ASP	CA-CB-CG	8.46	121.06	112.60
17	T	31	LYS	CA-C-N	8.46	132.43	120.42
17	T	31	LYS	C-N-CA	8.46	132.43	120.42
13	6	67	ALA	CA-C-N	8.45	131.61	120.28
13	6	67	ALA	C-N-CA	8.45	131.61	120.28
8	h	198	TYR	CA-C-N	8.45	128.58	119.28
8	h	198	TYR	C-N-CA	8.45	128.58	119.28
5	E	33	LEU	CA-C-N	8.45	128.03	119.92
5	E	33	LEU	C-N-CA	8.45	128.03	119.92
2	b	53	SER	O-C-N	-8.45	113.38	121.57
7	g	48	PHE	CA-CB-CG	-8.45	105.35	113.80
20	Z	727	GLU	CA-CB-CG	8.44	130.98	114.10
3	c	46	LEU	CA-C-O	8.44	129.47	120.36
28	H	270	THR	CA-C-O	-8.44	111.30	120.92
29	I	194	ILE	N-CA-C	-8.43	104.93	113.10
5	e	50	VAL	N-CA-C	-8.42	97.23	108.35
14	n	44	VAL	CA-C-O	-8.41	111.13	120.72
21	N	306	ASN	CA-CB-CG	-8.41	104.19	112.60
4	D	107	GLU	CA-C-O	-8.41	111.99	120.82
1	A	147	ASP	CA-CB-CG	-8.40	104.20	112.60
14	7	209	ALA	CA-C-N	8.40	131.31	120.56
14	7	209	ALA	C-N-CA	8.40	131.31	120.56
24	Q	67	THR	N-CA-CB	8.40	124.68	110.49
28	H	56	LEU	CA-C-N	8.40	132.37	120.28
28	H	56	LEU	C-N-CA	8.40	132.37	120.28
3	C	216	ILE	CA-C-O	8.39	128.56	120.25
5	E	15	PHE	CA-C-N	8.39	136.80	121.70
5	E	15	PHE	C-N-CA	8.39	136.80	121.70
16	V	91	MET	N-CA-C	-8.39	102.22	111.36
25	R	338	TYR	CB-CG-CD1	8.39	133.38	120.80
4	d	42	VAL	O-C-N	-8.38	114.23	123.03
12	5	153	ALA	O-C-N	-8.38	112.03	122.17
13	6	133	PHE	CA-CB-CG	-8.38	105.42	113.80
30	K	276	SER	CA-C-N	8.38	131.94	120.46
30	K	276	SER	C-N-CA	8.38	131.94	120.46
20	Z	727	GLU	CA-C-O	-8.38	111.25	121.89
28	H	115	THR	N-CA-C	-8.38	101.13	112.94
3	C	216	ILE	O-C-N	-8.37	114.41	123.03
8	1	108	VAL	O-C-N	-8.37	114.22	123.26
7	G	93	ARG	NH1-CZ-NH2	8.34	130.15	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	7	121	GLU	CA-C-N	8.34	128.83	119.32
14	7	121	GLU	C-N-CA	8.34	128.83	119.32
30	K	131	LEU	CA-C-O	8.34	129.50	120.24
2	B	53	SER	CA-C-N	8.34	129.05	120.04
2	B	53	SER	C-N-CA	8.34	129.05	120.04
32	M	291	PHE	CA-CB-CG	8.34	122.14	113.80
32	M	175	LYS	CA-C-N	8.34	128.39	119.89
32	M	175	LYS	C-N-CA	8.34	128.39	119.89
26	U	289	ASP	CA-CB-CG	8.33	120.93	112.60
3	c	125	HIS	CG-CD2-NE2	8.33	115.53	107.20
9	2	85	THR	CA-C-N	8.33	131.26	120.44
9	2	85	THR	C-N-CA	8.33	131.26	120.44
10	j	36	VAL	N-CA-C	-8.32	105.16	111.90
31	L	351	LEU	CA-C-N	8.32	128.83	119.93
31	L	351	LEU	C-N-CA	8.32	128.83	119.93
31	L	173	PHE	CA-CB-CG	-8.32	105.48	113.80
5	e	245	GLU	N-CA-C	-8.31	101.46	111.69
31	L	222	GLY	CA-C-N	8.31	125.64	119.66
31	L	222	GLY	C-N-CA	8.31	125.64	119.66
17	T	119	THR	CA-C-N	8.31	131.24	120.44
17	T	119	THR	C-N-CA	8.31	131.24	120.44
21	N	263	SER	CA-C-N	8.30	131.93	120.63
21	N	263	SER	C-N-CA	8.30	131.93	120.63
13	m	104	LEU	CA-C-N	8.30	131.60	120.65
13	m	104	LEU	C-N-CA	8.30	131.60	120.65
32	M	85	VAL	N-CA-C	-8.30	95.77	107.80
25	R	256	THR	CA-C-N	8.29	129.36	119.99
25	R	256	THR	C-N-CA	8.29	129.36	119.99
23	P	337	HIS	N-CA-C	-8.29	103.36	113.97
24	Q	98	LYS	O-C-N	-8.29	113.53	122.07
29	I	351	GLU	CA-C-N	8.28	132.67	120.83
29	I	351	GLU	C-N-CA	8.28	132.67	120.83
7	G	209	GLU	N-CA-C	-8.28	100.81	113.89
8	1	157	LYS	CA-C-N	8.27	132.88	120.31
8	1	157	LYS	C-N-CA	8.27	132.88	120.31
22	S	422	MET	CB-CA-C	-8.27	97.90	110.88
24	Q	115	ILE	CA-C-N	8.27	131.19	120.44
24	Q	115	ILE	C-N-CA	8.27	131.19	120.44
3	c	183	ASP	N-CA-CB	8.26	123.99	110.69
5	e	16	SER	N-CA-CB	8.26	124.54	110.50
28	H	271	PHE	CA-CB-CG	-8.26	105.54	113.80
17	T	60	ARG	NE-CZ-NH2	-8.25	111.77	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	17	ASN	CB-CA-C	-8.25	97.61	110.81
22	S	180	ASN	CA-CB-CG	8.24	120.84	112.60
27	O	76	LEU	CA-C-N	8.24	131.32	120.28
27	O	76	LEU	C-N-CA	8.24	131.32	120.28
14	7	182	HIS	CB-CG-CD2	-8.24	120.49	131.20
30	K	427	TYR	N-CA-C	-8.23	102.26	112.88
11	k	136	SER	CA-C-N	8.23	129.24	120.03
11	k	136	SER	C-N-CA	8.23	129.24	120.03
13	6	202	ARG	NE-CZ-NH2	-8.22	111.80	119.20
21	N	768	ILE	CA-C-O	-8.22	114.30	119.15
25	R	132	GLN	O-C-N	-8.22	112.16	122.27
13	6	85	PHE	CA-CB-CG	8.22	122.02	113.80
6	f	43	HIS	CB-CG-CD2	-8.21	120.52	131.20
32	M	267	PHE	CA-CB-CG	-8.21	105.59	113.80
31	L	353	ASN	CA-CB-CG	-8.21	104.39	112.60
21	N	321	LEU	CA-C-N	8.20	133.14	120.75
21	N	321	LEU	C-N-CA	8.20	133.14	120.75
13	6	162	VAL	N-CA-C	-8.20	104.51	111.56
24	Q	188	LEU	N-CA-C	-8.20	103.28	113.28
6	F	213	ILE	N-CA-C	-8.19	96.44	108.89
14	7	124	TYR	CA-C-N	8.19	131.69	120.46
14	7	124	TYR	C-N-CA	8.19	131.69	120.46
15	W	97	THR	O-C-N	8.19	130.51	122.07
1	A	35	THR	N-CA-C	-8.19	102.32	112.88
29	I	343	ARG	N-CA-C	-8.19	100.82	113.02
14	n	110	ASP	CA-CB-CG	-8.18	104.42	112.60
2	B	94	HIS	CE1-NE2-CD2	-8.18	100.82	109.00
5	E	22	PHE	CA-CB-CG	-8.17	105.63	113.80
17	T	86	LYS	CA-C-N	8.17	128.27	119.28
17	T	86	LYS	C-N-CA	8.17	128.27	119.28
33	J	386	VAL	N-CA-C	-8.17	102.28	110.62
27	O	285	SER	CA-C-O	-8.16	111.90	120.55
33	J	307	PRO	CA-C-O	-8.15	112.43	121.32
4	d	17	ILE	CA-C-N	8.15	131.54	120.54
4	d	17	ILE	C-N-CA	8.15	131.54	120.54
27	O	358	ILE	CA-C-O	8.15	128.50	120.27
10	j	183	TRP	CB-CG-CD2	-8.15	115.39	126.80
1	A	193	HIS	ND1-CE1-NE2	8.15	116.55	108.40
27	O	133	ILE	CB-CA-C	-8.14	100.98	112.22
30	K	313	LYS	N-CA-CB	8.14	122.15	109.69
6	F	55	GLU	N-CA-C	8.14	120.23	111.36
30	K	259	ARG	CA-C-N	8.14	131.18	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	259	ARG	C-N-CA	8.14	131.18	120.28
31	L	72	ASP	CA-CB-CG	-8.14	104.46	112.60
6	F	182	ILE	N-CA-C	-8.13	96.78	108.17
6	F	125	GLY	O-C-N	-8.13	114.25	122.86
27	O	53	LYS	N-CA-C	-8.13	103.15	113.72
24	Q	386	PHE	CA-CB-CG	8.12	121.92	113.80
12	I	258	ASP	N-CA-C	-8.12	102.94	112.92
32	M	23	LEU	CA-C-N	8.12	131.48	120.44
32	M	23	LEU	C-N-CA	8.12	131.48	120.44
21	N	129	ILE	CA-C-O	-8.11	113.07	121.67
29	I	97	GLU	N-CA-C	8.10	120.19	111.36
23	P	201	ARG	NH1-CZ-NH2	-8.10	108.78	119.30
7	G	97	ALA	O-C-N	-8.09	113.54	122.12
2	b	170	ALA	CA-C-N	8.09	131.12	120.28
2	b	170	ALA	C-N-CA	8.09	131.12	120.28
1	A	140	ILE	CA-C-O	-8.09	111.92	120.57
19	Y	85	LYS	CA-C-N	8.09	131.12	120.28
19	Y	85	LYS	C-N-CA	8.09	131.12	120.28
26	U	156	HIS	N-CA-CB	8.08	122.03	109.83
6	f	56	LEU	N-CA-C	-8.07	103.45	113.38
1	A	192	ASP	CA-CB-CG	8.07	120.67	112.60
29	I	242	ALA	N-CA-C	-8.07	96.81	109.07
1	a	36	ASN	N-CA-C	-8.06	102.75	112.59
30	K	244	HIS	CA-CB-CG	-8.06	105.74	113.80
7	G	22	PHE	CA-CB-CG	-8.06	105.74	113.80
22	S	412	ASN	CA-CB-CG	-8.06	104.54	112.60
25	R	269	LYS	CA-C-O	-8.06	112.40	120.70
15	W	9	VAL	N-CA-CB	8.05	122.11	111.64
21	N	625	LEU	CA-C-N	8.05	128.88	119.94
21	N	625	LEU	C-N-CA	8.05	128.88	119.94
27	O	147	ARG	NE-CZ-NH2	8.04	126.44	119.20
28	H	117	THR	N-CA-C	-8.04	100.92	110.41
1	a	149	GLU	N-CA-C	-8.04	103.94	114.31
24	Q	425	GLN	CA-C-N	8.04	131.05	120.28
24	Q	425	GLN	C-N-CA	8.04	131.05	120.28
12	I	92	ASP	N-CA-C	-8.03	98.33	110.14
32	M	42	ARG	CA-C-N	8.03	131.83	120.42
32	M	42	ARG	C-N-CA	8.03	131.83	120.42
25	R	374	ASN	CA-CB-CG	-8.02	104.58	112.60
5	e	188	HIS	CG-CD2-NE2	8.01	115.21	107.20
17	T	84	GLN	OE1-CD-NE2	-8.01	114.59	122.60
32	M	140	LEU	CA-C-O	8.01	129.22	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	71	MET	CA-C-O	-8.01	113.09	119.66
23	P	141	LYS	CA-C-N	8.01	131.66	120.29
23	P	141	LYS	C-N-CA	8.01	131.66	120.29
15	W	36	ILE	CA-C-N	8.00	131.32	120.44
15	W	36	ILE	C-N-CA	8.00	131.32	120.44
8	h	69	GLN	CA-C-N	8.00	131.31	120.44
8	h	69	GLN	C-N-CA	8.00	131.31	120.44
12	5	163	TYR	CA-C-N	7.99	131.90	120.79
12	5	163	TYR	C-N-CA	7.99	131.90	120.79
16	V	159	ILE	CA-C-N	7.99	132.57	120.82
16	V	159	ILE	C-N-CA	7.99	132.57	120.82
14	n	211	VAL	CA-C-O	-7.99	113.11	121.41
3	C	237	ASP	CA-CB-CG	-7.98	104.62	112.60
17	T	245	TYR	O-C-N	-7.98	113.66	122.12
33	J	170	HIS	CB-CA-C	-7.98	100.67	110.81
6	F	174	ARG	NE-CZ-NH1	-7.98	113.52	121.50
21	N	883	SER	CA-C-N	7.97	132.11	120.95
21	N	883	SER	C-N-CA	7.97	132.11	120.95
11	k	20	ALA	N-CA-CB	7.97	121.69	109.97
26	U	216	ASN	CA-CB-CG	7.97	120.57	112.60
25	R	86	ASP	N-CA-CB	7.97	123.69	110.47
3	c	86	ILE	CA-C-N	7.96	132.42	120.31
3	c	86	ILE	C-N-CA	7.96	132.42	120.31
3	C	231	LYS	N-CA-C	-7.96	99.31	110.29
8	h	140	SER	N-CA-C	-7.95	102.62	112.88
3	C	19	LEU	CA-C-N	7.95	132.75	120.82
3	C	19	LEU	C-N-CA	7.95	132.75	120.82
33	J	179	ILE	N-CA-C	-7.95	97.86	108.35
22	S	475	TYR	CA-C-N	7.95	130.77	120.44
22	S	475	TYR	C-N-CA	7.95	130.77	120.44
29	I	180	SER	N-CA-C	-7.95	97.66	108.86
6	f	67	ASP	CA-CB-CG	-7.95	104.66	112.60
12	l	184	GLY	O-C-N	-7.94	113.83	121.77
21	N	312	GLY	CA-C-O	7.94	128.82	119.45
7	G	111	ALA	CA-C-O	7.94	129.16	119.79
33	J	290	ILE	N-CA-CB	7.93	121.58	111.83
13	m	30	VAL	N-CA-CB	7.92	123.09	111.52
14	7	146	ALA	N-CA-C	-7.92	96.49	109.40
16	V	242	LYS	N-CA-C	7.92	119.55	111.07
9	2	73	ALA	CA-C-N	7.92	127.03	121.65
9	2	73	ALA	C-N-CA	7.92	127.03	121.65
13	m	80	VAL	CA-C-N	7.92	131.23	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	80	VAL	C-N-CA	7.92	131.23	120.54
15	W	121	SER	CA-C-N	7.92	130.73	120.44
15	W	121	SER	C-N-CA	7.92	130.73	120.44
15	W	181	LEU	CA-C-O	-7.92	112.16	120.55
23	P	249	ALA	N-CA-C	7.92	120.61	111.11
6	f	146	GLU	N-CA-C	-7.92	95.38	108.76
23	P	271	SER	CA-C-O	-7.92	112.07	120.70
24	Q	160	ASP	CA-C-N	7.91	130.88	120.28
24	Q	160	ASP	C-N-CA	7.91	130.88	120.28
32	M	419	ILE	N-CA-C	-7.91	103.09	110.53
21	N	57	ASP	N-CA-C	-7.91	102.94	112.59
23	P	341	LEU	CA-C-N	7.90	130.71	120.44
23	P	341	LEU	C-N-CA	7.90	130.71	120.44
3	c	7	ASP	CA-CB-CG	7.90	120.50	112.60
15	W	188	SER	CA-C-O	-7.90	112.03	120.88
28	H	232	PRO	N-CA-C	-7.90	104.57	114.68
22	S	191	HIS	ND1-CE1-NE2	7.90	116.30	108.40
6	F	116	ALA	CA-C-N	7.89	130.86	120.28
6	F	116	ALA	C-N-CA	7.89	130.86	120.28
25	R	308	LEU	CA-C-N	7.89	131.49	120.29
25	R	308	LEU	C-N-CA	7.89	131.49	120.29
27	O	255	LEU	CB-CA-C	-7.89	97.44	110.85
17	T	85	LEU	CA-C-N	7.88	134.00	121.62
17	T	85	LEU	C-N-CA	7.88	134.00	121.62
17	T	183	SER	CA-C-N	7.88	130.84	120.28
17	T	183	SER	C-N-CA	7.88	130.84	120.28
8	h	113	ASP	CA-C-N	7.88	131.63	120.28
8	h	113	ASP	C-N-CA	7.88	131.63	120.28
11	4	113	LYS	CA-C-N	7.88	127.93	119.89
11	4	113	LYS	C-N-CA	7.88	127.93	119.89
25	R	164	THR	CA-C-N	7.88	128.89	119.99
25	R	164	THR	C-N-CA	7.88	128.89	119.99
11	4	131	GLY	N-CA-C	-7.87	99.18	110.91
25	R	115	GLU	CA-C-N	7.87	130.67	120.44
25	R	115	GLU	C-N-CA	7.87	130.67	120.44
5	e	91	HIS	N-CA-C	7.87	119.86	111.28
5	e	20	ARG	NE-CZ-NH2	-7.87	112.12	119.20
4	D	155	ILE	N-CA-C	-7.87	97.12	108.53
1	a	240	ASN	CA-C-N	7.87	131.59	120.42
1	a	240	ASN	C-N-CA	7.87	131.59	120.42
22	S	473	ASP	CA-C-N	7.87	130.82	120.28
22	S	473	ASP	C-N-CA	7.87	130.82	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	232	GLY	CA-C-N	7.86	131.72	120.79
12	l	232	GLY	C-N-CA	7.86	131.72	120.79
16	V	33	ALA	CA-C-N	7.86	131.15	120.38
16	V	33	ALA	C-N-CA	7.86	131.15	120.38
16	V	76	THR	N-CA-C	-7.86	101.31	113.02
23	P	66	LEU	CA-C-N	7.86	130.81	120.28
23	P	66	LEU	C-N-CA	7.86	130.81	120.28
32	M	349	PHE	CB-CA-C	-7.86	100.89	109.85
20	Z	746	ILE	CB-CA-C	7.86	124.97	112.16
31	L	375	ASP	N-CA-C	-7.86	100.34	112.99
7	g	116	LEU	CA-C-N	7.85	128.66	119.94
7	g	116	LEU	C-N-CA	7.85	128.66	119.94
17	T	53	ASN	CA-C-N	7.85	132.25	120.31
17	T	53	ASN	C-N-CA	7.85	132.25	120.31
32	M	284	ASP	N-CA-C	-7.85	104.59	114.56
17	T	259	ILE	CA-C-N	7.85	130.45	120.56
17	T	259	ILE	C-N-CA	7.85	130.45	120.56
14	7	172	SER	O-C-N	-7.85	115.71	121.83
21	N	52	ASP	CA-CB-CG	7.85	120.45	112.60
22	S	275	TYR	CA-C-N	7.85	131.13	120.54
22	S	275	TYR	C-N-CA	7.85	131.13	120.54
2	b	100	ILE	N-CA-C	-7.84	104.24	113.42
11	4	60	ILE	CB-CA-C	7.84	122.73	112.14
14	7	233	ILE	N-CA-C	-7.84	95.76	107.37
22	S	261	HIS	CA-CB-CG	-7.84	105.96	113.80
8	h	159	GLU	CA-C-N	7.83	131.68	120.79
8	h	159	GLU	C-N-CA	7.83	131.68	120.79
10	3	3	ASP	CA-C-N	7.83	128.25	119.32
10	3	3	ASP	C-N-CA	7.83	128.25	119.32
17	T	240	LYS	CA-C-N	7.83	130.78	120.28
17	T	240	LYS	C-N-CA	7.83	130.78	120.28
14	n	129	LEU	CA-C-N	7.83	133.65	121.19
14	n	129	LEU	C-N-CA	7.83	133.65	121.19
3	C	65	LYS	N-CA-C	-7.83	105.69	114.62
5	E	17	PRO	N-CA-C	-7.83	105.60	114.92
3	c	187	ASP	CA-C-N	7.83	131.41	120.29
3	c	187	ASP	C-N-CA	7.83	131.41	120.29
27	O	193	LEU	N-CA-CB	7.83	121.75	110.16
22	S	339	GLN	CA-C-N	7.83	130.62	120.44
22	S	339	GLN	C-N-CA	7.83	130.62	120.44
25	R	100	ASN	CA-CB-CG	-7.83	104.77	112.60
32	M	182	ASP	N-CA-C	-7.83	102.78	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	218	ASP	N-CA-C	-7.82	103.25	114.12
23	P	170	SER	CA-C-N	7.82	136.47	121.54
23	P	170	SER	C-N-CA	7.82	136.47	121.54
16	V	69	PHE	CA-CB-CG	7.81	121.61	113.80
30	K	320	ARG	NE-CZ-NH2	-7.81	112.17	119.20
13	6	30	VAL	N-CA-C	-7.81	96.76	108.17
20	Z	251	ALA	O-C-N	7.81	130.40	122.12
22	S	177	ASN	CA-C-O	-7.81	112.27	120.55
22	S	271	ARG	CA-C-N	7.81	130.59	120.44
22	S	271	ARG	C-N-CA	7.81	130.59	120.44
27	O	93	ASP	CA-C-N	7.81	130.74	120.28
27	O	93	ASP	C-N-CA	7.81	130.74	120.28
9	i	209	ILE	CA-C-N	7.81	134.36	120.77
9	i	209	ILE	C-N-CA	7.81	134.36	120.77
21	N	422	TYR	CB-CG-CD2	-7.81	109.09	120.80
29	I	117	HIS	CA-C-O	7.81	129.81	121.45
30	K	207	ARG	CA-C-N	7.80	130.47	120.64
30	K	207	ARG	C-N-CA	7.80	130.47	120.64
11	4	141	PHE	CA-CB-CG	-7.80	106.00	113.80
14	7	231	ALA	CA-C-O	7.80	129.12	120.70
14	n	69	PHE	CA-CB-CG	-7.80	106.00	113.80
6	F	80	ASP	CA-CB-CG	-7.80	104.80	112.60
23	P	182	GLU	CA-C-N	7.80	131.36	120.29
23	P	182	GLU	C-N-CA	7.80	131.36	120.29
21	N	163	LEU	CA-C-N	7.79	130.72	120.28
21	N	163	LEU	C-N-CA	7.79	130.72	120.28
33	J	351	ASN	N-CA-C	-7.79	104.94	114.75
22	S	40	GLU	N-CA-C	7.79	119.40	111.07
16	V	279	HIS	ND1-CE1-NE2	7.79	116.19	108.40
12	l	147	GLU	N-CA-C	-7.78	94.23	110.80
8	h	116	LYS	CA-C-N	7.78	127.73	120.34
8	h	116	LYS	C-N-CA	7.78	127.73	120.34
24	Q	248	ASN	CA-CB-CG	-7.78	104.82	112.60
13	m	48	GLU	N-CA-C	-7.78	92.62	109.81
25	R	408	ASP	CA-C-N	7.78	128.55	120.00
25	R	408	ASP	C-N-CA	7.78	128.55	120.00
13	m	16	ASN	CA-CB-CG	-7.77	104.83	112.60
12	l	149	ILE	CA-C-O	-7.77	113.81	121.58
14	n	198	ILE	CA-C-O	-7.77	112.25	118.85
3	C	131	PHE	CA-CB-CG	7.77	121.57	113.80
8	l	182	ILE	N-CA-C	-7.76	97.26	108.36
30	K	268	ILE	N-CA-C	-7.76	97.25	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	112	LEU	CA-C-O	7.76	128.77	120.55
7	G	210	LYS	CA-C-O	7.76	129.13	121.14
16	V	190	HIS	CA-CB-CG	7.76	121.56	113.80
16	V	200	ASN	OD1-CG-ND2	7.76	130.36	122.60
21	N	623	PHE	N-CA-C	7.76	119.73	111.28
26	U	289	ASP	CA-C-N	7.75	130.67	120.28
26	U	289	ASP	C-N-CA	7.75	130.67	120.28
15	W	158	ILE	CA-C-N	7.75	130.66	120.28
15	W	158	ILE	C-N-CA	7.75	130.66	120.28
28	H	392	HIS	ND1-CE1-NE2	7.75	116.15	108.40
24	Q	114	GLN	CA-C-N	7.74	131.07	120.46
24	Q	114	GLN	C-N-CA	7.74	131.07	120.46
28	H	379	LEU	CA-C-N	7.74	127.79	119.90
28	H	379	LEU	C-N-CA	7.74	127.79	119.90
27	O	93	ASP	CA-C-O	7.73	128.62	120.42
15	W	104	LYS	N-CA-C	-7.73	102.36	112.41
23	P	201	ARG	NE-CZ-NH2	7.73	126.16	119.20
25	R	419	ALA	CA-C-O	7.73	128.75	120.55
4	d	210	ILE	CB-CA-C	7.72	120.48	110.91
24	Q	97	LEU	CA-C-N	7.72	130.48	120.44
24	Q	97	LEU	C-N-CA	7.72	130.48	120.44
29	I	200	LEU	O-C-N	-7.72	112.44	121.32
18	X	42	GLU	N-CA-C	-7.72	102.91	113.18
29	I	376	ASN	CA-CB-CG	-7.71	104.89	112.60
14	n	107	ASN	CA-C-O	7.71	128.59	120.42
20	Z	744	ALA	N-CA-C	-7.71	102.88	111.28
23	P	260	VAL	CA-C-N	7.71	130.61	120.28
23	P	260	VAL	C-N-CA	7.71	130.61	120.28
27	O	150	LEU	N-CA-CB	7.71	121.57	110.16
4	D	186	ALA	N-CA-C	7.70	120.75	111.82
23	P	113	ASN	N-CA-C	-7.70	102.97	111.36
1	a	34	ALA	N-CA-C	-7.70	100.60	112.99
14	n	92	ASP	CA-C-N	7.70	130.59	120.28
14	n	92	ASP	C-N-CA	7.70	130.59	120.28
10	3	6	SER	CA-C-N	7.70	131.35	120.42
10	3	6	SER	C-N-CA	7.70	131.35	120.42
5	E	136	ARG	CA-C-N	7.69	127.62	119.85
5	E	136	ARG	C-N-CA	7.69	127.62	119.85
17	T	146	ILE	N-CA-CB	7.69	120.41	110.57
26	U	19	LEU	CA-C-O	7.69	128.57	120.42
11	4	124	THR	CA-C-O	-7.69	112.09	120.24
14	n	169	THR	CA-C-O	-7.69	112.40	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	525	ASN	CA-CB-CG	-7.69	104.91	112.60
3	c	109	GLU	CA-C-N	7.68	130.24	120.56
3	c	109	GLU	C-N-CA	7.68	130.24	120.56
27	O	312	ASP	CA-C-N	7.68	131.33	120.42
27	O	312	ASP	C-N-CA	7.68	131.33	120.42
6	f	116	ALA	O-C-N	7.68	130.91	122.15
16	V	31	SER	CA-C-N	7.68	130.23	120.56
16	V	31	SER	C-N-CA	7.68	130.23	120.56
21	N	178	SER	CA-C-N	7.68	130.57	120.28
21	N	178	SER	C-N-CA	7.68	130.57	120.28
11	k	149	ARG	O-C-N	-7.67	116.80	121.71
21	N	340	HIS	CE1-NE2-CD2	-7.67	101.33	109.00
9	2	249	ILE	CA-C-N	7.67	131.33	120.28
9	2	249	ILE	C-N-CA	7.67	131.33	120.28
23	P	30	ASN	CA-CB-CG	-7.67	104.93	112.60
2	b	91	LYS	CA-C-O	-7.67	112.29	120.42
21	N	710	GLY	CA-C-N	7.66	133.62	122.36
21	N	710	GLY	C-N-CA	7.66	133.62	122.36
2	b	139	HIS	CE1-NE2-CD2	-7.66	101.34	109.00
21	N	111	GLN	CA-C-N	7.66	130.54	120.28
21	N	111	GLN	C-N-CA	7.66	130.54	120.28
1	a	104	PHE	O-C-N	7.66	129.96	122.07
21	N	148	SER	N-CA-CB	7.66	123.43	110.49
13	6	52	PHE	CA-CB-CG	-7.65	106.15	113.80
17	T	157	TYR	CA-C-N	7.65	130.87	120.54
17	T	157	TYR	C-N-CA	7.65	130.87	120.54
11	k	55	GLN	N-CA-C	7.65	119.25	111.07
6	F	108	ALA	CA-C-O	7.65	128.79	119.31
21	N	315	ASN	CB-CG-ND2	-7.65	104.93	116.40
21	N	131	PRO	CA-C-N	7.65	130.53	120.28
21	N	131	PRO	C-N-CA	7.65	130.53	120.28
14	7	198	ILE	N-CA-CB	-7.64	105.68	110.50
16	V	279	HIS	CA-C-N	7.64	130.53	120.28
16	V	279	HIS	C-N-CA	7.64	130.53	120.28
22	S	302	HIS	ND1-CE1-NE2	7.64	116.04	108.40
11	4	109	LYS	N-CA-C	-7.64	102.17	112.94
21	N	780	ASP	N-CA-C	-7.64	102.15	113.61
28	H	229	LEU	CA-C-N	7.64	130.82	120.44
28	H	229	LEU	C-N-CA	7.64	130.82	120.44
21	N	144	CYS	N-CA-C	-7.63	103.04	111.36
3	C	226	TYR	N-CA-C	-7.63	96.29	108.73
31	L	124	GLY	O-C-N	-7.63	114.14	121.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	206	GLY	O-C-N	-7.63	114.44	122.60
27	O	286	PHE	CA-C-N	7.63	130.50	120.28
27	O	286	PHE	C-N-CA	7.63	130.50	120.28
4	d	79	ASN	CA-CB-CG	-7.62	104.98	112.60
21	N	270	LEU	N-CA-C	7.62	119.67	111.36
7	G	154	SER	N-CA-C	-7.62	103.98	113.28
30	K	420	THR	N-CA-C	-7.62	105.15	114.75
14	n	197	ASP	CA-C-N	7.62	125.04	120.24
14	n	197	ASP	C-N-CA	7.62	125.04	120.24
14	7	187	LEU	CA-C-O	7.62	128.62	120.55
23	P	315	GLN	CA-C-N	7.62	130.49	120.28
23	P	315	GLN	C-N-CA	7.62	130.49	120.28
25	R	110	ILE	CA-C-N	7.61	130.33	120.44
25	R	110	ILE	C-N-CA	7.61	130.33	120.44
17	T	58	THR	N-CA-C	-7.61	102.92	111.14
10	j	40	PHE	N-CA-C	-7.61	94.60	110.80
25	R	275	GLU	CA-C-O	-7.61	112.87	120.70
1	a	37	GLN	OE1-CD-NE2	7.60	130.20	122.60
18	X	37	PRO	N-CA-C	-7.60	103.88	114.98
17	T	244	ASP	N-CA-CB	7.60	121.03	110.01
23	P	338	TRP	N-CA-C	-7.60	103.08	111.36
31	L	399	GLY	N-CA-C	-7.60	102.63	115.62
3	C	94	HIS	CE1-NE2-CD2	-7.60	101.40	109.00
1	A	204	GLU	CA-C-O	-7.60	112.84	120.82
5	e	226	ASP	CA-CB-CG	7.59	120.19	112.60
3	C	91	ALA	N-CA-C	7.59	119.56	111.28
6	F	210	ASN	N-CA-C	-7.59	104.62	114.04
21	N	444	HIS	CE1-NE2-CD2	-7.59	101.41	109.00
24	Q	71	LYS	CA-C-N	7.59	131.07	120.29
24	Q	71	LYS	C-N-CA	7.59	131.07	120.29
20	Z	614	VAL	N-CA-C	-7.59	103.54	111.58
9	2	114	GLN	CB-CG-CD	-7.59	99.70	112.60
10	3	131	ASP	N-CA-C	-7.58	94.64	107.99
21	N	878	GLN	CA-C-O	-7.58	110.16	119.18
28	H	118	ASP	CA-CB-CG	-7.58	105.02	112.60
29	I	227	THR	N-CA-CB	7.58	121.02	110.56
12	l	89	VAL	N-CA-C	-7.58	97.50	108.11
7	G	94	GLU	CA-C-N	7.58	130.44	120.28
7	G	94	GLU	C-N-CA	7.58	130.44	120.28
24	Q	379	GLN	CA-C-N	7.58	130.44	120.28
24	Q	379	GLN	C-N-CA	7.58	130.44	120.28
10	j	162	ASP	CA-C-N	7.57	130.43	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	162	ASP	C-N-CA	7.57	130.43	120.28
10	j	184	GLY	CA-C-O	-7.57	115.97	121.88
9	2	221	THR	CA-C-O	-7.57	113.02	119.76
5	E	226	ASP	N-CA-C	-7.57	103.13	114.64
12	5	266	HIS	CA-CB-CG	-7.57	106.23	113.80
22	S	143	GLN	CA-C-N	7.57	130.42	120.28
22	S	143	GLN	C-N-CA	7.57	130.42	120.28
28	H	80	HIS	ND1-CE1-NE2	7.57	115.97	108.40
5	e	26	TYR	CA-C-N	7.57	130.42	120.28
5	e	26	TYR	C-N-CA	7.57	130.42	120.28
5	e	50	VAL	CA-C-O	7.57	129.00	120.90
20	Z	153	TYR	CA-C-N	7.57	130.83	120.46
20	Z	153	TYR	C-N-CA	7.57	130.83	120.46
28	H	312	ASP	O-C-N	-7.57	113.92	122.09
1	a	46	ARG	NE-CZ-NH1	-7.56	113.94	121.50
31	L	256	ILE	CA-C-O	7.56	129.34	120.72
20	Z	738	TYR	CD1-CE1-CZ	7.56	133.20	119.60
32	M	38	ASP	N-CA-C	-7.56	102.40	111.69
24	Q	145	HIS	CA-C-O	-7.55	112.41	120.42
21	N	448	LEU	CA-C-N	7.55	128.32	119.94
21	N	448	LEU	C-N-CA	7.55	128.32	119.94
32	M	199	LEU	CA-C-O	-7.55	109.81	120.16
18	X	44	GLY	N-CA-C	-7.55	104.90	115.32
6	f	112	LEU	CA-C-N	7.55	130.39	120.28
6	f	112	LEU	C-N-CA	7.55	130.39	120.28
5	E	103	TYR	N-CA-C	-7.55	105.24	114.75
15	W	192	LEU	N-CA-C	-7.55	103.38	112.59
16	V	88	GLN	CA-C-N	7.54	130.39	120.28
16	V	88	GLN	C-N-CA	7.54	130.39	120.28
6	F	186	PRO	CA-C-N	7.54	130.72	120.54
6	F	186	PRO	C-N-CA	7.54	130.72	120.54
23	P	11	LYS	CA-C-N	7.54	130.25	120.44
23	P	11	LYS	C-N-CA	7.54	130.25	120.44
33	J	325	ALA	CA-C-O	-7.54	110.89	119.79
13	m	43	ILE	N-CA-CB	7.54	120.03	111.21
11	4	38	LEU	N-CA-C	-7.54	102.65	112.68
17	T	46	ILE	O-C-N	-7.54	116.41	122.97
18	X	71	GLY	N-CA-C	-7.54	104.92	115.32
1	A	187	LYS	N-CA-C	-7.54	102.42	111.69
11	k	146	HIS	CG-CD2-NE2	7.54	114.73	107.20
7	g	142	ASP	N-CA-CB	7.53	123.31	110.65
21	N	373	VAL	CA-C-N	7.53	130.05	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	373	VAL	C-N-CA	7.53	130.05	120.56
24	Q	28	LEU	CA-C-N	7.53	130.38	120.28
24	Q	28	LEU	C-N-CA	7.53	130.38	120.28
32	M	197	ILE	CB-CA-C	-7.53	104.28	111.44
33	J	360	GLY	CA-C-N	7.53	131.12	120.42
33	J	360	GLY	C-N-CA	7.53	131.12	120.42
29	I	64	ARG	N-CA-C	7.53	119.49	111.28
10	3	155	GLU	N-CA-C	-7.53	96.30	109.48
23	P	202	LYS	CB-CA-C	-7.53	98.05	110.85
17	T	186	ARG	NE-CZ-NH2	-7.53	112.42	119.20
21	N	810	ALA	CA-C-N	7.53	130.71	120.54
21	N	810	ALA	C-N-CA	7.53	130.71	120.54
2	B	13	SER	CA-C-N	7.53	127.16	119.56
2	B	13	SER	C-N-CA	7.53	127.16	119.56
12	l	192	SER	CA-C-N	7.53	130.37	120.28
12	l	192	SER	C-N-CA	7.53	130.37	120.28
22	S	43	LYS	N-CA-CB	7.53	121.27	110.13
22	S	457	PRO	CA-C-N	7.53	130.97	120.29
22	S	457	PRO	C-N-CA	7.53	130.97	120.29
5	E	233	ASN	CA-C-N	7.52	130.36	120.28
5	E	233	ASN	C-N-CA	7.52	130.36	120.28
3	C	84	ALA	N-CA-C	7.52	119.48	111.28
32	M	425	ARG	NE-CZ-NH1	-7.52	113.98	121.50
10	j	183	TRP	CB-CG-CD1	7.52	138.18	126.90
1	A	20	SER	CA-C-N	7.52	127.19	119.82
1	A	20	SER	C-N-CA	7.52	127.19	119.82
24	Q	181	GLU	CA-C-N	7.52	130.36	120.28
24	Q	181	GLU	C-N-CA	7.52	130.36	120.28
2	B	85	LEU	N-CA-C	-7.52	103.91	113.23
4	d	208	LYS	N-CA-C	7.52	119.47	111.28
11	4	96	ARG	CB-CA-C	-7.51	103.68	110.44
8	1	46	VAL	N-CA-C	-7.51	106.17	113.53
20	Z	244	ARG	CA-C-O	-7.51	112.94	120.82
21	N	864	LYS	CA-C-O	-7.50	113.77	119.32
28	H	404	TRP	N-CA-C	-7.50	104.27	113.50
30	K	235	ILE	CA-C-N	7.50	132.98	122.41
30	K	235	ILE	C-N-CA	7.50	132.98	122.41
13	m	153	LEU	N-CA-C	-7.50	103.08	112.90
4	d	84	ILE	CA-C-O	-7.49	112.69	120.71
13	6	40	ASP	CB-CA-C	-7.49	107.92	116.54
20	Z	248	TYR	N-CA-CB	7.49	121.13	110.12
25	R	333	MET	CA-C-N	7.49	130.93	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	333	MET	C-N-CA	7.49	130.93	120.29
7	g	35	THR	CA-C-N	7.48	131.37	120.82
7	g	35	THR	C-N-CA	7.48	131.37	120.82
12	5	237	LEU	CA-C-N	7.48	130.17	120.44
12	5	237	LEU	C-N-CA	7.48	130.17	120.44
13	6	84	HIS	CE1-NE2-CD2	-7.48	101.52	109.00
31	L	69	ARG	NE-CZ-NH1	7.48	128.98	121.50
21	N	279	ALA	N-CA-C	-7.48	102.81	112.23
32	M	420	SER	CA-C-N	7.47	130.90	120.29
32	M	420	SER	C-N-CA	7.47	130.90	120.29
5	E	9	ASP	CA-CB-CG	7.47	120.07	112.60
8	1	70	TYR	N-CA-CB	-7.47	98.71	110.22
33	J	170	HIS	ND1-CE1-NE2	7.47	115.87	108.40
5	e	248	ALA	N-CA-C	-7.47	102.40	112.26
21	N	340	HIS	CB-CG-CD2	-7.45	121.51	131.20
28	H	293	GLU	N-CA-C	7.45	119.48	111.36
32	M	131	MET	CA-C-N	7.45	130.49	120.50
32	M	131	MET	C-N-CA	7.45	130.49	120.50
21	N	436	ASP	CA-C-N	7.45	130.87	120.29
21	N	436	ASP	C-N-CA	7.45	130.87	120.29
4	d	221	ILE	CA-C-O	-7.45	112.56	120.53
10	j	55	GLY	CA-C-N	7.45	131.29	120.71
10	j	55	GLY	C-N-CA	7.45	131.29	120.71
2	b	64	VAL	CA-C-N	7.45	134.28	122.59
2	b	64	VAL	C-N-CA	7.45	134.28	122.59
3	c	65	LYS	N-CA-C	-7.44	106.13	114.62
10	3	118	LYS	CB-CA-C	-7.44	101.36	109.85
16	V	236	SER	CA-C-N	7.44	130.56	120.44
16	V	236	SER	C-N-CA	7.44	130.56	120.44
21	N	766	GLN	N-CA-CB	7.44	123.06	110.49
21	N	826	GLU	CA-C-N	7.44	130.56	120.44
21	N	826	GLU	C-N-CA	7.44	130.56	120.44
2	b	43	VAL	N-CA-CB	7.44	123.65	111.45
9	2	101	ARG	N-CA-C	-7.44	98.01	109.24
25	R	104	LYS	CA-C-N	7.43	130.58	120.54
25	R	104	LYS	C-N-CA	7.43	130.58	120.54
5	e	103	TYR	N-CA-C	-7.43	103.34	114.64
6	f	13	PHE	CA-C-N	7.43	135.07	121.70
6	f	13	PHE	C-N-CA	7.43	135.07	121.70
13	m	172	THR	N-CA-C	-7.43	104.06	113.72
27	O	115	ARG	CA-C-N	7.43	130.54	120.44
27	O	115	ARG	C-N-CA	7.43	130.54	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	80	VAL	CA-C-O	7.43	128.27	120.25
27	O	85	SER	N-CA-C	7.43	120.25	111.71
1	a	199	TRP	CA-C-N	7.42	130.09	120.44
1	a	199	TRP	C-N-CA	7.42	130.09	120.44
33	J	15	HIS	CA-CB-CG	7.42	121.22	113.80
24	Q	111	LEU	CA-C-N	7.42	132.99	121.19
24	Q	111	LEU	C-N-CA	7.42	132.99	121.19
30	K	410	ALA	CA-C-N	7.42	130.83	120.29
30	K	410	ALA	C-N-CA	7.42	130.83	120.29
14	n	121	GLU	CA-C-N	7.42	127.28	119.05
14	n	121	GLU	C-N-CA	7.42	127.28	119.05
12	5	216	ASP	CA-C-N	7.42	130.22	120.28
12	5	216	ASP	C-N-CA	7.42	130.22	120.28
27	O	245	ASP	CA-C-N	7.42	130.54	120.38
27	O	245	ASP	C-N-CA	7.42	130.54	120.38
31	L	262	ILE	CB-CA-C	-7.42	102.47	111.97
7	G	84	ASP	CA-C-N	7.42	129.64	120.22
7	G	84	ASP	C-N-CA	7.42	129.64	120.22
33	J	275	LEU	CA-C-N	7.42	130.96	120.28
33	J	275	LEU	C-N-CA	7.42	130.96	120.28
23	P	48	GLN	N-CA-C	7.42	119.00	111.07
24	Q	407	ALA	N-CA-C	7.41	119.44	111.36
25	R	352	SER	CA-C-N	7.41	130.52	120.44
25	R	352	SER	C-N-CA	7.41	130.52	120.44
28	H	319	PHE	CA-CB-CG	-7.41	106.39	113.80
14	7	76	ILE	N-CA-C	-7.41	99.47	107.77
32	M	129	LEU	N-CA-C	-7.41	97.50	109.58
1	A	144	VAL	CA-CB-CG1	-7.41	97.81	110.40
33	J	45	GLU	N-CA-C	-7.41	102.16	112.45
12	l	270	GLU	CA-C-N	7.40	130.80	120.29
12	l	270	GLU	C-N-CA	7.40	130.80	120.29
15	W	14	GLU	N-CA-C	-7.40	101.50	113.19
24	Q	75	ARG	CA-C-N	7.40	131.92	120.82
24	Q	75	ARG	C-N-CA	7.40	131.92	120.82
28	H	259	CYS	N-CA-C	-7.40	104.25	113.28
31	L	364	HIS	CE1-NE2-CD2	-7.40	101.60	109.00
13	6	116	HIS	CE1-NE2-CD2	-7.40	101.60	109.00
1	A	211	ILE	N-CA-C	-7.39	103.58	110.53
31	L	414	ASP	CA-CB-CG	-7.39	105.21	112.60
22	S	191	HIS	CE1-NE2-CD2	-7.39	101.61	109.00
4	d	126	VAL	N-CA-C	-7.39	97.48	108.12
10	3	100	PHE	N-CA-C	-7.38	97.18	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	n	57	ALA	N-CA-C	-7.38	97.49	108.79
25	R	336	LYS	N-CA-C	7.38	119.33	111.28
8	1	181	VAL	N-CA-C	-7.38	102.01	110.05
18	X	18	ASN	CA-CB-CG	-7.38	105.22	112.60
13	m	133	PHE	CA-CB-CG	7.38	121.18	113.80
1	A	90	ALA	CA-C-N	7.37	130.76	120.29
1	A	90	ALA	C-N-CA	7.37	130.76	120.29
29	I	196	GLU	CA-C-O	7.37	126.82	119.08
16	V	277	LYS	CA-C-N	7.37	130.46	120.44
16	V	277	LYS	C-N-CA	7.37	130.46	120.44
11	4	111	LYS	N-CA-C	-7.36	103.25	112.90
24	Q	384	LYS	N-CA-CB	7.36	122.93	110.49
31	L	370	LYS	CA-C-N	7.36	131.02	120.79
31	L	370	LYS	C-N-CA	7.36	131.02	120.79
33	J	383	GLU	N-CA-C	-7.36	103.19	111.14
15	W	86	HIS	CA-C-N	7.36	130.74	120.29
15	W	86	HIS	C-N-CA	7.36	130.74	120.29
3	c	200	THR	CA-C-O	7.36	127.10	118.79
2	B	127	VAL	N-CA-C	-7.36	97.90	108.42
21	N	649	VAL	CA-C-N	7.36	130.14	120.28
21	N	649	VAL	C-N-CA	7.36	130.14	120.28
30	K	406	ASP	CB-CA-C	-7.36	98.34	110.85
9	2	190	ALA	N-CA-C	-7.36	103.77	112.89
32	M	150	LYS	N-CA-C	-7.36	102.64	111.69
16	V	46	PRO	CA-C-N	7.35	131.15	120.71
16	V	46	PRO	C-N-CA	7.35	131.15	120.71
6	f	143	HIS	N-CA-C	-7.35	97.45	108.99
22	S	302	HIS	CE1-NE2-CD2	-7.35	101.65	109.00
30	K	136	SER	CA-C-N	-7.34	114.63	121.97
30	K	136	SER	C-N-CA	-7.34	114.63	121.97
33	J	190	PRO	CA-C-O	-7.34	109.91	120.56
15	W	178	PRO	O-C-N	7.34	131.32	123.10
21	N	450	ILE	CA-C-N	7.33	128.08	119.94
21	N	450	ILE	C-N-CA	7.33	128.08	119.94
21	N	884	PHE	N-CA-CB	7.33	120.78	109.85
1	A	28	VAL	CA-C-N	7.33	130.10	120.28
1	A	28	VAL	C-N-CA	7.33	130.10	120.28
21	N	819	LYS	CB-CA-C	-7.33	98.39	110.85
26	U	177	ASP	N-CA-C	7.33	120.32	110.35
29	I	331	ILE	O-C-N	7.33	129.53	122.20
10	j	157	ASN	N-CA-C	7.32	120.17	111.02
6	F	77	LEU	N-CA-C	7.32	121.48	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	127	ASN	CA-CB-CG	-7.32	105.28	112.60
15	W	92	GLN	OE1-CD-NE2	-7.32	115.28	122.60
1	A	94	ALA	CA-C-O	-7.32	113.16	120.70
30	K	358	SER	CA-C-N	7.32	130.40	120.44
30	K	358	SER	C-N-CA	7.32	130.40	120.44
1	A	51	THR	CA-C-O	-7.32	112.24	120.66
25	R	59	MET	N-CA-C	-7.32	104.37	112.72
21	N	544	GLU	CA-C-O	7.32	128.93	120.80
17	T	159	LYS	CA-C-N	7.32	130.08	120.28
17	T	159	LYS	C-N-CA	7.32	130.08	120.28
27	O	313	ILE	CA-C-N	7.32	129.95	120.44
27	O	313	ILE	C-N-CA	7.32	129.95	120.44
11	k	146	HIS	CB-CG-ND1	7.32	133.67	122.70
7	G	184	PRO	N-CA-C	-7.31	104.31	114.98
18	X	75	TRP	CA-C-O	7.31	128.40	120.43
30	K	262	ARG	CA-C-O	-7.31	112.67	120.42
21	N	705	ILE	N-CA-C	-7.31	103.34	110.72
24	Q	6	SER	CA-C-N	7.31	129.94	120.44
24	Q	6	SER	C-N-CA	7.31	129.94	120.44
7	g	200	ILE	CA-C-N	7.31	131.42	120.31
7	g	200	ILE	C-N-CA	7.31	131.42	120.31
26	U	171	VAL	O-C-N	7.31	129.50	121.90
27	O	294	MET	CA-C-N	7.31	130.07	120.28
27	O	294	MET	C-N-CA	7.31	130.07	120.28
33	J	233	LEU	CA-C-N	7.31	129.94	120.44
33	J	233	LEU	C-N-CA	7.31	129.94	120.44
25	R	131	ALA	CA-C-N	7.30	131.41	120.31
25	R	131	ALA	C-N-CA	7.30	131.41	120.31
1	a	111	ASP	CA-C-N	7.30	130.58	120.65
1	a	111	ASP	C-N-CA	7.30	130.58	120.65
17	T	230	ASN	CB-CA-C	7.30	121.56	111.63
19	Y	30	GLU	N-CA-C	-7.30	103.34	112.90
23	P	175	GLU	N-CA-C	7.30	119.31	111.36
25	R	64	LYS	CA-C-N	7.30	130.06	120.28
25	R	64	LYS	C-N-CA	7.30	130.06	120.28
5	e	82	THR	CA-CB-OG1	7.30	120.54	109.60
3	C	54	SER	N-CA-C	-7.30	97.23	108.76
30	K	179	MET	CA-C-O	-7.30	112.81	120.55
1	A	122	ALA	N-CA-C	7.29	119.22	111.28
14	n	163	VAL	O-C-N	-7.28	114.88	122.82
11	4	180	ILE	CB-CA-C	-7.28	101.88	110.91
21	N	919	THR	N-CA-C	7.28	120.51	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	89	PHE	CA-C-N	7.28	131.37	120.31
21	N	89	PHE	C-N-CA	7.28	131.37	120.31
21	N	882	ILE	CA-C-N	7.28	132.75	121.76
21	N	882	ILE	C-N-CA	7.28	132.75	121.76
28	H	187	LEU	CA-C-N	7.28	127.87	120.38
28	H	187	LEU	C-N-CA	7.28	127.87	120.38
31	L	283	VAL	N-CA-CB	7.28	118.90	110.82
27	O	216	ASP	CA-C-N	7.27	130.02	120.28
27	O	216	ASP	C-N-CA	7.27	130.02	120.28
30	K	382	VAL	O-C-N	-7.27	114.08	122.07
32	M	117	ALA	O-C-N	7.27	131.77	123.27
12	5	141	HIS	CG-CD2-NE2	7.26	114.47	107.20
21	N	45	ASP	N-CA-C	-7.26	103.44	111.36
18	X	57	VAL	CA-C-O	7.26	129.17	120.67
28	H	151	GLN	N-CA-C	-7.26	104.41	113.20
8	h	18	LYS	O-C-N	-7.26	114.43	122.12
1	A	162	TYR	N-CA-C	-7.26	99.74	110.48
8	h	159	GLU	CB-CA-C	-7.25	99.49	110.88
4	D	60	THR	CA-C-N	7.25	127.66	119.83
4	D	60	THR	C-N-CA	7.25	127.66	119.83
19	Y	11	GLN	OE1-CD-NE2	-7.25	115.35	122.60
28	H	339	GLN	CA-C-N	7.25	129.87	120.44
28	H	339	GLN	C-N-CA	7.25	129.87	120.44
31	L	176	GLY	N-CA-C	-7.25	104.14	115.67
28	H	446	ALA	N-CA-C	7.25	119.26	111.36
5	e	192	THR	CA-C-N	7.24	129.99	120.28
5	e	192	THR	C-N-CA	7.24	129.99	120.28
22	S	261	HIS	CB-CG-CD2	-7.24	121.79	131.20
29	I	376	ASN	N-CA-CB	7.24	121.85	110.84
11	4	53	THR	CA-CB-OG1	7.24	120.46	109.60
21	N	445	GLY	CA-C-O	7.24	128.26	120.30
27	O	349	THR	N-CA-C	-7.24	95.18	107.99
9	i	166	VAL	CB-CA-C	-7.23	102.24	112.22
21	N	139	ARG	CD-NE-CZ	-7.23	114.28	124.40
1	A	25	LEU	CA-C-N	7.23	129.96	120.28
1	A	25	LEU	C-N-CA	7.23	129.96	120.28
30	K	353	PHE	N-CA-CB	7.22	120.74	110.12
21	N	12	LEU	N-CA-C	7.22	119.15	111.28
21	N	545	SER	N-CA-C	7.22	120.01	111.71
8	1	137	GLY	N-CA-C	-7.22	102.63	112.52
28	H	265	ASN	CA-CB-CG	-7.22	105.38	112.60
7	g	115	ARG	CA-C-O	-7.21	113.27	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	146	HIS	CE1-NE2-CD2	-7.21	101.79	109.00
21	N	621	THR	N-CA-C	-7.21	103.35	111.14
22	S	218	LEU	CA-C-N	7.21	129.94	120.28
22	S	218	LEU	C-N-CA	7.21	129.94	120.28
33	J	339	ARG	O-C-N	-7.21	114.35	122.86
21	N	315	ASN	CA-C-N	7.21	129.81	120.44
21	N	315	ASN	C-N-CA	7.21	129.81	120.44
21	N	832	HIS	ND1-CE1-NE2	7.21	115.61	108.40
21	N	726	ASP	CA-C-N	7.21	129.94	120.28
21	N	726	ASP	C-N-CA	7.21	129.94	120.28
11	k	89	ALA	N-CA-CB	7.21	120.46	110.01
26	U	131	GLY	O-C-N	-7.21	115.83	122.96
31	L	377	GLU	CA-C-N	7.21	130.25	120.38
31	L	377	GLU	C-N-CA	7.21	130.25	120.38
33	J	10	ILE	CA-C-N	7.21	134.94	121.97
33	J	10	ILE	C-N-CA	7.21	134.94	121.97
7	g	90	ASN	CA-CB-CG	7.20	119.80	112.60
29	I	200	LEU	CA-C-N	7.20	128.84	119.84
29	I	200	LEU	C-N-CA	7.20	128.84	119.84
8	h	63	ALA	N-CA-C	7.20	119.75	111.11
25	R	215	GLY	CA-C-N	7.20	130.64	120.42
25	R	215	GLY	C-N-CA	7.20	130.64	120.42
21	N	870	ASN	CA-C-N	7.19	135.28	121.54
21	N	870	ASN	C-N-CA	7.19	135.28	121.54
9	i	187	ALA	N-CA-CB	7.19	120.80	110.16
1	A	211	ILE	N-CA-CB	7.19	119.77	110.57
12	l	266	HIS	CB-CA-C	-7.19	98.64	110.14
26	U	67	PHE	CA-CB-CG	7.19	120.99	113.80
7	g	136	THR	N-CA-C	-7.19	98.52	109.95
21	N	778	LYS	CA-C-N	7.18	135.26	121.54
21	N	778	LYS	C-N-CA	7.18	135.26	121.54
30	K	408	GLU	CA-C-N	7.18	130.49	120.29
30	K	408	GLU	C-N-CA	7.18	130.49	120.29
7	g	73	HIS	CA-CB-CG	7.18	120.98	113.80
21	N	232	LEU	O-C-N	-7.18	112.55	122.46
1	a	130	GLN	N-CA-C	-7.18	105.44	114.56
21	N	330	THR	CA-C-N	7.18	129.90	120.28
21	N	330	THR	C-N-CA	7.18	129.90	120.28
5	e	91	HIS	CA-CB-CG	7.18	120.98	113.80
2	b	142	PHE	CA-CB-CG	-7.17	106.63	113.80
8	h	182	ILE	CA-C-N	7.17	133.33	122.93
8	h	182	ILE	C-N-CA	7.17	133.33	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	250	GLY	CA-C-O	-7.17	111.26	121.52
2	B	145	PHE	CA-CB-CG	-7.17	106.63	113.80
3	c	205	ALA	N-CA-C	-7.17	97.73	108.99
24	Q	51	ARG	N-CA-C	7.17	126.07	110.80
5	e	211	LYS	N-CA-C	-7.17	97.74	108.99
1	A	244	ARG	N-CA-CB	7.17	120.77	110.16
7	G	40	ILE	N-CA-C	-7.17	97.41	107.80
17	T	96	LEU	N-CA-CB	7.17	122.60	110.49
21	N	330	THR	CA-CB-CG2	7.17	122.69	110.50
24	Q	51	ARG	CA-C-N	7.17	129.89	120.28
24	Q	51	ARG	C-N-CA	7.17	129.89	120.28
8	h	171	ALA	CA-C-N	7.17	129.59	120.56
8	h	171	ALA	C-N-CA	7.17	129.59	120.56
4	d	11	PHE	CA-CB-CG	-7.16	106.64	113.80
4	d	216	LYS	N-CA-C	-7.16	99.14	110.10
23	P	264	ILE	CA-C-N	7.16	130.27	120.46
23	P	264	ILE	C-N-CA	7.16	130.27	120.46
14	n	166	LEU	N-CA-CB	-7.16	101.07	110.59
25	R	32	LEU	CA-C-N	7.16	129.87	120.28
25	R	32	LEU	C-N-CA	7.16	129.87	120.28
21	N	904	VAL	N-CA-CB	7.16	118.52	110.72
30	K	166	LYS	CA-C-O	-7.16	111.57	120.23
13	6	99	ARG	CA-C-N	7.16	129.74	120.44
13	6	99	ARG	C-N-CA	7.16	129.74	120.44
14	7	95	HIS	CA-CB-CG	7.16	120.95	113.80
4	d	67	ILE	N-CA-C	-7.15	104.80	111.45
33	J	281	GLY	O-C-N	7.15	132.00	122.70
21	N	283	ASP	CA-C-O	-7.15	113.08	120.02
32	M	126	THR	N-CA-C	-7.15	98.15	109.23
12	5	235	SER	N-CA-CB	7.14	120.73	110.16
14	7	244	ASN	CA-C-N	7.14	132.15	120.94
14	7	244	ASN	C-N-CA	7.14	132.15	120.94
6	f	169	LYS	CB-CA-C	-7.14	96.97	110.67
7	g	115	ARG	NE-CZ-NH1	7.14	128.64	121.50
27	O	285	SER	O-C-N	7.14	129.69	122.12
21	N	168	SER	CA-C-N	7.13	129.72	120.44
21	N	168	SER	C-N-CA	7.13	129.72	120.44
30	K	305	GLY	CA-C-N	7.13	132.01	120.60
30	K	305	GLY	C-N-CA	7.13	132.01	120.60
3	c	205	ALA	CA-C-N	7.13	131.93	122.30
3	c	205	ALA	C-N-CA	7.13	131.93	122.30
8	1	99	LYS	N-CA-CB	7.13	120.83	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	578	ASP	N-CA-CB	7.13	121.93	110.16
15	W	77	HIS	CE1-NE2-CD2	-7.13	101.87	109.00
10	j	146	LEU	N-CA-C	7.13	123.13	111.37
13	m	166	ASN	CA-CB-CG	-7.13	105.47	112.60
6	F	155	GLU	N-CA-C	-7.13	98.12	109.59
3	c	66	LEU	N-CA-CB	7.12	122.04	110.43
3	c	94	HIS	N-CA-CB	7.12	120.59	110.12
5	E	2	PHE	CA-CB-CG	7.12	120.92	113.80
19	Y	54	VAL	CA-C-N	7.12	135.15	121.54
19	Y	54	VAL	C-N-CA	7.12	135.15	121.54
22	S	139	HIS	ND1-CE1-NE2	7.12	115.52	108.40
23	P	124	VAL	CA-C-O	7.12	128.36	120.95
33	J	236	MET	CA-C-O	7.12	127.97	120.42
3	C	174	THR	CA-C-N	7.12	129.82	120.28
3	C	174	THR	C-N-CA	7.12	129.82	120.28
6	F	233	TYR	N-CA-C	-7.12	104.74	113.50
31	L	211	GLY	N-CA-C	-7.12	105.39	115.43
33	J	355	GLY	CA-C-N	7.12	131.13	120.31
33	J	355	GLY	C-N-CA	7.12	131.13	120.31
18	X	75	TRP	CG-CD2-CE3	-7.12	126.78	133.90
25	R	415	GLN	CB-CG-CD	-7.12	100.50	112.60
21	N	674	GLN	N-CA-CB	7.11	121.99	110.40
21	N	133	LEU	CA-C-N	7.11	129.68	120.44
21	N	133	LEU	C-N-CA	7.11	129.68	120.44
6	f	143	HIS	CE1-NE2-CD2	-7.11	101.89	109.00
24	Q	80	HIS	ND1-CE1-NE2	7.11	115.51	108.40
29	I	77	SER	N-CA-C	7.11	121.05	112.38
22	S	182	LYS	N-CA-C	-7.11	105.14	113.88
10	j	192	LYS	N-CA-C	-7.10	104.18	112.92
1	A	193	HIS	CE1-NE2-CD2	-7.10	101.90	109.00
3	C	161	LYS	N-CA-C	-7.10	104.76	113.50
23	P	394	ASN	OD1-CG-ND2	-7.10	115.50	122.60
24	Q	178	HIS	CA-C-N	7.10	129.79	120.28
24	Q	178	HIS	C-N-CA	7.10	129.79	120.28
29	I	373	GLU	CA-C-O	-7.09	110.51	119.31
10	j	45	HIS	CE1-NE2-CD2	-7.09	101.91	109.00
11	k	41	HIS	CA-CB-CG	-7.09	106.71	113.80
19	Y	7	ALA	CB-CA-C	-7.09	98.80	110.85
23	P	162	GLU	CA-C-N	7.09	130.11	120.54
23	P	162	GLU	C-N-CA	7.09	130.11	120.54
30	K	74	HIS	ND1-CE1-NE2	7.09	115.49	108.40
4	d	241	GLN	CA-C-N	7.09	129.78	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	241	GLN	C-N-CA	7.09	129.78	120.28
24	Q	30	LEU	CA-C-N	7.09	132.46	121.19
24	Q	30	LEU	C-N-CA	7.09	132.46	121.19
6	f	207	THR	N-CA-C	-7.09	97.95	108.79
11	k	8	ARG	NE-CZ-NH2	-7.09	112.82	119.20
22	S	481	TYR	CA-C-N	7.09	127.08	119.28
22	S	481	TYR	C-N-CA	7.09	127.08	119.28
30	K	201	ILE	CA-C-O	-7.09	113.34	120.85
10	j	86	THR	N-CA-CB	7.08	120.53	110.12
7	G	124	THR	CA-CB-OG1	7.08	120.22	109.60
21	N	88	ARG	N-CA-CB	7.08	122.46	110.49
2	b	127	VAL	O-C-N	7.08	130.80	122.95
12	5	263	HIS	CA-CB-CG	-7.08	106.72	113.80
32	M	159	LEU	O-C-N	-7.07	117.18	121.71
2	B	224	TYR	N-CA-C	-7.07	97.39	108.14
14	7	204	GLN	OE1-CD-NE2	7.07	129.67	122.60
20	Z	747	ALA	CA-C-O	-7.07	113.06	120.55
28	H	251	PRO	N-CA-C	7.07	119.32	110.70
29	I	104	LEU	N-CA-C	-7.07	97.00	108.52
16	V	175	SER	N-CA-CB	7.07	123.55	112.46
22	S	234	ILE	CA-C-O	-7.07	113.60	120.95
16	V	212	MET	CG-SD-CE	-7.06	85.36	100.90
3	c	125	HIS	CB-CG-ND1	7.06	133.29	122.70
20	Z	915	ALA	N-CA-C	-7.06	104.60	112.57
16	V	138	ALA	N-CA-CB	7.06	123.01	110.80
9	2	108	ALA	CA-C-N	7.05	130.31	120.29
9	2	108	ALA	C-N-CA	7.05	130.31	120.29
21	N	288	ASN	CA-C-N	7.05	129.44	120.56
21	N	288	ASN	C-N-CA	7.05	129.44	120.56
23	P	13	TYR	CB-CG-CD2	-7.05	110.22	120.80
27	O	255	LEU	N-CA-CB	7.05	120.60	110.16
28	H	120	ASN	CA-C-O	7.05	126.28	118.52
3	c	4	ARG	N-CA-CB	7.05	120.48	110.12
5	E	115	SER	N-CA-C	7.05	119.82	111.71
7	G	206	ASP	CA-CB-CG	-7.05	105.55	112.60
14	7	115	ASP	CA-CB-CG	7.05	119.65	112.60
26	U	228	LYS	CA-C-N	7.05	130.30	120.29
26	U	228	LYS	C-N-CA	7.05	130.30	120.29
5	E	207	VAL	O-C-N	-7.04	115.75	122.09
22	S	37	VAL	CA-C-N	7.04	129.60	120.44
22	S	37	VAL	C-N-CA	7.04	129.60	120.44
28	H	66	LYS	CA-C-O	-7.04	111.87	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	200	LEU	CA-C-N	7.04	127.45	119.92
17	T	200	LEU	C-N-CA	7.04	127.45	119.92
25	R	179	PHE	CA-C-N	7.04	129.71	120.28
25	R	179	PHE	C-N-CA	7.04	129.71	120.28
10	j	57	ALA	CA-C-N	7.03	129.71	120.28
10	j	57	ALA	C-N-CA	7.03	129.71	120.28
12	5	256	THR	CA-C-N	7.03	130.40	120.28
12	5	256	THR	C-N-CA	7.03	130.40	120.28
14	n	262	GLY	N-CA-C	-7.03	104.49	116.01
23	P	328	ALA	O-C-N	-7.03	113.24	122.59
23	P	350	LEU	CA-C-O	-7.03	112.16	120.10
16	V	146	SER	N-CA-C	-7.03	103.28	112.41
24	Q	34	ASP	CA-CB-CG	-7.02	105.58	112.60
30	K	274	VAL	CA-C-N	7.02	129.69	120.28
30	K	274	VAL	C-N-CA	7.02	129.69	120.28
15	W	113	PHE	CA-CB-CG	7.02	120.82	113.80
19	Y	78	LYS	CA-C-N	7.02	129.57	120.44
19	Y	78	LYS	C-N-CA	7.02	129.57	120.44
22	S	122	ASN	OD1-CG-ND2	-7.02	115.58	122.60
28	H	89	GLN	CA-C-N	7.02	130.39	120.28
28	H	89	GLN	C-N-CA	7.02	130.39	120.28
7	G	38	ILE	CB-CA-C	-7.02	100.80	110.90
8	1	47	HIS	ND1-CE1-NE2	7.02	115.42	108.40
14	7	69	PHE	CA-CB-CG	-7.02	106.78	113.80
32	M	175	LYS	CA-C-O	-7.02	112.78	119.80
1	A	22	GLU	N-CA-C	-7.01	104.33	113.17
10	3	44	PHE	N-CA-C	-7.01	98.75	109.41
13	6	95	ASN	CA-C-O	-7.01	113.11	120.55
32	M	18	LEU	N-CA-CB	7.01	121.92	110.55
33	J	341	ILE	N-CA-C	-7.01	98.33	108.36
26	U	227	GLY	CA-C-N	7.01	129.68	120.28
26	U	227	GLY	C-N-CA	7.01	129.68	120.28
29	I	307	LEU	CA-C-N	7.01	129.56	120.44
29	I	307	LEU	C-N-CA	7.01	129.56	120.44
3	c	92	ARG	CA-C-O	-7.01	113.46	120.82
29	I	259	ASP	CA-C-O	7.01	128.00	119.31
14	7	182	HIS	CE1-NE2-CD2	-7.00	102.00	109.00
5	e	71	ASP	CA-CB-CG	-7.00	105.60	112.60
13	m	203	HIS	CB-CG-CD2	-7.00	122.10	131.20
4	D	138	PHE	CA-C-O	-7.00	113.20	121.11
8	1	37	ASN	CA-C-O	-7.00	112.17	120.43
16	V	221	TRP	N-CA-CB	7.00	120.78	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	745	LEU	CB-CG-CD1	-7.00	89.70	110.70
21	N	773	MET	N-CA-C	-7.00	98.52	109.72
26	U	5	HIS	CG-CD2-NE2	7.00	114.20	107.20
28	H	80	HIS	CE1-NE2-CD2	-7.00	102.00	109.00
31	L	75	LYS	CA-C-N	7.00	129.96	120.44
31	L	75	LYS	C-N-CA	7.00	129.96	120.44
14	n	153	GLN	OE1-CD-NE2	-7.00	115.60	122.60
20	Z	726	GLU	CA-C-N	7.00	134.77	122.67
20	Z	726	GLU	C-N-CA	7.00	134.77	122.67
22	S	73	THR	CA-C-N	7.00	129.53	120.44
22	S	73	THR	C-N-CA	7.00	129.53	120.44
14	7	134	TYR	O-C-N	6.99	129.36	122.09
21	N	879	SER	CA-C-N	6.99	130.35	120.28
21	N	879	SER	C-N-CA	6.99	130.35	120.28
25	R	380	VAL	N-CA-C	-6.99	98.59	108.80
16	V	223	SER	O-C-N	-6.99	113.95	122.20
14	n	70	ASN	CA-CB-CG	-6.99	105.61	112.60
13	6	28	PHE	CA-CB-CG	-6.99	106.81	113.80
26	U	37	ILE	N-CA-C	-6.99	98.39	108.53
18	X	124	LYS	N-CA-CB	6.99	120.14	110.01
22	S	93	LEU	CA-C-N	6.99	129.95	120.38
22	S	93	LEU	C-N-CA	6.99	129.95	120.38
28	H	184	GLU	O-C-N	6.99	130.35	122.32
2	B	12	PHE	CA-CB-CG	-6.98	106.82	113.80
15	W	48	THR	CA-CB-OG1	6.98	120.07	109.60
25	R	48	GLU	N-CA-CB	-6.98	99.86	110.12
23	P	363	LEU	CA-C-N	6.98	129.63	120.28
23	P	363	LEU	C-N-CA	6.98	129.63	120.28
32	M	362	GLN	OE1-CD-NE2	6.97	129.57	122.60
11	k	5	LEU	CA-C-N	6.97	126.98	121.61
11	k	5	LEU	C-N-CA	6.97	126.98	121.61
30	K	255	ARG	CA-C-N	6.97	130.19	120.29
30	K	255	ARG	C-N-CA	6.97	130.19	120.29
11	4	95	ARG	N-CA-C	6.97	118.96	111.36
25	R	269	LYS	O-C-N	6.97	129.62	122.09
31	L	386	PHE	CA-CB-CG	6.97	120.77	113.80
8	h	19	ASP	O-C-N	-6.97	113.63	122.34
21	N	224	THR	CA-CB-CG2	-6.96	98.66	110.50
26	U	52	PHE	CA-C-O	-6.96	113.19	120.99
28	H	308	PHE	O-C-N	6.96	132.01	122.41
21	N	671	LEU	N-CA-C	-6.96	106.69	114.62
21	N	311	ILE	CA-CB-CG1	6.96	122.23	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	103	HIS	CE1-NE2-CD2	-6.96	102.05	109.00
13	6	190	LYS	CG-CD-CE	6.96	127.30	111.30
30	K	76	LYS	N-CA-C	-6.96	103.14	111.69
4	D	110	THR	CA-CB-CG2	6.95	122.32	110.50
9	i	140	PHE	CA-CB-CG	6.95	120.75	113.80
12	l	88	ILE	N-CA-C	-6.95	98.57	108.58
30	K	116	MET	N-CA-C	-6.95	97.25	109.06
8	1	135	ILE	CA-C-O	6.95	128.40	120.76
16	V	87	PHE	CA-C-O	-6.95	113.06	120.42
24	Q	167	LYS	N-CA-C	-6.95	103.80	112.90
12	5	236	ILE	CA-C-N	6.94	129.47	120.44
12	5	236	ILE	C-N-CA	6.94	129.47	120.44
2	b	244	ASN	CA-C-N	6.94	130.15	120.29
2	b	244	ASN	C-N-CA	6.94	130.15	120.29
11	k	88	LEU	CB-CA-C	-6.94	97.34	110.67
10	3	171	LEU	CA-C-N	6.94	129.91	120.54
10	3	171	LEU	C-N-CA	6.94	129.91	120.54
28	H	270	THR	CA-C-N	-6.94	113.42	123.00
28	H	270	THR	C-N-CA	-6.94	113.42	123.00
3	C	136	ILE	N-CA-CB	6.94	120.20	111.46
22	S	39	ASN	CA-CB-CG	-6.94	105.66	112.60
22	S	339	GLN	N-CA-CB	6.94	120.32	110.12
31	L	117	TYR	CB-CG-CD2	-6.94	110.39	120.80
3	c	135	PHE	CB-CA-C	-6.94	96.89	109.38
8	1	111	TYR	O-C-N	6.94	131.55	123.30
2	b	93	ALA	O-C-N	6.93	131.62	122.33
7	g	239	ALA	N-CA-C	-6.93	103.65	111.14
12	l	113	ASN	N-CA-C	-6.93	101.90	108.07
13	6	62	ALA	N-CA-CB	6.93	121.61	110.65
24	Q	209	TYR	CA-C-N	6.93	130.03	120.39
24	Q	209	TYR	C-N-CA	6.93	130.03	120.39
21	N	188	TYR	N-CA-CB	6.93	120.31	110.12
25	R	359	VAL	CA-C-N	6.93	135.87	121.32
25	R	359	VAL	C-N-CA	6.93	135.87	121.32
12	l	134	LEU	N-CA-C	-6.93	103.73	111.28
24	Q	150	GLN	CA-C-O	6.93	129.30	120.57
3	c	202	ASP	N-CA-C	-6.92	104.64	113.23
14	n	217	LEU	CA-C-N	6.92	129.56	120.28
14	n	217	LEU	C-N-CA	6.92	129.56	120.28
14	7	213	ALA	CA-C-O	-6.92	113.55	120.82
17	T	181	LEU	CA-C-N	6.92	129.56	120.28
17	T	181	LEU	C-N-CA	6.92	129.56	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	353	LEU	CA-C-O	-6.92	111.62	118.34
33	J	37	LYS	CA-C-N	6.92	129.44	120.44
33	J	37	LYS	C-N-CA	6.92	129.44	120.44
7	G	204	HIS	ND1-CE1-NE2	6.92	115.32	108.40
30	K	350	ARG	NE-CZ-NH1	6.92	128.42	121.50
2	B	52	SER	CB-CA-C	-6.92	100.01	110.88
23	P	127	GLU	N-CA-C	-6.92	104.83	112.72
24	Q	404	ASN	CA-CB-CG	-6.92	105.68	112.60
32	M	24	ASN	OD1-CG-ND2	-6.92	115.68	122.60
29	I	430	GLU	CB-CG-CD	-6.92	100.84	112.60
6	f	58	SER	O-C-N	6.92	130.69	121.83
10	j	205	ASP	CA-CB-CG	-6.92	105.68	112.60
10	3	116	SER	CB-CA-C	-6.92	100.23	109.16
13	6	71	ALA	CA-C-O	6.92	127.75	120.42
23	P	253	ASP	N-CA-CB	6.92	121.58	110.16
24	Q	431	SER	N-CA-CB	6.92	120.40	110.16
31	L	279	PHE	O-C-N	-6.92	115.33	123.22
26	U	71	ASN	CA-C-N	6.92	129.55	120.28
26	U	71	ASN	C-N-CA	6.92	129.55	120.28
27	O	91	ASP	CA-CB-CG	-6.92	105.68	112.60
21	N	355	TRP	O-C-N	6.92	129.45	122.12
21	N	550	GLY	O-C-N	6.92	129.82	122.28
25	R	148	ASP	CA-CB-CG	-6.92	105.69	112.60
30	K	253	MET	CA-C-N	6.92	130.24	120.42
30	K	253	MET	C-N-CA	6.92	130.24	120.42
24	Q	186	HIS	CB-CG-CD2	-6.91	122.21	131.20
4	D	144	GLU	CA-C-N	6.91	126.67	119.76
4	D	144	GLU	C-N-CA	6.91	126.67	119.76
17	T	155	GLY	N-CA-C	-6.91	105.33	115.63
6	f	187	ASP	CA-C-N	6.91	130.10	120.29
6	f	187	ASP	C-N-CA	6.91	130.10	120.29
21	N	221	ASP	N-CA-C	-6.91	100.76	110.50
27	O	16	MET	CA-C-O	6.91	127.82	120.70
12	5	195	THR	N-CA-C	-6.91	100.06	110.28
23	P	209	LYS	N-CA-C	-6.91	105.00	113.50
8	1	39	VAL	N-CA-C	-6.91	106.08	112.43
1	a	158	ASP	CA-C-N	6.90	126.53	119.56
1	a	158	ASP	C-N-CA	6.90	126.53	119.56
7	g	8	TYR	CA-CB-CG	-6.90	101.48	113.90
1	A	12	TYR	N-CA-C	-6.90	97.99	108.96
11	4	119	ILE	CA-C-O	6.90	127.24	120.27
23	P	351	ARG	CA-C-N	6.90	129.39	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	351	ARG	C-N-CA	6.90	129.39	120.56
3	c	234	GLU	CA-C-N	6.90	130.21	120.42
3	c	234	GLU	C-N-CA	6.90	130.21	120.42
30	K	406	ASP	O-C-N	6.89	130.01	122.15
6	f	220	THR	CA-C-O	-6.89	113.45	119.72
25	R	169	ASP	CA-C-N	6.89	129.90	120.46
25	R	169	ASP	C-N-CA	6.89	129.90	120.46
14	n	172	SER	N-CA-CB	-6.89	104.19	111.29
14	7	163	VAL	CB-CA-C	6.89	121.94	110.30
30	K	200	GLN	CB-CG-CD	-6.89	100.89	112.60
16	V	201	ILE	N-CA-C	-6.89	98.20	108.46
7	g	234	ASP	CA-CB-CG	-6.88	105.72	112.60
8	l	90	VAL	N-CA-C	-6.88	104.06	110.53
11	k	122	LEU	O-C-N	-6.88	114.66	122.09
17	T	28	PRO	CA-C-O	-6.88	110.59	120.56
17	T	132	HIS	CE1-NE2-CD2	-6.88	102.12	109.00
2	b	81	ASP	CA-CB-CG	-6.88	105.72	112.60
12	l	144	ARG	CD-NE-CZ	-6.88	114.77	124.40
23	P	84	LYS	CA-C-N	6.88	132.12	121.19
23	P	84	LYS	C-N-CA	6.88	132.12	121.19
23	P	282	HIS	CE1-NE2-CD2	-6.88	102.12	109.00
17	T	195	LEU	CA-C-N	6.88	129.49	120.28
17	T	195	LEU	C-N-CA	6.88	129.49	120.28
7	g	60	VAL	CB-CA-C	-6.87	103.28	111.18
6	f	123	TYR	N-CA-C	-6.87	98.06	109.46
13	m	62	ALA	CA-C-O	6.87	127.61	120.40
11	4	68	SER	CA-C-N	6.87	130.56	120.74
11	4	68	SER	C-N-CA	6.87	130.56	120.74
22	S	244	ASN	CA-CB-CG	-6.87	105.73	112.60
27	O	131	SER	O-C-N	6.87	129.40	122.12
1	A	154	ILE	N-CA-C	-6.87	98.23	108.12
32	M	29	GLU	N-CA-CB	6.87	120.32	110.16
11	k	113	LYS	O-C-N	-6.86	116.49	121.84
1	A	225	VAL	CA-C-N	6.86	126.32	121.65
1	A	225	VAL	C-N-CA	6.86	126.32	121.65
33	J	201	ALA	CA-C-N	6.86	130.17	120.42
33	J	201	ALA	C-N-CA	6.86	130.17	120.42
17	T	204	ASN	CA-C-N	6.86	129.86	120.46
17	T	204	ASN	C-N-CA	6.86	129.86	120.46
31	L	245	PHE	N-CA-CB	6.86	122.08	110.49
33	J	304	LEU	N-CA-C	-6.86	104.94	113.38
5	E	151	ASP	N-CA-C	-6.86	103.46	114.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	4	126	VAL	CA-C-N	6.86	130.61	120.87
11	4	126	VAL	C-N-CA	6.86	130.61	120.87
29	I	160	LEU	N-CA-C	-6.86	106.11	114.75
30	K	80	LYS	N-CA-C	-6.86	103.73	111.07
21	N	884	PHE	CA-CB-CG	-6.86	106.94	113.80
29	I	187	LEU	N-CA-CB	6.86	122.08	110.49
30	K	403	LEU	N-CA-C	-6.86	100.31	110.46
7	G	47	VAL	O-C-N	-6.85	116.38	123.03
9	2	145	HIS	N-CA-C	-6.85	106.12	114.75
17	T	191	LYS	CA-C-N	6.85	130.15	120.28
17	T	191	LYS	C-N-CA	6.85	130.15	120.28
5	E	160	PRO	N-CA-C	-6.85	105.61	114.03
23	P	436	GLU	N-CA-CB	6.85	120.90	110.28
7	g	16	SER	CB-CA-C	-6.85	98.81	109.22
24	Q	354	PHE	CA-CB-CG	-6.85	106.95	113.80
5	e	24	VAL	O-C-N	6.84	128.78	121.87
3	C	194	LEU	N-CA-CB	6.84	119.93	110.01
27	O	98	TYR	CA-C-O	-6.84	113.17	120.42
6	f	143	HIS	CA-C-N	6.84	132.41	122.77
6	f	143	HIS	C-N-CA	6.84	132.41	122.77
16	V	161	THR	CA-C-N	6.84	128.75	120.13
16	V	161	THR	C-N-CA	6.84	128.75	120.13
26	U	255	ILE	CB-CA-C	6.84	121.37	112.14
32	M	140	LEU	O-C-N	-6.84	115.31	123.31
4	d	157	SER	N-CA-C	-6.84	98.63	109.23
25	R	350	LEU	CA-C-O	-6.84	113.17	120.42
9	i	133	ASP	CA-C-N	6.84	128.39	119.84
9	i	133	ASP	C-N-CA	6.84	128.39	119.84
20	Z	738	TYR	CE1-CZ-CE2	-6.84	106.63	120.30
24	Q	80	HIS	CA-CB-CG	6.83	120.63	113.80
30	K	57	GLU	CA-C-O	6.83	127.86	119.11
7	g	8	TYR	N-CA-C	-6.83	102.07	110.61
12	5	270	GLU	CB-CG-CD	-6.83	100.98	112.60
23	P	241	LEU	CA-C-N	6.83	129.43	120.28
23	P	241	LEU	C-N-CA	6.83	129.43	120.28
29	I	162	ASP	CA-CB-CG	-6.83	105.77	112.60
12	l	189	TYR	CB-CA-C	6.83	121.54	109.72
25	R	193	ALA	CA-C-O	-6.83	112.39	120.10
31	L	114	GLU	N-CA-C	-6.83	103.98	112.72
14	7	252	TRP	CG-CD2-CE3	-6.82	127.08	133.90
25	R	422	ARG	CA-C-N	6.82	129.42	120.28
25	R	422	ARG	C-N-CA	6.82	129.42	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	338	TYR	CB-CA-C	-6.82	99.26	110.85
22	S	114	TYR	CA-C-O	-6.82	112.67	120.03
22	S	299	LYS	CA-C-N	6.82	130.39	120.51
22	S	299	LYS	C-N-CA	6.82	130.39	120.51
25	R	360	SER	CA-C-N	6.82	130.10	120.42
25	R	360	SER	C-N-CA	6.82	130.10	120.42
1	a	110	TYR	CA-C-N	6.81	130.43	120.82
1	a	110	TYR	C-N-CA	6.81	130.43	120.82
7	G	93	ARG	N-CA-CB	6.81	120.55	110.33
28	H	464	MET	CA-C-N	6.81	134.55	121.54
28	H	464	MET	C-N-CA	6.81	134.55	121.54
29	I	220	ILE	N-CA-C	-6.81	98.31	108.12
4	d	139	ASP	CA-C-N	6.81	127.05	119.90
4	d	139	ASP	C-N-CA	6.81	127.05	119.90
26	U	4	GLN	N-CA-C	-6.81	103.67	113.21
2	b	115	ALA	CA-C-O	6.81	127.24	119.27
25	R	263	ARG	NE-CZ-NH1	6.81	128.31	121.50
32	M	117	ALA	CB-CA-C	-6.81	99.25	110.14
3	c	66	LEU	O-C-N	-6.81	115.58	123.27
13	6	71	ALA	N-CA-C	6.81	118.78	111.36
15	W	131	THR	N-CA-CB	6.81	120.23	110.16
29	I	80	GLU	CA-C-N	6.81	129.79	120.46
29	I	80	GLU	C-N-CA	6.81	129.79	120.46
21	N	436	ASP	CA-CB-CG	-6.81	105.79	112.60
6	F	148	GLN	O-C-N	-6.80	115.08	121.20
21	N	589	ILE	CA-C-N	6.80	129.40	120.28
21	N	589	ILE	C-N-CA	6.80	129.40	120.28
32	M	346	LYS	CA-C-N	6.80	131.50	122.93
32	M	346	LYS	C-N-CA	6.80	131.50	122.93
4	D	93	ALA	N-CA-C	-6.80	103.95	111.36
15	W	35	PHE	CA-CB-CG	6.80	120.60	113.80
21	N	893	VAL	N-CA-CB	6.80	119.79	110.54
23	P	37	ASP	CA-C-O	6.80	127.76	120.55
23	P	222	ASN	N-CA-CB	6.80	120.12	110.12
2	b	113	GLU	N-CA-CB	6.80	120.12	110.12
22	S	225	HIS	CE1-NE2-CD2	-6.80	102.20	109.00
5	e	146	GLY	O-C-N	-6.80	117.01	123.81
1	a	103	GLU	O-C-N	6.79	129.32	122.12
9	i	173	GLN	CA-C-N	6.79	134.52	121.54
9	i	173	GLN	C-N-CA	6.79	134.52	121.54
23	P	288	ASN	CA-CB-CG	-6.79	105.81	112.60
2	B	7	PHE	N-CA-CB	6.79	119.95	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	184	MET	CA-C-N	6.79	129.38	120.28
23	P	184	MET	C-N-CA	6.79	129.38	120.28
24	Q	227	CYS	CA-C-N	6.79	130.06	120.28
24	Q	227	CYS	C-N-CA	6.79	130.06	120.28
30	K	238	ASN	OD1-CG-ND2	6.79	129.39	122.60
9	i	125	ALA	CA-C-O	6.79	128.03	120.70
25	R	25	GLU	CA-C-N	6.79	129.76	120.46
25	R	25	GLU	C-N-CA	6.79	129.76	120.46
28	H	240	ILE	CB-CA-C	-6.79	102.51	111.13
22	S	86	SER	CA-C-N	6.79	129.26	120.44
22	S	86	SER	C-N-CA	6.79	129.26	120.44
23	P	215	SER	N-CA-C	-6.79	103.96	111.36
9	2	38	ASN	CA-CB-CG	-6.79	105.81	112.60
7	g	158	TRP	N-CA-C	-6.78	98.76	109.07
8	1	57	SER	CA-C-N	6.78	129.37	120.28
8	1	57	SER	C-N-CA	6.78	129.37	120.28
21	N	140	MET	O-C-N	6.78	130.61	122.27
25	R	100	ASN	OD1-CG-ND2	-6.78	115.82	122.60
30	K	44	ASN	CA-CB-CG	-6.78	105.82	112.60
15	W	97	THR	CA-C-O	-6.78	113.70	120.82
9	i	209	ILE	N-CA-CB	6.78	118.65	110.31
22	S	387	VAL	CA-C-N	6.78	130.05	120.42
22	S	387	VAL	C-N-CA	6.78	130.05	120.42
27	O	297	ILE	CA-C-N	6.78	129.66	120.44
27	O	297	ILE	C-N-CA	6.78	129.66	120.44
31	L	203	ASN	O-C-N	6.78	129.12	121.32
31	L	159	LEU	CA-C-N	6.78	127.70	120.11
31	L	159	LEU	C-N-CA	6.78	127.70	120.11
17	T	78	PHE	CA-C-N	6.78	129.69	120.54
17	T	78	PHE	C-N-CA	6.78	129.69	120.54
26	U	260	ASN	OD1-CG-ND2	6.78	129.38	122.60
2	b	230	ASP	CA-CB-CG	-6.78	105.83	112.60
15	W	50	GLY	O-C-N	-6.78	118.73	123.95
22	S	480	ARG	NE-CZ-NH1	-6.78	114.72	121.50
25	R	384	VAL	N-CA-C	6.78	117.56	110.72
20	Z	918	ASP	N-CA-CB	6.77	120.15	110.13
21	N	146	LYS	CB-CA-C	-6.77	99.34	110.85
28	H	422	VAL	N-CA-CB	6.77	120.27	110.52
11	k	73	TYR	N-CA-C	-6.77	98.43	108.79
27	O	47	LYS	CA-C-O	-6.77	113.71	120.82
21	N	291	SER	N-CA-C	-6.77	103.36	111.69
26	U	252	HIS	CG-CD2-NE2	6.77	113.97	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	206	VAL	CB-CA-C	-6.77	101.78	111.19
17	T	83	ASN	CA-CB-CG	-6.77	105.83	112.60
21	N	126	LYS	N-CA-C	-6.77	99.56	110.32
22	S	276	LEU	CB-CA-C	-6.77	99.98	110.81
16	V	250	GLN	CA-C-N	6.77	130.59	120.31
16	V	250	GLN	C-N-CA	6.77	130.59	120.31
24	Q	302	VAL	CA-C-N	6.77	129.35	120.28
24	Q	302	VAL	C-N-CA	6.77	129.35	120.28
33	J	235	VAL	CA-C-O	-6.77	113.16	120.47
11	k	82	SER	CA-C-N	6.76	129.24	120.44
11	k	82	SER	C-N-CA	6.76	129.24	120.44
17	T	86	LYS	CA-C-O	-6.76	112.08	118.44
9	i	89	GLY	CA-C-N	6.76	129.89	120.29
9	i	89	GLY	C-N-CA	6.76	129.89	120.29
17	T	261	GLU	CA-C-N	6.76	129.23	120.44
17	T	261	GLU	C-N-CA	6.76	129.23	120.44
3	C	173	GLN	CB-CG-CD	-6.76	101.11	112.60
24	Q	158	ILE	N-CA-C	6.76	117.51	110.62
11	4	193	ASP	CA-C-N	6.76	130.30	120.71
11	4	193	ASP	C-N-CA	6.76	130.30	120.71
25	R	409	GLY	CA-C-N	6.76	129.88	120.29
25	R	409	GLY	C-N-CA	6.76	129.88	120.29
29	I	376	ASN	CB-CA-C	-6.75	100.42	110.62
29	I	126	PRO	N-CA-CB	6.75	109.18	103.17
7	G	144	ASN	N-CA-C	-6.75	104.92	113.02
11	k	128	LEU	CB-CA-C	-6.75	99.51	109.97
17	T	255	GLN	CA-C-N	6.75	129.87	120.29
17	T	255	GLN	C-N-CA	6.75	129.87	120.29
7	g	145	GLY	CA-C-O	-6.74	115.58	122.26
25	R	364	LEU	N-CA-C	6.74	118.63	111.28
22	S	468	ALA	CA-C-N	6.74	129.31	120.28
22	S	468	ALA	C-N-CA	6.74	129.31	120.28
28	H	121	ASN	N-CA-C	-6.74	104.67	113.17
4	d	140	PRO	N-CA-CB	6.74	109.29	103.36
7	g	56	SER	N-CA-CB	6.74	123.19	111.39
26	U	156	HIS	CA-C-O	-6.74	113.78	121.19
1	A	87	ILE	O-C-N	-6.74	113.42	121.10
1	A	135	ARG	NE-CZ-NH1	6.73	128.23	121.50
22	S	459	GLN	N-CA-CB	6.73	120.12	110.16
31	L	253	ASP	CA-CB-CG	-6.73	105.87	112.60
1	A	19	PHE	CB-CG-CD2	6.73	132.14	120.70
16	V	80	VAL	CA-C-N	6.73	129.97	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	80	VAL	C-N-CA	6.73	129.97	120.28
22	S	85	SER	N-CA-C	6.73	118.62	111.28
33	J	173	LEU	CA-C-N	6.73	130.54	120.31
33	J	173	LEU	C-N-CA	6.73	130.54	120.31
3	c	120	GLN	CA-C-N	6.72	127.44	119.98
3	c	120	GLN	C-N-CA	6.72	127.44	119.98
7	g	173	LYS	N-CA-C	-6.72	104.03	111.36
12	5	104	GLN	CB-CG-CD	-6.72	101.17	112.60
5	e	15	PHE	CA-C-N	6.72	133.80	121.70
5	e	15	PHE	C-N-CA	6.72	133.80	121.70
21	N	212	ASP	CA-CB-CG	-6.72	105.88	112.60
3	c	35	ALA	O-C-N	-6.72	115.20	123.33
7	G	144	ASN	CA-CB-CG	-6.72	105.88	112.60
8	1	98	ASN	CA-CB-CG	6.72	119.32	112.60
3	C	141	ASP	N-CA-C	-6.72	99.09	109.24
21	N	788	TYR	N-CA-CB	6.72	121.81	111.46
23	P	104	LEU	CA-C-O	6.72	127.67	120.55
24	Q	67	THR	CA-C-N	6.72	133.80	121.70
24	Q	67	THR	C-N-CA	6.72	133.80	121.70
5	E	50	VAL	CA-C-O	6.72	128.09	120.90
6	f	87	TYR	CA-C-N	6.72	129.17	120.44
6	f	87	TYR	C-N-CA	6.72	129.17	120.44
6	f	110	HIS	CA-CB-CG	-6.71	107.09	113.80
3	C	229	ILE	CA-C-O	6.71	128.53	120.74
21	N	749	LEU	CA-C-N	6.71	129.95	120.28
21	N	749	LEU	C-N-CA	6.71	129.95	120.28
30	K	151	PRO	CB-CA-C	6.71	119.11	110.92
30	K	152	PRO	CA-C-N	6.71	129.17	120.44
30	K	152	PRO	C-N-CA	6.71	129.17	120.44
9	2	84	VAL	N-CA-CB	6.71	122.27	112.07
19	Y	5	VAL	CA-C-O	-6.71	112.83	120.95
16	V	20	ARG	CA-C-N	6.71	130.51	120.31
16	V	20	ARG	C-N-CA	6.71	130.51	120.31
26	U	110	PHE	CA-CB-CG	-6.71	107.09	113.80
4	d	214	VAL	N-CA-CB	6.71	120.67	111.41
9	i	158	SER	N-CA-C	-6.71	105.22	113.41
12	l	266	HIS	CE1-NE2-CD2	-6.71	102.29	109.00
4	D	79	ASN	N-CA-C	-6.71	103.44	111.69
7	g	22	PHE	CB-CG-CD1	-6.71	109.30	120.70
8	1	45	ARG	O-C-N	-6.71	115.42	123.13
4	d	188	VAL	O-C-N	6.71	128.38	121.87
25	R	412	THR	CA-C-N	6.71	129.81	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	412	THR	C-N-CA	6.71	129.81	120.29
32	M	334	ASP	CA-C-O	-6.71	113.39	120.70
13	m	39	THR	N-CA-C	-6.71	95.94	107.61
21	N	786	ARG	CA-C-N	6.71	133.66	122.87
21	N	786	ARG	C-N-CA	6.71	133.66	122.87
28	H	332	THR	CA-C-N	6.71	129.16	120.44
28	H	332	THR	C-N-CA	6.71	129.16	120.44
14	7	149	VAL	N-CA-C	-6.70	97.96	107.75
3	C	10	THR	CA-C-O	6.70	127.19	119.35
21	N	496	GLU	CA-C-N	6.70	129.56	120.44
21	N	496	GLU	C-N-CA	6.70	129.56	120.44
14	7	110	ASP	CA-CB-CG	-6.70	105.90	112.60
27	O	163	ILE	CA-C-O	-6.70	114.31	119.20
27	O	189	TYR	CA-C-O	-6.70	113.45	120.55
13	m	178	LYS	CA-C-N	6.69	126.45	119.76
13	m	178	LYS	C-N-CA	6.69	126.45	119.76
11	k	96	ARG	N-CA-C	-6.69	99.92	109.62
12	l	104	GLN	CB-CG-CD	-6.69	101.22	112.60
17	T	213	ASN	N-CA-C	-6.69	97.31	108.75
13	6	178	LYS	CA-C-N	6.69	127.23	120.14
13	6	178	LYS	C-N-CA	6.69	127.23	120.14
30	K	219	LYS	CB-CA-C	-6.69	100.38	110.88
1	a	106	TYR	CB-CG-CD2	-6.69	110.77	120.80
3	C	31	HIS	CB-CG-CD2	-6.69	122.50	131.20
24	Q	376	LYS	CA-C-N	6.69	129.24	120.28
24	Q	376	LYS	C-N-CA	6.69	129.24	120.28
10	3	122	ALA	CB-CA-C	-6.69	99.23	109.99
23	P	409	SER	CA-C-N	6.69	129.13	120.44
23	P	409	SER	C-N-CA	6.69	129.13	120.44
32	M	139	LYS	CA-C-N	6.69	133.04	122.74
32	M	139	LYS	C-N-CA	6.69	133.04	122.74
27	O	87	LYS	N-CA-C	-6.68	103.81	112.23
22	S	164	ILE	O-C-N	-6.68	113.48	121.10
31	L	226	THR	CA-C-N	6.68	134.03	120.80
31	L	226	THR	C-N-CA	6.68	134.03	120.80
14	7	182	HIS	CB-CG-ND1	6.68	132.72	122.70
22	S	357	LEU	CA-C-N	6.68	129.23	120.28
22	S	357	LEU	C-N-CA	6.68	129.23	120.28
32	M	416	VAL	N-CA-CB	-6.68	98.68	110.77
22	S	431	VAL	O-C-N	-6.68	115.36	121.91
27	O	378	GLU	CA-C-N	6.68	129.77	120.29
27	O	378	GLU	C-N-CA	6.68	129.77	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	13	ILE	O-C-N	-6.68	114.30	122.18
3	C	121	GLY	N-CA-C	6.67	120.97	112.83
21	N	624	ALA	CA-C-O	6.67	127.83	120.82
11	k	114	PRO	N-CA-C	-6.67	99.73	112.01
14	n	188	LEU	N-CA-C	6.67	118.55	111.28
4	D	203	VAL	O-C-N	-6.67	115.07	121.94
18	X	117	LYS	N-CA-C	-6.67	98.93	109.07
25	R	357	PHE	CA-C-N	6.67	130.73	121.26
25	R	357	PHE	C-N-CA	6.67	130.73	121.26
10	j	162	ASP	CA-CB-CG	-6.67	105.93	112.60
21	N	410	LEU	N-CA-CB	6.67	119.68	110.01
24	Q	336	ASN	CA-C-O	6.67	127.49	120.42
21	N	425	ASN	CB-CG-ND2	-6.67	106.40	116.40
11	k	160	LEU	CA-C-N	6.66	129.75	120.29
11	k	160	LEU	C-N-CA	6.66	129.75	120.29
17	T	7	LEU	CA-C-N	6.66	130.44	120.31
17	T	7	LEU	C-N-CA	6.66	130.44	120.31
23	P	192	ASP	CA-C-N	6.66	130.44	120.31
23	P	192	ASP	C-N-CA	6.66	130.44	120.31
7	g	204	HIS	CE1-NE2-CD2	-6.66	102.34	109.00
14	n	40	THR	CA-CB-OG1	6.66	119.59	109.60
1	A	94	ALA	N-CA-C	-6.66	103.95	111.14
17	T	252	GLU	CA-C-N	6.66	129.10	120.44
17	T	252	GLU	C-N-CA	6.66	129.10	120.44
15	W	28	ALA	CA-C-O	6.66	127.48	120.42
20	Z	746	ILE	CA-C-N	6.66	129.20	120.28
20	Z	746	ILE	C-N-CA	6.66	129.20	120.28
25	R	393	PRO	N-CA-CB	6.66	107.42	101.83
33	J	207	ASP	N-CA-CB	6.66	121.74	110.49
2	b	188	ALA	CA-C-O	-6.66	113.49	120.55
5	e	64	ILE	N-CA-C	-6.66	98.60	108.45
4	D	112	TYR	O-C-N	6.66	129.74	122.15
5	e	116	VAL	N-CA-C	-6.66	103.25	112.50
25	R	147	LYS	CA-C-N	6.66	129.09	120.44
25	R	147	LYS	C-N-CA	6.66	129.09	120.44
26	U	196	SER	CA-C-N	6.66	129.20	120.28
26	U	196	SER	C-N-CA	6.66	129.20	120.28
16	V	111	HIS	CE1-NE2-CD2	-6.65	102.35	109.00
31	L	149	ASP	N-CA-CB	6.65	120.53	110.42
31	L	183	ILE	N-CA-CB	6.65	118.97	110.99
7	g	21	ASN	N-CA-CB	6.65	121.63	110.79
9	i	178	GLU	N-CA-C	6.65	119.36	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	241	GLU	N-CA-C	6.65	118.53	111.28
23	P	99	LYS	N-CA-CB	6.65	120.46	110.22
8	1	47	HIS	CA-CB-CG	6.65	120.45	113.80
14	7	35	GLN	OE1-CD-NE2	6.65	129.25	122.60
22	S	157	GLU	CA-C-N	6.65	129.08	120.44
22	S	157	GLU	C-N-CA	6.65	129.08	120.44
9	i	66	ILE	N-CA-CB	6.64	117.86	110.62
29	I	215	PRO	CA-C-N	6.64	128.15	119.84
29	I	215	PRO	C-N-CA	6.64	128.15	119.84
23	P	158	ASP	CA-CB-CG	-6.64	105.96	112.60
27	O	174	THR	N-CA-CB	6.64	119.99	110.16
30	K	303	MET	N-CA-C	-6.64	103.52	111.69
26	U	149	SER	CA-C-N	6.64	134.22	121.54
26	U	149	SER	C-N-CA	6.64	134.22	121.54
30	K	116	MET	CA-C-N	6.64	132.54	122.65
30	K	116	MET	C-N-CA	6.64	132.54	122.65
1	a	216	THR	CA-C-N	6.64	134.22	121.54
1	a	216	THR	C-N-CA	6.64	134.22	121.54
22	S	158	PHE	CA-C-N	6.64	129.18	120.28
22	S	158	PHE	C-N-CA	6.64	129.18	120.28
22	S	455	GLU	CA-C-N	6.64	128.39	120.09
22	S	455	GLU	C-N-CA	6.64	128.39	120.09
14	7	63	TYR	N-CA-C	-6.64	96.69	109.24
20	Z	780	MET	CA-C-N	6.64	127.35	119.98
20	Z	780	MET	C-N-CA	6.64	127.35	119.98
10	3	137	ILE	N-CA-C	-6.63	98.63	108.45
20	Z	861	THR	N-CA-C	-6.63	107.06	114.62
22	S	295	ALA	N-CA-C	6.63	118.17	111.07
24	Q	153	ASP	CA-CB-CG	-6.63	105.97	112.60
24	Q	302	VAL	N-CA-C	-6.63	104.02	110.72
28	H	451	ILE	O-C-N	6.63	128.66	121.83
20	Z	735	GLU	CB-CG-CD	6.63	123.88	112.60
21	N	625	LEU	O-C-N	6.63	129.15	122.12
28	H	411	CYS	O-C-N	-6.63	114.23	121.53
1	a	147	ASP	CA-CB-CG	-6.63	105.97	112.60
23	P	148	LYS	O-C-N	6.63	128.90	122.07
13	6	155	MET	O-C-N	-6.63	115.69	120.27
16	V	74	SER	N-CA-C	-6.63	99.08	108.96
27	O	237	PRO	O-C-N	6.63	129.86	122.24
31	L	394	CYS	CA-C-N	6.63	129.70	120.29
31	L	394	CYS	C-N-CA	6.63	129.70	120.29
5	e	169	ALA	N-CA-CB	6.63	121.69	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	79	ALA	N-CA-C	6.63	118.58	111.36
18	X	81	SER	N-CA-CB	6.63	121.69	110.49
6	f	6	TYR	CA-C-O	6.62	126.34	119.05
22	S	273	PHE	CB-CG-CD1	6.62	131.96	120.70
27	O	289	GLN	CA-C-N	6.62	129.16	120.28
27	O	289	GLN	C-N-CA	6.62	129.16	120.28
28	H	193	PRO	N-CA-CB	6.62	109.49	103.33
20	Z	736	LEU	CA-C-N	6.62	129.81	120.28
20	Z	736	LEU	C-N-CA	6.62	129.81	120.28
27	O	237	PRO	CA-C-N	6.62	129.87	120.53
27	O	237	PRO	C-N-CA	6.62	129.87	120.53
28	H	126	ASN	N-CA-C	-6.62	103.15	113.02
9	i	178	GLU	CA-C-N	6.62	129.44	120.44
9	i	178	GLU	C-N-CA	6.62	129.44	120.44
5	E	12	VAL	CA-C-N	6.62	130.60	121.33
5	E	12	VAL	C-N-CA	6.62	130.60	121.33
12	5	234	ARG	N-CA-C	6.62	119.34	111.33
27	O	318	HIS	ND1-CE1-NE2	6.62	115.02	108.40
14	7	216	VAL	O-C-N	-6.62	115.01	121.83
21	N	64	ILE	N-CA-C	-6.62	104.06	110.42
27	O	242	ILE	CA-C-N	6.62	133.88	121.97
27	O	242	ILE	C-N-CA	6.62	133.88	121.97
6	F	20	PHE	CA-C-O	6.62	127.01	119.27
22	S	203	SER	CA-C-N	6.62	131.90	120.58
22	S	203	SER	C-N-CA	6.62	131.90	120.58
4	D	178	ASN	OD1-CG-ND2	-6.62	115.98	122.60
10	3	35	GLY	CA-C-O	-6.62	115.40	120.76
21	N	475	ALA	O-C-N	-6.62	115.11	122.12
26	U	225	ILE	CA-CB-CG1	-6.62	99.16	110.40
29	I	231	LEU	N-CA-CB	6.62	120.49	110.30
30	K	290	ARG	CD-NE-CZ	-6.61	115.14	124.40
12	l	148	ARG	CA-C-N	6.61	129.54	120.35
12	l	148	ARG	C-N-CA	6.61	129.54	120.35
15	W	44	ASN	CA-C-N	-6.61	112.89	120.89
15	W	44	ASN	C-N-CA	-6.61	112.89	120.89
16	V	274	GLN	N-CA-CB	6.61	122.84	112.46
14	7	38	ILE	O-C-N	6.61	127.07	121.98
4	D	8	LEU	N-CA-C	-6.61	104.53	112.59
23	P	5	ALA	CA-C-N	6.61	126.85	119.32
23	P	5	ALA	C-N-CA	6.61	126.85	119.32
29	I	76	VAL	N-CA-C	-6.61	104.05	110.72
22	S	309	PHE	CA-CB-CG	6.61	120.41	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	126	LEU	N-CA-C	-6.61	99.90	110.14
6	F	222	PHE	CA-C-O	6.60	128.29	120.70
10	3	114	SER	CA-C-O	6.60	127.07	119.35
13	m	63	ASN	CA-CB-CG	6.60	119.20	112.60
4	D	185	PRO	N-CA-CB	6.60	108.58	103.30
9	2	135	THR	N-CA-C	-6.60	104.61	114.64
25	R	326	ALA	CA-C-N	6.60	129.66	120.29
25	R	326	ALA	C-N-CA	6.60	129.66	120.29
13	m	131	TYR	N-CA-C	-6.60	98.22	109.24
15	W	141	ILE	N-CA-C	-6.60	98.23	107.80
18	X	102	GLN	OE1-CD-NE2	6.60	129.20	122.60
32	M	315	PHE	CA-CB-CG	-6.60	107.20	113.80
14	7	211	VAL	N-CA-C	6.60	117.28	110.36
32	M	391	LEU	CA-C-N	6.60	129.78	120.28
32	M	391	LEU	C-N-CA	6.60	129.78	120.28
9	i	122	HIS	ND1-CE1-NE2	6.59	114.99	108.40
2	B	141	GLU	CA-C-N	-6.59	110.51	121.92
2	B	141	GLU	C-N-CA	-6.59	110.51	121.92
13	6	155	MET	CA-C-O	-6.59	113.06	119.13
21	N	314	LEU	N-CA-C	6.59	118.55	111.36
25	R	49	PHE	CB-CA-C	-6.59	99.64	110.85
27	O	8	ASP	CA-CB-CG	-6.59	106.00	112.60
22	S	43	LYS	CA-C-N	6.59	134.13	121.54
22	S	43	LYS	C-N-CA	6.59	134.13	121.54
7	g	72	ARG	CB-CA-C	-6.59	99.58	110.72
13	6	192	VAL	O-C-N	6.59	128.26	121.87
25	R	340	GLN	CA-C-N	6.59	129.11	120.28
25	R	340	GLN	C-N-CA	6.59	129.11	120.28
8	h	91	PHE	CA-C-O	-6.59	113.56	120.55
14	n	190	LYS	CA-C-N	6.59	128.92	120.88
14	n	190	LYS	C-N-CA	6.59	128.92	120.88
5	E	97	VAL	CA-C-N	6.59	129.11	120.28
5	E	97	VAL	C-N-CA	6.59	129.11	120.28
26	U	157	LEU	N-CA-C	-6.59	100.19	110.14
14	7	248	GLU	CA-C-N	6.59	132.79	122.78
14	7	248	GLU	C-N-CA	6.59	132.79	122.78
23	P	76	ASN	N-CA-CB	6.59	119.91	110.16
10	j	184	GLY	O-C-N	6.59	128.59	122.47
7	G	71	ASP	CA-CB-CG	6.59	119.19	112.60
17	T	142	LEU	CA-C-N	6.59	130.00	120.38
17	T	142	LEU	C-N-CA	6.59	130.00	120.38
17	T	247	ASP	CA-CB-CG	-6.59	106.01	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	175	VAL	CA-C-N	6.59	129.10	120.28
24	Q	175	VAL	C-N-CA	6.59	129.10	120.28
25	R	400	TYR	CA-C-N	6.59	129.10	120.28
25	R	400	TYR	C-N-CA	6.59	129.10	120.28
28	H	174	VAL	CA-C-N	6.59	127.94	121.62
28	H	174	VAL	C-N-CA	6.59	127.94	121.62
33	J	302	PRO	CA-C-N	6.58	132.70	122.49
33	J	302	PRO	C-N-CA	6.58	132.70	122.49
4	d	80	ALA	N-CA-C	-6.58	102.56	112.04
9	i	171	TRP	CE2-CD2-CE3	6.58	125.38	118.80
21	N	222	TYR	N-CA-C	-6.58	104.87	113.17
25	R	129	GLU	N-CA-C	6.58	118.53	111.36
32	M	286	ILE	CB-CA-C	-6.58	103.62	111.65
21	N	93	GLU	N-CA-C	-6.58	105.07	113.23
27	O	175	ASN	CA-C-N	6.58	128.99	120.44
27	O	175	ASN	C-N-CA	6.58	128.99	120.44
12	5	285	VAL	CA-C-N	6.58	130.06	120.91
12	5	285	VAL	C-N-CA	6.58	130.06	120.91
24	Q	161	LEU	O-C-N	-6.58	115.15	122.12
27	O	46	THR	CA-C-N	6.58	128.99	120.44
27	O	46	THR	C-N-CA	6.58	128.99	120.44
30	K	298	GLU	CA-C-O	-6.58	113.58	120.55
23	P	43	GLU	CB-CA-C	-6.58	98.19	110.36
30	K	243	VAL	N-CA-C	6.58	118.06	109.58
14	n	198	ILE	CA-CB-CG2	6.58	121.68	110.50
25	R	294	ILE	N-CA-C	-6.58	103.83	111.00
14	7	121	GLU	O-C-N	6.57	126.55	121.88
17	T	129	LEU	N-CA-CB	6.57	120.34	110.22
23	P	210	ASN	OD1-CG-ND2	6.57	129.17	122.60
28	H	379	LEU	N-CA-C	-6.57	101.78	109.93
21	N	518	ALA	CA-C-O	6.57	127.52	120.55
2	b	139	HIS	CG-CD2-NE2	6.57	113.77	107.20
9	i	186	ASP	CA-C-N	6.57	129.62	120.29
9	i	186	ASP	C-N-CA	6.57	129.62	120.29
19	Y	53	ALA	CA-C-O	6.57	125.68	118.65
15	W	82	GLU	N-CA-C	-6.57	105.19	113.72
16	V	56	GLU	N-CA-C	-6.57	99.33	109.24
23	P	420	ASP	CA-C-N	6.57	130.29	120.31
23	P	420	ASP	C-N-CA	6.57	130.29	120.31
24	Q	296	ILE	CA-C-N	6.57	129.08	120.28
24	Q	296	ILE	C-N-CA	6.57	129.08	120.28
28	H	436	LYS	CA-C-N	6.57	129.29	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	H	436	LYS	C-N-CA	6.57	129.29	122.27
33	J	362	CYS	CA-C-O	6.57	127.38	120.42
1	A	125	SER	CA-C-N	6.56	129.08	120.28
1	A	125	SER	C-N-CA	6.56	129.08	120.28
28	H	211	VAL	N-CA-C	-6.56	98.43	107.75
9	i	232	TYR	CA-C-N	6.56	130.19	120.87
9	i	232	TYR	C-N-CA	6.56	130.19	120.87
21	N	84	ALA	N-CA-C	-6.56	105.43	113.50
32	M	43	ILE	N-CA-C	-6.56	104.09	110.72
5	E	3	LEU	CA-C-N	6.56	130.13	120.95
5	E	3	LEU	C-N-CA	6.56	130.13	120.95
22	S	484	ASP	CA-C-O	6.56	127.38	120.42
7	G	228	HIS	CE1-NE2-CD2	-6.56	102.44	109.00
33	J	98	VAL	CA-C-N	6.56	132.62	120.95
33	J	98	VAL	C-N-CA	6.56	132.62	120.95
9	2	174	ASP	CA-CB-CG	-6.56	106.04	112.60
13	6	203	HIS	CB-CG-CD2	-6.56	122.67	131.20
32	M	198	VAL	CB-CA-C	-6.56	103.17	112.22
13	6	214	ILE	N-CA-C	-6.56	98.99	108.17
12	5	249	SER	N-CA-C	-6.55	99.11	109.07
29	I	428	VAL	CA-C-O	-6.55	114.00	119.97
5	e	181	ALA	CA-C-O	6.55	127.37	120.42
2	B	205	ASN	N-CA-C	-6.55	99.62	108.86
16	V	204	HIS	CG-CD2-NE2	6.55	113.75	107.20
21	N	798	LYS	N-CA-C	6.55	118.42	111.28
25	R	383	ARG	CA-C-N	6.55	129.72	120.42
25	R	383	ARG	C-N-CA	6.55	129.72	120.42
27	O	172	TYR	CB-CG-CD1	6.55	130.63	120.80
6	f	111	LEU	N-CA-C	6.55	118.42	111.28
4	D	233	VAL	CA-C-O	-6.55	114.23	121.17
22	S	122	ASN	CA-C-N	6.55	129.59	120.29
22	S	122	ASN	C-N-CA	6.55	129.59	120.29
24	Q	91	SER	CA-C-O	-6.55	113.61	120.55
29	I	267	ILE	N-CA-CB	6.55	119.45	110.54
30	K	47	ILE	CA-C-N	6.55	128.96	120.44
30	K	47	ILE	C-N-CA	6.55	128.96	120.44
8	h	203	GLU	CA-C-N	6.55	129.59	120.29
8	h	203	GLU	C-N-CA	6.55	129.59	120.29
33	J	370	LEU	CA-C-O	6.55	127.36	120.42
5	e	236	THR	N-CA-C	-6.55	104.22	111.36
10	3	198	ARG	CA-C-O	6.55	127.18	120.24
21	N	520	GLY	CA-C-N	6.55	129.59	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	520	GLY	C-N-CA	6.55	129.59	120.29
21	N	834	GLU	O-C-N	6.55	129.06	122.12
27	O	244	ASN	CA-CB-CG	-6.55	106.05	112.60
16	V	100	ARG	N-CA-C	-6.54	104.53	113.30
22	S	334	HIS	CB-CG-CD2	-6.54	122.69	131.20
14	7	55	ILE	N-CA-C	-6.54	98.71	108.46
16	V	94	MET	CA-C-N	6.54	131.64	120.72
16	V	94	MET	C-N-CA	6.54	131.64	120.72
21	N	807	THR	N-CA-C	6.54	118.41	111.28
30	K	268	ILE	N-CA-CB	6.54	120.44	111.41
30	K	318	THR	CA-C-N	6.54	129.04	120.28
30	K	318	THR	C-N-CA	6.54	129.04	120.28
12	5	128	GLN	CA-C-N	6.54	129.28	120.65
12	5	128	GLN	C-N-CA	6.54	129.28	120.65
15	W	131	THR	N-CA-C	-6.54	104.23	111.36
22	S	483	GLU	CA-C-N	6.54	129.58	120.29
22	S	483	GLU	C-N-CA	6.54	129.58	120.29
28	H	205	ASP	CA-CB-CG	-6.54	106.06	112.60
23	P	415	TRP	CA-C-N	6.54	128.94	120.44
23	P	415	TRP	C-N-CA	6.54	128.94	120.44
6	f	71	GLY	CA-C-O	6.54	128.49	121.37
3	c	221	ASN	CA-C-N	6.53	131.42	122.34
3	c	221	ASN	C-N-CA	6.53	131.42	122.34
5	e	64	ILE	CA-C-O	-6.53	113.57	120.76
7	g	163	ALA	N-CA-C	-6.53	99.38	109.24
27	O	197	SER	N-CA-C	6.53	118.06	111.07
27	O	278	PRO	CA-C-N	6.53	129.70	120.42
27	O	278	PRO	C-N-CA	6.53	129.70	120.42
27	O	376	GLN	CA-C-O	-6.53	113.62	120.55
29	I	89	GLN	CA-C-N	6.53	129.33	120.44
29	I	89	GLN	C-N-CA	6.53	129.33	120.44
31	L	297	ALA	N-CA-CB	6.53	120.28	110.22
19	Y	88	ASN	CA-CB-CG	-6.53	106.07	112.60
11	4	40	PRO	N-CA-C	6.53	122.40	113.98
21	N	235	ALA	CA-C-N	6.53	127.18	120.00
21	N	235	ALA	C-N-CA	6.53	127.18	120.00
30	K	338	ILE	CA-C-N	6.53	130.61	120.75
30	K	338	ILE	C-N-CA	6.53	130.61	120.75
4	D	18	PHE	CA-C-O	6.53	127.68	120.63
28	H	107	LYS	CA-C-N	6.53	128.51	120.22
28	H	107	LYS	C-N-CA	6.53	128.51	120.22
19	Y	5	VAL	O-C-N	6.53	130.17	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L	268	ALA	O-C-N	6.53	128.79	122.07
2	B	238	LEU	N-CA-CB	6.53	121.06	110.42
8	1	135	ILE	O-C-N	-6.53	115.81	123.05
21	N	329	HIS	ND1-CE1-NE2	6.53	114.92	108.40
30	K	236	ARG	CA-C-N	-6.53	115.11	122.48
30	K	236	ARG	C-N-CA	-6.53	115.11	122.48
5	E	12	VAL	N-CA-C	-6.52	106.37	112.83
13	6	186	GLU	N-CA-C	6.52	118.39	111.28
21	N	494	LYS	O-C-N	6.52	126.73	121.38
31	L	164	ASP	CA-C-N	6.52	126.45	119.28
31	L	164	ASP	C-N-CA	6.52	126.45	119.28
6	F	183	ASP	CA-CB-CG	-6.52	106.08	112.60
31	L	203	ASN	CA-CB-CG	6.52	119.12	112.60
1	A	114	CYS	CA-C-N	6.52	129.31	120.38
1	A	114	CYS	C-N-CA	6.52	129.31	120.38
17	T	141	LEU	CA-C-N	6.52	131.61	120.72
17	T	141	LEU	C-N-CA	6.52	131.61	120.72
28	H	76	LEU	CA-C-N	6.52	128.99	120.26
28	H	76	LEU	C-N-CA	6.52	128.99	120.26
17	T	212	ASN	N-CA-C	-6.52	103.59	113.89
29	I	415	ASP	N-CA-CB	6.52	119.80	110.16
33	J	383	GLU	CA-C-N	6.52	129.54	120.29
33	J	383	GLU	C-N-CA	6.52	129.54	120.29
5	e	63	SER	N-CA-C	-6.51	103.94	112.41
13	m	49	PRO	N-CA-C	6.51	121.30	111.14
31	L	131	VAL	N-CA-C	-6.51	98.75	108.46
33	J	245	ILE	N-CA-CB	6.51	119.09	111.66
9	2	67	SER	O-C-N	-6.51	113.83	121.32
11	4	29	LYS	CA-C-O	6.51	127.73	120.70
29	I	192	GLN	N-CA-CB	6.51	120.40	110.70
30	K	352	ILE	CA-C-N	6.51	129.00	120.28
30	K	352	ILE	C-N-CA	6.51	129.00	120.28
9	i	65	ARG	NH1-CZ-NH2	-6.51	110.84	119.30
1	A	185	HIS	CB-CG-ND1	6.51	132.47	122.70
4	d	117	GLN	CA-C-N	6.51	129.00	120.28
4	d	117	GLN	C-N-CA	6.51	129.00	120.28
14	n	166	LEU	N-CA-C	-6.51	105.88	113.88
21	N	187	ASN	CA-C-N	6.51	129.00	120.28
21	N	187	ASN	C-N-CA	6.51	129.00	120.28
23	P	173	MET	N-CA-C	-6.51	104.11	111.07
26	U	247	ILE	CB-CA-C	-6.51	103.64	111.97
5	e	242	GLU	CA-C-O	6.50	127.44	119.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	95	SER	CA-C-O	6.50	127.52	120.43
24	Q	141	LEU	O-C-N	6.50	129.56	122.15
9	2	149	ASP	CA-C-N	6.50	131.81	122.45
9	2	149	ASP	C-N-CA	6.50	131.81	122.45
10	3	91	VAL	CA-C-N	6.50	129.32	120.54
10	3	91	VAL	C-N-CA	6.50	129.32	120.54
24	Q	10	GLU	CA-C-N	6.50	128.99	120.28
24	Q	10	GLU	C-N-CA	6.50	128.99	120.28
23	P	92	SER	CA-C-N	6.50	129.37	120.46
23	P	92	SER	C-N-CA	6.50	129.37	120.46
7	G	109	ILE	CA-C-N	6.50	126.19	119.56
7	G	109	ILE	C-N-CA	6.50	126.19	119.56
13	m	141	ARG	N-CA-C	6.50	119.14	109.59
33	J	310	ILE	N-CA-C	-6.50	98.69	108.17
18	X	36	LYS	O-C-N	6.49	127.62	121.71
18	X	72	GLU	N-CA-C	-6.49	104.02	114.09
27	O	181	PHE	N-CA-C	-6.49	103.70	111.69
33	J	205	HIS	CE1-NE2-CD2	-6.49	102.51	109.00
10	j	148	GLY	O-C-N	6.49	128.42	122.19
5	e	196	ALA	N-CA-C	-6.49	104.29	111.36
6	F	92	CYS	CA-C-N	6.49	131.71	120.68
6	F	92	CYS	C-N-CA	6.49	131.71	120.68
17	T	261	GLU	N-CA-CB	6.49	119.66	110.12
25	R	273	SER	CA-C-O	-6.49	113.61	120.23
6	f	177	ASP	N-CA-C	-6.49	105.37	113.28
21	N	314	LEU	CA-C-N	6.49	129.50	120.29
21	N	314	LEU	C-N-CA	6.49	129.50	120.29
7	g	160	TYR	N-CA-C	-6.49	98.81	108.99
29	I	193	GLU	CA-C-O	-6.49	111.60	119.32
10	3	183	TRP	CA-C-N	6.48	129.89	121.85
10	3	183	TRP	C-N-CA	6.48	129.89	121.85
17	T	170	ASN	N-CA-C	-6.48	98.67	109.24
31	L	152	THR	N-CA-C	-6.48	105.39	113.55
9	i	93	GLU	N-CA-C	6.48	118.42	111.36
20	Z	748	LEU	CB-CA-C	6.48	121.86	110.85
22	S	117	SER	N-CA-C	-6.48	104.69	112.59
29	I	299	GLU	CA-C-N	6.48	128.86	120.44
29	I	299	GLU	C-N-CA	6.48	128.86	120.44
11	k	39	SER	N-CA-C	-6.48	100.74	108.25
8	h	71	HIS	CG-CD2-NE2	6.47	113.67	107.20
11	k	172	MET	N-CA-CB	6.47	119.03	110.29
5	E	71	ASP	CA-CB-CG	-6.47	106.12	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	112	ILE	CA-C-N	6.47	130.60	121.02
10	3	112	ILE	C-N-CA	6.47	130.60	121.02
21	N	11	ALA	CA-C-N	6.47	128.96	120.28
21	N	11	ALA	C-N-CA	6.47	128.96	120.28
25	R	102	LEU	CA-C-N	6.47	128.86	120.44
25	R	102	LEU	C-N-CA	6.47	128.86	120.44
7	G	137	ILE	N-CA-CB	6.47	120.62	111.82
22	S	103	SER	N-CA-C	-6.47	103.04	111.71
29	I	285	ASP	CA-C-O	6.47	126.88	119.18
6	F	36	VAL	O-C-N	-6.47	116.21	123.20
13	m	39	THR	N-CA-CB	6.47	120.60	110.71
5	E	16	SER	O-C-N	-6.47	112.65	123.00
9	2	247	VAL	N-CA-C	-6.47	99.81	108.35
21	N	472	ASN	CA-C-N	6.47	133.89	121.54
21	N	472	ASN	C-N-CA	6.47	133.89	121.54
21	N	616	HIS	CA-CB-CG	-6.47	107.33	113.80
6	f	80	ASP	CA-C-N	6.46	128.94	120.28
6	f	80	ASP	C-N-CA	6.46	128.94	120.28
4	D	194	LEU	N-CA-C	-6.46	104.08	112.23
24	Q	101	ILE	N-CA-C	6.46	117.21	110.62
5	e	200	VAL	CA-C-O	-6.46	114.32	121.17
9	i	65	ARG	NE-CZ-NH2	6.46	125.02	119.20
23	P	214	GLU	N-CA-CB	6.46	119.62	110.12
7	G	216	ILE	N-CA-C	-6.46	98.34	108.81
2	b	179	TRP	O-C-N	-6.46	115.49	122.85
12	5	102	ALA	N-CA-C	6.46	118.12	111.14
17	T	269	SER	CA-C-N	6.46	128.70	120.56
17	T	269	SER	C-N-CA	6.46	128.70	120.56
24	Q	254	SER	N-CA-C	-6.46	105.15	113.16
26	U	14	VAL	CA-C-O	-6.46	114.23	120.95
29	I	215	PRO	N-CA-C	-6.46	102.82	110.70
30	K	163	GLU	N-CA-C	-6.46	106.36	114.56
13	m	53	ASP	CA-C-O	-6.46	113.25	120.54
3	C	244	ILE	N-CA-C	-6.46	104.56	110.82
26	U	185	GLY	O-C-N	-6.46	117.26	122.81
33	J	38	THR	CA-C-N	6.46	129.26	120.54
33	J	38	THR	C-N-CA	6.46	129.26	120.54
21	N	601	THR	CA-CB-OG1	6.46	119.28	109.60
22	S	269	GLU	N-CA-C	-6.46	104.32	111.36
16	V	120	SER	CA-C-N	6.45	129.30	120.46
16	V	120	SER	C-N-CA	6.45	129.30	120.46
26	U	43	SER	N-CA-C	-6.45	99.30	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	164	ILE	CA-C-N	6.45	129.17	120.65
8	1	164	ILE	C-N-CA	6.45	129.17	120.65
16	V	82	ALA	CA-C-N	6.45	129.75	120.98
16	V	82	ALA	C-N-CA	6.45	129.75	120.98
14	n	260	GLY	CA-C-N	6.45	132.97	122.65
14	n	260	GLY	C-N-CA	6.45	132.97	122.65
29	I	346	ARG	N-CA-CB	6.45	120.38	109.87
32	M	23	LEU	CB-CA-C	-6.45	100.71	110.90
32	M	277	ILE	N-CA-CB	6.45	120.59	111.82
25	R	34	THR	O-C-N	6.45	128.80	122.09
4	d	16	HIS	CB-CG-CD2	-6.45	122.82	131.20
30	K	220	THR	CA-C-N	6.45	128.92	120.28
30	K	220	THR	C-N-CA	6.45	128.92	120.28
21	N	99	GLU	CA-C-N	6.45	129.21	120.44
21	N	99	GLU	C-N-CA	6.45	129.21	120.44
23	P	397	ALA	N-CA-CB	6.45	121.38	110.49
30	K	89	ILE	CA-CB-CG1	6.45	121.36	110.40
2	b	90	ARG	N-CA-CB	6.44	119.70	110.16
2	b	172	LYS	CA-C-O	6.44	127.38	119.97
3	C	31	HIS	N-CA-C	-6.44	105.34	113.72
10	3	158	LEU	N-CA-CB	6.44	119.66	110.44
12	5	277	GLU	CB-CG-CD	6.44	123.56	112.60
21	N	470	LEU	CA-C-N	6.44	132.42	121.14
21	N	470	LEU	C-N-CA	6.44	132.42	121.14
3	C	193	ALA	CA-C-N	6.44	128.82	120.44
3	C	193	ALA	C-N-CA	6.44	128.82	120.44
24	Q	1	MET	CA-C-N	6.44	129.20	120.44
24	Q	1	MET	C-N-CA	6.44	129.20	120.44
26	U	301	ILE	N-CA-C	-6.44	104.21	110.72
22	S	316	LEU	N-CA-C	6.44	118.30	111.28
28	H	185	LEU	CA-C-N	6.44	126.81	119.92
28	H	185	LEU	C-N-CA	6.44	126.81	119.92
20	Z	152	GLU	N-CA-C	6.44	118.38	111.36
7	g	144	ASN	N-CA-C	-6.44	104.58	112.88
1	A	66	PRO	O-C-N	6.44	131.33	122.38
7	g	180	VAL	CA-CB-CG1	6.44	121.34	110.40
33	J	36	SER	CA-C-N	6.44	129.43	120.29
33	J	36	SER	C-N-CA	6.44	129.43	120.29
21	N	17	GLN	N-CA-C	-6.43	97.09	110.80
9	2	233	LYS	N-CA-C	-6.43	100.04	110.20
23	P	199	LEU	CA-C-O	6.43	127.24	120.42
27	O	124	ASP	N-CA-C	-6.43	103.78	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	150	ALA	N-CA-CB	-6.43	101.69	110.56
13	m	203	HIS	CE1-NE2-CD2	-6.43	102.57	109.00
9	2	119	TYR	N-CA-C	-6.43	105.44	113.28
11	4	36	ARG	O-C-N	-6.43	115.33	123.24
24	Q	255	TYR	N-CA-CB	6.43	119.39	110.07
16	V	173	THR	CB-CA-C	-6.43	99.86	110.72
25	R	46	ALA	O-C-N	6.43	129.48	122.15
27	O	103	LYS	CA-C-N	6.42	128.89	120.28
27	O	103	LYS	C-N-CA	6.42	128.89	120.28
28	H	265	ASN	CA-C-O	-6.42	114.08	120.70
19	Y	74	THR	CA-C-N	6.42	129.53	120.28
19	Y	74	THR	C-N-CA	6.42	129.53	120.28
25	R	178	GLY	CA-C-N	6.42	128.89	120.28
25	R	178	GLY	C-N-CA	6.42	128.89	120.28
5	e	67	ILE	CB-CA-C	6.42	118.87	110.91
10	3	159	GLU	CA-C-N	6.42	126.34	119.28
10	3	159	GLU	C-N-CA	6.42	126.34	119.28
18	X	50	TRP	N-CA-C	-6.42	101.02	110.52
24	Q	292	GLN	N-CA-C	-6.42	97.60	108.26
10	3	173	ASN	CA-CB-CG	-6.42	106.18	112.60
21	N	106	ILE	N-CA-C	6.42	117.20	110.72
27	O	332	ILE	O-C-N	-6.42	115.22	121.83
18	X	125	MET	CA-C-N	6.42	129.25	120.46
18	X	125	MET	C-N-CA	6.42	129.25	120.46
12	5	147	GLU	CA-C-N	6.42	129.82	120.71
12	5	147	GLU	C-N-CA	6.42	129.82	120.71
24	Q	200	ALA	CA-C-N	6.42	129.16	120.44
24	Q	200	ALA	C-N-CA	6.42	129.16	120.44
27	O	161	ASP	CA-CB-CG	-6.42	106.18	112.60
8	h	151	PHE	CA-C-N	6.41	131.30	122.77
8	h	151	PHE	C-N-CA	6.41	131.30	122.77
25	R	385	ASN	CA-CB-CG	-6.41	106.19	112.60
9	2	59	ASN	CA-CB-CG	-6.41	106.19	112.60
11	4	118	GLN	CA-C-O	6.41	127.16	120.30
22	S	218	LEU	CA-C-O	-6.41	113.76	120.55
30	K	157	SER	CA-C-N	6.41	132.31	122.25
30	K	157	SER	C-N-CA	6.41	132.31	122.25
30	K	287	GLY	O-C-N	6.41	129.03	122.24
32	M	277	ILE	CB-CA-C	-6.41	101.77	110.42
3	c	181	LYS	N-CA-C	-6.41	99.77	109.95
9	2	92	ILE	CA-C-O	-6.41	114.06	120.85
27	O	293	LEU	CA-C-N	6.41	128.86	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	293	LEU	C-N-CA	6.41	128.86	120.28
9	i	163	ALA	N-CA-CB	6.40	119.55	109.82
11	4	65	GLN	CA-C-N	6.40	128.76	120.44
11	4	65	GLN	C-N-CA	6.40	128.76	120.44
22	S	438	HIS	ND1-CE1-NE2	6.40	114.80	108.40
4	d	174	PHE	CA-C-O	-6.40	113.77	120.55
7	g	54	ILE	N-CA-CB	-6.40	103.41	111.41
6	F	69	HIS	CB-CG-CD2	-6.40	122.88	131.20
10	3	146	LEU	CA-C-N	6.40	129.15	120.38
10	3	146	LEU	C-N-CA	6.40	129.15	120.38
11	4	151	ASP	CA-CB-CG	6.40	119.00	112.60
15	W	58	ASN	CA-C-N	6.40	127.84	119.84
15	W	58	ASN	C-N-CA	6.40	127.84	119.84
23	P	51	ASP	CA-CB-CG	-6.40	106.20	112.60
31	L	435	GLN	N-CA-CB	-6.40	101.25	111.43
13	6	139	TYR	CB-CG-CD1	-6.40	111.20	120.80
8	h	85	GLU	CA-C-N	6.40	128.76	120.44
8	h	85	GLU	C-N-CA	6.40	128.76	120.44
14	7	44	VAL	CA-CB-CG2	6.40	121.28	110.40
17	T	99	SER	CA-C-N	6.40	128.85	120.28
17	T	99	SER	C-N-CA	6.40	128.85	120.28
30	K	62	THR	N-CA-C	-6.40	104.52	112.90
14	7	65	SER	O-C-N	6.40	128.66	122.07
26	U	89	LEU	N-CA-CB	6.40	119.47	109.69
15	W	72	ILE	O-C-N	6.39	128.42	121.83
21	N	398	ARG	CA-C-N	6.39	128.85	120.28
21	N	398	ARG	C-N-CA	6.39	128.85	120.28
29	I	353	PRO	N-CA-CB	6.39	108.91	103.35
10	j	149	MET	CA-C-N	6.39	128.85	120.28
10	j	149	MET	C-N-CA	6.39	128.85	120.28
28	H	435	ARG	N-CA-C	-6.39	98.98	109.40
29	I	208	TYR	N-CA-C	-6.39	105.12	113.17
32	M	86	MET	N-CA-C	-6.39	105.23	114.12
13	m	35	THR	N-CA-C	-6.39	104.74	113.30
4	D	44	LEU	N-CA-CB	6.39	120.62	110.65
7	G	108	PRO	CA-C-O	-6.39	113.90	122.08
8	1	127	SER	N-CA-C	-6.39	99.01	108.79
16	V	124	ASN	N-CA-CB	6.39	119.62	110.16
17	T	180	ILE	CA-C-N	6.39	130.02	120.31
17	T	180	ILE	C-N-CA	6.39	130.02	120.31
28	H	435	ARG	CA-C-O	6.39	127.60	120.70
30	K	179	MET	O-C-N	6.39	128.89	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	202	VAL	CA-CB-CG1	-6.39	99.54	110.40
6	F	105	VAL	N-CA-C	-6.39	104.27	110.72
31	L	213	LYS	CA-C-O	-6.39	113.53	120.17
31	L	338	LEU	N-CA-C	-6.39	104.80	112.59
11	k	36	ARG	CA-C-N	6.38	130.43	121.24
11	k	36	ARG	C-N-CA	6.38	130.43	121.24
5	E	90	GLU	CA-C-N	6.38	128.84	120.28
5	E	90	GLU	C-N-CA	6.38	128.84	120.28
23	P	394	ASN	CB-CG-OD1	6.38	133.57	120.80
24	Q	229	ASP	CA-C-N	6.38	133.76	123.93
24	Q	229	ASP	C-N-CA	6.38	133.76	123.93
4	D	117	GLN	CA-C-N	6.38	128.83	120.28
4	D	117	GLN	C-N-CA	6.38	128.83	120.28
12	5	256	THR	N-CA-C	-6.38	100.76	109.95
21	N	12	LEU	CA-C-N	6.38	128.83	120.28
21	N	12	LEU	C-N-CA	6.38	128.83	120.28
22	S	387	VAL	N-CA-CB	6.38	118.02	110.55
23	P	300	VAL	CA-C-N	6.38	129.47	120.28
23	P	300	VAL	C-N-CA	6.38	129.47	120.28
30	K	74	HIS	CE1-NE2-CD2	-6.38	102.62	109.00
15	W	96	LEU	CA-C-N	6.38	128.73	120.44
15	W	96	LEU	C-N-CA	6.38	128.73	120.44
21	N	75	TYR	CA-C-N	6.38	128.73	120.44
21	N	75	TYR	C-N-CA	6.38	128.73	120.44
11	4	34	LYS	N-CA-C	-6.38	102.72	112.99
31	L	176	GLY	O-C-N	-6.38	115.39	122.47
17	T	210	PHE	N-CA-C	6.37	118.37	110.91
21	N	314	LEU	CA-C-O	6.37	127.18	120.42
27	O	75	GLN	CA-C-N	6.37	129.34	120.29
27	O	75	GLN	C-N-CA	6.37	129.34	120.29
14	n	54	ILE	CB-CA-C	-6.37	101.13	110.62
5	E	50	VAL	N-CA-C	-6.37	99.94	108.35
1	A	70	SER	N-CA-CB	6.37	121.24	111.56
21	N	36	TRP	N-CA-C	6.37	118.22	111.28
1	a	126	GLN	CA-C-O	6.37	127.30	120.55
4	d	169	LYS	N-CA-C	-6.37	104.42	111.36
18	X	116	ALA	N-CA-CB	6.37	121.25	110.49
30	K	142	HIS	CA-C-O	6.37	127.77	120.00
2	b	139	HIS	ND1-CE1-NE2	6.36	114.76	108.40
4	d	85	LEU	CB-CA-C	-6.36	98.45	110.67
16	V	300	VAL	CA-C-N	6.36	128.81	120.28
16	V	300	VAL	C-N-CA	6.36	128.81	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	132	PHE	CA-C-N	6.36	129.09	120.44
24	Q	132	PHE	C-N-CA	6.36	129.09	120.44
24	Q	379	GLN	N-CA-C	6.36	118.22	111.28
31	L	299	ARG	NE-CZ-NH2	-6.36	113.47	119.20
21	N	761	ILE	O-C-N	-6.36	116.56	123.18
24	Q	148	LYS	N-CA-C	-6.36	105.52	113.28
18	X	92	SER	N-CA-CB	6.36	121.03	110.85
7	g	151	LEU	CA-C-N	6.36	131.20	121.03
7	g	151	LEU	C-N-CA	6.36	131.20	121.03
2	B	234	ARG	CA-C-O	6.36	126.14	119.14
10	3	200	LEU	O-C-N	6.36	130.06	122.94
22	S	388	ILE	CA-C-N	6.36	129.12	120.54
22	S	388	ILE	C-N-CA	6.36	129.12	120.54
24	Q	145	HIS	CA-CB-CG	-6.36	107.44	113.80
31	L	369	LYS	N-CA-C	-6.36	99.33	109.76
1	A	146	VAL	N-CA-C	-6.36	98.31	107.78
12	l	286	ILE	CA-CB-CG1	6.35	121.20	110.40
2	B	29	LYS	CA-C-N	6.35	132.51	122.60
2	B	29	LYS	C-N-CA	6.35	132.51	122.60
9	2	248	ASN	CA-C-O	6.35	127.07	120.40
14	7	179	PHE	CA-CB-CG	-6.35	107.45	113.80
12	l	105	THR	N-CA-CB	6.35	121.22	110.49
9	2	90	SER	CA-C-N	6.35	129.31	120.29
9	2	90	SER	C-N-CA	6.35	129.31	120.29
21	N	186	ILE	CA-C-N	6.35	128.69	120.44
21	N	186	ILE	C-N-CA	6.35	128.69	120.44
21	N	466	LEU	CA-C-N	6.35	129.42	120.28
21	N	466	LEU	C-N-CA	6.35	129.42	120.28
22	S	49	ASP	CA-C-O	-6.35	112.69	118.79
11	k	147	HIS	CE1-NE2-CD2	-6.35	102.65	109.00
3	C	108	VAL	CA-C-N	6.35	128.69	120.44
3	C	108	VAL	C-N-CA	6.35	128.69	120.44
5	E	67	ILE	N-CA-C	-6.35	99.44	108.58
19	Y	56	GLN	OE1-CD-NE2	-6.35	116.25	122.60
21	N	109	TYR	CA-C-N	6.35	129.15	120.46
21	N	109	TYR	C-N-CA	6.35	129.15	120.46
10	j	91	VAL	N-CA-C	-6.34	104.15	110.62
7	g	23	GLN	CA-C-N	6.34	129.15	120.46
7	g	23	GLN	C-N-CA	6.34	129.15	120.46
7	g	130	ARG	N-CA-C	-6.34	100.75	110.32
7	g	229	LYS	N-CA-C	-6.34	99.77	109.41
14	n	141	ASN	CA-CB-CG	6.34	118.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	238	GLN	CA-C-N	6.34	128.78	120.28
17	T	238	GLN	C-N-CA	6.34	128.78	120.28
23	P	376	THR	CA-C-O	-6.34	113.83	120.55
31	L	288	GLY	CA-C-N	6.34	133.65	121.54
31	L	288	GLY	C-N-CA	6.34	133.65	121.54
17	T	128	TYR	CA-C-N	6.34	129.41	120.28
17	T	128	TYR	C-N-CA	6.34	129.41	120.28
1	A	174	LYS	CA-C-N	6.34	131.30	120.72
1	A	174	LYS	C-N-CA	6.34	131.30	120.72
12	5	193	ASP	CA-CB-CG	-6.33	106.27	112.60
4	D	12	SER	CA-C-N	6.33	126.88	120.04
4	D	12	SER	C-N-CA	6.33	126.88	120.04
6	F	120	THR	CA-C-O	6.33	125.87	118.90
7	G	91	ARG	NE-CZ-NH1	6.33	127.83	121.50
22	S	337	ASN	N-CA-C	-6.33	103.90	112.26
33	J	306	ARG	CA-C-N	6.33	126.71	119.93
33	J	306	ARG	C-N-CA	6.33	126.71	119.93
7	G	171	SER	CB-CA-C	-6.33	100.09	110.85
21	N	338	PHE	CA-C-N	6.33	128.76	120.28
21	N	338	PHE	C-N-CA	6.33	128.76	120.28
22	S	63	LEU	CA-C-N	6.33	129.01	120.65
22	S	63	LEU	C-N-CA	6.33	129.01	120.65
24	Q	234	THR	O-C-N	-6.33	115.41	122.12
28	H	452	SER	CA-C-N	6.33	126.97	120.00
28	H	452	SER	C-N-CA	6.33	126.97	120.00
31	L	80	ASN	OD1-CG-ND2	6.33	128.93	122.60
25	R	370	LYS	CA-C-N	6.33	131.44	120.68
25	R	370	LYS	C-N-CA	6.33	131.44	120.68
29	I	285	ASP	CA-CB-CG	6.33	118.93	112.60
11	4	53	THR	N-CA-C	6.33	118.18	111.28
13	6	194	ASP	O-C-N	-6.33	115.55	122.07
7	g	105	THR	CA-C-N	6.33	126.28	119.76
7	g	105	THR	C-N-CA	6.33	126.28	119.76
33	J	16	GLU	N-CA-C	-6.33	103.91	112.26
3	c	14	SER	CA-C-O	-6.33	115.45	121.08
6	F	164	ARG	CA-C-N	6.33	129.93	120.31
6	F	164	ARG	C-N-CA	6.33	129.93	120.31
14	7	90	ILE	O-C-N	6.33	128.01	121.87
24	Q	116	PHE	CA-CB-CG	6.33	120.13	113.80
32	M	34	ALA	N-CA-C	6.33	118.98	111.71
8	h	178	SER	O-C-N	-6.32	115.78	123.30
5	E	98	THR	CA-C-N	6.32	129.27	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	98	THR	C-N-CA	6.32	129.27	120.29
10	3	111	GLY	CA-C-O	-6.32	114.97	121.61
1	a	106	TYR	CB-CG-CD1	6.32	130.28	120.80
7	g	165	THR	N-CA-C	-6.32	99.37	108.60
12	l	119	THR	N-CA-CB	6.32	120.69	110.77
10	3	77	LYS	N-CA-C	6.32	117.96	111.14
12	5	264	GLY	O-C-N	6.32	129.18	122.86
23	P	316	LYS	CA-C-N	6.32	129.07	120.54
23	P	316	LYS	C-N-CA	6.32	129.07	120.54
33	J	111	GLN	CA-C-N	6.32	129.80	120.95
33	J	111	GLN	C-N-CA	6.32	129.80	120.95
7	g	153	PRO	N-CA-C	-6.32	105.74	114.27
13	m	107	GLY	N-CA-C	-6.32	104.85	112.49
10	3	102	PRO	N-CA-C	-6.32	101.97	111.57
23	P	378	THR	O-C-N	6.32	128.58	122.07
27	O	257	ALA	CA-C-N	6.32	128.74	120.28
27	O	257	ALA	C-N-CA	6.32	128.74	120.28
4	d	56	ASP	CA-CB-CG	-6.31	106.29	112.60
32	M	187	ASP	N-CA-CB	6.31	119.40	110.12
33	J	23	PHE	O-C-N	6.31	128.81	122.12
30	K	160	VAL	CA-C-N	6.31	133.59	121.54
30	K	160	VAL	C-N-CA	6.31	133.59	121.54
6	f	181	LYS	N-CA-CB	-6.31	101.30	110.70
16	V	64	ASN	CA-CB-CG	-6.31	106.29	112.60
22	S	404	LEU	CA-C-N	6.31	130.28	120.82
22	S	404	LEU	C-N-CA	6.31	130.28	120.82
24	Q	5	GLY	CA-C-N	6.31	128.74	120.28
24	Q	5	GLY	C-N-CA	6.31	128.74	120.28
29	I	190	GLN	N-CA-C	-6.31	104.89	112.59
31	L	131	VAL	CA-C-O	6.31	127.74	120.67
10	3	44	PHE	CA-CB-CG	-6.31	107.49	113.80
15	W	95	GLN	OE1-CD-NE2	6.31	128.91	122.60
25	R	317	ILE	CA-C-O	-6.31	111.50	119.95
27	O	236	HIS	CE1-NE2-CD2	-6.31	102.69	109.00
7	g	230	PHE	O-C-N	-6.31	115.85	123.10
8	1	143	ILE	CA-C-N	6.31	130.28	120.82
8	1	143	ILE	C-N-CA	6.31	130.28	120.82
18	X	89	LEU	CA-C-N	6.31	130.38	122.43
18	X	89	LEU	C-N-CA	6.31	130.38	122.43
29	I	172	LYS	N-CA-CB	6.31	119.58	110.06
14	n	161	ARG	CA-C-N	6.30	132.40	122.94
14	n	161	ARG	C-N-CA	6.30	132.40	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	4	147	HIS	CA-CB-CG	6.30	120.11	113.80
14	7	184	ALA	CA-C-N	6.30	130.30	120.97
14	7	184	ALA	C-N-CA	6.30	130.30	120.97
4	D	96	HIS	CB-CG-ND1	6.30	132.15	122.70
31	L	256	ILE	N-CA-C	-6.30	99.39	108.53
10	3	186	VAL	CA-C-O	-6.30	113.62	120.67
21	N	625	LEU	CA-C-O	-6.30	113.87	120.55
33	J	270	ARG	CA-C-N	6.30	128.63	120.44
33	J	270	ARG	C-N-CA	6.30	128.63	120.44
12	5	196	ARG	N-CA-C	-6.30	97.54	108.69
11	k	125	LYS	O-C-N	-6.30	115.58	123.01
17	T	222	LEU	CB-CA-C	-6.30	100.34	110.79
23	P	246	GLN	CG-CD-NE2	-6.30	106.95	116.40
27	O	33	TYR	N-CA-C	6.30	118.14	111.28
13	6	16	ASN	CA-CB-CG	-6.29	106.31	112.60
17	T	129	LEU	CB-CA-C	-6.29	98.99	110.63
23	P	289	ASN	CA-C-N	6.29	129.88	120.31
23	P	289	ASN	C-N-CA	6.29	129.88	120.31
4	D	139	ASP	CA-CB-CG	6.29	118.89	112.60
14	7	78	VAL	N-CA-CB	6.29	120.38	111.82
22	S	76	PHE	CA-CB-CG	6.29	120.09	113.80
31	L	168	TYR	N-CA-CB	6.29	120.65	110.40
2	b	244	ASN	O-C-N	-6.29	114.53	122.27
7	G	182	HIS	N-CA-CB	6.29	119.19	110.07
12	5	87	ILE	N-CA-C	-6.29	99.14	108.45
3	C	61	THR	N-CA-C	-6.29	105.92	113.97
21	N	138	GLU	CB-CG-CD	-6.29	101.91	112.60
23	P	13	TYR	CA-C-N	6.29	128.61	120.44
23	P	13	TYR	C-N-CA	6.29	128.61	120.44
26	U	215	ILE	CA-C-O	6.29	126.14	119.91
2	b	96	SER	O-C-N	-6.29	114.05	122.22
2	b	128	ARG	CA-C-O	-6.29	114.72	120.50
5	e	155	LEU	N-CA-C	-6.29	97.56	108.69
6	f	182	ILE	N-CA-C	-6.29	98.69	107.80
12	l	118	GLY	N-CA-C	-6.29	101.28	110.90
12	5	153	ALA	CA-C-N	6.29	129.53	120.79
12	5	153	ALA	C-N-CA	6.29	129.53	120.79
12	5	266	HIS	ND1-CE1-NE2	6.29	114.69	108.40
27	O	209	GLU	CA-C-N	6.29	129.22	120.29
27	O	209	GLU	C-N-CA	6.29	129.22	120.29
12	l	202	PHE	CA-CB-CG	-6.28	107.52	113.80
3	C	222	ASP	N-CA-CB	6.28	121.11	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	4	171	ARG	NE-CZ-NH2	-6.28	113.55	119.20
21	N	702	ALA	CB-CA-C	-6.28	100.17	110.85
28	H	453	GLY	CA-C-N	6.28	128.99	120.44
28	H	453	GLY	C-N-CA	6.28	128.99	120.44
29	I	373	GLU	CA-C-N	6.28	128.61	120.44
29	I	373	GLU	C-N-CA	6.28	128.61	120.44
27	O	236	HIS	CB-CA-C	6.28	117.41	108.68
33	J	257	ARG	CD-NE-CZ	-6.28	115.61	124.40
23	P	349	ASN	CA-C-O	-6.28	113.85	120.63
26	U	84	ASN	O-C-N	-6.28	115.73	123.33
28	H	303	ALA	N-CA-CB	6.28	121.10	110.49
6	f	15	PRO	N-CA-C	-6.28	106.64	114.68
12	l	91	VAL	N-CA-CB	6.28	121.71	112.35
3	C	112	VAL	N-CA-C	-6.28	104.38	110.72
18	X	87	PHE	CA-CB-CG	6.28	120.08	113.80
7	g	238	GLU	CA-C-N	6.28	128.98	120.44
7	g	238	GLU	C-N-CA	6.28	128.98	120.44
18	X	128	VAL	N-CA-C	-6.28	104.22	110.62
5	e	120	ALA	CA-C-O	-6.28	113.90	120.55
6	f	57	SER	N-CA-C	-6.28	101.23	110.52
6	F	94	TYR	N-CA-C	6.28	118.93	111.71
21	N	673	PRO	CB-CA-C	-6.28	102.52	111.68
25	R	32	LEU	N-CA-CB	-6.28	100.89	110.12
4	D	160	SER	CA-C-O	6.27	127.26	120.55
9	2	106	VAL	CA-C-N	6.27	129.20	120.29
9	2	106	VAL	C-N-CA	6.27	129.20	120.29
2	b	68	THR	CA-CB-OG1	6.27	119.01	109.60
6	F	93	ASN	OD1-CG-ND2	-6.27	116.33	122.60
11	4	61	GLN	N-CA-CB	6.27	119.34	110.12
21	N	729	SER	CA-C-O	-6.27	114.24	120.70
3	c	97	ASN	CA-C-N	6.27	128.59	120.44
3	c	97	ASN	C-N-CA	6.27	128.59	120.44
31	L	364	HIS	N-CA-CB	6.27	120.94	110.41
20	Z	254	PRO	CA-C-N	6.27	132.64	122.67
20	Z	254	PRO	C-N-CA	6.27	132.64	122.67
22	S	464	ARG	CG-CD-NE	-6.27	98.20	112.00
27	O	217	LEU	N-CA-C	6.27	118.11	111.28
31	L	404	ARG	NE-CZ-NH1	6.27	127.77	121.50
32	M	410	VAL	CA-C-O	6.27	127.38	120.48
10	j	95	LEU	CA-C-N	6.27	131.19	120.72
10	j	95	LEU	C-N-CA	6.27	131.19	120.72
10	j	180	LEU	N-CA-C	-6.27	105.21	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	58	LEU	N-CA-C	-6.27	105.63	113.28
7	G	235	LEU	CA-C-N	6.27	128.96	120.44
7	G	235	LEU	C-N-CA	6.27	128.96	120.44
33	J	120	TYR	N-CA-CB	6.27	121.08	110.49
12	I	225	VAL	CA-C-N	6.27	129.19	120.29
12	I	225	VAL	C-N-CA	6.27	129.19	120.29
21	N	207	LEU	N-CA-C	6.27	117.78	111.07
5	e	58	LEU	O-C-N	6.26	128.86	122.09
27	O	133	ILE	N-CA-CB	6.26	119.98	110.58
31	L	150	ILE	N-CA-C	-6.26	106.22	112.17
33	J	19	ILE	N-CA-C	-6.26	106.63	112.83
5	e	70	ILE	CB-CA-C	-6.26	104.05	111.94
15	W	34	GLU	N-CA-CB	6.26	119.43	110.16
21	N	170	LEU	CA-C-O	-6.26	113.78	120.42
3	C	157	TYR	CB-CG-CD2	-6.26	111.41	120.80
5	E	184	LEU	CA-C-O	-6.26	113.03	120.10
23	P	70	ASN	CA-C-N	6.26	132.10	121.14
23	P	70	ASN	C-N-CA	6.26	132.10	121.14
27	O	124	ASP	CA-C-N	6.26	126.89	120.00
27	O	124	ASP	C-N-CA	6.26	126.89	120.00
27	O	152	ASP	CA-C-N	6.26	128.67	120.28
27	O	152	ASP	C-N-CA	6.26	128.67	120.28
31	L	375	ASP	O-C-N	6.26	129.25	122.05
32	M	288	THR	N-CA-CB	6.26	119.18	109.85
32	M	77	TYR	N-CA-CB	6.26	123.16	111.52
13	6	70	ASP	N-CA-C	-6.26	105.47	113.23
21	N	664	LEU	N-CA-C	-6.26	105.50	112.57
27	O	328	VAL	N-CA-C	-6.26	104.24	110.62
6	F	112	LEU	CA-C-N	6.25	128.57	120.44
6	F	112	LEU	C-N-CA	6.25	128.57	120.44
20	Z	741	LEU	CA-C-N	6.25	126.92	119.98
20	Z	741	LEU	C-N-CA	6.25	126.92	119.98
29	I	385	ASP	O-C-N	-6.25	115.01	123.14
6	f	47	VAL	O-C-N	-6.25	116.97	123.03
3	C	15	PRO	O-C-N	6.25	130.62	122.24
27	O	202	SER	N-CA-C	-6.25	98.34	108.41
3	c	203	SER	CA-C-N	6.25	130.60	120.60
3	c	203	SER	C-N-CA	6.25	130.60	120.60
5	E	241	LYS	N-CA-C	6.25	119.07	111.82
15	W	163	ASN	N-CA-C	-6.25	101.00	108.25
31	L	427	LYS	CA-C-N	6.25	129.17	120.29
31	L	427	LYS	C-N-CA	6.25	129.17	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	184	PRO	N-CA-CB	6.25	109.14	103.08
7	g	144	ASN	OD1-CG-ND2	6.25	128.85	122.60
22	S	33	GLU	CA-C-N	6.25	128.56	120.44
22	S	33	GLU	C-N-CA	6.25	128.56	120.44
27	O	19	ASP	CA-C-N	6.25	126.15	119.28
27	O	19	ASP	C-N-CA	6.25	126.15	119.28
29	I	414	GLU	N-CA-CB	6.25	119.41	110.16
2	B	78	MET	CA-C-N	6.25	131.68	121.87
2	B	78	MET	C-N-CA	6.25	131.68	121.87
21	N	676	ALA	CA-C-N	6.25	129.16	120.29
21	N	676	ALA	C-N-CA	6.25	129.16	120.29
23	P	400	VAL	N-CA-C	-6.25	98.63	107.75
12	5	104	GLN	N-CA-C	-6.25	103.11	112.54
24	Q	292	GLN	OE1-CD-NE2	6.25	128.84	122.60
32	M	64	ASP	CA-CB-CG	6.25	118.84	112.60
6	f	152	ASN	N-CA-C	-6.24	99.52	109.76
11	k	7	ILE	N-CA-C	-6.24	99.72	108.27
11	k	184	VAL	N-CA-C	-6.24	98.63	107.75
22	S	88	PHE	CA-CB-CG	6.24	120.04	113.80
20	Z	250	VAL	CA-C-O	-6.24	114.23	120.85
23	P	238	ALA	CA-C-O	-6.24	113.80	120.42
29	I	335	ASP	CA-C-N	6.24	126.36	119.87
29	I	335	ASP	C-N-CA	6.24	126.36	119.87
24	Q	80	HIS	CE1-NE2-CD2	-6.24	102.76	109.00
32	M	127	VAL	N-CA-CB	6.24	121.69	111.58
7	g	96	ALA	CA-C-N	6.24	128.64	120.28
7	g	96	ALA	C-N-CA	6.24	128.64	120.28
21	N	510	HIS	CE1-NE2-CD2	-6.24	102.76	109.00
22	S	271	ARG	N-CA-C	6.24	117.75	111.07
28	H	194	SER	CB-CA-C	-6.24	98.00	110.42
33	J	306	ARG	CA-C-O	-6.24	114.01	120.87
6	F	203	ASP	CA-CB-CG	-6.24	106.36	112.60
15	W	81	ILE	N-CA-C	-6.24	106.91	112.90
21	N	565	ASN	CA-C-N	6.24	128.64	120.28
21	N	565	ASN	C-N-CA	6.24	128.64	120.28
25	R	331	ARG	N-CA-C	6.24	118.08	111.28
27	O	175	ASN	N-CA-CB	6.24	119.39	110.16
1	a	244	ARG	NE-CZ-NH2	-6.24	113.59	119.20
21	N	295	THR	CA-C-N	6.24	129.14	120.29
21	N	295	THR	C-N-CA	6.24	129.14	120.29
24	Q	112	ASP	N-CA-CB	6.24	120.32	109.72
24	Q	330	LEU	CA-C-N	6.24	128.96	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	330	LEU	C-N-CA	6.24	128.96	120.54
29	I	126	PRO	N-CD-CG	6.24	112.55	103.20
4	D	150	THR	N-CA-C	-6.23	100.00	109.85
15	W	9	VAL	N-CA-C	-6.23	98.65	107.75
26	U	145	ASP	CA-CB-CG	-6.23	106.37	112.60
26	U	272	GLU	CA-C-N	6.23	128.54	120.44
26	U	272	GLU	C-N-CA	6.23	128.54	120.44
27	O	296	LEU	CA-C-N	6.23	130.52	120.30
27	O	296	LEU	C-N-CA	6.23	130.52	120.30
3	C	202	ASP	N-CA-C	-6.23	105.43	113.16
6	F	185	ASN	OD1-CG-ND2	6.23	128.83	122.60
12	l	119	THR	CA-C-N	6.23	130.71	122.42
12	l	119	THR	C-N-CA	6.23	130.71	122.42
1	A	172	GLY	CA-C-N	6.23	125.80	119.19
1	A	172	GLY	C-N-CA	6.23	125.80	119.19
21	N	169	ALA	N-CA-C	6.23	117.74	111.07
21	N	234	ASP	CA-CB-CG	6.23	118.83	112.60
32	M	138	ASP	N-CA-C	-6.23	105.50	113.23
32	M	416	VAL	CA-C-O	-6.23	113.74	120.47
4	D	135	ILE	N-CA-C	-6.23	99.39	108.11
16	V	281	SER	CA-C-N	6.23	128.95	120.54
16	V	281	SER	C-N-CA	6.23	128.95	120.54
17	T	58	THR	CA-C-N	6.23	128.63	120.28
17	T	58	THR	C-N-CA	6.23	128.63	120.28
21	N	147	ALA	O-C-N	6.23	130.78	122.43
1	a	134	MET	CG-SD-CE	-6.23	87.20	100.90
1	A	96	ARG	NE-CZ-NH1	6.23	127.73	121.50
6	F	80	ASP	N-CA-C	-6.23	104.38	112.23
29	I	364	ILE	O-C-N	6.23	128.24	121.83
10	j	81	ALA	CA-C-N	6.22	130.25	121.66
10	j	81	ALA	C-N-CA	6.22	130.25	121.66
14	n	113	LEU	CA-C-O	6.22	126.59	119.18
21	N	439	VAL	CB-CA-C	-6.22	103.74	112.14
29	I	428	VAL	N-CA-C	-6.22	106.70	112.43
8	h	87	ALA	CA-C-N	6.22	128.62	120.28
8	h	87	ALA	C-N-CA	6.22	128.62	120.28
4	D	104	VAL	CB-CA-C	-6.22	101.93	111.08
11	4	76	SER	O-C-N	-6.22	114.89	121.30
21	N	451	GLY	O-C-N	6.22	128.15	122.18
32	M	344	ASP	CA-CB-CG	6.22	118.82	112.60
1	a	169	THR	CA-C-N	6.22	132.31	122.36
1	a	169	THR	C-N-CA	6.22	132.31	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	W	156	GLU	N-CA-C	6.22	119.03	111.82
19	Y	60	TRP	N-CA-C	-6.22	99.87	109.14
22	S	374	ASP	CA-CB-CG	-6.22	106.38	112.60
24	Q	14	LEU	CA-C-N	6.22	128.52	120.56
24	Q	14	LEU	C-N-CA	6.22	128.52	120.56
27	O	38	TRP	CB-CG-CD2	-6.22	118.09	126.80
12	l	236	ILE	O-C-N	-6.22	115.43	121.83
3	C	212	GLU	N-CA-C	-6.22	99.58	109.59
5	E	188	HIS	CE1-NE2-CD2	-6.22	102.78	109.00
4	d	127	ARG	CA-C-N	6.22	126.57	119.92
4	d	127	ARG	C-N-CA	6.22	126.57	119.92
4	d	205	THR	CA-CB-OG1	6.22	118.93	109.60
3	C	170	SER	O-C-N	6.22	128.71	122.12
25	R	287	GLN	N-CA-C	6.22	118.85	111.33
33	J	284	THR	CA-C-N	6.22	133.41	121.54
33	J	284	THR	C-N-CA	6.22	133.41	121.54
4	D	68	ASP	N-CA-C	-6.21	100.04	108.24
4	D	179	TYR	N-CA-C	-6.21	99.78	109.72
9	2	88	ILE	CA-C-N	6.21	126.84	119.94
9	2	88	ILE	C-N-CA	6.21	126.84	119.94
17	T	252	GLU	N-CA-C	-6.21	106.33	114.04
22	S	99	ASN	OD1-CG-ND2	-6.21	116.39	122.60
23	P	402	PHE	CA-C-O	-6.21	113.61	120.38
3	c	217	ARG	NH1-CZ-NH2	6.21	127.38	119.30
4	D	191	CYS	CA-C-N	6.21	128.97	120.46
4	D	191	CYS	C-N-CA	6.21	128.97	120.46
10	3	172	LEU	O-C-N	-6.21	115.63	122.09
13	6	206	VAL	N-CA-C	-6.21	99.17	108.12
3	C	125	HIS	CE1-NE2-CD2	-6.21	102.79	109.00
4	D	235	GLN	CA-C-N	6.21	128.97	120.46
4	D	235	GLN	C-N-CA	6.21	128.97	120.46
22	S	52	TYR	N-CA-CB	6.21	119.35	110.16
25	R	415	GLN	N-CA-CB	6.21	119.25	110.12
4	d	158	SER	N-CA-C	-6.21	100.80	110.42
11	k	76	SER	CA-C-N	6.21	126.67	119.47
11	k	76	SER	C-N-CA	6.21	126.67	119.47
14	n	102	ASP	N-CA-CB	6.21	119.34	110.16
10	3	7	ILE	N-CA-C	-6.21	104.45	110.72
31	L	106	GLY	O-C-N	6.20	130.76	122.70
20	Z	247	GLN	CA-CB-CG	6.20	126.50	114.10
21	N	365	PHE	CA-C-N	6.20	128.59	120.28
21	N	365	PHE	C-N-CA	6.20	128.59	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	311	GLU	CA-C-O	6.20	127.12	120.55
28	H	188	PRO	CA-C-O	-6.20	111.57	120.56
5	e	15	PHE	CA-CB-CG	-6.20	107.60	113.80
21	N	57	ASP	CA-C-N	6.20	128.59	120.28
21	N	57	ASP	C-N-CA	6.20	128.59	120.28
26	U	226	LEU	CA-C-N	6.20	126.86	119.98
26	U	226	LEU	C-N-CA	6.20	126.86	119.98
32	M	241	ALA	N-CA-C	-6.20	98.50	108.55
9	i	251	ASP	N-CA-CB	6.20	119.12	110.26
4	D	198	SER	CA-C-N	6.20	129.09	120.29
4	D	198	SER	C-N-CA	6.20	129.09	120.29
8	l	197	PHE	CA-C-O	6.20	127.20	120.32
17	T	62	LEU	CA-C-N	6.20	128.50	120.44
17	T	62	LEU	C-N-CA	6.20	128.50	120.44
21	N	582	ASP	CA-C-N	6.20	129.22	120.42
21	N	582	ASP	C-N-CA	6.20	129.22	120.42
31	L	131	VAL	N-CA-CB	6.20	121.61	111.44
31	L	145	ARG	CA-C-O	6.20	127.94	120.81
32	M	180	TYR	N-CA-C	-6.20	104.88	112.88
33	J	72	VAL	CB-CA-C	-6.20	101.97	110.77
33	J	257	ARG	N-CA-C	-6.20	105.76	113.38
7	G	22	PHE	CA-C-N	6.20	131.04	121.19
7	G	22	PHE	C-N-CA	6.20	131.04	121.19
6	f	87	TYR	O-C-N	-6.20	115.69	122.07
2	B	216	ASP	CA-CB-CG	-6.20	106.40	112.60
17	T	53	ASN	CA-C-O	6.20	126.99	120.42
11	k	128	LEU	CA-C-O	-6.19	114.64	120.34
14	n	223	ARG	NH1-CZ-NH2	-6.19	111.25	119.30
27	O	358	ILE	N-CA-C	-6.19	98.60	107.77
9	i	81	THR	N-CA-CB	6.19	119.17	110.07
10	j	88	THR	CA-C-N	6.19	128.58	120.28
10	j	88	THR	C-N-CA	6.19	128.58	120.28
26	U	298	ASN	OD1-CG-ND2	-6.19	116.41	122.60
28	H	429	PHE	N-CA-C	-6.19	105.21	112.89
24	Q	113	ASP	CA-C-N	6.19	128.90	120.54
24	Q	113	ASP	C-N-CA	6.19	128.90	120.54
27	O	47	LYS	CA-C-N	6.19	128.57	120.28
27	O	47	LYS	C-N-CA	6.19	128.57	120.28
5	E	157	HIS	N-CA-CB	6.19	120.30	110.65
16	V	269	ARG	NE-CZ-NH2	-6.19	113.63	119.20
17	T	102	LYS	N-CA-C	6.19	118.02	111.28
21	N	477	SER	N-CA-C	-6.19	105.69	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	74	ASN	CA-C-N	6.19	128.57	120.28
27	O	74	ASN	C-N-CA	6.19	128.57	120.28
7	g	90	ASN	CA-C-N	6.18	129.19	120.28
7	g	90	ASN	C-N-CA	6.18	129.19	120.28
21	N	425	ASN	OD1-CG-ND2	6.18	128.78	122.60
26	U	192	ASN	CA-C-N	6.18	128.57	120.28
26	U	192	ASN	C-N-CA	6.18	128.57	120.28
1	a	141	LEU	N-CA-CB	6.18	120.64	110.69
21	N	72	LEU	CA-C-O	-6.18	114.33	120.70
21	N	568	VAL	N-CA-C	-6.18	104.26	111.00
18	X	28	PRO	O-C-N	6.18	130.39	122.85
27	O	251	LEU	CA-C-N	6.18	129.71	120.31
27	O	251	LEU	C-N-CA	6.18	129.71	120.31
31	L	364	HIS	CG-CD2-NE2	6.18	113.38	107.20
5	e	226	ASP	N-CA-CB	6.18	119.14	110.98
9	2	143	HIS	N-CA-C	-6.18	100.36	109.81
10	3	68	ARG	CA-C-N	6.18	128.56	120.28
10	3	68	ARG	C-N-CA	6.18	128.56	120.28
13	6	123	ASP	CA-C-N	6.18	133.41	121.18
13	6	123	ASP	C-N-CA	6.18	133.41	121.18
22	S	177	ASN	O-C-N	6.18	128.67	122.12
27	O	120	LYS	N-CA-CB	6.18	120.94	110.49
30	K	127	ASP	CA-CB-CG	-6.18	106.42	112.60
4	d	34	VAL	O-C-N	-6.18	116.51	123.18
28	H	358	PRO	N-CA-C	-6.18	106.77	114.68
5	e	188	HIS	CE1-NE2-CD2	-6.18	102.82	109.00
31	L	301	ILE	CA-C-N	6.18	128.56	120.28
31	L	301	ILE	C-N-CA	6.18	128.56	120.28
1	a	15	HIS	CA-C-N	6.17	130.60	122.51
1	a	15	HIS	C-N-CA	6.17	130.60	122.51
3	c	209	ASP	CA-CB-CG	6.17	118.77	112.60
21	N	582	ASP	N-CA-CB	6.17	119.73	110.22
30	K	35	ASN	OD1-CG-ND2	6.17	128.77	122.60
30	K	242	PHE	N-CA-C	-6.17	104.35	113.61
30	K	375	ASN	CB-CG-OD1	6.17	133.15	120.80
2	B	225	THR	CA-C-O	-6.17	114.60	121.51
21	N	607	GLN	CA-C-N	6.17	128.47	120.44
21	N	607	GLN	C-N-CA	6.17	128.47	120.44
2	b	172	LYS	N-CA-C	6.17	118.98	111.82
10	j	155	GLU	O-C-N	-6.17	114.51	121.79
9	2	130	ALA	N-CA-C	-6.17	99.85	109.72
19	Y	32	ASP	CA-CB-CG	-6.17	106.43	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	373	GLU	CA-C-N	6.17	128.46	120.44
23	P	373	GLU	C-N-CA	6.17	128.46	120.44
4	d	162	GLN	CG-CD-NE2	-6.17	107.14	116.40
9	i	92	ILE	CA-C-O	-6.17	113.59	120.25
11	k	23	ARG	N-CA-C	-6.17	98.22	108.34
21	N	701	VAL	N-CA-C	6.17	116.95	110.72
26	U	53	ALA	N-CA-CB	6.17	119.67	110.29
26	U	105	LYS	N-CA-C	-6.17	104.64	111.36
5	e	184	LEU	N-CA-CB	6.17	119.72	110.22
20	Z	361	HIS	CA-C-N	6.17	129.16	120.28
20	Z	361	HIS	C-N-CA	6.17	129.16	120.28
25	R	230	LEU	CA-C-O	-6.17	113.88	120.42
30	K	125	THR	N-CA-C	-6.17	105.06	112.58
31	L	406	ASP	CA-CB-CG	-6.17	106.43	112.60
33	J	314	ILE	CA-C-O	-6.17	113.45	120.66
25	R	258	LEU	CA-C-N	6.17	128.46	120.44
25	R	258	LEU	C-N-CA	6.17	128.46	120.44
6	f	144	LEU	CA-C-O	6.16	126.77	120.24
3	C	30	SER	N-CA-C	-6.16	105.62	113.02
3	C	94	HIS	CG-CD2-NE2	6.16	113.36	107.20
6	F	193	GLY	CA-C-N	6.16	128.33	120.56
6	F	193	GLY	C-N-CA	6.16	128.33	120.56
10	3	35	GLY	N-CA-C	-6.16	99.29	111.31
17	T	111	LEU	CA-C-O	-6.16	114.02	120.55
17	T	138	ASP	CA-CB-CG	6.16	118.76	112.60
17	T	226	TRP	N-CA-C	-6.16	99.54	109.40
21	N	335	ALA	CA-C-N	6.16	128.54	120.28
21	N	335	ALA	C-N-CA	6.16	128.54	120.28
22	S	263	ASP	CA-CB-CG	-6.16	106.44	112.60
11	k	163	LEU	N-CA-C	-6.16	104.47	112.23
21	N	384	LYS	N-CA-C	6.16	118.00	111.28
23	P	402	PHE	CA-C-N	-6.16	111.26	121.80
23	P	402	PHE	C-N-CA	-6.16	111.26	121.80
3	C	125	HIS	ND1-CE1-NE2	6.16	114.56	108.40
20	Z	413	ASP	CA-C-N	6.16	126.82	119.98
20	Z	413	ASP	C-N-CA	6.16	126.82	119.98
24	Q	150	GLN	O-C-N	-6.16	113.60	122.96
26	U	9	THR	N-CA-CB	6.16	120.68	110.52
33	J	168	VAL	CB-CA-C	-6.16	103.97	112.04
11	4	166	GLN	N-CA-C	6.16	117.99	111.28
16	V	176	ASN	OD1-CG-ND2	6.16	128.76	122.60
13	6	200	THR	CA-C-O	6.16	126.95	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	92	ASP	CA-CB-CG	-6.16	106.44	112.60
27	O	354	GLN	O-C-N	-6.16	115.95	121.31
7	G	48	PHE	CA-CB-CG	-6.16	107.64	113.80
28	H	233	GLU	CB-CG-CD	-6.16	102.14	112.60
9	i	227	GLU	CA-C-N	6.15	131.27	120.87
9	i	227	GLU	C-N-CA	6.15	131.27	120.87
12	l	141	HIS	CE1-NE2-CD2	-6.15	102.85	109.00
28	H	307	PHE	CA-CB-CG	6.15	119.95	113.80
28	H	335	GLU	N-CA-C	-6.15	104.68	111.82
32	M	173	ASP	N-CA-C	-6.15	106.37	114.31
16	V	303	VAL	CA-C-N	6.15	128.81	120.44
16	V	303	VAL	C-N-CA	6.15	128.81	120.44
21	N	187	ASN	OD1-CG-ND2	-6.15	116.45	122.60
21	N	628	ALA	N-CA-C	6.15	118.07	111.36
22	S	172	ASN	N-CA-C	6.15	119.15	110.23
27	O	36	LYS	N-CA-CB	6.15	120.89	110.49
29	I	290	LYS	N-CA-C	-6.15	98.97	109.24
6	f	18	ARG	N-CA-C	-6.15	101.67	110.59
21	N	649	VAL	CB-CA-C	6.15	119.15	111.15
22	S	467	PHE	CA-CB-CG	-6.15	107.65	113.80
27	O	93	ASP	CA-CB-CG	-6.15	106.45	112.60
33	J	3	ALA	N-CA-CB	6.15	120.89	110.49
10	3	147	PHE	CA-CB-CG	-6.15	107.65	113.80
22	S	258	GLU	N-CA-C	-6.15	104.60	113.21
14	n	106	GLU	CA-C-N	6.15	129.02	120.29
14	n	106	GLU	C-N-CA	6.15	129.02	120.29
6	F	80	ASP	CA-C-N	6.15	129.66	120.31
6	F	80	ASP	C-N-CA	6.15	129.66	120.31
14	7	215	ARG	O-C-N	6.15	128.48	122.09
26	U	5	HIS	CE1-NE2-CD2	-6.15	102.85	109.00
29	I	70	LEU	O-C-N	6.15	128.63	122.12
33	J	86	VAL	N-CA-C	-6.15	99.50	108.11
11	4	125	LYS	N-CA-CB	6.15	119.63	110.29
21	N	23	TYR	O-C-N	6.15	128.63	122.12
12	5	193	ASP	N-CA-C	-6.14	105.82	113.38
19	Y	35	PHE	N-CA-C	-6.14	103.10	112.99
21	N	71	ASN	CA-C-N	6.14	128.80	120.44
21	N	71	ASN	C-N-CA	6.14	128.80	120.44
11	k	98	TYR	N-CA-C	-6.14	100.90	110.42
16	V	56	GLU	CA-C-N	6.14	131.43	122.77
16	V	56	GLU	C-N-CA	6.14	131.43	122.77
21	N	284	PRO	N-CA-C	-6.14	106.47	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	297	ILE	CA-C-N	6.14	129.01	120.29
22	S	297	ILE	C-N-CA	6.14	129.01	120.29
22	S	343	LEU	CA-C-N	6.14	125.70	119.19
22	S	343	LEU	C-N-CA	6.14	125.70	119.19
10	3	171	LEU	N-CA-C	6.14	118.89	111.40
14	7	214	MET	N-CA-C	6.14	117.64	111.07
20	Z	968	ASP	N-CA-C	-6.14	98.40	108.41
23	P	103	TYR	CA-C-N	6.14	128.51	120.28
23	P	103	TYR	C-N-CA	6.14	128.51	120.28
23	P	110	LEU	N-CA-CB	6.14	119.00	109.48
24	Q	215	VAL	CA-C-N	6.14	128.51	120.28
24	Q	215	VAL	C-N-CA	6.14	128.51	120.28
31	L	60	PHE	CA-C-N	6.14	128.51	120.28
31	L	60	PHE	C-N-CA	6.14	128.51	120.28
6	F	96	SER	CA-C-N	6.14	130.96	120.71
6	F	96	SER	C-N-CA	6.14	130.96	120.71
16	V	111	HIS	CA-CB-CG	-6.14	107.66	113.80
25	R	160	LYS	N-CA-CB	6.14	119.10	109.83
14	n	57	ALA	O-C-N	-6.14	116.85	123.42
28	H	151	GLN	CB-CG-CD	-6.14	102.17	112.60
2	b	86	VAL	CA-CB-CG1	6.13	120.83	110.40
12	5	273	TRP	CD2-CE2-CZ2	-6.13	116.27	122.40
17	T	55	LEU	CA-C-N	6.13	128.50	120.28
17	T	55	LEU	C-N-CA	6.13	128.50	120.28
22	S	289	ALA	CA-C-N	6.13	128.42	120.44
22	S	289	ALA	C-N-CA	6.13	128.42	120.44
31	L	54	ASN	CA-CB-CG	6.13	118.73	112.60
21	N	851	GLU	N-CA-CB	6.13	120.86	110.49
29	I	60	LEU	N-CA-C	6.13	117.97	111.28
32	M	91	ILE	N-CA-CB	-6.13	104.28	111.39
1	a	73	PHE	CA-CB-CG	-6.13	107.67	113.80
25	R	70	TYR	CA-C-N	6.13	128.50	120.28
25	R	70	TYR	C-N-CA	6.13	128.50	120.28
9	i	164	MET	CA-C-N	6.13	128.81	120.54
9	i	164	MET	C-N-CA	6.13	128.81	120.54
33	J	121	MET	CA-C-N	6.13	129.46	120.82
33	J	121	MET	C-N-CA	6.13	129.46	120.82
5	E	52	LYS	O-C-N	-6.13	115.62	122.12
6	F	176	LEU	CB-CA-C	-6.13	100.62	110.79
23	P	4	ASP	CA-C-N	6.13	127.75	120.09
23	P	4	ASP	C-N-CA	6.13	127.75	120.09
5	E	100	ASN	CA-CB-CG	-6.13	106.47	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	7	159	PHE	CA-CB-CG	-6.13	107.67	113.80
21	N	608	LEU	CA-C-N	6.13	129.62	120.31
21	N	608	LEU	C-N-CA	6.13	129.62	120.31
30	K	111	SER	N-CA-CB	6.13	120.17	110.55
21	N	183	VAL	O-C-N	6.12	128.14	121.83
5	E	131	GLU	N-CA-C	-6.12	99.29	109.46
15	W	158	ILE	O-C-N	6.12	127.81	121.87
8	h	33	ALA	N-CA-C	-6.12	105.10	113.30
31	L	339	ARG	CA-C-O	-6.12	114.79	119.32
11	4	20	ALA	N-CA-CB	6.12	118.98	110.17
29	I	121	THR	N-CA-C	-6.12	98.43	108.41
9	i	159	GLY	CA-C-N	6.12	133.22	121.54
9	i	159	GLY	C-N-CA	6.12	133.22	121.54
4	D	185	PRO	CA-C-N	6.12	129.61	120.31
4	D	185	PRO	C-N-CA	6.12	129.61	120.31
15	W	77	HIS	O-C-N	6.12	129.13	122.15
20	Z	257	PRO	CA-C-N	6.12	126.68	120.38
20	Z	257	PRO	C-N-CA	6.12	126.68	120.38
32	M	209	ASP	CA-C-N	6.12	128.48	120.28
32	M	209	ASP	C-N-CA	6.12	128.48	120.28
6	F	43	HIS	CA-CB-CG	-6.12	107.68	113.80
13	6	14	GLY	N-CA-C	-6.12	105.45	112.79
30	K	340	PHE	CA-C-O	-6.12	114.82	119.59
14	n	145	ASN	CA-C-O	-6.11	114.66	121.51
6	F	138	ASP	CA-CB-CG	6.11	118.71	112.60
11	k	69	ILE	CA-C-N	6.11	128.97	120.29
11	k	69	ILE	C-N-CA	6.11	128.97	120.29
22	S	31	VAL	CA-C-N	6.11	128.38	120.44
22	S	31	VAL	C-N-CA	6.11	128.38	120.44
23	P	213	TYR	CA-C-N	6.11	128.47	120.28
23	P	213	TYR	C-N-CA	6.11	128.47	120.28
7	g	220	SER	N-CA-C	-6.11	99.76	109.23
9	i	142	ILE	CA-C-O	-6.11	114.20	120.25
15	W	43	SER	O-C-N	6.11	129.12	122.15
23	P	53	ALA	N-CA-C	6.11	117.94	111.28
23	P	96	MET	N-CA-CB	-6.11	101.15	110.01
23	P	161	CYS	N-CA-CB	6.11	118.87	110.01
23	P	425	HIS	ND1-CE1-NE2	6.11	114.51	108.40
27	O	282	GLN	N-CA-C	-6.11	105.31	112.89
23	P	240	TYR	CA-C-N	6.11	129.59	120.31
23	P	240	TYR	C-N-CA	6.11	129.59	120.31
23	P	280	LEU	O-C-N	-6.11	115.49	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I	83	LYS	CA-C-O	-6.11	111.79	120.16
2	B	94	HIS	CA-CB-CG	-6.11	107.69	113.80
13	6	65	PHE	CA-C-N	6.11	129.07	120.28
13	6	65	PHE	C-N-CA	6.11	129.07	120.28
21	N	239	LEU	O-C-N	6.11	129.11	122.15
6	f	197	ILE	CA-C-N	6.11	129.59	120.31
6	f	197	ILE	C-N-CA	6.11	129.59	120.31
6	F	207	THR	N-CA-C	-6.11	101.17	110.14
21	N	601	THR	CA-C-O	-6.11	111.74	119.31
13	m	116	HIS	CE1-NE2-CD2	-6.10	102.90	109.00
6	F	41	ASN	OD1-CG-ND2	6.10	128.70	122.60
27	O	326	HIS	CB-CG-CD2	-6.10	123.27	131.20
1	a	59	VAL	N-CA-C	-6.10	95.70	108.88
2	b	54	PRO	N-CA-C	-6.10	106.03	114.27
8	1	122	ILE	CA-C-N	6.10	127.47	119.84
8	1	122	ILE	C-N-CA	6.10	127.47	119.84
30	K	39	ALA	CA-C-O	6.10	128.79	121.65
13	m	70	ASP	CB-CA-C	-6.10	101.22	110.92
10	j	70	LYS	CA-C-N	6.10	128.37	120.44
10	j	70	LYS	C-N-CA	6.10	128.37	120.44
10	j	198	ARG	NE-CZ-NH2	6.10	124.69	119.20
1	a	143	PHE	CA-CB-CG	-6.10	107.70	113.80
6	f	100	ASN	CA-C-O	6.09	128.91	121.84
14	n	184	ALA	CA-C-N	6.09	128.43	120.26
14	n	184	ALA	C-N-CA	6.09	128.43	120.26
1	A	37	GLN	N-CA-C	-6.09	107.07	114.75
33	J	320	SER	N-CA-CB	6.09	118.54	110.25
24	Q	360	SER	N-CA-CB	6.09	119.08	110.12
9	i	82	GLU	N-CA-C	6.09	118.71	111.71
22	S	139	HIS	CA-C-N	6.09	128.44	120.28
22	S	139	HIS	C-N-CA	6.09	128.44	120.28
30	K	349	ARG	CA-C-N	6.09	128.36	120.44
30	K	349	ARG	C-N-CA	6.09	128.36	120.44
33	J	199	ALA	N-CA-C	-6.09	104.76	111.82
1	a	218	PHE	CA-C-O	6.09	128.16	121.40
3	c	23	GLU	CA-C-O	6.09	127.00	120.55
9	i	208	GLU	N-CA-C	-6.09	98.71	109.06
14	n	243	LYS	CA-C-N	6.09	130.77	122.07
14	n	243	LYS	C-N-CA	6.09	130.77	122.07
16	V	165	ILE	N-CA-C	-6.09	104.57	110.72
4	D	107	GLU	O-C-N	6.08	128.34	122.07
8	1	166	HIS	ND1-CE1-NE2	6.08	114.48	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	49	PHE	CA-C-N	6.08	128.43	120.28
30	K	49	PHE	C-N-CA	6.08	128.43	120.28
9	2	48	ARG	N-CA-CB	6.08	119.78	109.87
2	B	101	TYR	CA-CB-CG	-6.08	102.96	113.90
23	P	361	THR	N-CA-C	-6.08	101.48	110.48
30	K	55	GLU	CA-C-N	6.08	131.02	120.68
30	K	55	GLU	C-N-CA	6.08	131.02	120.68
21	N	490	LEU	N-CA-C	6.08	119.64	110.64
21	N	832	HIS	CE1-NE2-CD2	-6.08	102.92	109.00
24	Q	130	ARG	CA-C-N	6.08	128.79	120.46
24	Q	130	ARG	C-N-CA	6.08	128.79	120.46
28	H	220	LYS	CA-C-N	6.08	128.43	120.28
28	H	220	LYS	C-N-CA	6.08	128.43	120.28
30	K	89	ILE	N-CA-C	-6.08	104.74	113.07
32	M	170	MET	N-CA-C	-6.08	104.21	111.69
33	J	215	GLY	O-C-N	6.08	130.11	122.39
21	N	438	ASP	N-CA-CB	6.08	118.88	110.07
29	I	326	MET	CA-C-O	6.08	126.92	120.36
12	l	151	VAL	CA-C-N	6.07	128.70	120.38
12	l	151	VAL	C-N-CA	6.07	128.70	120.38
1	A	32	PHE	CA-CB-CG	-6.07	107.73	113.80
2	B	32	VAL	CA-CB-CG1	-6.07	100.08	110.40
14	7	90	ILE	CA-C-N	6.07	128.34	120.44
14	7	90	ILE	C-N-CA	6.07	128.34	120.44
21	N	137	PHE	CA-C-O	6.07	126.99	120.55
21	N	733	LEU	CA-C-O	-6.07	112.62	119.79
23	P	251	LYS	CB-CA-C	-6.07	100.53	110.85
33	J	365	ALA	O-C-N	-6.07	115.68	122.12
15	W	100	HIS	CG-CD2-NE2	6.07	113.27	107.20
23	P	178	GLN	CA-C-N	6.07	128.41	120.28
23	P	178	GLN	C-N-CA	6.07	128.41	120.28
24	Q	182	SER	CA-C-N	6.07	128.41	120.28
24	Q	182	SER	C-N-CA	6.07	128.41	120.28
27	O	388	GLY	CA-C-N	6.07	128.70	120.38
27	O	388	GLY	C-N-CA	6.07	128.70	120.38
28	H	86	GLY	N-CA-C	-6.07	106.08	115.73
31	L	307	GLU	N-CA-CB	-6.07	101.19	110.12
3	C	177	GLN	N-CA-C	6.07	118.69	111.71
13	6	192	VAL	CA-C-O	-6.07	114.64	120.95
22	S	139	HIS	CE1-NE2-CD2	-6.07	102.93	109.00
25	R	338	TYR	CB-CG-CD2	-6.07	111.70	120.80
7	g	204	HIS	ND1-CE1-NE2	6.07	114.47	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	7	138	SER	N-CA-CB	6.07	119.03	110.12
18	X	69	ILE	CA-C-N	6.07	126.42	119.93
18	X	69	ILE	C-N-CA	6.07	126.42	119.93
31	L	97	ALA	CA-C-N	6.07	128.90	120.29
31	L	97	ALA	C-N-CA	6.07	128.90	120.29
31	L	189	GLN	N-CA-CB	6.07	119.64	110.30
4	d	71	VAL	O-C-N	-6.06	116.78	123.03
3	C	207	THR	CA-C-N	6.06	128.41	120.28
3	C	207	THR	C-N-CA	6.06	128.41	120.28
16	V	135	ARG	N-CA-C	-6.06	104.39	112.94
17	T	100	ASP	CA-CB-CG	-6.06	106.54	112.60
32	M	111	THR	N-CA-CB	6.06	120.73	110.49
3	c	80	LEU	CA-C-O	-6.06	113.41	120.62
3	c	94	HIS	CG-CD2-NE2	6.06	113.26	107.20
5	e	125	GLU	N-CA-C	-6.06	106.05	113.50
5	e	157	HIS	CB-CG-CD2	6.06	139.08	131.20
6	f	216	VAL	N-CA-C	-6.06	100.35	108.35
23	P	6	PRO	CA-C-N	6.06	128.11	120.72
23	P	6	PRO	C-N-CA	6.06	128.11	120.72
33	J	29	GLU	CA-C-N	6.06	129.52	120.31
33	J	29	GLU	C-N-CA	6.06	129.52	120.31
10	j	158	LEU	N-CA-CB	6.06	120.28	110.41
8	1	44	THR	CA-CB-OG1	6.06	118.69	109.60
10	3	89	GLN	OE1-CD-NE2	6.06	128.66	122.60
20	Z	248	TYR	CB-CA-C	-6.06	100.74	110.79
24	Q	190	ASN	N-CA-C	-6.06	99.12	109.24
32	M	89	ASN	CA-CB-CG	-6.06	106.54	112.60
32	M	389	ALA	N-CA-C	6.06	118.84	111.82
2	b	207	ASP	CA-CB-CG	-6.05	106.55	112.60
13	6	39	THR	N-CA-CB	6.05	120.58	110.59
25	R	100	ASN	N-CA-C	6.05	118.38	111.11
30	K	246	TYR	N-CA-CB	6.05	121.12	111.56
8	h	179	GLY	N-CA-C	-6.05	102.64	110.69
21	N	899	ASN	CA-C-N	6.05	131.99	120.97
21	N	899	ASN	C-N-CA	6.05	131.99	120.97
13	6	159	ASP	CA-CB-CG	-6.05	106.55	112.60
15	W	191	ILE	O-C-N	-6.05	115.01	122.57
19	Y	10	ALA	CA-C-O	-6.05	114.00	120.42
22	S	242	LEU	CA-C-N	6.05	128.39	120.28
22	S	242	LEU	C-N-CA	6.05	128.39	120.28
13	m	103	HIS	CG-CD2-NE2	6.05	113.25	107.20
6	F	159	THR	CA-CB-CG2	6.05	120.78	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	45	THR	CA-CB-OG1	6.05	118.67	109.60
6	f	143	HIS	CA-CB-CG	-6.05	107.75	113.80
19	Y	64	TRP	CA-C-O	-6.05	114.21	121.40
21	N	414	GLY	N-CA-C	6.05	123.40	115.36
25	R	36	SER	CA-C-N	6.05	132.47	122.73
25	R	36	SER	C-N-CA	6.05	132.47	122.73
28	H	221	LEU	CA-C-O	6.05	126.96	120.55
32	M	354	GLU	CA-C-O	6.05	127.17	120.82
4	d	233	VAL	CA-C-N	6.04	128.38	120.28
4	d	233	VAL	C-N-CA	6.04	128.38	120.28
6	f	102	LYS	N-CA-CB	6.04	118.86	109.97
21	N	625	LEU	N-CA-C	6.04	117.87	111.28
24	Q	15	VAL	N-CA-CB	6.04	118.31	110.57
25	R	331	ARG	NE-CZ-NH1	6.04	127.55	121.50
13	m	103	HIS	N-CA-C	-6.04	104.81	111.82
15	W	163	ASN	OD1-CG-ND2	6.04	128.64	122.60
18	X	62	ASP	CA-C-N	6.04	126.36	119.83
18	X	62	ASP	C-N-CA	6.04	126.36	119.83
27	O	23	HIS	CE1-NE2-CD2	-6.04	102.96	109.00
30	K	57	GLU	O-C-N	-6.04	113.61	122.43
30	K	272	ASP	CA-CB-CG	-6.04	106.56	112.60
31	L	168	TYR	N-CA-C	-6.04	105.39	112.89
2	b	234	ARG	CD-NE-CZ	6.04	132.86	124.40
29	I	95	GLN	CB-CG-CD	-6.04	102.33	112.60
32	M	174	GLU	CA-C-N	6.04	128.76	120.67
32	M	174	GLU	C-N-CA	6.04	128.76	120.67
2	B	94	HIS	CB-CG-CD2	-6.04	123.35	131.20
30	K	307	ASP	CA-CB-CG	-6.04	106.56	112.60
8	h	120	TYR	CA-CB-CG	-6.04	103.03	113.90
9	i	48	ARG	N-CA-CB	6.04	120.31	110.17
17	T	237	ASN	CA-C-N	6.04	128.37	120.28
17	T	237	ASN	C-N-CA	6.04	128.37	120.28
27	O	357	ILE	O-C-N	-6.04	115.02	122.57
3	c	39	MET	CG-SD-CE	-6.04	87.62	100.90
10	j	109	VAL	N-CA-C	-6.04	99.72	108.17
10	j	142	ALA	N-CA-C	-6.04	104.29	112.26
12	l	153	ALA	CA-C-O	-6.04	113.54	120.24
5	E	54	ALA	CA-C-O	-6.04	113.98	120.92
16	V	183	ALA	N-CA-CB	6.04	119.94	110.71
18	X	61	LEU	O-C-N	6.04	129.98	122.86
22	S	290	ASN	N-CA-CB	6.04	118.76	110.01
30	K	288	SER	CA-C-O	-6.04	112.67	119.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	168	SER	N-CA-CB	6.03	118.82	110.07
2	B	219	PRO	N-CA-C	-6.03	106.13	114.27
7	G	230	PHE	CA-C-O	-6.03	114.16	121.28
12	5	258	ASP	CA-CB-CG	6.03	118.63	112.60
13	6	200	THR	CA-CB-OG1	6.03	118.65	109.60
14	7	219	TYR	O-C-N	-6.03	114.87	122.17
22	S	266	SER	CA-C-N	6.03	128.28	120.44
22	S	266	SER	C-N-CA	6.03	128.28	120.44
28	H	397	SER	CA-C-N	6.03	131.51	122.58
28	H	397	SER	C-N-CA	6.03	131.51	122.58
23	P	198	VAL	N-CA-C	6.03	116.77	110.62
12	l	181	ARG	CA-C-O	6.03	126.41	119.35
11	4	174	MET	CA-C-O	-6.03	113.63	120.32
25	R	79	LEU	CA-C-O	-6.03	112.21	119.27
25	R	367	ASP	CA-C-N	6.03	128.36	120.28
25	R	367	ASP	C-N-CA	6.03	128.36	120.28
27	O	247	ASN	N-CA-C	-6.03	105.78	113.02
20	Z	340	LEU	N-CA-C	-6.03	104.66	112.68
21	N	152	LEU	CB-CA-C	-6.03	100.78	110.79
24	Q	12	ARG	CB-CA-C	6.03	120.80	110.79
25	R	406	GLN	CA-C-N	6.03	127.88	120.22
25	R	406	GLN	C-N-CA	6.03	127.88	120.22
16	V	178	GLY	CA-C-O	6.03	126.55	119.19
17	T	251	HIS	CA-CB-CG	6.03	119.83	113.80
19	Y	65	ASP	CA-C-N	6.03	131.02	121.44
19	Y	65	ASP	C-N-CA	6.03	131.02	121.44
25	R	91	TRP	CA-C-N	6.03	131.92	122.70
25	R	91	TRP	C-N-CA	6.03	131.92	122.70
2	b	218	ASN	CA-C-O	-6.03	113.77	119.55
2	B	191	ILE	O-C-N	6.03	128.17	121.90
27	O	138	LEU	O-C-N	-6.03	114.40	122.23
27	O	368	ASP	O-C-N	6.03	128.51	122.12
21	N	642	ASP	CA-C-O	-6.02	111.91	120.16
2	B	119	GLN	O-C-N	-6.02	115.74	122.12
18	X	123	ASN	CA-C-O	6.02	126.93	120.55
28	H	204	PRO	N-CA-CB	-6.02	97.74	103.34
30	K	169	VAL	O-C-N	6.02	129.73	123.05
23	P	41	VAL	N-CA-C	-6.02	104.87	110.53
20	Z	85	VAL	CA-C-O	-6.02	111.89	119.95
21	N	669	GLU	N-CA-C	-6.02	105.52	112.92
16	V	87	PHE	O-C-N	6.01	129.01	122.15
19	Y	32	ASP	CA-C-N	6.01	131.66	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Y	32	ASP	C-N-CA	6.01	131.66	121.14
23	P	343	LYS	CA-C-N	6.01	128.83	120.29
23	P	343	LYS	C-N-CA	6.01	128.83	120.29
26	U	29	GLU	CB-CA-C	6.01	120.71	111.39
27	O	88	ASP	CA-C-O	6.01	126.31	119.27
30	K	322	ASP	N-CA-CB	6.01	121.12	111.20
31	L	302	GLN	OE1-CD-NE2	6.01	128.62	122.60
32	M	184	GLY	N-CA-C	-6.01	98.92	113.18
5	e	55	THR	CA-CB-OG1	6.01	118.62	109.60
7	g	127	ASN	CB-CG-ND2	-6.01	107.38	116.40
21	N	224	THR	O-C-N	6.01	129.00	122.15
21	N	247	GLU	CA-C-O	6.01	126.58	119.48
25	R	34	THR	CA-C-O	-6.01	114.47	120.90
32	M	302	GLN	OE1-CD-NE2	6.01	128.61	122.60
17	T	216	GLU	CA-C-N	6.01	128.33	120.28
17	T	216	GLU	C-N-CA	6.01	128.33	120.28
18	X	122	TYR	CA-C-N	6.01	128.33	120.28
18	X	122	TYR	C-N-CA	6.01	128.33	120.28
21	N	777	ALA	CA-C-N	6.01	132.52	121.70
21	N	777	ALA	C-N-CA	6.01	132.52	121.70
31	L	66	GLU	N-CA-CB	6.01	118.72	110.01
8	h	121	THR	CA-C-N	6.01	133.25	122.13
8	h	121	THR	C-N-CA	6.01	133.25	122.13
21	N	357	GLY	CA-C-N	6.01	128.82	120.29
21	N	357	GLY	C-N-CA	6.01	128.82	120.29
22	S	21	SER	N-CA-C	6.01	118.32	111.11
26	U	25	THR	CA-C-O	-6.01	112.53	119.14
11	k	133	HIS	CB-CG-CD2	-6.01	123.39	131.20
27	O	97	LYS	CA-C-N	6.01	128.82	120.29
27	O	97	LYS	C-N-CA	6.01	128.82	120.29
10	j	200	LEU	CA-C-N	6.00	130.94	121.99
10	j	200	LEU	C-N-CA	6.00	130.94	121.99
26	U	61	LYS	O-C-N	6.00	130.04	122.23
7	G	103	TYR	CA-C-N	6.00	130.88	122.36
7	G	103	TYR	C-N-CA	6.00	130.88	122.36
9	2	164	MET	CG-SD-CE	-6.00	87.69	100.90
22	S	437	ASN	OD1-CG-ND2	6.00	128.60	122.60
25	R	81	HIS	ND1-CE1-NE2	6.00	114.40	108.40
15	W	108	GLN	N-CA-CB	6.00	120.01	110.65
11	k	171	ARG	NE-CZ-NH2	6.00	124.60	119.20
4	D	89	ALA	CA-C-N	6.00	128.81	120.29
4	D	89	ALA	C-N-CA	6.00	128.81	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	217	LYS	N-CA-C	-6.00	105.96	113.28
21	N	89	PHE	CA-C-O	6.00	125.39	118.55
27	O	283	HIS	CA-C-N	6.00	128.24	120.44
27	O	283	HIS	C-N-CA	6.00	128.24	120.44
7	G	31	VAL	CA-C-O	6.00	127.28	119.85
18	X	27	ILE	N-CA-C	-6.00	101.18	107.84
21	N	224	THR	CA-CB-OG1	6.00	118.59	109.60
21	N	538	LYS	N-CA-C	6.00	117.90	111.36
22	S	316	LEU	CA-C-O	6.00	126.91	120.55
24	Q	416	VAL	CA-C-N	6.00	126.77	119.99
24	Q	416	VAL	C-N-CA	6.00	126.77	119.99
28	H	93	GLU	CA-C-O	6.00	126.72	120.30
14	7	83	VAL	N-CA-C	-6.00	99.85	108.48
14	7	130	ALA	N-CA-C	6.00	118.30	111.11
28	H	250	GLY	CA-C-N	6.00	126.56	120.38
28	H	250	GLY	C-N-CA	6.00	126.56	120.38
6	f	64	ILE	CA-C-O	-5.99	114.10	120.39
28	H	196	THR	N-CA-C	-5.99	106.01	113.38
32	M	79	VAL	CA-C-O	-5.99	114.01	120.36
4	d	238	GLN	OE1-CD-NE2	5.99	128.59	122.60
4	d	105	THR	N-CA-C	-5.99	101.14	110.42
4	d	245	GLU	CA-C-O	-5.99	114.07	120.42
14	n	172	SER	O-C-N	-5.99	115.63	121.56
19	Y	47	GLU	CA-C-N	5.99	130.91	121.99
19	Y	47	GLU	C-N-CA	5.99	130.91	121.99
24	Q	259	CYS	CB-CA-C	-5.99	101.47	110.88
30	K	256	ASP	CA-C-O	-5.99	114.07	120.42
32	M	62	ILE	CB-CA-C	-5.99	103.95	112.22
21	N	580	ASN	OD1-CG-ND2	-5.99	116.61	122.60
24	Q	274	LEU	N-CA-C	-5.99	98.65	108.41
27	O	248	TYR	N-CA-C	-5.99	103.50	112.54
32	M	98	GLU	CB-CG-CD	-5.99	102.42	112.60
12	l	160	ASN	CA-CB-CG	-5.99	106.61	112.60
24	Q	10	GLU	CA-C-O	-5.99	114.53	120.82
13	m	81	LYS	N-CA-CB	5.99	118.86	109.94
4	D	5	ASP	CA-CB-CG	5.99	118.59	112.60
14	7	54	ILE	N-CA-CB	5.99	119.67	111.41
21	N	437	GLU	CA-C-O	5.99	126.77	120.42
26	U	54	LEU	N-CA-C	-5.99	101.10	110.14
27	O	109	LEU	N-CA-C	5.99	117.88	111.36
3	C	112	VAL	CA-CB-CG2	-5.98	100.23	110.40
19	Y	54	VAL	O-C-N	-5.98	115.77	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	63	THR	N-CA-C	-5.98	98.55	109.56
21	N	210	SER	CA-C-O	-5.98	114.21	120.55
30	K	87	LYS	N-CA-C	5.98	118.76	111.82
32	M	250	GLN	CA-C-N	5.98	128.30	120.28
32	M	250	GLN	C-N-CA	5.98	128.30	120.28
21	N	45	ASP	CA-C-O	-5.98	114.08	120.42
27	O	166	ARG	CA-C-N	5.98	128.10	120.56
27	O	166	ARG	C-N-CA	5.98	128.10	120.56
20	Z	24	THR	CA-C-O	-5.98	111.97	120.16
20	Z	738	TYR	CB-CG-CD2	5.98	129.77	120.80
24	Q	251	THR	CA-C-O	5.98	126.90	120.38
30	K	196	ASP	CA-C-N	5.98	128.29	120.28
30	K	196	ASP	C-N-CA	5.98	128.29	120.28
31	L	435	GLN	N-CA-C	5.98	118.50	109.41
1	a	246	VAL	CA-CB-CG1	5.98	120.56	110.40
5	e	91	HIS	CE1-NE2-CD2	-5.98	103.02	109.00
9	i	185	SER	CA-C-O	-5.98	114.21	120.55
14	n	256	LYS	N-CA-C	-5.98	105.31	114.16
3	C	63	THR	CA-CB-OG1	5.98	118.56	109.60
21	N	340	HIS	ND1-CE1-NE2	5.98	114.38	108.40
24	Q	114	GLN	N-CA-C	5.98	118.28	111.11
30	K	421	VAL	CA-C-N	5.98	129.20	120.71
30	K	421	VAL	C-N-CA	5.98	129.20	120.71
12	l	209	THR	CA-C-N	5.97	131.60	121.14
12	l	209	THR	C-N-CA	5.97	131.60	121.14
11	4	39	SER	N-CA-CB	5.97	121.01	110.37
11	4	82	SER	CA-C-O	-5.97	114.55	120.82
23	P	181	LEU	CA-C-O	5.97	126.88	120.55
33	J	384	LEU	CA-C-O	-5.97	114.09	120.42
8	h	195	LEU	N-CA-C	-5.97	100.26	109.52
1	A	48	LYS	N-CA-C	-5.97	106.33	113.97
21	N	297	ASP	N-CA-C	5.97	117.79	111.28
2	b	89	SER	N-CA-C	-5.97	104.77	111.28
13	m	155	MET	CA-C-O	-5.97	113.06	118.79
12	5	225	VAL	N-CA-C	5.97	116.15	110.42
1	A	16	ILE	CA-C-O	-5.97	115.34	121.67
1	A	238	ALA	CA-C-N	5.97	128.77	120.29
1	A	238	ALA	C-N-CA	5.97	128.77	120.29
4	D	6	ARG	CA-C-N	5.97	129.32	120.90
4	D	6	ARG	C-N-CA	5.97	129.32	120.90
23	P	232	ARG	CA-C-O	-5.97	114.67	121.65
2	b	30	GLN	OE1-CD-NE2	5.97	128.57	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	141	ASP	N-CA-CB	5.97	122.08	111.69
17	T	132	HIS	CA-CB-CG	5.97	119.77	113.80
4	d	127	ARG	N-CA-C	-5.97	102.63	110.39
4	d	251	LYS	N-CA-C	5.97	117.78	111.28
12	l	121	ALA	N-CA-C	-5.97	100.07	108.96
9	2	177	LYS	N-CA-C	-5.97	105.83	113.23
12	5	109	VAL	N-CA-C	-5.97	99.89	108.48
2	b	59	GLU	CA-C-N	5.96	132.19	122.65
2	b	59	GLU	C-N-CA	5.96	132.19	122.65
9	2	102	GLU	CB-CG-CD	-5.96	102.46	112.60
1	a	31	ALA	N-CA-C	-5.96	104.69	111.07
17	T	85	LEU	N-CA-C	5.96	117.45	111.07
24	Q	52	ASN	CA-C-O	-5.96	114.23	120.55
9	i	105	VAL	CA-CB-CG1	5.96	120.53	110.40
9	2	115	HIS	CE1-NE2-CD2	-5.96	103.04	109.00
20	Z	725	GLU	N-CA-C	5.96	117.58	111.14
23	P	3	ARG	N-CA-CB	5.96	121.27	111.08
3	C	31	HIS	CB-CG-ND1	5.96	131.64	122.70
28	H	231	SER	O-C-N	5.96	124.85	121.27
4	d	106	VAL	CA-C-N	5.96	128.26	120.28
4	d	106	VAL	C-N-CA	5.96	128.26	120.28
3	C	133	VAL	O-C-N	-5.96	116.21	123.00
5	E	232	ASP	O-C-N	-5.96	115.38	122.65
8	l	34	TYR	CB-CG-CD2	-5.96	111.86	120.80
23	P	399	ILE	CB-CG1-CD1	-5.96	101.29	113.80
24	Q	404	ASN	N-CA-C	-5.96	105.19	112.88
4	d	181	ARG	NH1-CZ-NH2	5.96	127.04	119.30
7	g	242	PHE	CA-C-N	5.96	128.26	120.28
7	g	242	PHE	C-N-CA	5.96	128.26	120.28
10	j	89	GLN	CA-C-N	5.96	128.75	120.29
10	j	89	GLN	C-N-CA	5.96	128.75	120.29
13	m	36	ARG	NE-CZ-NH1	-5.96	115.54	121.50
12	5	144	ARG	NE-CZ-NH2	5.96	124.56	119.20
13	6	144	CYS	N-CA-CB	5.96	121.79	111.13
31	L	86	LYS	N-CA-CB	5.96	118.97	110.16
11	k	193	ASP	N-CA-C	-5.95	106.02	113.28
2	B	105	PRO	CA-C-N	5.95	127.28	119.84
2	B	105	PRO	C-N-CA	5.95	127.28	119.84
25	R	354	ALA	N-CA-C	-5.95	104.87	111.36
4	D	190	GLU	N-CA-CB	-5.95	101.37	110.12
9	2	98	TYR	N-CA-C	-5.95	105.85	113.23
27	O	45	LEU	N-CA-CB	5.95	118.87	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	J	203	ALA	N-CA-C	5.95	119.64	112.38
5	e	226	ASP	N-CA-C	-5.95	105.76	114.39
11	k	139	TYR	CB-CA-C	-5.95	98.46	109.29
8	1	147	CYS	N-CA-CB	5.95	118.64	110.01
32	M	418	GLY	CA-C-N	5.95	128.18	120.56
32	M	418	GLY	C-N-CA	5.95	128.18	120.56
4	D	57	THR	CA-C-N	5.95	128.53	120.44
4	D	57	THR	C-N-CA	5.95	128.53	120.44
14	7	129	LEU	N-CA-C	-5.95	104.71	111.07
27	O	112	LYS	O-C-N	5.95	128.93	122.15
12	l	119	THR	CA-C-O	5.95	126.54	120.24
3	C	129	ARG	NE-CZ-NH2	-5.95	113.85	119.20
1	A	147	ASP	N-CA-C	-5.95	100.92	110.14
13	6	154	ILE	O-C-N	5.95	130.00	122.57
18	X	65	SER	N-CA-CB	5.95	119.92	110.65
30	K	382	VAL	N-CA-C	-5.95	105.96	112.80
31	L	218	VAL	CA-C-N	5.95	131.37	122.99
31	L	218	VAL	C-N-CA	5.95	131.37	122.99
13	m	171	GLY	CA-C-O	5.94	125.62	119.02
4	D	74	SER	CB-CA-C	5.94	121.42	110.24
17	T	46	ILE	CA-C-O	5.94	125.95	120.96
1	a	85	GLY	O-C-N	5.94	127.71	121.77
8	1	31	THR	N-CA-CB	5.94	119.87	110.84
12	5	194	GLY	CA-C-N	5.94	129.31	120.87
12	5	194	GLY	C-N-CA	5.94	129.31	120.87
14	7	53	VAL	O-C-N	-5.94	116.44	123.04
21	N	428	VAL	N-CA-C	5.94	118.52	111.09
24	Q	336	ASN	N-CA-C	5.94	117.84	111.36
14	n	154	SER	N-CA-C	-5.94	104.88	111.36
9	2	41	VAL	N-CA-C	-5.94	100.46	108.06
9	2	71	TRP	CE3-CZ3-CH2	-5.94	113.38	121.10
27	O	77	SER	N-CA-CB	5.94	118.85	110.12
28	H	61	ALA	CA-C-N	5.94	128.24	120.28
28	H	61	ALA	C-N-CA	5.94	128.24	120.28
7	G	219	CYS	CA-C-O	-5.94	113.92	120.33
12	5	238	ALA	O-C-N	5.94	128.19	122.07
21	N	65	ALA	CA-C-N	5.94	128.16	120.44
21	N	65	ALA	C-N-CA	5.94	128.16	120.44
23	P	398	LYS	CA-CB-CG	5.94	125.97	114.10
23	P	411	LEU	N-CA-CB	5.94	118.85	110.12
26	U	59	ASP	CA-CB-CG	5.94	118.54	112.60
32	M	324	LEU	N-CA-CB	5.94	120.35	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	14	PRO	N-CA-C	-5.94	106.44	113.86
15	W	115	CYS	CB-CA-C	-5.94	99.66	109.99
21	N	912	GLU	CA-C-O	-5.94	115.26	120.60
24	Q	72	ASP	CA-C-O	-5.94	114.13	120.42
1	a	57	LYS	N-CA-C	-5.93	98.41	108.26
4	d	60	THR	O-C-N	-5.93	112.94	121.54
14	n	182	HIS	CE1-NE2-CD2	-5.93	103.07	109.00
14	7	64	GLY	CA-C-N	5.93	128.16	120.44
14	7	64	GLY	C-N-CA	5.93	128.16	120.44
28	H	122	SER	N-CA-C	-5.93	104.90	113.21
10	j	44	PHE	CA-CB-CG	-5.93	107.87	113.80
14	n	153	GLN	CA-C-N	5.93	128.71	120.29
14	n	153	GLN	C-N-CA	5.93	128.71	120.29
1	A	149	GLU	N-CA-C	-5.93	106.38	113.97
17	T	172	SER	CA-C-N	5.93	132.87	121.54
17	T	172	SER	C-N-CA	5.93	132.87	121.54
24	Q	157	LEU	CA-C-N	5.93	128.59	120.46
24	Q	157	LEU	C-N-CA	5.93	128.59	120.46
10	j	163	LEU	N-CA-C	-5.93	104.81	111.28
6	F	14	SER	N-CA-CB	5.93	120.58	110.50
13	m	47	TYR	N-CA-C	-5.93	98.62	108.34
13	6	122	LEU	CA-C-O	-5.93	114.43	121.66
18	X	81	SER	CB-CA-C	-5.93	98.62	110.42
23	P	294	GLU	CA-C-N	5.93	128.23	120.28
23	P	294	GLU	C-N-CA	5.93	128.23	120.28
25	R	100	ASN	CA-C-N	5.93	128.54	120.54
25	R	100	ASN	C-N-CA	5.93	128.54	120.54
25	R	232	VAL	CA-CB-CG1	5.93	120.48	110.40
28	H	423	CYS	N-CA-C	5.93	117.41	111.07
30	K	236	ARG	CA-C-O	-5.93	115.43	122.13
32	M	216	LYS	CB-CA-C	5.93	120.93	110.85
3	c	141	ASP	CA-CB-CG	5.93	118.53	112.60
3	C	157	TYR	CB-CG-CD1	5.93	129.69	120.80
21	N	468	GLU	N-CA-C	-5.93	104.40	111.69
30	K	37	ASN	OD1-CG-ND2	5.93	128.53	122.60
13	m	43	ILE	N-CA-C	-5.92	99.34	107.99
14	n	232	ILE	CB-CA-C	5.92	119.18	110.77
14	n	255	ALA	CB-CA-C	-5.92	103.62	111.74
7	G	162	GLY	N-CA-C	-5.92	99.14	113.18
9	2	242	LEU	N-CA-C	-5.92	104.22	112.45
21	N	371	LEU	N-CA-CB	5.92	118.83	110.12
21	N	567	ALA	CA-C-N	5.92	130.03	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	567	ALA	C-N-CA	5.92	130.03	120.55
23	P	431	HIS	CB-CG-CD2	-5.92	123.50	131.20
26	U	156	HIS	CA-CB-CG	5.92	119.72	113.80
31	L	276	CYS	CA-C-O	5.92	127.62	120.99
3	c	189	ALA	CA-C-N	5.92	128.57	120.46
3	c	189	ALA	C-N-CA	5.92	128.57	120.46
28	H	132	GLN	CA-C-O	-5.92	114.53	121.16
31	L	182	GLY	O-C-N	-5.92	118.53	121.85
1	a	39	ASN	N-CA-CB	5.92	120.50	110.49
2	B	151	ASP	O-C-N	-5.92	116.88	121.14
2	B	183	LEU	N-CA-C	-5.92	98.75	108.76
4	D	58	ARG	CB-CA-C	-5.92	101.55	110.90
21	N	831	GLU	CA-C-O	-5.92	112.04	120.51
23	P	297	GLU	O-C-N	-5.92	115.84	122.12
1	A	123	ASN	N-CA-C	-5.92	104.77	112.23
5	E	213	ASP	N-CA-C	-5.92	99.14	108.14
11	4	73	TYR	CA-C-N	5.92	129.24	120.95
11	4	73	TYR	C-N-CA	5.92	129.24	120.95
21	N	514	THR	N-CA-CB	5.92	118.82	110.12
1	a	148	GLU	N-CA-C	-5.92	105.71	113.17
3	c	202	ASP	CA-CB-CG	-5.92	106.68	112.60
9	i	62	LYS	N-CA-C	-5.92	106.39	113.97
9	2	170	HIS	CE1-NE2-CD2	-5.92	103.08	109.00
11	4	13	VAL	N-CA-C	-5.92	99.82	108.11
20	Z	743	ILE	CA-C-N	5.92	128.21	120.28
20	Z	743	ILE	C-N-CA	5.92	128.21	120.28
25	R	60	ALA	O-C-N	-5.92	114.51	121.32
25	R	192	GLU	CA-C-N	5.92	128.80	120.28
25	R	192	GLU	C-N-CA	5.92	128.80	120.28
28	H	128	ASN	OD1-CG-ND2	5.92	128.52	122.60
28	H	288	ALA	CA-C-N	5.92	128.53	120.54
28	H	288	ALA	C-N-CA	5.92	128.53	120.54
29	I	245	LEU	O-C-N	-5.92	116.29	123.10
1	a	161	GLY	CA-C-O	5.92	124.33	118.77
11	4	118	GLN	N-CA-CB	5.92	119.88	110.65
16	V	95	LEU	CB-CA-C	-5.92	97.95	110.31
17	T	28	PRO	N-CA-C	5.92	117.92	110.70
31	L	141	LYS	CA-C-O	-5.92	115.11	121.38
31	L	197	ILE	CA-C-N	5.92	130.74	120.68
31	L	197	ILE	C-N-CA	5.92	130.74	120.68
25	R	373	PRO	CA-C-N	5.92	128.69	120.29
25	R	373	PRO	C-N-CA	5.92	128.69	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	W	12	ASN	N-CA-C	-5.91	98.64	108.34
16	V	53	MET	CG-SD-CE	-5.91	87.89	100.90
21	N	804	LEU	O-C-N	5.91	128.39	122.12
23	P	37	ASP	N-CA-C	5.91	117.73	111.28
32	M	331	ASP	N-CA-C	-5.91	106.11	113.38
9	2	122	HIS	CE1-NE2-CD2	-5.91	103.09	109.00
16	V	84	ASP	N-CA-C	-5.91	98.77	108.76
21	N	547	LEU	CA-C-O	5.91	126.65	119.38
22	S	146	LEU	N-CA-CB	5.91	118.58	110.01
6	F	122	SER	CB-CA-C	5.91	119.49	109.50
13	6	39	THR	N-CA-C	-5.91	97.96	108.13
17	T	258	ASN	CA-CB-CG	-5.91	106.69	112.60
21	N	248	GLU	CA-C-O	-5.91	114.29	120.32
23	P	76	ASN	CA-CB-CG	-5.91	106.69	112.60
26	U	134	THR	CA-C-O	5.91	126.88	120.32
30	K	158	ILE	N-CA-C	-5.91	100.55	108.35
32	M	247	ALA	N-CA-C	-5.91	99.27	108.90
33	J	204	HIS	CA-C-N	5.91	128.68	120.29
33	J	204	HIS	C-N-CA	5.91	128.68	120.29
33	J	282	PHE	CA-C-N	5.91	132.83	121.54
33	J	282	PHE	C-N-CA	5.91	132.83	121.54
4	d	90	ARG	CA-C-O	-5.91	114.29	120.55
1	A	130	GLN	N-CA-C	-5.91	106.71	114.04
10	3	135	ASP	N-CA-C	-5.91	104.20	112.12
18	X	126	ILE	CA-C-N	5.91	127.72	120.22
18	X	126	ILE	C-N-CA	5.91	127.72	120.22
24	Q	423	VAL	CA-C-O	-5.91	114.25	120.57
25	R	265	ASP	N-CA-C	5.91	117.39	111.07
28	H	164	SER	N-CA-CB	5.91	117.18	110.03
19	Y	85	LYS	N-CA-CB	5.91	118.80	110.12
13	m	189	ILE	CA-CB-CG2	5.91	120.54	110.50
7	G	60	VAL	N-CA-CB	5.91	118.52	111.08
16	V	104	VAL	CA-CB-CG2	-5.91	100.36	110.40
16	V	242	LYS	CA-C-N	5.91	128.67	120.29
16	V	242	LYS	C-N-CA	5.91	128.67	120.29
21	N	124	TYR	CA-C-O	5.91	125.29	118.97
21	N	707	ASN	CA-CB-CG	-5.91	106.69	112.60
24	Q	250	THR	N-CA-CB	5.91	118.72	110.04
27	O	184	ASP	CA-C-N	5.91	128.47	120.44
27	O	184	ASP	C-N-CA	5.91	128.47	120.44
3	C	3	SER	N-CA-C	5.90	117.39	111.07
2	B	47	THR	CA-CB-OG1	5.90	118.45	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	132	THR	CA-CB-OG1	5.90	118.45	109.60
18	X	82	LYS	N-CA-C	-5.90	103.86	113.19
21	N	653	ARG	CA-C-O	-5.90	114.29	120.55
33	J	376	HIS	CE1-NE2-CD2	-5.90	103.10	109.00
4	d	135	ILE	N-CA-C	-5.90	99.85	108.11
4	d	174	PHE	CA-CB-CG	-5.90	107.90	113.80
2	B	170	ALA	CA-C-N	5.90	128.19	120.28
2	B	170	ALA	C-N-CA	5.90	128.19	120.28
4	D	57	THR	N-CA-C	-5.90	105.92	114.12
6	F	67	ASP	O-C-N	-5.90	116.68	122.99
8	h	31	THR	N-CA-CB	5.90	120.38	110.77
2	B	19	GLY	CA-C-N	5.90	130.71	120.68
2	B	19	GLY	C-N-CA	5.90	130.71	120.68
27	O	175	ASN	O-C-N	-5.90	115.43	122.15
21	N	782	PHE	N-CA-CB	5.90	120.45	110.49
23	P	86	HIS	N-CA-C	-5.90	107.32	114.75
24	Q	15	VAL	N-CA-C	-5.90	104.99	110.53
5	E	73	HIS	CB-CG-CD2	-5.89	123.54	131.20
20	Z	353	VAL	N-CA-CB	5.89	114.21	110.50
20	Z	455	ILE	CA-C-N	5.89	126.65	119.99
20	Z	455	ILE	C-N-CA	5.89	126.65	119.99
20	Z	470	ALA	CA-C-N	5.89	128.50	120.54
20	Z	470	ALA	C-N-CA	5.89	128.50	120.54
21	N	597	ARG	CB-CA-C	-5.89	101.62	110.88
25	R	232	VAL	CA-C-N	5.89	128.18	120.28
25	R	232	VAL	C-N-CA	5.89	128.18	120.28
26	U	252	HIS	CE1-NE2-CD2	-5.89	103.11	109.00
1	a	130	GLN	O-C-N	-5.89	115.86	122.10
3	c	220	ALA	N-CA-C	-5.89	100.58	109.95
3	C	191	GLU	CB-CG-CD	-5.89	102.58	112.60
12	5	97	ALA	CB-CA-C	-5.89	103.70	111.42
13	6	56	ASP	CA-CB-CG	-5.89	106.71	112.60
22	S	33	GLU	CA-C-O	5.89	126.67	120.42
27	O	187	SER	N-CA-CB	5.89	118.88	110.16
9	i	153	TYR	N-CA-C	-5.89	98.00	108.13
10	3	11	ILE	CB-CA-C	-5.89	101.59	110.55
29	I	353	PRO	CA-C-O	-5.89	114.73	121.56
7	g	179	LEU	N-CA-C	-5.89	105.19	112.90
30	K	44	ASN	OD1-CG-ND2	5.89	128.49	122.60
14	7	141	ASN	OD1-CG-ND2	5.89	128.49	122.60
22	S	333	PHE	CB-CG-CD1	-5.89	110.69	120.70
5	e	9	ASP	CA-C-N	5.89	131.44	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	9	ASP	C-N-CA	5.89	131.44	122.08
6	f	51	ARG	N-CA-CB	5.89	120.48	110.71
7	g	28	VAL	CA-C-N	5.89	128.17	120.28
7	g	28	VAL	C-N-CA	5.89	128.17	120.28
25	R	217	HIS	CA-CB-CG	-5.89	107.91	113.80
25	R	307	TYR	CA-C-N	5.89	128.65	120.29
25	R	307	TYR	C-N-CA	5.89	128.65	120.29
25	R	311	THR	N-CA-CB	5.89	119.28	110.22
31	L	206	ILE	CA-C-O	5.89	126.01	119.42
31	L	296	SER	CA-C-N	5.89	128.76	120.28
31	L	296	SER	C-N-CA	5.89	128.76	120.28
33	J	102	ILE	O-C-N	5.89	129.24	122.82
33	J	250	ILE	CB-CA-C	-5.89	104.35	112.24
1	a	40	ILE	N-CA-C	-5.88	99.82	109.12
1	a	237	SER	N-CA-CB	5.88	118.86	110.44
2	b	23	TYR	CB-CA-C	-5.88	101.02	110.79
12	l	203	CYS	N-CA-C	-5.88	98.82	108.41
4	D	199	LEU	N-CA-C	-5.88	104.95	111.36
7	G	210	LYS	CA-C-N	5.88	131.83	122.59
7	G	210	LYS	C-N-CA	5.88	131.83	122.59
14	7	120	LEU	N-CA-CB	5.88	121.07	110.83
15	W	147	ILE	CB-CA-C	-5.88	104.10	112.22
21	N	103	SER	CA-C-N	5.88	128.16	120.28
21	N	103	SER	C-N-CA	5.88	128.16	120.28
27	O	24	PRO	CA-C-N	5.88	128.16	120.28
27	O	24	PRO	C-N-CA	5.88	128.16	120.28
31	L	77	ARG	O-C-N	-5.88	114.44	122.33
9	i	170	HIS	CE1-NE2-CD2	-5.88	103.12	109.00
25	R	328	PHE	N-CA-CB	-5.88	101.46	110.16
9	2	160	SER	O-C-N	5.88	128.21	122.09
12	5	84	GLN	CA-C-O	5.88	126.65	120.42
12	l	241	HIS	CG-CD2-NE2	5.88	113.08	107.20
25	R	99	TYR	CA-CB-CG	5.88	124.48	113.90
9	i	247	VAL	CA-C-O	5.87	127.42	120.72
12	5	256	THR	N-CA-CB	5.87	119.53	110.60
13	6	194	ASP	CA-C-N	5.87	128.07	120.44
13	6	194	ASP	C-N-CA	5.87	128.07	120.44
18	X	56	PRO	CA-C-O	-5.87	114.92	121.32
22	S	121	VAL	O-C-N	5.87	127.67	121.91
22	S	133	GLU	CA-C-O	-5.87	114.32	120.55
1	A	140	ILE	N-CA-CB	5.87	118.04	110.99
13	6	229	ARG	NE-CZ-NH2	-5.87	113.92	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	19	LEU	CA-C-N	5.87	132.75	121.54
3	c	19	LEU	C-N-CA	5.87	132.75	121.54
14	n	181	ALA	CA-C-N	5.87	130.71	121.08
14	n	181	ALA	C-N-CA	5.87	130.71	121.08
3	C	13	PHE	N-CA-CB	5.87	118.62	110.17
15	W	2	VAL	CA-C-O	-5.87	115.28	121.44
2	b	189	ILE	O-C-N	-5.87	116.18	121.87
17	T	65	GLY	CA-C-N	5.87	128.42	120.44
17	T	65	GLY	C-N-CA	5.87	128.42	120.44
23	P	207	THR	CA-C-O	-5.87	113.44	120.65
26	U	86	LYS	N-CA-C	-5.87	104.78	112.41
30	K	175	GLY	CA-C-N	5.87	129.93	121.54
30	K	175	GLY	C-N-CA	5.87	129.93	121.54
1	a	104	PHE	CA-C-O	-5.86	114.66	120.82
3	c	134	SER	N-CA-C	-5.86	98.31	108.69
2	B	128	ARG	N-CA-C	-5.86	99.40	108.55
27	O	271	LYS	CA-C-N	5.86	127.87	120.72
27	O	271	LYS	C-N-CA	5.86	127.87	120.72
33	J	54	LYS	N-CA-CB	5.86	118.57	110.07
7	G	121	GLN	OE1-CD-NE2	5.86	128.46	122.60
21	N	60	MET	CA-C-N	5.86	128.62	120.29
21	N	60	MET	C-N-CA	5.86	128.62	120.29
2	b	167	GLY	CA-C-N	5.86	128.13	120.28
2	b	167	GLY	C-N-CA	5.86	128.13	120.28
23	P	196	ALA	CA-C-O	5.86	126.71	119.97
23	P	21	PHE	N-CA-CB	5.86	119.03	110.30
8	1	56	GLY	CA-C-O	-5.86	114.45	121.83
11	4	185	ASP	CA-CB-CG	5.86	118.46	112.60
23	P	123	ARG	CA-C-O	-5.86	114.34	120.55
24	Q	361	HIS	CA-C-N	5.86	128.49	120.46
24	Q	361	HIS	C-N-CA	5.86	128.49	120.46
30	K	228	ASN	N-CA-C	-5.86	105.03	111.82
5	e	153	TYR	CA-CB-CG	-5.86	103.36	113.90
4	D	23	ALA	CA-C-N	5.86	128.60	120.29
4	D	23	ALA	C-N-CA	5.86	128.60	120.29
4	D	182	LYS	N-CA-C	5.86	117.46	111.14
28	H	308	PHE	CA-C-N	-5.86	112.06	122.07
28	H	308	PHE	C-N-CA	-5.86	112.06	122.07
29	I	143	PRO	N-CA-C	5.86	124.53	112.47
31	L	226	THR	O-C-N	-5.86	114.88	122.37
5	e	27	SER	N-CA-C	5.85	117.66	111.28
10	j	179	ALA	N-CA-C	-5.85	105.80	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	173	GLY	N-CA-C	-5.85	102.05	110.60
12	l	277	GLU	N-CA-C	5.85	117.33	111.07
25	R	401	HIS	CG-CD2-NE2	5.85	113.05	107.20
30	K	365	GLU	N-CA-CB	5.85	118.56	110.07
32	M	210	MET	O-C-N	-5.85	115.92	122.12
5	e	158	ALA	CB-CA-C	-5.85	99.60	109.72
11	k	13	VAL	N-CA-CB	5.85	119.48	111.41
26	U	245	ASP	CA-CB-CG	-5.85	106.75	112.60
1	a	107	LYS	N-CA-C	-5.85	106.30	113.50
12	l	100	TRP	N-CA-C	-5.85	100.41	109.24
22	S	261	HIS	N-CA-C	-5.85	104.69	112.94
7	g	40	ILE	N-CA-CB	5.85	118.72	111.41
7	G	217	SER	N-CA-C	-5.85	100.18	109.07
23	P	372	THR	N-CA-C	-5.85	101.55	110.14
29	I	122	SER	CA-C-N	5.85	125.55	119.82
29	I	122	SER	C-N-CA	5.85	125.55	119.82
32	M	274	ALA	CA-C-O	-5.85	112.15	120.16
6	f	184	GLY	CA-C-N	5.84	128.94	122.74
6	f	184	GLY	C-N-CA	5.84	128.94	122.74
12	l	219	TYR	N-CA-C	-5.84	98.76	108.34
15	W	166	GLU	CA-C-N	5.84	131.01	122.77
15	W	166	GLU	C-N-CA	5.84	131.01	122.77
22	S	91	ASN	OD1-CG-ND2	5.84	128.44	122.60
22	S	393	ARG	CA-C-O	5.84	126.62	120.42
29	I	112	ILE	CA-CB-CG2	-5.84	100.57	110.50
32	M	18	LEU	N-CA-C	-5.84	100.65	108.19
33	J	1	MET	CA-C-N	5.84	132.71	121.54
33	J	1	MET	C-N-CA	5.84	132.71	121.54
4	d	127	ARG	CD-NE-CZ	-5.84	116.22	124.40
2	B	169	VAL	CA-C-N	5.84	128.38	120.44
2	B	169	VAL	C-N-CA	5.84	128.38	120.44
21	N	813	ARG	CA-C-N	5.84	128.59	120.29
21	N	813	ARG	C-N-CA	5.84	128.59	120.29
24	Q	246	TYR	N-CA-CB	5.84	118.90	110.20
27	O	99	LEU	CA-C-N	5.84	129.19	120.31
27	O	99	LEU	C-N-CA	5.84	129.19	120.31
30	K	142	HIS	O-C-N	-5.84	113.69	122.28
5	e	57	PRO	CA-C-N	5.84	128.38	120.44
5	e	57	PRO	C-N-CA	5.84	128.38	120.44
6	f	103	LEU	N-CA-CB	5.84	119.50	110.21
8	h	55	SER	N-CA-C	-5.84	99.53	108.76
17	T	78	PHE	N-CA-CB	5.84	118.64	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	743	ILE	N-CA-C	5.84	116.02	110.53
26	U	17	SER	CA-C-N	5.84	128.10	120.28
26	U	17	SER	C-N-CA	5.84	128.10	120.28
27	O	351	SER	O-C-N	-5.84	116.17	122.19
11	k	130	TYR	O-C-N	-5.84	117.17	123.42
1	A	221	ASN	N-CA-C	-5.84	105.48	113.30
4	D	45	GLY	O-C-N	-5.84	117.07	123.49
21	N	686	ILE	N-CA-C	-5.84	104.83	110.72
24	Q	264	TYR	O-C-N	5.83	130.15	122.33
32	M	173	ASP	O-C-N	5.83	128.76	122.34
6	f	10	THR	CB-CA-C	-5.83	101.93	111.50
13	m	66	ALA	N-CA-C	5.83	118.39	111.33
2	B	139	HIS	CA-CB-CG	5.83	119.63	113.80
12	5	131	GLU	CA-C-N	5.83	128.02	120.44
12	5	131	GLU	C-N-CA	5.83	128.02	120.44
14	7	158	GLN	CB-CG-CD	5.83	122.52	112.60
21	N	600	THR	O-C-N	-5.83	115.79	122.09
27	O	379	LYS	CA-C-O	5.83	126.60	120.42
31	L	186	LEU	N-CA-C	-5.83	103.64	111.87
4	D	236	ILE	N-CA-C	-5.83	104.67	110.62
16	V	221	TRP	CA-C-N	5.83	132.68	121.54
16	V	221	TRP	C-N-CA	5.83	132.68	121.54
22	S	20	HIS	CE1-NE2-CD2	-5.83	103.17	109.00
22	S	338	MET	CA-C-N	5.83	128.09	120.28
22	S	338	MET	C-N-CA	5.83	128.09	120.28
29	I	253	ILE	N-CA-C	-5.83	100.02	108.36
31	L	223	PRO	CA-C-O	-5.83	116.12	120.73
32	M	74	GLN	CB-CG-CD	-5.83	102.69	112.60
24	Q	145	HIS	N-CA-C	5.83	117.71	111.36
7	g	106	PRO	N-CD-CG	5.83	111.94	103.20
14	n	160	LEU	N-CA-C	-5.83	98.58	108.26
4	D	66	LYS	CA-C-O	5.83	127.33	120.69
7	G	79	SER	CA-C-O	5.83	127.99	121.40
14	7	145	ASN	OD1-CG-ND2	-5.83	116.77	122.60
24	Q	177	VAL	CA-C-O	-5.83	114.67	120.85
32	M	55	ASN	CA-CB-CG	-5.83	106.77	112.60
32	M	94	LYS	N-CA-CB	5.83	118.34	110.59
3	c	208	TYR	N-CA-C	-5.83	104.93	111.28
20	Z	634	ASP	CB-CA-C	-5.83	101.69	110.90
21	N	569	LYS	CA-C-O	5.83	126.72	120.55
26	U	165	GLU	CA-C-N	5.83	128.56	120.29
26	U	165	GLU	C-N-CA	5.83	128.56	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	81	TYR	CA-C-N	5.83	128.67	120.28
27	O	81	TYR	C-N-CA	5.83	128.67	120.28
29	I	366	THR	O-C-N	-5.83	115.06	122.34
7	g	188	SER	N-CA-C	-5.82	101.86	110.48
1	A	104	PHE	CA-C-N	5.82	128.09	120.28
1	A	104	PHE	C-N-CA	5.82	128.09	120.28
13	6	97	ALA	N-CA-C	5.82	118.10	111.11
26	U	129	GLY	CA-C-N	5.82	129.81	121.02
26	U	129	GLY	C-N-CA	5.82	129.81	121.02
6	F	148	GLN	CA-C-O	5.82	127.33	120.87
15	W	69	PHE	CA-C-N	5.82	127.61	120.22
15	W	69	PHE	C-N-CA	5.82	127.61	120.22
24	Q	406	ASP	CA-CB-CG	-5.82	106.78	112.60
1	a	158	ASP	CA-C-O	-5.82	115.26	120.56
2	b	236	ARG	CB-CA-C	-5.82	103.49	110.94
5	e	119	LEU	CA-C-N	5.82	128.08	120.28
5	e	119	LEU	C-N-CA	5.82	128.08	120.28
11	k	33	ASP	CA-CB-CG	5.82	118.42	112.60
10	3	71	THR	N-CA-C	-5.82	105.67	112.89
15	W	196	SER	N-CA-C	-5.82	105.55	114.16
17	T	68	ALA	CA-C-O	5.82	126.59	120.42
17	T	239	SER	N-CA-CB	5.82	118.68	110.12
24	Q	331	THR	CA-CB-OG1	5.82	118.33	109.60
33	J	72	VAL	CA-C-O	5.82	126.44	120.39
11	4	182	LYS	N-CA-C	-5.82	99.17	109.06
28	H	309	ASP	CA-CB-CG	5.82	118.42	112.60
12	l	268	VAL	CA-CB-CG1	5.82	120.29	110.40
2	B	52	SER	N-CA-CB	5.82	118.44	110.01
11	4	19	LYS	O-C-N	-5.82	115.81	122.09
21	N	427	ILE	CA-C-O	-5.82	114.59	121.05
24	Q	344	GLU	N-CA-C	5.82	117.70	111.36
28	H	409	ARG	NE-CZ-NH2	5.82	124.44	119.20
29	I	422	ARG	CA-C-N	5.82	128.68	120.42
29	I	422	ARG	C-N-CA	5.82	128.68	120.42
3	C	190	ILE	N-CA-C	-5.82	104.69	110.62
8	1	74	LEU	O-C-N	-5.82	115.12	122.27
20	Z	739	ALA	CA-C-O	-5.82	114.26	120.42
28	H	390	ARG	NH1-CZ-NH2	-5.82	111.74	119.30
31	L	213	LYS	CA-C-N	5.82	126.37	120.38
31	L	213	LYS	C-N-CA	5.82	126.37	120.38
24	Q	20	TYR	CA-C-O	5.81	126.66	119.97
7	G	206	ASP	N-CA-C	-5.81	104.74	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	270	LEU	N-CA-C	5.81	119.98	113.01
27	O	291	ILE	CA-C-N	5.81	128.54	120.29
27	O	291	ILE	C-N-CA	5.81	128.54	120.29
27	O	368	ASP	N-CA-CB	5.81	118.66	110.12
29	I	165	ASP	N-CA-C	-5.81	102.78	110.40
30	K	100	LEU	CA-C-O	5.81	127.59	120.56
30	K	375	ASN	CB-CG-ND2	-5.81	107.68	116.40
1	a	130	GLN	N-CA-CB	5.81	118.73	111.00
11	k	172	MET	N-CA-C	-5.81	102.75	110.07
14	n	124	TYR	CA-C-N	5.81	127.88	120.56
14	n	124	TYR	C-N-CA	5.81	127.88	120.56
4	D	99	THR	N-CA-C	-5.81	106.73	113.88
24	Q	208	ILE	CA-CB-CG2	-5.81	100.62	110.50
24	Q	320	GLN	CB-CG-CD	-5.81	102.72	112.60
27	O	233	LEU	CB-CA-C	-5.81	101.15	110.79
6	f	64	ILE	CA-C-N	5.81	129.60	121.24
6	f	64	ILE	C-N-CA	5.81	129.60	121.24
7	g	107	ILE	N-CA-CB	5.81	116.62	110.17
16	V	31	SER	CA-C-O	-5.81	114.26	120.42
18	X	75	TRP	O-C-N	-5.81	116.71	123.27
23	P	228	SER	CA-C-N	5.81	128.06	120.28
23	P	228	SER	C-N-CA	5.81	128.06	120.28
33	J	31	GLU	O-C-N	5.81	129.01	122.22
33	J	229	MET	N-CA-CB	5.81	120.31	110.49
5	e	188	HIS	CB-CG-ND1	5.81	131.41	122.70
1	A	185	HIS	CE1-NE2-CD2	-5.81	103.19	109.00
9	2	70	ILE	N-CA-CB	-5.81	105.12	112.15
22	S	241	PHE	CA-C-N	5.81	128.06	120.28
22	S	241	PHE	C-N-CA	5.81	128.06	120.28
3	c	169	THR	CA-C-N	5.80	128.06	120.28
3	c	169	THR	C-N-CA	5.80	128.06	120.28
4	d	70	HIS	CG-CD2-NE2	5.80	113.00	107.20
12	l	284	ASN	CA-CB-CG	5.80	118.41	112.60
2	B	207	ASP	N-CA-C	-5.80	106.16	113.18
17	T	81	TYR	CA-C-N	5.80	127.99	120.44
17	T	81	TYR	C-N-CA	5.80	127.99	120.44
18	X	34	GLU	CB-CG-CD	-5.80	102.73	112.60
20	Z	251	ALA	CB-CA-C	-5.80	101.16	110.79
21	N	425	ASN	CB-CA-C	-5.80	101.15	110.79
21	N	835	LYS	O-C-N	5.80	130.15	122.95
25	R	35	GLN	N-CA-CB	5.80	118.57	110.04
23	P	126	THR	N-CA-C	-5.80	105.04	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	H	394	LYS	N-CA-C	-5.80	105.09	111.82
3	c	226	TYR	CA-C-N	5.80	129.07	120.95
3	c	226	TYR	C-N-CA	5.80	129.07	120.95
6	f	89	ARG	CB-CA-C	-5.80	101.16	110.79
1	A	237	SER	CA-C-N	5.80	128.63	120.28
1	A	237	SER	C-N-CA	5.80	128.63	120.28
21	N	709	GLY	O-C-N	-5.80	115.16	122.41
23	P	225	VAL	N-CA-C	5.80	115.99	110.42
25	R	50	VAL	CB-CA-C	-5.80	104.55	111.97
26	U	92	TRP	CD2-CE2-CZ2	-5.80	116.60	122.40
27	O	58	ARG	O-C-N	5.80	128.04	122.07
27	O	208	ALA	CA-C-N	5.80	128.53	120.29
27	O	208	ALA	C-N-CA	5.80	128.53	120.29
6	f	161	ILE	N-CA-C	-5.80	100.13	108.42
12	l	273	TRP	CD2-CE3-CZ3	5.80	126.14	118.60
11	4	50	ALA	CB-CA-C	-5.80	101.14	109.84
24	Q	129	LYS	N-CA-CB	5.80	119.75	111.05
24	Q	178	HIS	CE1-NE2-CD2	-5.80	103.20	109.00
27	O	181	PHE	N-CA-CB	5.80	118.84	110.20
27	O	216	ASP	CA-CB-CG	-5.80	106.80	112.60
33	J	223	ILE	N-CA-CB	5.80	120.80	111.23
15	W	150	ASN	CA-CB-CG	5.80	118.40	112.60
26	U	84	ASN	CA-CB-CG	-5.80	106.80	112.60
11	k	79	ALA	CA-C-N	5.80	129.63	120.47
11	k	79	ALA	C-N-CA	5.80	129.63	120.47
12	l	87	ILE	CA-C-O	5.80	126.12	120.27
7	G	171	SER	N-CA-CB	5.80	118.74	110.16
20	Z	916	LEU	N-CA-C	-5.80	105.40	112.88
23	P	262	SER	CA-C-N	5.80	128.05	120.28
23	P	262	SER	C-N-CA	5.80	128.05	120.28
26	U	147	GLY	CA-C-N	5.80	130.48	122.77
26	U	147	GLY	C-N-CA	5.80	130.48	122.77
30	K	50	LYS	CA-C-N	5.80	128.05	120.28
30	K	50	LYS	C-N-CA	5.80	128.05	120.28
33	J	7	SER	CA-C-N	5.80	128.99	120.82
33	J	7	SER	C-N-CA	5.80	128.99	120.82
5	E	228	PHE	CA-C-O	5.79	126.92	120.43
15	W	192	LEU	CA-C-N	5.79	129.06	120.95
15	W	192	LEU	C-N-CA	5.79	129.06	120.95
4	d	229	ILE	CA-C-N	5.79	128.04	120.28
4	d	229	ILE	C-N-CA	5.79	128.04	120.28
6	f	111	LEU	CA-C-N	5.79	128.04	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	111	LEU	C-N-CA	5.79	128.04	120.28
6	f	118	LYS	CA-C-N	-5.79	112.60	122.56
6	f	118	LYS	C-N-CA	-5.79	112.60	122.56
8	h	129	HIS	N-CA-C	-5.79	98.17	108.13
5	E	138	PHE	CA-CB-CG	-5.79	108.01	113.80
14	7	212	ASN	CA-C-N	5.79	127.97	120.44
14	7	212	ASN	C-N-CA	5.79	127.97	120.44
15	W	80	GLN	CA-C-O	5.79	127.32	120.66
23	P	418	ASN	O-C-N	5.79	128.12	122.09
32	M	234	ALA	CB-CA-C	-5.79	101.00	110.85
33	J	5	VAL	O-C-N	5.79	127.49	121.87
33	J	70	SER	N-CA-C	-5.79	98.17	108.13
1	A	212	ASP	N-CA-CB	5.79	118.41	110.01
16	V	39	LYS	N-CA-C	-5.79	104.89	111.14
18	X	18	ASN	CB-CA-C	-5.79	100.11	109.72
24	Q	161	LEU	CA-C-O	5.79	126.69	120.55
25	R	413	LYS	CB-CA-C	-5.79	101.00	110.85
33	J	123	HIS	CA-C-N	5.79	131.68	122.59
33	J	123	HIS	C-N-CA	5.79	131.68	122.59
7	g	235	LEU	N-CA-C	5.79	117.59	111.28
24	Q	194	SER	CA-C-N	5.79	128.04	120.28
24	Q	194	SER	C-N-CA	5.79	128.04	120.28
32	M	343	LEU	CA-C-N	5.79	130.48	120.58
32	M	343	LEU	C-N-CA	5.79	130.48	120.58
4	d	247	ASP	N-CA-C	-5.79	104.57	111.69
13	m	152	SER	N-CA-CB	-5.79	101.04	110.42
6	F	147	PHE	CA-C-O	5.79	126.69	120.38
23	P	32	CYS	N-CA-C	5.79	118.37	111.71
25	R	283	THR	CA-C-N	5.79	127.96	120.44
25	R	283	THR	C-N-CA	5.79	127.96	120.44
27	O	240	GLU	CA-C-N	5.79	130.52	120.68
27	O	240	GLU	C-N-CA	5.79	130.52	120.68
2	b	240	SER	CA-C-N	5.79	128.03	120.28
2	b	240	SER	C-N-CA	5.79	128.03	120.28
7	g	89	VAL	CA-C-N	5.79	128.03	120.28
7	g	89	VAL	C-N-CA	5.79	128.03	120.28
6	F	230	VAL	CA-C-N	5.79	130.38	120.72
6	F	230	VAL	C-N-CA	5.79	130.38	120.72
10	3	177	ARG	NE-CZ-NH2	5.79	124.41	119.20
14	7	36	GLN	CA-C-N	5.79	125.72	119.76
14	7	36	GLN	C-N-CA	5.79	125.72	119.76
14	7	164	ASN	O-C-N	-5.79	116.80	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	42	GLY	CA-C-O	-5.78	116.14	121.63
7	G	236	LEU	CA-C-O	-5.78	114.74	120.70
6	f	20	PHE	CA-CB-CG	-5.78	108.02	113.80
25	R	134	TRP	CZ3-CH2-CZ2	-5.78	113.98	121.50
11	4	146	HIS	CG-CD2-NE2	5.78	112.98	107.20
12	5	121	ALA	N-CA-C	-5.78	100.28	109.07
8	1	67	ILE	O-C-N	-5.78	115.27	121.80
13	6	73	VAL	N-CA-C	-5.78	105.45	111.58
29	I	91	GLU	CA-C-O	5.78	126.67	120.55
2	b	244	ASN	CA-C-O	5.78	126.61	119.97
3	C	187	ASP	CA-C-N	5.78	128.49	120.29
3	C	187	ASP	C-N-CA	5.78	128.49	120.29
4	D	7	ALA	N-CA-C	5.78	118.39	110.24
14	7	257	ASP	N-CA-C	-5.78	106.27	113.38
21	N	646	LYS	CA-C-N	5.78	129.44	120.60
21	N	646	LYS	C-N-CA	5.78	129.44	120.60
22	S	294	ILE	CB-CA-C	-5.78	104.34	112.14
30	K	219	LYS	N-CA-CB	5.78	118.39	110.01
32	M	241	ALA	CA-C-N	5.78	129.57	121.02
32	M	241	ALA	C-N-CA	5.78	129.57	121.02
3	c	3	SER	CA-C-N	5.78	128.02	120.28
3	c	3	SER	C-N-CA	5.78	128.02	120.28
21	N	24	ALA	CA-C-N	5.78	128.34	120.54
21	N	24	ALA	C-N-CA	5.78	128.34	120.54
23	P	32	CYS	CA-C-N	5.78	128.49	120.29
23	P	32	CYS	C-N-CA	5.78	128.49	120.29
25	R	324	ARG	NE-CZ-NH1	-5.78	115.72	121.50
12	5	241	HIS	CA-CB-CG	-5.77	108.03	113.80
29	I	264	CYS	CA-C-N	5.77	128.02	120.28
29	I	264	CYS	C-N-CA	5.77	128.02	120.28
17	T	233	VAL	N-CA-C	-5.77	101.43	109.45
21	N	588	VAL	N-CA-C	-5.77	104.71	111.00
23	P	3	ARG	NE-CZ-NH1	-5.77	115.73	121.50
25	R	371	PHE	CB-CG-CD1	5.77	130.51	120.70
21	N	377	GLY	O-C-N	-5.77	117.42	122.90
21	N	665	ILE	O-C-N	5.77	128.84	122.66
23	P	33	ASN	CA-CB-CG	-5.77	106.83	112.60
23	P	311	TRP	O-C-N	-5.77	115.34	120.48
23	P	361	THR	CA-C-N	5.77	128.48	120.29
23	P	361	THR	C-N-CA	5.77	128.48	120.29
25	R	112	GLU	N-CA-C	5.77	118.06	111.02
33	J	84	VAL	CA-CB-CG1	-5.77	100.59	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	60	GLN	CB-CG-CD	-5.77	102.79	112.60
13	6	15	ASP	N-CA-C	-5.77	100.38	109.50
21	N	561	GLY	CA-C-O	5.77	125.46	119.00
21	N	774	ASN	CA-C-O	5.77	127.06	120.54
30	K	159	SER	CA-C-N	5.77	129.11	120.69
30	K	159	SER	C-N-CA	5.77	129.11	120.69
4	d	135	ILE	CA-CB-CG2	-5.77	100.70	110.50
10	j	126	LEU	N-CA-CB	5.77	118.53	109.94
16	V	237	ASN	CA-CB-CG	-5.77	106.83	112.60
20	Z	151	HIS	N-CA-C	-5.77	106.16	113.43
22	S	295	ALA	O-C-N	5.77	128.01	122.07
24	Q	281	ILE	N-CA-CB	5.77	118.38	110.54
25	R	366	ASN	O-C-N	-5.77	116.01	122.12
16	V	31	SER	N-CA-C	-5.77	105.08	111.36
25	R	353	MET	CA-C-N	5.77	128.48	120.29
25	R	353	MET	C-N-CA	5.77	128.48	120.29
27	O	65	PHE	N-CA-CB	5.77	118.60	110.12
8	1	41	ASP	CA-C-O	-5.76	114.70	121.16
14	7	123	SER	N-CA-C	5.76	118.34	111.71
27	O	119	SER	CA-C-O	-5.76	114.76	121.10
27	O	318	HIS	CE1-NE2-CD2	-5.76	103.24	109.00
28	H	442	ASP	CA-CB-CG	5.76	118.36	112.60
4	D	121	THR	N-CA-CB	5.76	118.28	110.10
22	S	263	ASP	N-CA-C	-5.76	98.69	108.26
31	L	54	ASN	OD1-CG-ND2	-5.76	116.84	122.60
3	c	63	THR	CA-CB-OG1	5.76	118.24	109.60
6	f	29	ILE	CA-C-O	5.76	126.96	120.85
13	m	44	ASN	OD1-CG-ND2	5.76	128.36	122.60
3	C	60	ASP	CA-CB-CG	-5.76	106.84	112.60
11	4	194	ASP	CB-CA-C	5.76	119.28	109.72
28	H	227	LEU	CA-C-O	-5.76	112.27	120.16
28	H	293	GLU	CA-C-N	5.76	128.00	120.28
28	H	293	GLU	C-N-CA	5.76	128.00	120.28
1	a	204	GLU	CA-C-N	5.76	128.00	120.28
1	a	204	GLU	C-N-CA	5.76	128.00	120.28
3	C	125	HIS	CG-CD2-NE2	5.76	112.96	107.20
19	Y	43	TRP	O-C-N	5.76	129.94	122.86
20	Z	64	TYR	N-CA-C	-5.76	106.17	113.43
27	O	235	HIS	CE1-NE2-CD2	-5.76	103.24	109.00
11	k	2	ASP	CA-C-N	5.76	128.81	120.98
11	k	2	ASP	C-N-CA	5.76	128.81	120.98
14	n	212	ASN	CA-CB-CG	-5.76	106.84	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	ASP	CA-CB-CG	5.76	118.36	112.60
6	F	177	ASP	N-CA-C	-5.76	106.25	113.28
26	U	57	GLU	N-CA-C	-5.76	99.03	108.76
9	2	77	THR	CA-C-N	5.76	127.99	120.28
9	2	77	THR	C-N-CA	5.76	127.99	120.28
9	2	116	LEU	N-CA-CB	5.76	118.68	110.16
1	A	155	TYR	CA-C-O	-5.75	114.14	120.36
7	g	148	LEU	O-C-N	-5.75	116.68	123.41
11	k	51	GLY	CA-C-N	5.75	128.46	120.29
11	k	51	GLY	C-N-CA	5.75	128.46	120.29
10	3	191	LYS	N-CA-C	-5.75	101.94	110.46
16	V	278	LYS	O-C-N	5.75	128.30	122.09
25	R	50	VAL	N-CA-CB	5.75	117.28	110.55
7	g	71	ASP	CA-CB-CG	5.75	118.35	112.60
14	n	127	GLU	CB-CG-CD	-5.75	102.82	112.60
21	N	658	ILE	CA-C-N	5.75	127.99	120.28
21	N	658	ILE	C-N-CA	5.75	127.99	120.28
29	I	215	PRO	CB-CA-C	-5.75	103.90	110.92
32	M	106	VAL	N-CA-CB	5.75	120.72	111.23
32	M	317	SER	N-CA-C	-5.75	103.34	111.56
8	h	82	PRO	O-C-N	5.75	130.16	123.14
12	l	239	ALA	N-CA-CB	5.75	118.57	110.12
1	A	33	LYS	N-CA-CB	5.75	118.95	110.56
28	H	357	ARG	O-C-N	-5.75	116.27	121.39
4	d	93	ALA	O-C-N	5.75	128.70	122.15
12	l	199	GLY	CA-C-O	-5.75	115.97	121.83
5	E	24	VAL	O-C-N	-5.75	116.30	121.87
24	Q	260	GLN	N-CA-C	5.75	117.63	111.36
25	R	268	SER	N-CA-CB	5.75	118.30	109.91
13	m	27	ASP	CA-C-N	5.75	132.13	121.62
13	m	27	ASP	C-N-CA	5.75	132.13	121.62
1	A	113	PRO	CA-C-N	5.75	127.98	120.28
1	A	113	PRO	C-N-CA	5.75	127.98	120.28
6	F	185	ASN	O-C-N	5.75	126.05	121.17
6	F	220	THR	CA-C-O	-5.75	114.34	119.86
16	V	49	VAL	CA-C-O	-5.75	116.20	121.72
24	Q	375	GLY	CA-C-N	5.75	128.45	120.29
24	Q	375	GLY	C-N-CA	5.75	128.45	120.29
29	I	317	ASP	CA-C-N	5.75	131.13	122.68
29	I	317	ASP	C-N-CA	5.75	131.13	122.68
31	L	128	ILE	CA-C-N	5.75	131.19	122.92
31	L	128	ILE	C-N-CA	5.75	131.19	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	173	GLN	CA-C-O	-5.75	115.33	121.94
33	J	81	ASP	O-C-N	5.75	130.30	122.37
3	c	46	LEU	N-CA-C	-5.74	99.54	108.90
8	h	12	ILE	N-CA-CB	5.74	120.86	111.44
2	B	130	PHE	CA-C-O	-5.74	114.87	121.19
6	F	161	ILE	CA-CB-CG2	-5.74	100.73	110.50
6	F	228	GLU	CB-CG-CD	-5.74	102.84	112.60
7	G	52	LYS	O-C-N	-5.74	115.54	123.12
23	P	213	TYR	N-CA-CB	5.74	119.31	110.46
28	H	359	ASN	N-CA-CB	5.74	119.18	110.28
29	I	374	ASP	N-CA-CB	5.74	118.34	110.01
33	J	91	GLU	CA-C-O	-5.74	112.30	120.51
5	E	225	GLN	CA-C-O	-5.74	112.84	119.56
22	S	247	VAL	CB-CA-C	5.74	120.14	112.22
24	Q	260	GLN	OE1-CD-NE2	5.74	128.34	122.60
6	f	29	ILE	CB-CA-C	-5.74	104.30	112.22
8	1	39	VAL	CB-CA-C	5.74	118.65	111.65
11	4	31	SER	N-CA-CB	5.74	120.06	110.59
22	S	144	LEU	CA-C-N	5.74	128.29	120.54
22	S	144	LEU	C-N-CA	5.74	128.29	120.54
31	L	307	GLU	CB-CG-CD	5.74	122.36	112.60
11	k	19	LYS	CA-C-O	5.74	126.61	120.24
14	n	102	ASP	CB-CA-C	-5.74	101.09	110.85
14	7	124	TYR	O-C-N	5.74	128.29	122.09
19	Y	57	THR	O-C-N	5.74	129.82	122.93
25	R	47	ALA	O-C-N	5.74	128.20	122.12
30	K	348	GLU	CB-CG-CD	-5.74	102.85	112.60
6	f	13	PHE	N-CA-C	-5.74	100.35	109.59
17	T	238	GLN	O-C-N	5.74	128.20	122.12
21	N	874	ILE	CA-C-O	-5.74	114.37	120.39
23	P	12	ASP	CA-CB-CG	5.74	118.34	112.60
29	I	191	ILE	O-C-N	-5.74	116.94	122.16
30	K	36	ASN	N-CA-C	-5.74	106.63	113.97
31	L	308	LEU	CB-CA-C	-5.74	100.02	110.63
31	L	352	PRO	N-CA-CB	5.74	108.35	103.19
1	a	135	ARG	N-CA-C	-5.74	100.32	109.04
12	5	270	GLU	CA-C-N	5.74	128.54	120.28
12	5	270	GLU	C-N-CA	5.74	128.54	120.28
17	T	51	TYR	CA-C-N	5.74	129.03	120.31
17	T	51	TYR	C-N-CA	5.74	129.03	120.31
14	7	105	THR	N-CA-CB	-5.73	101.69	110.12
20	Z	432	GLY	CA-C-N	5.73	128.75	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	432	GLY	C-N-CA	5.73	128.75	120.38
24	Q	38	SER	N-CA-C	5.73	117.20	111.07
5	e	45	GLY	N-CA-C	-5.73	105.77	111.85
4	D	237	GLU	CA-C-O	-5.73	114.80	120.82
10	3	45	HIS	CB-CG-CD2	-5.73	123.75	131.20
18	X	19	GLU	N-CA-C	-5.73	105.67	114.16
23	P	21	PHE	O-C-N	-5.73	115.38	120.48
25	R	171	MET	CG-SD-CE	-5.73	88.29	100.90
31	L	114	GLU	CB-CA-C	-5.73	100.97	110.37
1	a	113	PRO	CA-N-CD	-5.73	103.98	112.00
13	m	110	PHE	CA-CB-CG	-5.73	108.07	113.80
4	D	48	ARG	NE-CZ-NH1	-5.73	115.77	121.50
9	2	166	VAL	N-CA-CB	5.73	117.91	110.57
30	K	227	ALA	N-CA-C	5.73	117.61	111.36
31	L	299	ARG	CB-CA-C	-5.73	99.68	109.65
23	P	74	ASP	CA-C-O	5.73	126.56	119.97
27	O	77	SER	CB-CA-C	-5.73	101.28	110.79
22	S	52	TYR	CA-C-N	5.73	128.31	120.46
22	S	52	TYR	C-N-CA	5.73	128.31	120.46
24	Q	432	VAL	CA-C-N	5.73	127.96	120.28
24	Q	432	VAL	C-N-CA	5.73	127.96	120.28
25	R	244	THR	CA-C-N	5.73	132.48	121.54
25	R	244	THR	C-N-CA	5.73	132.48	121.54
27	O	324	VAL	CA-C-N	5.73	128.42	120.29
27	O	324	VAL	C-N-CA	5.73	128.42	120.29
33	J	117	SER	CA-C-N	5.73	132.48	121.54
33	J	117	SER	C-N-CA	5.73	132.48	121.54
33	J	246	PHE	CA-CB-CG	5.73	119.53	113.80
8	h	70	TYR	N-CA-CB	-5.72	101.77	110.07
8	h	145	GLY	CA-C-O	5.72	126.22	120.09
5	E	13	SER	CB-CA-C	-5.72	104.33	111.43
21	N	781	ALA	N-CA-CB	5.72	119.90	110.97
22	S	230	LYS	CA-C-N	5.72	128.22	120.44
22	S	230	LYS	C-N-CA	5.72	128.22	120.44
25	R	238	PHE	CA-C-O	5.72	127.47	120.60
32	M	125	GLN	CA-C-O	-5.72	115.19	121.31
12	l	189	TYR	N-CA-C	-5.72	99.86	109.07
7	G	234	ASP	CA-CB-CG	-5.72	106.88	112.60
18	X	9	LYS	O-C-N	-5.72	116.49	123.19
22	S	190	SER	N-CA-C	-5.72	105.04	111.28
25	R	182	ASN	CA-CB-CG	5.72	118.32	112.60
27	O	279	ILE	CB-CA-C	-5.72	104.32	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	H	368	PRO	N-CA-C	-5.72	106.67	114.80
1	A	128	TYR	N-CA-C	5.72	119.52	112.54
12	5	141	HIS	CE1-NE2-CD2	-5.72	103.28	109.00
17	T	158	GLN	N-CA-C	5.72	117.97	111.11
23	P	153	ILE	CA-C-N	5.72	128.41	120.29
23	P	153	ILE	C-N-CA	5.72	128.41	120.29
27	O	184	ASP	N-CA-C	-5.72	98.42	108.20
21	N	234	ASP	CA-C-O	5.72	126.77	120.71
25	R	241	ILE	CB-CA-C	5.72	116.93	110.41
28	H	102	CYS	N-CA-CB	5.72	118.37	109.85
32	M	202	LYS	CA-C-O	-5.72	114.43	120.55
11	k	155	GLU	N-CA-C	-5.72	105.80	112.89
1	A	72	ILE	N-CA-CB	5.72	118.88	111.67
8	1	115	ASN	OD1-CG-ND2	5.72	128.32	122.60
10	3	183	TRP	CE2-CD2-CE3	5.72	124.52	118.80
16	V	291	ASN	CA-CB-CG	-5.72	106.88	112.60
25	R	287	GLN	OE1-CD-NE2	5.72	128.32	122.60
27	O	95	SER	O-C-N	5.72	128.18	122.12
4	d	87	GLU	N-CA-CB	5.72	118.62	110.16
12	l	230	TYR	N-CA-C	-5.72	105.03	112.23
9	2	104	ARG	NE-CZ-NH1	-5.72	115.78	121.50
31	L	89	ASP	N-CA-C	-5.72	105.03	112.23
3	c	94	HIS	CB-CA-C	-5.71	101.30	110.79
20	Z	254	PRO	O-C-N	5.71	130.35	122.35
21	N	204	SER	CA-C-N	5.71	128.41	120.29
21	N	204	SER	C-N-CA	5.71	128.41	120.29
21	N	270	LEU	CA-C-N	5.71	127.94	120.28
21	N	270	LEU	C-N-CA	5.71	127.94	120.28
21	N	603	PRO	O-C-N	5.71	130.54	122.37
24	Q	418	GLN	OE1-CD-NE2	5.71	128.31	122.60
29	I	427	LYS	CB-CG-CD	5.71	124.44	111.30
5	e	162	GLY	N-CA-C	-5.71	106.59	115.67
4	d	251	LYS	CA-C-N	5.71	128.73	120.79
4	d	251	LYS	C-N-CA	5.71	128.73	120.79
13	m	203	HIS	CB-CG-ND1	5.71	131.27	122.70
18	X	51	ARG	N-CA-CB	5.71	121.47	111.19
2	B	174	PHE	CA-C-N	5.71	130.26	120.72
2	B	174	PHE	C-N-CA	5.71	130.26	120.72
17	T	222	LEU	N-CA-CB	5.71	118.51	110.12
24	Q	108	PRO	CB-CA-C	-5.71	104.45	111.64
2	b	86	VAL	CA-C-O	-5.71	114.80	120.85
11	k	82	SER	CB-CA-C	-5.71	101.15	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	903	VAL	CA-C-O	5.71	125.90	120.25
30	K	290	ARG	NE-CZ-NH2	5.71	124.34	119.20
32	M	189	GLN	N-CA-CB	-5.71	101.71	110.16
8	1	167	SER	CA-C-N	5.71	131.12	121.14
8	1	167	SER	C-N-CA	5.71	131.12	121.14
15	W	182	TYR	N-CA-C	5.71	118.44	111.82
23	P	70	ASN	CA-CB-CG	-5.71	106.89	112.60
25	R	22	PRO	CA-C-N	5.71	127.93	120.28
25	R	22	PRO	C-N-CA	5.71	127.93	120.28
25	R	271	ILE	N-CA-C	-5.71	108.29	113.71
13	m	89	ASP	CA-C-N	5.71	128.97	120.87
13	m	89	ASP	C-N-CA	5.71	128.97	120.87
30	K	148	ASP	N-CA-C	-5.71	100.27	108.60
6	f	187	ASP	CA-CB-CG	-5.70	106.90	112.60
13	m	103	HIS	CB-CG-CD2	-5.70	123.79	131.20
21	N	195	THR	CA-CB-OG1	5.70	118.16	109.60
21	N	714	THR	CA-CB-OG1	5.70	118.16	109.60
22	S	53	ILE	CA-C-O	-5.70	115.02	120.95
33	J	331	HIS	N-CA-CB	-5.70	101.52	110.30
33	J	390	MET	CA-C-N	5.70	128.39	120.29
33	J	390	MET	C-N-CA	5.70	128.39	120.29
7	G	210	LYS	N-CA-C	-5.70	101.27	108.45
8	1	17	PHE	CA-CB-CG	5.70	119.50	113.80
24	Q	281	ILE	CA-C-N	5.70	129.36	120.75
24	Q	281	ILE	C-N-CA	5.70	129.36	120.75
25	R	249	ILE	CB-CA-C	-5.70	104.35	112.22
5	e	88	MET	CA-C-O	-5.70	114.38	120.42
7	g	81	LEU	CA-C-N	5.70	123.83	120.24
7	g	81	LEU	C-N-CA	5.70	123.83	120.24
13	m	115	VAL	CA-C-N	5.70	129.65	121.50
13	m	115	VAL	C-N-CA	5.70	129.65	121.50
5	E	26	TYR	CA-C-N	5.70	127.92	120.28
5	E	26	TYR	C-N-CA	5.70	127.92	120.28
20	Z	735	GLU	N-CA-CB	5.70	119.00	110.22
21	N	209	LYS	CA-C-N	5.70	127.92	120.28
21	N	209	LYS	C-N-CA	5.70	127.92	120.28
21	N	831	GLU	CA-CB-CG	5.70	125.50	114.10
24	Q	63	GLN	CA-C-N	5.70	127.85	120.44
24	Q	63	GLN	C-N-CA	5.70	127.85	120.44
31	L	413	ASP	CB-CA-C	-5.70	100.27	110.70
3	C	94	HIS	ND1-CE1-NE2	5.70	114.10	108.40
9	2	123	ILE	N-CA-C	-5.70	99.43	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	55	GLY	CA-C-N	5.70	128.85	120.82
10	3	55	GLY	C-N-CA	5.70	128.85	120.82
12	5	118	GLY	N-CA-C	-5.70	100.95	111.04
14	7	187	LEU	CD1-CG-CD2	5.70	123.33	110.80
17	T	54	ASP	CA-CB-CG	-5.70	106.90	112.60
17	T	226	TRP	CA-C-N	5.70	126.96	119.84
17	T	226	TRP	C-N-CA	5.70	126.96	119.84
21	N	495	PRO	CA-C-N	5.70	127.92	120.28
21	N	495	PRO	C-N-CA	5.70	127.92	120.28
22	S	352	VAL	CA-CB-CG1	5.70	120.09	110.40
25	R	363	PHE	CA-C-N	5.70	127.92	120.28
25	R	363	PHE	C-N-CA	5.70	127.92	120.28
29	I	228	GLY	CA-C-N	5.70	128.19	120.38
29	I	228	GLY	C-N-CA	5.70	128.19	120.38
31	L	136	ASP	CA-CB-CG	-5.70	106.90	112.60
32	M	190	ILE	O-C-N	5.70	127.70	121.83
12	5	202	PHE	CA-CB-CG	-5.70	108.10	113.80
21	N	352	ASN	CA-C-N	5.70	127.21	120.09
21	N	352	ASN	C-N-CA	5.70	127.21	120.09
10	j	21	VAL	O-C-N	-5.70	116.73	123.00
13	m	203	HIS	CG-CD2-NE2	5.70	112.89	107.20
16	V	220	GLN	OE1-CD-NE2	5.70	128.29	122.60
23	P	83	SER	CA-C-N	5.70	128.38	120.29
23	P	83	SER	C-N-CA	5.70	128.38	120.29
33	J	229	MET	CG-SD-CE	-5.70	88.37	100.90
10	j	8	ASN	CB-CA-C	-5.69	101.71	109.28
1	a	18	ILE	CA-C-N	5.69	128.95	120.87
1	a	18	ILE	C-N-CA	5.69	128.95	120.87
2	b	187	ASP	CA-CB-CG	5.69	118.29	112.60
9	2	224	VAL	N-CA-C	-5.69	100.23	108.71
10	3	92	SER	CA-C-N	5.69	128.37	120.29
10	3	92	SER	C-N-CA	5.69	128.37	120.29
16	V	266	LEU	N-CA-C	-5.69	105.16	111.36
29	I	152	LYS	CA-C-N	5.69	128.92	120.95
29	I	152	LYS	C-N-CA	5.69	128.92	120.95
31	L	361	PHE	CA-CB-CG	-5.69	108.11	113.80
2	b	221	LEU	N-CA-C	-5.69	106.00	113.17
21	N	55	PHE	N-CA-C	-5.69	100.65	109.24
21	N	835	LYS	CA-C-N	5.69	130.72	122.36
21	N	835	LYS	C-N-CA	5.69	130.72	122.36
22	S	123	THR	N-CA-CB	5.69	118.58	110.16
25	R	47	ALA	CA-C-N	5.69	127.91	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	47	ALA	C-N-CA	5.69	127.91	120.28
28	H	241	ASP	CA-C-N	5.69	126.24	120.38
28	H	241	ASP	C-N-CA	5.69	126.24	120.38
7	g	105	THR	O-C-N	-5.69	116.14	121.72
21	N	16	ASN	CA-CB-CG	-5.69	106.91	112.60
22	S	243	ASN	N-CA-C	5.69	117.48	111.28
26	U	134	THR	N-CA-C	-5.69	99.15	108.76
3	c	119	LYS	CA-C-N	5.69	127.90	120.28
3	c	119	LYS	C-N-CA	5.69	127.90	120.28
8	h	182	ILE	N-CA-CB	5.69	117.81	110.99
1	A	209	HIS	CA-C-N	5.69	128.96	120.31
1	A	209	HIS	C-N-CA	5.69	128.96	120.31
22	S	213	THR	CA-C-O	-5.69	114.84	120.70
22	S	222	SER	N-CA-CB	5.69	118.32	110.07
6	F	35	THR	N-CA-C	-5.69	100.42	109.23
15	W	180	LEU	CA-C-N	5.69	127.90	120.28
15	W	180	LEU	C-N-CA	5.69	127.90	120.28
18	X	60	GLU	N-CA-C	-5.69	105.16	111.36
20	Z	740	VAL	CB-CA-C	-5.69	104.37	112.22
10	j	85	GLU	CB-CA-C	-5.68	101.96	110.88
11	k	165	VAL	N-CA-C	5.68	116.33	110.36
14	n	191	VAL	N-CA-CB	5.68	117.46	110.64
10	3	198	ARG	O-C-N	-5.68	116.62	123.27
32	M	26	SER	N-CA-C	-5.68	101.28	110.32
5	e	146	GLY	CA-C-O	5.68	127.55	121.75
8	h	182	ILE	O-C-N	-5.68	116.72	123.03
9	2	69	LYS	N-CA-C	-5.68	106.39	113.38
23	P	12	ASP	N-CA-C	-5.68	104.99	111.07
25	R	42	GLN	CA-C-N	5.68	128.36	120.29
25	R	42	GLN	C-N-CA	5.68	128.36	120.29
3	C	110	ILE	N-CA-CB	5.68	117.84	110.57
1	A	209	HIS	N-CA-CB	-5.68	101.48	110.28
2	B	63	LYS	N-CA-C	-5.68	105.09	113.61
4	D	168	SER	CA-C-N	5.68	128.36	120.29
4	D	168	SER	C-N-CA	5.68	128.36	120.29
10	3	187	VAL	N-CA-C	-5.68	99.36	107.77
22	S	155	LEU	CA-C-N	5.68	127.72	120.56
22	S	155	LEU	C-N-CA	5.68	127.72	120.56
22	S	354	LEU	N-CA-C	-5.68	106.35	113.28
13	m	80	VAL	CB-CA-C	-5.68	104.55	111.87
13	m	85	PHE	CA-C-O	-5.68	114.85	120.70
12	5	157	ILE	CA-C-N	5.68	128.16	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	157	ILE	C-N-CA	5.68	128.16	120.38
29	I	209	GLU	N-CA-C	-5.68	105.46	112.90
4	D	119	ARG	NE-CZ-NH1	-5.68	115.82	121.50
5	E	55	THR	CA-CB-OG1	5.68	118.12	109.60
16	V	26	THR	N-CA-C	-5.68	99.93	108.96
16	V	212	MET	N-CA-CB	5.68	118.47	110.12
22	S	326	ASP	N-CA-CB	5.68	119.05	110.42
30	K	234	PHE	N-CA-C	-5.68	100.08	108.99
32	M	413	GLU	CB-CG-CD	-5.68	102.95	112.60
10	j	133	ALA	N-CA-C	-5.67	100.72	108.38
12	l	254	HIS	CG-CD2-NE2	5.67	112.87	107.20
6	F	97	LEU	CA-C-N	5.67	130.05	121.65
6	F	97	LEU	C-N-CA	5.67	130.05	121.65
32	M	342	ARG	N-CA-C	-5.67	98.71	110.80
33	J	276	LEU	CA-C-N	5.67	127.89	120.28
33	J	276	LEU	C-N-CA	5.67	127.89	120.28
12	5	82	ARG	NH1-CZ-NH2	-5.67	111.92	119.30
9	i	133	ASP	CA-C-O	-5.67	112.39	120.16
11	k	39	SER	CB-CA-C	-5.67	101.18	109.97
21	N	23	TYR	CA-C-O	-5.67	114.54	120.55
21	N	120	ASP	CA-CB-CG	-5.67	106.93	112.60
24	Q	141	LEU	CA-C-O	-5.67	114.41	120.42
7	g	147	HIS	CE1-NE2-CD2	-5.67	103.33	109.00
8	1	73	GLU	CA-C-N	5.67	128.93	120.31
8	1	73	GLU	C-N-CA	5.67	128.93	120.31
10	3	50	PHE	N-CA-CB	5.67	120.70	110.83
22	S	452	TYR	CA-CB-CG	-5.67	103.69	113.90
14	7	217	LEU	CA-C-N	5.67	128.93	120.31
14	7	217	LEU	C-N-CA	5.67	128.93	120.31
16	V	151	VAL	N-CA-CB	5.67	116.90	110.72
17	T	164	LEU	N-CA-C	5.67	117.46	111.28
21	N	289	ILE	CB-CA-C	-5.67	104.72	111.97
22	S	198	SER	O-C-N	5.67	130.13	122.59
6	F	59	TYR	N-CA-C	-5.67	100.94	109.95
23	P	175	GLU	CB-CA-C	-5.67	101.22	110.85
23	P	431	HIS	CB-CG-ND1	5.67	131.20	122.70
30	K	219	LYS	CA-C-O	5.67	126.77	120.82
33	J	316	PHE	CA-C-O	-5.67	115.17	119.59
1	A	140	ILE	N-CA-C	-5.67	100.26	108.36
14	7	220	ARG	N-CA-C	5.67	120.31	113.17
1	A	124	LEU	N-CA-CB	5.66	118.94	110.22
12	5	124	ALA	N-CA-CB	5.66	118.22	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	67	THR	N-CA-C	-5.66	98.73	110.80
25	R	27	SER	CA-C-N	5.66	128.14	120.44
25	R	27	SER	C-N-CA	5.66	128.14	120.44
32	M	65	ASN	OD1-CG-ND2	-5.66	116.94	122.60
11	k	142	SER	N-CA-C	-5.66	105.10	112.23
21	N	20	VAL	CA-C-N	5.66	128.33	120.29
21	N	20	VAL	C-N-CA	5.66	128.33	120.29
2	b	63	LYS	CA-C-N	5.66	130.63	123.10
2	b	63	LYS	C-N-CA	5.66	130.63	123.10
13	m	187	GLU	N-CA-CB	5.66	118.44	110.12
7	G	167	LYS	CA-C-O	5.66	126.76	120.82
13	6	31	LEU	CA-C-O	5.66	126.24	120.24
21	N	480	ALA	CA-C-O	5.66	126.48	119.97
25	R	144	ILE	CA-CB-CG1	5.66	120.02	110.40
27	O	279	ILE	N-CA-CB	5.66	119.07	110.58
11	k	120	ASP	CA-C-N	5.66	128.43	120.28
11	k	120	ASP	C-N-CA	5.66	128.43	120.28
8	1	37	ASN	O-C-N	5.66	129.93	123.48
15	W	91	LEU	CA-C-N	5.66	128.32	120.29
15	W	91	LEU	C-N-CA	5.66	128.32	120.29
16	V	269	ARG	N-CA-C	5.66	117.12	111.07
21	N	421	ASP	CA-C-N	5.66	127.80	120.44
21	N	421	ASP	C-N-CA	5.66	127.80	120.44
21	N	422	TYR	CB-CG-CD1	5.66	129.29	120.80
21	N	792	SER	CA-C-O	5.66	125.91	119.18
22	S	131	THR	N-CA-C	-5.66	104.73	111.69
33	J	171	PRO	N-CA-CB	5.66	109.05	102.88
9	i	117	PHE	CA-CB-CG	-5.66	108.14	113.80
5	e	29	GLU	CA-C-N	5.66	131.25	122.49
5	e	29	GLU	C-N-CA	5.66	131.25	122.49
10	j	49	VAL	N-CA-C	-5.66	100.20	108.97
9	2	155	SER	N-CA-C	-5.66	99.08	108.75
21	N	289	ILE	CA-C-O	-5.66	115.17	121.17
22	S	286	TYR	CA-C-O	5.65	125.05	118.77
24	Q	253	ASN	CA-CB-CG	-5.65	106.95	112.60
26	U	62	ASN	CA-CB-CG	-5.65	106.95	112.60
27	O	29	PHE	N-CA-CB	5.65	118.21	110.01
32	M	291	PHE	N-CA-CB	5.65	120.05	110.49
13	6	61	SER	CA-C-N	5.65	131.32	123.07
13	6	61	SER	C-N-CA	5.65	131.32	123.07
17	T	238	GLN	CA-C-O	-5.65	114.56	120.55
21	N	534	ASP	CA-CB-CG	5.65	118.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	377	TYR	CB-CG-CD2	5.65	129.28	120.80
23	P	149	GLU	CA-C-N	5.65	131.13	121.29
23	P	149	GLU	C-N-CA	5.65	131.13	121.29
23	P	348	HIS	N-CA-C	-5.65	103.90	112.04
26	U	284	SER	CA-C-N	5.65	128.20	120.46
26	U	284	SER	C-N-CA	5.65	128.20	120.46
27	O	202	SER	N-CA-CB	5.65	119.20	110.21
3	C	100	LYS	CA-C-O	5.65	126.41	120.42
12	5	263	HIS	N-CA-C	5.65	120.17	112.88
24	Q	34	ASP	CB-CA-C	-5.65	101.41	110.79
24	Q	400	TYR	N-CA-CB	5.65	119.64	110.77
8	1	26	ASP	N-CA-C	-5.65	98.31	108.48
22	S	54	TRP	O-C-N	-5.65	116.13	122.12
22	S	483	GLU	CB-CG-CD	-5.65	103.00	112.60
27	O	37	LEU	CA-C-O	-5.65	114.67	120.54
3	c	74	ALA	N-CA-C	-5.65	100.93	109.85
8	1	83	SER	O-C-N	-5.65	116.41	122.85
22	S	105	PRO	CA-C-N	5.65	130.31	122.29
22	S	105	PRO	C-N-CA	5.65	130.31	122.29
27	O	73	ILE	O-C-N	-5.65	115.51	122.57
27	O	376	GLN	CB-CG-CD	-5.65	103.00	112.60
10	3	99	ARG	NE-CZ-NH1	-5.65	115.85	121.50
21	N	506	GLN	OE1-CD-NE2	-5.65	116.95	122.60
28	H	190	ARG	NE-CZ-NH2	5.65	124.28	119.20
31	L	209	ARG	CA-C-O	-5.65	114.56	120.55
5	e	188	HIS	N-CA-C	-5.64	100.55	108.96
6	f	52	ASN	CA-C-O	5.64	128.38	121.72
13	m	46	ARG	O-C-N	5.64	128.12	122.03
20	Z	629	VAL	N-CA-C	5.64	116.42	110.72
27	O	253	GLN	CA-C-N	5.64	127.84	120.28
27	O	253	GLN	C-N-CA	5.64	127.84	120.28
5	e	183	LEU	CA-C-N	5.64	128.40	120.28
5	e	183	LEU	C-N-CA	5.64	128.40	120.28
14	7	169	THR	N-CA-CB	5.64	119.63	110.77
17	T	172	SER	N-CA-C	-5.64	98.78	110.80
28	H	129	SER	N-CA-C	-5.64	104.98	113.89
4	d	243	GLN	CA-C-N	5.64	127.84	120.28
4	d	243	GLN	C-N-CA	5.64	127.84	120.28
6	f	89	ARG	N-CA-CB	5.64	118.41	110.12
2	B	139	HIS	ND1-CE1-NE2	5.64	114.04	108.40
10	3	142	ALA	CA-C-N	5.64	128.88	120.31
10	3	142	ALA	C-N-CA	5.64	128.88	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	129	ALA	N-CA-C	-5.64	99.47	109.06
3	C	39	MET	N-CA-CB	5.64	119.41	110.55
12	5	99	ASN	CA-CB-CG	5.64	118.24	112.60
23	P	20	GLU	N-CA-C	-5.64	106.06	113.17
27	O	106	PHE	CA-CB-CG	5.64	119.44	113.80
14	7	139	LYS	N-CA-C	-5.64	105.22	111.36
17	T	150	ARG	NE-CZ-NH2	-5.64	114.13	119.20
21	N	315	ASN	CA-C-O	-5.64	114.44	120.42
1	a	203	VAL	N-CA-CB	5.64	119.03	110.58
4	d	171	VAL	CA-C-O	-5.64	114.88	120.85
9	i	170	HIS	ND1-CE1-NE2	5.64	114.04	108.40
10	j	104	PHE	N-CA-C	-5.64	98.80	110.80
5	E	16	SER	N-CA-CB	5.64	120.08	110.50
9	2	254	GLU	O-C-N	-5.64	114.73	122.23
16	V	64	ASN	N-CA-C	-5.64	99.54	108.73
18	X	87	PHE	N-CA-C	-5.64	100.63	109.25
22	S	334	HIS	CB-CG-ND1	5.64	131.15	122.70
23	P	122	ILE	CA-C-N	5.64	127.83	120.28
23	P	122	ILE	C-N-CA	5.64	127.83	120.28
29	I	247	ILE	CA-CB-CG1	5.64	119.98	110.40
9	2	212	ASP	CA-CB-CG	-5.63	106.97	112.60
21	N	682	PHE	CA-C-N	5.63	128.39	120.28
21	N	682	PHE	C-N-CA	5.63	128.39	120.28
26	U	276	ILE	N-CA-CB	5.63	118.20	110.54
30	K	80	LYS	N-CA-CB	5.63	118.18	110.01
11	k	126	VAL	N-CA-CB	5.63	121.54	111.63
7	G	44	ASP	N-CA-C	-5.63	106.76	113.97
21	N	694	LEU	CA-C-N	5.63	128.29	120.29
21	N	694	LEU	C-N-CA	5.63	128.29	120.29
24	Q	245	SER	CB-CA-C	-5.63	102.00	110.90
26	U	173	HIS	CG-CD2-NE2	5.63	112.83	107.20
29	I	382	THR	CA-C-O	-5.63	114.91	120.82
31	L	260	ALA	N-CA-C	-5.63	104.76	111.69
4	d	88	LYS	CB-CA-C	-5.63	101.45	110.79
2	B	187	ASP	CA-C-N	5.63	127.82	120.28
2	B	187	ASP	C-N-CA	5.63	127.82	120.28
3	C	188	ASP	N-CA-C	-5.63	105.22	111.36
21	N	69	TYR	CA-C-N	5.63	128.28	120.29
21	N	69	TYR	C-N-CA	5.63	128.28	120.29
21	N	477	SER	N-CA-CB	5.63	119.87	110.41
21	N	594	VAL	CA-C-O	-5.63	115.09	120.95
25	R	67	CYS	CA-C-N	5.63	127.82	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	67	CYS	C-N-CA	5.63	127.82	120.28
25	R	91	TRP	N-CA-C	-5.63	104.59	112.25
27	O	337	LEU	N-CA-C	-5.63	100.74	109.24
32	M	207	PHE	CA-CB-CG	-5.63	108.17	113.80
2	b	233	PRO	N-CA-C	-5.63	102.36	111.19
3	c	83	ASP	N-CA-CB	5.63	118.49	110.16
14	7	238	GLY	O-C-N	-5.63	117.55	122.90
8	1	62	GLN	CA-C-N	5.62	128.38	120.28
8	1	62	GLN	C-N-CA	5.62	128.38	120.28
27	O	119	SER	CA-C-N	5.62	132.28	121.54
27	O	119	SER	C-N-CA	5.62	132.28	121.54
28	H	45	TYR	CA-C-N	5.62	128.28	120.29
28	H	45	TYR	C-N-CA	5.62	128.28	120.29
7	g	172	ALA	N-CA-CB	5.62	118.17	110.01
19	Y	83	ARG	N-CA-CB	5.62	118.32	109.94
21	N	788	TYR	CB-CA-C	-5.62	100.15	111.17
24	Q	378	SER	CA-C-N	5.62	127.82	120.28
24	Q	378	SER	C-N-CA	5.62	127.82	120.28
26	U	290	ASP	CA-CB-CG	-5.62	106.98	112.60
12	l	148	ARG	N-CA-C	5.62	118.14	110.55
14	n	66	LEU	N-CA-C	-5.62	101.33	109.59
1	A	185	HIS	ND1-CE1-NE2	5.62	114.02	108.40
24	Q	252	HIS	CE1-NE2-CD2	-5.62	103.38	109.00
26	U	52	PHE	O-C-N	5.62	129.68	123.33
27	O	304	ASN	N-CA-C	-5.62	106.42	113.28
33	J	106	ASP	CA-CB-CG	-5.62	106.98	112.60
3	C	223	GLY	O-C-N	5.62	127.68	122.57
12	5	242	ARG	CB-CA-C	-5.62	99.41	109.24
22	S	248	ASP	CA-C-N	5.62	128.27	120.29
22	S	248	ASP	C-N-CA	5.62	128.27	120.29
26	U	171	VAL	N-CA-C	-5.62	105.25	110.53
3	c	236	LYS	CA-C-O	5.62	126.51	120.55
3	C	211	LEU	N-CA-CB	5.62	119.59	110.43
7	G	242	PHE	CA-C-O	5.62	126.72	120.82
15	W	144	PHE	CA-C-O	5.62	124.70	118.52
16	V	40	HIS	CB-CG-CD2	-5.62	123.90	131.20
22	S	475	TYR	N-CA-C	5.62	117.08	111.07
28	H	235	PHE	N-CA-C	-5.62	106.42	113.28
1	a	100	GLU	N-CA-C	5.62	118.34	111.82
14	n	144	TRP	CB-CG-CD2	-5.62	118.94	126.80
27	O	116	ASN	OD1-CG-ND2	-5.62	116.98	122.60
29	I	209	GLU	CA-C-N	5.62	127.81	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I	209	GLU	C-N-CA	5.62	127.81	120.28
3	c	118	ILE	CA-C-N	5.62	127.80	120.28
3	c	118	ILE	C-N-CA	5.62	127.80	120.28
12	5	241	HIS	ND1-CE1-NE2	5.62	114.02	108.40
14	7	169	THR	CA-CB-OG1	5.62	118.02	109.60
18	X	75	TRP	CE2-CD2-CE3	5.62	124.42	118.80
21	N	146	LYS	CA-C-N	5.62	130.10	120.72
21	N	146	LYS	C-N-CA	5.62	130.10	120.72
21	N	421	ASP	O-C-N	5.62	128.07	122.12
21	N	796	VAL	N-CA-C	5.62	116.35	110.62
28	H	94	GLU	N-CA-CB	5.62	119.98	110.49
30	K	286	THR	CA-C-N	5.62	127.16	120.14
30	K	286	THR	C-N-CA	5.62	127.16	120.14
32	M	337	LEU	N-CA-C	-5.62	104.32	113.19
2	B	221	LEU	N-CA-C	-5.61	106.28	113.02
33	J	149	MET	CG-SD-CE	-5.61	88.55	100.90
18	X	13	GLY	CA-C-N	5.61	130.21	121.85
18	X	13	GLY	C-N-CA	5.61	130.21	121.85
18	X	69	ILE	CB-CA-C	-5.61	104.40	110.85
23	P	292	LYS	N-CA-C	-5.61	106.02	112.92
18	X	121	ILE	N-CA-C	-5.61	104.89	111.00
24	Q	216	ALA	N-CA-C	-5.61	105.16	111.28
25	R	162	ILE	CA-C-N	5.61	129.22	120.75
25	R	162	ILE	C-N-CA	5.61	129.22	120.75
26	U	240	GLY	CA-C-N	5.61	130.59	122.29
26	U	240	GLY	C-N-CA	5.61	130.59	122.29
21	N	774	ASN	O-C-N	-5.61	116.83	123.22
30	K	249	GLU	N-CA-C	5.61	117.47	111.36
31	L	349	ILE	N-CA-C	-5.61	101.33	107.73
1	a	191	ILE	CB-CA-C	5.61	120.49	111.29
13	6	93	SER	CA-C-N	5.61	127.83	120.60
13	6	93	SER	C-N-CA	5.61	127.83	120.60
25	R	422	ARG	CA-C-O	5.61	126.42	119.97
32	M	246	LEU	N-CA-C	-5.61	99.53	109.06
33	J	278	GLN	CA-C-O	5.61	127.09	120.70
4	D	162	GLN	CA-CB-CG	5.61	125.31	114.10
5	E	15	PHE	CA-C-O	-5.61	114.64	120.70
10	3	144	ASP	CA-C-O	5.61	126.49	120.55
16	V	25	GLU	N-CA-CB	5.61	118.28	110.04
21	N	283	ASP	N-CA-C	5.61	116.05	109.60
27	O	16	MET	CA-C-N	5.61	128.83	120.31
27	O	16	MET	C-N-CA	5.61	128.83	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	305	ILE	CA-C-O	-5.61	114.91	121.80
30	K	393	ARG	CA-C-N	5.61	128.35	120.28
30	K	393	ARG	C-N-CA	5.61	128.35	120.28
2	b	150	VAL	N-CA-C	-5.60	100.35	108.36
13	m	154	ILE	CA-C-N	5.60	126.73	119.78
13	m	154	ILE	C-N-CA	5.60	126.73	119.78
7	G	72	ARG	CA-C-O	-5.60	113.28	119.78
13	6	230	ASP	CA-CB-CG	-5.60	107.00	112.60
14	7	50	ASP	CA-CB-CG	5.60	118.20	112.60
22	S	490	ASN	CA-CB-CG	-5.60	107.00	112.60
27	O	43	GLU	CB-CA-C	-5.60	101.32	110.85
28	H	391	ILE	N-CA-C	-5.60	105.06	110.72
29	I	91	GLU	O-C-N	-5.60	116.18	122.12
13	m	122	LEU	N-CA-C	-5.60	99.89	109.24
5	E	64	ILE	CA-C-O	-5.60	114.55	120.48
16	V	111	HIS	CB-CG-CD2	-5.60	123.92	131.20
21	N	510	HIS	CG-CD2-NE2	5.60	112.80	107.20
29	I	200	LEU	CA-C-O	-5.60	112.49	120.16
32	M	364	HIS	ND1-CE1-NE2	5.60	114.00	108.40
33	J	344	ARG	CA-C-N	5.60	128.24	120.29
33	J	344	ARG	C-N-CA	5.60	128.24	120.29
5	e	160	PRO	N-CA-C	-5.60	107.35	114.35
21	N	878	GLN	CA-C-N	5.60	128.24	120.29
21	N	878	GLN	C-N-CA	5.60	128.24	120.29
22	S	234	ILE	O-C-N	5.60	127.30	121.87
24	Q	272	LEU	CA-C-O	5.60	126.42	120.10
28	H	377	PHE	N-CA-C	-5.60	100.58	109.76
33	J	184	GLY	CA-C-O	-5.60	116.49	121.64
7	g	203	ALA	CA-C-N	5.60	130.72	121.99
7	g	203	ALA	C-N-CA	5.60	130.72	121.99
23	P	114	THR	N-CA-C	-5.60	105.08	111.07
23	P	373	GLU	O-C-N	-5.60	116.19	122.12
2	B	90	ARG	NE-CZ-NH1	5.59	127.09	121.50
5	E	153	TYR	N-CA-C	-5.59	100.58	109.76
16	V	261	LEU	CA-C-N	5.59	132.23	121.54
16	V	261	LEU	C-N-CA	5.59	132.23	121.54
28	H	167	ASP	N-CA-CB	5.59	119.24	110.46
32	M	59	LEU	CA-C-O	-5.59	113.78	120.10
1	A	95	LEU	N-CA-C	5.59	117.06	111.07
24	Q	192	ALA	N-CA-CB	5.59	118.34	110.12
4	d	105	THR	O-C-N	-5.59	116.71	123.03
5	e	230	ILE	CB-CA-C	-5.59	104.19	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	26	ALA	CA-C-N	5.59	129.91	120.29
4	D	26	ALA	C-N-CA	5.59	129.91	120.29
21	N	623	PHE	CA-CB-CG	-5.59	108.21	113.80
25	R	81	HIS	CA-C-N	5.59	129.04	120.82
25	R	81	HIS	C-N-CA	5.59	129.04	120.82
5	e	130	GLU	CA-CB-CG	5.59	125.28	114.10
8	h	67	ILE	N-CA-C	5.59	116.36	110.72
12	l	273	TRP	CE2-CD2-CE3	-5.59	113.21	118.80
14	7	95	HIS	CA-C-O	5.59	126.24	119.31
16	V	261	LEU	O-C-N	-5.59	116.72	123.03
21	N	482	ALA	N-CA-C	5.59	117.37	111.28
23	P	23	LYS	CA-C-N	5.59	128.12	120.46
23	P	23	LYS	C-N-CA	5.59	128.12	120.46
3	c	47	ALA	CB-CA-C	-5.59	99.87	109.65
6	f	194	VAL	O-C-N	5.59	127.29	121.87
9	2	160	SER	N-CA-C	5.59	117.82	111.11
21	N	199	ASN	N-CA-CB	5.59	118.61	109.95
7	g	22	PHE	N-CA-C	-5.59	105.27	111.36
12	l	209	THR	O-C-N	-5.59	115.78	122.15
10	3	49	VAL	N-CA-C	-5.59	100.38	108.87
14	7	201	THR	N-CA-C	-5.59	100.07	109.07
17	T	123	HIS	O-C-N	-5.59	115.78	122.15
20	Z	287	ARG	CG-CD-NE	-5.59	99.71	112.00
22	S	347	HIS	CA-CB-CG	5.59	119.39	113.80
25	R	417	TYR	N-CA-CB	5.59	118.43	110.16
26	U	116	ASN	OD1-CG-ND2	5.59	128.19	122.60
29	I	404	LEU	CB-CA-C	-5.59	100.48	110.70
31	L	375	ASP	CA-C-N	5.59	127.77	120.28
31	L	375	ASP	C-N-CA	5.59	127.77	120.28
32	M	357	ARG	CA-C-N	5.59	127.77	120.28
32	M	357	ARG	C-N-CA	5.59	127.77	120.28
9	2	148	THR	CA-C-O	5.58	127.08	120.66
21	N	483	LEU	CA-C-N	5.58	126.14	120.00
21	N	483	LEU	C-N-CA	5.58	126.14	120.00
29	I	318	ASP	O-C-N	5.58	129.73	122.86
16	V	186	GLN	CA-C-N	5.58	128.03	120.38
16	V	186	GLN	C-N-CA	5.58	128.03	120.38
17	T	18	GLY	N-CA-C	-5.58	107.40	115.27
28	H	387	ASN	CA-CB-CG	-5.58	107.02	112.60
30	K	246	TYR	N-CA-C	-5.58	100.64	108.96
32	M	173	ASP	CA-CB-CG	5.58	118.18	112.60
10	3	87	PHE	CA-CB-CG	-5.58	108.22	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	186	GLU	CA-C-N	5.58	128.22	120.29
13	6	186	GLU	C-N-CA	5.58	128.22	120.29
30	K	106	ASN	OD1-CG-ND2	-5.58	117.02	122.60
32	M	426	LYS	N-CA-CB	5.58	119.08	110.21
1	A	37	GLN	CB-CA-C	-5.58	101.96	109.16
14	7	145	ASN	CA-C-O	-5.58	115.47	121.38
30	K	398	ASN	CA-CB-CG	-5.58	107.02	112.60
32	M	154	LEU	O-C-N	-5.58	116.55	123.36
33	J	190	PRO	N-CA-C	5.58	117.51	110.70
6	F	210	ASN	CA-C-N	5.58	130.06	122.19
6	F	210	ASN	C-N-CA	5.58	130.06	122.19
13	6	166	ASN	OD1-CG-ND2	-5.58	117.02	122.60
21	N	478	GLY	CA-C-O	-5.58	114.17	120.30
24	Q	183	LYS	CA-C-N	5.58	127.59	120.56
24	Q	183	LYS	C-N-CA	5.58	127.59	120.56
3	C	196	THR	CA-C-O	-5.58	114.96	120.70
23	P	24	ILE	CA-C-N	5.58	128.21	120.29
23	P	24	ILE	C-N-CA	5.58	128.21	120.29
25	R	327	ASP	N-CA-C	-5.58	105.28	111.36
33	J	338	THR	CA-C-N	5.58	129.69	120.94
33	J	338	THR	C-N-CA	5.58	129.69	120.94
5	e	89	ILE	CA-C-N	5.57	127.75	120.28
5	e	89	ILE	C-N-CA	5.57	127.75	120.28
5	e	157	HIS	CA-CB-CG	-5.57	108.23	113.80
2	B	36	GLY	N-CA-C	-5.57	99.97	113.18
11	4	28	LEU	O-C-N	5.57	128.91	122.17
13	6	114	TYR	CA-C-N	5.57	131.49	122.68
13	6	114	TYR	C-N-CA	5.57	131.49	122.68
17	T	226	TRP	O-C-N	-5.57	116.43	121.39
17	T	75	PHE	CA-CB-CG	-5.57	108.23	113.80
29	I	198	VAL	N-CA-C	-5.57	97.75	109.34
5	E	57	PRO	N-CA-CB	5.57	108.86	103.51
6	F	145	LEU	N-CA-C	-5.57	101.09	109.95
13	6	36	ARG	CA-CB-CG	5.57	125.24	114.10
23	P	299	LEU	N-CA-C	5.57	117.16	111.14
30	K	104	ASP	N-CA-CB	5.57	120.04	111.24
6	F	229	ALA	N-CA-C	-5.57	105.13	111.14
8	1	192	VAL	CA-CB-CG2	5.57	119.87	110.40
22	S	106	GLY	N-CA-C	-5.57	107.33	115.63
2	b	173	THR	CA-C-N	5.57	128.01	120.44
2	b	173	THR	C-N-CA	5.57	128.01	120.44
10	j	105	VAL	N-CA-CB	5.57	120.42	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	71	ALA	O-C-N	5.57	128.02	122.12
1	A	195	ASN	CA-CB-CG	-5.57	107.03	112.60
17	T	81	TYR	N-CA-CB	5.57	118.08	110.01
22	S	20	HIS	CA-C-N	5.57	128.06	120.54
22	S	20	HIS	C-N-CA	5.57	128.06	120.54
22	S	362	SER	CA-C-N	5.57	127.68	120.44
22	S	362	SER	C-N-CA	5.57	127.68	120.44
25	R	136	ASN	CA-C-N	5.57	128.19	120.29
25	R	136	ASN	C-N-CA	5.57	128.19	120.29
3	c	90	THR	N-CA-CB	5.57	118.40	110.16
13	m	203	HIS	ND1-CE1-NE2	5.57	113.97	108.40
21	N	84	ALA	CA-C-O	5.57	125.26	119.14
21	N	134	THR	CA-C-O	-5.57	114.98	120.82
30	K	106	ASN	CA-CB-CG	-5.57	107.03	112.60
1	a	61	ASP	N-CA-C	-5.56	100.85	109.14
4	d	243	GLN	N-CA-CB	5.56	118.36	110.13
7	G	125	LEU	CB-CA-C	-5.56	100.77	110.17
9	2	84	VAL	N-CA-C	-5.56	106.38	113.22
15	W	140	ASP	CA-CB-CG	5.56	118.16	112.60
33	J	246	PHE	CA-C-O	-5.56	115.97	122.37
7	g	22	PHE	CB-CG-CD2	5.56	130.16	120.70
8	h	37	ASN	N-CA-C	-5.56	99.24	108.75
10	j	17	GLY	N-CA-C	-5.56	100.00	113.18
13	m	124	GLU	CA-C-O	5.56	126.01	119.28
3	C	84	ALA	CA-C-N	5.56	128.29	120.28
3	C	84	ALA	C-N-CA	5.56	128.29	120.28
16	V	128	SER	O-C-N	5.56	127.80	122.07
30	K	337	LYS	N-CA-CB	-5.56	100.53	110.82
3	c	112	VAL	CA-C-N	5.56	128.76	120.31
3	c	112	VAL	C-N-CA	5.56	128.76	120.31
9	i	57	ASP	O-C-N	-5.56	116.60	123.44
7	g	182	HIS	CA-C-O	-5.56	114.60	120.55
5	E	55	THR	O-C-N	5.56	128.92	122.25
26	U	253	ASP	CA-CB-CG	-5.56	107.04	112.60
28	H	392	HIS	CE1-NE2-CD2	-5.56	103.44	109.00
29	I	180	SER	CA-C-N	5.56	129.15	120.75
29	I	180	SER	C-N-CA	5.56	129.15	120.75
30	K	291	GLU	N-CA-C	5.56	117.42	111.36
2	b	58	SER	N-CA-C	-5.56	105.85	113.30
6	f	137	TYR	N-CA-CB	-5.56	101.71	110.77
10	j	53	ILE	O-C-N	-5.56	117.20	123.20
21	N	702	ALA	N-CA-C	5.56	117.42	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	74	ASP	CA-C-N	5.56	127.73	120.28
23	P	74	ASP	C-N-CA	5.56	127.73	120.28
30	K	143	SER	N-CA-C	-5.56	104.04	112.04
31	L	320	GLN	N-CA-C	-5.56	105.11	112.94
1	a	95	LEU	CB-CA-C	-5.56	102.12	110.90
6	f	151	GLY	CA-C-O	5.56	123.99	118.77
22	S	285	ASP	N-CA-CB	5.56	119.32	110.65
22	S	372	LEU	CA-C-N	5.56	127.72	120.28
22	S	372	LEU	C-N-CA	5.56	127.72	120.28
23	P	404	LYS	CB-CA-C	-5.56	100.55	108.88
30	K	414	GLN	CA-C-N	5.56	128.31	120.42
30	K	414	GLN	C-N-CA	5.56	128.31	120.42
3	c	4	ARG	O-C-N	5.55	128.01	122.12
3	C	50	ARG	NE-CZ-NH1	-5.55	115.94	121.50
3	C	210	ARG	CD-NE-CZ	-5.55	116.62	124.40
11	4	190	ARG	N-CA-C	-5.55	100.83	109.72
16	V	302	SER	O-C-N	-5.55	116.09	122.09
17	T	92	ASN	OD1-CG-ND2	5.55	128.16	122.60
21	N	55	PHE	CA-CB-CG	-5.55	108.25	113.80
32	M	143	ASN	N-CA-CB	5.55	119.88	110.49
9	i	171	TRP	CA-C-O	5.55	127.44	121.55
33	J	297	LEU	CA-C-O	5.55	125.73	119.18
2	B	218	ASN	CA-C-N	5.55	126.03	120.04
2	B	218	ASN	C-N-CA	5.55	126.03	120.04
3	C	195	LYS	CA-C-O	-5.55	114.53	120.42
12	5	260	TRP	CA-C-O	5.55	127.30	120.92
17	T	140	SER	N-CA-C	-5.55	108.29	114.62
25	R	206	ARG	N-CA-C	-5.55	106.55	113.38
27	O	7	ILE	CA-CB-CG1	5.55	119.84	110.40
30	K	69	LYS	N-CA-CB	5.55	118.38	110.16
31	L	144	VAL	CA-CB-CG2	-5.55	100.96	110.40
31	L	413	ASP	N-CA-CB	5.55	118.47	110.20
6	f	159	THR	O-C-N	-5.55	116.43	122.92
5	E	216	ASN	CA-CB-CG	-5.55	107.05	112.60
14	7	221	ASP	N-CA-C	-5.55	100.35	109.40
16	V	283	THR	CA-C-N	5.55	127.66	120.44
16	V	283	THR	C-N-CA	5.55	127.66	120.44
32	M	253	GLN	N-CA-C	-5.55	100.64	109.07
4	d	148	TYR	N-CA-C	-5.55	100.92	109.52
4	d	232	TYR	CB-CG-CD1	5.55	129.12	120.80
12	l	153	ALA	CA-C-N	5.55	127.65	120.44
12	l	153	ALA	C-N-CA	5.55	127.65	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	187	ILE	O-C-N	-5.55	117.19	123.18
22	S	487	THR	CA-C-N	5.55	127.65	120.44
22	S	487	THR	C-N-CA	5.55	127.65	120.44
25	R	187	VAL	N-CA-C	5.55	115.75	110.42
26	U	108	GLU	CA-C-N	5.55	128.17	120.29
26	U	108	GLU	C-N-CA	5.55	128.17	120.29
28	H	361	LEU	N-CA-C	-5.55	100.50	108.60
10	j	17	GLY	CA-C-N	5.55	130.56	122.85
10	j	17	GLY	C-N-CA	5.55	130.56	122.85
9	2	104	ARG	NH1-CZ-NH2	5.55	126.51	119.30
21	N	652	VAL	CA-C-N	5.55	127.71	120.28
21	N	652	VAL	C-N-CA	5.55	127.71	120.28
22	S	155	LEU	O-C-N	5.55	128.47	122.15
28	H	49	LEU	N-CA-C	-5.55	104.63	111.40
9	i	82	GLU	O-C-N	5.54	128.71	122.22
12	l	161	LEU	O-C-N	5.54	127.78	122.07
19	Y	41	ASP	CA-CB-CG	-5.54	107.06	112.60
10	j	21	VAL	N-CA-C	-5.54	100.71	108.80
9	2	34	GLY	N-CA-C	-5.54	100.04	113.18
10	3	159	GLU	CA-C-O	-5.54	114.93	120.64
21	N	308	ASN	CA-CB-CG	-5.54	107.06	112.60
24	Q	32	ASP	N-CA-CB	5.54	118.05	110.01
31	L	309	LEU	CA-C-N	5.54	127.71	120.28
31	L	309	LEU	C-N-CA	5.54	127.71	120.28
13	m	70	ASP	N-CA-C	5.54	117.78	111.02
7	G	116	LEU	N-CA-CB	5.54	118.36	110.16
18	X	64	ILE	CA-C-N	5.54	130.81	123.00
18	X	64	ILE	C-N-CA	5.54	130.81	123.00
21	N	861	TYR	N-CA-CB	5.54	118.11	109.85
22	S	43	LYS	N-CA-C	-5.54	104.64	111.40
26	U	43	SER	CB-CA-C	5.54	120.96	109.38
5	e	196	ALA	O-C-N	-5.54	115.83	122.15
9	2	94	LEU	CB-CA-C	-5.54	101.94	110.81
22	S	308	GLY	N-CA-C	5.54	119.34	112.64
13	6	56	ASP	CA-C-O	-5.54	114.69	121.28
18	X	59	ARG	CA-C-N	5.54	128.16	120.29
18	X	59	ARG	C-N-CA	5.54	128.16	120.29
19	Y	31	GLU	N-CA-CB	5.54	119.85	110.49
26	U	52	PHE	CB-CG-CD1	-5.54	111.28	120.70
33	J	185	VAL	N-CA-C	-5.54	99.57	107.77
33	J	404	PHE	CA-CB-CG	5.54	119.34	113.80
2	b	238	LEU	N-CA-C	-5.54	99.70	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	429	ILE	CA-C-N	5.54	127.06	120.14
23	P	429	ILE	C-N-CA	5.54	127.06	120.14
6	F	110	HIS	CB-CG-CD2	-5.54	124.00	131.20
10	3	112	ILE	N-CA-CB	5.54	119.35	111.82
21	N	717	LEU	CA-C-O	-5.54	114.09	120.24
6	f	85	SER	CA-C-N	5.53	127.69	120.28
6	f	85	SER	C-N-CA	5.53	127.69	120.28
6	F	22	VAL	CA-C-N	5.53	127.69	120.28
6	F	22	VAL	C-N-CA	5.53	127.69	120.28
6	F	203	ASP	N-CA-C	-5.53	103.77	111.52
11	4	22	THR	CA-C-O	5.53	126.11	120.24
29	I	181	TYR	CA-C-N	5.53	130.43	122.35
29	I	181	TYR	C-N-CA	5.53	130.43	122.35
33	J	264	GLY	CA-C-N	5.53	130.09	120.68
33	J	264	GLY	C-N-CA	5.53	130.09	120.68
11	4	176	PHE	CA-CB-CG	5.53	119.33	113.80
27	O	263	PHE	CA-C-N	5.53	128.15	120.29
27	O	263	PHE	C-N-CA	5.53	128.15	120.29
11	k	39	SER	CA-C-N	5.53	126.75	119.84
11	k	39	SER	C-N-CA	5.53	126.75	119.84
8	1	67	ILE	CA-C-N	5.53	128.27	120.42
8	1	67	ILE	C-N-CA	5.53	128.27	120.42
20	Z	727	GLU	CA-C-N	5.53	132.10	121.54
20	Z	727	GLU	C-N-CA	5.53	132.10	121.54
30	K	393	ARG	CD-NE-CZ	5.53	132.14	124.40
31	L	300	GLU	CA-C-N	5.53	127.73	120.60
31	L	300	GLU	C-N-CA	5.53	127.73	120.60
5	e	9	ASP	N-CA-C	-5.53	99.02	110.80
11	4	154	THR	O-C-N	5.53	127.98	122.12
1	a	74	CYS	CA-C-N	-5.53	112.02	121.97
1	a	74	CYS	C-N-CA	-5.53	112.02	121.97
11	4	135	TYR	CA-C-N	5.53	128.14	120.29
11	4	135	TYR	C-N-CA	5.53	128.14	120.29
16	V	111	HIS	ND1-CE1-NE2	5.53	113.93	108.40
19	Y	54	VAL	N-CA-C	-5.53	106.92	112.17
21	N	637	ALA	CA-C-N	5.53	128.03	120.46
21	N	637	ALA	C-N-CA	5.53	128.03	120.46
3	c	158	THR	O-C-N	-5.53	116.94	123.41
13	m	189	ILE	N-CA-C	5.53	115.72	110.42
10	3	153	LEU	CA-C-N	5.53	130.18	121.56
10	3	153	LEU	C-N-CA	5.53	130.18	121.56
16	V	121	VAL	N-CA-C	5.53	116.26	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	518	ALA	O-C-N	-5.53	116.26	122.12
29	I	115	ASP	CA-CB-CG	5.53	118.13	112.60
29	I	337	ALA	N-CA-C	-5.53	105.75	112.88
6	F	26	LEU	N-CA-C	-5.52	106.50	113.18
28	H	75	GLY	CA-C-O	-5.52	112.89	119.02
26	U	260	ASN	CA-C-N	5.52	128.13	120.29
26	U	260	ASN	C-N-CA	5.52	128.13	120.29
30	K	347	ARG	CA-C-O	-5.52	112.46	119.31
3	c	59	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	A	108	TYR	CA-CB-CG	-5.52	103.96	113.90
23	P	257	TRP	O-C-N	5.52	129.06	122.27
26	U	76	MET	CA-C-O	-5.52	114.70	120.55
26	U	254	ARG	CA-C-N	5.52	128.02	120.46
26	U	254	ARG	C-N-CA	5.52	128.02	120.46
5	e	121	LEU	CA-C-O	-5.52	115.02	120.98
9	i	88	ILE	CA-C-O	5.52	125.60	119.42
9	2	190	ALA	CA-C-N	5.52	127.23	120.22
9	2	190	ALA	C-N-CA	5.52	127.23	120.22
22	S	259	TYR	CA-C-O	-5.52	114.28	119.80
29	I	366	THR	CA-C-N	5.52	128.70	120.31
29	I	366	THR	C-N-CA	5.52	128.70	120.31
31	L	362	LYS	N-CA-CB	5.52	118.80	110.30
32	M	367	LYS	CA-C-O	-5.52	115.03	120.82
3	c	125	HIS	CE1-NE2-CD2	-5.52	103.48	109.00
4	d	226	SER	CA-C-N	5.52	127.67	120.28
4	d	226	SER	C-N-CA	5.52	127.67	120.28
10	j	195	VAL	N-CA-C	-5.52	100.54	108.48
11	k	41	HIS	ND1-CE1-NE2	5.52	113.92	108.40
1	A	234	PHE	N-CA-C	-5.52	100.97	109.52
3	C	86	ILE	CB-CG1-CD1	5.52	125.39	113.80
25	R	132	GLN	CA-C-N	5.52	128.13	120.29
25	R	132	GLN	C-N-CA	5.52	128.13	120.29
2	b	88	LYS	CB-CA-C	-5.52	100.08	110.67
2	b	209	ILE	N-CA-C	-5.52	99.70	107.75
22	S	261	HIS	CA-C-N	5.52	129.16	120.89
22	S	261	HIS	C-N-CA	5.52	129.16	120.89
26	U	175	LEU	N-CA-C	-5.52	101.37	109.81
1	a	120	ARG	CB-CA-C	-5.51	101.48	110.85
1	a	146	VAL	N-CA-CB	5.51	119.32	111.82
7	g	73	HIS	CA-C-O	5.51	124.87	119.08
13	m	103	HIS	CE1-NE2-CD2	-5.51	103.49	109.00
1	A	21	PRO	N-CA-CB	5.51	108.76	103.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	HIS	CB-CG-CD2	-5.51	124.03	131.20
8	1	197	PHE	CA-CB-CG	-5.51	108.29	113.80
10	3	118	LYS	CA-C-N	5.51	125.44	119.76
10	3	118	LYS	C-N-CA	5.51	125.44	119.76
22	S	100	HIS	ND1-CE1-NE2	5.51	113.92	108.40
27	O	79	VAL	CA-C-N	5.51	128.22	120.28
27	O	79	VAL	C-N-CA	5.51	128.22	120.28
33	J	214	SER	CB-CA-C	-5.51	98.31	110.99
7	G	28	VAL	CA-C-N	5.51	128.22	120.28
7	G	28	VAL	C-N-CA	5.51	128.22	120.28
13	6	164	PHE	CA-CB-CG	-5.51	108.29	113.80
1	a	15	HIS	CE1-NE2-CD2	-5.51	103.49	109.00
7	g	165	THR	CA-CB-OG1	5.51	117.87	109.60
7	g	176	LEU	CA-C-N	5.51	128.12	120.29
7	g	176	LEU	C-N-CA	5.51	128.12	120.29
7	g	243	ALA	O-C-N	-5.51	116.28	122.12
9	i	196	LEU	N-CA-C	5.51	118.00	111.33
21	N	93	GLU	CA-C-N	5.51	131.20	122.60
21	N	93	GLU	C-N-CA	5.51	131.20	122.60
27	O	249	ASP	N-CA-CB	5.51	119.80	110.49
29	I	78	ASN	CA-CB-CG	-5.51	107.09	112.60
2	b	49	LYS	N-CA-C	-5.51	99.75	108.73
8	1	29	THR	CA-C-O	5.51	127.19	120.25
22	S	462	ASP	CA-C-N	5.51	128.11	120.29
22	S	462	ASP	C-N-CA	5.51	128.11	120.29
28	H	60	GLU	CA-C-N	5.51	127.66	120.28
28	H	60	GLU	C-N-CA	5.51	127.66	120.28
30	K	169	VAL	CA-CB-CG1	5.51	119.77	110.40
11	k	146	HIS	N-CA-C	5.51	116.96	111.07
23	P	109	SER	CA-C-N	5.51	128.93	121.05
23	P	109	SER	C-N-CA	5.51	128.93	121.05
30	K	420	THR	CA-C-N	5.51	130.06	121.85
30	K	420	THR	C-N-CA	5.51	130.06	121.85
14	n	251	LYS	N-CA-C	-5.51	100.43	109.40
15	W	77	HIS	CG-CD2-NE2	5.51	112.71	107.20
26	U	14	VAL	O-C-N	5.51	127.21	121.87
1	a	66	PRO	O-C-N	5.50	130.07	122.64
13	m	208	ASP	N-CA-CB	5.50	119.79	110.49
13	m	229	ARG	CD-NE-CZ	-5.50	116.69	124.40
17	T	101	LYS	N-CA-C	5.50	117.28	111.28
18	X	21	SER	N-CA-C	-5.50	105.93	113.30
19	Y	27	LYS	O-C-N	5.50	128.42	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	137	PHE	CA-C-N	5.50	127.66	120.28
22	S	137	PHE	C-N-CA	5.50	127.66	120.28
23	P	402	PHE	O-C-N	5.50	129.78	123.29
25	R	179	PHE	N-CA-CB	5.50	118.21	110.12
2	b	176	GLU	CB-CG-CD	-5.50	103.25	112.60
11	4	174	MET	CA-C-N	5.50	130.74	120.95
11	4	174	MET	C-N-CA	5.50	130.74	120.95
20	Z	247	GLN	N-CA-CB	-5.50	101.75	110.28
23	P	83	SER	N-CA-CB	5.50	118.21	110.12
9	2	233	LYS	CG-CD-CE	5.50	123.95	111.30
12	5	263	HIS	CB-CG-CD2	-5.50	124.05	131.20
22	S	468	ALA	CA-C-O	-5.50	114.59	120.42
24	Q	227	CYS	CB-CA-C	-5.50	101.50	110.85
33	J	316	PHE	CB-CA-C	-5.50	101.98	110.62
33	J	385	ALA	CA-C-N	5.50	128.00	120.46
33	J	385	ALA	C-N-CA	5.50	128.00	120.46
13	m	38	ILE	CA-C-O	-5.50	116.19	121.63
22	S	147	TRP	CA-C-N	5.50	127.96	120.54
22	S	147	TRP	C-N-CA	5.50	127.96	120.54
22	S	375	ASP	CA-C-N	5.50	132.29	122.06
22	S	375	ASP	C-N-CA	5.50	132.29	122.06
22	S	431	VAL	CA-CB-CG1	5.50	119.75	110.40
23	P	312	PRO	CA-C-N	5.50	129.17	122.63
23	P	312	PRO	C-N-CA	5.50	129.17	122.63
24	Q	189	ARG	NE-CZ-NH2	5.50	124.15	119.20
29	I	354	ASP	CA-C-N	5.50	127.65	120.28
29	I	354	ASP	C-N-CA	5.50	127.65	120.28
14	n	167	GLY	CA-C-N	5.50	127.94	120.63
14	n	167	GLY	C-N-CA	5.50	127.94	120.63
12	5	130	TRP	CE2-CD2-CE3	5.50	124.30	118.80
15	W	68	GLU	CA-C-N	5.50	128.66	120.31
15	W	68	GLU	C-N-CA	5.50	128.66	120.31
17	T	127	GLN	CA-C-N	5.50	128.09	120.29
17	T	127	GLN	C-N-CA	5.50	128.09	120.29
22	S	34	LEU	CA-C-N	5.50	127.58	120.44
22	S	34	LEU	C-N-CA	5.50	127.58	120.44
1	A	59	VAL	CA-C-O	-5.50	112.59	119.95
5	E	10	ARG	CA-C-O	-5.50	114.14	120.24
25	R	116	LYS	N-CA-CB	5.50	117.98	110.01
11	4	195	PHE	CA-CB-CG	-5.49	108.31	113.80
23	P	95	TYR	N-CA-C	5.49	118.45	111.69
5	e	73	HIS	CG-CD2-NE2	5.49	112.69	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	30	GLN	CG-CD-NE2	-5.49	108.16	116.40
10	3	50	PHE	N-CA-C	-5.49	100.45	109.40
14	7	50	ASP	CA-C-O	-5.49	114.73	120.55
25	R	43	ARG	CB-CA-C	-5.49	101.52	110.85
26	U	225	ILE	N-CA-C	-5.49	105.02	111.00
26	U	294	ASN	OD1-CG-ND2	-5.49	117.11	122.60
27	O	202	SER	CA-C-N	5.49	129.04	120.75
27	O	202	SER	C-N-CA	5.49	129.04	120.75
28	H	44	PRO	N-CA-CB	5.49	109.32	103.39
4	d	190	GLU	N-CA-C	5.49	117.26	111.28
7	G	83	PRO	CA-C-N	5.49	128.65	120.31
7	G	83	PRO	C-N-CA	5.49	128.65	120.31
17	T	122	PHE	CA-CB-CG	-5.49	108.31	113.80
22	S	273	PHE	CB-CG-CD2	-5.49	111.37	120.70
31	L	293	GLU	CA-C-O	5.49	125.85	119.32
2	b	206	GLY	O-C-N	-5.49	114.94	122.68
10	j	19	ASP	CA-CB-CG	-5.49	107.11	112.60
1	A	46	ARG	NE-CZ-NH2	5.49	124.14	119.20
16	V	237	ASN	N-CA-CB	5.49	118.03	110.07
18	X	28	PRO	CA-C-O	-5.49	115.34	121.32
21	N	213	PHE	CA-C-N	5.49	128.08	120.29
21	N	213	PHE	C-N-CA	5.49	128.08	120.29
23	P	257	TRP	CA-C-O	-5.49	113.66	119.97
2	b	133	SER	N-CA-CB	5.49	119.18	110.57
8	h	170	GLN	N-CA-C	-5.49	105.38	111.36
11	k	114	PRO	N-CA-CB	5.49	108.54	102.72
1	A	170	ALA	N-CA-C	-5.49	100.97	109.14
2	B	171	ALA	CB-CA-C	-5.49	101.68	110.79
5	E	54	ALA	N-CA-CB	5.49	119.12	110.23
15	W	40	LYS	CA-C-N	5.49	128.08	120.29
15	W	40	LYS	C-N-CA	5.49	128.08	120.29
21	N	390	LEU	CA-C-N	5.49	125.48	119.89
21	N	390	LEU	C-N-CA	5.49	125.48	119.89
21	N	757	THR	N-CA-C	-5.49	100.18	108.52
24	Q	177	VAL	O-C-N	5.49	127.48	121.83
30	K	247	LEU	N-CA-C	5.48	118.27	110.10
14	n	157	ASP	N-CA-C	-5.48	100.10	108.76
9	2	54	ILE	N-CA-CB	-5.48	102.99	110.56
9	2	89	GLY	CA-C-N	5.48	127.57	120.44
9	2	89	GLY	C-N-CA	5.48	127.57	120.44
13	6	97	ALA	CB-CA-C	-5.48	102.04	110.81
16	V	188	LEU	CA-C-N	5.48	128.21	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	188	LEU	C-N-CA	5.48	128.21	120.42
18	X	8	ILE	CA-CB-CG1	5.48	119.72	110.40
23	P	263	HIS	CB-CG-CD2	-5.48	124.07	131.20
24	Q	315	ASN	CA-C-N	5.48	128.07	120.29
24	Q	315	ASN	C-N-CA	5.48	128.07	120.29
25	R	67	CYS	CA-C-O	5.48	126.28	119.97
32	M	190	ILE	N-CA-C	-5.48	105.18	110.72
33	J	248	ASP	CA-CB-CG	5.48	118.08	112.60
3	c	63	THR	N-CA-C	-5.48	97.17	108.18
21	N	422	TYR	CA-C-O	5.48	126.57	120.82
28	H	247	LEU	N-CA-C	-5.48	100.77	109.59
29	I	368	LYS	CA-C-N	5.48	133.09	122.07
29	I	368	LYS	C-N-CA	5.48	133.09	122.07
2	b	121	ALA	N-CA-C	-5.48	106.64	113.38
7	g	107	ILE	CA-C-N	5.48	125.42	119.78
7	g	107	ILE	C-N-CA	5.48	125.42	119.78
8	l	62	GLN	OE1-CD-NE2	5.48	128.08	122.60
23	P	33	ASN	N-CA-C	-5.48	105.39	111.36
21	N	81	TYR	N-CA-C	5.48	118.17	111.82
27	O	8	ASP	CA-C-N	5.48	128.07	120.29
27	O	8	ASP	C-N-CA	5.48	128.07	120.29
13	m	213	LEU	CB-CA-C	-5.48	100.71	109.75
1	A	111	ASP	CA-CB-CG	-5.48	107.12	112.60
16	V	194	ARG	NE-CZ-NH2	-5.48	114.27	119.20
29	I	158	GLY	N-CA-C	-5.48	102.69	110.63
7	g	109	ILE	O-C-N	-5.47	114.86	121.10
9	2	119	TYR	CA-C-N	5.47	130.34	122.35
9	2	119	TYR	C-N-CA	5.47	130.34	122.35
21	N	299	TYR	CA-C-O	-5.47	114.75	120.55
22	S	145	PHE	CA-CB-CG	5.47	119.27	113.80
29	I	325	ILE	O-C-N	-5.47	117.49	123.18
8	h	157	LYS	CA-C-N	5.47	128.06	120.29
8	h	157	LYS	C-N-CA	5.47	128.06	120.29
10	j	125	ASP	O-C-N	5.47	129.32	122.43
10	j	164	PHE	N-CA-C	5.47	118.00	111.71
3	C	77	VAL	N-CA-C	-5.47	100.60	108.48
7	G	237	GLN	O-C-N	-5.47	115.10	122.43
24	Q	64	LEU	N-CA-C	5.47	116.93	111.07
30	K	420	THR	CA-C-O	5.47	124.71	118.47
11	k	31	SER	N-CA-C	-5.47	106.06	114.16
5	E	155	LEU	CA-C-N	5.47	131.15	122.62
5	E	155	LEU	C-N-CA	5.47	131.15	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	453	ASP	N-CA-C	-5.47	107.61	114.56
28	H	363	PRO	CA-C-O	5.47	123.54	118.29
7	g	17	PRO	N-CA-C	-5.47	105.45	114.75
14	n	252	TRP	CB-CG-CD2	-5.47	119.14	126.80
17	T	88	TYR	N-CA-CB	5.47	117.94	110.01
21	N	448	LEU	N-CA-C	5.47	117.32	111.36
21	N	892	PRO	CA-C-N	5.47	127.95	120.46
21	N	892	PRO	C-N-CA	5.47	127.95	120.46
23	P	99	LYS	O-C-N	-5.47	115.82	122.22
24	Q	171	LYS	O-C-N	-5.47	114.64	121.70
27	O	151	ASP	CA-CB-CG	-5.47	107.13	112.60
33	J	155	LYS	CA-C-N	5.47	127.61	120.28
33	J	155	LYS	C-N-CA	5.47	127.61	120.28
16	V	72	PRO	N-CA-C	5.47	123.73	112.47
19	Y	89	GLN	N-CA-CB	5.47	119.80	110.50
7	g	199	ILE	CA-C-O	-5.47	113.41	119.20
20	Z	743	ILE	CA-CB-CG1	-5.47	101.11	110.40
22	S	437	ASN	CA-C-N	5.47	128.05	120.29
22	S	437	ASN	C-N-CA	5.47	128.05	120.29
23	P	254	GLU	N-CA-C	5.47	116.92	111.07
28	H	359	ASN	N-CA-C	-5.47	105.48	111.82
5	e	13	SER	CB-CA-C	-5.46	104.28	112.09
5	e	25	GLU	CA-C-N	5.46	127.60	120.28
5	e	25	GLU	C-N-CA	5.46	127.60	120.28
1	A	49	ASP	CA-C-N	5.46	131.15	121.80
1	A	49	ASP	C-N-CA	5.46	131.15	121.80
1	A	158	ASP	CA-C-N	5.46	125.17	119.82
1	A	158	ASP	C-N-CA	5.46	125.17	119.82
2	B	208	THR	N-CA-CB	5.46	118.27	111.00
5	E	210	GLU	N-CA-C	-5.46	99.16	110.80
10	3	107	PRO	CA-C-O	-5.46	114.75	121.31
21	N	94	LYS	CA-C-N	5.46	130.26	122.72
21	N	94	LYS	C-N-CA	5.46	130.26	122.72
26	U	177	ASP	CA-C-N	5.46	129.64	121.77
26	U	177	ASP	C-N-CA	5.46	129.64	121.77
9	i	37	PHE	CA-C-N	5.46	127.86	120.38
9	i	37	PHE	C-N-CA	5.46	127.86	120.38
9	2	162	ALA	N-CA-CB	5.46	118.75	110.28
10	3	173	ASN	CA-C-N	5.46	128.61	120.31
10	3	173	ASN	C-N-CA	5.46	128.61	120.31
11	4	7	ILE	N-CA-CB	5.46	120.07	111.99
15	W	126	ILE	O-C-N	5.46	127.58	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	56	SER	N-CA-C	-5.46	105.24	112.94
25	R	208	ASN	CB-CA-C	-5.46	101.72	110.79
30	K	188	VAL	N-CA-C	-5.46	106.48	111.67
2	b	49	LYS	N-CA-CB	5.46	119.32	110.42
13	6	116	HIS	CG-CD2-NE2	5.46	112.66	107.20
24	Q	247	HIS	CE1-NE2-CD2	-5.46	103.54	109.00
32	M	19	ASP	N-CA-C	-5.46	106.57	113.18
4	d	135	ILE	CA-C-O	-5.46	114.66	120.39
22	S	305	LYS	N-CA-C	-5.46	106.78	113.50
27	O	236	HIS	N-CA-C	-5.46	102.78	110.31
28	H	169	GLU	N-CA-CB	5.46	121.31	111.37
29	I	354	ASP	N-CA-CB	5.46	118.92	110.46
7	g	22	PHE	CA-C-N	5.46	129.87	121.19
7	g	22	PHE	C-N-CA	5.46	129.87	121.19
21	N	888	ASP	N-CA-CB	5.46	118.75	110.45
33	J	229	MET	N-CA-C	-5.46	99.18	110.80
3	c	184	MET	CA-C-N	5.46	133.03	122.07
3	c	184	MET	C-N-CA	5.46	133.03	122.07
4	d	91	VAL	N-CA-C	-5.46	105.06	110.62
23	P	210	ASN	CB-CA-C	-5.46	101.18	108.87
5	e	114	GLN	CG-CD-NE2	-5.45	108.22	116.40
8	h	50	ILE	N-CA-C	-5.45	98.00	109.34
5	E	157	HIS	CA-CB-CG	5.45	119.25	113.80
24	Q	252	HIS	ND1-CE1-NE2	5.45	113.85	108.40
28	H	230	LEU	CA-C-O	5.45	126.32	120.70
28	H	239	GLY	CA-C-N	5.45	128.75	120.13
28	H	239	GLY	C-N-CA	5.45	128.75	120.13
32	M	289	LYS	CA-C-N	5.45	128.61	120.87
32	M	289	LYS	C-N-CA	5.45	128.61	120.87
17	T	43	ASP	N-CA-CB	5.45	120.76	112.47
21	N	444	HIS	CA-CB-CG	5.45	119.25	113.80
6	F	146	GLU	CA-C-O	-5.45	114.47	120.36
9	2	58	LYS	CA-C-O	-5.45	114.19	120.24
14	7	215	ARG	CD-NE-CZ	5.45	132.03	124.40
18	X	69	ILE	CA-C-O	-5.45	114.39	119.62
21	N	355	TRP	CD2-CE2-CZ2	-5.45	116.95	122.40
32	M	256	ILE	N-CA-C	-5.45	100.21	108.17
3	c	117	ASP	CA-CB-CG	-5.45	107.15	112.60
8	h	17	PHE	CA-CB-CG	5.45	119.25	113.80
22	S	235	ASN	OD1-CG-ND2	5.45	128.05	122.60
24	Q	383	ASP	O-C-N	5.45	127.90	122.12
3	C	162	ALA	N-CA-C	-5.45	99.44	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	94	HIS	CE1-NE2-CD2	-5.45	103.55	109.00
9	2	107	SER	CA-C-N	5.45	127.52	120.44
9	2	107	SER	C-N-CA	5.45	127.52	120.44
12	5	283	ASN	N-CA-C	-5.45	105.34	111.28
15	W	13	SER	CA-C-N	5.45	130.11	121.18
15	W	13	SER	C-N-CA	5.45	130.11	121.18
21	N	209	LYS	N-CA-CB	5.45	118.22	110.16
32	M	247	ALA	CA-C-N	5.45	126.90	120.09
32	M	247	ALA	C-N-CA	5.45	126.90	120.09
6	F	228	GLU	CA-C-N	5.44	127.84	120.44
6	F	228	GLU	C-N-CA	5.44	127.84	120.44
21	N	662	MET	N-CA-CB	5.44	118.31	110.20
2	b	26	THR	CA-C-N	5.44	129.81	120.72
2	b	26	THR	C-N-CA	5.44	129.81	120.72
8	h	111	TYR	O-C-N	-5.44	116.27	123.13
13	m	103	HIS	CB-CG-ND1	5.44	130.86	122.70
18	X	116	ALA	CA-C-O	-5.44	112.73	120.51
32	M	353	SER	CB-CA-C	-5.44	100.67	110.36
1	A	15	HIS	CE1-NE2-CD2	-5.44	103.56	109.00
11	4	40	PRO	CA-C-N	5.44	129.31	120.23
11	4	40	PRO	C-N-CA	5.44	129.31	120.23
24	Q	315	ASN	CA-CB-CG	5.44	118.04	112.60
30	K	189	GLU	N-CA-CB	5.44	118.21	110.16
9	i	122	HIS	CB-CG-CD2	-5.44	124.13	131.20
20	Z	168	GLN	CA-C-N	5.44	127.52	120.56
20	Z	168	GLN	C-N-CA	5.44	127.52	120.56
21	N	216	ASN	O-C-N	-5.44	116.35	122.12
2	b	64	VAL	O-C-N	-5.44	117.44	123.20
5	e	91	HIS	CG-CD2-NE2	5.44	112.64	107.20
12	l	253	TYR	O-C-N	5.44	129.99	123.36
17	T	225	ASN	N-CA-CB	5.44	119.68	110.49
23	P	275	ASN	N-CA-C	-5.44	104.89	112.45
24	Q	87	GLN	CA-C-N	5.44	127.84	120.44
24	Q	87	GLN	C-N-CA	5.44	127.84	120.44
25	R	129	GLU	CA-C-O	-5.44	114.66	120.42
5	e	20	ARG	N-CA-C	-5.44	100.91	109.50
10	3	150	CYS	N-CA-CB	5.44	117.89	110.01
23	P	372	THR	CA-C-N	5.44	127.56	120.28
23	P	372	THR	C-N-CA	5.44	127.56	120.28
27	O	85	SER	CB-CA-C	-5.44	100.57	110.63
10	j	169	GLN	CA-CB-CG	-5.43	103.23	114.10
18	X	109	LEU	CA-C-N	5.43	125.44	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	X	109	LEU	C-N-CA	5.43	125.44	119.90
1	A	22	GLU	N-CA-CB	5.43	118.53	110.49
5	E	44	GLU	CA-C-N	-5.43	114.71	122.64
5	E	44	GLU	C-N-CA	-5.43	114.71	122.64
15	W	2	VAL	N-CA-CB	5.43	118.57	112.32
20	Z	927	VAL	N-CA-C	-5.43	100.30	108.12
7	G	99	PHE	N-CA-CB	5.43	118.20	110.16
21	N	343	THR	O-C-N	-5.43	117.06	123.41
24	Q	82	THR	CA-C-N	5.43	129.87	120.58
24	Q	82	THR	C-N-CA	5.43	129.87	120.58
2	B	218	ASN	CA-CB-CG	-5.43	107.17	112.60
22	S	456	ASP	CA-C-O	-5.43	113.07	118.34
24	Q	337	ALA	CA-C-O	5.43	126.52	120.82
27	O	138	LEU	CA-C-O	5.43	126.27	120.24
32	M	420	SER	N-CA-C	5.43	118.37	111.69
4	d	138	PHE	CA-CB-CG	-5.43	108.37	113.80
11	k	146	HIS	ND1-CE1-NE2	5.43	113.83	108.40
6	F	108	ALA	CA-C-N	5.43	125.97	120.00
6	F	108	ALA	C-N-CA	5.43	125.97	120.00
21	N	221	ASP	CA-CB-CG	-5.43	107.17	112.60
30	K	314	VAL	N-CA-C	5.43	120.63	109.34
8	h	46	VAL	N-CA-CB	-5.43	105.87	112.33
8	h	166	HIS	ND1-CE1-NE2	5.43	113.83	108.40
11	k	63	ASN	CB-CA-C	-5.43	101.63	110.85
17	T	83	ASN	OD1-CG-ND2	5.43	128.03	122.60
33	J	315	GLU	N-CA-C	-5.43	101.69	110.32
13	m	223	GLU	N-CA-C	-5.42	99.44	108.34
2	B	161	ALA	N-CA-CB	5.42	119.66	110.49
15	W	20	ASP	N-CA-C	-5.42	107.92	114.75
26	U	299	LYS	O-C-N	-5.42	115.97	122.15
31	L	60	PHE	CA-CB-CG	-5.42	108.38	113.80
21	N	484	GLY	CA-C-N	5.42	127.49	120.44
21	N	484	GLY	C-N-CA	5.42	127.49	120.44
32	M	141	LYS	N-CA-C	-5.42	99.65	109.09
6	f	59	TYR	N-CA-C	-5.42	101.44	110.17
13	m	120	ALA	O-C-N	-5.42	116.87	123.10
6	F	174	ARG	NE-CZ-NH2	5.42	124.08	119.20
22	S	92	LEU	CA-C-N	5.42	127.55	120.28
22	S	92	LEU	C-N-CA	5.42	127.55	120.28
25	R	325	HIS	CG-CD2-NE2	5.42	112.62	107.20
3	C	230	PHE	CA-CB-CG	5.42	119.22	113.80
7	G	190	ARG	NE-CZ-NH1	-5.42	116.08	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	W	72	ILE	CA-C-N	5.42	127.99	120.29
15	W	72	ILE	C-N-CA	5.42	127.99	120.29
22	S	473	ASP	CB-CA-C	-5.42	102.34	110.90
28	H	202	GLU	CB-CG-CD	5.42	121.81	112.60
31	L	78	ARG	NE-CZ-NH2	-5.42	114.32	119.20
7	g	65	VAL	N-CA-CB	5.42	120.82	111.39
13	m	166	ASN	OD1-CG-ND2	5.42	128.02	122.60
14	n	242	LYS	CG-CD-CE	5.42	123.76	111.30
6	F	185	ASN	CA-C-O	-5.42	114.93	121.22
16	V	67	ASP	CA-C-O	-5.42	115.64	121.38
21	N	210	SER	N-CA-CB	5.42	118.08	110.12
22	S	110	LEU	N-CA-CB	5.42	118.79	110.61
3	c	55	THR	N-CA-C	-5.42	106.26	112.92
5	e	196	ALA	CA-C-N	5.42	127.48	120.44
5	e	196	ALA	C-N-CA	5.42	127.48	120.44
10	j	42	LYS	N-CA-C	-5.42	105.49	113.61
11	k	21	VAL	CA-CB-CG2	-5.42	101.19	110.40
11	k	77	PRO	O-C-N	5.42	128.72	122.17
1	A	156	LYS	N-CA-CB	5.42	119.05	110.55
24	Q	27	TYR	N-CA-C	5.42	117.18	111.28
25	R	355	SER	CA-C-N	5.42	127.48	120.44
25	R	355	SER	C-N-CA	5.42	127.48	120.44
26	U	252	HIS	N-CA-CB	5.42	118.18	110.16
27	O	156	THR	CA-C-N	5.42	127.54	120.28
27	O	156	THR	C-N-CA	5.42	127.54	120.28
13	m	19	THR	CA-C-O	-5.42	114.92	120.99
22	S	373	LYS	CA-C-N	5.42	132.13	122.06
22	S	373	LYS	C-N-CA	5.42	132.13	122.06
11	k	33	ASP	N-CA-CB	5.41	118.85	110.46
1	A	142	THR	N-CA-C	-5.41	100.36	109.07
3	C	194	LEU	CA-C-N	5.41	127.98	120.29
3	C	194	LEU	C-N-CA	5.41	127.98	120.29
4	D	118	GLN	O-C-N	-5.41	116.38	122.12
8	1	30	THR	CA-CB-OG1	5.41	117.72	109.60
11	4	133	HIS	CG-CD2-NE2	5.41	112.61	107.20
29	I	320	GLY	CA-C-O	5.41	129.99	120.57
33	J	308	GLY	O-C-N	-5.41	115.51	122.39
1	A	98	LYS	CG-CD-CE	5.41	123.75	111.30
18	X	107	GLY	CA-C-N	5.41	131.85	122.32
18	X	107	GLY	C-N-CA	5.41	131.85	122.32
19	Y	52	ASN	CA-C-N	5.41	128.50	120.17
19	Y	52	ASN	C-N-CA	5.41	128.50	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	480	ARG	CA-C-N	5.41	126.49	119.78
22	S	480	ARG	C-N-CA	5.41	126.49	119.78
27	O	256	ASN	N-CA-CB	5.41	118.67	110.28
33	J	337	LEU	CA-C-N	5.41	131.50	122.73
33	J	337	LEU	C-N-CA	5.41	131.50	122.73
5	e	138	PHE	CA-CB-CG	-5.41	108.39	113.80
7	g	211	ASP	CA-CB-CG	5.41	118.01	112.60
14	n	73	GLU	N-CA-CB	-5.41	101.61	110.43
14	n	236	ASN	CA-CB-CG	-5.41	107.19	112.60
5	E	144	ILE	CB-CA-C	5.41	117.07	111.23
17	T	232	LYS	CA-C-O	5.41	127.19	120.54
20	Z	747	ALA	O-C-N	5.41	127.86	122.12
24	Q	43	GLY	N-CA-C	-5.41	105.56	114.76
28	H	348	ASN	CA-CB-CG	5.41	118.01	112.60
29	I	278	ILE	N-CA-C	-5.41	99.76	107.77
5	e	107	ILE	CA-CB-CG2	5.41	119.69	110.50
8	1	132	PRO	N-CD-CG	5.41	111.31	103.20
8	1	197	PHE	O-C-N	-5.41	116.98	123.31
21	N	175	ASP	CA-CB-CG	5.41	118.01	112.60
13	6	84	HIS	CB-CG-CD2	-5.41	124.17	131.20
13	6	168	TYR	CA-CB-CG	-5.41	104.17	113.90
33	J	295	ASN	CA-C-O	-5.41	113.27	119.60
6	f	184	GLY	N-CA-C	-5.41	106.75	115.08
8	h	137	GLY	N-CA-C	-5.41	100.37	113.18
11	k	83	PHE	CA-C-O	-5.41	115.14	120.82
12	l	120	MET	N-CA-C	-5.41	99.71	108.41
2	B	64	VAL	N-CA-C	-5.41	99.86	107.75
11	4	30	ASP	N-CA-CB	5.41	118.77	110.61
11	4	180	ILE	CA-C-O	-5.41	114.60	120.71
12	5	280	GLY	CA-C-O	5.41	124.36	118.95
20	Z	524	ALA	CA-C-N	5.41	129.33	120.63
20	Z	524	ALA	C-N-CA	5.41	129.33	120.63
24	Q	334	HIS	CG-CD2-NE2	5.41	112.61	107.20
24	Q	420	ASN	CA-CB-CG	-5.41	107.19	112.60
26	U	219	LEU	CA-C-O	-5.41	114.83	120.88
27	O	356	ARG	NE-CZ-NH1	5.41	126.91	121.50
32	M	74	GLN	CA-C-N	5.41	134.99	121.80
32	M	74	GLN	C-N-CA	5.41	134.99	121.80
12	l	124	ALA	CB-CA-C	-5.40	102.17	110.81
13	6	203	HIS	CE1-NE2-CD2	-5.40	103.60	109.00
31	L	118	ILE	N-CA-CB	5.40	117.16	111.00
2	b	173	THR	N-CA-CB	5.40	118.15	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	85	SER	N-CA-CB	5.40	118.15	110.16
8	h	31	THR	N-CA-C	-5.40	99.29	108.26
13	m	64	GLY	N-CA-C	-5.40	100.38	113.18
14	7	111	ASN	O-C-N	-5.40	115.11	121.32
21	N	193	ALA	CA-C-N	5.40	128.09	120.42
21	N	193	ALA	C-N-CA	5.40	128.09	120.42
21	N	234	ASP	CA-C-N	5.40	129.86	120.68
21	N	234	ASP	C-N-CA	5.40	129.86	120.68
23	P	88	GLN	CB-CA-C	-5.40	102.56	111.36
27	O	44	SER	N-CA-CB	5.40	118.15	110.16
32	M	141	LYS	O-C-N	-5.40	117.34	121.55
33	J	166	LEU	CA-C-O	-5.40	112.76	120.16
5	e	2	PHE	CA-CB-CG	-5.40	108.40	113.80
30	K	58	TYR	N-CA-C	-5.40	106.74	113.38
4	d	139	ASP	CA-CB-CG	-5.40	107.20	112.60
7	g	187	LEU	N-CA-CB	5.40	120.01	111.43
4	D	203	VAL	CB-CA-C	-5.40	105.06	111.81
21	N	232	LEU	CD1-CG-CD2	5.40	122.67	110.80
21	N	433	THR	N-CA-C	-5.40	100.86	109.23
21	N	503	THR	O-C-N	5.40	128.91	122.27
24	Q	48	ASP	CA-CB-CG	-5.40	107.20	112.60
25	R	363	PHE	N-CA-CB	5.40	118.24	110.20
25	R	396	LYS	CA-C-N	5.40	127.51	120.28
25	R	396	LYS	C-N-CA	5.40	127.51	120.28
3	C	181	LYS	CA-C-N	5.40	127.51	120.28
3	C	181	LYS	C-N-CA	5.40	127.51	120.28
9	2	92	ILE	N-CA-CB	5.40	118.67	110.58
21	N	747	HIS	CA-CB-CG	-5.40	108.40	113.80
29	I	236	VAL	CA-C-O	-5.40	113.05	119.58
30	K	375	ASN	N-CA-CB	5.40	119.48	110.85
3	c	105	ASP	CA-C-N	5.39	130.57	120.11
3	c	105	ASP	C-N-CA	5.39	130.57	120.11
9	i	249	ILE	O-C-N	5.39	127.59	122.20
14	7	137	ARG	CA-CB-CG	5.39	124.89	114.10
26	U	300	LYS	CA-C-N	5.39	128.08	120.42
26	U	300	LYS	C-N-CA	5.39	128.08	120.42
11	k	118	GLN	OE1-CD-NE2	5.39	127.99	122.60
2	B	94	HIS	CB-CG-ND1	5.39	130.79	122.70
3	C	58	GLU	CA-C-O	5.39	126.13	120.36
8	1	120	TYR	O-C-N	-5.39	116.18	123.19
12	5	126	ASP	CA-C-O	5.39	126.27	120.55
15	W	143	ASN	CB-CA-C	-5.39	100.39	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	27	VAL	CB-CA-C	5.39	117.48	110.96
23	P	58	VAL	CA-C-O	-5.39	115.13	120.85
28	H	330	GLN	N-CA-C	-5.39	106.54	113.01
32	M	42	ARG	O-C-N	-5.39	116.00	122.15
1	A	189	SER	CA-C-N	5.39	130.22	122.35
1	A	189	SER	C-N-CA	5.39	130.22	122.35
12	5	123	GLY	CA-C-N	5.39	127.45	120.44
12	5	123	GLY	C-N-CA	5.39	127.45	120.44
27	O	71	ASP	CA-C-O	5.39	124.42	118.65
28	H	104	LYS	CA-C-N	5.39	129.35	121.80
28	H	104	LYS	C-N-CA	5.39	129.35	121.80
33	J	170	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
7	g	227	LEU	N-CA-C	-5.39	101.38	109.95
2	B	238	LEU	N-CA-C	-5.39	99.94	108.73
7	G	52	LYS	CB-CA-C	-5.39	102.06	110.74
7	G	81	LEU	N-CA-CB	5.39	118.66	109.87
14	7	81	ASN	N-CA-C	-5.39	104.99	113.02
22	S	150	LYS	N-CA-CB	5.39	119.60	110.49
27	O	294	MET	N-CA-C	-5.39	105.41	111.28
29	I	188	GLU	N-CA-CB	5.39	119.12	111.25
2	b	214	ILE	N-CA-C	-5.39	98.13	109.34
2	b	143	ASN	CA-C-N	5.39	129.01	120.07
2	b	143	ASN	C-N-CA	5.39	129.01	120.07
7	G	58	LEU	N-CA-C	-5.39	106.75	113.38
7	G	106	PRO	CA-C-N	5.39	130.54	119.72
7	G	106	PRO	C-N-CA	5.39	130.54	119.72
10	3	95	LEU	CB-CA-C	-5.39	101.85	110.79
14	7	203	VAL	N-CA-C	-5.39	106.59	113.22
23	P	182	GLU	CA-C-O	5.39	126.26	120.55
25	R	339	ALA	CA-C-N	5.39	127.44	120.44
25	R	339	ALA	C-N-CA	5.39	127.44	120.44
28	H	131	GLN	CA-C-O	5.39	125.73	119.32
30	K	82	ALA	O-C-N	5.39	129.55	122.33
30	K	111	SER	CA-C-N	5.39	129.97	120.87
30	K	111	SER	C-N-CA	5.39	129.97	120.87
2	b	84	VAL	O-C-N	5.38	127.88	121.80
10	j	106	GLY	CA-C-N	5.38	125.68	119.92
10	j	106	GLY	C-N-CA	5.38	125.68	119.92
3	C	64	GLU	CA-C-O	5.38	125.86	119.56
17	T	112	ASN	CA-C-O	-5.38	114.84	120.55
28	H	241	ASP	CA-C-O	-5.38	114.74	120.23
30	K	292	VAL	N-CA-CB	5.38	116.85	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L	354	GLU	CA-C-O	-5.38	115.14	120.90
2	b	204	PHE	CB-CG-CD1	-5.38	111.55	120.70
17	T	11	LEU	CA-C-N	5.38	127.49	120.28
17	T	11	LEU	C-N-CA	5.38	127.49	120.28
29	I	437	LEU	CB-CA-C	-5.38	99.87	110.10
2	b	69	PRO	N-CA-CB	5.38	108.47	103.41
13	m	102	GLN	OE1-CD-NE2	5.38	127.98	122.60
14	n	258	ILE	CA-CB-CG2	-5.38	101.35	110.50
3	C	128	LEU	CA-C-O	5.38	128.16	121.81
20	Z	237	VAL	CA-C-N	5.38	128.89	120.82
20	Z	237	VAL	C-N-CA	5.38	128.89	120.82
20	Z	733	VAL	CA-C-N	5.38	127.93	120.29
20	Z	733	VAL	C-N-CA	5.38	127.93	120.29
22	S	417	GLN	OE1-CD-NE2	5.38	127.98	122.60
28	H	118	ASP	N-CA-CB	-5.38	102.22	111.21
28	H	365	LEU	CA-C-N	5.38	129.22	120.23
28	H	365	LEU	C-N-CA	5.38	129.22	120.23
33	J	122	LEU	CA-C-N	5.38	131.82	121.54
33	J	122	LEU	C-N-CA	5.38	131.82	121.54
8	h	87	ALA	CB-CA-C	-5.38	101.70	110.85
1	A	209	HIS	ND1-CE1-NE2	5.38	113.78	108.40
9	2	194	ASN	CA-CB-CG	-5.38	107.22	112.60
29	I	322	VAL	CA-C-N	-5.38	111.27	121.54
29	I	322	VAL	C-N-CA	-5.38	111.27	121.54
3	c	163	ILE	N-CA-C	5.38	116.78	108.44
5	e	61	SER	CB-CA-C	-5.38	101.41	110.44
5	E	4	THR	N-CA-CB	5.38	117.86	109.85
5	E	238	GLU	CA-C-N	5.38	127.49	120.28
5	E	238	GLU	C-N-CA	5.38	127.49	120.28
24	Q	398	TYR	CA-C-O	-5.38	114.83	120.80
24	Q	413	LEU	N-CA-CB	5.38	118.62	110.28
25	R	274	PRO	CA-C-N	5.38	127.75	120.44
25	R	274	PRO	C-N-CA	5.38	127.75	120.44
30	K	397	LYS	CA-C-N	5.38	131.81	121.54
30	K	397	LYS	C-N-CA	5.38	131.81	121.54
3	c	52	VAL	N-CA-CB	5.38	121.88	111.93
1	A	120	ARG	CA-C-O	5.38	126.21	120.24
8	1	98	ASN	N-CA-C	-5.38	102.37	110.06
21	N	218	PRO	N-CA-C	-5.38	107.01	114.27
22	S	95	PHE	O-C-N	5.38	127.61	122.07
23	P	91	LEU	CA-C-N	5.38	128.26	120.79
23	P	91	LEU	C-N-CA	5.38	128.26	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	174	SER	CA-C-O	-5.38	114.85	120.55
26	U	135	ASP	N-CA-C	-5.38	101.12	109.72
26	U	256	ASN	N-CA-C	5.38	116.82	111.07
28	H	222	ARG	CD-NE-CZ	-5.38	116.87	124.40
30	K	164	ASN	CB-CG-ND2	-5.38	108.33	116.40
1	a	203	VAL	N-CA-C	-5.38	105.29	110.72
14	n	207	GLU	CA-C-N	5.38	127.80	120.54
14	n	207	GLU	C-N-CA	5.38	127.80	120.54
28	H	462	ARG	CB-CA-C	-5.38	101.07	109.72
33	J	385	ALA	N-CA-CB	5.38	118.11	110.16
4	d	160	SER	N-CA-CB	5.37	118.57	110.30
5	e	153	TYR	CB-CA-C	-5.37	100.66	109.53
9	i	246	ILE	CA-C-O	-5.37	114.38	120.67
8	l	118	GLU	N-CA-CB	5.37	121.53	111.53
12	5	144	ARG	CB-CA-C	-5.37	100.35	110.67
17	T	158	GLN	CB-CA-C	-5.37	102.21	110.81
21	N	443	LEU	N-CA-C	-5.37	105.46	112.23
23	P	98	GLN	CA-C-N	5.37	128.02	120.28
23	P	98	GLN	C-N-CA	5.37	128.02	120.28
24	Q	139	ILE	CA-C-O	-5.37	115.16	120.85
32	M	64	ASP	CB-CA-C	-5.37	102.44	110.88
4	d	49	ARG	CD-NE-CZ	-5.37	116.88	124.40
4	D	83	ARG	CA-C-N	5.37	129.53	120.29
4	D	83	ARG	C-N-CA	5.37	129.53	120.29
9	2	162	ALA	CA-C-O	-5.37	113.79	119.97
29	I	128	TYR	CG-CD2-CE2	-5.37	113.14	121.20
33	J	139	VAL	O-C-N	5.37	127.08	121.87
10	j	5	SER	CA-C-N	5.37	131.28	123.12
10	j	5	SER	C-N-CA	5.37	131.28	123.12
1	a	71	TYR	CB-CG-CD2	-5.37	112.75	120.80
1	A	43	LEU	N-CA-C	-5.37	99.57	108.75
5	E	73	HIS	CA-C-O	-5.37	112.78	119.28
21	N	322	ASP	CA-CB-CG	-5.37	107.23	112.60
22	S	47	THR	N-CA-C	5.37	122.23	110.80
22	S	368	LYS	CG-CD-CE	5.37	123.65	111.30
3	c	125	HIS	ND1-CG-CD2	-5.37	100.73	106.10
23	P	178	GLN	N-CA-C	-5.37	105.33	111.07
8	h	119	VAL	N-CA-C	-5.37	100.47	108.46
9	2	209	ILE	O-C-N	5.37	129.07	122.95
20	Z	800	SER	CA-C-N	5.37	127.78	120.54
20	Z	800	SER	C-N-CA	5.37	127.78	120.54
23	P	349	ASN	OD1-CG-ND2	-5.37	117.23	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	378	THR	CA-C-O	-5.37	115.19	120.82
25	R	131	ALA	N-CA-C	-5.37	105.51	111.36
27	O	351	SER	CA-C-O	5.37	124.86	118.69
30	K	214	PRO	CB-CA-C	5.37	117.47	110.92
33	J	397	ALA	CA-C-O	-5.37	113.55	119.08
20	Z	250	VAL	CB-CA-C	-5.36	104.82	112.22
26	U	109	LEU	CA-C-O	-5.36	114.73	120.42
10	j	67	PHE	CA-C-O	5.36	125.97	119.11
14	n	122	PRO	N-CA-CB	5.36	109.23	103.33
24	Q	251	THR	O-C-N	-5.36	116.96	123.29
11	k	17	SER	N-CA-CB	5.36	120.88	111.55
21	N	648	PRO	CA-CB-CG	-5.36	94.31	104.50
22	S	226	ASP	CA-CB-CG	-5.36	107.24	112.60
32	M	190	ILE	CA-C-O	-5.36	115.17	120.85
2	b	95	THR	N-CA-CB	5.36	119.14	110.40
2	b	170	ALA	N-CA-CB	5.36	117.84	110.07
8	h	175	ASP	O-C-N	-5.36	117.05	123.27
6	F	233	TYR	CA-CB-CG	-5.36	104.25	113.90
17	T	30	ILE	CA-C-N	5.36	127.90	120.29
17	T	30	ILE	C-N-CA	5.36	127.90	120.29
31	L	212	ILE	CA-C-N	5.36	127.84	120.39
31	L	212	ILE	C-N-CA	5.36	127.84	120.39
1	a	203	VAL	CA-C-N	5.36	127.41	120.44
1	a	203	VAL	C-N-CA	5.36	127.41	120.44
9	i	81	THR	CA-CB-OG1	5.36	117.64	109.60
10	j	26	ASP	CA-CB-CG	-5.36	107.24	112.60
13	m	189	ILE	CA-C-N	5.36	127.77	120.54
13	m	189	ILE	C-N-CA	5.36	127.77	120.54
9	2	239	THR	N-CA-C	-5.36	102.82	110.59
20	Z	761	PHE	CB-CA-C	-5.36	101.90	110.79
21	N	444	HIS	CG-CD2-NE2	5.36	112.56	107.20
5	e	7	GLU	CB-CA-C	-5.36	101.43	110.64
5	e	140	VAL	O-C-N	5.36	129.30	123.09
11	k	171	ARG	O-C-N	-5.36	115.07	122.46
6	F	89	ARG	N-CA-C	5.36	116.80	111.07
24	Q	134	LYS	CB-CA-C	-5.36	102.47	110.88
32	M	286	ILE	N-CA-C	-5.36	107.50	112.43
33	J	189	GLY	CA-C-O	-5.36	113.86	121.52
33	J	343	LEU	N-CA-C	-5.36	106.33	112.92
30	K	215	PRO	O-C-N	5.35	129.71	122.37
4	d	206	GLY	CA-C-O	5.35	129.50	122.06
1	A	70	SER	CB-CA-C	-5.35	101.44	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	161	LYS	CA-C-O	-5.35	113.25	119.14
21	N	66	SER	CA-C-O	-5.35	115.20	120.82
21	N	735	MET	CG-SD-CE	-5.35	89.12	100.90
22	S	300	ALA	CA-C-N	5.35	125.27	119.76
22	S	300	ALA	C-N-CA	5.35	125.27	119.76
27	O	316	ALA	O-C-N	5.35	128.25	122.15
32	M	371	ASP	N-CA-C	-5.35	102.83	110.59
33	J	388	LYS	N-CA-CB	5.35	118.08	110.16
3	c	50	ARG	CD-NE-CZ	-5.35	116.91	124.40
10	3	160	PRO	CA-C-N	5.35	129.73	120.58
10	3	160	PRO	C-N-CA	5.35	129.73	120.58
18	X	119	LYS	N-CA-C	-5.35	106.01	112.54
29	I	320	GLY	O-C-N	-5.35	115.74	122.70
6	f	71	GLY	O-C-N	-5.35	118.58	123.56
9	i	52	GLY	CA-C-O	-5.35	113.87	121.52
1	A	148	GLU	N-CA-C	-5.35	106.80	113.38
22	S	421	TYR	CB-CA-C	-5.35	101.76	110.85
24	Q	114	GLN	OE1-CD-NE2	-5.35	117.25	122.60
27	O	160	LYS	CA-C-N	5.35	127.39	120.44
27	O	160	LYS	C-N-CA	5.35	127.39	120.44
28	H	391	ILE	CA-C-N	5.35	129.77	120.68
28	H	391	ILE	C-N-CA	5.35	129.77	120.68
33	J	131	ASP	CA-C-N	5.35	125.04	119.64
33	J	131	ASP	C-N-CA	5.35	125.04	119.64
5	e	167	TYR	CA-CB-CG	-5.35	104.28	113.90
6	f	106	GLU	CB-CG-CD	-5.35	103.51	112.60
15	W	100	HIS	CE1-NE2-CD2	-5.35	103.65	109.00
23	P	73	ASP	CB-CA-C	-5.35	101.76	110.85
24	Q	211	PRO	CA-C-N	5.35	127.45	120.28
24	Q	211	PRO	C-N-CA	5.35	127.45	120.28
28	H	186	PRO	N-CA-CB	5.35	108.42	103.39
33	J	88	VAL	CA-C-N	5.35	126.78	120.09
33	J	88	VAL	C-N-CA	5.35	126.78	120.09
28	H	300	THR	N-CA-C	-5.35	105.53	111.36
3	c	76	ALA	CA-C-O	-5.34	115.04	120.71
1	A	136	PRO	N-CA-CB	5.34	108.00	103.35
4	D	39	LYS	N-CA-C	-5.34	107.13	113.97
6	F	211	LEU	N-CA-C	-5.34	100.59	109.46
16	V	170	PRO	CA-C-N	5.34	128.44	120.31
16	V	170	PRO	C-N-CA	5.34	128.44	120.31
24	Q	313	ASP	CA-CB-CG	-5.34	107.25	112.60
28	H	377	PHE	CA-CB-CG	-5.34	108.45	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	H	450	VAL	CA-C-N	5.34	128.01	120.42
28	H	450	VAL	C-N-CA	5.34	128.01	120.42
29	I	221	LEU	N-CA-C	-5.34	100.53	109.24
3	c	18	ARG	N-CA-C	-5.34	101.17	109.24
4	d	20	VAL	CA-CB-CG2	-5.34	101.32	110.40
9	i	170	HIS	CA-CB-CG	-5.34	108.46	113.80
13	6	141	ARG	NE-CZ-NH2	5.34	124.01	119.20
24	Q	318	LEU	N-CA-C	-5.34	106.72	113.18
24	Q	434	TYR	CB-CG-CD2	-5.34	112.79	120.80
32	M	21	GLU	O-C-N	-5.34	115.66	122.34
33	J	331	HIS	CE1-NE2-CD2	-5.34	103.66	109.00
8	h	170	GLN	N-CA-CB	5.34	118.06	110.16
16	V	260	GLU	O-C-N	-5.34	115.49	122.59
29	I	420	LYS	CA-C-O	-5.34	114.76	120.42
32	M	109	ASP	CA-CB-CG	5.34	117.94	112.60
2	b	151	ASP	N-CA-C	-5.34	103.41	110.40
8	h	174	TRP	CB-CG-CD2	-5.34	119.32	126.80
10	j	44	PHE	N-CA-C	-5.34	100.95	109.07
5	E	190	SER	N-CA-C	-5.34	105.04	112.30
8	1	42	LYS	CB-CA-C	-5.34	100.41	109.38
9	2	205	CYS	CA-C-N	5.34	130.37	123.11
9	2	205	CYS	C-N-CA	5.34	130.37	123.11
18	X	25	THR	N-CA-C	-5.34	100.86	109.40
20	Z	385	PHE	CA-C-N	5.34	128.91	120.47
20	Z	385	PHE	C-N-CA	5.34	128.91	120.47
21	N	43	LEU	CA-C-N	5.34	124.85	119.19
21	N	43	LEU	C-N-CA	5.34	124.85	119.19
21	N	817	THR	CA-C-O	-5.34	114.76	120.42
23	P	413	ASN	N-CA-CB	5.34	117.97	110.12
28	H	197	MET	N-CA-C	-5.34	106.54	113.16
29	I	402	LEU	O-C-N	-5.34	116.06	122.15
1	a	201	LYS	CA-C-O	-5.34	112.28	119.11
12	5	140	LEU	CB-CA-C	-5.34	101.17	110.09
1	a	184	ASN	OD1-CG-ND2	5.34	127.94	122.60
6	f	183	ASP	CA-C-N	5.34	130.62	121.07
6	f	183	ASP	C-N-CA	5.34	130.62	121.07
7	g	80	GLY	N-CA-C	-5.34	100.53	113.18
13	m	141	ARG	CA-CB-CG	5.34	124.77	114.10
8	1	24	GLY	N-CA-C	-5.34	101.67	110.80
15	W	39	ALA	CB-CA-C	-5.34	101.93	110.79
27	O	376	GLN	O-C-N	5.34	127.78	122.12
28	H	329	VAL	N-CA-C	-5.34	105.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I	133	LEU	O-C-N	-5.34	117.17	123.41
32	M	331	ASP	O-C-N	5.34	129.41	122.42
33	J	373	ARG	O-C-N	5.34	129.69	122.59
24	Q	107	VAL	CA-C-N	5.33	125.59	119.83
24	Q	107	VAL	C-N-CA	5.33	125.59	119.83
30	K	42	ASN	N-CA-CB	5.33	118.46	110.19
2	b	201	GLU	CB-CA-C	-5.33	101.16	110.17
3	c	18	ARG	CB-CG-CD	5.33	123.57	111.30
4	d	83	ARG	CA-C-N	5.33	129.08	120.55
4	d	83	ARG	C-N-CA	5.33	129.08	120.55
5	e	186	GLU	N-CA-CB	5.33	118.37	110.53
12	5	211	ALA	N-CA-C	5.33	116.78	111.07
16	V	22	ASP	CB-CA-C	-5.33	103.69	112.06
20	Z	793	PHE	CA-CB-CG	-5.33	108.47	113.80
25	R	323	ASN	N-CA-C	-5.33	105.55	111.36
28	H	268	ASP	N-CA-CB	5.33	119.59	111.70
33	J	124	LYS	N-CA-C	-5.33	101.25	109.52
2	b	196	LEU	CA-C-O	5.33	125.98	119.05
3	c	4	ARG	NE-CZ-NH1	5.33	126.83	121.50
5	e	39	GLY	N-CA-C	-5.33	100.55	113.18
6	F	16	THR	CA-CB-OG1	5.33	117.60	109.60
21	N	711	ARG	NE-CZ-NH1	5.33	126.83	121.50
2	b	17	LYS	CA-C-N	5.33	130.51	123.00
2	b	17	LYS	C-N-CA	5.33	130.51	123.00
6	f	47	VAL	CA-C-O	5.33	125.53	120.31
3	C	43	GLY	CA-C-O	-5.33	115.78	121.38
9	2	234	PHE	CA-C-N	5.33	125.33	119.89
9	2	234	PHE	C-N-CA	5.33	125.33	119.89
21	N	17	GLN	N-CA-CB	5.33	119.50	110.49
26	U	122	ILE	N-CA-C	-5.33	99.80	107.37
27	O	193	LEU	N-CA-C	-5.33	105.55	111.36
1	a	146	VAL	O-C-N	5.33	128.72	123.18
2	b	96	SER	CA-C-O	5.33	126.40	119.95
10	j	112	ILE	N-CA-C	-5.33	100.39	108.17
2	B	241	GLN	N-CA-C	5.33	117.09	111.28
5	E	66	LYS	N-CA-C	-5.33	106.09	112.59
19	Y	19	LYS	N-CA-C	5.33	117.17	111.36
21	N	235	ALA	N-CA-CB	5.33	118.51	110.30
27	O	373	TRP	N-CA-C	-5.33	105.64	111.82
32	M	400	MET	CA-C-N	5.33	128.89	120.47
32	M	400	MET	C-N-CA	5.33	128.89	120.47
2	B	151	ASP	CA-C-O	-5.33	116.34	121.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	194	ARG	CD-NE-CZ	5.33	131.86	124.40
20	Z	285	ALA	CA-C-N	5.33	127.76	120.46
20	Z	285	ALA	C-N-CA	5.33	127.76	120.46
6	f	24	TYR	CB-CA-C	-5.33	101.95	110.79
11	k	100	VAL	N-CA-CB	5.33	119.06	111.82
1	A	85	GLY	CA-C-N	5.33	125.33	119.90
1	A	85	GLY	C-N-CA	5.33	125.33	119.90
6	F	136	GLY	O-C-N	5.33	129.73	123.61
22	S	136	CYS	CA-C-N	5.33	127.42	120.28
22	S	136	CYS	C-N-CA	5.33	127.42	120.28
23	P	406	LYS	N-CA-CB	5.33	119.38	110.59
27	O	29	PHE	CB-CA-C	-5.33	102.52	110.88
32	M	369	THR	CA-CB-OG1	5.33	117.59	109.60
2	b	177	LYS	CB-CA-C	-5.32	98.97	109.67
3	c	123	THR	CA-C-N	5.32	127.68	120.44
3	c	123	THR	C-N-CA	5.32	127.68	120.44
10	j	43	ILE	N-CA-C	-5.32	100.72	108.97
14	n	254	PHE	CA-CB-CG	5.32	119.12	113.80
27	O	326	HIS	CE1-NE2-CD2	-5.32	103.68	109.00
29	I	211	MET	N-CA-C	-5.32	106.29	112.89
31	L	128	ILE	N-CA-C	-5.32	100.66	108.11
31	L	387	ASN	N-CA-CB	5.32	118.51	110.42
33	J	331	HIS	ND1-CE1-NE2	5.32	113.72	108.40
2	b	225	THR	O-C-N	5.32	129.32	123.25
7	g	60	VAL	CA-C-O	5.32	125.69	119.89
25	R	346	LYS	N-CA-C	-5.32	106.84	113.55
2	b	5	TYR	N-CA-CB	5.32	118.29	109.88
5	e	91	HIS	CB-CA-C	-5.32	101.96	110.79
14	n	134	TYR	CA-C-O	-5.32	115.21	120.90
11	4	189	ILE	CA-C-O	5.32	125.52	120.31
14	7	83	VAL	O-C-N	-5.32	117.43	123.18
20	Z	351	PRO	CA-C-N	5.32	127.84	120.29
20	Z	351	PRO	C-N-CA	5.32	127.84	120.29
22	S	364	ILE	CA-C-N	5.32	127.68	120.44
22	S	364	ILE	C-N-CA	5.32	127.68	120.44
22	S	474	GLU	N-CA-C	5.32	117.08	111.28
23	P	350	LEU	O-C-N	5.32	128.44	122.22
24	Q	282	LEU	N-CA-CB	5.32	117.86	110.04
26	U	303	GLU	O-C-N	-5.32	116.59	122.07
31	L	91	THR	N-CA-C	-5.32	106.95	113.50
4	d	24	LEU	CA-C-N	5.32	127.84	120.29
4	d	24	LEU	C-N-CA	5.32	127.84	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	27	SER	CA-C-N	5.32	127.26	120.56
21	N	27	SER	C-N-CA	5.32	127.26	120.56
24	Q	44	ALA	CA-C-N	5.32	131.70	121.54
24	Q	44	ALA	C-N-CA	5.32	131.70	121.54
24	Q	231	ASP	CA-CB-CG	-5.32	107.28	112.60
31	L	117	TYR	CA-CB-CG	-5.32	104.33	113.90
4	d	91	VAL	CA-CB-CG2	-5.32	101.36	110.40
11	k	61	GLN	OE1-CD-NE2	5.32	127.92	122.60
2	B	111	VAL	CA-CB-CG2	-5.32	101.36	110.40
5	E	151	ASP	O-C-N	-5.32	116.29	122.09
11	4	98	TYR	CB-CG-CD1	5.32	128.78	120.80
20	Z	196	SER	CA-C-N	5.32	127.41	120.28
20	Z	196	SER	C-N-CA	5.32	127.41	120.28
24	Q	369	ASP	CA-CB-CG	-5.32	107.28	112.60
29	I	150	HIS	CG-CD2-NE2	5.32	112.52	107.20
5	e	42	THR	CA-C-N	5.32	130.89	122.60
5	e	42	THR	C-N-CA	5.32	130.89	122.60
4	D	112	TYR	CA-C-O	-5.32	114.78	120.42
5	E	120	ALA	CA-C-O	-5.32	114.92	120.55
21	N	240	GLN	CA-C-N	5.32	127.40	120.28
21	N	240	GLN	C-N-CA	5.32	127.40	120.28
23	P	175	GLU	CA-C-O	-5.32	114.79	120.42
28	H	98	GLN	CA-C-O	-5.32	114.32	120.49
29	I	90	GLU	N-CA-C	-5.32	105.40	111.14
33	J	30	THR	CA-C-O	-5.32	113.86	119.97
8	h	154	ASN	N-CA-CB	5.31	119.47	110.49
30	K	62	THR	CA-C-O	-5.31	113.38	119.60
8	h	10	THR	N-CA-C	-5.31	96.12	111.00
7	G	32	GLU	O-C-N	-5.31	114.67	122.43
21	N	257	ILE	CA-CB-CG1	5.31	119.43	110.40
33	J	379	GLN	CB-CG-CD	-5.31	103.57	112.60
3	c	200	THR	O-C-N	-5.31	116.30	122.09
5	e	147	HIS	ND1-CE1-NE2	5.31	113.71	108.40
10	j	23	ILE	CB-CA-C	5.31	119.19	110.69
21	N	35	LEU	N-CA-C	-5.31	105.45	112.94
21	N	799	VAL	CA-C-N	-5.31	113.16	120.28
21	N	799	VAL	C-N-CA	-5.31	113.16	120.28
9	i	145	HIS	CE1-NE2-CD2	-5.31	103.69	109.00
20	Z	256	LEU	O-C-N	5.31	127.43	121.32
22	S	139	HIS	O-C-N	-5.31	116.49	122.12
25	R	132	GLN	N-CA-C	-5.31	105.66	111.82
28	H	218	ILE	CA-C-O	5.31	126.00	119.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L	191	ARG	CA-C-N	5.31	127.83	120.29
31	L	191	ARG	C-N-CA	5.31	127.83	120.29
8	h	195	LEU	N-CA-CB	5.31	120.79	111.55
10	j	137	ILE	N-CA-C	-5.31	100.83	108.42
11	k	189	ILE	N-CA-CB	5.31	118.89	112.10
2	B	157	PHE	CB-CA-C	-5.31	103.10	110.16
4	D	44	LEU	CA-C-O	5.31	125.98	120.30
23	P	372	THR	N-CA-CB	5.31	118.61	110.70
24	Q	136	SER	CA-C-N	5.31	128.38	120.31
24	Q	136	SER	C-N-CA	5.31	128.38	120.31
24	Q	359	ILE	CA-C-N	5.31	127.39	120.28
24	Q	359	ILE	C-N-CA	5.31	127.39	120.28
3	C	9	ARG	CD-NE-CZ	5.31	131.83	124.40
16	V	287	THR	CA-CB-OG1	5.31	117.56	109.60
25	R	161	ALA	CA-C-O	5.31	126.37	120.43
31	L	84	LEU	CA-C-N	5.31	127.66	120.44
31	L	84	LEU	C-N-CA	5.31	127.66	120.44
8	l	201	GLU	CA-C-O	5.30	126.22	120.55
15	W	103	ASN	N-CA-CB	5.30	120.67	111.39
21	N	117	TYR	N-CA-CB	5.30	118.79	110.46
22	S	20	HIS	ND1-CE1-NE2	5.30	113.70	108.40
26	U	304	GLN	CB-CG-CD	5.30	121.62	112.60
30	K	178	ASP	CA-C-O	-5.30	113.87	119.97
7	g	183	HIS	CE1-NE2-CD2	-5.30	103.70	109.00
11	k	126	VAL	CA-CB-CG1	-5.30	101.39	110.40
16	V	176	ASN	CA-CB-CG	-5.30	107.30	112.60
21	N	345	ASP	CB-CA-C	-5.30	99.87	110.42
23	P	219	GLU	CA-C-N	5.30	127.33	120.44
23	P	219	GLU	C-N-CA	5.30	127.33	120.44
30	K	381	ALA	CA-C-N	5.30	129.16	121.52
30	K	381	ALA	C-N-CA	5.30	129.16	121.52
3	c	68	LYS	N-CA-CB	5.30	118.17	109.95
8	h	78	GLN	N-CA-C	-5.30	107.47	114.04
11	k	194	ASP	O-C-N	5.30	129.45	122.93
14	n	49	TYR	CA-C-O	-5.30	115.51	121.40
5	E	167	TYR	CB-CG-CD2	-5.30	112.85	120.80
9	2	99	THR	CA-C-N	5.30	129.67	122.19
9	2	99	THR	C-N-CA	5.30	129.67	122.19
16	V	300	VAL	CA-C-O	-5.30	115.16	121.05
17	T	177	PHE	CA-C-N	5.30	127.82	120.29
17	T	177	PHE	C-N-CA	5.30	127.82	120.29
25	R	305	PHE	CA-C-N	5.30	124.93	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	305	PHE	C-N-CA	5.30	124.93	119.05
30	K	38	SER	CA-C-N	5.30	129.71	122.34
30	K	38	SER	C-N-CA	5.30	129.71	122.34
12	l	204	VAL	CA-CB-CG2	-5.30	101.39	110.40
22	S	360	PHE	CA-CB-CG	-5.30	108.50	113.80
24	Q	23	ALA	CA-C-N	5.30	127.64	120.38
24	Q	23	ALA	C-N-CA	5.30	127.64	120.38
25	R	157	SER	CA-C-N	5.30	127.38	120.28
25	R	157	SER	C-N-CA	5.30	127.38	120.28
2	B	64	VAL	CA-CB-CG1	-5.30	101.39	110.40
8	l	71	HIS	CE1-NE2-CD2	-5.30	103.70	109.00
32	M	168	LYS	N-CA-C	-5.30	106.32	112.89
1	a	235	THR	N-CA-C	-5.30	100.77	109.40
6	f	219	ASP	N-CA-C	-5.30	105.47	112.94
9	i	85	THR	CA-C-O	-5.30	114.81	120.42
3	C	217	ARG	NE-CZ-NH1	5.30	126.80	121.50
18	X	91	PHE	CA-CB-CG	-5.30	108.50	113.80
25	R	271	ILE	CB-CA-C	5.30	115.61	110.63
26	U	266	THR	CA-C-N	5.30	127.94	120.42
26	U	266	THR	C-N-CA	5.30	127.94	120.42
28	H	406	LEU	O-C-N	5.30	127.52	122.07
30	K	335	ASP	CA-C-O	5.30	126.93	120.31
12	l	243	ASP	CA-C-N	5.29	127.38	120.28
12	l	243	ASP	C-N-CA	5.29	127.38	120.28
3	C	83	ASP	CA-CB-CG	-5.29	107.31	112.60
16	V	234	GLU	CB-CG-CD	-5.29	103.60	112.60
21	N	340	HIS	N-CA-CB	-5.29	102.83	110.56
1	a	125	SER	CA-C-N	5.29	127.37	120.28
1	a	125	SER	C-N-CA	5.29	127.37	120.28
12	l	134	LEU	N-CA-CB	5.29	117.90	110.12
24	Q	252	HIS	CB-CG-ND1	5.29	130.64	122.70
25	R	214	TYR	N-CA-C	5.29	117.13	111.36
28	H	144	LYS	N-CA-C	-5.29	101.36	109.41
5	e	10	ARG	CA-C-N	-5.29	115.26	122.03
5	e	10	ARG	C-N-CA	-5.29	115.26	122.03
8	h	194	ARG	NH1-CZ-NH2	-5.29	112.42	119.30
13	m	67	ALA	N-CA-C	5.29	117.05	111.28
6	F	138	ASP	CA-C-N	5.29	129.56	120.72
6	F	138	ASP	C-N-CA	5.29	129.56	120.72
22	S	21	SER	O-C-N	5.29	127.59	122.09
23	P	104	LEU	N-CA-C	5.29	117.05	111.28
24	Q	308	ASN	CA-C-O	-5.29	114.94	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	326	SER	CA-C-N	5.29	127.80	120.29
21	N	326	SER	C-N-CA	5.29	127.80	120.29
23	P	229	LEU	CA-C-N	5.29	127.80	120.29
23	P	229	LEU	C-N-CA	5.29	127.80	120.29
9	i	149	ASP	N-CA-CB	5.29	120.19	111.62
9	i	154	LEU	CA-C-O	-5.29	115.42	121.40
9	i	173	GLN	O-C-N	5.29	129.44	122.93
7	G	228	HIS	CA-CB-CG	-5.29	108.51	113.80
12	5	227	ASP	CA-C-N	5.29	127.37	120.28
12	5	227	ASP	C-N-CA	5.29	127.37	120.28
15	W	110	ILE	N-CA-C	-5.29	100.86	108.48
21	N	312	GLY	O-C-N	-5.29	116.05	122.71
22	S	240	ASP	CA-CB-CG	-5.29	107.31	112.60
24	Q	287	THR	CA-C-O	5.29	124.64	118.77
24	Q	359	ILE	CB-CG1-CD1	5.29	124.91	113.80
25	R	229	LYS	N-CA-C	5.29	117.12	111.36
2	b	82	TYR	CA-C-O	5.29	126.15	120.55
1	A	222	ASP	N-CA-C	-5.29	106.22	113.30
6	F	47	VAL	CB-CA-C	5.29	117.86	110.99
25	R	135	ILE	CA-C-N	5.29	127.89	120.28
25	R	135	ILE	C-N-CA	5.29	127.89	120.28
11	4	19	LYS	CA-C-O	5.29	126.14	120.70
12	5	166	LYS	CA-C-N	5.29	131.84	121.06
12	5	166	LYS	C-N-CA	5.29	131.84	121.06
17	T	113	LEU	CA-C-O	-5.29	114.82	120.42
25	R	176	ARG	CB-CG-CD	5.29	123.46	111.30
27	O	341	ILE	CA-C-O	5.29	125.94	120.39
29	I	303	GLN	CA-C-N	5.29	127.67	120.54
29	I	303	GLN	C-N-CA	5.29	127.67	120.54
30	K	283	ASP	N-CA-CB	5.29	117.61	110.10
30	K	332	GLY	N-CA-C	-5.29	108.05	114.92
4	d	49	ARG	N-CA-CB	5.28	118.27	109.60
5	e	116	VAL	CA-C-N	5.28	127.79	120.29
5	e	116	VAL	C-N-CA	5.28	127.79	120.29
6	f	116	ALA	CA-C-O	-5.28	114.82	120.42
3	C	89	ASN	CA-C-O	-5.28	112.76	119.31
11	4	86	GLN	CA-C-N	5.28	127.79	120.29
11	4	86	GLN	C-N-CA	5.28	127.79	120.29
23	P	162	GLU	O-C-N	5.28	127.72	122.12
30	K	320	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	a	131	ARG	NE-CZ-NH2	5.28	123.95	119.20
7	G	172	ALA	CA-C-O	-5.28	114.95	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	39	VAL	CA-C-N	5.28	129.23	120.94
8	h	39	VAL	C-N-CA	5.28	129.23	120.94
13	6	31	LEU	N-CA-C	-5.28	99.68	108.34
23	P	323	ASN	N-CA-C	-5.28	106.81	113.20
23	P	345	VAL	CA-C-N	5.28	127.21	120.56
23	P	345	VAL	C-N-CA	5.28	127.21	120.56
24	Q	209	TYR	N-CA-CB	-5.28	102.68	110.49
27	O	66	VAL	CB-CA-C	-5.28	105.01	112.14
30	K	297	ILE	CB-CA-C	-5.28	105.01	112.14
32	M	295	LYS	CA-C-O	-5.28	115.59	122.14
23	P	51	ASP	CB-CA-C	-5.28	102.03	110.79
31	L	67	HIS	CG-CD2-NE2	5.28	112.48	107.20
33	J	388	LYS	CB-CA-C	-5.28	101.88	110.85
1	A	51	THR	CA-C-N	5.28	130.28	122.94
1	A	51	THR	C-N-CA	5.28	130.28	122.94
6	F	170	THR	CA-C-N	5.28	127.35	120.28
6	F	170	THR	C-N-CA	5.28	127.35	120.28
11	4	75	LEU	CA-C-N	5.28	127.73	120.39
11	4	75	LEU	C-N-CA	5.28	127.73	120.39
11	4	153	THR	CA-CB-OG1	5.28	117.52	109.60
15	W	99	LYS	CB-CA-C	-5.28	101.64	110.56
22	S	98	SER	N-CA-C	5.28	117.53	110.35
25	R	82	ASP	CA-C-O	5.28	127.14	121.44
28	H	57	LYS	N-CA-CB	5.28	118.35	110.22
28	H	362	ASP	CA-C-O	-5.28	115.20	120.64
4	d	90	ARG	CA-C-N	5.28	127.69	120.46
4	d	90	ARG	C-N-CA	5.28	127.69	120.46
4	d	123	SER	N-CA-C	-5.28	102.24	110.42
8	h	142	PHE	CA-CB-CG	-5.28	108.53	113.80
10	j	112	ILE	O-C-N	5.28	128.77	123.07
1	A	242	GLU	CA-C-N	5.28	127.35	120.28
1	A	242	GLU	C-N-CA	5.28	127.35	120.28
2	B	190	HIS	ND1-CE1-NE2	5.28	113.68	108.40
7	G	33	ASN	OD1-CG-ND2	5.28	127.88	122.60
14	7	53	VAL	CA-C-O	5.28	127.21	121.67
21	N	211	PHE	CA-CB-CG	-5.28	108.52	113.80
21	N	738	GLN	N-CA-C	-5.28	100.13	108.73
24	Q	205	ALA	N-CA-C	-5.28	106.07	112.88
24	Q	363	SER	N-CA-C	5.28	117.03	111.28
28	H	89	GLN	N-CA-C	-5.28	105.99	112.90
6	f	122	SER	N-CA-CB	5.27	119.23	110.63
14	n	132	VAL	N-CA-C	5.27	115.48	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	84	THR	CA-CB-CG2	5.27	119.47	110.50
30	K	180	GLN	CA-C-O	5.27	125.86	119.11
31	L	413	ASP	N-CA-C	-5.27	105.20	111.69
32	M	233	ARG	CB-CA-C	-5.27	102.03	110.79
1	a	157	THR	N-CA-CB	5.27	118.63	110.46
3	C	209	ASP	N-CA-C	-5.27	106.80	113.18
4	D	111	ARG	CD-NE-CZ	5.27	131.78	124.40
15	W	40	LYS	N-CA-C	5.27	117.11	111.36
19	Y	40	ILE	CA-C-O	-5.27	115.20	121.05
23	P	15	GLN	CA-C-O	-5.27	114.83	120.42
24	Q	375	GLY	O-C-N	-5.27	117.08	122.19
28	H	108	GLY	O-C-N	-5.27	116.53	122.28
15	W	120	ASP	CA-C-N	5.27	128.25	120.82
15	W	120	ASP	C-N-CA	5.27	128.25	120.82
6	f	162	GLY	CA-C-N	5.27	130.20	122.77
6	f	162	GLY	C-N-CA	5.27	130.20	122.77
1	A	181	ASN	O-C-N	5.27	127.78	122.09
2	B	197	LYS	CA-C-O	-5.27	113.57	119.79
16	V	117	TRP	N-CA-CB	5.27	119.39	110.49
28	H	168	ILE	CA-C-N	5.27	130.84	122.62
28	H	168	ILE	C-N-CA	5.27	130.84	122.62
5	e	167	TYR	CB-CA-C	-5.27	100.34	110.24
10	j	23	ILE	N-CA-C	-5.27	100.27	108.86
9	2	48	ARG	NE-CZ-NH2	-5.27	114.46	119.20
20	Z	191	SER	CA-C-N	5.27	125.79	120.00
20	Z	191	SER	C-N-CA	5.27	125.79	120.00
27	O	385	GLU	N-CA-C	-5.27	105.62	111.36
29	I	84	PRO	N-CA-C	-5.27	107.16	114.27
31	L	69	ARG	N-CA-C	-5.27	106.90	113.38
1	a	193	HIS	CA-C-N	5.27	128.23	120.91
1	a	193	HIS	C-N-CA	5.27	128.23	120.91
3	C	103	ASN	CA-C-O	-5.27	115.01	121.28
3	C	229	ILE	N-CA-C	-5.26	99.67	107.51
5	E	42	THR	CA-CB-OG1	5.26	117.50	109.60
13	6	172	THR	CA-C-N	5.26	129.66	122.34
13	6	172	THR	C-N-CA	5.26	129.66	122.34
15	W	148	GLU	CB-CA-C	-5.26	102.05	110.79
22	S	214	MET	CA-C-N	5.26	127.33	120.28
22	S	214	MET	C-N-CA	5.26	127.33	120.28
23	P	88	GLN	CA-C-O	-5.26	114.11	120.32
24	Q	252	HIS	CG-CD2-NE2	5.26	112.46	107.20
30	K	278	ALA	CA-C-N	5.26	131.21	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	278	ALA	C-N-CA	5.26	131.21	121.94
16	V	253	LYS	CA-C-N	5.26	127.76	120.29
16	V	253	LYS	C-N-CA	5.26	127.76	120.29
17	T	108	LEU	N-CA-C	5.26	117.10	111.36
20	Z	253	VAL	CG1-CB-CG2	-5.26	99.22	110.80
4	d	121	THR	CA-C-N	5.26	129.02	120.60
4	d	121	THR	C-N-CA	5.26	129.02	120.60
12	l	77	THR	CA-CB-OG1	5.26	117.49	109.60
6	F	16	THR	N-CA-CB	5.26	118.04	110.20
9	2	58	LYS	CG-CD-CE	5.26	123.40	111.30
14	7	124	TYR	CB-CG-CD1	5.26	128.69	120.80
16	V	114	PHE	N-CA-C	-5.26	101.41	109.41
21	N	548	ARG	O-C-N	5.26	128.15	122.15
27	O	301	PHE	CA-CB-CG	-5.26	108.54	113.80
1	a	68	THR	N-CA-C	-5.26	106.37	112.89
9	i	67	SER	O-C-N	-5.26	117.81	121.65
3	C	112	VAL	CA-C-O	-5.26	115.28	120.85
3	C	203	SER	N-CA-C	-5.26	101.31	109.72
6	F	93	ASN	N-CA-C	-5.26	105.60	112.23
8	1	65	ALA	CA-C-O	-5.26	114.16	120.10
17	T	85	LEU	N-CA-CB	-5.26	102.38	110.01
23	P	337	HIS	CE1-NE2-CD2	-5.26	103.74	109.00
31	L	234	ALA	CA-C-O	-5.26	113.92	119.97
16	V	60	ASP	CA-C-N	5.26	131.58	121.54
16	V	60	ASP	C-N-CA	5.26	131.58	121.54
2	b	226	GLY	N-CA-C	-5.26	107.97	115.64
4	d	214	VAL	CA-C-O	-5.26	114.87	120.39
9	i	217	ARG	NE-CZ-NH2	-5.26	114.47	119.20
14	n	51	ASN	O-C-N	-5.26	115.99	122.25
1	A	200	GLU	CB-CG-CD	-5.26	103.67	112.60
19	Y	65	ASP	N-CA-C	-5.26	99.89	109.56
21	N	308	ASN	N-CA-C	-5.26	99.53	108.26
26	U	123	VAL	CB-CA-C	-5.26	103.95	111.31
2	b	211	LEU	CA-C-O	5.25	126.38	120.70
12	5	130	TRP	CG-CD2-CE3	-5.25	128.65	133.90
18	X	8	ILE	N-CA-CB	5.25	118.08	111.46
24	Q	408	THR	CA-C-N	5.25	127.32	120.28
24	Q	408	THR	C-N-CA	5.25	127.32	120.28
30	K	140	HIS	CA-CB-CG	-5.25	108.55	113.80
6	f	135	ILE	CB-CA-C	-5.25	104.56	111.70
14	7	125	ILE	CA-C-N	5.25	127.59	120.65
14	7	125	ILE	C-N-CA	5.25	127.59	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	7	133	MET	CA-C-N	5.25	127.63	120.54
14	7	133	MET	C-N-CA	5.25	127.63	120.54
23	P	118	VAL	CA-C-O	-5.25	115.28	120.85
27	O	240	GLU	N-CA-CB	5.25	117.63	110.01
28	H	154	LYS	CB-CA-C	-5.25	100.66	109.48
32	M	88	MET	N-CA-C	-5.25	100.74	108.99
4	d	181	ARG	NE-CZ-NH1	-5.25	116.25	121.50
8	h	178	SER	CA-C-O	5.25	126.03	120.36
13	m	202	ARG	NE-CZ-NH2	-5.25	114.47	119.20
10	3	129	CYS	N-CA-CB	5.25	119.36	110.49
25	R	230	LEU	CA-C-N	5.25	130.33	121.14
25	R	230	LEU	C-N-CA	5.25	130.33	121.14
26	U	172	GLU	CA-C-N	5.25	127.75	120.29
26	U	172	GLU	C-N-CA	5.25	127.75	120.29
28	H	120	ASN	N-CA-C	-5.25	106.39	114.16
28	H	408	SER	CA-C-O	5.25	125.99	120.42
31	L	50	GLN	CG-CD-NE2	5.25	124.28	116.40
31	L	95	ILE	N-CA-CB	5.25	118.46	110.58
11	k	133	HIS	CA-CB-CG	-5.25	108.55	113.80
1	A	183	GLU	CA-C-N	5.25	127.31	120.28
1	A	183	GLU	C-N-CA	5.25	127.31	120.28
6	F	159	THR	O-C-N	-5.25	116.78	122.92
15	W	77	HIS	ND1-CE1-NE2	5.25	113.65	108.40
22	S	332	PHE	CA-CB-CG	5.25	119.05	113.80
26	U	200	LEU	CA-C-N	5.25	127.31	120.28
26	U	200	LEU	C-N-CA	5.25	127.31	120.28
20	Z	29	ASP	CA-C-N	5.25	127.62	120.54
20	Z	29	ASP	C-N-CA	5.25	127.62	120.54
25	R	110	ILE	N-CA-CB	5.25	116.13	110.62
29	I	117	HIS	O-C-N	-5.25	117.06	123.10
33	J	357	ASP	N-CA-CB	5.25	117.93	110.16
3	c	11	THR	N-CA-CB	5.25	118.36	110.65
1	A	147	ASP	CB-CA-C	-5.25	100.27	109.71
4	D	117	GLN	OE1-CD-NE2	-5.25	117.35	122.60
8	1	123	PRO	N-CD-CG	5.25	111.07	103.20
12	5	111	GLU	CA-C-N	5.25	128.94	120.55
12	5	111	GLU	C-N-CA	5.25	128.94	120.55
20	Z	444	GLU	CA-C-N	5.25	124.91	119.56
20	Z	444	GLU	C-N-CA	5.25	124.91	119.56
21	N	90	ASP	N-CA-C	-5.25	105.73	111.82
22	S	73	THR	CA-CB-OG1	5.25	117.47	109.60
2	b	246	ARG	CD-NE-CZ	-5.25	117.06	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	35	LEU	N-CA-CB	5.25	117.61	110.01
30	K	49	PHE	CA-CB-CG	5.25	119.05	113.80
31	L	232	ALA	CB-CA-C	-5.25	101.93	110.85
32	M	144	ASP	CA-C-O	5.25	126.96	121.19
33	J	47	GLN	CG-CD-NE2	-5.25	108.53	116.40
6	f	66	CYS	N-CA-C	-5.24	106.57	113.12
8	h	35	ILE	N-CA-C	-5.24	100.21	108.23
14	n	133	MET	CA-C-N	5.24	127.62	120.54
14	n	133	MET	C-N-CA	5.24	127.62	120.54
3	C	110	ILE	CB-CA-C	-5.24	105.15	112.02
11	4	168	LEU	N-CA-C	-5.24	105.68	111.71
21	N	119	LYS	O-C-N	5.24	129.35	122.33
28	H	302	LYS	CA-C-N	5.24	131.56	121.54
28	H	302	LYS	C-N-CA	5.24	131.56	121.54
30	K	211	LEU	N-CA-C	-5.24	100.63	109.07
4	d	91	VAL	CA-CB-CG1	-5.24	101.49	110.40
4	D	145	PRO	N-CA-CB	5.24	108.21	103.34
16	V	30	SER	N-CA-CB	5.24	117.42	110.29
22	S	97	THR	N-CA-CB	5.24	119.34	110.49
25	R	74	ASN	CB-CA-C	-5.24	100.61	110.51
32	M	395	THR	CA-C-O	5.24	125.97	120.42
1	a	251	GLN	N-CA-CB	5.24	119.41	110.50
2	b	18	LEU	CA-C-N	5.24	125.79	119.98
2	b	18	LEU	C-N-CA	5.24	125.79	119.98
4	d	137	GLY	N-CA-C	-5.24	102.94	110.38
10	j	100	PHE	N-CA-C	-5.24	99.87	108.41
3	C	31	HIS	N-CA-CB	5.24	118.35	110.65
4	D	63	LYS	CA-C-O	5.24	126.03	119.59
27	O	289	GLN	OE1-CD-NE2	-5.24	117.36	122.60
14	7	184	ALA	N-CA-CB	5.24	117.91	110.16
25	R	95	ASP	N-CA-CB	5.24	120.04	111.08
25	R	362	ALA	N-CA-CB	-5.24	102.42	110.12
30	K	53	LYS	N-CA-CB	5.24	117.88	110.13
6	f	204	GLU	CA-C-N	5.24	131.54	121.54
6	f	204	GLU	C-N-CA	5.24	131.54	121.54
7	g	51	GLU	CB-CG-CD	-5.24	103.70	112.60
12	5	282	PHE	CA-C-N	5.24	127.30	120.28
12	5	282	PHE	C-N-CA	5.24	127.30	120.28
15	W	97	THR	N-CA-C	-5.24	105.47	111.07
21	N	367	ALA	CB-CA-C	-5.24	101.95	110.85
24	Q	21	ASN	CA-C-O	-5.24	115.00	120.55
24	Q	356	CYS	CA-C-N	5.24	128.89	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	356	CYS	C-N-CA	5.24	128.89	121.66
27	O	205	ILE	N-CA-C	-5.24	100.11	107.75
14	7	121	GLU	CA-C-O	-5.23	114.89	120.28
4	d	118	GLN	CA-C-O	-5.23	115.00	120.55
6	f	210	ASN	CA-C-N	5.23	129.57	122.19
6	f	210	ASN	C-N-CA	5.23	129.57	122.19
8	h	192	VAL	CA-C-O	5.23	124.88	120.22
14	7	156	GLY	N-CA-C	-5.23	108.03	115.30
14	7	241	PHE	CA-C-O	-5.23	113.98	120.57
16	V	32	ILE	N-CA-CB	5.23	116.67	110.55
20	Z	298	PHE	CA-C-N	5.23	127.29	120.28
20	Z	298	PHE	C-N-CA	5.23	127.29	120.28
23	P	213	TYR	CB-CG-CD2	-5.23	112.95	120.80
25	R	130	GLN	CB-CA-C	-5.23	101.95	110.85
28	H	162	ARG	CA-C-N	5.23	129.60	122.90
28	H	162	ARG	C-N-CA	5.23	129.60	122.90
4	D	195	THR	N-CA-CB	5.23	118.36	110.30
9	2	138	HIS	CE1-NE2-CD2	-5.23	103.77	109.00
12	5	236	ILE	N-CA-CB	5.23	118.43	110.58
19	Y	7	ALA	N-CA-C	5.23	117.06	111.36
23	P	328	ALA	CA-C-O	5.23	127.99	120.51
24	Q	166	LYS	N-CA-C	-5.23	106.95	113.38
24	Q	252	HIS	CB-CG-CD2	-5.23	124.40	131.20
32	M	326	ALA	N-CA-C	-5.23	101.35	109.72
33	J	296	ARG	NE-CZ-NH2	-5.23	114.49	119.20
7	g	43	ASN	CA-CB-CG	-5.23	107.37	112.60
12	l	206	SER	N-CA-C	-5.23	105.75	111.82
5	E	117	CYS	N-CA-CB	5.23	117.90	110.16
14	7	80	ASP	CA-CB-CG	5.23	117.83	112.60
7	G	244	GLN	CA-CB-CG	5.23	124.56	114.10
16	V	196	TYR	N-CA-CB	5.23	119.74	111.43
23	P	48	GLN	N-CA-CB	5.23	117.59	110.01
24	Q	265	MET	CA-C-O	-5.23	115.01	120.55
24	Q	271	MET	CA-C-N	5.23	127.81	120.28
24	Q	271	MET	C-N-CA	5.23	127.81	120.28
26	U	185	GLY	CA-C-N	5.23	127.23	120.44
26	U	185	GLY	C-N-CA	5.23	127.23	120.44
29	I	128	TYR	CA-C-N	5.23	130.71	122.34
29	I	128	TYR	C-N-CA	5.23	130.71	122.34
1	a	99	ALA	O-C-N	-5.23	116.69	122.07
1	a	162	TYR	CB-CG-CD2	-5.23	112.96	120.80
10	j	20	CYS	CA-C-O	-5.23	113.04	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	254	GLU	CA-C-N	5.23	131.11	121.70
9	2	254	GLU	C-N-CA	5.23	131.11	121.70
33	J	213	VAL	N-CA-C	-5.23	100.87	108.97
1	a	19	PHE	N-CA-CB	5.22	117.65	109.97
7	g	41	LYS	N-CA-C	-5.22	100.00	108.41
11	k	147	HIS	CB-CG-CD2	5.22	137.99	131.20
12	5	78	THR	N-CA-CB	5.22	119.28	110.77
17	T	21	ALA	CA-C-N	5.22	128.25	120.31
17	T	21	ALA	C-N-CA	5.22	128.25	120.31
22	S	22	GLU	CB-CA-C	-5.22	101.97	110.85
22	S	365	THR	N-CA-CB	5.22	117.64	110.07
28	H	54	ASN	CA-C-N	5.22	127.28	120.28
28	H	54	ASN	C-N-CA	5.22	127.28	120.28
31	L	75	LYS	O-C-N	-5.22	115.30	122.46
32	M	220	MET	CA-C-O	5.22	125.89	120.30
6	f	85	SER	O-C-N	-5.22	116.20	122.15
7	g	87	HIS	CE1-NE2-CD2	-5.22	103.78	109.00
13	m	91	LYS	O-C-N	5.22	129.17	123.01
12	5	260	TRP	CB-CG-CD2	-5.22	119.49	126.80
20	Z	925	VAL	CA-C-N	5.22	131.52	121.54
20	Z	925	VAL	C-N-CA	5.22	131.52	121.54
21	N	697	PHE	CA-C-N	5.22	126.85	120.22
21	N	697	PHE	C-N-CA	5.22	126.85	120.22
23	P	82	LEU	CA-C-N	5.22	127.28	120.28
23	P	82	LEU	C-N-CA	5.22	127.28	120.28
27	O	216	ASP	N-CA-CB	5.22	117.80	110.12
28	H	168	ILE	CA-CB-CG1	5.22	119.28	110.40
33	J	230	VAL	CA-C-N	5.22	127.28	120.28
33	J	230	VAL	C-N-CA	5.22	127.28	120.28
1	a	100	GLU	CA-C-O	5.22	125.97	119.97
1	a	218	PHE	N-CA-C	-5.22	101.50	108.86
3	C	216	ILE	CA-C-N	5.22	131.01	122.81
3	C	216	ILE	C-N-CA	5.22	131.01	122.81
23	P	101	MET	CA-C-N	5.22	127.59	120.54
23	P	101	MET	C-N-CA	5.22	127.59	120.54
23	P	156	ALA	N-CA-C	5.22	116.97	111.28
29	I	179	GLU	N-CA-CB	5.22	117.69	110.17
32	M	364	HIS	CB-CA-C	-5.22	101.14	110.70
12	l	215	LEU	N-CA-C	5.22	116.78	111.14
14	n	116	ALA	N-CA-C	-5.22	105.03	111.40
4	D	184	PRO	N-CA-C	-5.22	104.33	110.70
22	S	253	PHE	CA-CB-CG	-5.22	108.58	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	407	ILE	CA-CB-CG2	-5.22	101.63	110.50
14	7	197	ASP	CA-C-O	-5.22	113.20	119.15
15	W	44	ASN	N-CA-CB	-5.22	102.30	111.17
21	N	157	ALA	N-CA-C	5.22	117.87	111.82
30	K	48	TYR	CA-C-N	5.22	127.27	120.28
30	K	48	TYR	C-N-CA	5.22	127.27	120.28
7	g	99	PHE	CA-CB-CG	-5.22	108.58	113.80
14	n	83	VAL	N-CA-CB	5.22	118.61	111.41
1	A	33	LYS	N-CA-C	-5.22	106.50	112.92
15	W	54	GLY	CA-C-N	5.22	128.62	120.75
15	W	54	GLY	C-N-CA	5.22	128.62	120.75
25	R	266	LEU	CA-C-N	5.22	127.27	120.28
25	R	266	LEU	C-N-CA	5.22	127.27	120.28
33	J	33	LYS	CA-C-N	5.22	128.86	120.30
33	J	33	LYS	C-N-CA	5.22	128.86	120.30
3	c	11	THR	N-CA-C	-5.21	106.94	113.72
7	G	29	LYS	CA-C-N	5.21	127.69	120.29
7	G	29	LYS	C-N-CA	5.21	127.69	120.29
9	2	140	PHE	N-CA-C	-5.21	101.48	109.41
15	W	65	PHE	CA-CB-CG	-5.21	108.58	113.80
20	Z	369	PHE	CA-CB-CG	-5.21	108.58	113.80
21	N	113	ALA	CA-C-N	5.21	127.79	120.28
21	N	113	ALA	C-N-CA	5.21	127.79	120.28
27	O	80	LYS	CB-CA-C	-5.21	100.98	110.63
23	P	194	SER	CA-C-N	5.21	127.27	120.28
23	P	194	SER	C-N-CA	5.21	127.27	120.28
28	H	321	ASP	N-CA-CB	-5.21	103.09	110.81
7	g	147	HIS	ND1-CE1-NE2	5.21	113.61	108.40
8	h	151	PHE	N-CA-CB	5.21	118.37	109.87
13	m	99	ARG	N-CA-C	5.21	117.64	111.33
5	E	148	ASP	CA-CB-CG	5.21	117.81	112.60
8	1	69	GLN	CA-C-N	5.21	127.79	120.28
8	1	69	GLN	C-N-CA	5.21	127.79	120.28
17	T	76	ASP	CA-C-N	5.21	127.26	120.28
17	T	76	ASP	C-N-CA	5.21	127.26	120.28
25	R	109	LYS	CA-C-N	5.21	127.60	120.77
25	R	109	LYS	C-N-CA	5.21	127.60	120.77
27	O	44	SER	CA-C-N	5.21	127.27	120.28
27	O	44	SER	C-N-CA	5.21	127.27	120.28
31	L	124	GLY	CA-C-N	5.21	125.62	119.99
31	L	124	GLY	C-N-CA	5.21	125.62	119.99
10	j	138	VAL	CB-CA-C	-5.21	101.10	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	108	ASP	CA-CB-CG	-5.21	107.39	112.60
5	E	21	LEU	O-C-N	-5.21	116.40	122.81
23	P	2	SER	N-CA-C	-5.21	108.19	114.75
25	R	213	TYR	CA-C-N	5.21	127.69	120.29
25	R	213	TYR	C-N-CA	5.21	127.69	120.29
27	O	367	LYS	CB-CA-C	-5.21	102.70	110.88
33	J	375	ILE	CA-C-N	5.21	128.61	120.75
33	J	375	ILE	C-N-CA	5.21	128.61	120.75
1	a	213	ALA	N-CA-C	5.21	117.03	111.36
13	6	53	ASP	CB-CA-C	5.21	119.12	109.54
14	7	150	ALA	O-C-N	5.21	129.50	123.41
23	P	394	ASN	CA-CB-CG	5.21	117.81	112.60
28	H	162	ARG	CB-CG-CD	5.21	123.28	111.30
29	I	209	GLU	CA-C-O	-5.21	113.51	119.60
33	J	40	ASN	N-CA-C	5.21	117.03	111.36
7	G	132	PHE	CA-C-O	-5.21	115.47	121.19
24	Q	139	ILE	N-CA-C	-5.21	105.46	110.72
25	R	124	ASP	N-CA-CB	5.21	117.72	109.71
30	K	404	GLN	N-CA-C	-5.21	106.88	113.18
11	k	18	SER	CA-C-N	5.20	129.48	120.58
11	k	18	SER	C-N-CA	5.20	129.48	120.58
13	m	201	GLU	CB-CG-CD	-5.20	103.75	112.60
3	C	183	ASP	O-C-N	-5.20	117.11	123.30
8	1	11	SER	N-CA-CB	5.20	119.36	110.57
10	3	200	LEU	CA-C-N	5.20	128.94	121.50
10	3	200	LEU	C-N-CA	5.20	128.94	121.50
26	U	292	ILE	CA-C-N	5.20	127.68	120.29
26	U	292	ILE	C-N-CA	5.20	127.68	120.29
28	H	444	LEU	N-CA-C	5.20	116.95	111.28
31	L	137	ARG	N-CA-CB	5.20	117.86	110.16
32	M	431	SER	CA-C-O	-5.20	114.71	120.38
8	h	71	HIS	CE1-NE2-CD2	-5.20	103.80	109.00
12	l	282	PHE	CA-CB-CG	-5.20	108.60	113.80
6	F	126	ARG	NH1-CZ-NH2	-5.20	112.54	119.30
22	S	417	GLN	O-C-N	5.20	128.08	122.15
25	R	225	LYS	N-CA-CB	5.20	117.86	110.16
29	I	321	ASP	CA-CB-CG	5.20	117.80	112.60
30	K	88	ARG	NE-CZ-NH2	5.20	123.88	119.20
31	L	51	GLU	N-CA-CB	5.20	118.86	110.85
33	J	303	ALA	CA-C-O	5.20	125.51	119.32
1	a	164	VAL	O-C-N	-5.20	118.45	122.97
2	b	41	ASN	OD1-CG-ND2	5.20	127.80	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	212	ILE	N-CA-CB	5.20	120.00	111.58
14	n	110	ASP	CA-C-N	5.20	129.18	120.86
14	n	110	ASP	C-N-CA	5.20	129.18	120.86
1	A	185	HIS	CG-CD2-NE2	5.20	112.40	107.20
7	G	161	LYS	N-CA-C	-5.20	106.99	113.38
8	1	123	PRO	N-CA-CB	-5.20	97.79	103.25
13	6	165	LYS	O-C-N	5.20	129.32	122.93
16	V	69	PHE	N-CA-CB	5.20	121.19	111.52
17	T	267	ALA	N-CA-CB	5.20	117.76	110.12
24	Q	278	VAL	N-CA-C	-5.20	105.64	110.53
25	R	184	GLN	N-CA-C	-5.20	105.69	111.36
30	K	283	ASP	CB-CA-C	-5.20	103.12	111.39
1	a	141	LEU	CA-C-O	-5.20	115.20	120.71
4	D	144	GLU	N-CA-C	-5.20	102.02	109.24
11	4	7	ILE	N-CA-C	-5.20	100.04	107.78
12	5	145	GLU	CA-C-N	5.20	129.93	122.40
12	5	145	GLU	C-N-CA	5.20	129.93	122.40
17	T	150	ARG	N-CA-C	-5.20	105.70	111.36
17	T	213	ASN	N-CA-CB	5.20	120.53	111.13
24	Q	228	GLU	N-CA-C	5.20	117.68	111.71
27	O	129	ILE	N-CA-CB	5.20	116.63	110.55
30	K	189	GLU	O-C-N	-5.20	116.23	122.15
5	e	170	LYS	N-CA-C	-5.19	100.14	108.55
6	F	112	LEU	O-C-N	-5.19	116.61	122.12
14	7	118	GLU	CA-C-N	5.19	127.50	120.38
14	7	118	GLU	C-N-CA	5.19	127.50	120.38
17	T	189	ILE	O-C-N	5.19	127.18	121.83
10	j	157	ASN	CA-C-O	-5.19	115.70	122.45
12	l	113	ASN	CA-C-N	5.19	126.33	119.84
12	l	113	ASN	C-N-CA	5.19	126.33	119.84
14	n	206	ALA	CA-C-N	5.19	128.01	120.79
14	n	206	ALA	C-N-CA	5.19	128.01	120.79
6	F	29	ILE	O-C-N	5.19	127.18	121.83
9	2	81	THR	CA-C-O	-5.19	115.55	120.90
15	W	120	ASP	N-CA-C	-5.19	101.23	109.59
23	P	440	HIS	CA-CB-CG	5.19	118.99	113.80
29	I	125	MET	N-CA-CB	5.19	119.61	110.37
2	b	57	MET	CA-C-O	5.19	125.91	120.36
2	b	192	ALA	CA-C-N	5.19	127.24	120.28
2	b	192	ALA	C-N-CA	5.19	127.24	120.28
6	f	25	ALA	N-CA-C	-5.19	106.21	112.54
3	C	233	GLN	N-CA-C	-5.19	107.00	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	73	HIS	O-C-N	5.19	129.53	122.37
7	G	183	HIS	CE1-NE2-CD2	-5.19	103.81	109.00
20	Z	960	GLY	N-CA-C	-5.19	107.89	115.63
27	O	97	LYS	CA-C-O	-5.19	115.37	120.82
27	O	303	LYS	N-CA-CB	5.19	118.87	110.41
27	O	304	ASN	N-CA-CB	5.19	118.61	110.46
29	I	181	TYR	N-CA-C	5.19	117.41	110.35
2	b	178	ARG	CD-NE-CZ	-5.19	117.14	124.40
4	d	66	LYS	CA-C-O	5.19	126.51	120.49
9	i	170	HIS	CG-CD2-NE2	5.19	112.39	107.20
8	l	69	GLN	CB-CG-CD	-5.19	103.78	112.60
12	5	172	MET	CA-C-O	-5.19	113.09	120.51
22	S	440	ASP	CA-CB-CG	-5.19	107.41	112.60
28	H	220	LYS	CB-CA-C	-5.19	102.03	110.85
5	e	173	GLY	O-C-N	-5.19	117.65	123.10
10	j	41	GLU	CB-CA-C	-5.19	101.81	109.90
10	j	71	THR	N-CA-C	-5.19	105.52	111.07
3	C	12	ILE	CA-CB-CG2	-5.19	101.68	110.50
13	6	122	LEU	O-C-N	5.19	128.89	123.03
14	7	250	MET	N-CA-CB	5.19	118.63	110.23
22	S	207	ASN	O-C-N	5.19	127.62	122.12
31	L	333	LEU	N-CA-C	5.19	117.23	110.43
5	e	82	THR	O-C-N	-5.19	115.05	122.41
11	k	50	ALA	CA-C-O	5.19	126.77	120.81
10	3	12	VAL	CA-CB-CG1	5.19	119.22	110.40
24	Q	25	GLN	CB-CA-C	-5.19	102.03	110.85
2	b	64	VAL	N-CA-C	-5.18	100.18	107.75
14	n	155	ASN	CA-CB-CG	5.18	117.78	112.60
1	A	91	ARG	CG-CD-NE	-5.18	100.59	112.00
2	B	72	GLY	N-CA-C	-5.18	102.55	111.57
3	C	146	TYR	CA-CB-CG	-5.18	104.57	113.90
23	P	315	GLN	OE1-CD-NE2	-5.18	117.42	122.60
29	I	274	ASN	N-CA-C	-5.18	105.42	112.26
30	K	79	LEU	CA-C-N	5.18	127.18	120.44
30	K	79	LEU	C-N-CA	5.18	127.18	120.44
32	M	52	SER	CB-CA-C	-5.18	102.04	110.85
2	b	224	TYR	CA-C-O	5.18	126.78	121.23
4	d	174	PHE	O-C-N	5.18	127.61	122.12
10	3	183	TRP	CG-CD2-CE3	-5.18	128.72	133.90
14	7	105	THR	CA-CB-OG1	5.18	117.37	109.60
21	N	58	ARG	CA-C-N	5.18	127.49	120.44
21	N	58	ARG	C-N-CA	5.18	127.49	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	334	VAL	CA-CB-CG2	-5.18	101.59	110.40
21	N	539	MET	CA-C-N	5.18	128.19	120.31
21	N	539	MET	C-N-CA	5.18	128.19	120.31
21	N	776	TYR	CA-C-N	5.18	129.65	121.56
21	N	776	TYR	C-N-CA	5.18	129.65	121.56
5	e	173	GLY	CA-C-N	5.18	127.65	120.29
5	e	173	GLY	C-N-CA	5.18	127.65	120.29
8	h	67	ILE	CA-C-N	5.18	127.19	120.56
8	h	67	ILE	C-N-CA	5.18	127.19	120.56
7	G	63	LYS	N-CA-C	-5.18	105.96	113.21
7	G	194	LYS	N-CA-C	-5.18	106.91	113.18
8	1	133	TYR	CB-CG-CD2	5.18	128.57	120.80
21	N	819	LYS	CA-C-N	5.18	129.44	120.58
21	N	819	LYS	C-N-CA	5.18	129.44	120.58
11	4	21	VAL	N-CA-C	-5.18	100.66	108.12
22	S	167	LEU	O-C-N	5.18	128.06	122.15
23	P	113	ASN	N-CA-CB	5.18	117.83	110.16
26	U	30	ASN	N-CA-CB	5.18	119.25	110.49
27	O	294	MET	N-CA-CB	5.18	117.73	110.12
24	Q	140	LYS	CA-C-N	5.18	127.64	120.29
24	Q	140	LYS	C-N-CA	5.18	127.64	120.29
6	f	126	ARG	N-CA-CB	5.18	119.97	111.17
2	B	51	SER	N-CA-C	-5.18	101.25	108.96
14	7	216	VAL	CA-C-O	5.18	126.34	120.85
20	Z	364	ASN	O-C-N	-5.18	116.50	122.09
21	N	444	HIS	ND1-CE1-NE2	5.18	113.58	108.40
31	L	145	ARG	O-C-N	-5.18	116.56	122.93
6	F	72	LEU	CA-C-N	5.17	131.27	122.37
6	F	72	LEU	C-N-CA	5.17	131.27	122.37
20	Z	531	ALA	CA-C-N	5.17	127.21	120.28
20	Z	531	ALA	C-N-CA	5.17	127.21	120.28
23	P	79	LEU	N-CA-C	5.17	119.91	111.37
23	P	272	PRO	CA-C-O	-5.17	115.64	121.43
24	Q	219	ASP	CA-CB-CG	-5.17	107.43	112.60
27	O	60	ARG	O-C-N	5.17	127.47	122.09
27	O	117	ASN	OD1-CG-ND2	5.17	127.77	122.60
27	O	392	TRP	CA-C-O	-5.17	115.53	122.31
10	j	108	VAL	N-CA-C	-5.17	100.62	108.17
21	N	396	SER	CA-C-N	5.17	131.01	121.85
21	N	396	SER	C-N-CA	5.17	131.01	121.85
31	L	89	ASP	CA-C-N	5.17	128.17	120.31
31	L	89	ASP	C-N-CA	5.17	128.17	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	14	SER	N-CA-CB	5.17	119.29	110.50
14	n	241	PHE	CB-CA-C	5.17	120.11	111.22
12	5	219	TYR	CA-C-O	-5.17	114.79	120.69
17	T	53	ASN	O-C-N	-5.17	116.25	122.15
23	P	428	THR	N-CA-CB	5.17	118.30	110.28
24	Q	67	THR	O-C-N	-5.17	115.71	122.59
25	R	116	LYS	CA-C-N	5.17	127.55	120.46
25	R	116	LYS	C-N-CA	5.17	127.55	120.46
25	R	349	SER	O-C-N	-5.17	117.19	123.03
26	U	223	HIS	CA-C-N	5.17	127.63	120.29
26	U	223	HIS	C-N-CA	5.17	127.63	120.29
30	K	64	GLN	CA-C-N	5.17	127.16	120.44
30	K	64	GLN	C-N-CA	5.17	127.16	120.44
33	J	364	GLU	N-CA-C	5.17	117.00	111.36
2	B	90	ARG	CB-CA-C	-5.17	102.06	110.85
12	5	110	ILE	N-CA-C	-5.17	100.12	107.77
20	Z	610	GLY	N-CA-C	-5.17	107.67	115.32
32	M	353	SER	CA-C-N	5.17	127.16	120.44
32	M	353	SER	C-N-CA	5.17	127.16	120.44
4	d	250	LYS	N-CA-C	-5.17	105.65	111.28
15	W	177	GLY	CA-C-O	-5.17	117.45	122.46
21	N	597	ARG	CA-C-N	5.17	130.20	122.86
21	N	597	ARG	C-N-CA	5.17	130.20	122.86
27	O	250	TRP	CG-CD2-CE3	-5.17	128.73	133.90
28	H	57	LYS	CA-C-N	5.17	127.21	120.28
28	H	57	LYS	C-N-CA	5.17	127.21	120.28
32	M	27	THR	CB-CA-C	-5.17	99.80	109.72
33	J	106	ASP	N-CA-C	-5.17	106.56	112.92
8	h	41	ASP	N-CA-C	-5.17	99.87	108.34
9	i	92	ILE	CA-C-N	5.17	127.62	120.29
9	i	92	ILE	C-N-CA	5.17	127.62	120.29
1	A	96	ARG	O-C-N	5.17	127.60	122.12
3	C	48	ALA	CA-C-O	5.17	127.16	121.11
4	D	117	GLN	CG-CD-OE1	5.17	131.13	120.80
15	W	140	ASP	N-CA-C	-5.17	99.99	108.41
24	Q	154	SER	CA-C-O	-5.17	114.94	120.42
25	R	420	ALA	N-CA-C	5.17	116.91	111.28
26	U	215	ILE	CA-CB-CG1	5.17	119.18	110.40
29	I	65	ILE	CA-C-N	5.17	127.63	120.29
29	I	65	ILE	C-N-CA	5.17	127.63	120.29
30	K	360	MET	CA-C-N	5.17	128.81	121.42
30	K	360	MET	C-N-CA	5.17	128.81	121.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	105	LEU	CA-C-N	5.17	127.20	120.28
13	6	105	LEU	C-N-CA	5.17	127.20	120.28
26	U	8	VAL	N-CA-CB	5.17	118.41	111.90
2	b	32	VAL	O-C-N	-5.16	116.12	122.57
9	i	122	HIS	N-CA-C	-5.16	106.98	113.28
5	E	120	ALA	O-C-N	5.16	127.59	122.12
9	2	107	SER	N-CA-CB	5.16	117.80	110.16
16	V	169	GLU	CB-CG-CD	-5.16	103.82	112.60
21	N	251	GLU	N-CA-C	5.16	116.99	111.36
22	S	278	LYS	N-CA-CB	5.16	117.56	110.07
23	P	34	SER	CA-C-O	5.16	125.89	120.42
26	U	247	ILE	N-CA-CB	5.16	116.59	110.55
32	M	263	VAL	CB-CA-C	-5.16	105.36	111.97
10	3	147	PHE	CB-CA-C	-5.16	101.90	110.68
17	T	171	ILE	CA-C-N	5.16	131.40	121.54
17	T	171	ILE	C-N-CA	5.16	131.40	121.54
21	N	665	ILE	N-CA-C	5.16	115.90	108.93
32	M	249	PRO	CA-C-N	5.16	128.16	120.31
32	M	249	PRO	C-N-CA	5.16	128.16	120.31
14	7	78	VAL	N-CA-C	-5.16	100.13	107.77
20	Z	731	GLY	CA-C-N	5.16	127.81	120.53
20	Z	731	GLY	C-N-CA	5.16	127.81	120.53
21	N	506	GLN	CG-CD-OE1	5.16	131.12	120.80
30	K	101	GLU	O-C-N	5.16	126.41	121.71
30	K	108	GLY	N-CA-C	-5.16	103.43	111.12
3	c	141	ASP	N-CA-C	-5.16	101.45	109.24
9	i	219	TYR	O-C-N	5.16	127.38	122.07
2	B	77	GLY	N-CA-C	-5.16	100.95	113.18
2	B	99	ARG	N-CA-C	-5.16	108.01	114.56
5	E	13	SER	N-CA-CB	5.16	118.80	110.86
16	V	299	GLY	CA-C-O	5.16	125.61	120.09
23	P	258	LYS	CA-C-N	5.16	124.47	118.85
23	P	258	LYS	C-N-CA	5.16	124.47	118.85
24	Q	418	GLN	CA-C-N	5.16	127.61	120.29
24	Q	418	GLN	C-N-CA	5.16	127.61	120.29
33	J	340	GLY	O-C-N	-5.16	116.42	122.45
16	V	278	LYS	CA-C-N	-5.16	112.97	120.29
16	V	278	LYS	C-N-CA	-5.16	112.97	120.29
25	R	130	GLN	OE1-CD-NE2	-5.16	117.44	122.60
29	I	57	LEU	N-CA-C	5.16	116.90	111.28
5	e	237	ALA	O-C-N	5.16	127.58	122.12
4	D	154	GLY	CA-C-N	5.16	129.75	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	154	GLY	C-N-CA	5.16	129.75	123.10
31	L	212	ILE	CB-CA-C	-5.16	105.92	111.59
9	2	228	LYS	O-C-N	-5.15	117.14	122.96
21	N	873	ARG	N-CA-C	-5.15	100.68	108.67
23	P	306	ASN	CA-CB-CG	-5.15	107.45	112.60
24	Q	410	ASP	CA-CB-CG	-5.15	107.45	112.60
27	O	123	GLY	N-CA-C	-5.15	108.57	115.32
31	L	192	GLU	CB-CG-CD	-5.15	103.84	112.60
3	c	91	ALA	N-CA-C	5.15	116.90	111.28
11	k	166	GLN	CA-C-N	5.15	127.14	120.44
11	k	166	GLN	C-N-CA	5.15	127.14	120.44
7	G	240	ILE	O-C-N	5.15	127.09	121.94
16	V	262	THR	CA-C-N	5.15	127.14	120.44
16	V	262	THR	C-N-CA	5.15	127.14	120.44
25	R	263	ARG	CA-C-N	5.15	129.38	121.19
25	R	263	ARG	C-N-CA	5.15	129.38	121.19
29	I	97	GLU	CA-C-N	5.15	127.70	120.28
29	I	97	GLU	C-N-CA	5.15	127.70	120.28
31	L	158	ILE	O-C-N	5.15	128.80	122.72
31	L	403	ILE	CA-C-N	5.15	127.14	120.44
31	L	403	ILE	C-N-CA	5.15	127.14	120.44
4	d	83	ARG	O-C-N	-5.15	116.19	122.22
2	B	118	MET	CA-C-N	5.15	127.44	120.38
2	B	118	MET	C-N-CA	5.15	127.44	120.38
2	B	245	ASP	CA-C-N	5.15	130.15	121.14
2	B	245	ASP	C-N-CA	5.15	130.15	121.14
14	7	152	VAL	N-CA-CB	5.15	119.90	111.45
21	N	152	LEU	CA-C-N	5.15	127.18	120.28
21	N	152	LEU	C-N-CA	5.15	127.18	120.28
28	H	152	ILE	CA-C-N	5.15	130.00	121.86
28	H	152	ILE	C-N-CA	5.15	130.00	121.86
28	H	333	MET	O-C-N	5.15	127.38	122.07
30	K	113	THR	CA-CB-OG1	5.15	117.33	109.60
10	j	118	LYS	CA-C-O	-5.15	114.92	119.86
12	l	266	HIS	CG-CD2-NE2	5.15	112.35	107.20
13	m	198	SER	N-CA-C	5.15	116.58	110.97
5	E	44	GLU	CB-CA-C	-5.15	101.78	110.64
27	O	215	TYR	N-CA-C	5.15	116.58	111.07
33	J	186	ILE	N-CA-CB	5.15	116.87	111.00
3	c	7	ASP	CA-C-N	5.15	129.38	120.58
3	c	7	ASP	C-N-CA	5.15	129.38	120.58
1	A	87	ILE	CA-C-N	5.15	124.76	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ILE	C-N-CA	5.15	124.76	119.05
1	A	165	GLY	CA-C-O	-5.15	115.25	122.51
7	G	73	HIS	CE1-NE2-CD2	-5.15	103.85	109.00
24	Q	138	SER	N-CA-C	5.15	117.79	111.82
26	U	24	ARG	N-CA-C	-5.15	106.68	113.17
28	H	133	SER	CA-C-O	5.15	125.25	119.18
31	L	118	ILE	N-CA-C	-5.15	100.35	108.23
32	M	278	ILE	CA-CB-CG2	-5.15	101.75	110.50
32	M	409	SER	N-CA-C	-5.15	100.91	108.99
1	A	190	LYS	N-CA-CB	5.15	120.54	112.46
8	1	122	ILE	N-CA-CB	5.15	118.41	111.21
4	d	95	SER	CA-C-N	5.14	127.17	120.28
4	d	95	SER	C-N-CA	5.14	127.17	120.28
9	i	208	GLU	CB-CG-CD	-5.14	103.86	112.60
14	n	65	SER	CA-C-O	-5.14	115.10	120.55
17	T	245	TYR	N-CA-C	5.14	117.56	111.33
21	N	823	PRO	CB-CA-C	5.14	119.16	111.85
27	O	286	PHE	CA-CB-CG	-5.14	108.66	113.80
28	H	177	ASP	CA-CB-CG	5.14	117.74	112.60
32	M	110	ASN	CA-CB-CG	-5.14	107.45	112.60
33	J	144	ASP	CA-CB-CG	5.14	117.75	112.60
4	d	187	THR	CA-CB-OG1	5.14	117.31	109.60
6	f	72	LEU	CA-C-O	5.14	127.03	121.06
6	f	114	ASP	O-C-N	-5.14	115.36	122.46
11	4	162	LYS	CB-CA-C	-5.14	101.12	110.63
26	U	62	ASN	CA-C-N	5.14	130.44	122.26
26	U	62	ASN	C-N-CA	5.14	130.44	122.26
30	K	244	HIS	CA-C-O	-5.14	115.53	121.19
31	L	55	LYS	CA-C-O	5.14	125.88	119.97
32	M	216	LYS	CA-C-O	-5.14	114.97	120.42
33	J	337	LEU	N-CA-CB	5.14	117.34	109.94
1	a	202	VAL	CA-C-N	5.14	127.72	120.42
1	a	202	VAL	C-N-CA	5.14	127.72	120.42
14	n	177	THR	CA-C-O	-5.14	115.59	121.40
10	3	153	LEU	N-CA-C	5.14	116.74	111.03
19	Y	34	GLU	CB-CA-C	5.14	118.62	111.63
28	H	267	THR	CA-C-N	5.14	129.66	122.36
28	H	267	THR	C-N-CA	5.14	129.66	122.36
13	m	26	GLU	N-CA-C	-5.14	105.69	112.94
7	G	20	ARG	NE-CZ-NH1	5.14	126.64	121.50
11	4	125	LYS	N-CA-C	-5.14	102.87	110.48
16	V	221	TRP	N-CA-C	-5.14	106.60	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	152	ASP	CA-C-O	-5.14	115.42	120.82
29	I	306	MET	N-CA-CB	5.14	117.60	109.94
30	K	204	ASP	N-CA-C	-5.14	103.59	110.07
33	J	13	GLU	CA-C-N	5.14	129.61	121.44
33	J	13	GLU	C-N-CA	5.14	129.61	121.44
4	d	64	VAL	N-CA-C	-5.14	100.17	107.77
12	5	218	ASN	OD1-CG-ND2	5.14	127.74	122.60
17	T	79	GLU	CA-C-O	-5.14	115.40	120.90
24	Q	318	LEU	N-CA-CB	5.14	119.04	110.41
13	m	73	VAL	CA-C-N	5.14	127.58	120.29
13	m	73	VAL	C-N-CA	5.14	127.58	120.29
20	Z	611	THR	CA-CB-CG2	5.14	119.23	110.50
21	N	135	SER	N-CA-C	5.14	116.88	111.28
23	P	48	GLN	CB-CA-C	-5.14	102.82	110.88
30	K	287	GLY	CA-C-O	-5.14	114.85	120.40
4	D	237	GLU	O-C-N	5.13	127.36	122.07
5	E	187	TRP	N-CA-C	-5.13	102.16	110.32
21	N	801	THR	CA-C-N	5.13	127.42	120.44
21	N	801	THR	C-N-CA	5.13	127.42	120.44
23	P	136	ARG	CA-C-N	5.13	127.16	120.28
23	P	136	ARG	C-N-CA	5.13	127.16	120.28
27	O	166	ARG	N-CA-CB	5.13	117.46	110.01
28	H	335	GLU	CB-CG-CD	-5.13	103.87	112.60
13	m	171	GLY	O-C-N	-5.13	115.87	122.39
21	N	202	PHE	CA-CB-CG	-5.13	108.67	113.80
24	Q	273	ASN	N-CA-CB	5.13	119.16	110.49
9	2	104	ARG	CA-C-N	5.13	127.13	120.56
9	2	104	ARG	C-N-CA	5.13	127.13	120.56
10	3	199	TYR	CB-CA-C	-5.13	101.38	109.80
12	5	260	TRP	CG-CD2-CE3	-5.13	128.77	133.90
13	6	17	GLY	CA-C-N	5.13	128.21	121.85
13	6	17	GLY	C-N-CA	5.13	128.21	121.85
14	7	70	ASN	CA-C-O	-5.13	115.31	121.11
17	T	88	TYR	CA-CB-CG	-5.13	104.66	113.90
18	X	116	ALA	N-CA-C	-5.13	99.87	110.80
21	N	61	ALA	CA-C-O	-5.13	114.98	120.42
21	N	521	LEU	N-CA-C	-5.13	105.77	111.36
23	P	362	LEU	CA-C-N	5.13	127.16	120.28
23	P	362	LEU	C-N-CA	5.13	127.16	120.28
25	R	262	GLU	N-CA-C	-5.13	101.74	109.85
26	U	46	ILE	N-CA-C	-5.13	101.02	108.36
28	H	254	THR	N-CA-C	-5.13	106.61	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	78	GLN	CA-C-N	5.13	129.93	122.08
8	h	78	GLN	C-N-CA	5.13	129.93	122.08
18	X	45	PHE	CA-CB-CG	-5.13	108.67	113.80
23	P	314	VAL	CA-C-N	5.13	127.92	120.79
23	P	314	VAL	C-N-CA	5.13	127.92	120.79
30	K	107	THR	N-CA-CB	5.13	120.31	111.13
3	c	176	LEU	CA-C-N	5.13	127.66	120.28
3	c	176	LEU	C-N-CA	5.13	127.66	120.28
6	f	196	ALA	CA-C-O	5.13	125.86	120.42
8	h	53	CYS	CA-CB-SG	5.13	126.20	114.40
12	l	162	VAL	CA-C-N	5.13	127.15	120.28
12	l	162	VAL	C-N-CA	5.13	127.15	120.28
6	F	98	VAL	N-CA-CB	5.13	118.52	110.31
21	N	430	ASN	CA-CB-CG	-5.13	107.47	112.60
22	S	376	THR	N-CA-C	-5.13	107.02	113.28
22	S	438	HIS	CE1-NE2-CD2	-5.13	103.87	109.00
24	Q	37	GLN	N-CA-CB	5.13	117.66	110.12
25	R	118	GLN	CA-C-N	5.13	127.57	120.29
25	R	118	GLN	C-N-CA	5.13	127.57	120.29
28	H	101	ARG	CA-C-N	5.13	128.13	120.95
28	H	101	ARG	C-N-CA	5.13	128.13	120.95
32	M	233	ARG	N-CA-CB	5.13	117.66	110.12
3	c	115	LEU	O-C-N	5.13	127.55	122.12
4	d	88	LYS	N-CA-CB	5.13	117.66	110.12
5	e	38	ILE	CB-CA-C	5.13	118.71	110.82
5	e	172	ILE	CA-CB-CG2	-5.13	101.78	110.50
2	B	87	ASP	N-CA-CB	5.13	117.75	110.16
6	F	6	TYR	N-CA-C	-5.13	106.03	113.21
9	2	143	HIS	CA-CB-CG	-5.13	108.67	113.80
10	3	194	GLU	N-CA-C	5.13	116.31	108.52
11	4	83	PHE	CA-C-N	5.13	127.70	120.42
11	4	83	PHE	C-N-CA	5.13	127.70	120.42
25	R	113	LEU	N-CA-C	5.13	116.87	111.28
28	H	448	ASP	CA-C-N	5.13	127.10	120.44
28	H	448	ASP	C-N-CA	5.13	127.10	120.44
14	7	59	ASN	CB-CA-C	-5.12	102.49	110.74
15	W	123	ASP	CA-C-O	-5.12	115.09	120.63
16	V	268	THR	CA-CB-CG2	-5.12	101.79	110.50
28	H	175	GLY	CA-C-O	5.12	124.91	120.76
28	H	439	THR	CA-C-N	5.12	127.57	120.29
28	H	439	THR	C-N-CA	5.12	127.57	120.29
31	L	389	ALA	CA-C-O	5.12	125.66	119.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	M	42	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	A	175	GLN	N-CA-CB	5.12	118.90	110.39
2	B	209	ILE	N-CA-C	-5.12	100.37	107.80
11	4	193	ASP	O-C-N	5.12	128.44	122.24
23	P	8	LYS	N-CA-CB	5.12	117.75	110.06
25	R	189	GLU	N-CA-C	5.12	116.94	111.36
26	U	100	ARG	CA-C-O	5.12	127.25	121.51
27	O	256	ASN	CB-CA-C	-5.12	100.83	110.67
31	L	251	ILE	CA-CB-CG2	-5.12	101.79	110.50
1	a	27	GLN	CA-C-O	5.12	125.98	120.55
15	W	58	ASN	CA-CB-CG	5.12	117.72	112.60
22	S	22	GLU	O-C-N	-5.12	116.31	122.15
29	I	214	LYS	CA-C-O	-5.12	115.36	120.64
31	L	257	GLY	N-CA-C	-5.12	108.18	115.30
6	F	105	VAL	CA-C-O	-5.12	115.42	120.85
21	N	427	ILE	O-C-N	5.12	127.22	121.90
21	N	753	PHE	N-CA-C	-5.12	102.28	109.96
25	R	88	LEU	N-CA-C	-5.12	106.72	113.17
2	b	177	LYS	CB-CG-CD	5.12	123.07	111.30
3	c	82	ALA	N-CA-C	-5.12	105.61	111.14
9	i	170	HIS	CB-CG-ND1	5.12	130.38	122.70
10	j	152	SER	O-C-N	5.12	127.62	122.09
1	A	32	PHE	N-CA-CB	5.12	119.35	110.39
2	B	53	SER	CA-C-O	-5.12	115.57	120.64
6	F	198	SER	N-CA-CB	5.12	118.18	110.30
6	F	199	GLN	O-C-N	5.12	129.52	122.46
23	P	191	GLY	N-CA-C	-5.12	107.99	115.72
24	Q	308	ASN	N-CA-C	-5.12	105.70	111.28
31	L	131	VAL	O-C-N	-5.12	117.62	123.10
27	O	139	LEU	CB-CA-C	-5.12	99.61	110.31
28	H	59	ILE	CA-C-O	-5.12	115.37	121.05
31	L	165	PRO	CA-C-O	-5.12	111.77	119.55
2	b	244	ASN	N-CA-C	-5.12	105.89	111.82
7	g	173	LYS	CB-CA-C	-5.12	102.16	110.85
11	k	72	ASP	CA-C-O	5.12	127.47	121.54
21	N	182	ASN	O-C-N	-5.12	116.70	122.12
22	S	229	THR	CA-CB-OG1	-5.12	101.93	109.60
23	P	269	VAL	CA-CB-CG1	5.12	119.10	110.40
30	K	330	ARG	NE-CZ-NH1	5.12	126.61	121.50
31	L	299	ARG	N-CA-C	-5.12	107.09	113.38
33	J	66	GLN	OE1-CD-NE2	-5.12	117.48	122.60
8	h	98	ASN	CB-CG-OD1	-5.11	110.57	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	123	GLY	CA-C-N	5.11	127.44	120.54
12	l	123	GLY	C-N-CA	5.11	127.44	120.54
5	E	20	ARG	CA-C-N	5.11	128.47	120.75
5	E	20	ARG	C-N-CA	5.11	128.47	120.75
5	E	188	HIS	CG-CD2-NE2	5.11	112.31	107.20
8	1	150	ASN	CA-C-N	-5.11	115.52	122.93
8	1	150	ASN	C-N-CA	-5.11	115.52	122.93
9	2	122	HIS	ND1-CE1-NE2	5.11	113.51	108.40
11	4	124	THR	CA-C-N	5.11	129.88	121.39
11	4	124	THR	C-N-CA	5.11	129.88	121.39
16	V	279	HIS	CG-CD2-NE2	5.11	112.31	107.20
17	T	232	LYS	N-CA-C	-5.11	100.01	108.75
26	U	252	HIS	O-C-N	-5.11	116.32	122.15
28	H	292	ARG	NE-CZ-NH2	-5.11	114.60	119.20
33	J	220	GLN	O-C-N	-5.11	117.18	122.96
25	R	163	SER	CA-C-N	5.11	127.13	120.28
25	R	163	SER	C-N-CA	5.11	127.13	120.28
29	I	221	LEU	CA-C-O	5.11	126.00	120.43
29	I	374	ASP	CB-CA-C	-5.11	102.85	110.88
3	c	218	LYS	N-CA-C	-5.11	104.45	111.81
13	m	116	HIS	CG-CD2-NE2	5.11	112.31	107.20
2	B	194	LEU	CD1-CG-CD2	5.11	122.04	110.80
5	E	222	ILE	CA-C-N	5.11	130.83	122.81
5	E	222	ILE	C-N-CA	5.11	130.83	122.81
24	Q	117	VAL	CB-CA-C	-5.11	105.33	112.02
3	c	84	ALA	O-C-N	-5.11	116.24	122.22
1	A	79	ILE	N-CA-C	-5.11	100.29	107.75
4	D	213	THR	CA-C-O	-5.11	114.81	120.38
19	Y	66	ASP	N-CA-C	-5.11	106.17	114.09
9	i	254	GLU	CA-C-O	-5.11	115.53	121.15
7	G	151	LEU	CA-C-N	5.11	128.44	120.68
7	G	151	LEU	C-N-CA	5.11	128.44	120.68
17	T	72	THR	N-CA-C	-5.11	106.64	112.92
21	N	236	GLY	CA-C-N	5.11	127.54	120.29
21	N	236	GLY	C-N-CA	5.11	127.54	120.29
21	N	237	LEU	O-C-N	5.11	127.97	122.15
21	N	268	GLN	N-CA-C	5.11	116.93	111.36
27	O	25	LEU	N-CA-CB	5.11	117.63	110.12
30	K	407	LEU	O-C-N	-5.11	115.99	122.27
32	M	126	THR	N-CA-CB	5.11	121.03	111.53
3	c	34	THR	N-CA-CB	-5.11	102.35	110.06
4	d	217	PRO	N-CA-C	5.11	119.23	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	252	SER	N-CA-CB	5.11	117.58	109.82
7	g	144	ASN	CB-CG-ND2	-5.11	108.74	116.40
1	A	13	ASP	CA-CB-CG	5.11	117.70	112.60
9	2	202	VAL	N-CA-C	-5.11	100.54	107.99
11	4	141	PHE	N-CA-CB	5.11	117.72	110.06
26	U	116	ASN	CB-CG-ND2	-5.11	108.74	116.40
27	O	47	LYS	O-C-N	5.11	127.33	122.07
33	J	186	ILE	CB-CA-C	-5.11	104.78	110.96
6	F	226	ASP	CA-C-O	-5.10	115.77	121.23
21	N	910	PRO	CB-CA-C	5.10	118.50	110.49
2	b	129	PRO	N-CA-CB	5.10	107.79	103.35
7	g	48	PHE	O-C-N	-5.10	117.35	123.06
1	A	150	LEU	O-C-N	5.10	127.45	122.19
1	A	167	LYS	O-C-N	5.10	129.60	122.36
3	C	95	ALA	CA-C-N	5.10	127.54	120.29
3	C	95	ALA	C-N-CA	5.10	127.54	120.29
9	2	81	THR	N-CA-C	-5.10	105.36	111.03
25	R	208	ASN	N-CA-CB	5.10	117.62	110.12
26	U	167	GLU	CA-C-O	-5.10	115.14	120.55
2	b	55	LEU	CA-C-N	5.10	127.95	120.71
2	b	55	LEU	C-N-CA	5.10	127.95	120.71
6	f	43	HIS	CE1-NE2-CD2	-5.10	103.90	109.00
12	5	218	ASN	CA-C-O	5.10	125.53	119.56
29	I	326	MET	O-C-N	-5.10	117.23	123.30
32	M	160	PRO	CA-C-O	-5.10	115.79	122.12
8	h	21	VAL	N-CA-CB	5.10	118.07	111.19
8	h	158	GLU	N-CA-C	-5.10	105.80	111.36
10	j	131	ASP	CA-C-N	5.10	128.11	120.87
10	j	131	ASP	C-N-CA	5.10	128.11	120.87
7	G	89	VAL	N-CA-C	5.10	115.87	110.72
11	4	145	ASP	CA-C-N	5.10	127.56	120.63
11	4	145	ASP	C-N-CA	5.10	127.56	120.63
12	5	119	THR	N-CA-CB	5.10	118.62	110.46
14	7	126	PHE	CB-CA-C	-5.10	103.11	110.96
17	T	217	THR	CA-C-N	5.10	129.30	120.58
17	T	217	THR	C-N-CA	5.10	129.30	120.58
19	Y	40	ILE	N-CA-C	5.10	115.32	110.53
20	Z	433	LEU	CA-C-N	5.10	127.53	120.29
20	Z	433	LEU	C-N-CA	5.10	127.53	120.29
22	S	327	ILE	CA-C-N	5.10	125.50	119.99
22	S	327	ILE	C-N-CA	5.10	125.50	119.99
24	Q	129	LYS	N-CA-C	-5.10	102.01	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	317	THR	N-CA-C	-5.10	107.11	113.38
14	7	97	GLU	CA-C-N	5.10	129.30	120.58
14	7	97	GLU	C-N-CA	5.10	129.30	120.58
25	R	255	VAL	CA-C-N	5.10	127.53	120.29
25	R	255	VAL	C-N-CA	5.10	127.53	120.29
28	H	132	GLN	N-CA-CB	5.10	117.46	109.97
9	i	52	GLY	CA-C-N	5.10	124.81	119.82
9	i	52	GLY	C-N-CA	5.10	124.81	119.82
2	B	5	TYR	CA-C-O	-5.10	116.24	122.41
8	1	177	SER	N-CA-CB	5.10	118.15	110.30
9	2	184	ALA	O-C-N	-5.10	116.82	122.07
18	X	47	ASP	N-CA-CB	5.10	118.57	110.57
31	L	324	ILE	N-CA-CB	5.10	118.27	111.64
5	E	187	TRP	CE2-CD2-CE3	5.09	123.89	118.80
11	4	149	ARG	CA-C-O	-5.09	115.81	120.50
21	N	438	ASP	CA-C-N	5.09	127.44	120.46
21	N	438	ASP	C-N-CA	5.09	127.44	120.46
28	H	246	ILE	CA-C-N	-5.09	115.54	122.93
28	H	246	ILE	C-N-CA	-5.09	115.54	122.93
33	J	40	ASN	CA-CB-CG	-5.09	107.50	112.60
11	k	49	GLU	CB-CG-CD	-5.09	103.94	112.60
9	2	164	MET	N-CA-C	5.09	116.83	111.28
13	m	179	PRO	N-CA-CB	5.09	108.07	103.34
3	C	100	LYS	O-C-N	-5.09	116.34	122.15
3	C	118	ILE	N-CA-CB	5.09	117.46	110.54
3	C	210	ARG	N-CA-C	-5.09	106.48	113.30
4	D	83	ARG	O-C-N	-5.09	115.77	122.39
5	E	171	ALA	N-CA-C	-5.09	101.58	109.72
5	E	215	ASN	N-CA-C	-5.09	106.38	112.59
6	F	175	THR	N-CA-C	-5.09	106.91	113.02
9	2	189	GLN	O-C-N	-5.09	116.72	122.12
21	N	622	ALA	N-CA-C	5.09	117.22	111.11
21	N	870	ASN	O-C-N	5.09	128.99	123.13
22	S	398	THR	N-CA-C	5.09	116.91	111.36
23	P	230	HIS	ND1-CE1-NE2	5.09	113.49	108.40
26	U	273	LEU	O-C-N	5.09	127.31	122.07
29	I	70	LEU	CA-C-N	5.09	127.06	120.44
29	I	70	LEU	C-N-CA	5.09	127.06	120.44
2	b	164	ILE	CA-C-O	-5.09	116.36	121.45
4	d	142	ASP	CA-CB-CG	-5.09	107.51	112.60
4	d	142	ASP	N-CA-CB	5.09	119.26	111.22
2	B	149	GLN	CB-CG-CD	-5.09	103.95	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	196	THR	O-C-N	5.09	127.59	122.09
11	4	57	ALA	N-CA-CB	5.09	117.45	110.07
14	7	246	GLN	N-CA-C	-5.09	102.02	109.81
16	V	230	TYR	N-CA-C	-5.09	107.12	113.38
17	T	111	LEU	N-CA-CB	5.09	117.60	110.12
4	d	42	VAL	N-CA-C	-5.09	101.01	108.85
5	e	217	ALA	O-C-N	5.09	129.49	123.33
7	g	94	GLU	CB-CA-C	-5.09	102.86	110.90
9	i	83	ALA	N-CA-CB	5.09	117.78	110.20
11	k	141	PHE	O-C-N	5.09	128.17	122.22
8	l	166	HIS	CE1-NE2-CD2	-5.09	103.91	109.00
20	Z	311	ALA	N-CA-C	5.09	116.83	111.28
1	A	206	ALA	CA-C-O	5.09	126.16	120.82
6	F	60	GLN	N-CA-C	-5.09	100.23	108.52
21	N	196	THR	N-CA-CB	5.09	119.37	110.27
22	S	450	ASN	N-CA-CB	5.09	119.69	111.65
23	P	57	GLU	CA-C-O	5.09	125.81	120.42
23	P	425	HIS	CE1-NE2-CD2	-5.09	103.91	109.00
24	Q	119	GLU	CB-CG-CD	5.09	121.25	112.60
26	U	134	THR	O-C-N	-5.09	117.36	123.31
27	O	134	ALA	CB-CA-C	-5.09	102.35	110.79
9	2	112	LEU	CA-C-N	5.08	127.05	120.44
9	2	112	LEU	C-N-CA	5.08	127.05	120.44
14	7	134	TYR	CA-C-O	-5.08	115.46	120.90
21	N	611	LYS	CA-C-N	5.08	128.43	120.75
21	N	611	LYS	C-N-CA	5.08	128.43	120.75
21	N	719	ASN	CA-CB-CG	-5.08	107.52	112.60
1	a	15	HIS	CB-CG-CD2	-5.08	124.59	131.20
6	f	26	LEU	CB-CA-C	5.08	120.07	109.95
9	i	80	ASP	N-CA-CB	5.08	118.69	110.40
12	l	104	GLN	N-CA-C	-5.08	104.26	110.61
7	G	70	VAL	O-C-N	-5.08	117.71	123.20
16	V	212	MET	CA-C-O	-5.08	115.16	120.55
16	V	300	VAL	CB-CA-C	-5.08	105.36	112.02
20	Z	24	THR	CA-C-N	5.08	126.19	119.84
20	Z	24	THR	C-N-CA	5.08	126.19	119.84
31	L	317	ASN	CA-CB-CG	-5.08	107.52	112.60
31	L	386	PHE	CA-C-O	5.08	126.10	120.71
4	d	77	GLY	CA-C-N	5.08	127.98	120.82
4	d	77	GLY	C-N-CA	5.08	127.98	120.82
12	l	141	HIS	CG-CD2-NE2	5.08	112.28	107.20
7	G	42	CYS	CA-C-N	5.08	127.80	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	42	CYS	C-N-CA	5.08	127.80	120.38
13	6	150	ALA	CA-C-O	5.08	125.95	119.95
18	X	63	PRO	CA-C-O	-5.08	115.79	121.23
27	O	172	TYR	CA-C-N	5.08	127.51	120.29
27	O	172	TYR	C-N-CA	5.08	127.51	120.29
28	H	137	ASP	CA-CB-CG	5.08	117.68	112.60
29	I	159	VAL	N-CA-C	-5.08	100.25	107.77
7	g	152	GLU	CA-C-N	5.08	125.53	120.04
7	g	152	GLU	C-N-CA	5.08	125.53	120.04
8	h	42	LYS	O-C-N	-5.08	115.80	122.20
3	C	236	LYS	O-C-N	5.08	127.50	122.12
13	6	131	TYR	N-CA-C	-5.08	101.59	109.72
5	e	181	ALA	CA-C-N	5.08	129.31	120.68
5	e	181	ALA	C-N-CA	5.08	129.31	120.68
14	n	45	ILE	N-CA-C	-5.08	101.39	108.80
8	1	129	HIS	CB-CG-ND1	5.08	130.32	122.70
20	Z	625	THR	CA-C-N	5.08	126.19	119.84
20	Z	625	THR	C-N-CA	5.08	126.19	119.84
21	N	106	ILE	CA-C-N	5.08	127.59	120.28
21	N	106	ILE	C-N-CA	5.08	127.59	120.28
21	N	504	TYR	CA-CB-CG	-5.08	104.76	113.90
21	N	786	ARG	NE-CZ-NH2	-5.08	114.63	119.20
23	P	46	THR	O-C-N	5.08	128.38	122.24
23	P	399	ILE	CA-CB-CG1	5.08	119.03	110.40
24	Q	35	SER	N-CA-C	5.08	116.82	111.28
25	R	243	LEU	CA-C-O	5.08	126.69	120.60
4	D	154	GLY	O-C-N	5.08	128.27	122.33
31	L	208	GLN	OE1-CD-NE2	-5.08	117.52	122.60
3	C	244	ILE	CA-CB-CG1	5.08	119.03	110.40
13	6	139	TYR	CB-CG-CD2	5.08	128.41	120.80
13	6	184	SER	CA-C-N	5.08	127.63	120.42
13	6	184	SER	C-N-CA	5.08	127.63	120.42
22	S	53	ILE	N-CA-CB	5.08	117.44	110.54
23	P	158	ASP	N-CA-CB	5.08	117.67	110.16
23	P	323	ASN	OD1-CG-ND2	5.08	127.68	122.60
32	M	178	GLU	CA-C-N	5.08	131.23	121.54
32	M	178	GLU	C-N-CA	5.08	131.23	121.54
32	M	231	LEU	N-CA-CB	5.08	117.37	110.01
3	C	58	GLU	O-C-N	-5.07	117.44	123.22
5	E	166	ARG	CA-C-O	-5.07	114.60	120.49
7	G	93	ARG	CD-NE-CZ	5.07	131.50	124.40
13	6	161	GLN	OE1-CD-NE2	5.07	127.67	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	617	ILE	CA-C-N	5.07	127.08	120.28
20	Z	617	ILE	C-N-CA	5.07	127.08	120.28
21	N	383	LYS	CA-C-N	5.07	127.08	120.28
21	N	383	LYS	C-N-CA	5.07	127.08	120.28
27	O	279	ILE	CA-CB-CG1	-5.07	101.77	110.40
6	f	170	THR	N-CA-C	-5.07	105.83	111.36
27	O	286	PHE	N-CA-CB	5.07	117.36	110.01
28	H	242	PRO	CA-C-N	5.07	124.83	119.76
28	H	242	PRO	C-N-CA	5.07	124.83	119.76
5	e	110	GLU	CB-CA-C	-5.07	102.23	110.85
5	e	241	LYS	N-CA-CB	5.07	118.14	110.28
6	f	224	ILE	N-CA-C	-5.07	101.01	108.11
7	g	214	LEU	CA-C-O	5.07	125.96	120.43
9	i	212	ASP	CA-C-N	5.07	129.15	122.30
9	i	212	ASP	C-N-CA	5.07	129.15	122.30
21	N	324	LYS	CG-CD-CE	5.07	122.96	111.30
29	I	89	GLN	N-CA-CB	5.07	119.06	110.49
6	f	100	ASN	O-C-N	-5.07	116.26	122.55
6	f	124	GLY	CA-C-O	5.07	124.43	118.96
9	i	41	VAL	N-CA-C	-5.07	101.17	108.42
14	7	215	ARG	CA-C-N	5.07	127.62	120.42
14	7	215	ARG	C-N-CA	5.07	127.62	120.42
5	e	14	THR	CA-CB-CG2	5.07	119.12	110.50
5	e	53	ARG	NE-CZ-NH1	5.07	126.57	121.50
8	1	160	THR	CA-C-N	5.07	127.40	120.46
8	1	160	THR	C-N-CA	5.07	127.40	120.46
12	5	236	ILE	CB-CA-C	-5.07	105.23	112.22
13	6	225	TYR	CA-CB-CG	-5.07	104.78	113.90
16	V	71	MET	CA-CB-CG	-5.07	103.96	114.10
17	T	47	GLN	CA-C-N	5.07	130.69	122.53
17	T	47	GLN	C-N-CA	5.07	130.69	122.53
20	Z	268	ALA	CB-CA-C	-5.07	102.38	110.79
22	S	370	LEU	N-CA-CB	5.07	117.66	110.16
25	R	139	GLU	N-CA-C	5.07	116.80	111.28
28	H	388	ILE	CA-C-N	5.07	129.18	120.72
28	H	388	ILE	C-N-CA	5.07	129.18	120.72
4	d	119	ARG	NE-CZ-NH1	5.07	126.56	121.50
1	A	244	ARG	CB-CA-C	-5.07	102.24	110.85
8	1	47	HIS	CE1-NE2-CD2	-5.07	103.93	109.00
11	4	189	ILE	O-C-N	-5.07	118.12	123.03
12	5	152	ALA	CA-C-O	-5.07	114.38	120.10
20	Z	727	GLU	CB-CG-CD	5.07	121.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	36	TRP	CB-CA-C	-5.07	102.38	110.79
21	N	266	SER	CA-C-N	5.07	127.58	120.28
21	N	266	SER	C-N-CA	5.07	127.58	120.28
24	Q	414	GLU	CA-C-N	5.07	127.03	120.44
24	Q	414	GLU	C-N-CA	5.07	127.03	120.44
25	R	264	THR	CB-CA-C	-5.07	102.43	110.84
7	g	177	GLU	CA-C-N	5.06	127.06	120.28
7	g	177	GLU	C-N-CA	5.06	127.06	120.28
12	5	253	TYR	N-CA-C	-5.06	101.38	109.23
33	J	379	GLN	CA-C-O	5.06	125.59	119.31
9	i	136	GLY	CA-C-N	5.06	128.66	121.42
9	i	136	GLY	C-N-CA	5.06	128.66	121.42
8	1	119	VAL	N-CA-C	-5.06	100.83	108.12
11	4	10	GLN	CG-CD-NE2	-5.06	108.81	116.40
21	N	46	ILE	CB-CA-C	-5.06	105.23	112.22
21	N	881	TYR	CA-C-N	5.06	127.28	120.50
21	N	881	TYR	C-N-CA	5.06	127.28	120.50
22	S	71	ALA	CA-C-N	5.06	128.01	120.31
22	S	71	ALA	C-N-CA	5.06	128.01	120.31
27	O	249	ASP	CA-C-N	5.06	131.21	121.54
27	O	249	ASP	C-N-CA	5.06	131.21	121.54
30	K	42	ASN	CA-CB-CG	-5.06	107.54	112.60
30	K	73	ARG	CA-C-N	5.06	127.48	120.29
30	K	73	ARG	C-N-CA	5.06	127.48	120.29
30	K	267	SER	N-CA-CB	5.06	119.41	111.56
12	5	283	ASN	O-C-N	5.06	127.48	122.12
22	S	309	PHE	CA-C-N	5.06	127.06	120.28
22	S	309	PHE	C-N-CA	5.06	127.06	120.28
23	P	13	TYR	CB-CG-CD1	5.06	128.39	120.80
33	J	20	LYS	CA-C-N	5.06	125.74	120.12
33	J	20	LYS	C-N-CA	5.06	125.74	120.12
33	J	144	ASP	CB-CA-C	5.06	119.76	110.24
7	g	73	HIS	CE1-NE2-CD2	-5.06	103.94	109.00
13	m	86	ASP	CB-CA-C	-5.06	100.84	109.65
25	R	326	ALA	CA-C-O	-5.06	115.19	120.55
26	U	256	ASN	CA-CB-CG	5.06	117.66	112.60
31	L	231	LEU	N-CA-CB	5.06	117.56	110.12
1	a	77	ARG	CD-NE-CZ	-5.06	117.32	124.40
11	k	72	ASP	N-CA-CB	5.06	119.38	111.84
14	n	231	ALA	O-C-N	5.06	129.46	123.24
5	E	239	LEU	N-CA-CB	-5.06	102.69	110.12
8	1	72	LEU	CA-C-N	5.06	127.06	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	72	LEU	C-N-CA	5.06	127.06	120.28
18	X	30	GLN	CA-C-O	-5.06	115.71	121.58
21	N	184	LYS	CA-C-N	5.06	127.60	120.42
21	N	184	LYS	C-N-CA	5.06	127.60	120.42
24	Q	57	SER	N-CA-C	5.06	116.79	111.28
25	R	321	TYR	N-CA-C	-5.06	106.80	113.17
27	O	250	TRP	CA-CB-CG	5.06	123.21	113.60
12	l	220	LYS	CA-C-O	5.06	126.50	120.28
3	C	32	ALA	N-CA-C	-5.06	102.58	110.42
27	O	357	ILE	CA-C-O	5.06	127.10	120.78
29	I	117	HIS	ND1-CE1-NE2	5.06	113.46	108.40
2	b	98	LYS	N-CA-CB	5.05	118.06	110.53
5	E	40	ILE	N-CA-C	-5.05	100.37	107.75
24	Q	13	ARG	CB-CA-C	-5.05	102.40	110.79
27	O	210	ARG	NH1-CZ-NH2	5.05	125.87	119.30
30	K	184	ILE	CA-CB-CG1	5.05	118.99	110.40
1	a	152	PRO	N-CA-CB	5.05	107.82	103.27
1	a	198	SER	N-CA-C	-5.05	100.17	108.41
6	F	143	HIS	CA-C-N	5.05	129.87	122.39
6	F	143	HIS	C-N-CA	5.05	129.87	122.39
8	1	37	ASN	OD1-CG-ND2	5.05	127.65	122.60
21	N	117	TYR	N-CA-C	-5.05	107.11	113.28
4	D	15	GLY	N-CA-C	-5.05	107.64	115.67
16	V	221	TRP	CA-C-O	5.05	125.47	119.56
17	T	14	ALA	CA-C-N	5.05	127.46	120.29
17	T	14	ALA	C-N-CA	5.05	127.46	120.29
29	I	190	GLN	OE1-CD-NE2	5.05	127.65	122.60
3	c	217	ARG	NE-CZ-NH1	-5.05	116.45	121.50
4	d	98	LEU	N-CA-CB	5.05	117.39	110.07
5	E	157	HIS	N-CA-C	-5.05	100.18	108.41
16	V	163	ALA	CA-C-N	5.05	127.46	120.29
16	V	163	ALA	C-N-CA	5.05	127.46	120.29
21	N	642	ASP	N-CA-CB	5.05	119.36	110.37
25	R	211	LYS	N-CA-CB	5.05	117.54	110.12
31	L	143	GLY	CA-C-N	5.05	128.88	122.37
31	L	143	GLY	C-N-CA	5.05	128.88	122.37
32	M	29	GLU	N-CA-C	-5.05	105.86	111.36
6	f	143	HIS	CG-CD2-NE2	5.05	112.25	107.20
21	N	239	LEU	CA-C-O	-5.05	115.07	120.42
21	N	714	THR	N-CA-CB	5.05	119.71	111.08
27	O	284	GLU	CB-CA-C	-5.05	102.95	110.88
33	J	258	VAL	O-C-N	5.05	127.18	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	244	GLN	CA-C-O	5.05	125.90	120.55
11	k	37	GLN	CB-CA-C	-5.05	102.69	110.26
4	D	20	VAL	N-CA-C	-5.05	105.24	112.35
6	F	160	ALA	CA-C-N	5.05	129.12	122.51
6	F	160	ALA	C-N-CA	5.05	129.12	122.51
7	G	39	GLY	N-CA-C	-5.05	101.22	113.18
9	2	143	HIS	N-CA-CB	5.05	118.62	111.05
12	5	164	GLN	CA-C-N	5.05	131.03	122.65
12	5	164	GLN	C-N-CA	5.05	131.03	122.65
17	T	206	LYS	CA-C-N	5.05	127.46	120.29
17	T	206	LYS	C-N-CA	5.05	127.46	120.29
22	S	402	ILE	CA-C-N	5.05	127.88	120.71
22	S	402	ILE	C-N-CA	5.05	127.88	120.71
28	H	297	MET	CG-SD-CE	-5.05	89.80	100.90
29	I	317	ASP	CA-CB-CG	-5.05	107.55	112.60
30	K	306	PHE	CA-CB-CG	5.05	118.85	113.80
32	M	191	GLU	N-CA-CB	5.05	117.63	110.16
11	k	84	VAL	N-CA-CB	5.04	117.40	110.54
16	V	221	TRP	CH2-CZ2-CE2	5.04	124.06	117.50
21	N	177	ASP	CB-CA-C	-5.04	102.42	110.79
11	k	167	GLU	O-C-N	5.04	127.27	122.07
6	F	174	ARG	N-CA-C	-5.04	105.25	111.40
9	2	81	THR	CA-C-N	5.04	127.04	120.28
9	2	81	THR	C-N-CA	5.04	127.04	120.28
14	7	190	LYS	CA-C-O	5.04	125.90	120.55
16	V	52	LEU	N-CA-CB	5.04	118.92	110.85
22	S	275	TYR	N-CA-CB	5.04	117.32	110.01
23	P	21	PHE	CA-C-O	-5.04	113.79	118.73
26	U	138	VAL	CA-C-O	-5.04	115.02	120.67
26	U	278	ILE	N-CA-CB	5.04	118.15	110.58
27	O	21	SER	N-CA-C	-5.04	107.08	113.18
2	b	5	TYR	CA-C-N	5.04	128.92	120.70
2	b	5	TYR	C-N-CA	5.04	128.92	120.70
4	d	59	ILE	N-CA-C	-5.04	108.06	112.90
7	g	201	TYR	CB-CG-CD1	-5.04	113.24	120.80
12	l	151	VAL	O-C-N	-5.04	116.64	121.83
13	6	84	HIS	N-CA-CB	5.04	117.98	110.22
22	S	141	LEU	N-CA-C	5.04	116.78	111.28
22	S	347	HIS	CB-CG-CD2	-5.04	124.65	131.20
22	S	462	ASP	CA-C-O	5.04	125.77	119.97
28	H	162	ARG	NE-CZ-NH2	-5.04	114.66	119.20
29	I	383	THR	CA-C-O	-5.04	115.53	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I	386	ASP	CA-C-N	5.04	131.28	122.81
29	I	386	ASP	C-N-CA	5.04	131.28	122.81
32	M	307	GLU	CA-C-N	5.04	127.30	120.44
32	M	307	GLU	C-N-CA	5.04	127.30	120.44
33	J	104	VAL	CA-C-N	5.04	131.44	122.06
33	J	104	VAL	C-N-CA	5.04	131.44	122.06
13	m	219	GLY	CA-C-O	-5.04	118.25	122.33
7	G	28	VAL	CB-CA-C	-5.04	104.09	112.26
11	4	181	VAL	O-C-N	5.04	128.27	122.93
15	W	136	ASN	N-CA-CB	5.04	120.13	112.47
16	V	143	PRO	N-CA-C	-5.04	106.18	114.75
20	Z	208	VAL	CA-C-O	-5.04	115.31	118.69
28	H	232	PRO	CA-C-N	5.04	127.45	120.29
28	H	232	PRO	C-N-CA	5.04	127.45	120.29
3	c	84	ALA	CB-CA-C	-5.04	101.31	110.63
9	i	92	ILE	CB-CA-C	-5.04	103.95	112.16
9	i	203	ASP	CA-CB-CG	-5.04	107.56	112.60
12	l	121	ALA	N-CA-CB	5.04	119.52	111.56
14	n	101	LYS	N-CA-C	5.04	117.50	111.71
12	5	120	MET	CA-C-O	-5.04	115.11	120.40
12	5	138	CYS	N-CA-C	-5.04	105.87	111.36
14	7	59	ASN	CB-CG-ND2	5.04	123.96	116.40
15	W	36	ILE	N-CA-CB	5.04	116.44	110.55
16	V	117	TRP	CD2-CE2-CZ2	-5.04	117.36	122.40
17	T	27	LEU	CA-C-N	5.04	125.57	120.38
17	T	27	LEU	C-N-CA	5.04	125.57	120.38
20	Z	476	ASP	CA-C-N	5.04	127.45	120.29
20	Z	476	ASP	C-N-CA	5.04	127.45	120.29
24	Q	88	PHE	CA-CB-CG	5.04	118.84	113.80
24	Q	206	ASN	CA-C-N	5.04	127.92	120.82
24	Q	206	ASN	C-N-CA	5.04	127.92	120.82
29	I	206	GLU	CA-C-N	5.04	127.44	120.29
29	I	206	GLU	C-N-CA	5.04	127.44	120.29
29	I	344	ILE	CA-CB-CG1	5.04	118.97	110.40
30	K	205	PRO	CA-C-N	5.04	125.03	119.89
30	K	205	PRO	C-N-CA	5.04	125.03	119.89
1	A	10	ALA	N-CA-CB	5.04	117.95	110.40
3	C	237	ASP	CB-CA-C	-5.04	102.94	110.90
15	W	158	ILE	CA-C-O	-5.04	115.71	120.95
21	N	316	LYS	CA-C-N	5.04	127.03	120.28
21	N	316	LYS	C-N-CA	5.04	127.03	120.28
23	P	63	VAL	N-CA-CB	5.04	117.39	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	72	ASP	CA-CB-CG	-5.04	107.56	112.60
33	J	15	HIS	N-CA-C	-5.04	106.98	114.64
11	k	179	VAL	CA-C-O	-5.04	117.70	121.68
13	m	167	GLN	N-CA-CB	5.04	120.11	111.00
6	F	120	THR	N-CA-C	-5.04	107.12	114.12
8	l	84	THR	CA-C-N	5.04	127.03	120.28
8	l	84	THR	C-N-CA	5.04	127.03	120.28
16	V	90	LYS	N-CA-C	5.04	116.85	111.36
20	Z	738	TYR	N-CA-C	-5.04	105.79	111.28
21	N	297	ASP	CB-CA-C	-5.04	102.43	110.79
24	Q	63	GLN	N-CA-C	-5.04	105.50	111.69
24	Q	323	LYS	CA-C-N	5.04	127.44	120.29
24	Q	323	LYS	C-N-CA	5.04	127.44	120.29
26	U	112	LYS	N-CA-C	5.04	116.46	111.07
26	U	194	LEU	CA-C-N	5.04	127.03	120.28
26	U	194	LEU	C-N-CA	5.04	127.03	120.28
29	I	75	PHE	CA-C-O	-5.04	115.53	120.82
29	I	352	ASN	CA-C-N	5.04	124.97	119.78
29	I	352	ASN	C-N-CA	5.04	124.97	119.78
1	a	116	VAL	CB-CA-C	-5.03	103.96	112.16
5	e	71	ASP	CA-C-N	5.03	127.03	120.28
5	e	71	ASP	C-N-CA	5.03	127.03	120.28
10	j	161	GLU	N-CA-C	-5.03	106.06	113.61
11	k	170	LYS	CB-CG-CD	5.03	122.88	111.30
11	4	25	ILE	CA-CB-CG1	5.03	118.96	110.40
24	Q	57	SER	N-CA-CB	5.03	117.52	110.12
1	a	131	ARG	CA-C-N	5.03	127.02	120.28
1	a	131	ARG	C-N-CA	5.03	127.02	120.28
1	A	227	VAL	CA-C-O	5.03	125.92	120.43
4	d	225	SER	N-CA-C	5.03	117.19	110.35
5	e	234	GLU	CA-C-N	5.03	127.95	120.31
5	e	234	GLU	C-N-CA	5.03	127.95	120.31
7	g	191	GLU	CB-CG-CD	-5.03	104.05	112.60
2	B	55	LEU	N-CA-C	-5.03	107.14	113.28
21	N	183	VAL	CA-C-O	-5.03	115.52	120.85
21	N	365	PHE	N-CA-CB	5.03	117.52	110.12
21	N	746	ALA	N-CA-C	5.03	118.68	112.54
22	S	61	SER	CA-C-N	5.03	126.98	120.44
22	S	61	SER	C-N-CA	5.03	126.98	120.44
22	S	213	THR	CA-CB-OG1	5.03	117.14	109.60
27	O	146	ALA	CA-C-N	5.03	127.33	120.54
27	O	146	ALA	C-N-CA	5.03	127.33	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	364	PRO	O-C-N	5.03	128.98	122.24
31	L	280	MET	CA-C-N	-5.03	116.06	123.00
31	L	280	MET	C-N-CA	-5.03	116.06	123.00
10	j	53	ILE	CA-C-N	5.03	128.80	122.16
10	j	53	ILE	C-N-CA	5.03	128.80	122.16
26	U	103	ASP	CA-CB-CG	5.03	117.63	112.60
6	f	46	LEU	O-C-N	5.03	129.28	123.30
12	l	200	ASP	CA-CB-CG	-5.03	107.57	112.60
12	5	112	ILE	N-CA-C	-5.03	105.52	111.00
15	W	32	SER	CA-C-N	5.03	126.89	120.56
15	W	32	SER	C-N-CA	5.03	126.89	120.56
20	Z	224	LEU	CA-C-N	5.03	127.33	120.54
20	Z	224	LEU	C-N-CA	5.03	127.33	120.54
21	N	446	ALA	N-CA-C	-5.03	105.88	111.36
25	R	51	LEU	CA-C-N	5.03	127.02	120.28
25	R	51	LEU	C-N-CA	5.03	127.02	120.28
25	R	100	ASN	CB-CG-OD1	5.03	130.86	120.80
30	K	183	GLU	CB-CG-CD	5.03	121.15	112.60
32	M	198	VAL	N-CA-CB	5.03	118.12	110.58
4	d	16	HIS	CB-CG-ND1	5.03	130.24	122.70
12	l	167	GLY	CA-C-O	5.03	124.84	119.06
13	6	219	GLY	CA-C-N	5.03	129.65	123.12
13	6	219	GLY	C-N-CA	5.03	129.65	123.12
17	T	54	ASP	N-CA-CB	5.03	118.07	110.28
21	N	655	ALA	N-CA-C	-5.03	105.88	111.36
32	M	423	GLN	OE1-CD-NE2	-5.03	117.57	122.60
10	j	83	GLU	CA-C-O	-5.02	115.47	120.64
12	5	220	LYS	CA-C-O	-5.02	114.57	120.60
2	b	6	SER	N-CA-C	-5.02	106.73	114.16
4	d	89	ALA	CA-C-N	5.02	127.01	120.28
4	d	89	ALA	C-N-CA	5.02	127.01	120.28
7	g	15	PHE	N-CA-C	-5.02	101.73	109.52
7	g	35	THR	O-C-N	-5.02	117.52	123.25
2	B	173	THR	CB-CA-C	5.02	119.39	110.85
3	C	80	LEU	O-C-N	5.02	129.27	122.59
5	E	249	ALA	CA-C-O	5.02	125.23	119.35
8	1	142	PHE	CB-CG-CD2	5.02	129.24	120.70
21	N	370	SER	CA-C-N	5.02	127.01	120.28
21	N	370	SER	C-N-CA	5.02	127.01	120.28
27	O	282	GLN	N-CA-CB	5.02	118.59	110.40
28	H	132	GLN	O-C-N	5.02	129.02	122.89
32	M	327	THR	CA-C-O	-5.02	115.37	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	224	GLU	CB-CA-C	-5.02	102.91	110.24
6	f	46	LEU	CA-C-O	-5.02	114.94	120.36
22	S	330	LEU	CA-C-N	5.02	127.51	120.28
22	S	330	LEU	C-N-CA	5.02	127.51	120.28
25	R	317	ILE	N-CA-C	5.02	119.73	108.88
30	K	160	VAL	N-CA-CB	5.02	116.68	110.05
1	a	62	LYS	CA-C-O	5.02	125.53	119.31
3	c	117	ASP	CB-CA-C	-5.02	101.03	110.67
6	f	59	TYR	CA-CB-CG	-5.02	104.87	113.90
14	n	225	SER	CA-C-N	5.02	127.94	120.31
14	n	225	SER	C-N-CA	5.02	127.94	120.31
2	B	115	ALA	N-CA-C	-5.02	105.91	112.23
5	E	95	ALA	CA-C-N	5.02	127.00	120.28
5	E	95	ALA	C-N-CA	5.02	127.00	120.28
5	E	160	PRO	N-CA-CB	5.02	108.13	103.41
9	2	103	PRO	O-C-N	5.02	129.24	123.01
14	7	139	LYS	N-CA-CB	5.02	117.59	110.16
17	T	78	PHE	CB-CG-CD1	5.02	129.23	120.70
17	T	137	GLU	N-CA-C	-5.02	107.21	113.38
21	N	448	LEU	CA-C-O	5.02	125.74	120.42
21	N	459	ASN	CA-CB-CG	-5.02	107.58	112.60
31	L	281	ASP	CA-CB-CG	5.02	117.62	112.60
6	f	191	LYS	N-CA-C	5.02	117.48	111.71
9	i	130	ALA	N-CA-C	-5.02	101.67	109.14
10	j	41	GLU	N-CA-CB	5.02	117.37	109.69
14	n	153	GLN	CG-CD-NE2	5.02	123.93	116.40
8	1	131	LEU	CA-C-N	5.02	125.84	120.47
8	1	131	LEU	C-N-CA	5.02	125.84	120.47
22	S	325	GLY	N-CA-C	-5.02	108.16	115.63
23	P	364	ARG	CA-C-N	5.02	127.42	120.29
23	P	364	ARG	C-N-CA	5.02	127.42	120.29
33	J	342	ASN	OD1-CG-ND2	5.02	127.62	122.60
13	m	40	ASP	CA-CB-CG	-5.02	107.58	112.60
13	6	221	ARG	CA-C-N	5.02	131.17	122.64
13	6	221	ARG	C-N-CA	5.02	131.17	122.64
14	7	174	THR	N-CA-C	-5.02	101.12	108.99
27	O	261	GLY	CA-C-N	5.02	129.46	121.99
27	O	261	GLY	C-N-CA	5.02	129.46	121.99
29	I	139	GLU	N-CA-C	-5.02	107.21	113.38
1	a	209	HIS	ND1-CE1-NE2	5.01	113.42	108.40
3	c	165	VAL	CA-CB-CG2	5.01	118.92	110.40
4	d	228	GLU	CB-CA-C	-5.01	103.01	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	13	VAL	CA-CB-CG1	-5.01	101.87	110.40
5	E	84	ASP	CA-C-N	5.01	129.20	120.68
5	E	84	ASP	C-N-CA	5.01	129.20	120.68
6	F	152	ASN	N-CA-C	-5.01	101.54	109.76
12	5	174	THR	O-C-N	5.01	129.41	123.24
22	S	49	ASP	CA-C-N	5.01	125.04	119.32
22	S	49	ASP	C-N-CA	5.01	125.04	119.32
22	S	334	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
23	P	389	ILE	CA-C-N	5.01	130.46	122.74
23	P	389	ILE	C-N-CA	5.01	130.46	122.74
33	J	205	HIS	ND1-CE1-NE2	5.01	113.41	108.40
5	E	193	LEU	CA-C-O	-5.01	115.24	120.55
16	V	23	THR	CA-C-O	-5.01	115.74	121.40
21	N	599	TYR	CA-C-N	5.01	127.26	120.44
21	N	599	TYR	C-N-CA	5.01	127.26	120.44
22	S	164	ILE	CA-C-N	5.01	124.67	119.56
22	S	164	ILE	C-N-CA	5.01	124.67	119.56
28	H	426	ALA	CA-C-N	5.01	126.66	120.34
28	H	426	ALA	C-N-CA	5.01	126.66	120.34
29	I	273	GLU	CA-C-O	-5.01	115.11	120.42
30	K	223	VAL	CA-C-N	5.01	127.00	120.28
30	K	223	VAL	C-N-CA	5.01	127.00	120.28
3	c	190	ILE	CA-C-N	5.01	127.25	120.44
3	c	190	ILE	C-N-CA	5.01	127.25	120.44
6	f	186	PRO	CA-C-N	5.01	127.25	120.38
6	f	186	PRO	C-N-CA	5.01	127.25	120.38
11	k	52	ASP	CA-C-O	5.01	125.73	120.42
14	n	98	ARG	NE-CZ-NH1	5.01	126.51	121.50
4	D	86	ILE	N-CA-C	-5.01	105.54	111.00
5	E	148	ASP	N-CA-C	-5.01	101.75	109.52
7	G	164	ALA	CA-C-O	5.01	126.69	121.38
9	2	124	GLY	CA-C-O	5.01	129.29	120.57
21	N	369	ALA	CA-C-O	-5.01	113.22	119.38
32	M	64	ASP	N-CA-C	5.01	116.43	111.07
12	l	111	GLU	CA-C-N	5.01	127.32	120.46
12	l	111	GLU	C-N-CA	5.01	127.32	120.46
13	m	197	THR	CA-C-O	-5.01	115.24	120.55
2	B	190	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
4	D	168	SER	CA-C-O	-5.01	114.21	119.97
16	V	126	GLN	CA-C-N	5.01	126.99	120.28
16	V	126	GLN	C-N-CA	5.01	126.99	120.28
16	V	270	TYR	N-CA-C	5.01	118.87	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	292	ILE	N-CA-CB	5.01	118.09	110.58
21	N	654	GLN	O-C-N	5.01	127.43	122.12
24	Q	258	ALA	O-C-N	5.01	127.86	122.15
25	R	422	ARG	O-C-N	-5.01	116.11	122.27
27	O	362	GLN	CA-C-O	-5.01	115.24	120.55
30	K	209	VAL	N-CA-C	-5.01	101.10	108.11
2	b	213	ILE	CA-CB-CG1	5.01	118.91	110.40
7	g	183	HIS	CA-C-N	5.01	124.70	119.64
7	g	183	HIS	C-N-CA	5.01	124.70	119.64
2	B	234	ARG	N-CA-C	-5.01	107.34	113.50
18	X	17	TYR	CA-C-N	5.01	127.82	120.71
18	X	17	TYR	C-N-CA	5.01	127.82	120.71
18	X	32	GLU	N-CA-C	-5.01	100.85	108.76
20	Z	151	HIS	CA-C-N	5.01	127.40	120.29
20	Z	151	HIS	C-N-CA	5.01	127.40	120.29
20	Z	913	ILE	N-CA-C	-5.01	106.27	111.58
24	Q	290	THR	N-CA-CB	5.01	117.48	110.12
2	b	128	ARG	NE-CZ-NH2	-5.01	114.69	119.20
13	m	122	LEU	CA-C-O	5.01	126.42	120.66
13	m	208	ASP	CA-CB-CG	-5.01	107.59	112.60
6	F	69	HIS	CB-CG-ND1	5.01	130.21	122.70
18	X	28	PRO	CB-CA-C	-5.01	105.28	111.64
24	Q	176	ASP	CA-C-N	5.01	127.53	120.42
24	Q	176	ASP	C-N-CA	5.01	127.53	120.42
25	R	270	VAL	CA-C-O	-5.01	114.95	119.91
26	U	218	GLU	CA-C-O	-5.01	116.03	121.84
29	I	173	MET	N-CA-CB	5.01	118.79	110.63
31	L	189	GLN	O-C-N	-5.01	115.62	122.33
13	m	228	LYS	O-C-N	-5.00	116.65	122.81
4	D	202	VAL	CB-CA-C	-5.00	105.63	111.94
9	2	224	VAL	CA-C-N	5.00	128.43	121.02
9	2	224	VAL	C-N-CA	5.00	128.43	121.02
16	V	282	GLU	O-C-N	5.00	127.30	122.09
6	f	119	ASN	CA-CB-CG	5.00	117.60	112.60
7	g	21	ASN	N-CA-C	-5.00	98.88	107.23
14	7	126	PHE	CA-C-O	-5.00	115.75	121.00
16	V	105	VAL	N-CA-C	-5.00	108.10	112.90
20	Z	919	GLU	N-CA-C	-5.00	105.83	111.28
21	N	284	PRO	N-CA-CB	-5.00	98.71	103.41
21	N	551	GLY	CA-C-N	5.00	126.98	120.28
21	N	551	GLY	C-N-CA	5.00	126.98	120.28
22	S	54	TRP	CA-C-O	5.00	125.85	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	130	ASP	N-CA-CB	5.00	117.92	110.22
1	a	192	ASP	CA-CB-CG	5.00	117.60	112.60
12	l	163	TYR	CB-CG-CD1	5.00	128.30	120.80
13	m	38	ILE	CA-CB-CG1	5.00	118.90	110.40
13	m	48	GLU	N-CA-CB	5.00	119.27	110.37
13	m	191	LEU	CA-C-N	5.00	126.86	120.56
13	m	191	LEU	C-N-CA	5.00	126.86	120.56
5	E	99	HIS	ND1-CE1-NE2	5.00	113.40	108.40
16	V	268	THR	N-CA-C	-5.00	105.54	111.69
17	T	261	GLU	O-C-N	-5.00	116.82	122.12
21	N	92	ASP	N-CA-C	-5.00	106.60	113.30
24	Q	185	TYR	CA-C-N	5.00	126.98	120.28
24	Q	185	TYR	C-N-CA	5.00	126.98	120.28
26	U	113	TYR	CA-C-N	5.00	130.07	120.97
26	U	113	TYR	C-N-CA	5.00	130.07	120.97

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	Z	748	LEU	CA

All (350) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	133	TYR	Sidechain
8	1	144	TYR	Sidechain
8	1	146	TYR	Sidechain
8	1	75	TYR	Sidechain
9	2	119	TYR	Sidechain
9	2	140	PHE	Sidechain
9	2	219	TYR	Sidechain
9	2	232	TYR	Sidechain
9	2	98	TYR	Sidechain
10	3	136	PHE	Sidechain
10	3	154	TYR	Sidechain
10	3	199	TYR	Sidechain
10	3	203	ARG	Sidechain
10	3	69	TYR	Sidechain
10	3	96	TYR	Sidechain
11	4	121	TYR	Sidechain
11	4	176	PHE	Sidechain
11	4	59	TYR	Sidechain

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Mol	Chain	Res	Type	Group
12	5	148	ARG	Sidechain
12	5	176	ILE	Mainchain
12	5	179	TYR	Sidechain
12	5	188	TYR	Sidechain
12	5	219	TYR	Sidechain
13	6	114	TYR	Sidechain
13	6	203	HIS	Sidechain
13	6	229	ARG	Peptide
13	6	47	TYR	Sidechain
13	6	75	ARG	Sidechain
13	6	83	TYR	Sidechain
13	6	99	ARG	Sidechain
14	7	124	TYR	Sidechain
14	7	162	TYR	Sidechain
14	7	170	TYR	Sidechain
14	7	179	PHE	Sidechain
14	7	223	ARG	Sidechain
14	7	49	TYR	Sidechain
14	7	63	TYR	Sidechain
1	A	110	TYR	Sidechain
1	A	131	ARG	Sidechain
1	A	244	ARG	Sidechain
1	A	71	TYR	Sidechain
1	A	91	ARG	Sidechain
2	B	104	TYR	Sidechain
2	B	178	ARG	Sidechain
2	B	23	TYR	Sidechain
2	B	235	PHE	Sidechain
2	B	236	ARG	Sidechain
2	B	5	TYR	Sidechain
2	B	90	ARG	Sidechain
2	B	97	TYR	Sidechain
3	C	131	PHE	Sidechain
3	C	140	TYR	Sidechain
3	C	157	TYR	Sidechain
3	C	180	TYR	Sidechain
3	C	226	TYR	Sidechain
3	C	4	ARG	Sidechain
4	D	112	TYR	Sidechain
4	D	172	ARG	Sidechain
4	D	179	TYR	Sidechain
4	D	41	CYS	Peptide

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Mol	Chain	Res	Type	Group
4	D	49	ARG	Sidechain
4	D	83	ARG	Sidechain
4	D	96	HIS	Sidechain
4	D	97	ARG	Sidechain
5	E	10	ARG	Sidechain
5	E	102	TYR	Sidechain
5	E	103	TYR	Sidechain
5	E	132	ARG	Sidechain
5	E	136	ARG	Sidechain
5	E	138	PHE	Sidechain
5	E	15	PHE	Sidechain
5	E	20	ARG	Sidechain
5	E	228	PHE	Sidechain
5	E	231	TYR	Sidechain
6	F	101	ARG	Sidechain
6	F	137	TYR	Sidechain
6	F	157	TYR	Sidechain
6	F	174	ARG	Sidechain
6	F	179	PHE	Sidechain
6	F	18	ARG	Peptide
6	F	233	TYR	Sidechain
6	F	51	ARG	Sidechain
6	F	89	ARG	Sidechain
6	F	94	TYR	Sidechain
7	G	149	TYR	Sidechain
7	G	16	SER	Peptide
7	G	190	ARG	Sidechain
7	G	201	TYR	Sidechain
7	G	21	ASN	Peptide
7	G	78	TYR	Sidechain
7	G	93	ARG	Sidechain
28	H	190	ARG	Sidechain
28	H	249	TYR	Sidechain
28	H	318	ARG	Sidechain
28	H	385	ARG	Sidechain
28	H	429	PHE	Sidechain
28	H	434	ARG	Sidechain
28	H	463	TYR	Sidechain
28	H	73	ASP	Peptide
29	I	181	TYR	Sidechain
29	I	208	TYR	Sidechain
29	I	340	ARG	Sidechain

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Mol	Chain	Res	Type	Group
29	I	408	ARG	Sidechain
29	I	422	ARG	Sidechain
29	I	429	GLU	Peptide
29	I	54	ARG	Sidechain
29	I	68	HIS	Sidechain
33	J	124	LYS	Peptide
33	J	147	TYR	Sidechain
33	J	22	TYR	Sidechain
33	J	222	TYR	Sidechain
33	J	270	ARG	Sidechain
33	J	286	LYS	Peptide
33	J	309	ARG	Sidechain
33	J	312	ARG	Sidechain
33	J	35	ARG	Sidechain
33	J	94	TYR	Sidechain
30	K	118	TYR	Sidechain
30	K	141	ARG	Sidechain
30	K	185	ARG	Sidechain
30	K	198	TYR	Sidechain
30	K	236	ARG	Sidechain,Mainchain
30	K	246	TYR	Sidechain
30	K	262	ARG	Sidechain
30	K	67	TYR	Sidechain
30	K	88	ARG	Sidechain
31	L	131	VAL	Peptide
31	L	168	TYR	Sidechain
31	L	209	ARG	Sidechain
31	L	243	PHE	Peptide,Mainchain
31	L	244	ILE	Peptide,Mainchain
31	L	255	TYR	Sidechain
31	L	261	ARG	Sidechain
31	L	264	ARG	Sidechain
31	L	303	ARG	Sidechain
31	L	315	PHE	Peptide
31	L	318	LEU	Peptide
31	L	342	ARG	Peptide
31	L	345	ARG	Sidechain
31	L	374	PHE	Sidechain
31	L	376	PHE	Peptide
31	L	407	ARG	Sidechain
31	L	409	HIS	Sidechain
31	L	434	TYR	Sidechain

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Mol	Chain	Res	Type	Group
31	L	62	ARG	Sidechain
31	L	70	TYR	Sidechain
31	L	77	ARG	Sidechain
32	M	124	ARG	Sidechain
32	M	153	TYR	Sidechain
32	M	213	ARG	Sidechain
32	M	291	PHE	Sidechain
32	M	314	GLY	Peptide
32	M	320	ARG	Sidechain
32	M	329	ARG	Sidechain
32	M	349	PHE	Sidechain
32	M	423	GLN	Peptide
21	N	109	TYR	Sidechain
21	N	139	ARG	Sidechain
21	N	161	TYR	Sidechain
21	N	202	PHE	Sidechain
21	N	282	TYR	Sidechain
21	N	329	HIS	Sidechain
21	N	348	PHE	Sidechain
21	N	389	TYR	Sidechain
21	N	412	TYR	Sidechain
21	N	415	PHE	Sidechain
21	N	471	TYR	Sidechain
21	N	549	TYR	Sidechain
21	N	599	TYR	Sidechain
21	N	653	ARG	Sidechain
21	N	69	TYR	Sidechain
21	N	762	ARG	Sidechain
21	N	771	PHE	Sidechain
21	N	782	PHE	Sidechain
21	N	784	TYR	Sidechain
21	N	788	TYR	Sidechain
21	N	81	TYR	Sidechain
21	N	884	PHE	Sidechain
21	N	889	ARG	Sidechain
21	N	894	ARG	Sidechain
27	O	15	ARG	Sidechain
27	O	172	TYR	Sidechain
27	O	195	TYR	Sidechain
27	O	32	PHE	Sidechain
27	O	58	ARG	Sidechain
23	P	138	ARG	Sidechain

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Mol	Chain	Res	Type	Group
23	P	21	PHE	Sidechain
23	P	213	TYR	Sidechain
23	P	220	TYR	Sidechain
23	P	310	ARG	Sidechain
23	P	351	ARG	Sidechain
23	P	356	TYR	Sidechain
23	P	47	ARG	Sidechain
24	Q	161	LEU	Peptide
24	Q	209	TYR	Sidechain
24	Q	232	TYR	Sidechain
24	Q	243	PHE	Sidechain
24	Q	246	TYR	Sidechain
24	Q	255	TYR	Sidechain
24	Q	264	TYR	Sidechain
24	Q	306	TYR	Sidechain
24	Q	321	TYR	Sidechain
24	Q	332	ARG	Sidechain
24	Q	400	TYR	Sidechain
24	Q	50	ARG	Sidechain
24	Q	67	THR	Peptide
24	Q	84	TYR	Sidechain
25	R	140	TYR	Sidechain
25	R	141	TYR	Sidechain
25	R	176	ARG	Sidechain
25	R	181	TYR	Sidechain
25	R	20	ARG	Sidechain
25	R	209	ARG	Sidechain
25	R	210	TYR	Sidechain
25	R	224	PHE	Sidechain
25	R	24	TYR	Sidechain
25	R	307	TYR	Sidechain
25	R	312	TYR	Sidechain
25	R	325	HIS	Sidechain
25	R	345	TYR	Sidechain
25	R	62	TYR	Sidechain
25	R	65	TYR	Sidechain
25	R	70	TYR	Peptide
25	R	99	TYR	Sidechain
22	S	185	PHE	Sidechain
22	S	186	TYR	Sidechain
22	S	197	SER	Peptide
22	S	211	ARG	Sidechain

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Mol	Chain	Res	Type	Group
22	S	259	TYR	Sidechain
22	S	272	TYR	Sidechain
22	S	345	TYR	Sidechain
22	S	442	PHE	Sidechain
22	S	481	TYR	Sidechain
22	S	64	ARG	Sidechain
22	S	76	PHE	Sidechain
22	S	82	TYR	Sidechain
17	T	144	TYR	Sidechain
17	T	251	HIS	Peptide
17	T	266	TYR	Sidechain
17	T	88	TYR	Sidechain
17	T	91	SER	Peptide
26	U	22	TYR	Sidechain
26	U	283	ARG	Sidechain
26	U	47	ARG	Sidechain
26	U	94	HIS	Sidechain
16	V	135	ARG	Sidechain
16	V	230	TYR	Sidechain
16	V	269	ARG	Sidechain
16	V	28	TYR	Sidechain
16	V	40	HIS	Sidechain
16	V	87	PHE	Sidechain
15	W	122	ARG	Sidechain
15	W	17	ARG	Sidechain
15	W	179	ARG	Sidechain
15	W	41	ARG	Sidechain
18	X	17	TYR	Sidechain
18	X	97	TYR	Sidechain
18	X	98	PHE	Sidechain
20	Z	248	TYR	Sidechain
20	Z	269	TYR	Sidechain
20	Z	287	ARG	Sidechain
20	Z	623	ARG	Sidechain
20	Z	738	TYR	Sidechain
1	a	108	TYR	Sidechain
1	a	110	TYR	Sidechain
1	a	209	HIS	Sidechain
1	a	26	TYR	Sidechain
1	a	71	TYR	Sidechain
1	a	77	ARG	Sidechain
2	b	178	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	b	90	ARG	Sidechain
2	b	97	TYR	Sidechain
3	c	140	TYR	Sidechain
3	c	143	ARG	Sidechain
3	c	157	TYR	Sidechain
3	c	18	ARG	Sidechain
3	c	210	ARG	Sidechain
3	c	217	ARG	Sidechain
3	c	5	ARG	Sidechain
3	c	6	TYR	Sidechain
4	d	108	TYR	Sidechain
4	d	11	PHE	Sidechain
4	d	22	TYR	Sidechain
4	d	49	ARG	Sidechain
4	d	83	ARG	Sidechain
5	e	10	ARG	Sidechain
5	e	136	ARG	Sidechain
5	e	138	PHE	Sidechain
5	e	164	PHE	Sidechain
5	e	165	TYR	Sidechain
5	e	86	ARG	Sidechain
5	e	91	HIS	Sidechain
6	f	12	THR	Peptide
6	f	137	TYR	Sidechain
6	f	147	PHE	Sidechain
6	f	18	ARG	Peptide
6	f	225	TYR	Sidechain
6	f	233	TYR	Sidechain
6	f	24	TYR	Sidechain
6	f	43	HIS	Sidechain
7	g	130	ARG	Sidechain
7	g	169	ARG	Sidechain
7	g	190	ARG	Sidechain
7	g	20	ARG	Sidechain
7	g	21	ASN	Peptide
7	g	72	ARG	Sidechain
7	g	8	TYR	Sidechain
8	h	111	TYR	Sidechain
8	h	133	TYR	Sidechain
8	h	142	PHE	Sidechain
8	h	144	TYR	Sidechain
8	h	34	TYR	Sidechain

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Mol	Chain	Res	Type	Group
8	h	45	ARG	Sidechain
8	h	96	TYR	Sidechain
9	i	145	HIS	Sidechain
9	i	215	TYR	Sidechain
9	i	219	TYR	Sidechain
10	j	103	TYR	Sidechain
10	j	177	ARG	Sidechain
10	j	188	TYR	Sidechain
10	j	44	PHE	Sidechain
10	j	46	TYR	Sidechain
10	j	69	TYR	Sidechain
10	j	74	TYR	Sidechain
11	k	139	TYR	Sidechain
11	k	56	PHE	Sidechain
11	k	67	TYR	Sidechain
11	k	8	ARG	Sidechain
12	l	144	ARG	Sidechain
12	l	179	TYR	Sidechain
12	l	210	PHE	Sidechain
12	l	253	TYR	Sidechain
12	l	81	PHE	Sidechain
13	m	106	TYR	Sidechain
13	m	113	TYR	Sidechain
13	m	114	TYR	Sidechain
13	m	13	TYR	Sidechain
13	m	182	TYR	Sidechain
13	m	225	TYR	Sidechain
13	m	41	TYR	Sidechain
13	m	83	TYR	Sidechain
14	n	136	ARG	Sidechain
14	n	162	TYR	Sidechain
14	n	189	ARG	Sidechain
14	n	226	ARG	Sidechain
14	n	49	TYR	Sidechain
14	n	63	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1913	0	1906	10	0
1	a	1913	0	1906	3	0
2	B	1907	0	1917	0	0
2	b	1907	0	1917	5	0
3	C	1905	0	1901	3	0
3	c	1905	0	1901	5	0
4	D	1859	0	1875	7	0
4	d	1982	0	1993	4	0
5	E	1926	0	1896	3	0
5	e	1926	0	1896	4	0
6	F	1773	0	1775	4	0
6	f	1773	0	1775	5	0
7	G	1886	0	1876	22	0
7	g	1886	0	1876	23	0
8	1	1512	0	1478	2	0
8	h	1512	0	1478	6	0
9	2	1720	0	1716	8	0
9	i	1720	0	1716	5	0
10	3	1581	0	1571	3	0
10	j	1581	0	1571	4	0
11	4	1562	0	1569	1	0
11	k	1562	0	1569	1	0
12	5	1644	0	1592	4	0
12	l	1644	0	1592	5	0
13	6	1757	0	1708	3	0
13	m	1757	0	1708	2	0
14	7	1790	0	1790	25	0
14	n	1816	0	1818	24	0
15	W	1535	0	1542	7	0
16	V	2274	0	2273	8	0
17	T	2193	0	2161	7	0
18	X	1033	0	1017	2	0
19	Y	731	0	675	2	0
20	Z	7006	0	6932	290	0
21	N	7158	0	7226	64	0
22	S	3895	0	3938	10	0
23	P	3609	0	3694	12	0
24	Q	3499	0	3524	10	0
25	R	3259	0	3263	4	0
26	U	2427	0	2462	8	0
27	O	3186	0	3213	7	0
28	H	3313	0	3318	65	0
29	I	3015	0	3082	259	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	K	3113	0	3168	28	0
31	L	3083	0	3157	24	0
32	M	3285	0	3321	25	0
33	J	3171	0	3310	32	0
34	H	31	0	10	40	0
34	I	31	0	10	23	0
34	K	31	0	12	24	0
34	L	31	0	11	8	0
34	M	31	0	11	19	0
35	H	1	0	0	0	0
35	I	1	0	0	1	0
35	J	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
36	J	27	0	9	17	0
All	All	110592	0	110625	754	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 3.

All (754) 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)
20:Z:748:LEU:CA	20:Z:748:LEU:CB	1.81	1.56
20:Z:728:LYS:CB	20:Z:728:LYS:CA	1.85	1.53
20:Z:728:LYS:CE	20:Z:728:LYS:NZ	1.69	1.50
20:Z:728:LYS:CB	20:Z:728:LYS:CG	1.87	1.49
14:n:109:TYR:CZ	14:n:109:TYR:CE1	2.02	1.48
14:n:109:TYR:CE1	14:n:109:TYR:CD1	1.99	1.48
14:7:109:TYR:CE2	14:7:109:TYR:CZ	2.02	1.47
14:n:109:TYR:CE2	14:n:109:TYR:CD2	2.02	1.46
14:7:109:TYR:CE2	14:7:109:TYR:CD2	2.04	1.46
14:7:109:TYR:CE1	14:7:109:TYR:CD1	2.01	1.46
29:I:393:GLN:NE2	34:I:501:ATP:H1'	1.28	1.45
14:n:109:TYR:CD2	14:n:109:TYR:CG	2.07	1.42
14:7:109:TYR:CD1	14:7:109:TYR:CG	2.06	1.40
34:K:501:ATP:H5'1	31:L:339:ARG:NH2	1.29	1.40
28:H:308:PHE:C	28:H:309:ASP:N	1.81	1.39
34:K:501:ATP:C5'	31:L:339:ARG:HH22	1.33	1.38
14:7:109:TYR:CZ	14:7:109:TYR:CE1	2.09	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:I:322:VAL:C	29:I:323:LYS:N	1.82	1.37
14:n:109:TYR:CZ	14:n:109:TYR:CE2	2.09	1.37
14:n:109:TYR:CD1	14:n:109:TYR:CG	2.11	1.37
14:7:109:TYR:CD2	14:7:109:TYR:CG	2.14	1.34
20:Z:728:LYS:CG	29:I:62:MET:H	1.45	1.30
20:Z:728:LYS:HD2	29:I:64:ARG:N	1.43	1.29
20:Z:748:LEU:CB	20:Z:748:LEU:CG	2.10	1.29
20:Z:748:LEU:CG	29:I:81:ILE:C	2.05	1.28
20:Z:728:LYS:CE	20:Z:728:LYS:CD	2.12	1.28
29:I:230:THR:HB	34:I:501:ATP:O2A	1.31	1.27
28:H:307:PHE:C	28:H:308:PHE:N	1.91	1.26
29:I:393:GLN:CD	34:I:501:ATP:H1'	1.60	1.26
20:Z:748:LEU:CD2	29:I:82:LEU:H	1.49	1.25
33:J:197:LEU:HG	36:J:501:ADP:O1A	1.26	1.25
28:H:257:THR:N	34:H:501:ATP:O2B	1.62	1.24
33:J:197:LEU:CG	36:J:501:ADP:O1A	1.85	1.24
28:H:211:VAL:O	34:H:501:ATP:C2	1.93	1.22
29:I:393:GLN:OE1	34:I:501:ATP:O4'	1.58	1.20
20:Z:635:ALA:CA	21:N:792:SER:H	1.56	1.19
32:M:227:GLY:HA2	34:M:501:ATP:PA	1.83	1.18
7:G:93:ARG:CZ	7:G:93:ARG:NH2	2.07	1.17
20:Z:728:LYS:CE	29:I:65:ILE:H	1.58	1.17
28:H:212:GLY:HA2	34:H:501:ATP:C5	1.78	1.17
30:K:221:MET:N	34:K:501:ATP:O1A	1.79	1.16
30:K:173:ASP:O	34:K:501:ATP:N1	1.78	1.16
28:H:213:GLY:CA	34:H:501:ATP:HN62	1.53	1.15
20:Z:635:ALA:HB3	21:N:793:GLY:N	1.62	1.13
7:g:93:ARG:CZ	7:g:93:ARG:NH2	2.12	1.12
20:Z:728:LYS:CD	29:I:62:MET:C	2.22	1.11
33:J:197:LEU:HD11	36:J:501:ADP:C3'	1.80	1.11
7:g:93:ARG:CZ	14:n:109:TYR:CD2	2.34	1.11
20:Z:728:LYS:HG3	29:I:62:MET:H	1.05	1.11
28:H:256:LYS:HB2	34:H:501:ATP:O2B	1.39	1.11
20:Z:728:LYS:CG	29:I:62:MET:N	2.14	1.10
7:g:93:ARG:CZ	14:n:109:TYR:CE1	2.35	1.10
7:G:93:ARG:NH2	14:7:109:TYR:CZ	2.19	1.10
20:Z:748:LEU:CG	29:I:83:LYS:H	1.64	1.10
7:G:93:ARG:CZ	14:7:109:TYR:CE2	2.35	1.09
20:Z:635:ALA:CB	21:N:793:GLY:H	1.64	1.09
20:Z:748:LEU:CG	29:I:83:LYS:N	2.14	1.09
20:Z:728:LYS:HG2	29:I:59:LEU:C	1.77	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:748:LEU:CG	29:I:80:GLU:O	1.99	1.09
33:J:197:LEU:CD1	36:J:501:ADP:H3'	1.81	1.09
20:Z:748:LEU:CD2	29:I:81:ILE:N	2.16	1.09
28:H:213:GLY:HA2	34:H:501:ATP:HN62	0.92	1.09
30:K:220:THR:HB	34:K:501:ATP:PA	1.93	1.08
28:H:212:GLY:HA2	34:H:501:ATP:C4	1.87	1.08
28:H:212:GLY:CA	34:H:501:ATP:C5	2.36	1.08
28:H:258:LEU:HB2	34:H:501:ATP:O2A	1.52	1.08
7:G:93:ARG:CZ	14:7:109:TYR:CZ	2.36	1.08
7:G:93:ARG:CZ	14:7:109:TYR:CD1	2.36	1.07
28:H:213:GLY:CA	34:H:501:ATP:N6	2.14	1.07
7:g:93:ARG:NH2	14:n:109:TYR:CE2	2.23	1.06
7:G:93:ARG:NH2	14:7:109:TYR:CG	2.23	1.06
20:Z:748:LEU:CG	29:I:84:PRO:CD	2.33	1.06
20:Z:728:LYS:CD	29:I:61:ARG:C	2.29	1.06
7:g:93:ARG:NH2	14:n:109:TYR:CG	2.24	1.06
20:Z:738:TYR:OH	20:Z:738:TYR:CZ	2.09	1.06
20:Z:748:LEU:CD2	29:I:82:LEU:N	2.18	1.06
7:g:93:ARG:NH2	14:n:109:TYR:CZ	2.24	1.05
20:Z:748:LEU:HD22	29:I:81:ILE:HB	1.36	1.05
7:g:93:ARG:CZ	14:n:109:TYR:CG	2.40	1.05
7:G:93:ARG:NH2	14:7:109:TYR:CD2	2.24	1.05
7:G:93:ARG:NH2	14:7:109:TYR:CE2	2.25	1.05
7:g:93:ARG:NH2	14:n:109:TYR:CD1	2.23	1.05
20:Z:728:LYS:CG	29:I:59:LEU:O	2.03	1.05
7:g:93:ARG:NH2	14:n:109:TYR:CD2	2.25	1.05
7:G:93:ARG:NH2	14:7:109:TYR:CD1	2.25	1.04
20:Z:748:LEU:CG	29:I:84:PRO:HD2	1.85	1.04
7:g:93:ARG:CZ	14:n:109:TYR:CD1	2.40	1.04
7:G:93:ARG:CZ	14:7:109:TYR:CD2	2.40	1.04
7:G:93:ARG:NH2	14:7:109:TYR:CE1	2.25	1.04
7:g:93:ARG:CZ	14:n:109:TYR:CE2	2.39	1.04
7:G:93:ARG:CZ	14:7:109:TYR:CG	2.40	1.04
20:Z:635:ALA:HA	21:N:790:GLU:CG	1.86	1.04
29:I:393:GLN:OE1	34:I:501:ATP:C1'	2.05	1.04
7:g:93:ARG:NH2	14:n:109:TYR:CE1	2.26	1.04
20:Z:255:LEU:HD21	29:I:61:ARG:HE	1.24	1.03
7:g:93:ARG:CZ	14:n:109:TYR:CZ	2.42	1.02
20:Z:728:LYS:CD	29:I:61:ARG:O	2.08	1.02
20:Z:728:LYS:HD3	29:I:60:LEU:O	1.59	1.02
20:Z:728:LYS:CD	29:I:60:LEU:O	2.07	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:748:LEU:HG	29:I:83:LYS:H	1.20	1.02
20:Z:748:LEU:HD11	29:I:82:LEU:C	1.84	1.01
29:I:393:GLN:NE2	34:I:501:ATP:C1'	2.22	1.01
33:J:197:LEU:CD2	36:J:501:ADP:O1A	2.08	1.01
20:Z:635:ALA:HB3	21:N:793:GLY:H	0.84	1.01
20:Z:738:TYR:CZ	29:I:66:LYS:HA	1.94	1.01
20:Z:728:LYS:CD	29:I:63:GLU:N	2.23	1.01
7:G:93:ARG:CZ	14:7:109:TYR:CE1	2.43	1.00
28:H:256:LYS:CB	34:H:501:ATP:O2B	1.99	1.00
29:I:312:GLN:OE1	29:I:319:ARG:NH2	1.93	1.00
20:Z:635:ALA:CB	21:N:790:GLU:HG2	1.92	0.99
20:Z:635:ALA:HB2	21:N:791:ALA:CA	1.90	0.99
20:Z:748:LEU:CD1	29:I:84:PRO:HD2	1.92	0.99
29:I:393:GLN:CD	34:I:501:ATP:C1'	2.34	0.99
20:Z:748:LEU:HG	29:I:83:LYS:N	1.76	0.99
20:Z:635:ALA:HA	21:N:790:GLU:HG2	1.44	0.99
20:Z:728:LYS:HE3	29:I:65:ILE:H	1.21	0.99
29:I:230:THR:CB	34:I:501:ATP:O2A	2.10	0.99
29:I:393:GLN:OE1	34:I:501:ATP:C4'	2.10	0.98
20:Z:254:PRO:HB3	20:Z:727:GLU:HB3	1.44	0.98
20:Z:728:LYS:CE	29:I:61:ARG:O	2.12	0.98
20:Z:728:LYS:HD2	29:I:64:ARG:H	0.94	0.98
28:H:213:GLY:HA2	34:H:501:ATP:N6	1.76	0.97
20:Z:728:LYS:HB3	29:I:59:LEU:HA	1.45	0.96
28:H:258:LEU:N	34:H:501:ATP:O2A	1.99	0.96
20:Z:728:LYS:CD	29:I:64:ARG:H	1.77	0.95
28:H:388:ILE:HD13	34:H:501:ATP:C6	2.00	0.95
30:K:221:MET:CE	34:K:501:ATP:N6	2.21	0.95
20:Z:728:LYS:CE	29:I:62:MET:O	2.13	0.95
20:Z:748:LEU:CG	29:I:81:ILE:O	2.16	0.94
20:Z:728:LYS:CD	29:I:64:ARG:N	2.31	0.94
29:I:268:PHE:CD2	29:I:322:VAL:HG11	2.02	0.94
28:H:388:ILE:CD1	34:H:501:ATP:C6	2.51	0.93
30:K:221:MET:HE1	34:K:501:ATP:N6	1.30	0.93
20:Z:728:LYS:HE3	29:I:65:ILE:CB	1.98	0.93
30:K:220:THR:HB	34:K:501:ATP:O1A	1.67	0.92
20:Z:748:LEU:HD13	29:I:85:PHE:CE1	2.04	0.92
20:Z:738:TYR:CZ	29:I:69:LEU:HB3	2.04	0.92
29:I:393:GLN:HE22	34:I:501:ATP:C1'	1.82	0.91
20:Z:728:LYS:HE3	29:I:65:ILE:N	1.85	0.91
20:Z:748:LEU:CD1	29:I:82:LEU:C	2.43	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:635:ALA:CA	21:N:790:GLU:CG	2.49	0.91
30:K:173:ASP:O	34:K:501:ATP:C2	2.22	0.91
20:Z:255:LEU:HD21	29:I:61:ARG:NE	1.85	0.91
32:M:184:GLY:H	34:M:501:ATP:HN62	1.10	0.91
20:Z:728:LYS:CE	29:I:65:ILE:N	2.32	0.91
20:Z:748:LEU:HD23	29:I:79:SER:C	1.95	0.90
28:H:388:ILE:HD11	34:H:501:ATP:N6	1.85	0.90
20:Z:728:LYS:CG	29:I:62:MET:HB2	2.02	0.90
28:H:258:LEU:CB	34:H:501:ATP:O2A	2.19	0.90
20:Z:728:LYS:CG	29:I:62:MET:CB	2.50	0.89
29:I:393:GLN:HE22	34:I:501:ATP:H1'	1.09	0.89
32:M:227:GLY:HA2	34:M:501:ATP:O3A	1.73	0.89
20:Z:748:LEU:CG	29:I:84:PRO:HD3	2.00	0.88
20:Z:635:ALA:HB2	21:N:791:ALA:HA	1.53	0.88
20:Z:728:LYS:HE3	29:I:65:ILE:HB	1.55	0.88
20:Z:635:ALA:CA	21:N:791:ALA:H	1.86	0.88
20:Z:748:LEU:CD1	29:I:81:ILE:O	2.22	0.87
7:G:93:ARG:NH1	14:7:109:TYR:CD2	2.43	0.86
20:Z:748:LEU:HD23	29:I:81:ILE:H	1.40	0.86
20:Z:728:LYS:CE	29:I:62:MET:C	2.49	0.85
20:Z:738:TYR:OH	29:I:66:LYS:CA	2.24	0.85
20:Z:748:LEU:HD11	29:I:82:LEU:O	1.76	0.85
20:Z:738:TYR:OH	29:I:66:LYS:HA	1.76	0.85
20:Z:748:LEU:CD2	29:I:81:ILE:H	1.85	0.85
20:Z:738:TYR:OH	29:I:66:LYS:C	2.19	0.85
20:Z:748:LEU:HB3	29:I:81:ILE:HA	1.56	0.85
20:Z:635:ALA:CA	21:N:791:ALA:N	2.40	0.84
20:Z:738:TYR:OH	29:I:69:LEU:HB3	1.77	0.84
28:H:257:THR:H	34:H:501:ATP:PB	2.00	0.84
28:H:256:LYS:C	34:H:501:ATP:O2B	2.13	0.84
7:g:93:ARG:NE	14:n:109:TYR:CE2	2.46	0.84
20:Z:728:LYS:HG2	29:I:59:LEU:O	1.66	0.84
20:Z:748:LEU:CD2	29:I:79:SER:C	2.52	0.83
20:Z:748:LEU:HG	29:I:84:PRO:HD3	1.60	0.83
20:Z:728:LYS:HD2	29:I:63:GLU:C	2.03	0.83
20:Z:748:LEU:CG	20:Z:748:LEU:CD1	2.57	0.83
31:L:229:THR:OG1	34:L:501:ATP:PA	2.37	0.83
32:M:184:GLY:O	34:M:501:ATP:N6	2.12	0.82
32:M:184:GLY:H	34:M:501:ATP:N6	1.78	0.82
20:Z:635:ALA:CB	21:N:792:SER:N	2.43	0.82
7:G:93:ARG:NE	14:7:109:TYR:CE1	2.47	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:728:LYS:CE	29:I:65:ILE:HB	2.09	0.81
20:Z:748:LEU:CD2	29:I:79:SER:O	2.27	0.81
7:g:93:ARG:NE	14:n:109:TYR:CZ	2.48	0.81
20:Z:738:TYR:OH	29:I:65:ILE:O	1.98	0.81
29:I:230:THR:HB	34:I:501:ATP:PA	2.20	0.81
20:Z:635:ALA:CB	21:N:791:ALA:CA	2.58	0.81
20:Z:748:LEU:CD2	29:I:81:ILE:CA	2.59	0.80
34:K:501:ATP:C5'	31:L:339:ARG:NH2	2.09	0.80
28:H:255:GLY:HA2	34:H:501:ATP:O3A	1.81	0.80
31:L:229:THR:OG1	34:L:501:ATP:O3A	1.99	0.80
20:Z:745:LEU:HD11	29:I:77:SER:OG	1.81	0.80
20:Z:748:LEU:HD21	29:I:82:LEU:HD13	1.62	0.80
30:K:221:MET:HE1	34:K:501:ATP:HN61	1.46	0.80
33:J:276:LEU:HD22	33:J:290:ILE:HD12	1.63	0.80
7:g:93:ARG:NH1	14:n:109:TYR:CG	2.50	0.79
20:Z:748:LEU:CG	29:I:82:LEU:N	2.44	0.79
20:Z:635:ALA:CB	21:N:791:ALA:N	2.45	0.79
33:J:327:ILE:HG23	36:J:501:ADP:C2	2.17	0.79
20:Z:635:ALA:HA	21:N:790:GLU:CA	2.14	0.78
20:Z:635:ALA:CB	21:N:791:ALA:C	2.55	0.78
20:Z:635:ALA:HA	21:N:791:ALA:N	1.99	0.78
20:Z:635:ALA:C	21:N:790:GLU:HG3	2.09	0.78
20:Z:738:TYR:CZ	29:I:66:LYS:O	2.37	0.77
32:M:228:LYS:HB2	34:M:501:ATP:O2B	1.83	0.77
20:Z:738:TYR:OH	29:I:69:LEU:CB	2.32	0.77
7:G:93:ARG:NH1	14:7:109:TYR:CG	2.52	0.77
20:Z:728:LYS:HE2	29:I:62:MET:O	1.83	0.77
20:Z:252:CYS:HA	20:Z:255:LEU:HB2	1.67	0.77
20:Z:738:TYR:CZ	29:I:66:LYS:CA	2.67	0.77
20:Z:635:ALA:CA	21:N:790:GLU:HG3	2.13	0.77
7:G:93:ARG:NE	14:7:109:TYR:CZ	2.52	0.76
20:Z:726:GLU:HB2	20:Z:727:GLU:HG3	1.67	0.76
20:Z:727:GLU:HB2	29:I:62:MET:CE	2.16	0.76
20:Z:748:LEU:HD22	29:I:81:ILE:CB	2.14	0.76
20:Z:635:ALA:CA	21:N:792:SER:N	2.41	0.76
29:I:229:LYS:HB2	34:I:501:ATP:O2B	1.86	0.75
20:Z:923:ILE:HD12	20:Z:925:VAL:H	1.51	0.75
7:g:93:ARG:NH1	14:n:109:TYR:CD1	2.54	0.75
28:H:258:LEU:CA	34:H:501:ATP:O2A	2.35	0.75
28:H:256:LYS:NZ	34:H:501:ATP:O3G	2.18	0.75
34:K:501:ATP:H5'1	31:L:339:ARG:HH22	0.60	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:I:230:THR:OG1	35:I:502:MG:MG	1.28	0.75
33:J:327:ILE:HG23	36:J:501:ADP:N3	2.00	0.75
20:Z:748:LEU:CD2	29:I:81:ILE:HB	2.14	0.74
20:Z:728:LYS:HG3	29:I:62:MET:N	1.87	0.74
20:Z:728:LYS:HG3	29:I:62:MET:HG2	1.69	0.74
32:M:228:LYS:H	34:M:501:ATP:PB	2.11	0.74
20:Z:748:LEU:HD21	29:I:79:SER:O	1.87	0.74
20:Z:635:ALA:CA	21:N:790:GLU:HA	2.18	0.74
20:Z:728:LYS:CB	20:Z:728:LYS:C	2.60	0.74
20:Z:745:LEU:O	20:Z:748:LEU:HA	1.87	0.73
20:Z:748:LEU:HD13	29:I:81:ILE:O	1.87	0.73
29:I:268:PHE:O	29:I:319:ARG:NE	2.21	0.73
20:Z:635:ALA:HB1	21:N:790:GLU:HG2	1.70	0.72
30:K:220:THR:HB	34:K:501:ATP:O3A	1.90	0.71
32:M:227:GLY:HA2	34:M:501:ATP:O2A	1.88	0.71
20:Z:251:ALA:HA	29:I:58:LYS:HB3	1.72	0.71
20:Z:748:LEU:CB	29:I:84:PRO:CD	2.69	0.71
20:Z:635:ALA:HA	21:N:790:GLU:C	2.15	0.71
20:Z:748:LEU:CD2	29:I:82:LEU:CD1	2.69	0.71
20:Z:728:LYS:HE3	29:I:65:ILE:CA	2.21	0.71
20:Z:738:TYR:OH	29:I:66:LYS:O	2.09	0.70
20:Z:748:LEU:HG	29:I:80:GLU:O	1.87	0.70
33:J:330:ILE:HD12	36:J:501:ADP:H2	1.56	0.70
20:Z:748:LEU:CB	29:I:80:GLU:O	2.39	0.70
20:Z:748:LEU:CD2	29:I:82:LEU:HD13	2.22	0.70
29:I:365:HIS:NE2	34:I:501:ATP:C2	2.60	0.70
20:Z:247:GLN:HG2	29:I:54:ARG:HE	1.57	0.70
20:Z:635:ALA:CB	21:N:790:GLU:C	2.65	0.70
20:Z:728:LYS:HD2	29:I:63:GLU:N	2.07	0.69
28:H:388:ILE:CD1	34:H:501:ATP:N6	2.55	0.69
32:M:184:GLY:N	34:M:501:ATP:HN62	1.88	0.69
33:J:197:LEU:HD11	36:J:501:ADP:H3'	0.87	0.69
28:H:212:GLY:O	34:H:501:ATP:N7	2.16	0.68
29:I:313:LEU:O	29:I:314:ASP:CB	2.12	0.68
20:Z:728:LYS:CG	29:I:62:MET:CA	2.71	0.68
20:Z:748:LEU:HD22	29:I:82:LEU:HD12	1.74	0.68
20:Z:748:LEU:HD12	29:I:84:PRO:HD2	1.73	0.68
20:Z:728:LYS:HE2	29:I:65:ILE:N	2.07	0.68
20:Z:728:LYS:HE2	29:I:65:ILE:H	1.56	0.68
28:H:257:THR:N	34:H:501:ATP:PB	2.64	0.67
29:I:268:PHE:HD2	29:I:322:VAL:HG11	1.56	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:I:272:GLY:HA2	29:I:320:GLY:HA3	1.75	0.67
20:Z:249:MET:HE3	20:Z:268:ALA:HB2	1.77	0.67
29:I:269:LYS:CG	29:I:319:ARG:HH21	2.08	0.67
20:Z:247:GLN:HE21	29:I:54:ARG:HB3	1.58	0.67
20:Z:247:GLN:HB3	29:I:54:ARG:HH21	1.59	0.67
28:H:308:PHE:CE2	28:H:336:LEU:CD2	2.78	0.66
28:H:388:ILE:HD11	34:H:501:ATP:C6	2.26	0.66
20:Z:728:LYS:CB	29:I:62:MET:HB2	2.25	0.66
20:Z:748:LEU:CD1	29:I:84:PRO:CD	2.71	0.66
20:Z:748:LEU:CD1	29:I:85:PHE:CD1	2.79	0.66
28:H:308:PHE:CZ	28:H:336:LEU:HD22	2.30	0.66
20:Z:635:ALA:CA	21:N:790:GLU:CA	2.73	0.65
28:H:308:PHE:HB3	28:H:311:ILE:HG12	1.79	0.65
20:Z:728:LYS:CB	29:I:62:MET:HG2	2.26	0.65
20:Z:748:LEU:HD23	29:I:81:ILE:N	2.01	0.65
34:K:501:ATP:O2G	31:L:342:ARG:NH2	2.27	0.65
29:I:268:PHE:C	29:I:319:ARG:HE	2.05	0.65
28:H:388:ILE:HD11	34:H:501:ATP:HN62	1.62	0.64
20:Z:249:MET:O	20:Z:253:VAL:HG23	1.96	0.64
20:Z:635:ALA:CB	20:Z:635:ALA:HA	2.28	0.64
28:H:308:PHE:CZ	28:H:336:LEU:CD2	2.81	0.64
30:K:96:ILE:HD11	31:L:128:ILE:HD11	1.80	0.64
20:Z:735:GLU:HG3	20:Z:738:TYR:CD2	2.32	0.64
33:J:197:LEU:HD21	36:J:501:ADP:O1A	1.98	0.63
20:Z:748:LEU:CD2	29:I:81:ILE:CB	2.75	0.63
29:I:311:ASN:O	29:I:315:GLY:HA3	1.99	0.63
30:K:220:THR:C	34:K:501:ATP:O1A	2.40	0.63
20:Z:738:TYR:CE1	29:I:66:LYS:O	2.51	0.63
29:I:334:LEU:HD13	29:I:338:LEU:HD22	1.81	0.63
15:W:125:LEU:HD23	15:W:128:LEU:HD12	1.82	0.62
20:Z:255:LEU:HD22	21:N:816:LYS:HG2	1.81	0.62
20:Z:748:LEU:HD22	29:I:82:LEU:CD1	2.29	0.62
32:M:227:GLY:CA	34:M:501:ATP:O3A	2.44	0.62
20:Z:727:GLU:HB2	29:I:62:MET:HE2	1.82	0.62
20:Z:728:LYS:CG	29:I:62:MET:HG2	2.29	0.62
20:Z:748:LEU:HG	29:I:84:PRO:CD	2.21	0.62
20:Z:728:LYS:HB3	29:I:59:LEU:CA	2.26	0.61
31:L:393:ASN:HD22	32:M:213:ARG:HH12	1.45	0.61
20:Z:255:LEU:HD23	21:N:813:ARG:NH1	2.15	0.61
20:Z:728:LYS:CA	29:I:62:MET:CG	2.78	0.61
29:I:279:VAL:HG23	29:I:322:VAL:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:K:501:ATP:PG	31:L:342:ARG:HH22	2.22	0.61
20:Z:728:LYS:HE3	29:I:65:ILE:CG1	2.31	0.61
29:I:268:PHE:CE2	29:I:322:VAL:HG11	2.36	0.61
29:I:268:PHE:HB3	29:I:319:ARG:HD2	1.82	0.61
20:Z:728:LYS:NZ	29:I:62:MET:HA	2.16	0.61
20:Z:748:LEU:HD21	29:I:82:LEU:CD1	2.29	0.61
29:I:268:PHE:HB3	29:I:319:ARG:CD	2.31	0.61
31:L:229:THR:OG1	34:L:501:ATP:PB	2.59	0.61
29:I:228:GLY:N	34:I:501:ATP:O1B	2.33	0.61
29:I:271:ALA:CB	29:I:322:VAL:HG22	2.31	0.61
29:I:322:VAL:C	29:I:323:LYS:CA	2.72	0.61
28:H:308:PHE:CE2	28:H:336:LEU:HD22	2.36	0.60
1:A:150:LEU:HD12	9:2:101:ARG:HH21	1.66	0.60
20:Z:748:LEU:CD1	29:I:85:PHE:CE1	2.81	0.60
29:I:269:LYS:HG2	29:I:319:ARG:HH21	1.67	0.60
20:Z:251:ALA:O	20:Z:255:LEU:HD12	2.00	0.60
28:H:308:PHE:C	28:H:309:ASP:CA	2.73	0.60
29:I:231:LEU:N	34:I:501:ATP:O1A	2.33	0.60
7:g:72:ARG:HE	14:n:105:THR:HG23	1.67	0.60
20:Z:728:LYS:HD3	29:I:61:ARG:C	2.21	0.60
20:Z:728:LYS:HD3	29:I:61:ARG:O	1.99	0.60
20:Z:635:ALA:HB2	21:N:791:ALA:N	2.11	0.60
20:Z:728:LYS:NZ	29:I:65:ILE:HB	2.16	0.60
28:H:258:LEU:HB2	34:H:501:ATP:PA	2.42	0.60
3:c:58:GLU:HG2	3:c:60:ASP:H	1.65	0.59
20:Z:748:LEU:CG	29:I:82:LEU:C	2.75	0.59
10:j:149:MET:HE3	10:j:153:LEU:HD11	1.82	0.59
20:Z:635:ALA:CA	21:N:790:GLU:HG2	2.21	0.59
20:Z:728:LYS:CA	29:I:62:MET:HG3	2.32	0.59
30:K:220:THR:CB	34:K:501:ATP:O1A	2.46	0.59
20:Z:728:LYS:CG	29:I:58:LYS:O	2.50	0.59
33:J:152:GLY:H	33:J:154:THR:HG23	1.66	0.59
20:Z:253:VAL:HG21	20:Z:287:ARG:HH12	1.68	0.59
20:Z:255:LEU:HD22	21:N:816:LYS:CG	2.32	0.59
20:Z:748:LEU:CG	29:I:80:GLU:C	2.74	0.59
33:J:196:THR:N	36:J:501:ADP:O3B	2.34	0.58
20:Z:745:LEU:CD1	29:I:77:SER:OG	2.51	0.58
20:Z:748:LEU:HD13	29:I:85:PHE:CD1	2.38	0.58
28:H:255:GLY:HA2	34:H:501:ATP:PA	2.44	0.58
20:Z:748:LEU:CA	29:I:84:PRO:CG	2.81	0.58
8:l:43:LEU:HD13	8:l:185:VAL:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:728:LYS:HE2	29:I:66:LYS:H	1.69	0.58
28:H:256:LYS:HG3	34:H:501:ATP:O1B	2.04	0.58
20:Z:635:ALA:HA	21:N:790:GLU:CB	2.33	0.58
20:Z:748:LEU:HG	29:I:83:LYS:CA	2.33	0.58
20:Z:748:LEU:HD12	29:I:84:PRO:CD	2.33	0.58
21:N:107:GLU:HG2	33:J:26:LYS:HE3	1.86	0.58
29:I:393:GLN:OE1	34:I:501:ATP:H4'	2.01	0.58
20:Z:728:LYS:CB	29:I:62:MET:CG	2.81	0.57
21:N:25:LEU:HD21	21:N:49:LEU:HD13	1.85	0.57
31:L:364:HIS:CE1	34:L:501:ATP:H2	2.21	0.57
29:I:268:PHE:C	29:I:319:ARG:NE	2.62	0.57
29:I:312:GLN:HA	29:I:319:ARG:HH12	1.69	0.57
33:J:327:ILE:HG22	33:J:331:HIS:CE1	2.40	0.57
12:5:128:GLN:HE22	13:6:99:ARG:HH12	1.52	0.57
20:Z:748:LEU:CB	29:I:84:PRO:HD2	2.34	0.57
20:Z:748:LEU:HD21	29:I:82:LEU:H	1.61	0.57
20:Z:621:LEU:HD22	21:N:803:VAL:HG22	1.86	0.57
28:H:308:PHE:CE2	28:H:336:LEU:HD21	2.40	0.57
29:I:312:GLN:OE1	29:I:319:ARG:CZ	2.53	0.57
20:Z:224:LEU:HD21	20:Z:248:TYR:CE2	2.40	0.56
7:G:70:VAL:HG22	7:G:93:ARG:HG3	1.87	0.56
20:Z:738:TYR:CE2	29:I:69:LEU:HD22	2.40	0.56
20:Z:748:LEU:CD2	29:I:82:LEU:HD12	2.34	0.56
20:Z:728:LYS:HD2	29:I:63:GLU:CA	2.35	0.56
29:I:271:ALA:HB1	29:I:322:VAL:HG22	1.87	0.56
29:I:313:LEU:O	29:I:314:ASP:OD1	2.23	0.56
20:Z:728:LYS:CG	29:I:62:MET:CG	2.84	0.56
20:Z:728:LYS:CD	29:I:62:MET:N	2.68	0.56
29:I:313:LEU:O	29:I:314:ASP:HB2	1.99	0.56
31:L:429:GLU:HG2	32:M:338:LEU:HD13	1.87	0.55
20:Z:739:ALA:HB2	20:Z:764:LEU:HD13	1.87	0.55
28:H:308:PHE:CA	28:H:309:ASP:N	2.63	0.55
20:Z:748:LEU:CD2	29:I:78:ASN:O	2.54	0.55
20:Z:738:TYR:CE2	29:I:69:LEU:CD2	2.90	0.55
31:L:229:THR:HG1	34:L:501:ATP:PA	2.29	0.55
28:H:211:VAL:O	34:H:501:ATP:N1	2.39	0.55
29:I:71:LEU:HD13	29:I:71:LEU:C	2.31	0.55
1:A:53:VAL:HG21	1:A:82:VAL:HG21	1.87	0.55
20:Z:635:ALA:N	21:N:792:SER:H	2.03	0.55
27:O:113:LYS:HD3	27:O:122:HIS:CE1	2.41	0.55
30:K:220:THR:CB	34:K:501:ATP:O3A	2.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:7:74:ARG:HH22	14:7:90:ILE:CD1	2.20	0.55
20:Z:635:ALA:H	21:N:792:SER:N	2.05	0.54
33:J:37:LYS:HE3	33:J:37:LYS:HA	1.89	0.54
20:Z:728:LYS:NZ	29:I:62:MET:O	2.41	0.54
20:Z:748:LEU:HB3	29:I:81:ILE:CA	2.32	0.54
20:Z:255:LEU:HB3	21:N:816:LYS:HG2	1.88	0.54
20:Z:728:LYS:CD	29:I:62:MET:CA	2.86	0.54
3:c:9:ARG:HE	3:c:12:ILE:HG21	1.72	0.54
14:7:148:ILE:HD11	14:7:177:THR:HG23	1.90	0.54
20:Z:257:PRO:HG3	20:Z:611:THR:HB	1.89	0.54
28:H:367:ARG:HH21	32:M:225:GLY:HA2	1.73	0.53
23:P:225:VAL:HG13	23:P:237:VAL:HG13	1.90	0.53
31:L:309:LEU:HB3	31:L:342:ARG:HH12	1.74	0.53
16:V:145:GLN:HG2	30:K:142:HIS:CD2	2.44	0.53
20:Z:728:LYS:HG3	29:I:62:MET:CG	2.36	0.53
20:Z:748:LEU:CD1	29:I:82:LEU:CA	2.86	0.53
24:Q:298:ALA:HA	24:Q:321:TYR:CD1	2.44	0.53
33:J:195:LYS:N	36:J:501:ADP:O1B	2.41	0.53
10:j:183:TRP:HE1	12:5:241:HIS:CE1	2.27	0.53
20:Z:728:LYS:CA	29:I:62:MET:HG2	2.39	0.53
7:g:16:SER:HB3	7:g:17:PRO:HD2	1.90	0.52
20:Z:748:LEU:CG	29:I:81:ILE:CA	2.83	0.52
20:Z:748:LEU:HD23	29:I:80:GLU:N	2.23	0.52
24:Q:191:LEU:HA	24:Q:194:SER:HB2	1.90	0.52
28:H:308:PHE:HE2	28:H:336:LEU:HD21	1.73	0.52
33:J:140:GLU:HG3	33:J:212:ARG:HH21	1.75	0.52
20:Z:738:TYR:CE2	29:I:66:LYS:HG2	2.44	0.52
20:Z:253:VAL:CG2	20:Z:287:ARG:HH12	2.23	0.52
20:Z:748:LEU:CB	29:I:81:ILE:HA	2.34	0.52
27:O:223:LEU:HD11	27:O:280:LEU:HD12	1.91	0.52
29:I:279:VAL:CG2	29:I:322:VAL:HG13	2.39	0.52
20:Z:738:TYR:CZ	29:I:66:LYS:C	2.88	0.52
29:I:269:LYS:HG3	29:I:319:ARG:HH21	1.73	0.52
20:Z:748:LEU:CD2	29:I:81:ILE:C	2.82	0.52
20:Z:748:LEU:C	29:I:84:PRO:HG3	2.34	0.52
21:N:545:SER:HA	21:N:548:ARG:HH21	1.74	0.52
33:J:197:LEU:HD12	36:J:501:ADP:C8	2.45	0.52
20:Z:256:LEU:HD13	20:Z:261:ASP:HA	1.92	0.52
20:Z:255:LEU:CD2	21:N:816:LYS:HG2	2.40	0.52
28:H:256:LYS:CG	34:H:501:ATP:O1B	2.58	0.52
3:C:201:THR:HG23	3:C:203:SER:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:635:ALA:H	21:N:792:SER:CB	2.22	0.51
21:N:832:HIS:CE1	21:N:833:GLU:HG2	2.44	0.51
21:N:498:ILE:HD11	21:N:525:ASN:HD21	1.75	0.51
28:H:388:ILE:CD1	34:H:501:ATP:N1	2.73	0.51
29:I:313:LEU:O	29:I:314:ASP:CG	2.53	0.51
19:Y:1:MET:HA	22:S:336:SER:HB3	1.91	0.51
20:Z:251:ALA:HA	29:I:58:LYS:CB	2.38	0.51
20:Z:728:LYS:HZ3	29:I:62:MET:HA	1.76	0.51
7:G:92:GLY:HA3	7:G:116:LEU:HD21	1.91	0.51
24:Q:282:LEU:HD23	24:Q:287:THR:HG21	1.93	0.51
24:Q:330:LEU:HD11	24:Q:334:HIS:CE1	2.46	0.51
20:Z:951:GLN:HE21	20:Z:951:GLN:HA	1.76	0.51
8:h:47:HIS:CD2	8:h:48:ASP:H	2.29	0.51
20:Z:728:LYS:HZ1	29:I:65:ILE:HB	1.76	0.51
28:H:255:GLY:CA	34:H:501:ATP:O3A	2.53	0.51
34:K:501:ATP:H5'2	31:L:339:ARG:NH2	2.18	0.51
20:Z:745:LEU:HB3	20:Z:746:ILE:HG13	1.92	0.51
28:H:212:GLY:CA	34:H:501:ATP:C6	2.49	0.51
15:W:179:ARG:HE	15:W:184:ASN:HD21	1.58	0.50
20:Z:635:ALA:N	21:N:792:SER:N	2.59	0.50
14:n:56:ALA:HA	14:n:75:LEU:HD11	1.94	0.50
20:Z:917:ASN:HA	29:I:58:LYS:HZ1	1.76	0.50
32:M:227:GLY:HA2	34:M:501:ATP:O5'	2.12	0.50
33:J:297:LEU:H	33:J:297:LEU:HD23	1.75	0.50
20:Z:247:GLN:CB	29:I:54:ARG:HH21	2.23	0.50
20:Z:253:VAL:C	20:Z:255:LEU:H	2.19	0.50
6:F:9:ASP:OD1	6:F:9:ASP:C	2.53	0.50
28:H:308:PHE:HD2	28:H:311:ILE:HG21	1.77	0.50
33:J:330:ILE:HD12	36:J:501:ADP:C2	2.43	0.50
15:W:179:ARG:HE	15:W:184:ASN:ND2	2.10	0.50
20:Z:728:LYS:CB	29:I:58:LYS:O	2.60	0.50
20:Z:748:LEU:HD23	29:I:78:ASN:O	2.10	0.50
21:N:398:ARG:H	21:N:398:ARG:HE	1.58	0.50
20:Z:255:LEU:CB	21:N:816:LYS:HG2	2.42	0.50
20:Z:728:LYS:CE	29:I:65:ILE:CA	2.86	0.50
29:I:393:GLN:HE22	34:I:501:ATP:C2'	2.25	0.50
16:V:25:GLU:CD	16:V:25:GLU:H	2.19	0.49
20:Z:738:TYR:CD2	29:I:69:LEU:HD23	2.47	0.49
20:Z:635:ALA:HB2	21:N:790:GLU:C	2.36	0.49
20:Z:736:LEU:HD13	20:Z:765:MET:HG2	1.93	0.49
26:U:14:VAL:HG21	26:U:48:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:17:LYS:H	3:c:28:SER:HB3	1.77	0.49
20:Z:171:LYS:H	20:Z:171:LYS:HD3	1.77	0.49
32:M:186:LEU:HD12	34:M:501:ATP:HN61	1.78	0.49
16:V:238:LEU:HD11	16:V:242:LYS:HE3	1.94	0.49
21:N:152:LEU:HD12	21:N:152:LEU:H	1.78	0.49
29:I:231:LEU:HD22	34:I:501:ATP:O2'	2.13	0.49
1:a:242:GLU:HA	1:a:245:LEU:HD12	1.94	0.49
20:Z:739:ALA:HB2	20:Z:764:LEU:CD1	2.43	0.49
23:P:431:HIS:CD2	26:U:156:HIS:CE1	3.01	0.49
29:I:427:LYS:HB2	29:I:428:VAL:HG23	1.95	0.49
30:K:161:MET:HE2	30:K:236:ARG:HG2	1.95	0.49
32:M:87:ASP:HA	32:M:116:ALA:H	1.78	0.49
5:E:214:GLU:CD	5:E:214:GLU:H	2.21	0.48
20:Z:728:LYS:CG	29:I:59:LEU:C	2.58	0.48
20:Z:738:TYR:HH	29:I:69:LEU:HB2	1.77	0.48
20:Z:748:LEU:O	29:I:84:PRO:HD3	2.12	0.48
8:h:75:TYR:CD1	8:h:82:PRO:HB3	2.48	0.48
13:6:37:ASN:HD22	13:6:44:ASN:HD22	1.58	0.48
20:Z:728:LYS:N	29:I:62:MET:HG3	2.29	0.48
20:Z:741:LEU:HD12	29:I:70:LEU:HD12	1.95	0.48
20:Z:918:ASP:H	29:I:58:LYS:HZ1	1.61	0.48
24:Q:67:THR:HB	24:Q:68:MET:HA	1.95	0.48
28:H:367:ARG:HH22	34:M:501:ATP:H5'1	1.78	0.48
32:M:364:HIS:HE1	34:M:501:ATP:N3	2.12	0.48
9:2:153:TYR:CE1	9:2:167:LEU:HG	2.49	0.48
20:Z:254:PRO:HG2	20:Z:255:LEU:HG	1.94	0.48
20:Z:728:LYS:N	29:I:62:MET:CG	2.76	0.48
16:V:218:LYS:HA	16:V:221:TRP:HE1	1.78	0.48
20:Z:253:VAL:N	20:Z:254:PRO:HD2	2.28	0.48
23:P:69:ARG:HE	23:P:69:ARG:HA	1.79	0.48
8:h:68:VAL:HG11	8:h:91:PHE:CE1	2.49	0.48
12:l:148:ARG:HH12	12:l:180:THR:HG22	1.79	0.48
11:4:101:ASN:HB3	11:4:133:HIS:CD2	2.49	0.48
20:Z:248:TYR:HB2	20:Z:249:MET:HE2	1.95	0.48
10:j:67:PHE:CZ	10:j:91:VAL:HG22	2.49	0.47
31:L:183:ILE:HD13	34:L:501:ATP:HN61	1.79	0.47
16:V:28:TYR:CE2	16:V:202:ASP:HB2	2.48	0.47
22:S:480:ARG:HB2	33:J:43:ARG:HG3	1.96	0.47
3:c:162:ALA:HB3	4:d:54:LEU:HD13	1.95	0.47
29:I:272:GLY:CA	29:I:320:GLY:HA3	2.42	0.47
2:b:85:LEU:HD23	2:b:134:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:157:HIS:CE1	5:E:159:GLU:HG2	2.48	0.47
20:Z:30:LYS:HG3	20:Z:37:GLN:HB3	1.97	0.47
20:Z:738:TYR:HH	29:I:69:LEU:CB	2.28	0.47
22:S:323:LEU:HD23	22:S:383:LEU:HD23	1.97	0.47
3:C:9:ARG:HH21	4:D:8:LEU:HA	1.79	0.47
4:D:192:VAL:O	4:D:196:VAL:HG23	2.15	0.47
4:D:199:LEU:HD13	4:D:210:ILE:HG23	1.97	0.47
10:3:3:ASP:HB2	10:3:4:PRO:HD2	1.95	0.47
21:N:25:LEU:HD21	21:N:49:LEU:CD1	2.45	0.47
29:I:312:GLN:HA	29:I:319:ARG:NH1	2.30	0.47
4:D:101:GLU:HG2	4:D:102:ASP:H	1.80	0.47
17:T:236:ASN:HD22	17:T:236:ASN:H	1.63	0.47
20:Z:739:ALA:CB	20:Z:764:LEU:HD13	2.45	0.47
27:O:134:ALA:HA	27:O:149:LEU:HD23	1.97	0.47
28:H:366:LEU:HG	28:H:366:LEU:O	2.15	0.47
22:S:99:ASN:O	22:S:100:HIS:CG	2.68	0.47
1:a:104:PHE:CD2	1:a:112:MET:HA	2.49	0.46
32:M:351:LEU:HD12	32:M:351:LEU:H	1.80	0.46
20:Z:738:TYR:CE1	29:I:69:LEU:HB3	2.46	0.46
27:O:207:LEU:HD13	27:O:210:ARG:HH21	1.80	0.46
32:M:364:HIS:CD2	32:M:392:LYS:HA	2.50	0.46
20:Z:253:VAL:HG12	20:Z:727:GLU:HG2	1.96	0.46
29:I:194:ILE:HD12	29:I:221:LEU:HD11	1.97	0.46
29:I:229:LYS:N	34:I:501:ATP:PB	2.89	0.46
8:1:68:VAL:HG21	8:1:91:PHE:CD2	2.50	0.46
14:7:114:ALA:O	14:7:119:ALA:HB2	2.14	0.46
1:A:80:GLY:HA3	1:A:233:PHE:CZ	2.50	0.46
21:N:329:HIS:CE1	21:N:355:TRP:CH2	3.02	0.46
1:A:147:ASP:CG	9:2:101:ARG:HH22	2.24	0.46
6:F:171:TYR:CD2	6:F:199:GLN:HG3	2.51	0.46
20:Z:747:ALA:O	29:I:84:PRO:HG2	2.15	0.46
20:Z:748:LEU:CA	29:I:84:PRO:HG2	2.45	0.46
2:b:193:LEU:CD2	2:b:209:ILE:HG21	2.46	0.46
6:f:13:PHE:HA	6:f:14:SER:HB3	1.98	0.46
20:Z:918:ASP:OD1	29:I:59:LEU:HD23	2.16	0.46
24:Q:68:MET:HB3	24:Q:74:LEU:HD12	1.98	0.46
28:H:213:GLY:N	34:H:501:ATP:C6	2.44	0.46
20:Z:728:LYS:CB	29:I:62:MET:CB	2.94	0.46
12:5:233:LYS:HG2	12:5:252:LEU:HD11	1.98	0.46
20:Z:728:LYS:CB	20:Z:728:LYS:HG3	2.24	0.46
23:P:415:TRP:HE1	26:U:237:PRO:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:H:388:ILE:CG2	28:H:392:HIS:CE1	2.99	0.46
6:f:45:VAL:HG22	6:f:215:ILE:HG22	1.98	0.45
9:i:36:LYS:HG3	9:i:139:LEU:HD22	1.98	0.45
29:I:268:PHE:HB3	29:I:319:ARG:NE	2.31	0.45
9:i:116:LEU:HD12	9:i:142:ILE:HD11	1.98	0.45
20:Z:253:VAL:CG1	20:Z:287:ARG:HH22	2.28	0.45
26:U:32:ARG:HD2	26:U:94:HIS:CE1	2.51	0.45
32:M:230:LEU:HB2	34:M:501:ATP:O2A	2.16	0.45
15:W:101:ARG:HH22	15:W:108:GLN:HE21	1.64	0.45
20:Z:741:LEU:HD13	29:I:74:GLU:HB2	1.97	0.45
21:N:398:ARG:H	21:N:398:ARG:NE	2.14	0.45
21:N:669:GLU:HB3	21:N:676:ALA:HB2	1.98	0.45
29:I:393:GLN:NE2	34:I:501:ATP:N3	2.65	0.45
7:g:137:ILE:HD11	7:g:165:THR:HG22	1.99	0.45
5:E:211:LYS:HG2	5:E:212:LEU:H	1.81	0.45
17:T:102:LYS:HA	17:T:105:LEU:HD12	1.97	0.45
21:N:782:PHE:H	21:N:873:ARG:HH21	1.65	0.45
23:P:285:GLN:HE21	23:P:304:THR:HG21	1.81	0.45
28:H:388:ILE:HG12	34:H:501:ATP:N1	2.32	0.45
10:j:56:LEU:HD12	10:j:57:ALA:H	1.82	0.45
9:2:233:LYS:HE3	9:2:233:LYS:HA	1.99	0.45
20:Z:635:ALA:N	21:N:792:SER:OG	2.49	0.45
21:N:567:ALA:HA	21:N:570:ARG:HH21	1.81	0.45
28:H:134:THR:HA	31:L:87:LEU:HD13	1.99	0.45
29:I:165:ASP:H	29:I:168:VAL:HG22	1.82	0.45
3:C:51:LYS:HG2	3:C:65:LYS:HZ1	1.81	0.45
20:Z:249:MET:C	20:Z:253:VAL:HG23	2.42	0.45
30:K:220:THR:CA	34:K:501:ATP:O1A	2.65	0.45
20:Z:728:LYS:C	20:Z:728:LYS:HB2	2.41	0.45
8:h:47:HIS:CE1	8:h:82:PRO:HD2	2.51	0.45
15:W:175:THR:HG22	15:W:177:GLY:H	1.82	0.45
28:H:337:ILE:HG23	28:H:370:ARG:HH22	1.82	0.45
11:k:60:ILE:HD12	11:k:84:VAL:HG22	1.98	0.45
4:d:149:GLN:C	4:d:149:GLN:HE21	2.25	0.44
29:I:271:ALA:HB3	29:I:322:VAL:CG2	2.47	0.44
9:i:61:ALA:HB2	9:i:217:ARG:HH12	1.83	0.44
33:J:276:LEU:HD22	33:J:290:ILE:CD1	2.42	0.44
7:g:40:ILE:HG22	7:g:42:CYS:SG	2.58	0.44
20:Z:728:LYS:CB	20:Z:728:LYS:HG2	2.24	0.44
23:P:421:GLU:O	23:P:425:HIS:CD2	2.70	0.44
20:Z:24:THR:HB	20:Z:25:PRO:CD	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:244:ARG:O	29:I:54:ARG:NH2	2.50	0.44
6:F:190:ILE:O	6:F:194:VAL:HG23	2.17	0.44
20:Z:918:ASP:N	29:I:58:LYS:HZ1	2.16	0.44
32:M:227:GLY:CA	34:M:501:ATP:O2A	2.62	0.44
20:Z:748:LEU:CB	29:I:81:ILE:CA	2.95	0.44
28:H:100:ALA:HB2	28:H:149:LEU:HD23	1.99	0.44
20:Z:728:LYS:CB	29:I:59:LEU:O	2.66	0.44
20:Z:728:LYS:HG2	29:I:58:LYS:O	2.17	0.44
23:P:165:VAL:HG12	30:K:399:ARG:HH22	1.83	0.44
28:H:367:ARG:HH22	34:M:501:ATP:C5'	2.30	0.44
31:L:119:VAL:HG21	31:L:148:LEU:HD11	1.99	0.44
32:M:228:LYS:N	34:M:501:ATP:PB	2.85	0.44
20:Z:743:ILE:HG21	20:Z:780:MET:CE	2.48	0.44
27:O:215:TYR:CD1	27:O:251:LEU:HD22	2.53	0.44
12:l:163:TYR:O	12:l:166:LYS:HB3	2.18	0.43
20:Z:631:GLY:HA3	21:N:795:GLU:HG2	2.00	0.43
20:Z:743:ILE:HD11	20:Z:761:PHE:HB2	2.00	0.43
21:N:665:ILE:HG21	21:N:715:ILE:H	1.82	0.43
20:Z:728:LYS:NZ	29:I:61:ARG:O	2.51	0.43
21:N:837:LYS:H	21:N:837:LYS:HG2	1.68	0.43
25:R:60:ALA:HB3	25:R:102:LEU:HD13	1.99	0.43
26:U:291:LEU:O	26:U:295:LYS:HG3	2.18	0.43
29:I:229:LYS:H	34:I:501:ATP:PB	2.41	0.43
29:I:268:PHE:CD2	29:I:322:VAL:CG1	2.88	0.43
1:A:181:ASN:HD21	1:A:212:ASP:HB2	1.83	0.43
29:I:268:PHE:CE2	29:I:322:VAL:CG1	3.00	0.43
24:Q:67:THR:H	24:Q:68:MET:HB2	1.82	0.43
24:Q:258:ALA:HB3	24:Q:291:TYR:CZ	2.52	0.43
24:Q:282:LEU:HD23	24:Q:287:THR:CG2	2.48	0.43
26:U:244:ASP:HA	26:U:247:ILE:HD12	1.99	0.43
28:H:149:LEU:HD13	28:H:151:GLN:HE21	1.84	0.43
33:J:194:GLY:N	36:J:501:ADP:O1B	2.51	0.43
17:T:85:LEU:HD21	17:T:105:LEU:HD13	1.99	0.43
23:P:193:TYR:CD2	23:P:230:HIS:CD2	3.07	0.43
28:H:275:ILE:HB	28:H:278:GLU:HB2	2.00	0.43
8:h:47:HIS:CG	8:h:48:ASP:H	2.35	0.43
20:Z:745:LEU:HD11	29:I:77:SER:HG	1.78	0.43
28:H:224:VAL:HA	28:H:243:PRO:HG2	2.00	0.43
30:K:95:VAL:HG23	31:L:127:TYR:CE2	2.54	0.43
31:L:244:ILE:HD13	31:L:244:ILE:N	2.34	0.43
33:J:303:ALA:O	33:J:306:ARG:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:15:PRO:HA	7:G:26:TYR:CE1	2.54	0.43
20:Z:748:LEU:HD12	29:I:84:PRO:N	2.34	0.43
29:I:322:VAL:C	29:I:323:LYS:C	2.86	0.43
30:K:177:LEU:HD12	34:K:501:ATP:HN61	1.84	0.43
31:L:178:ILE:HD12	31:L:178:ILE:HA	1.92	0.43
4:d:37:LYS:HE2	4:d:160:SER:HA	2.00	0.43
7:g:16:SER:HB3	7:g:17:PRO:CD	2.49	0.43
12:l:130:TRP:HA	12:l:130:TRP:CE3	2.54	0.43
20:Z:247:GLN:CG	29:I:54:ARG:HE	2.29	0.43
20:Z:745:LEU:HD11	29:I:80:GLU:OE2	2.18	0.43
20:Z:917:ASN:CA	29:I:58:LYS:HZ1	2.32	0.43
20:Z:741:LEU:O	20:Z:745:LEU:HD13	2.19	0.42
21:N:361:ASN:HA	21:N:399:PHE:CZ	2.54	0.42
33:J:85:LEU:HD21	33:J:93:LYS:HD3	2.00	0.42
23:P:346:ILE:HD13	23:P:371:LEU:HD11	2.01	0.42
29:I:186:GLY:H	29:I:188:GLU:HG3	1.83	0.42
33:J:330:ILE:CD1	36:J:501:ADP:H2	2.30	0.42
21:N:16:ASN:HD22	21:N:16:ASN:HA	1.70	0.42
32:M:143:ASN:C	32:M:143:ASN:HD22	2.26	0.42
15:W:101:ARG:HH22	15:W:108:GLN:NE2	2.16	0.42
20:Z:745:LEU:HD11	29:I:77:SER:CB	2.49	0.42
20:Z:738:TYR:CE2	29:I:69:LEU:HD23	2.54	0.42
17:T:108:LEU:HD21	17:T:173:GLU:HG3	2.01	0.42
20:Z:248:TYR:CB	20:Z:249:MET:HE2	2.50	0.42
20:Z:727:GLU:HB2	29:I:62:MET:HE1	1.97	0.42
31:L:183:ILE:HD13	34:L:501:ATP:N6	2.34	0.42
1:a:27:GLN:HE22	7:g:15:PHE:N	2.17	0.42
25:R:341:LEU:HD23	25:R:353:MET:HE3	2.02	0.42
27:O:113:LYS:HD3	27:O:122:HIS:HE1	1.83	0.42
28:H:308:PHE:N	28:H:352:MET:O	2.53	0.42
10:3:49:VAL:HG11	10:3:87:PHE:CD2	2.54	0.42
15:W:146:GLU:HG3	15:W:150:ASN:HD22	1.85	0.42
21:N:743:PHE:HB2	21:N:744:PRO:HD3	2.01	0.42
7:G:126:TYR:HB2	7:G:129:VAL:HG22	2.02	0.42
23:P:164:GLN:HB2	23:P:183:GLN:HE22	1.85	0.42
25:R:47:ALA:HB1	25:R:91:TRP:HB2	2.02	0.42
30:K:221:MET:SD	34:K:501:ATP:C2'	3.08	0.42
20:Z:748:LEU:CB	29:I:84:PRO:CG	2.97	0.41
20:Z:916:LEU:HA	29:I:55:CYS:SG	2.59	0.41
28:H:388:ILE:HG23	28:H:392:HIS:CE1	2.54	0.41
30:K:140:HIS:CE1	30:K:142:HIS:H	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:241:GLN:HA	2:b:244:ASN:HD22	1.85	0.41
1:A:87:ILE:HG22	1:A:88:PRO:HD3	2.02	0.41
19:Y:26:LYS:HZ1	22:S:270:ALA:HB3	1.86	0.41
30:K:177:LEU:CD1	34:K:501:ATP:HN61	2.33	0.41
33:J:133:LEU:HD13	33:J:236:MET:CB	2.51	0.41
13:m:25:GLY:HA2	13:m:183:LEU:HD22	2.03	0.41
21:N:556:ALA:HB1	21:N:593:PHE:HB2	2.03	0.41
22:S:413:LEU:HD13	22:S:419:VAL:HB	2.02	0.41
29:I:231:LEU:HB2	34:I:501:ATP:O1A	2.21	0.41
33:J:150:VAL:HA	36:J:501:ADP:C6	2.50	0.41
4:D:240:LYS:NZ	4:D:240:LYS:HB3	2.35	0.41
12:5:236:ILE:HG21	12:5:250:VAL:HG12	2.02	0.41
20:Z:728:LYS:HB2	29:I:62:MET:HB2	2.01	0.41
28:H:211:VAL:O	34:H:501:ATP:H2	1.84	0.41
5:e:31:ILE:O	5:e:31:ILE:HG22	2.20	0.41
6:f:78:ALA:HB3	6:f:79:PRO:HD3	2.03	0.41
30:K:221:MET:CG	34:K:501:ATP:H2'	2.51	0.41
3:c:184:MET:HB3	3:c:188:ASP:HB2	2.02	0.41
5:e:68:VAL:HG21	5:e:89:ILE:HG12	2.02	0.41
9:i:175:LEU:HD22	9:i:179:GLU:CD	2.46	0.41
16:V:47:MET:HE3	16:V:73:GLN:HE21	1.86	0.41
20:Z:728:LYS:HE3	29:I:65:ILE:HG13	2.02	0.41
21:N:186:ILE:HG21	21:N:214:LEU:HD11	2.03	0.41
32:M:184:GLY:C	34:M:501:ATP:HN62	2.24	0.41
8:h:122:ILE:N	8:h:122:ILE:HD12	2.36	0.41
1:A:25:LEU:HB3	1:A:28:VAL:HG23	2.03	0.41
1:A:108:TYR:HE1	9:2:111:MET:HE2	1.84	0.41
18:X:29:VAL:HG23	18:X:55:LYS:O	2.21	0.41
23:P:327:LEU:HD13	23:P:327:LEU:HA	1.96	0.41
30:K:161:MET:CB	30:K:236:ARG:HB3	2.51	0.41
2:b:214:ILE:HD12	2:b:214:ILE:N	2.35	0.41
5:e:36:THR:HG21	5:e:207:VAL:HG21	2.03	0.41
9:i:189:GLN:O	9:i:193:TRP:CD1	2.73	0.41
12:l:164:GLN:C	12:l:166:LYS:H	2.29	0.41
13:6:31:LEU:HD12	13:6:31:LEU:HA	1.96	0.41
20:Z:635:ALA:CA	20:Z:635:ALA:CB	2.98	0.41
20:Z:738:TYR:CD2	29:I:69:LEU:CD2	3.03	0.41
20:Z:745:LEU:HA	20:Z:745:LEU:HD12	1.72	0.41
25:R:120:LEU:HD22	25:R:129:GLU:HB2	2.03	0.41
28:H:388:ILE:HD13	34:H:501:ATP:N1	2.32	0.41
29:I:125:MET:HB3	29:I:126:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:128:GLN:HE22	13:m:139:TYR:H	1.69	0.41
27:O:193:LEU:HD23	27:O:193:LEU:HA	1.82	0.41
6:f:176:LEU:HA	6:f:179:PHE:CZ	2.56	0.40
9:2:109:LEU:HD22	9:2:140:PHE:CG	2.55	0.40
17:T:44:LEU:HD22	17:T:47:GLN:HE21	1.86	0.40
20:Z:713:LYS:HD2	20:Z:746:ILE:HD13	2.03	0.40
20:Z:743:ILE:HG21	20:Z:780:MET:HE1	2.03	0.40
30:K:362:LEU:HD23	30:K:402:ILE:HB	2.03	0.40
4:d:151:GLU:HB2	4:d:152:PRO:HD2	2.03	0.40
5:e:214:GLU:CD	5:e:214:GLU:H	2.29	0.40
4:D:32:CYS:HA	4:D:165:GLY:HA3	2.04	0.40
17:T:138:ASP:CG	17:T:139:ASP:H	2.29	0.40
18:X:117:LYS:H	18:X:121:ILE:HG13	1.86	0.40
20:Z:748:LEU:CB	29:I:81:ILE:C	2.95	0.40
20:Z:748:LEU:CB	29:I:84:PRO:HD3	2.47	0.40
22:S:263:ASP:C	22:S:264:VAL:HG13	2.46	0.40
24:Q:191:LEU:HA	24:Q:194:SER:CB	2.50	0.40
30:K:99:PHE:HA	30:K:110:VAL:HG12	2.03	0.40
32:M:18:LEU:HG	32:M:20:GLN:H	1.85	0.40
4:D:207:ALA:HB2	4:D:233:VAL:HG11	2.03	0.40
9:2:249:ILE:HD13	10:3:45:HIS:CG	2.57	0.40
21:N:531:LEU:HD23	21:N:531:LEU:HA	1.88	0.40
1:A:54:ILE:HD13	1:A:206:ALA:HB1	2.04	0.40
16:V:50:MET:HE2	16:V:78:VAL:HG22	2.02	0.40
17:T:123:HIS:CD2	22:S:284:LEU:HD21	2.56	0.40
22:S:46:LEU:O	22:S:50:PRO:HD2	2.21	0.40
23:P:69:ARG:HE	23:P:69:ARG:CA	2.34	0.40
26:U:37:ILE:CG2	26:U:48:VAL:HG13	2.52	0.40
28:H:258:LEU:HD13	34:H:501:ATP:O3'	2.22	0.40
30:K:194:GLN:HG2	30:K:196:ASP:H	1.85	0.40
31:L:364:HIS:NE2	34:L:501:ATP:C2	2.90	0.40
33:J:142:VAL:HG11	33:J:212:ARG:HB2	2.03	0.40
6:f:133:LEU:HD23	6:f:133:LEU:HA	1.89	0.40
1:A:15:HIS:CE1	7:G:8:TYR:CZ	3.09	0.40
9:2:252:ILE:HD13	9:2:252:ILE:HG21	1.92	0.40
16:V:222:GLN:HE22	26:U:203:LYS:HE2	1.87	0.40
20:Z:249:MET:O	20:Z:253:VAL:N	2.55	0.40
22:S:176:LEU:HD23	22:S:176:LEU:HA	1.73	0.40
30:K:203:ILE:HD11	33:J:367:MET:HE2	2.03	0.40
33:J:133:LEU:HD13	33:J:236:MET:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	240/242 (99%)	221 (92%)	18 (8%)	1 (0%)	30	67
1	a	240/242 (99%)	224 (93%)	15 (6%)	1 (0%)	30	67
2	B	247/249 (99%)	230 (93%)	16 (6%)	1 (0%)	30	67
2	b	247/249 (99%)	230 (93%)	13 (5%)	4 (2%)	7	37
3	C	242/244 (99%)	230 (95%)	11 (4%)	1 (0%)	30	67
3	c	242/244 (99%)	233 (96%)	8 (3%)	1 (0%)	30	67
4	D	235/251 (94%)	215 (92%)	17 (7%)	3 (1%)	9	41
4	d	249/251 (99%)	235 (94%)	9 (4%)	5 (2%)	6	31
5	E	247/249 (99%)	231 (94%)	10 (4%)	6 (2%)	4	27
5	e	247/249 (99%)	229 (93%)	13 (5%)	5 (2%)	6	31
6	F	229/231 (99%)	211 (92%)	16 (7%)	2 (1%)	14	49
6	f	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	5	29
7	G	240/242 (99%)	227 (95%)	13 (5%)	0	100	100
7	g	240/242 (99%)	231 (96%)	9 (4%)	0	100	100
8	1	194/196 (99%)	187 (96%)	6 (3%)	1 (0%)	24	63
8	h	194/196 (99%)	175 (90%)	16 (8%)	3 (2%)	8	38
9	2	224/226 (99%)	212 (95%)	12 (5%)	0	100	100
9	i	224/226 (99%)	203 (91%)	18 (8%)	3 (1%)	9	41
10	3	202/204 (99%)	183 (91%)	19 (9%)	0	100	100
10	j	202/204 (99%)	182 (90%)	15 (7%)	5 (2%)	4	26
11	4	193/195 (99%)	176 (91%)	13 (7%)	4 (2%)	5	30
11	k	193/195 (99%)	179 (93%)	13 (7%)	1 (0%)	24	63
12	5	210/212 (99%)	198 (94%)	11 (5%)	1 (0%)	24	63
12	l	210/212 (99%)	192 (91%)	14 (7%)	4 (2%)	6	32
13	6	220/222 (99%)	201 (91%)	16 (7%)	3 (1%)	9	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	m	220/222 (99%)	207 (94%)	10 (4%)	3 (1%)	9	39
14	7	227/232 (98%)	204 (90%)	20 (9%)	3 (1%)	9	41
14	n	230/232 (99%)	207 (90%)	21 (9%)	2 (1%)	14	49
15	W	195/197 (99%)	174 (89%)	18 (9%)	3 (2%)	8	38
16	V	94/289 (32%)	87 (93%)	5 (5%)	2 (2%)	5	30
17	T	221/266 (83%)	205 (93%)	9 (4%)	7 (3%)	3	21
18	X	125/127 (98%)	106 (85%)	15 (12%)	4 (3%)	3	21
19	Y	3/89 (3%)	2 (67%)	1 (33%)	0	100	100
20	Z	349/970 (36%)	327 (94%)	17 (5%)	5 (1%)	9	39
21	N	465/922 (50%)	438 (94%)	21 (4%)	6 (1%)	9	41
25	R	49/405 (12%)	44 (90%)	5 (10%)	0	100	100
26	U	302/304 (99%)	292 (97%)	8 (3%)	2 (1%)	18	55
27	O	68/388 (18%)	67 (98%)	1 (2%)	0	100	100
28	H	292/426 (68%)	261 (89%)	24 (8%)	7 (2%)	4	27
29	I	382/384 (100%)	335 (88%)	35 (9%)	12 (3%)	3	22
30	K	392/394 (100%)	361 (92%)	22 (6%)	9 (2%)	5	28
31	L	386/388 (100%)	355 (92%)	25 (6%)	6 (2%)	7	37
32	M	419/421 (100%)	375 (90%)	30 (7%)	14 (3%)	3	21
33	J	403/405 (100%)	342 (85%)	49 (12%)	12 (3%)	3	22
All	All	10462/12765 (82%)	9632 (92%)	673 (6%)	157 (2%)	11	38

All (157) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	d	101	GLU
5	e	16	SER
6	f	11	VAL
5	E	9	ASP
6	F	14	SER
12	5	172	MET
13	6	89	ASP
13	6	138	SER
16	V	73	GLN
17	T	92	ASN
17	T	96	LEU

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Mol	Chain	Res	Type
17	T	173	GLU
20	Z	728	LYS
21	N	175	ASP
28	H	458	SER
28	H	465	GLN
29	I	125	MET
29	I	142	GLU
29	I	213	ILE
30	K	314	VAL
31	L	245	PHE
31	L	246	SER
31	L	343	LEU
32	M	97	SER
32	M	316	SER
32	M	424	ALA
33	J	282	PHE
3	c	168	ASN
5	e	9	ASP
5	e	122	ARG
5	e	169	ALA
6	f	9	ASP
8	h	101	ASN
10	j	7	ILE
11	k	4	ILE
5	E	122	ARG
5	E	169	ALA
11	4	150	PRO
14	7	260	GLY
16	V	61	TYR
17	T	225	ASN
18	X	116	ALA
20	Z	612	GLY
21	N	120	ASP
21	N	148	SER
21	N	178	SER
21	N	395	ALA
26	U	150	THR
29	I	86	GLU
29	I	187	LEU
31	L	179	THR
32	M	92	GLU
32	M	124	ARG

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Mol	Chain	Res	Type
32	M	240	ASN
32	M	408	SER
32	M	433	TYR
33	J	2	THR
33	J	3	ALA
33	J	284	THR
2	b	4	ARG
2	b	17	LYS
6	f	14	SER
6	f	164	ARG
9	i	146	GLY
9	i	174	ASP
10	j	40	PHE
13	m	27	ASP
1	A	13	ASP
2	B	106	PRO
5	E	16	SER
5	E	128	SER
5	E	216	ASN
8	1	123	PRO
11	4	2	ASP
13	6	27	ASP
14	7	244	ASN
15	W	169	SER
17	T	138	ASP
18	X	77	PRO
20	Z	825	ALA
26	U	30	ASN
28	H	194	SER
29	I	143	PRO
29	I	291	ARG
30	K	41	SER
30	K	155	ASP
30	K	162	GLY
30	K	399	ARG
32	M	87	ASP
32	M	108	LEU
32	M	179	THR
32	M	427	SER
33	J	252	SER
5	e	53	ARG
10	j	116	SER

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Mol	Chain	Res	Type
10	j	194	GLU
12	l	147	GLU
12	l	281	SER
13	m	208	ASP
14	n	252	TRP
3	C	222	ASP
4	D	219	SER
11	4	11	ASP
15	W	179	ARG
18	X	38	ASN
20	Z	142	ASP
28	H	323	ALA
28	H	457	PHE
29	I	216	PRO
31	L	289	ARG
33	J	4	ALA
33	J	82	LYS
33	J	283	GLU
33	J	353	CYS
1	a	49	ASP
4	d	5	ASP
4	d	40	ASN
4	d	70	HIS
6	f	69	HIS
8	h	123	PRO
8	h	154	ASN
13	m	138	SER
14	n	249	ASN
4	D	101	GLU
4	D	208	LYS
6	F	41	ASN
11	4	176	PHE
14	7	114	ALA
17	T	95	LYS
17	T	257	THR
18	X	112	ASN
20	Z	557	GLU
21	N	86	LYS
29	I	198	VAL
29	I	283	GLU
29	I	292	TYR
30	K	167	PRO

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Mol	Chain	Res	Type
30	K	398	ASN
30	K	426	PHE
31	L	244	ILE
32	M	106	VAL
32	M	282	GLU
33	J	118	ASP
33	J	141	LYS
2	b	97	TYR
2	b	161	ALA
4	d	102	ASP
10	j	193	ASP
29	I	329	ASN
33	J	261	SER
12	l	106	VAL
12	l	173	GLY
28	H	191	ILE
28	H	314	VAL
30	K	175	GLY
9	i	222	PRO
15	W	164	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	
4	d	41/224 (18%)	40 (98%)	1 (2%)	43	63
5	e	33/205 (16%)	32 (97%)	1 (3%)	36	57
6	F	5/190 (3%)	5 (100%)	0	100	100
8	h	50/162 (31%)	50 (100%)	0	100	100
9	2	24/185 (13%)	24 (100%)	0	100	100
9	i	136/185 (74%)	136 (100%)	0	100	100
10	j	71/172 (41%)	69 (97%)	2 (3%)	38	59
11	k	135/173 (78%)	130 (96%)	5 (4%)	30	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	5	25/169 (15%)	24 (96%)	1 (4%)	28	49
12	l	169/169 (100%)	161 (95%)	8 (5%)	23	45
13	6	185/185 (100%)	181 (98%)	4 (2%)	45	64
13	m	179/185 (97%)	175 (98%)	4 (2%)	45	64
14	7	195/198 (98%)	193 (99%)	2 (1%)	68	76
14	n	128/198 (65%)	123 (96%)	5 (4%)	28	50
15	W	171/171 (100%)	164 (96%)	7 (4%)	27	49
16	V	253/253 (100%)	242 (96%)	11 (4%)	26	48
17	T	249/249 (100%)	243 (98%)	6 (2%)	43	63
18	X	116/116 (100%)	111 (96%)	5 (4%)	26	48
19	Y	81/81 (100%)	81 (100%)	0	100	100
20	Z	18/828 (2%)	18 (100%)	0	100	100
21	N	317/776 (41%)	312 (98%)	5 (2%)	55	69
22	S	447/447 (100%)	439 (98%)	8 (2%)	51	67
23	P	339/412 (82%)	335 (99%)	4 (1%)	63	73
24	Q	100/391 (26%)	98 (98%)	2 (2%)	48	65
25	R	324/356 (91%)	316 (98%)	8 (2%)	42	62
26	U	277/277 (100%)	270 (98%)	7 (2%)	42	62
27	O	351/363 (97%)	341 (97%)	10 (3%)	38	59
28	H	361/361 (100%)	346 (96%)	15 (4%)	26	48
29	I	341/341 (100%)	327 (96%)	14 (4%)	27	49
30	K	346/346 (100%)	334 (96%)	12 (4%)	32	53
31	L	332/332 (100%)	321 (97%)	11 (3%)	33	55
32	M	364/364 (100%)	350 (96%)	14 (4%)	29	51
33	J	352/352 (100%)	335 (95%)	17 (5%)	23	45
All	All	6515/9416 (69%)	6326 (97%)	189 (3%)	38	58

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	241	GLN
5	e	68	VAL
10	j	13	VAL

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Mol	Chain	Res	Type
10	j	84	PRO
11	k	53	THR
11	k	76	SER
11	k	85	ARG
11	k	126	VAL
11	k	141	PHE
12	l	79	LEU
12	l	105	THR
12	l	109	VAL
12	l	181	ARG
12	l	201	ILE
12	l	261	ILE
12	l	268	VAL
12	l	276	LYS
13	m	49	PRO
13	m	115	VAL
13	m	136	VAL
13	m	196	PHE
14	n	36	GLN
14	n	39	VAL
14	n	148	ILE
14	n	186	PRO
14	n	195	GLU
12	5	268	VAL
13	6	20	ILE
13	6	39	THR
13	6	73	VAL
13	6	125	ASP
14	7	39	VAL
14	7	185	ASN
15	W	58	ASN
15	W	59	PRO
15	W	76	LEU
15	W	79	THR
15	W	120	ASP
15	W	155	ASP
15	W	182	TYR
16	V	25	GLU
16	V	67	ASP
16	V	130	GLU
16	V	141	VAL
16	V	144	ILE

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Mol	Chain	Res	Type
16	V	160	ASP
16	V	192	LEU
16	V	196	TYR
16	V	199	LEU
16	V	274	GLN
16	V	278	LYS
17	T	9	LYS
17	T	27	LEU
17	T	46	ILE
17	T	193	THR
17	T	197	TYR
17	T	236	ASN
18	X	14	VAL
18	X	28	PRO
18	X	57	VAL
18	X	102	GLN
18	X	115	SER
21	N	669	GLU
21	N	670	LYS
21	N	876	PRO
21	N	888	ASP
21	N	902	VAL
22	S	54	TRP
22	S	81	LEU
22	S	128	ILE
22	S	161	LYS
22	S	165	PRO
22	S	393	ARG
22	S	407	ILE
22	S	486	LYS
23	P	145	GLU
23	P	149	GLU
23	P	163	LEU
23	P	258	LYS
24	Q	338	LEU
24	Q	406	ASP
25	R	68	GLU
25	R	71	LEU
25	R	95	ASP
25	R	124	ASP
25	R	188	LYS
25	R	306	PRO

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Mol	Chain	Res	Type
25	R	348	LEU
25	R	373	PRO
26	U	27	THR
26	U	79	MET
26	U	115	GLN
26	U	134	THR
26	U	140	ILE
26	U	176	ARG
26	U	190	LEU
27	O	79	VAL
27	O	102	LEU
27	O	237	PRO
27	O	243	VAL
27	O	271	LYS
27	O	308	LEU
27	O	341	ILE
27	O	346	GLU
27	O	348	VAL
27	O	387	ARG
28	H	76	LEU
28	H	82	TRP
28	H	94	GLU
28	H	95	HIS
28	H	162	ARG
28	H	194	SER
28	H	207	THR
28	H	221	LEU
28	H	273	ARG
28	H	281	GLN
28	H	311	ILE
28	H	314	VAL
28	H	331	ARG
28	H	450	VAL
28	H	464	MET
29	I	71	LEU
29	I	82	LEU
29	I	86	GLU
29	I	102	ASN
29	I	147	VAL
29	I	177	PRO
29	I	278	ILE
29	I	300	ARG

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Mol	Chain	Res	Type
29	I	328	THR
29	I	347	LYS
29	I	348	ILE
29	I	410	GLN
29	I	428	VAL
29	I	432	LEU
30	K	37	ASN
30	K	77	ARG
30	K	137	VAL
30	K	160	VAL
30	K	169	VAL
30	K	236	ARG
30	K	237	VAL
30	K	254	VAL
30	K	275	ASP
30	K	360	MET
30	K	382	VAL
30	K	405	SER
31	L	51	GLU
31	L	147	THR
31	L	174	GLU
31	L	196	VAL
31	L	199	LEU
31	L	244	ILE
31	L	246	SER
31	L	251	ILE
31	L	254	LYS
31	L	361	PHE
31	L	416	MET
32	M	18	LEU
32	M	36	LEU
32	M	75	LEU
32	M	127	VAL
32	M	143	ASN
32	M	173	ASP
32	M	252	VAL
32	M	278	ILE
32	M	291	PHE
32	M	335	PRO
32	M	342	ARG
32	M	343	LEU
32	M	352	PRO

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Mol	Chain	Res	Type
32	M	433	TYR
33	J	2	THR
33	J	12	LEU
33	J	34	ILE
33	J	37	LYS
33	J	101	ASP
33	J	125	VAL
33	J	179	ILE
33	J	222	TYR
33	J	244	ILE
33	J	261	SER
33	J	274	GLU
33	J	279	LEU
33	J	283	GLU
33	J	287	ASN
33	J	320	SER
33	J	358	VAL
33	J	400	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (171) such sidechains are listed below:

Mol	Chain	Res	Type
4	d	231	GLN
9	i	122	HIS
10	j	8	ASN
10	j	157	ASN
11	k	41	HIS
11	k	63	ASN
12	l	208	GLN
12	l	283	ASN
13	m	11	ASN
13	m	16	ASN
13	m	44	ASN
13	m	57	ASN
13	m	63	ASN
13	m	78	ASN
13	m	84	HIS
13	m	87	HIS
13	m	102	GLN
13	m	116	HIS
14	n	36	GLN
14	n	51	ASN

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Mol	Chain	Res	Type
14	n	107	ASN
14	n	227	ASN
14	n	236	ASN
9	2	114	GLN
9	2	189	GLN
13	6	37	ASN
13	6	102	GLN
13	6	163	ASN
14	7	81	ASN
14	7	107	ASN
14	7	182	HIS
14	7	236	ASN
15	W	18	ASN
15	W	92	GLN
15	W	106	GLN
15	W	108	GLN
15	W	150	ASN
15	W	162	ASN
15	W	184	ASN
16	V	73	GLN
16	V	111	HIS
16	V	124	ASN
16	V	193	ASN
16	V	217	HIS
16	V	250	GLN
17	T	47	GLN
17	T	71	GLN
17	T	80	ASN
17	T	123	HIS
17	T	132	HIS
17	T	158	GLN
17	T	192	ASN
17	T	225	ASN
17	T	236	ASN
18	X	18	ASN
18	X	102	GLN
19	Y	21	ASN
21	N	199	ASN
21	N	580	ASN
21	N	635	GLN
21	N	679	ASN
21	N	859	ASN

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Mol	Chain	Res	Type
21	N	870	ASN
21	N	878	GLN
22	S	19	HIS
22	S	20	HIS
22	S	79	ASN
22	S	112	ASN
22	S	159	ASN
22	S	180	ASN
22	S	191	HIS
22	S	205	ASN
22	S	225	HIS
22	S	311	GLN
22	S	312	GLN
22	S	369	GLN
22	S	417	GLN
22	S	459	GLN
22	S	469	ASN
23	P	29	GLN
23	P	38	GLN
23	P	164	GLN
23	P	178	GLN
23	P	183	GLN
23	P	195	GLN
23	P	210	ASN
23	P	230	HIS
23	P	263	HIS
23	P	285	GLN
23	P	296	GLN
23	P	306	ASN
23	P	334	ASN
23	P	349	ASN
24	Q	334	HIS
24	Q	405	GLN
25	R	42	GLN
25	R	96	GLN
25	R	182	ASN
25	R	208	ASN
25	R	223	ASN
25	R	395	ASN
25	R	401	HIS
25	R	406	GLN
26	U	5	HIS

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Mol	Chain	Res	Type
26	U	21	HIS
26	U	42	ASN
26	U	94	HIS
26	U	115	GLN
26	U	117	ASN
26	U	128	GLN
26	U	156	HIS
26	U	230	GLN
26	U	252	HIS
26	U	262	GLN
26	U	270	ASN
26	U	294	ASN
27	O	23	HIS
27	O	117	ASN
27	O	169	ASN
27	O	186	ASN
27	O	235	HIS
27	O	236	HIS
27	O	282	GLN
27	O	304	ASN
27	O	374	ASN
27	O	389	GLN
28	H	89	GLN
28	H	128	ASN
28	H	131	GLN
28	H	151	GLN
28	H	281	GLN
28	H	327	ASN
28	H	359	ASN
28	H	392	HIS
28	H	465	GLN
29	I	161	GLN
29	I	190	GLN
29	I	204	HIS
29	I	238	ASN
29	I	274	ASN
29	I	329	ASN
29	I	410	GLN
29	I	431	ASN
30	K	35	ASN
30	K	37	ASN
30	K	90	GLN

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Mol	Chain	Res	Type
30	K	142	HIS
30	K	180	GLN
30	K	244	HIS
30	K	398	ASN
31	L	59	GLN
31	L	80	ASN
31	L	103	GLN
31	L	175	GLN
31	L	302	GLN
31	L	387	ASN
31	L	393	ASN
31	L	411	ASN
32	M	65	ASN
32	M	102	GLN
32	M	107	ASN
32	M	110	ASN
32	M	125	GLN
32	M	143	ASN
32	M	364	HIS
32	M	387	ASN
32	M	423	GLN
33	J	128	ASN
33	J	156	GLN
33	J	287	ASN
33	J	376	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	ATP	I	501	35	32,33,33	3.34	6 (18%)	48,52,52	1.60	11 (22%)
34	ATP	H	501	35	32,33,33	4.17	8 (25%)	48,52,52	1.87	13 (27%)
34	ATP	L	501	35	32,33,33	3.56	7 (21%)	48,52,52	1.71	8 (16%)
34	ATP	M	501	35	32,33,33	2.96	8 (25%)	48,52,52	1.43	7 (14%)
36	ADP	J	501	35	28,29,29	1.80	6 (21%)	43,45,45	1.37	6 (13%)
34	ATP	K	501	35	32,33,33	4.25	4 (12%)	48,52,52	1.61	12 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	ATP	I	501	35	-	5/22/38/38	0/3/3/3
34	ATP	H	501	35	-	4/22/38/38	0/3/3/3
34	ATP	L	501	35	-	3/22/38/38	0/3/3/3
34	ATP	M	501	35	-	6/22/38/38	0/3/3/3
36	ADP	J	501	35	-	7/16/32/32	0/3/3/3
34	ATP	K	501	35	-	5/22/38/38	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	K	501	ATP	PB-O3A	19.30	1.80	1.59
34	H	501	ATP	PB-O3A	18.08	1.79	1.59
34	L	501	ATP	PB-O3A	13.00	1.73	1.59
34	M	501	ATP	PB-O3B	12.36	1.72	1.59
34	L	501	ATP	PA-O3A	11.59	1.72	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	I	501	ATP	PA-O3A	11.08	1.71	1.59
34	H	501	ATP	PA-O3A	10.46	1.70	1.59
34	I	501	ATP	PB-O3A	10.08	1.70	1.59
34	K	501	ATP	PB-O3B	9.89	1.70	1.59
34	I	501	ATP	PB-O3B	9.82	1.70	1.59
34	K	501	ATP	PA-O3A	8.74	1.68	1.59
34	H	501	ATP	PB-O3B	8.08	1.68	1.59
34	M	501	ATP	PB-O3A	8.06	1.68	1.59
34	L	501	ATP	PB-O3B	6.98	1.67	1.59
36	J	501	ADP	PA-O3A	6.92	1.67	1.59
34	L	501	ATP	C5'-C4'	3.77	1.62	1.51
34	M	501	ATP	C5-N7	-3.31	1.33	1.39
34	M	501	ATP	C2'-C1'	-3.16	1.43	1.53
34	H	501	ATP	C5-N7	-3.10	1.33	1.39
34	L	501	ATP	C2-N3	2.99	1.39	1.33
36	J	501	ADP	C8-N9	2.90	1.42	1.37
34	H	501	ATP	C4-N9	-2.71	1.32	1.37
34	H	501	ATP	C6-N6	2.64	1.40	1.34
34	M	501	ATP	PA-O2A	-2.44	1.44	1.55
34	I	501	ATP	O4'-C4'	2.37	1.50	1.45
34	H	501	ATP	PA-O2A	-2.32	1.44	1.55
34	I	501	ATP	C2-N3	2.27	1.38	1.33
34	M	501	ATP	C1'-N9	2.24	1.52	1.46
34	M	501	ATP	O2'-C2'	-2.23	1.37	1.43
34	M	501	ATP	C3'-C4'	-2.22	1.47	1.53
34	I	501	ATP	O2'-C2'	-2.21	1.37	1.43
34	L	501	ATP	O3'-C3'	-2.20	1.37	1.43
34	H	501	ATP	C5'-C4'	2.19	1.58	1.51
34	K	501	ATP	C6-N1	2.16	1.41	1.35
34	L	501	ATP	PA-O2A	-2.15	1.45	1.55
36	J	501	ADP	C5'-C4'	2.11	1.57	1.51
36	J	501	ADP	C8-N7	-2.08	1.27	1.31
36	J	501	ADP	C2-N1	2.07	1.37	1.33
36	J	501	ADP	C6-N1	2.04	1.41	1.35

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	K	501	ATP	C6-C5-C4	4.49	123.31	117.18
34	H	501	ATP	C6-C5-C4	4.36	123.14	117.18
34	L	501	ATP	N6-C6-N1	4.36	128.08	118.38
34	L	501	ATP	C4-C5-N7	-4.08	105.92	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	H	501	ATP	O4'-C1'-N9	4.07	115.90	108.09
34	H	501	ATP	N9-C8-N7	-3.99	108.28	113.94
34	H	501	ATP	N6-C6-N1	3.85	126.94	118.38
34	M	501	ATP	C6-C5-C4	3.83	122.40	117.18
34	K	501	ATP	N3-C2-N1	3.59	134.02	128.58
34	L	501	ATP	C6-C5-C4	3.58	122.06	117.18
36	J	501	ADP	C6-C5-C4	3.52	121.99	117.18
34	M	501	ATP	N9-C8-N7	-3.48	109.00	113.94
34	L	501	ATP	C5-N7-C8	3.41	108.80	103.45
34	I	501	ATP	N6-C6-N1	3.36	125.87	118.38
34	M	501	ATP	O2B-PB-O3A	3.33	116.27	107.27
34	M	501	ATP	C5-N7-C8	3.28	108.61	103.45
34	I	501	ATP	C5-C4-N9	3.26	109.36	105.81
34	L	501	ATP	O3B-PB-O1B	-3.19	101.10	110.70
34	I	501	ATP	C4-C5-N7	-3.14	106.99	110.58
34	I	501	ATP	C4-N9-C8	-3.12	102.46	105.74
34	H	501	ATP	C1'-N9-C8	-3.06	120.31	127.09
34	H	501	ATP	N3-C4-N9	2.99	132.24	127.17
34	H	501	ATP	C5-N7-C8	2.97	108.11	103.45
34	K	501	ATP	C2'-C1'-N9	-2.89	106.11	113.30
34	H	501	ATP	N3-C2-N1	2.88	132.94	128.58
34	K	501	ATP	C6-C5-N7	-2.83	126.64	132.09
34	H	501	ATP	C6-C5-N7	-2.82	126.65	132.09
34	H	501	ATP	C4-N9-C8	2.79	108.67	105.74
34	I	501	ATP	C1'-N9-C8	2.78	133.26	127.09
36	J	501	ADP	C5-N7-C8	2.65	107.62	103.45
34	L	501	ATP	C5-C4-N9	2.64	108.69	105.81
34	I	501	ATP	O2A-PA-O3A	-2.63	100.17	107.27
34	H	501	ATP	C5-C4-N3	-2.62	123.11	126.72
36	J	501	ADP	N6-C6-N1	2.60	124.17	118.38
34	K	501	ATP	N6-C6-N1	2.58	124.11	118.38
34	K	501	ATP	C5-C4-N3	-2.57	123.17	126.72
34	L	501	ATP	C5-C6-N6	-2.51	117.08	123.29
34	K	501	ATP	O4'-C4'-C5'	2.45	117.18	109.33
34	I	501	ATP	N3-C4-N9	-2.45	123.00	127.17
34	L	501	ATP	C1'-N9-C8	2.43	132.48	127.09
36	J	501	ADP	C5-C6-N1	-2.40	111.42	117.51
34	I	501	ATP	O4'-C1'-N9	2.36	112.63	108.09
34	K	501	ATP	O3G-PG-O1G	2.35	120.00	110.83
34	K	501	ATP	O2A-PA-O3A	2.28	113.44	107.27
34	M	501	ATP	O3G-PG-O3B	-2.25	97.08	104.64
34	K	501	ATP	O3B-PB-O1B	-2.18	104.14	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	K	501	ATP	C5-C6-N1	-2.16	112.02	117.51
34	K	501	ATP	C4-N9-C8	-2.14	103.49	105.74
34	M	501	ATP	C6-C5-N7	-2.13	127.97	132.09
34	H	501	ATP	C5'-C4'-C3'	-2.13	107.54	115.21
34	I	501	ATP	C2-N1-C6	2.08	122.14	118.73
34	I	501	ATP	C2'-C3'-C4'	-2.08	98.60	102.61
34	I	501	ATP	O3G-PG-O3B	2.07	111.57	104.64
34	M	501	ATP	C5-C6-N1	-2.03	112.36	117.51
36	J	501	ADP	O3B-PB-O3A	2.02	111.42	104.64
34	H	501	ATP	C5-C6-N6	-2.02	118.28	123.29
36	J	501	ADP	C4-C5-N7	-2.02	108.27	110.58

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	H	501	ATP	C5'-O5'-PA-O2A
34	H	501	ATP	C5'-O5'-PA-O3A
34	I	501	ATP	C5'-O5'-PA-O1A
34	I	501	ATP	C5'-O5'-PA-O2A
34	I	501	ATP	C5'-O5'-PA-O3A
34	L	501	ATP	C5'-O5'-PA-O2A
34	L	501	ATP	C5'-O5'-PA-O3A
34	M	501	ATP	PB-O3B-PG-O3G
36	J	501	ADP	PA-O3A-PB-O3B
36	J	501	ADP	C5'-O5'-PA-O1A
36	J	501	ADP	C5'-O5'-PA-O2A
36	J	501	ADP	C5'-O5'-PA-O3A
34	M	501	ATP	O4'-C4'-C5'-O5'
34	I	501	ATP	PA-O3A-PB-O1B
34	M	501	ATP	PG-O3B-PB-O1B
34	K	501	ATP	PB-O3B-PG-O1G
36	J	501	ADP	PA-O3A-PB-O2B
34	M	501	ATP	C3'-C4'-C5'-O5'
34	K	501	ATP	PG-O3B-PB-O1B
34	H	501	ATP	O4'-C4'-C5'-O5'
34	L	501	ATP	O4'-C4'-C5'-O5'
34	M	501	ATP	PG-O3B-PB-O2B
36	J	501	ADP	C4'-C5'-O5'-PA
34	M	501	ATP	PB-O3B-PG-O1G
34	I	501	ATP	PB-O3B-PG-O3G
34	K	501	ATP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
34	K	501	ATP	PB-O3B-PG-O3G
34	H	501	ATP	C2'-C1'-N9-C8
36	J	501	ADP	PA-O3A-PB-O1B
34	K	501	ATP	PG-O3B-PB-O2B

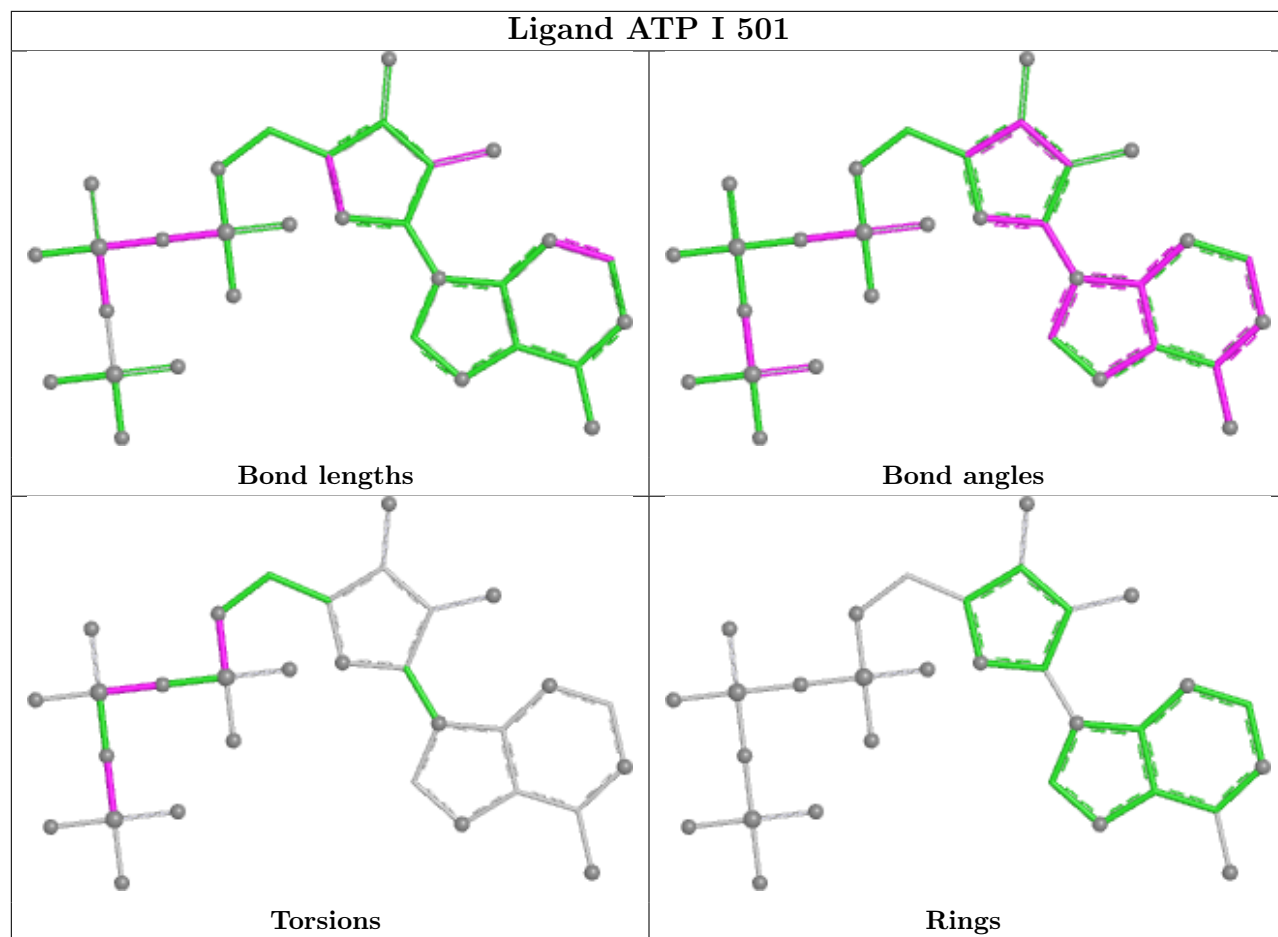
There are no ring outliers.

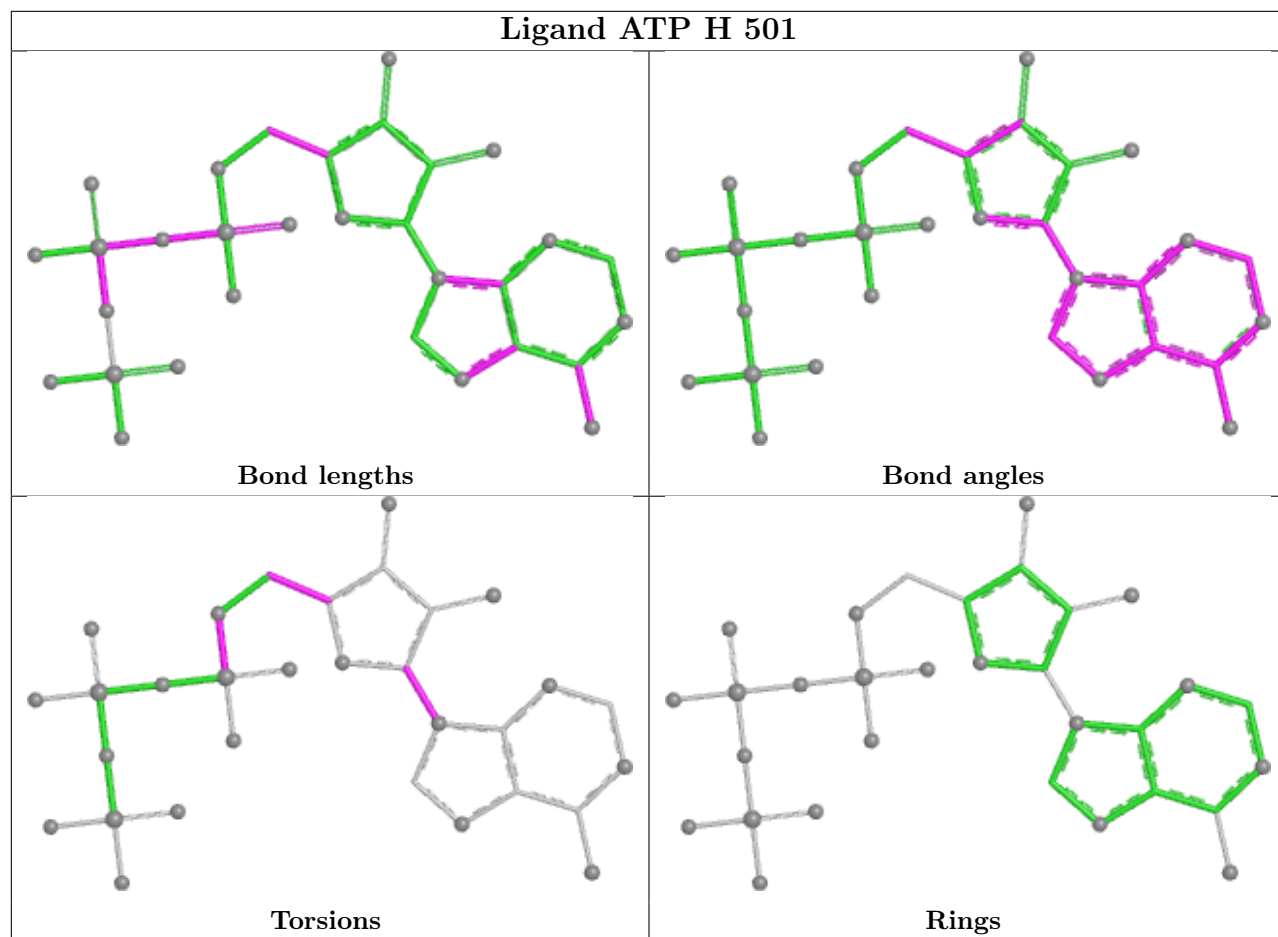
6 monomers are involved in 131 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	I	501	ATP	23	0
34	H	501	ATP	40	0
34	L	501	ATP	8	0
34	M	501	ATP	19	0
36	J	501	ADP	17	0
34	K	501	ATP	24	0

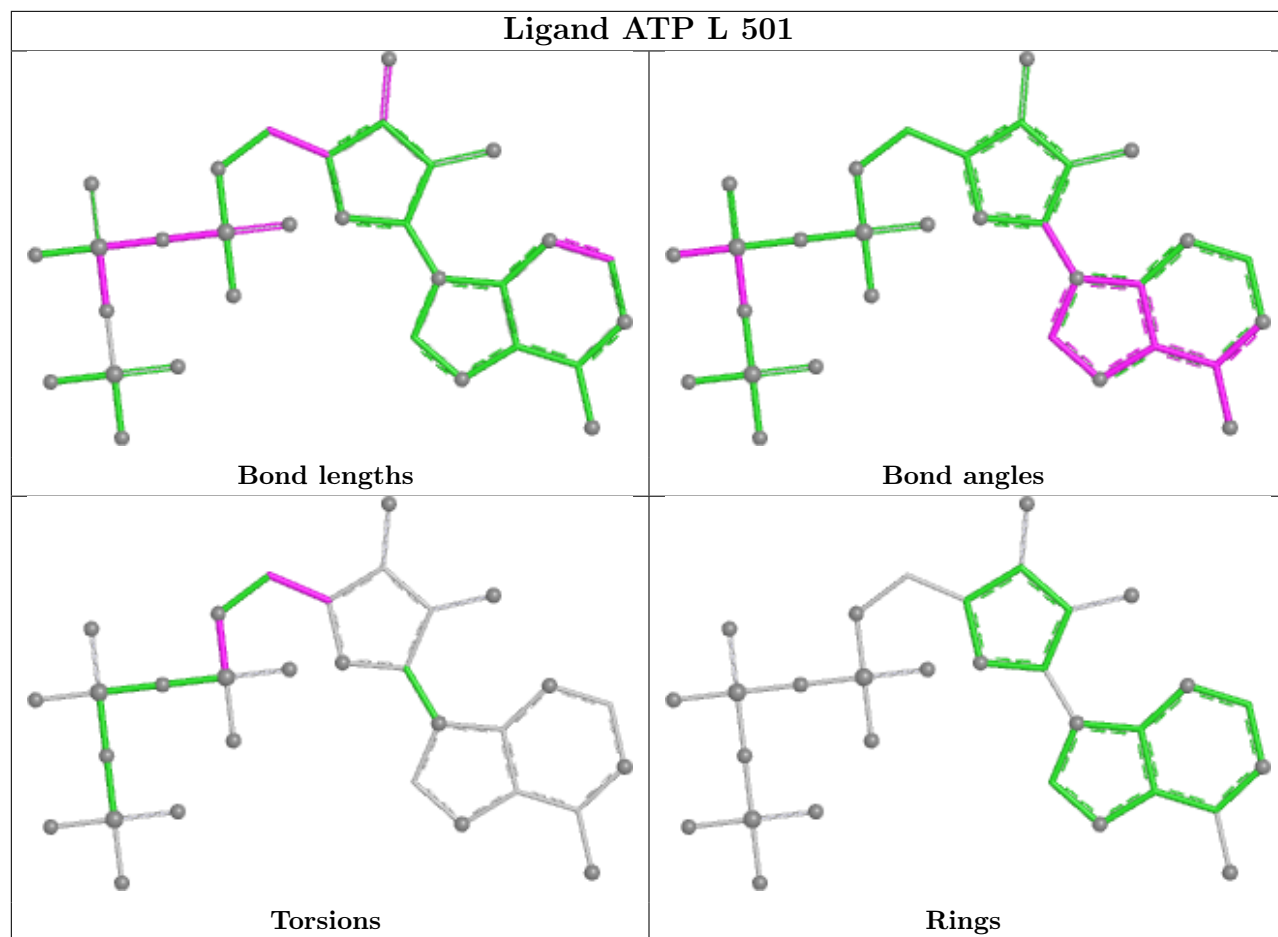
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

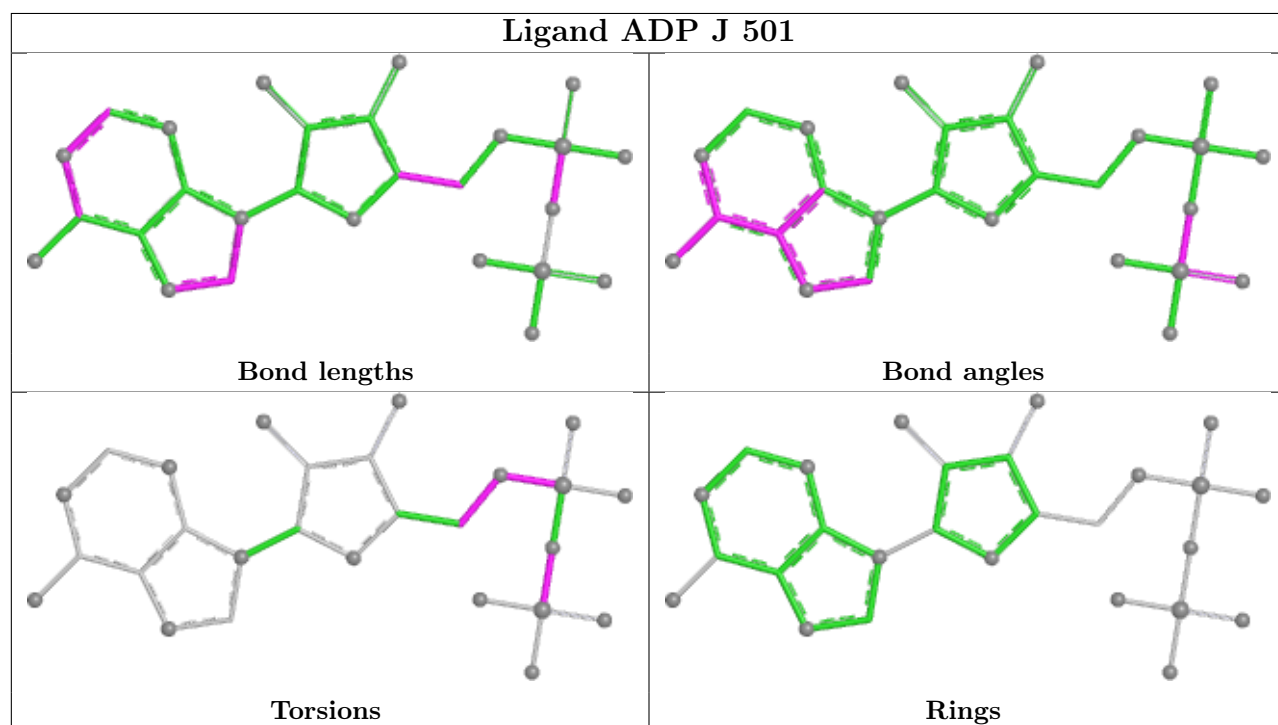
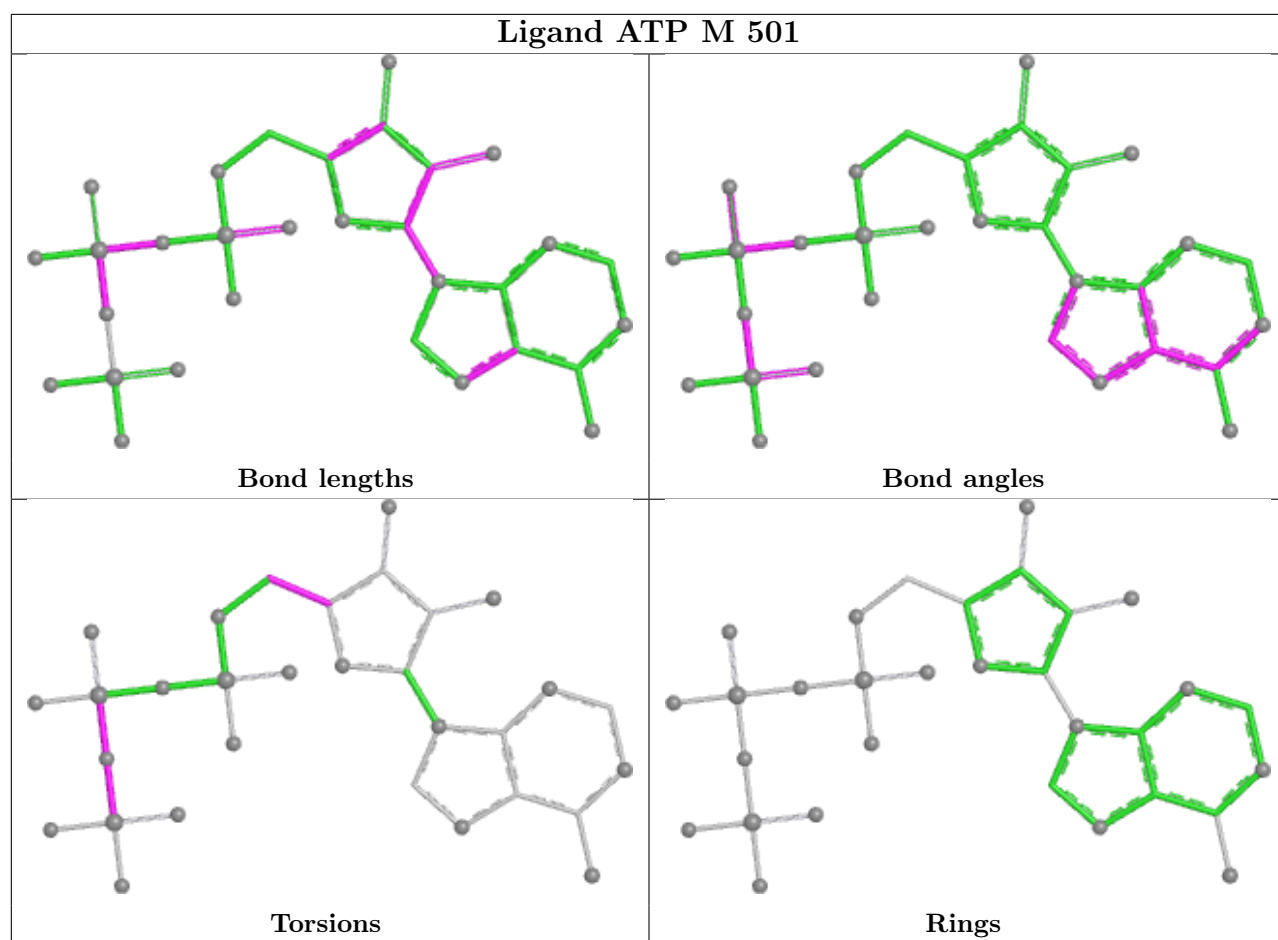
Ligand ATP I 501

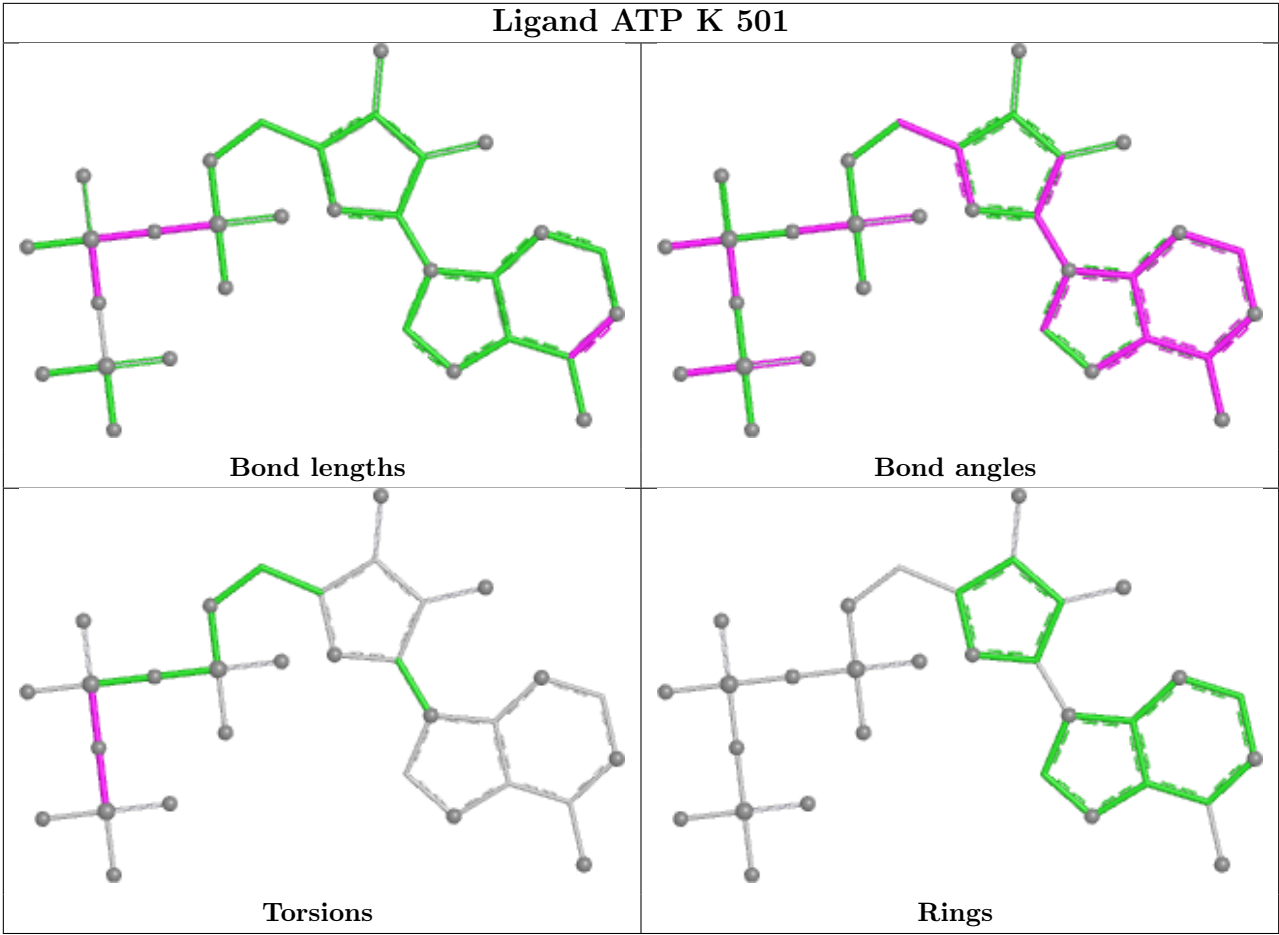




Ligand ATP L 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
28	H	2
29	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	307:PHE	C	308:PHE	N	1.91
1	I	322:VAL	C	323:LYS	N	1.82
1	H	308:PHE	C	309:ASP	N	1.81

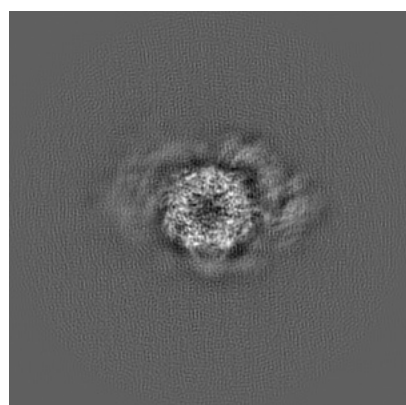
6 Map visualisation [i](#)

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

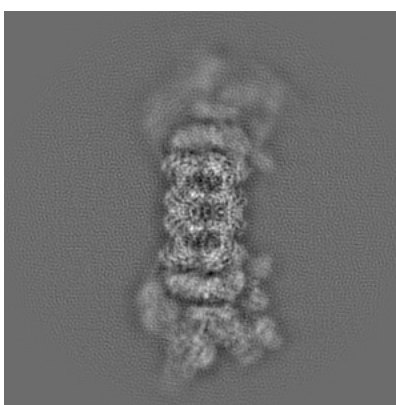
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

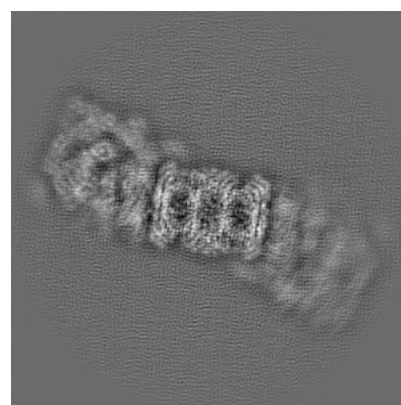
6.1.1 Primary map



X



Y

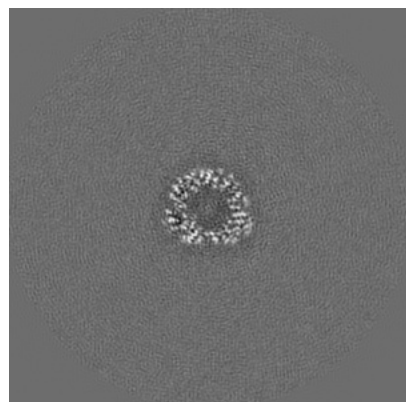


Z

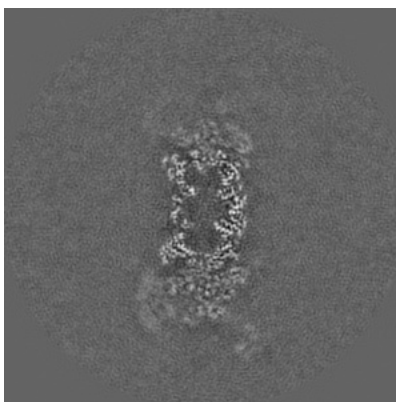
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

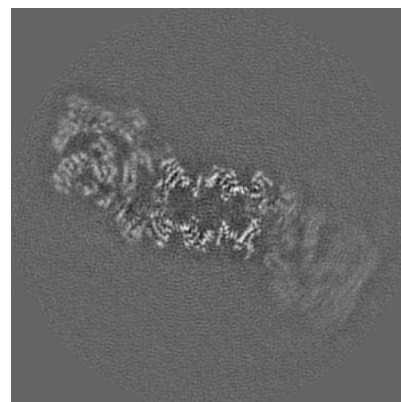
6.2.1 Primary map



X Index: 192



Y Index: 192

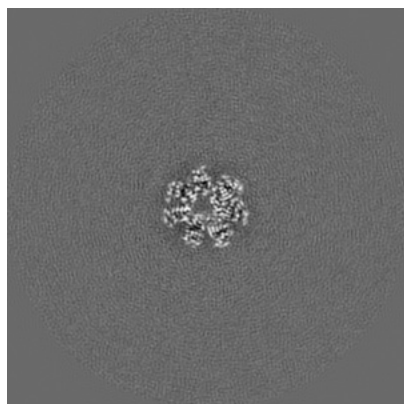


Z Index: 192

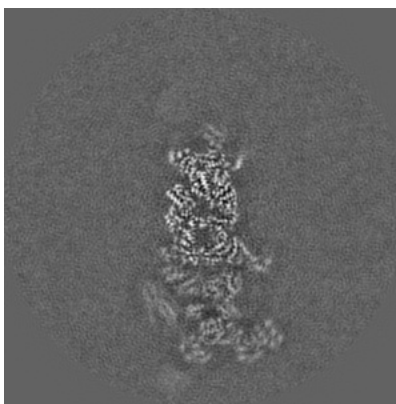
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

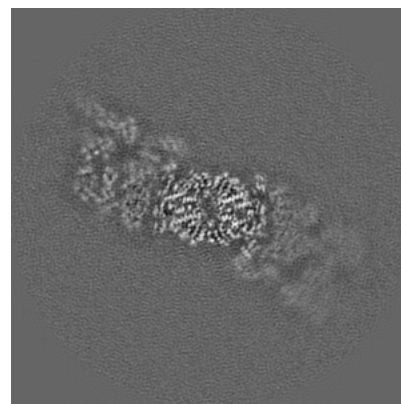
6.3.1 Primary map



X Index: 206



Y Index: 210

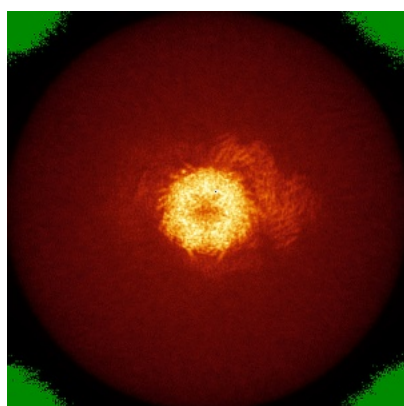


Z Index: 210

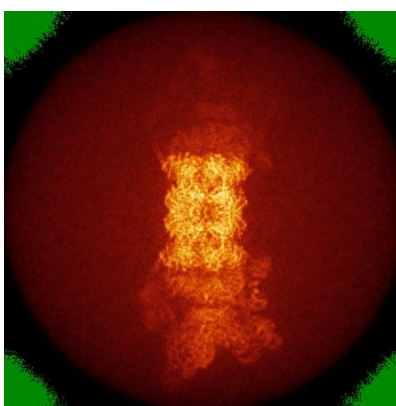
The images above show the largest variance slices of the map in three orthogonal directions.

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

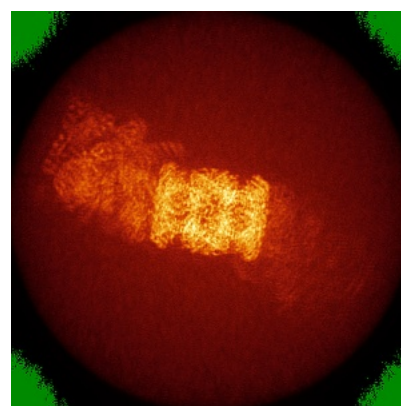
6.4.1 Primary map



X



Y

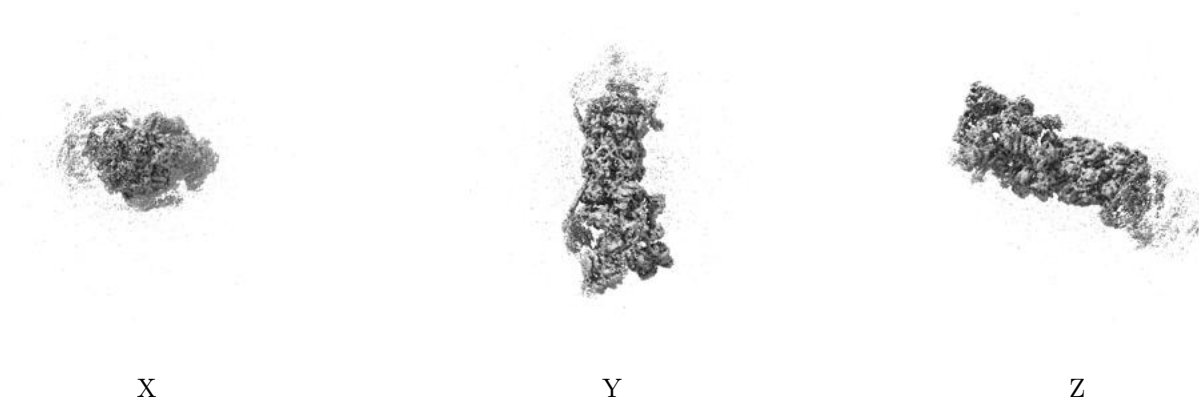


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

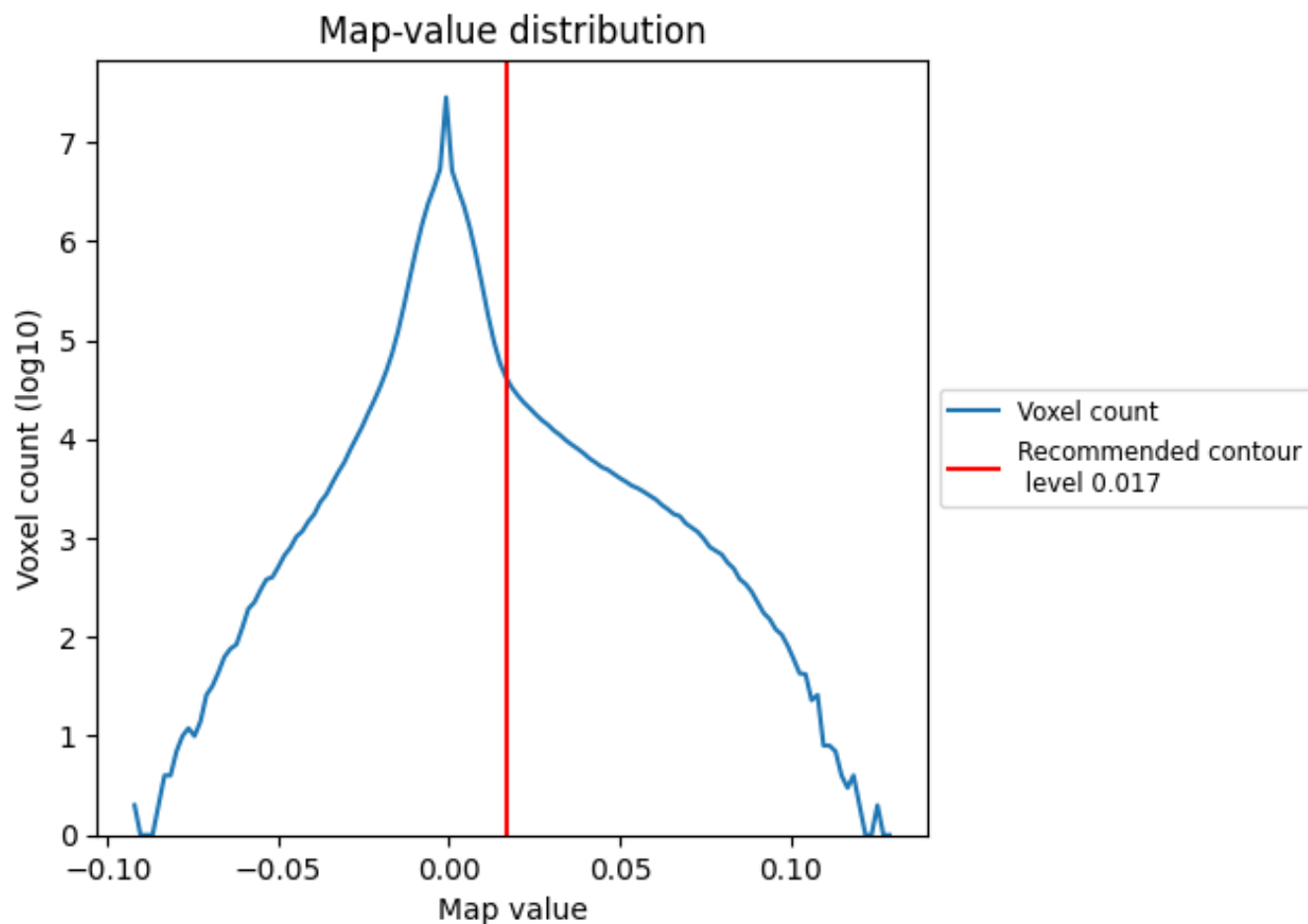
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

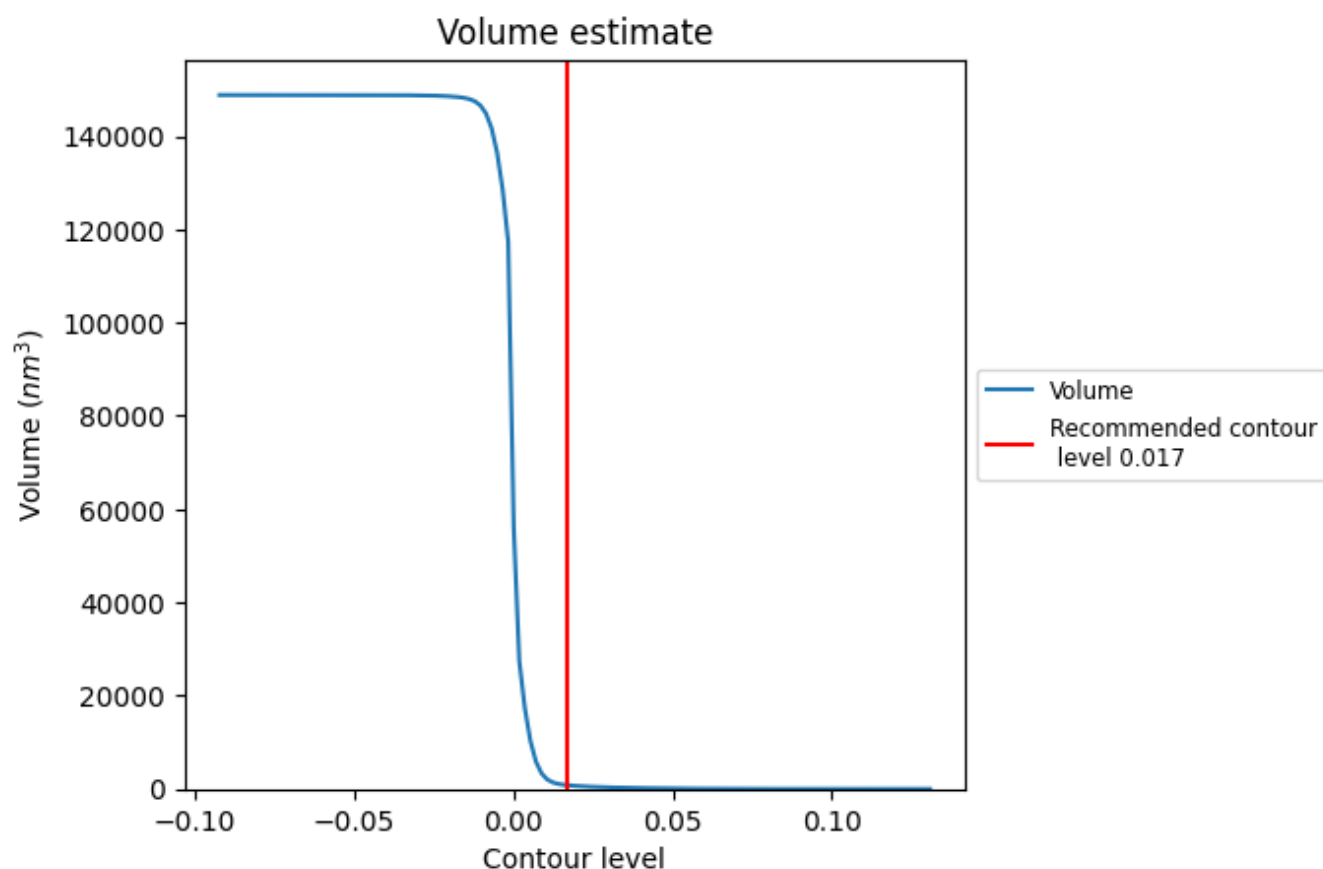
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

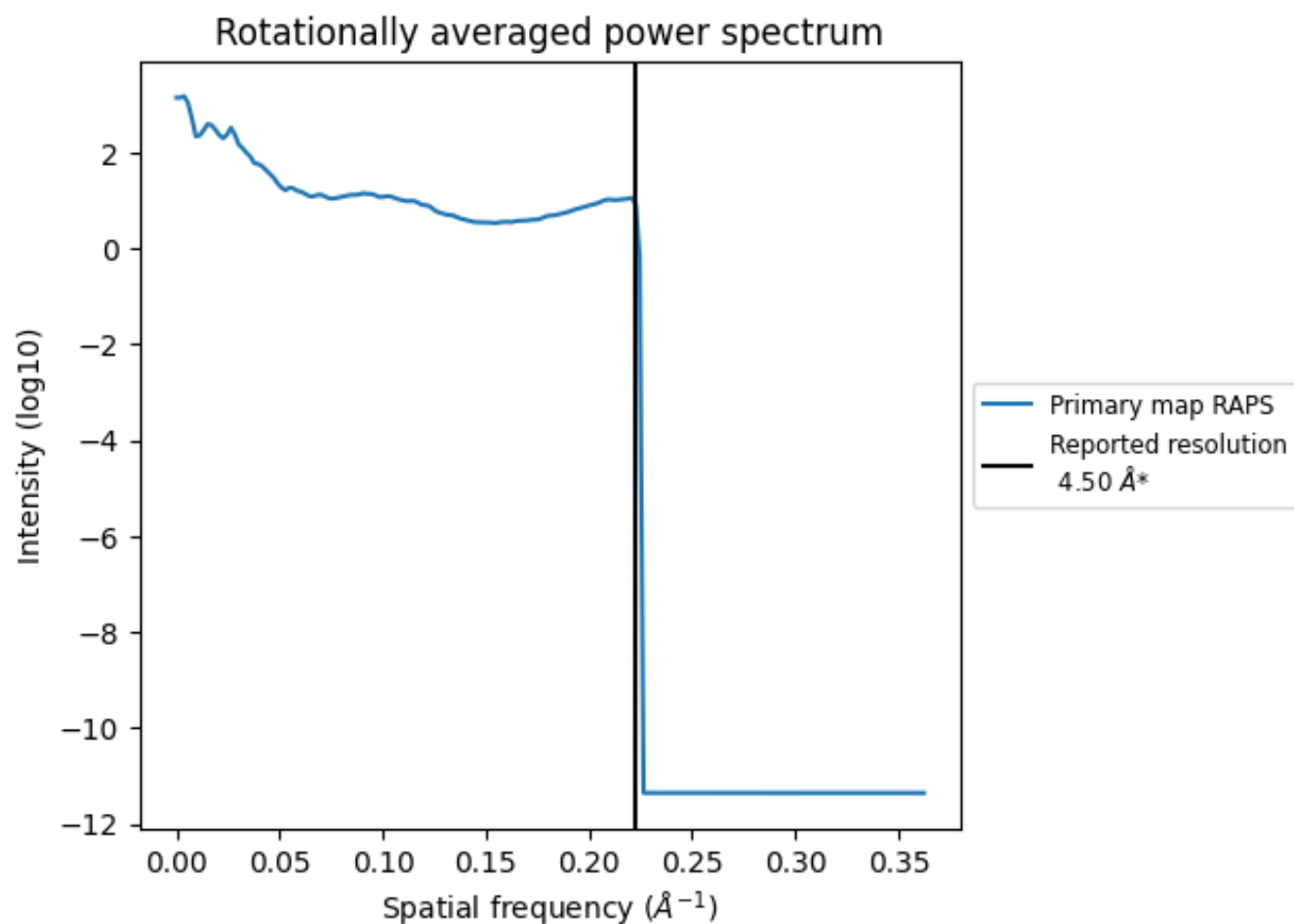
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ



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

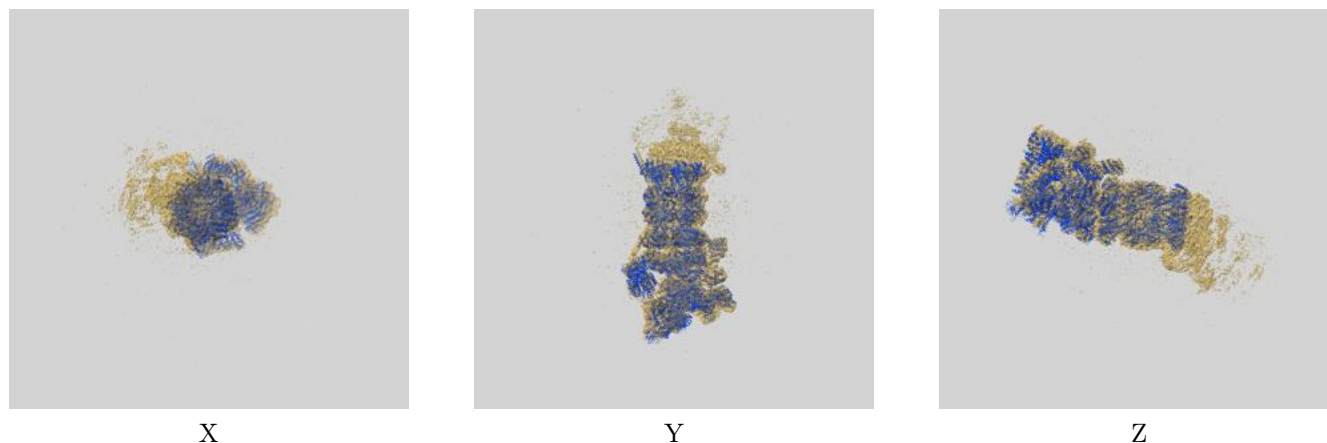
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

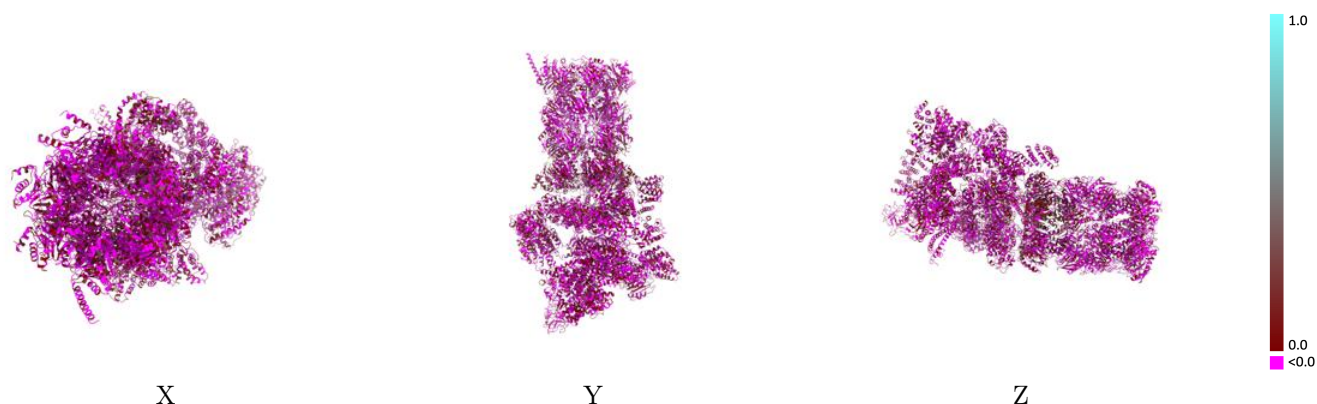
This section contains information regarding the fit between EMDB map EMD-3535 and PDB model 6FVU. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



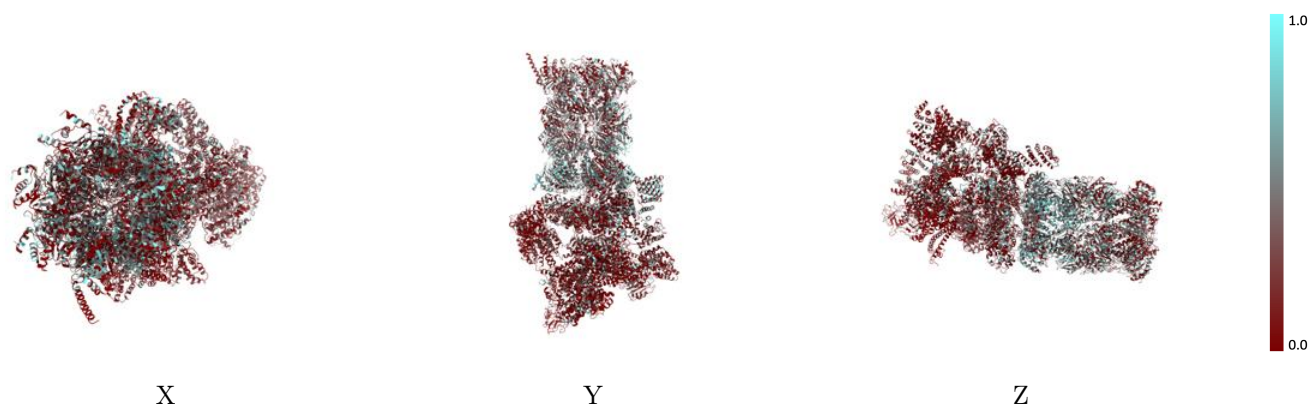
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



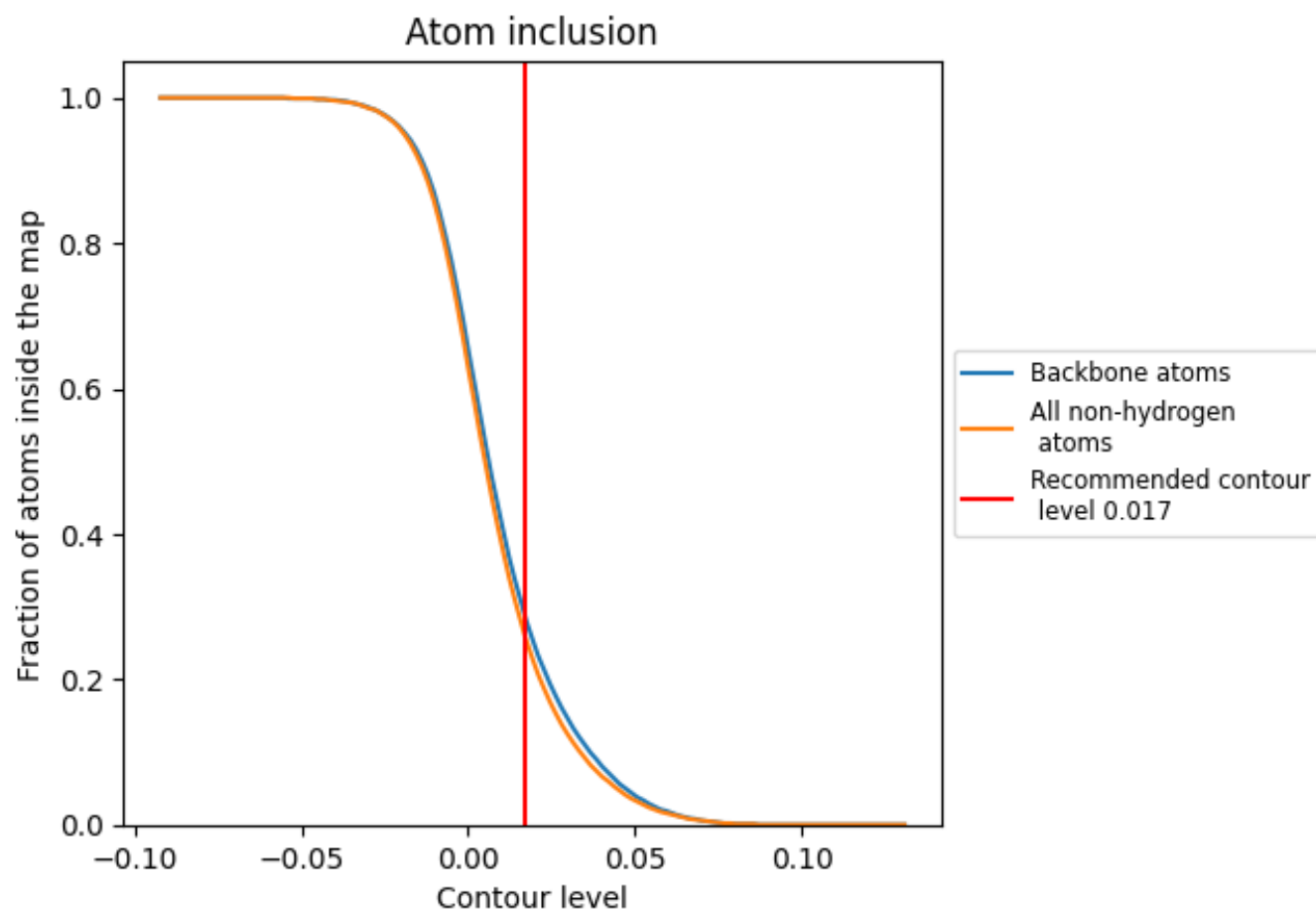
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 29% of all backbone atoms, 26% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.2600	 0.0040
1	 0.5100	 0.0490
2	 0.3850	 -0.0120
3	 0.3540	 -0.0510
4	 0.4600	 0.0150
5	 0.4510	 0.0080
6	 0.3900	 -0.0200
7	 0.3790	 -0.0460
A	 0.5480	 0.1340
B	 0.4570	 0.0990
C	 0.4360	 0.0400
D	 0.5720	 0.1650
E	 0.5240	 0.1260
F	 0.4120	 0.0270
G	 0.4260	 0.0230
H	 0.2040	 0.0000
I	 0.1900	 -0.0150
J	 0.1930	 0.0020
K	 0.2450	 0.0040
L	 0.2000	 -0.0180
M	 0.1930	 0.0090
N	 0.1600	 0.0000
O	 0.1770	 0.0090
P	 0.2650	 0.0170
Q	 0.2030	 -0.0040
R	 0.1730	 -0.0050
S	 0.1350	 -0.0030
T	 0.1010	 0.0060
U	 0.1760	 -0.0150
V	 0.1430	 -0.0180
W	 0.1360	 0.0160
X	 0.0060	 0.0150
Y	 0.2120	 0.0080
Z	 0.0570	 0.0060
a	 0.2950	 -0.0420



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Chain	Atom inclusion	Q-score
b	 0.2800	 -0.0060
c	 0.3260	 0.0140
d	 0.2580	 -0.0230
e	 0.2510	 -0.0090
f	 0.2780	 -0.0350
g	 0.3170	 -0.0010
h	 0.3000	 -0.0610
i	 0.3190	 -0.0170
j	 0.3250	 -0.0420
k	 0.3060	 -0.0220
l	 0.3290	 -0.0330
m	 0.3200	 -0.0410
n	 0.3400	 -0.0260