



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:15 AM UTC

PDB ID : 6FVV / pdb_00006fvv
EMDB ID : EMD-4321
Title : 26S proteasome, s3 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 : 5.40 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:

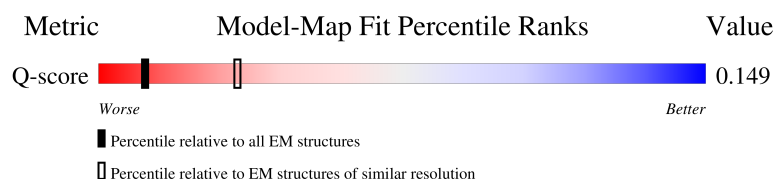
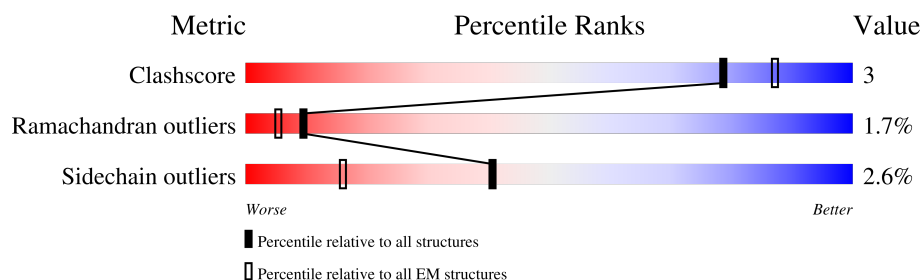
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 5.40 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	538 (4.90 - 5.90)

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	241	
1	a	241	
2	B	249	
2	b	249	

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Mol	Chain	Length	Quality of chain
3	C	244	
3	c	244	
4	D	251	
4	d	251	
5	E	244	
5	e	244	
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	417	
29	I	385	
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	ADP	H	501	-	-	X	-
36	ATP	I	501	-	-	X	-
36	ATP	K	501	-	-	X	-
36	ATP	L	501	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 110420 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	241	Total	C	N	O	S	0	0
			1908	1214	320	366	8		
1	A	241	Total	C	N	O	S	0	0
			1908	1214	320	366	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	244	Total	C	N	O	S	0	0
			1883	1176	316	384	7		
5	E	244	Total	C	N	O	S	0	0
			1883	1176	316	384	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	417	Total	C	N	O	S	0	0
			3234	2008	578	632	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	I	385	Total	C	N	O	S	0	0
			3022	1899	508	598	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		

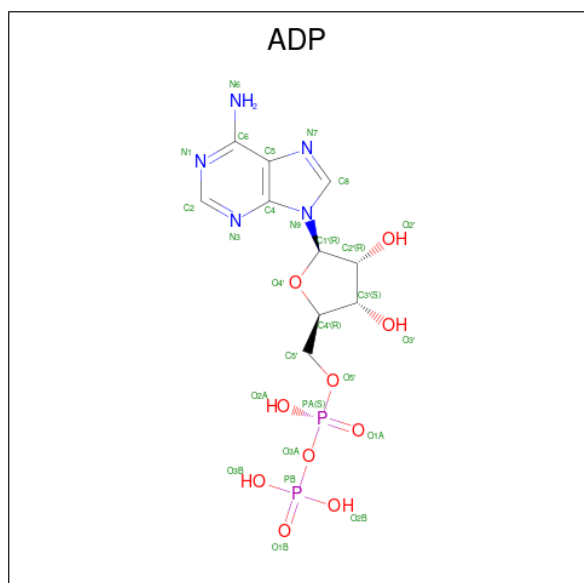
- Molecule 32 is a protein called 26S proteasome regulatory subunit 6A.

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'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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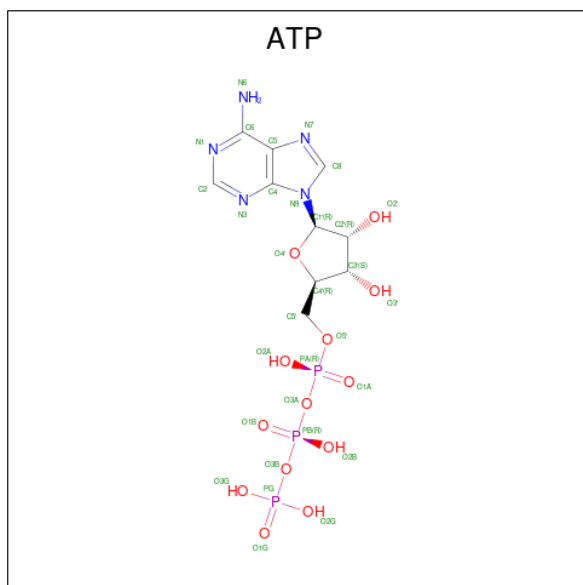
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Mol	Chain	Residues	Atoms					AltConf
34	M	1	Total	C	N	O	P	0
			27	10	5	10	2	

- 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'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

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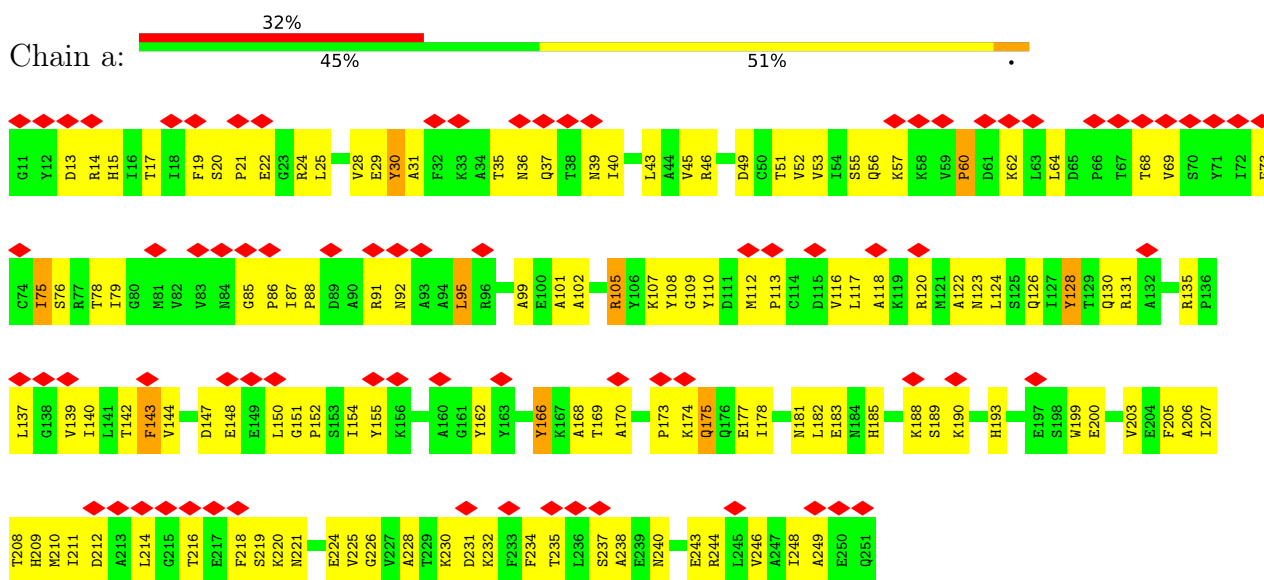
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Mol	Chain	Residues	Atoms					AltConf
36	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

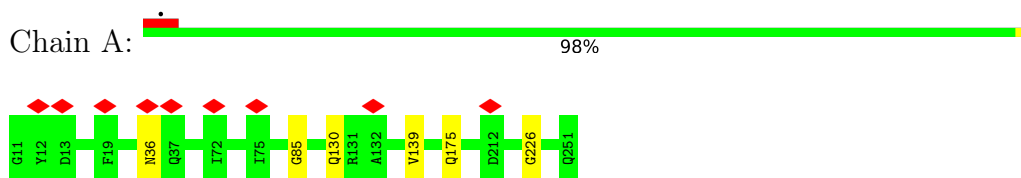
3 Residue-property plots

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.

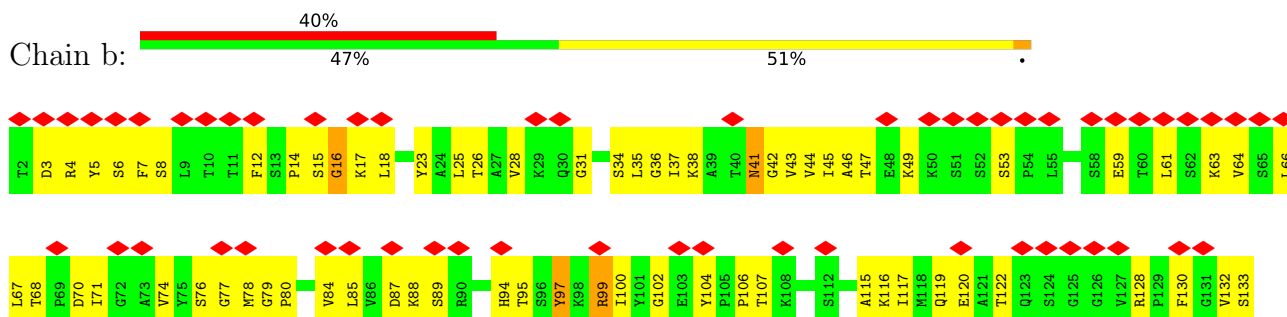
• Molecule 1: Proteasome subunit alpha type-1

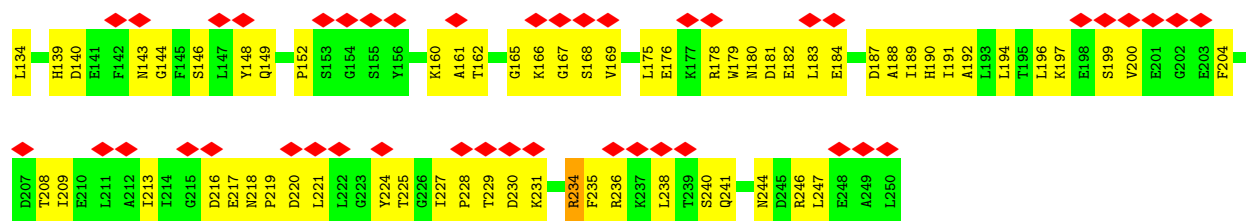


• Molecule 1: Proteasome subunit alpha type-1

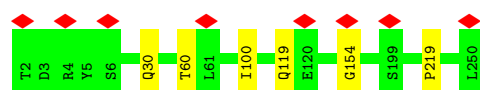


• Molecule 2: Proteasome subunit alpha type-2

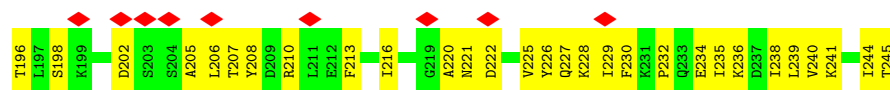
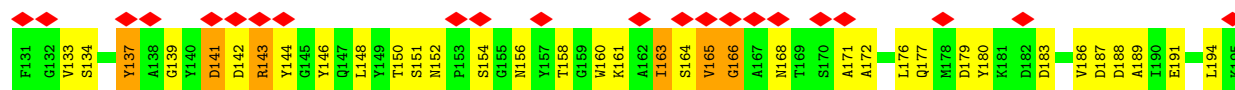
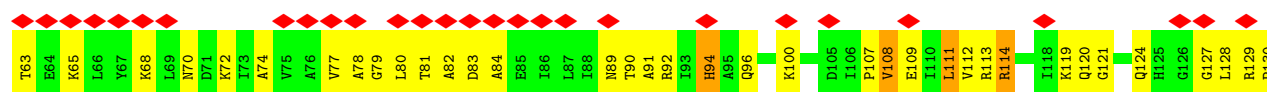
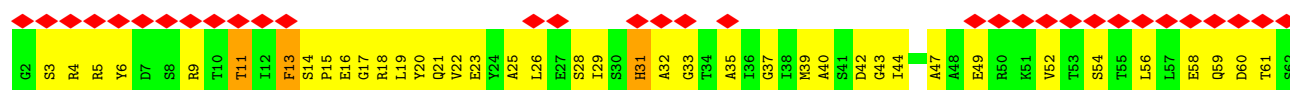




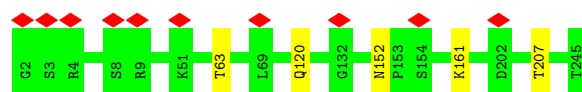
• Molecule 2: Proteasome subunit alpha type-2



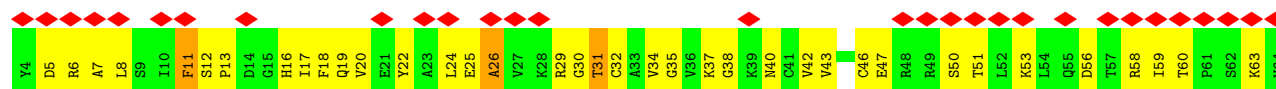
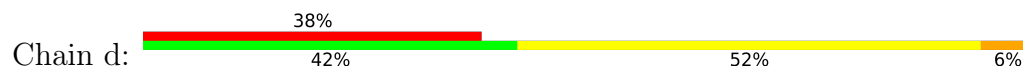
• Molecule 3: Proteasome subunit alpha type-3

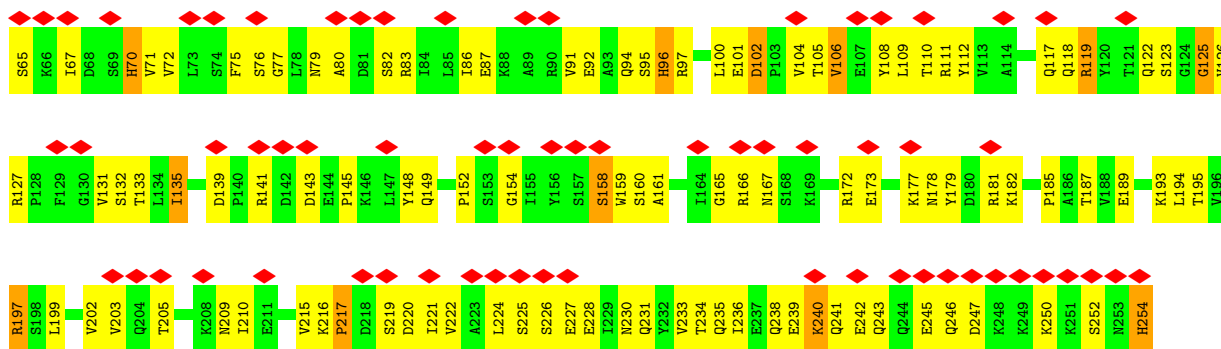


• Molecule 3: Proteasome subunit alpha type-3



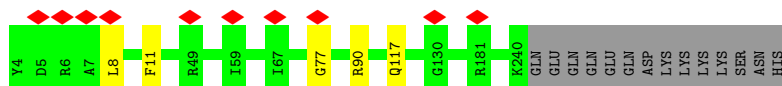
• Molecule 4: Proteasome subunit alpha type-4





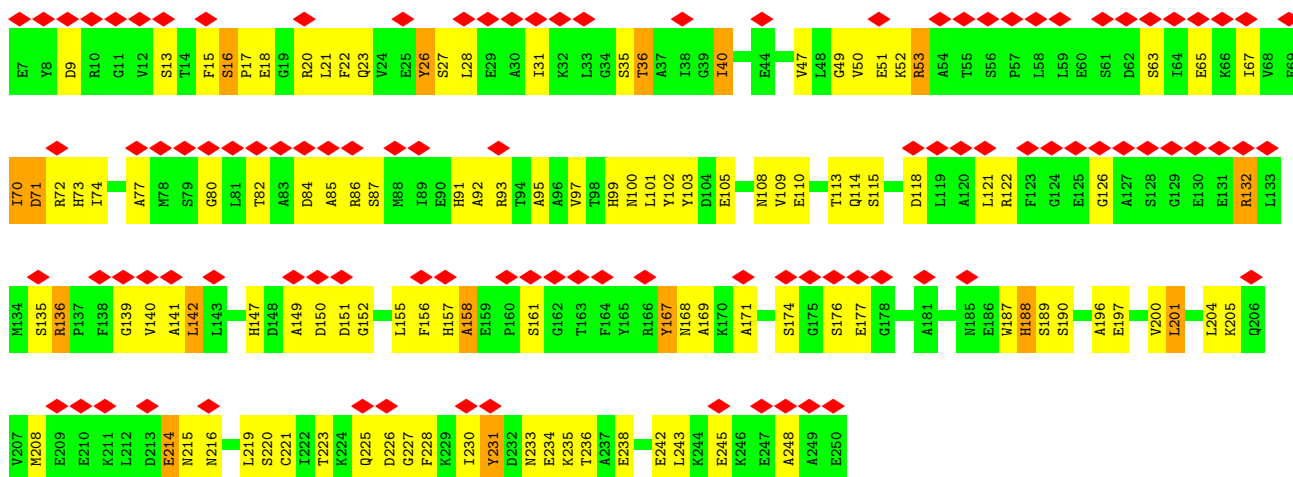
• Molecule 4: Proteasome subunit alpha type-4

Chain D: 92% • 6%



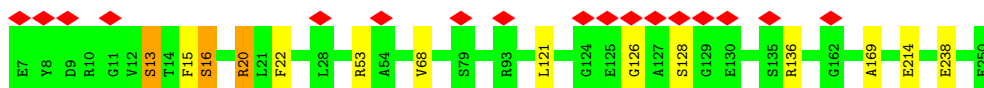
• Molecule 5: Proteasome subunit alpha type-5

Chain e: 42% 52% 41% 7%



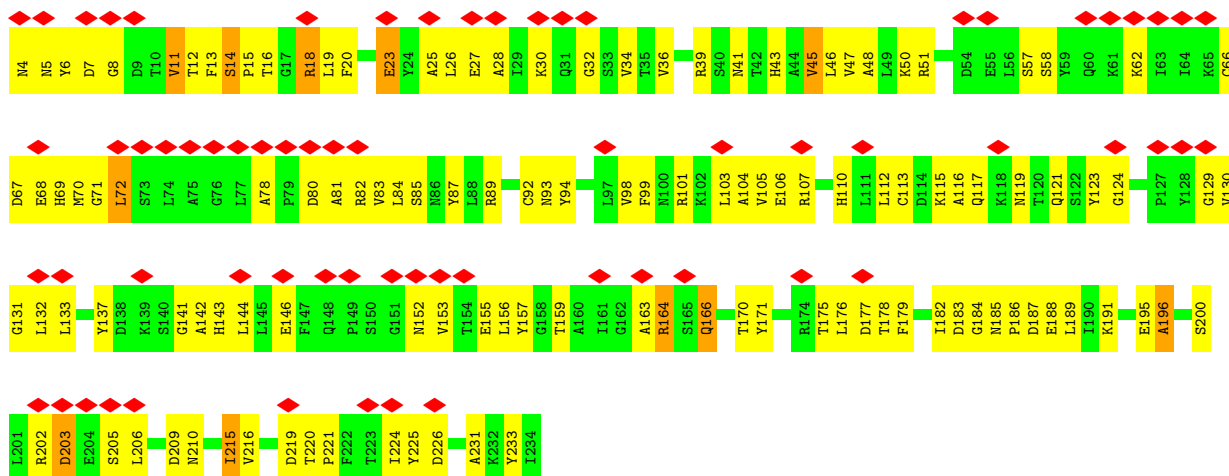
• Molecule 5: Proteasome subunit alpha type-5

Chain E: 7% 94% 5%



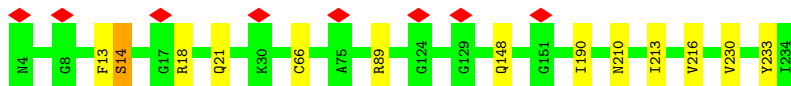
• Molecule 6: Proteasome subunit alpha type-6

Chain f: 29% 45% 50% 5%



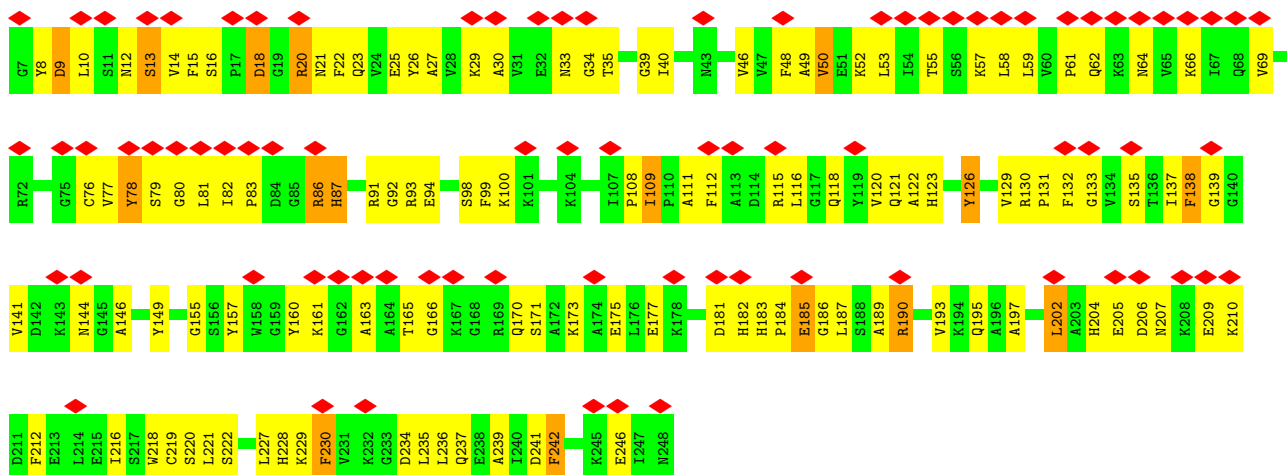
- Molecule 6: Proteasome subunit alpha type-6

Chain F: 94% 5%



- Molecule 7: Probable proteasome subunit alpha type-7

Chain g: 33% 46% 47% 7%

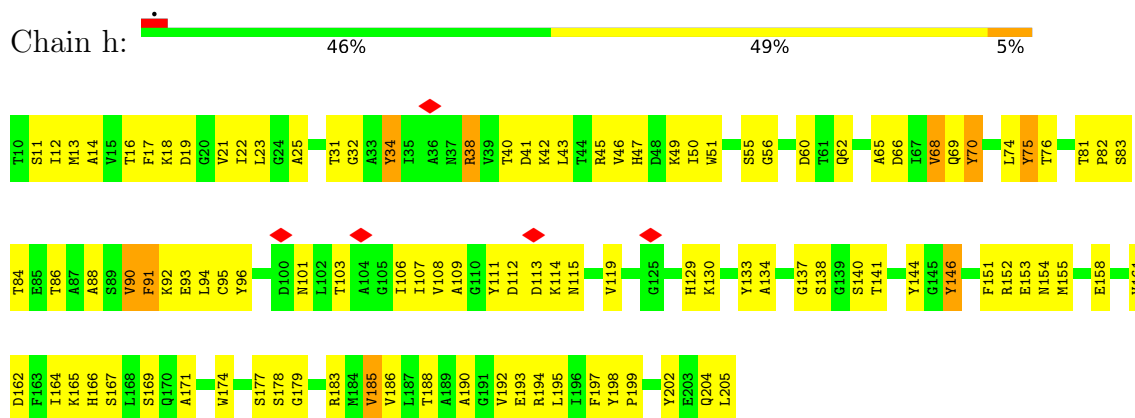


- Molecule 7: Probable proteasome subunit alpha type-7

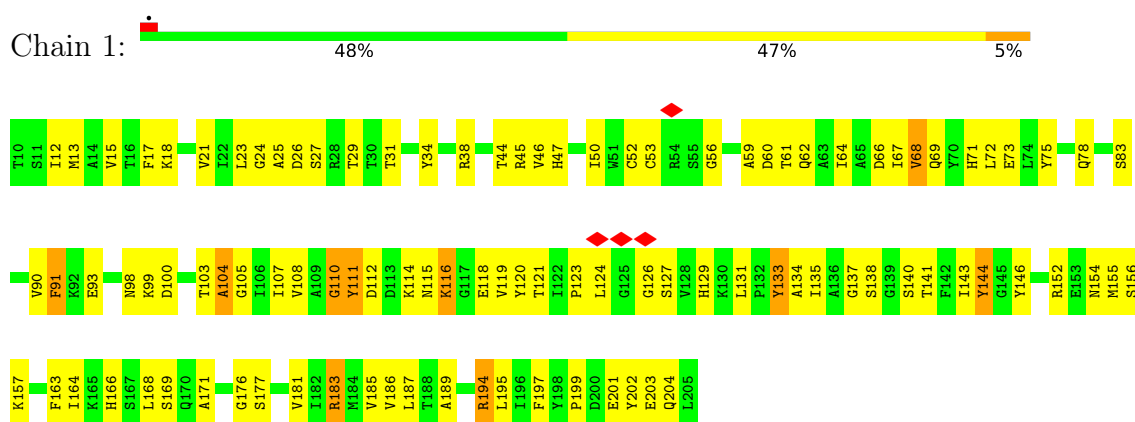
Chain G: 95% 5%



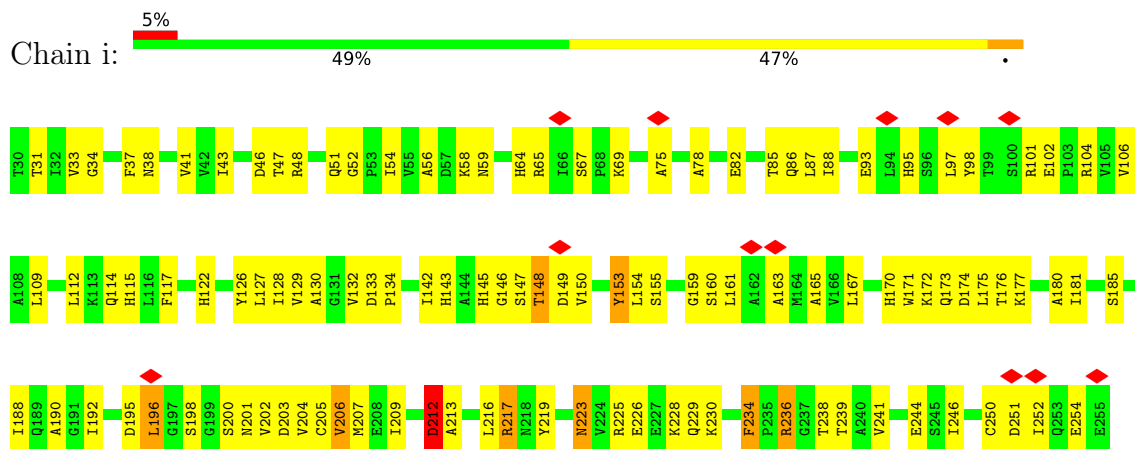
- Molecule 8: Proteasome subunit beta type-1



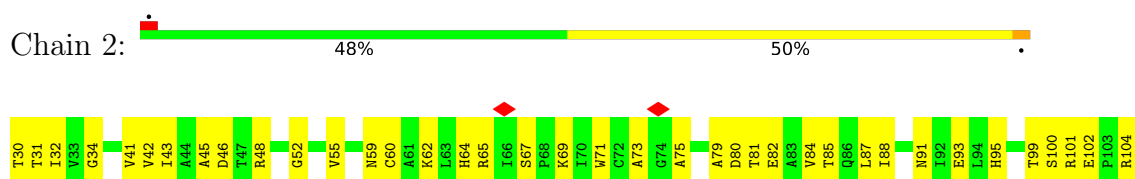
• Molecule 8: Proteasome subunit beta type-1

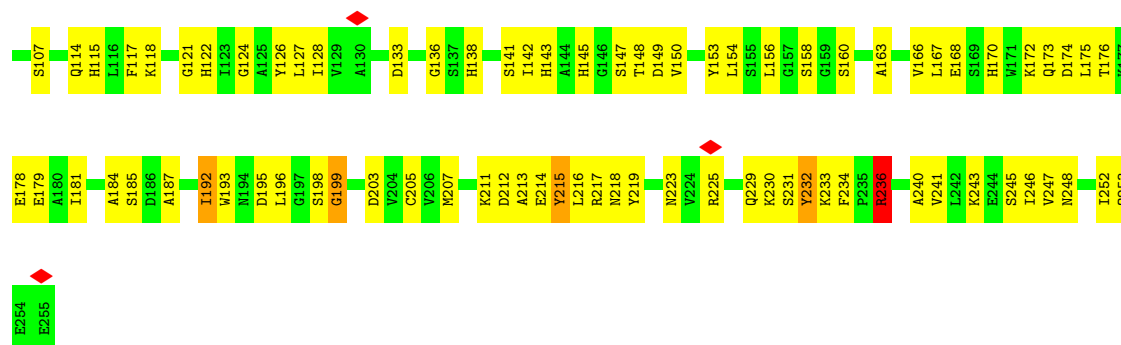


• Molecule 9: Proteasome subunit beta type-2

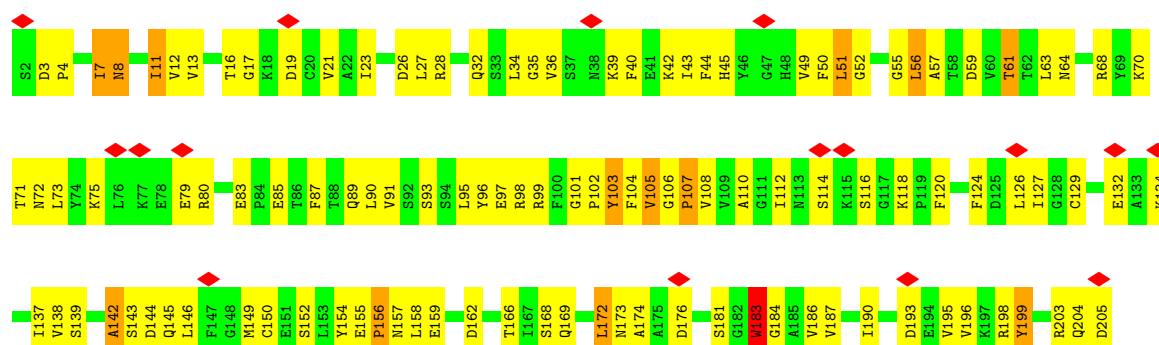
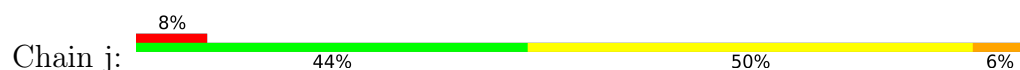


• Molecule 9: Proteasome subunit beta type-2

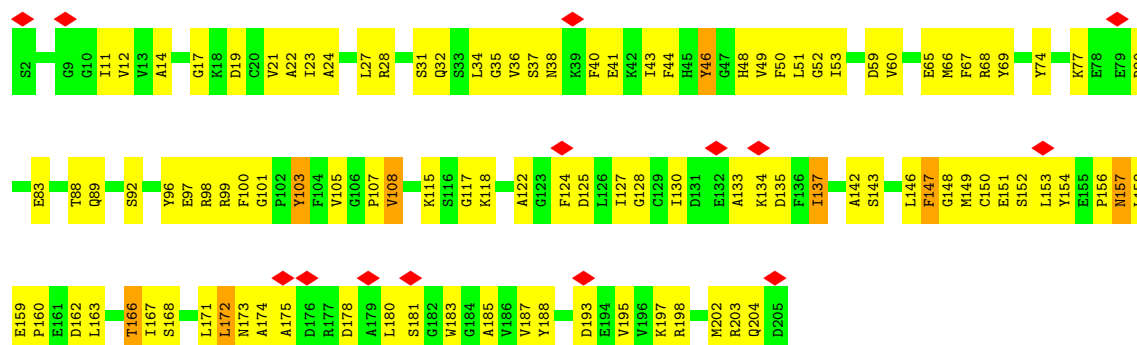




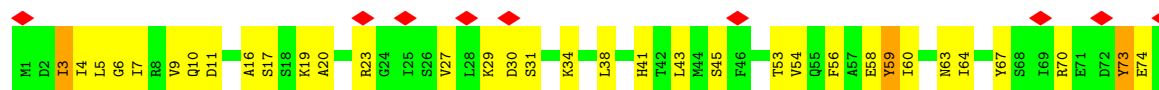
• Molecule 10: Proteasome subunit beta type-3

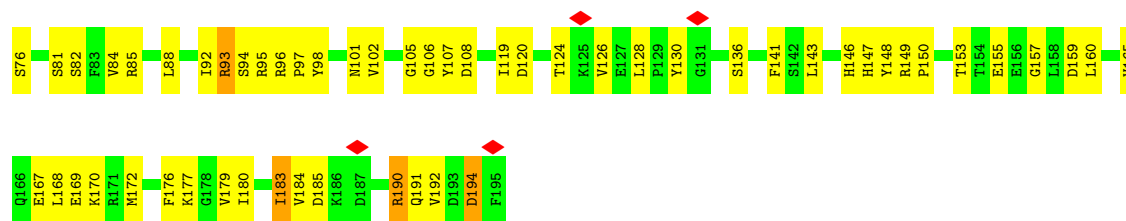


• Molecule 10: Proteasome subunit beta type-3

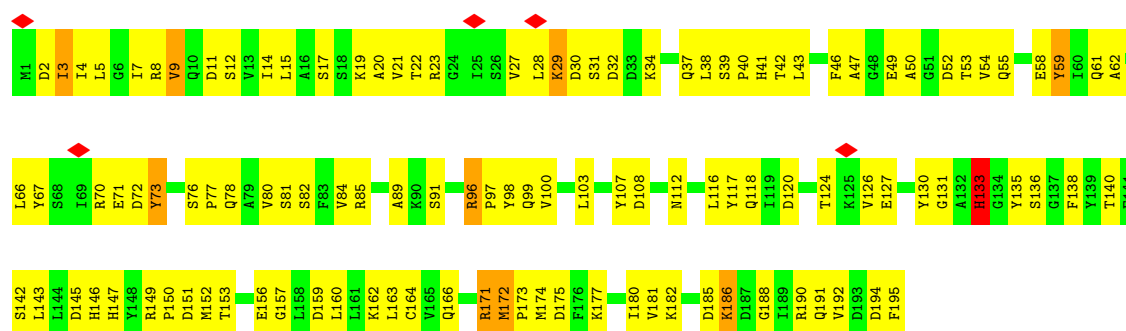


• Molecule 11: Proteasome subunit beta type-4

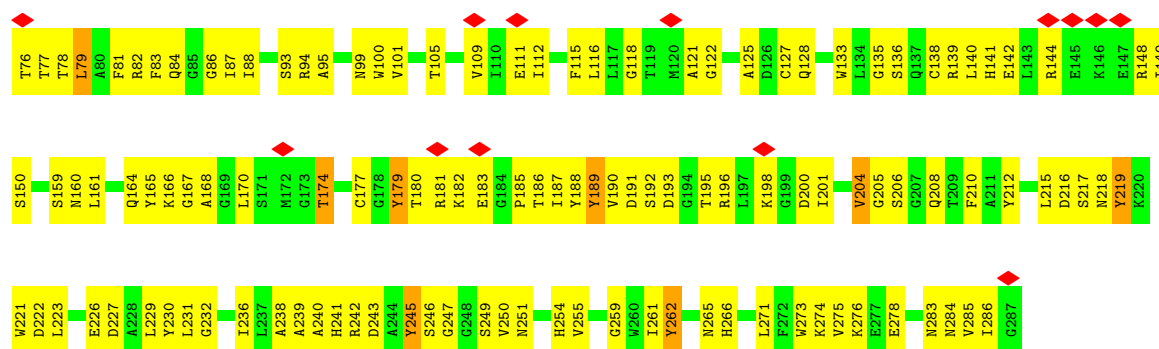




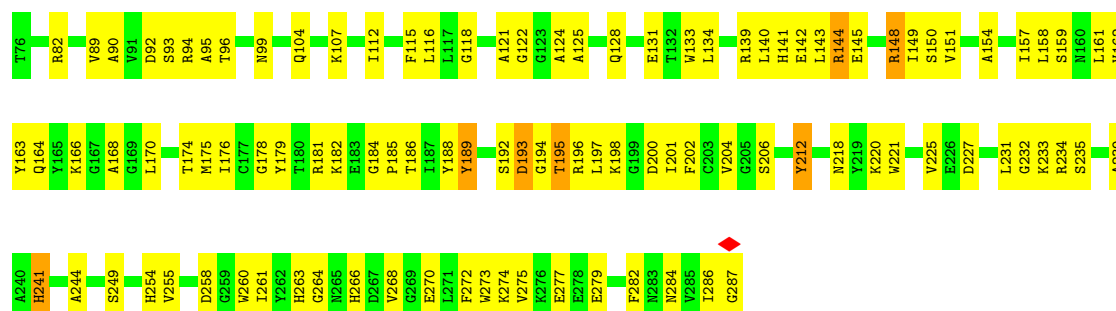
• Molecule 11: Proteasome subunit beta type-4



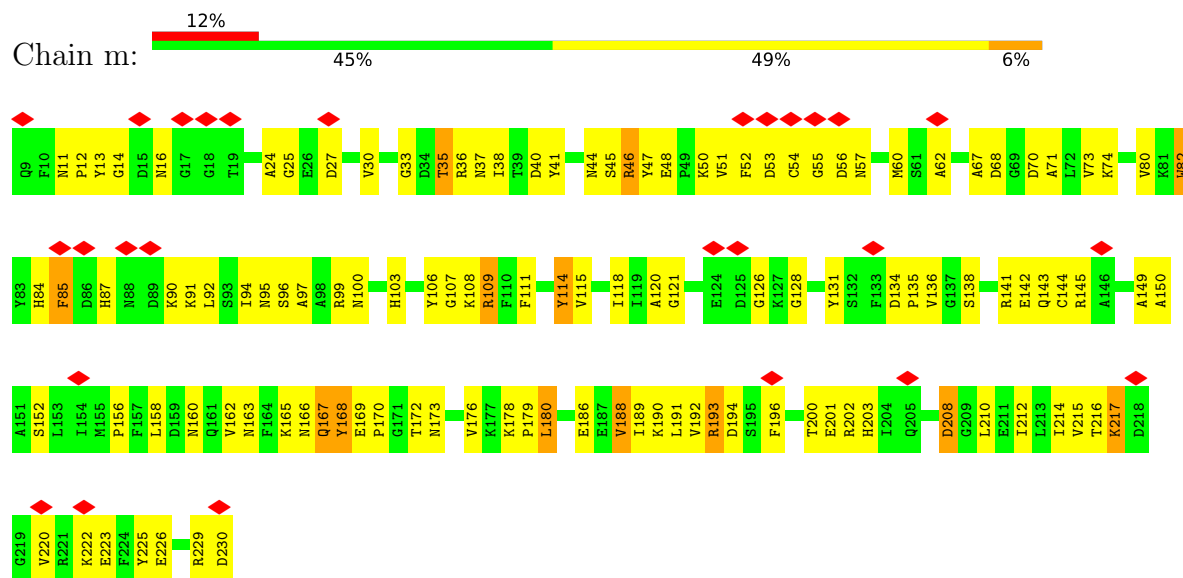
• Molecule 12: Proteasome subunit beta type-5



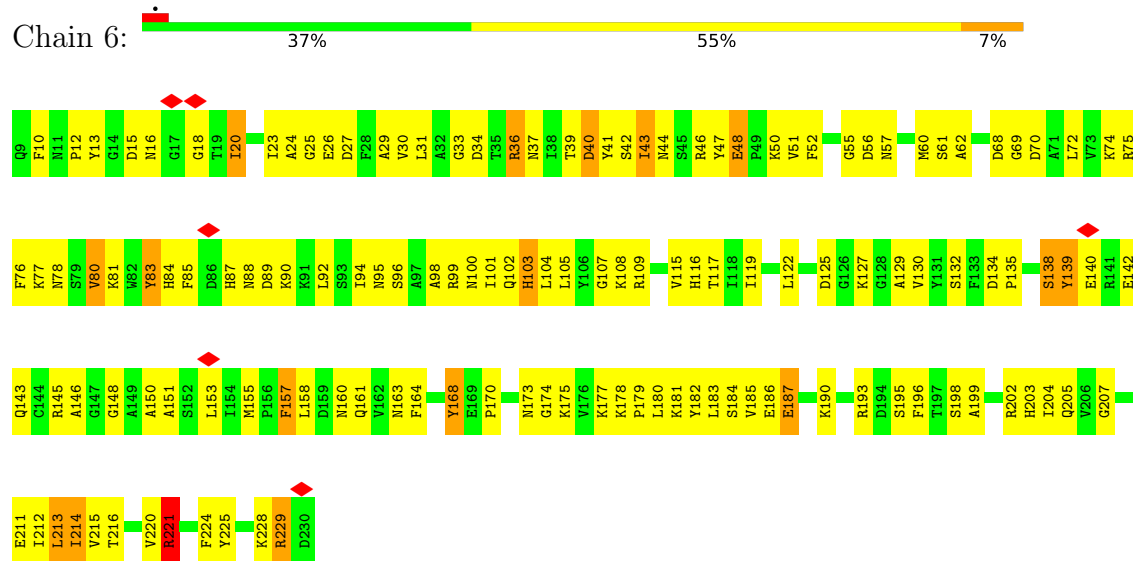
• Molecule 12: Proteasome subunit beta type-5



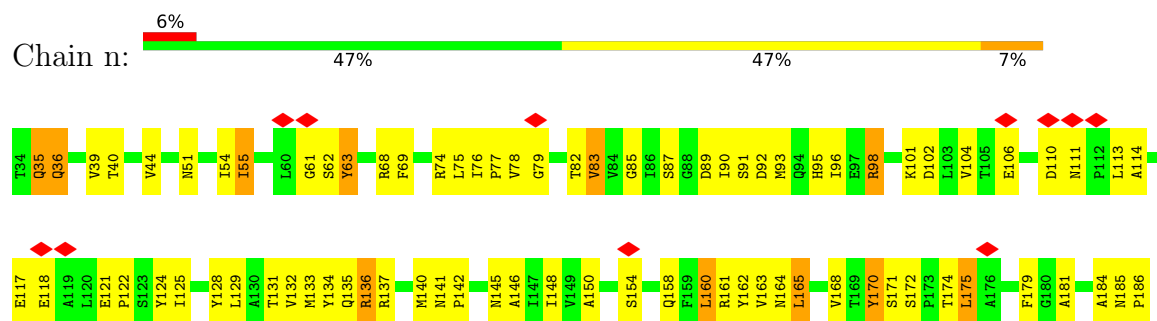
- Molecule 13: Proteasome subunit beta type-6



- Molecule 13: Proteasome subunit beta type-6



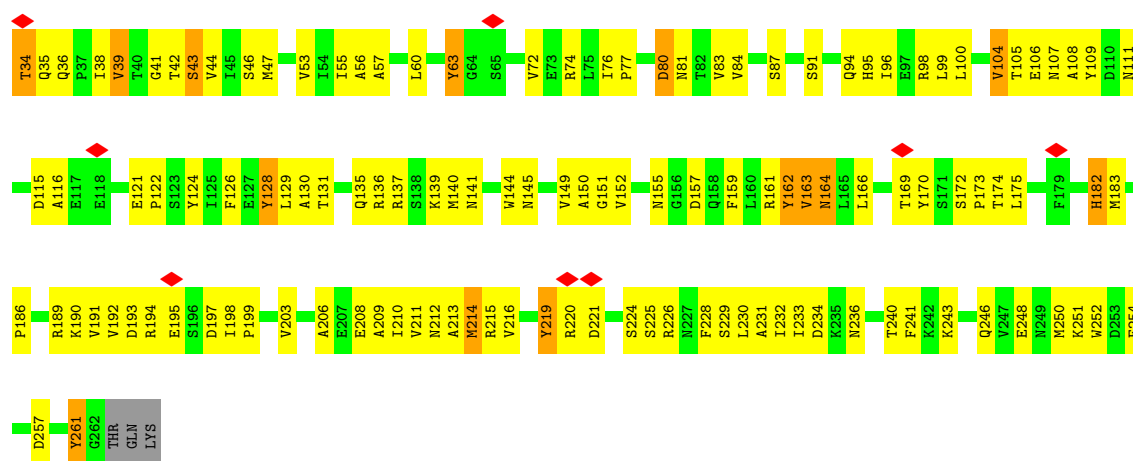
- Molecule 14: Proteasome subunit beta type-7





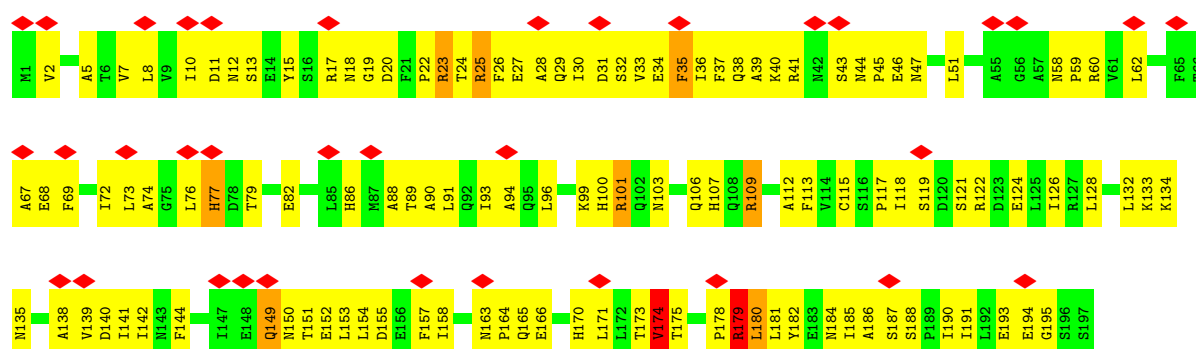
• Molecule 14: Proteasome subunit beta type-7

Chain 7: 45% 48% 6%



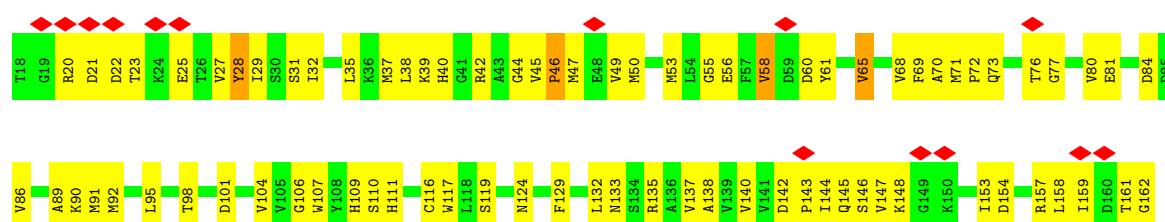
• Molecule 15: 26S proteasome regulatory subunit RPN10

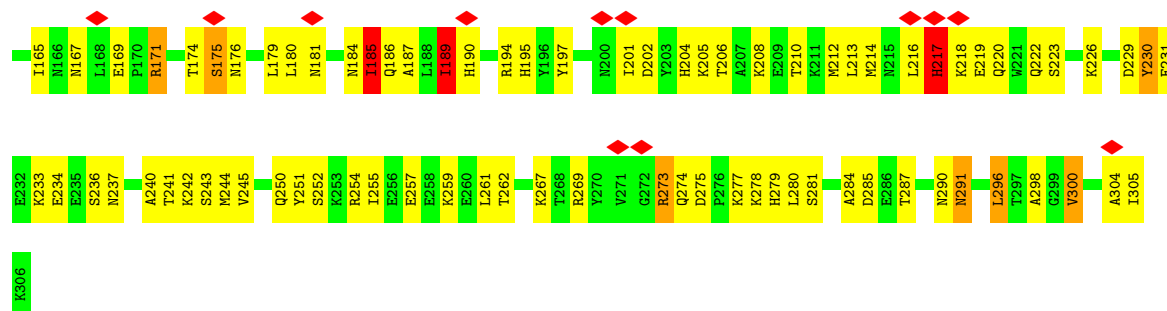
Chain W: 18% 38% 57%



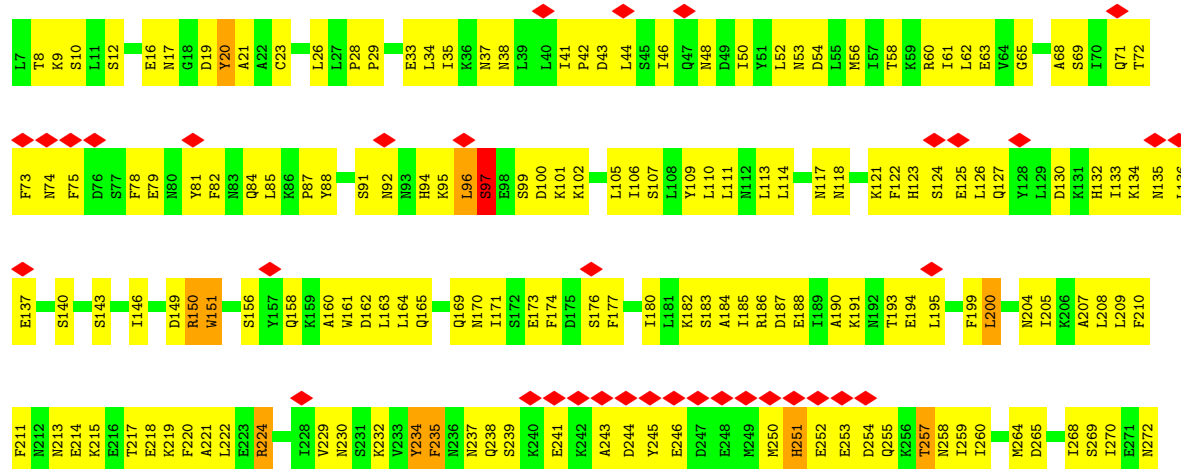
• Molecule 16: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain V: 9% 45% 50%

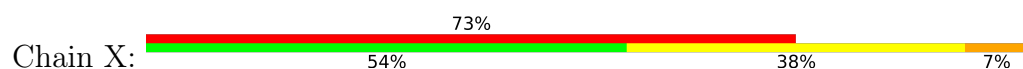




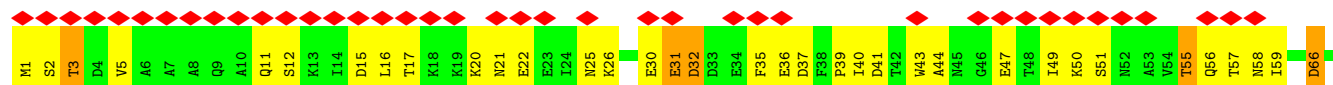
- Molecule 17: 26S proteasome regulatory subunit RPN12



- Molecule 18: 26S proteasome regulatory subunit RPN13

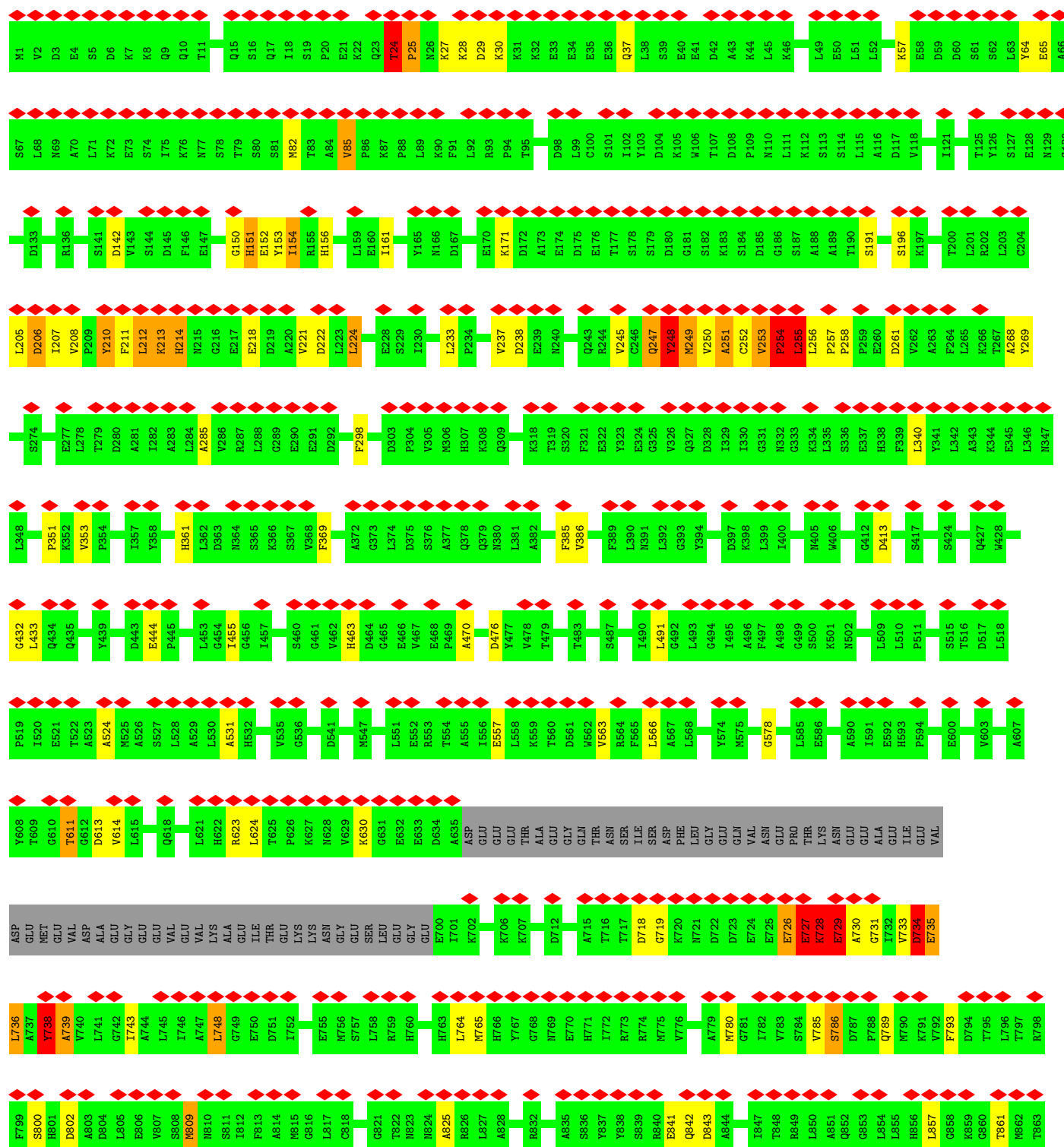
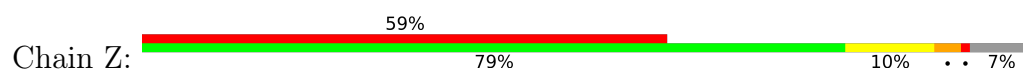


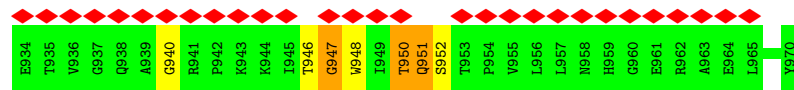
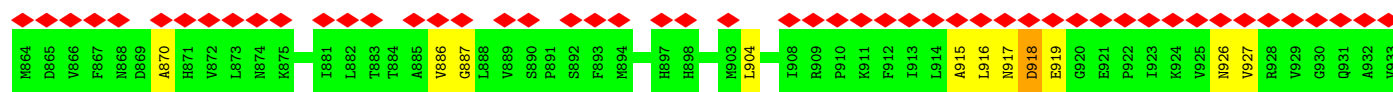
- Molecule 19: 26S proteasome complex subunit SEM1



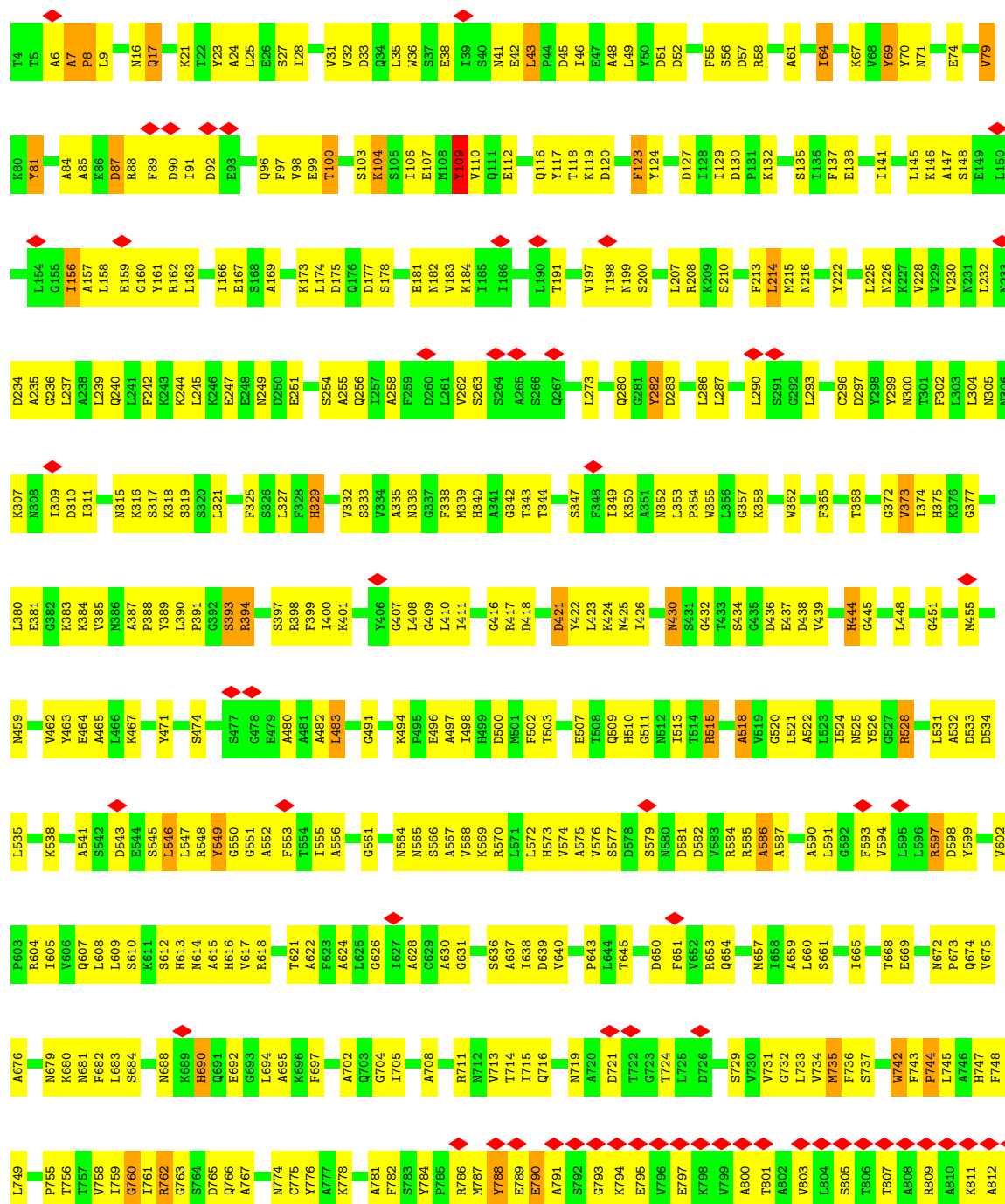


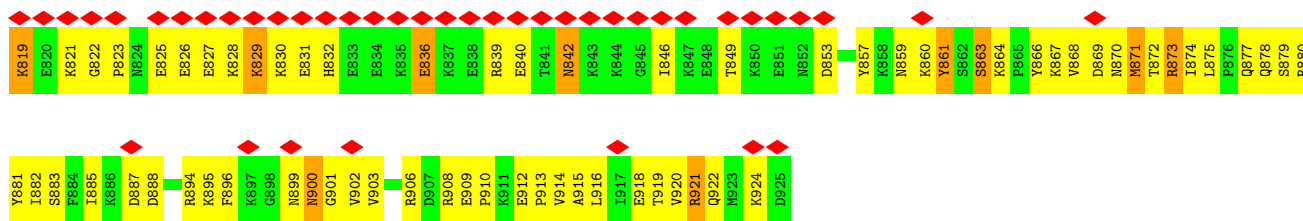
• Molecule 20: 26S proteasome regulatory subunit RPN1



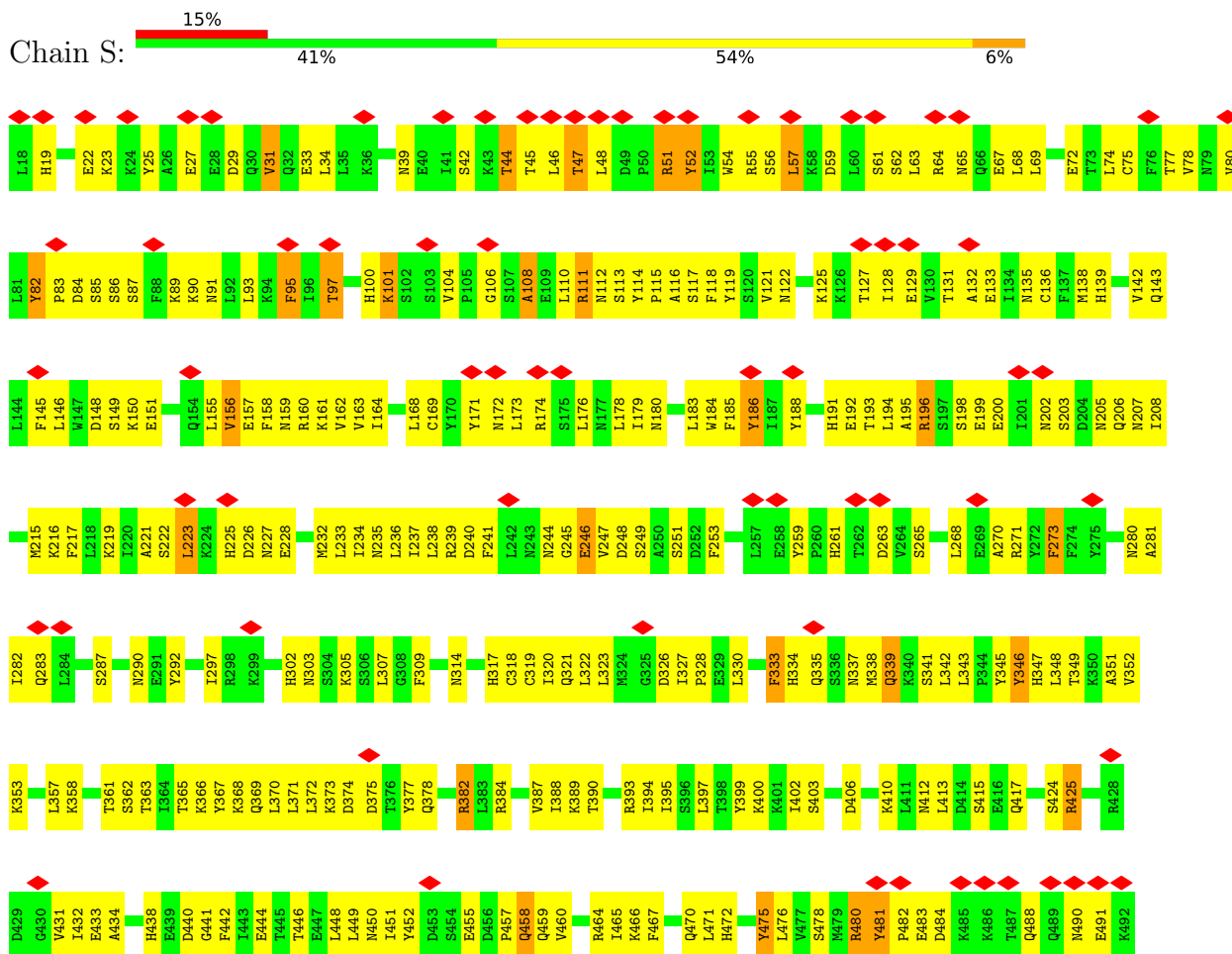


• Molecule 21: 26S proteasome regulatory subunit RPN2

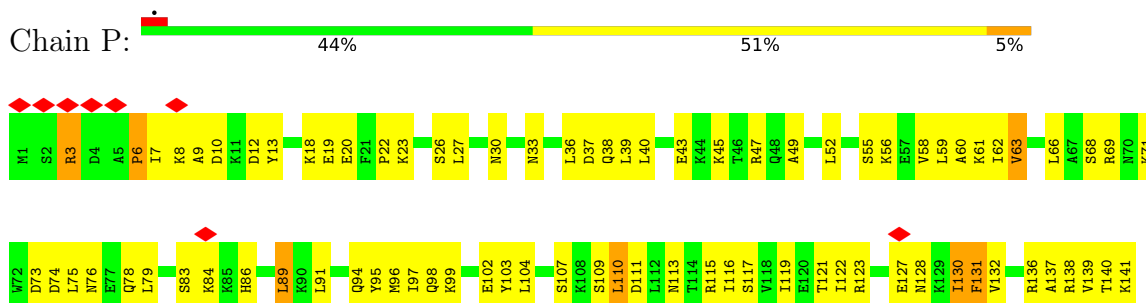


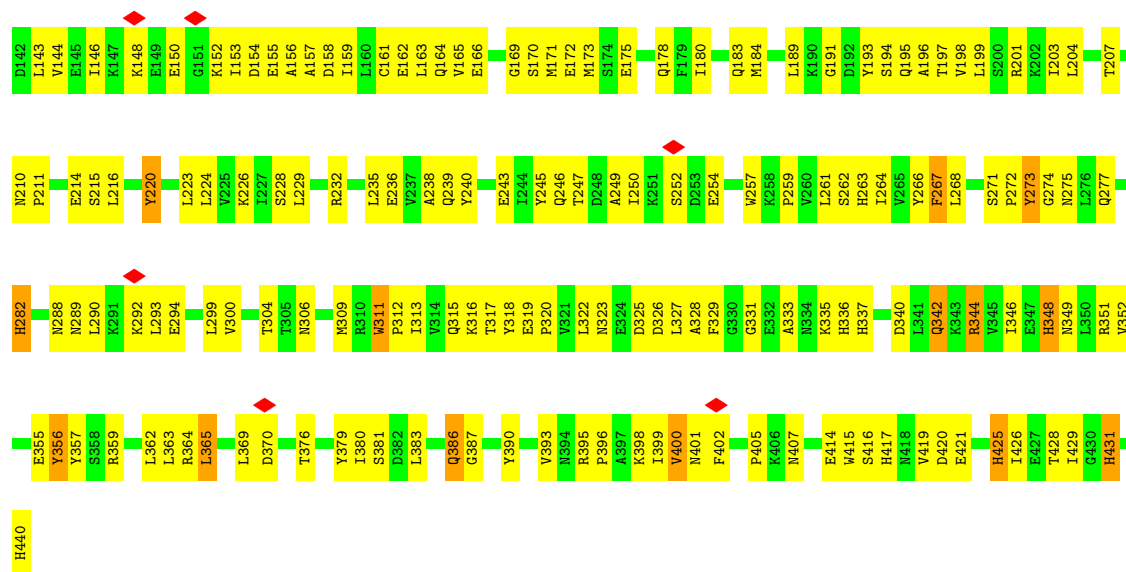


• Molecule 22: 26S proteasome regulatory subunit RPN3

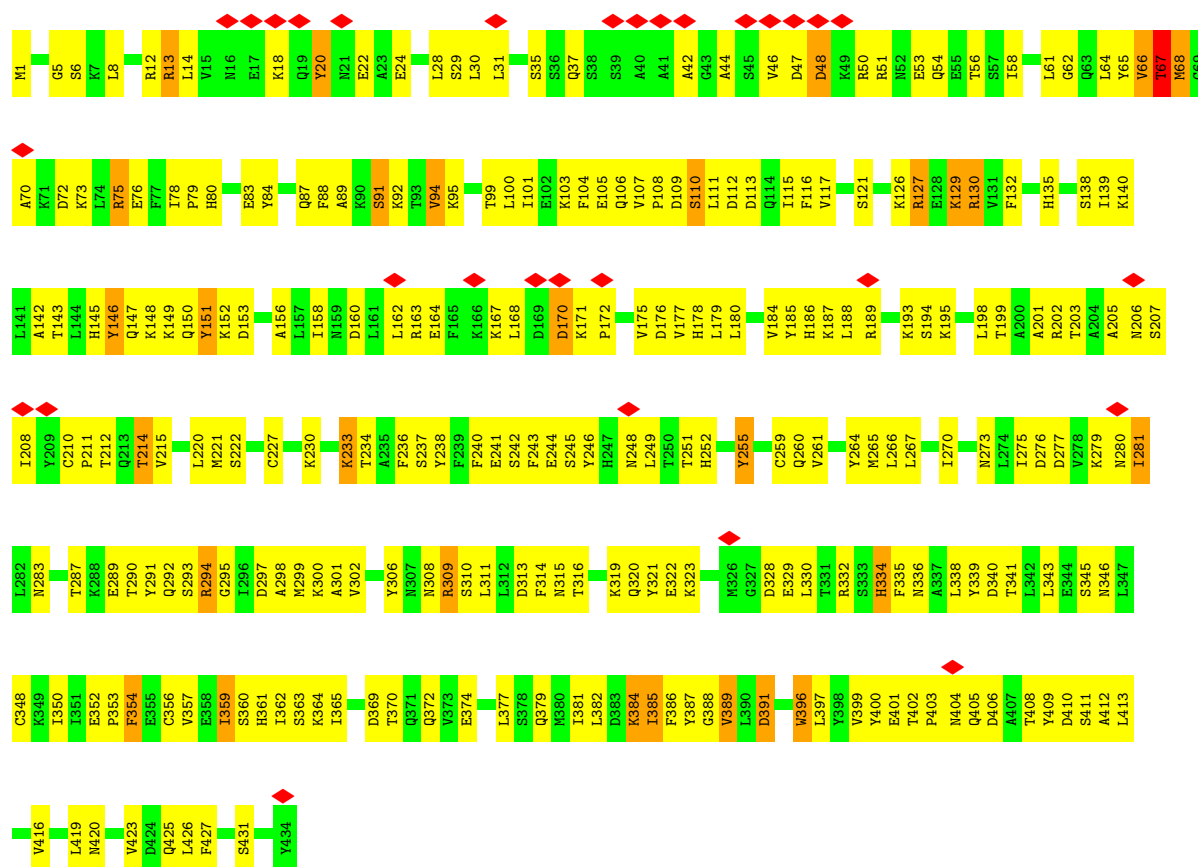


• Molecule 23: 26S proteasome regulatory subunit RPN5

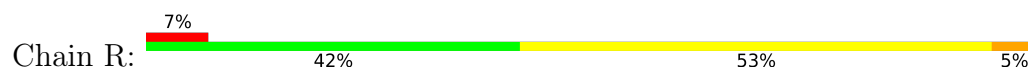


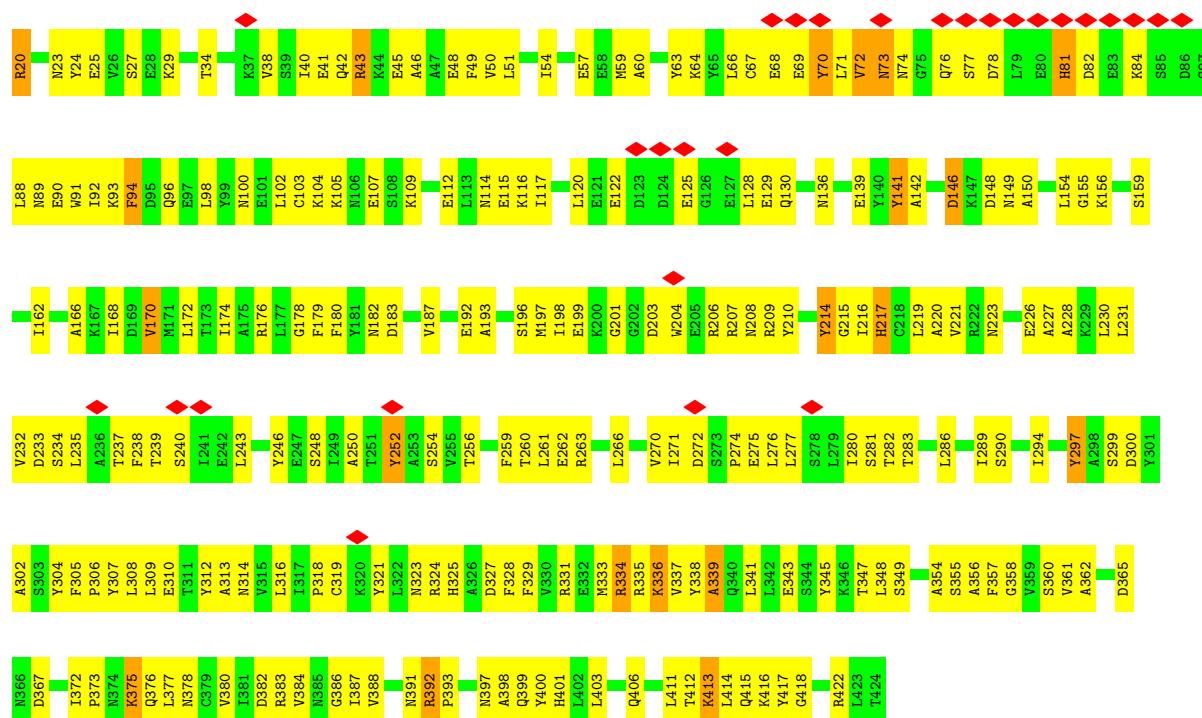


• Molecule 24: 26S proteasome regulatory subunit RPN6

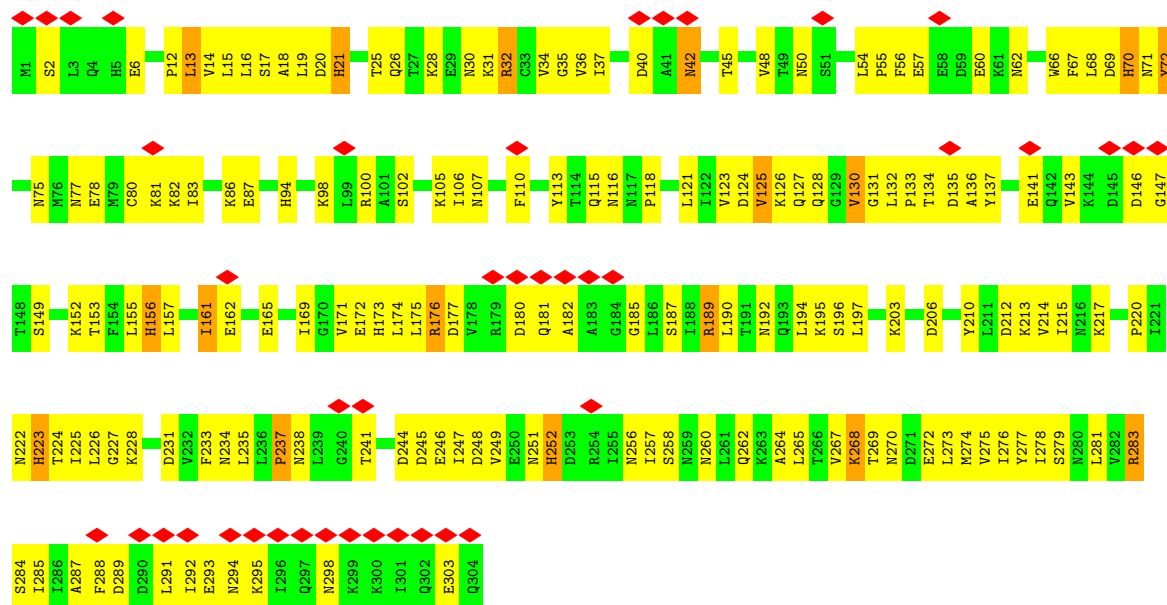
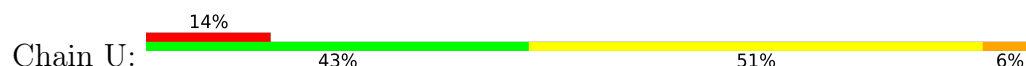


• Molecule 25: 26S proteasome regulatory subunit RPN7

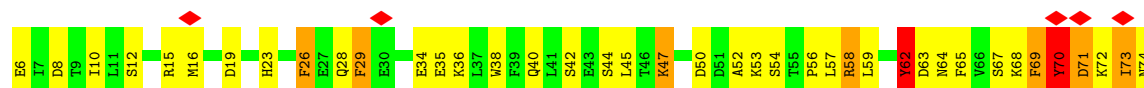


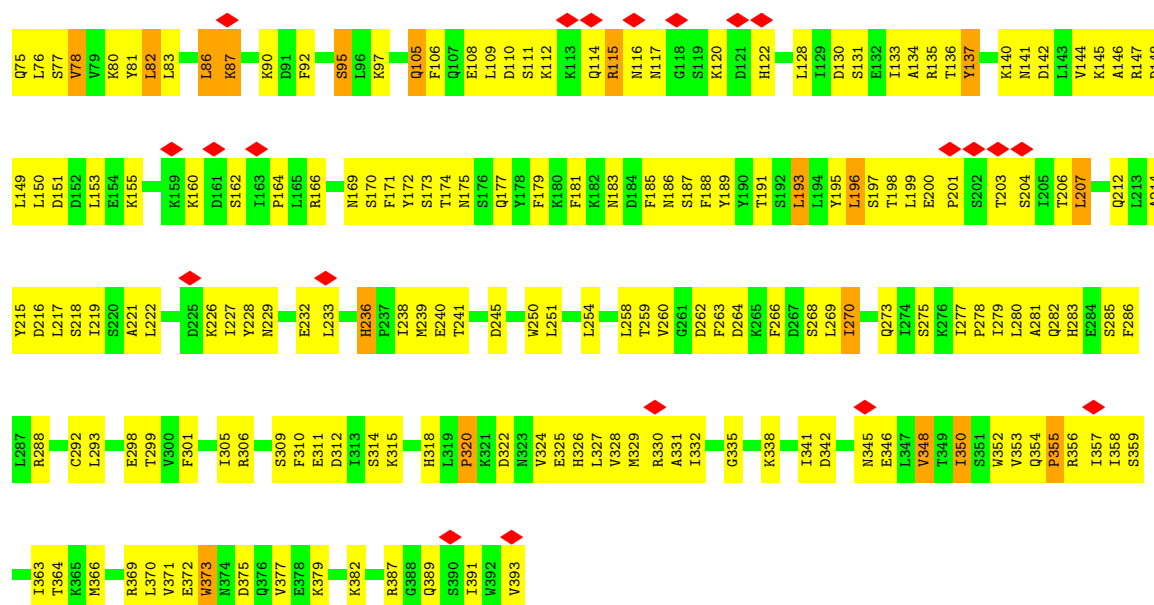


• Molecule 26: 26S proteasome regulatory subunit RPN8



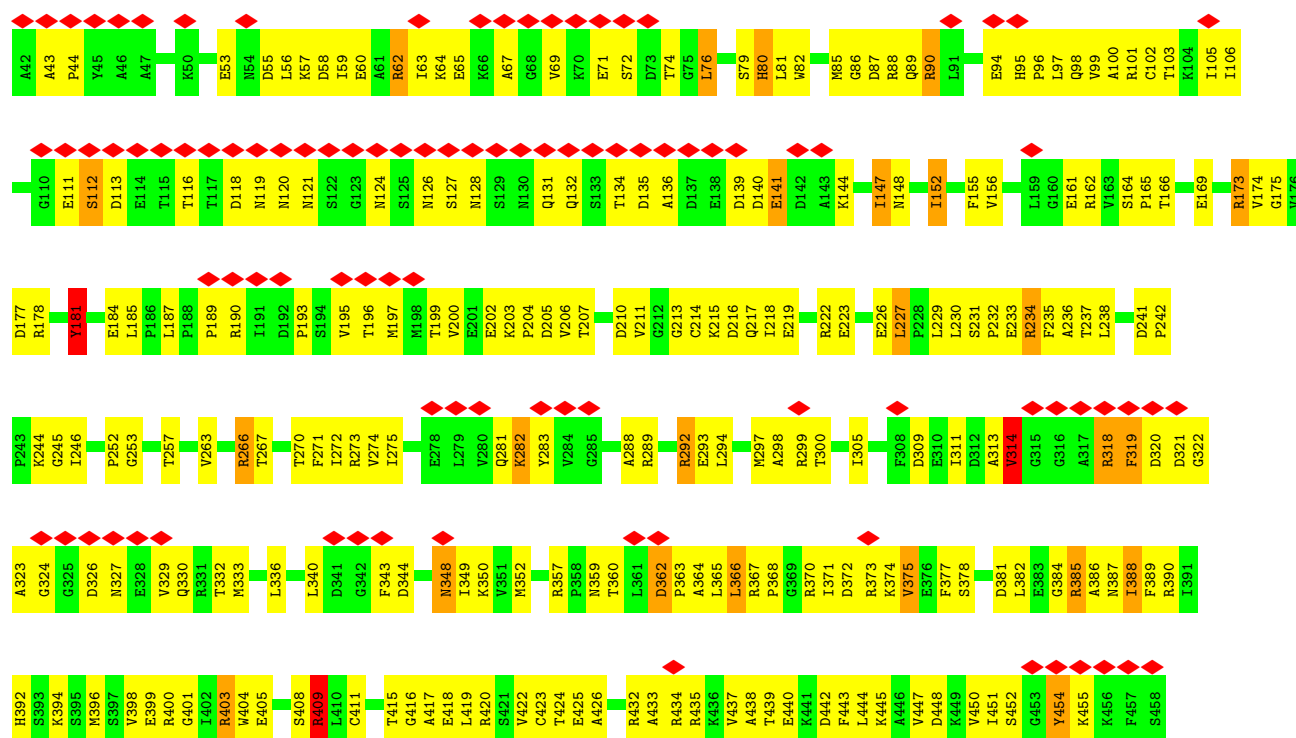
• Molecule 27: 26S proteasome regulatory subunit RPN9





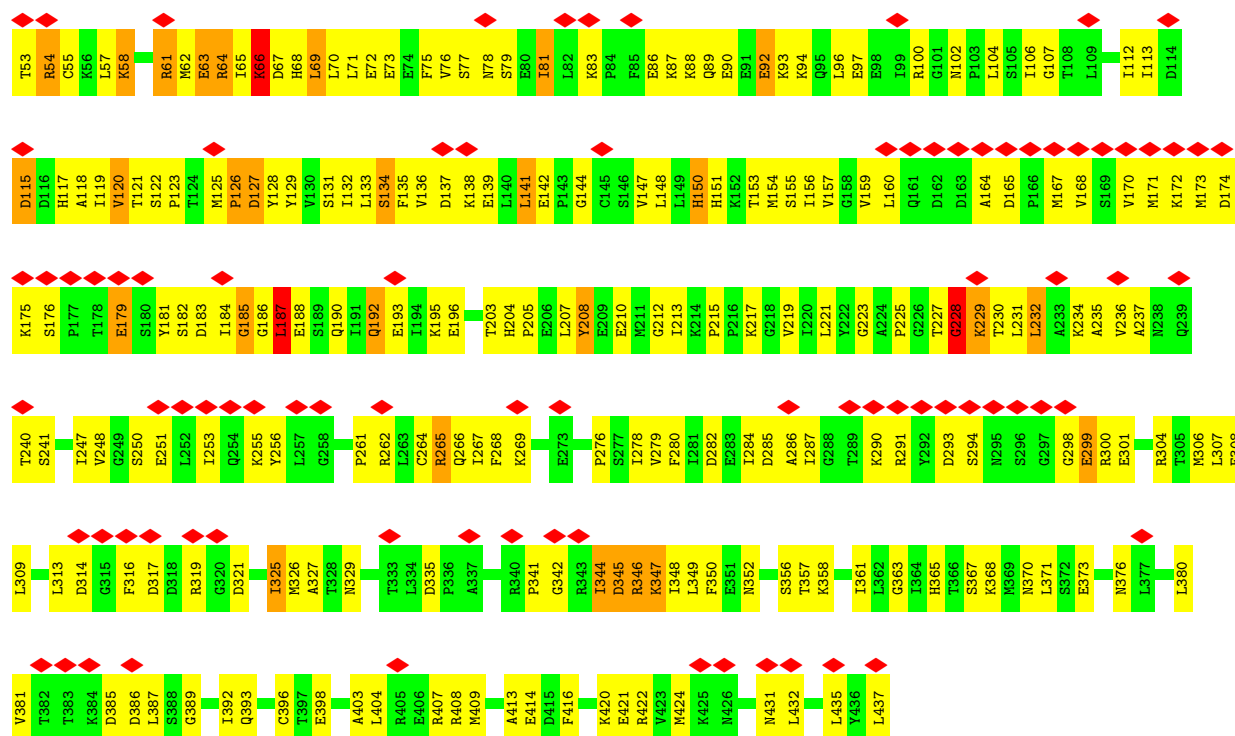
• Molecule 28: 26S proteasome regulatory subunit 7 homolog

Chain H: 23% 41% 52% 6% .

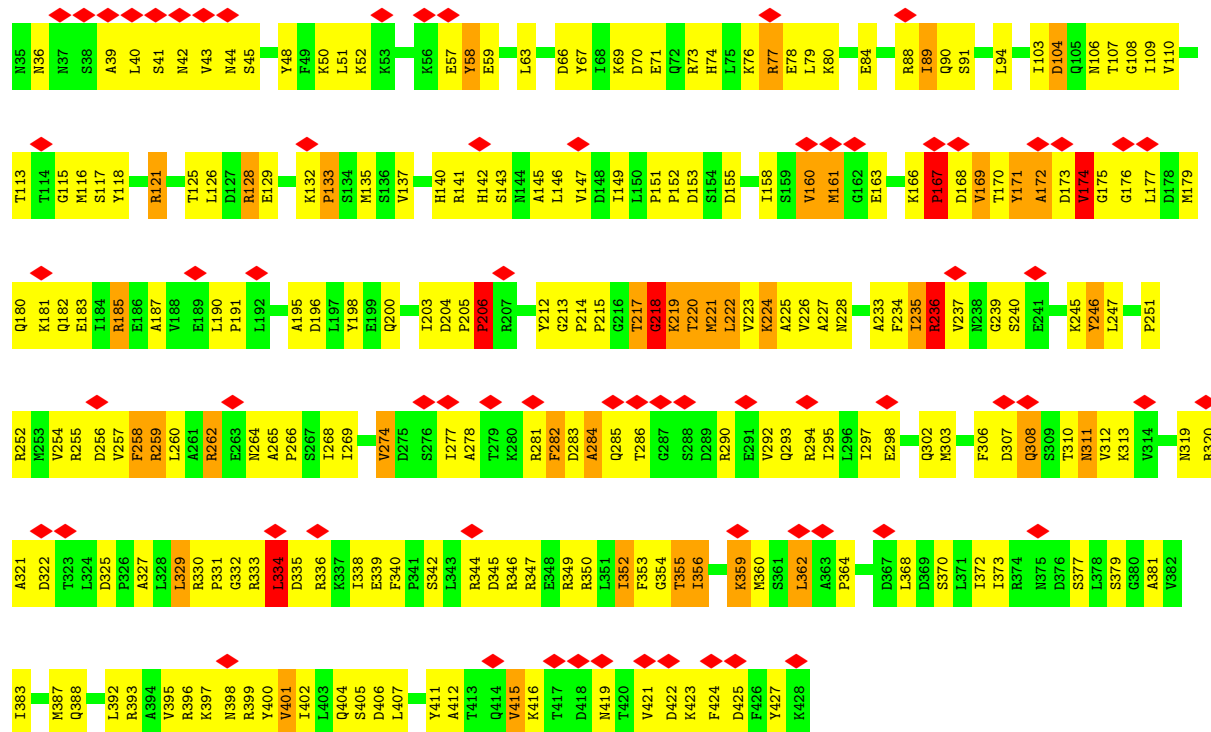


• Molecule 29: 26S proteasome regulatory subunit 4 homolog

Chain I: 23% 42% 50% 7% .

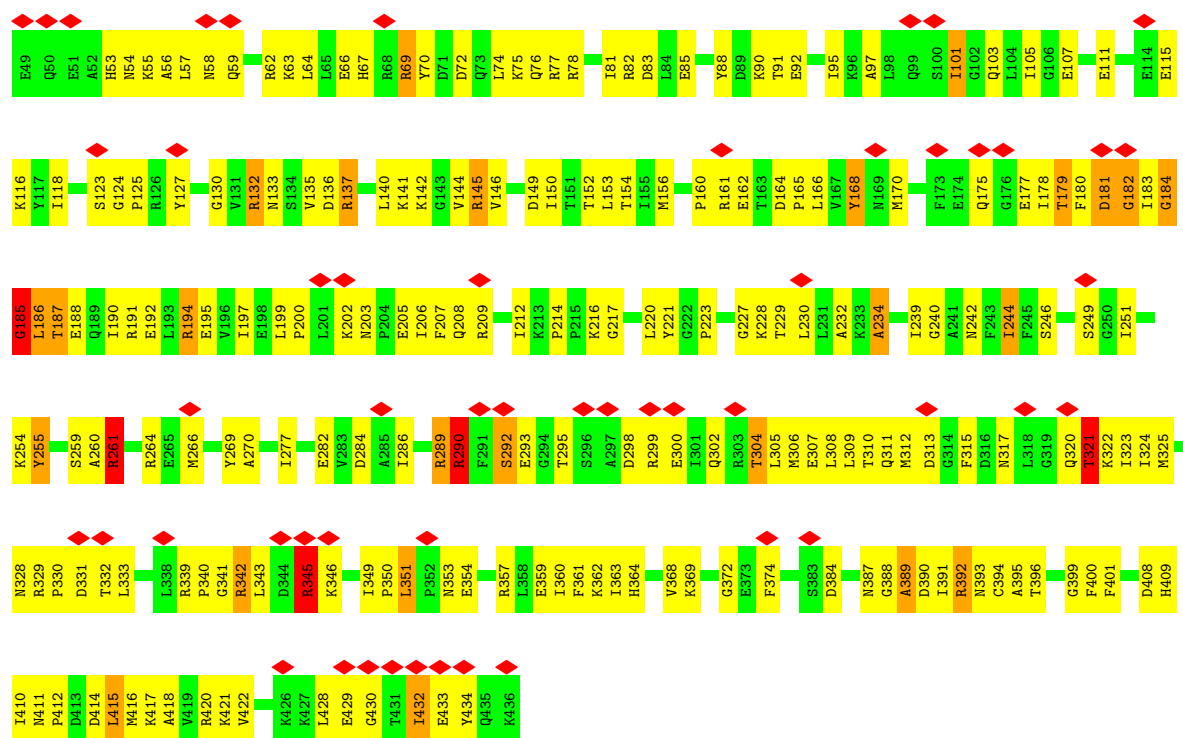


• Molecule 30: 26S proteasome regulatory subunit 6B homolog



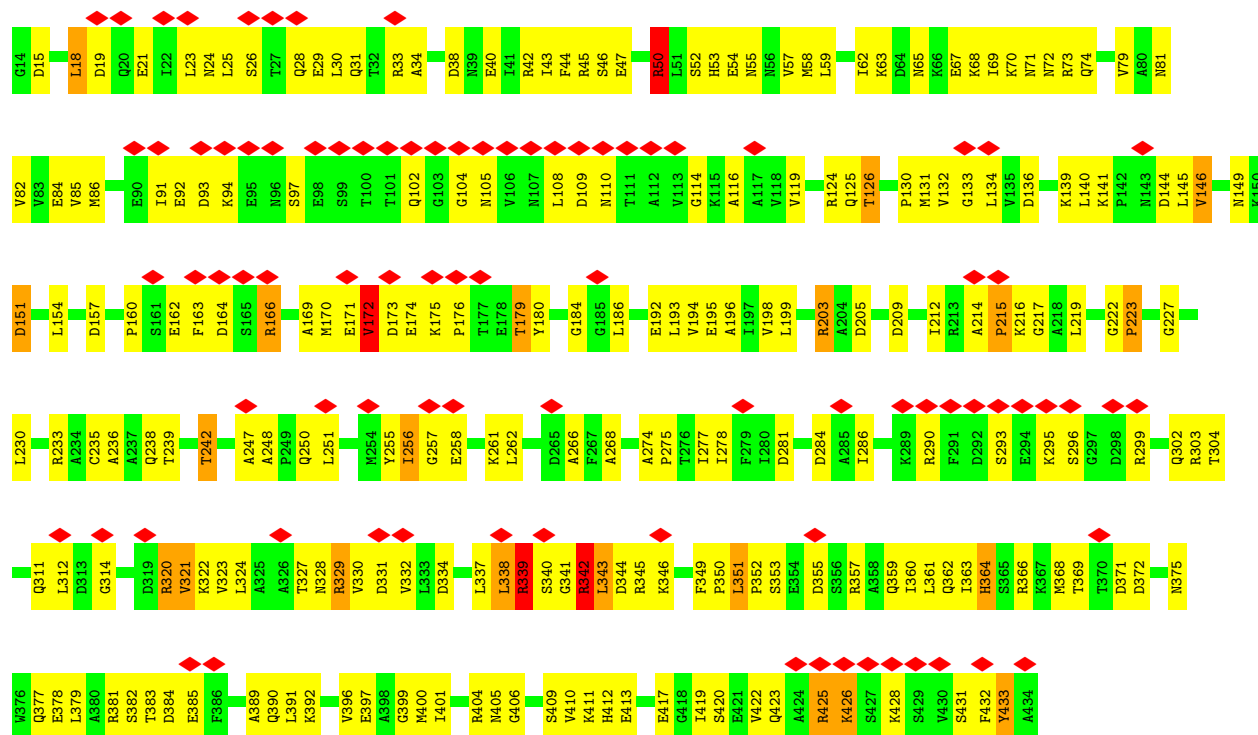
• Molecule 31: 26S proteasome subunit RPT4

Chain L: 13% 44% 48% 6%

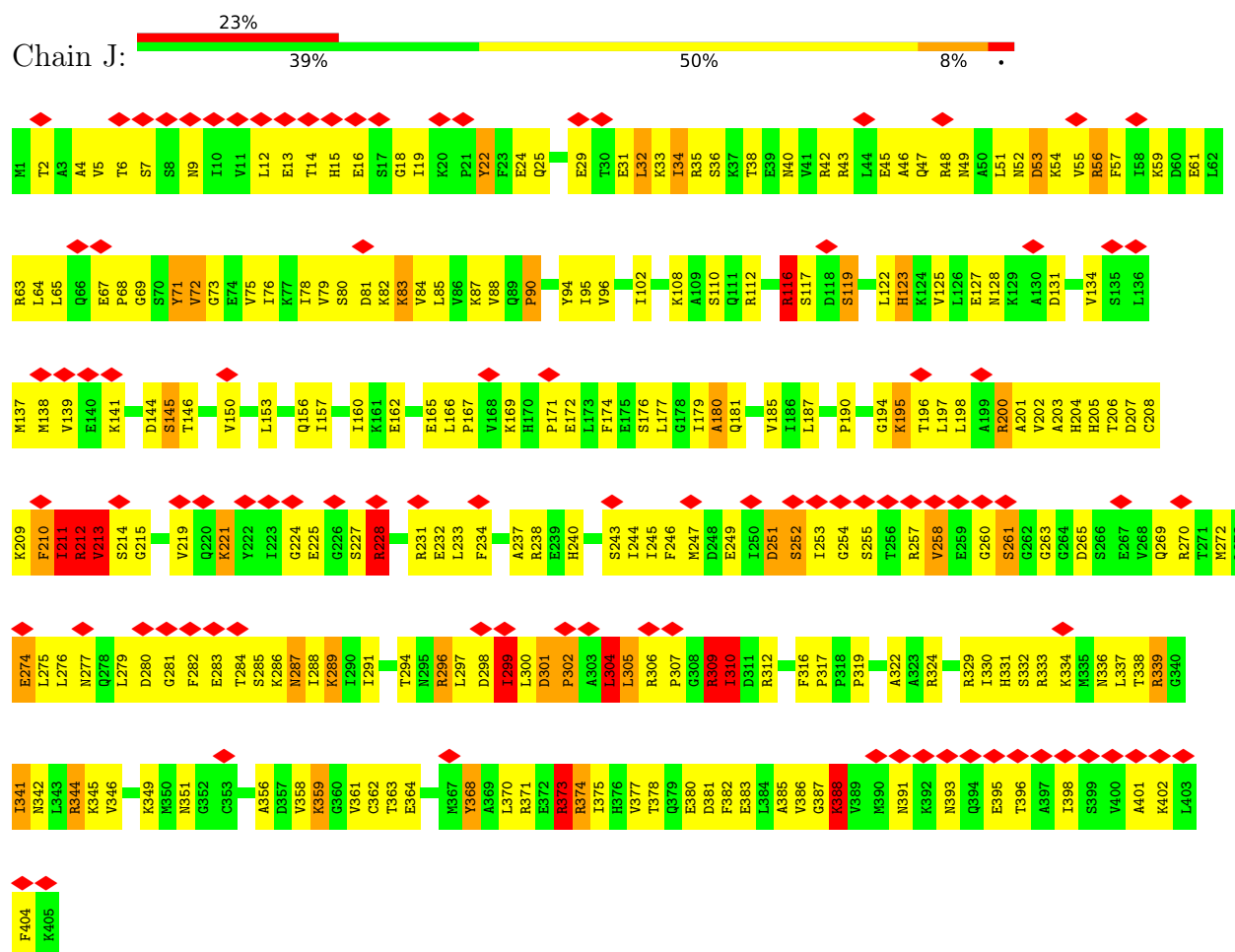


• Molecule 32: 26S proteasome regulatory subunit 6A

Chain M: 21% 45% 49% 5%



• Molecule 33: 26S proteasome regulatory subunit 8 homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	292279	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 ($e^-/\text{\AA}^2$)	35	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	0.086	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	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	1.19	0/1946	1.44	5/2634 (0.2%)
1	a	2.26	74/1946 (3.8%)	2.38	119/2634 (4.5%)
2	B	1.16	0/1944	1.41	5/2632 (0.2%)
2	b	2.29	77/1944 (4.0%)	2.36	114/2632 (4.3%)
3	C	1.20	0/1935	1.41	6/2618 (0.2%)
3	c	2.32	79/1935 (4.1%)	2.47	127/2618 (4.9%)
4	D	1.23	0/1888	1.45	4/2557 (0.2%)
4	d	2.34	87/2012 (4.3%)	2.44	128/2718 (4.7%)
5	E	2.07	2/1909 (0.1%)	1.60	10/2571 (0.4%)
5	e	2.24	64/1909 (3.4%)	2.36	96/2571 (3.7%)
6	F	1.22	0/1800	1.44	10/2433 (0.4%)
6	f	2.29	72/1800 (4.0%)	2.41	108/2433 (4.4%)
7	G	1.21	1/1926 (0.1%)	1.70	5/2599 (0.2%)
7	g	2.25	71/1926 (3.7%)	2.60	123/2599 (4.7%)
8	1	2.27	64/1541 (4.2%)	2.31	81/2087 (3.9%)
8	h	2.26	60/1541 (3.9%)	2.34	84/2087 (4.0%)
9	2	2.30	69/1751 (3.9%)	2.39	112/2373 (4.7%)
9	i	2.36	80/1751 (4.6%)	2.46	107/2373 (4.5%)
10	3	2.30	66/1611 (4.1%)	2.34	84/2174 (3.9%)
10	j	2.25	59/1611 (3.7%)	2.34	104/2174 (4.8%)
11	4	2.33	63/1590 (4.0%)	2.41	98/2142 (4.6%)
11	k	2.31	53/1590 (3.3%)	2.40	77/2142 (3.6%)
12	5	2.25	63/1681 (3.7%)	2.39	98/2274 (4.3%)
12	l	2.29	66/1681 (3.9%)	2.46	138/2274 (6.1%)
13	6	2.29	83/1795 (4.6%)	2.42	115/2420 (4.8%)
13	m	2.26	60/1795 (3.3%)	2.41	103/2420 (4.3%)
14	7	2.29	75/1821 (4.1%)	2.46	121/2470 (4.9%)
14	n	2.29	74/1847 (4.0%)	2.46	126/2503 (5.0%)
15	W	2.34	63/1558 (4.0%)	2.45	111/2111 (5.3%)
16	V	2.25	91/2309 (3.9%)	2.53	158/3115 (5.1%)
17	T	2.22	81/2236 (3.6%)	2.53	173/3017 (5.7%)
18	X	2.22	31/1059 (2.9%)	2.38	51/1432 (3.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	Y	2.08	18/741 (2.4%)	2.53	57/1000 (5.7%)
20	Z	1.65	23/7123 (0.3%)	1.98	176/9645 (1.8%)
21	N	2.27	270/7273 (3.7%)	2.50	489/9822 (5.0%)
22	S	2.26	144/3967 (3.6%)	2.51	302/5355 (5.6%)
23	P	2.18	113/3664 (3.1%)	2.53	278/4940 (5.6%)
24	Q	2.28	136/3556 (3.8%)	2.56	286/4787 (6.0%)
25	R	2.25	120/3314 (3.6%)	2.51	250/4469 (5.6%)
26	U	2.23	88/2461 (3.6%)	2.42	160/3327 (4.8%)
27	O	2.26	119/3247 (3.7%)	2.50	228/4380 (5.2%)
28	H	2.30	136/3282 (4.1%)	2.48	223/4423 (5.0%)
29	I	2.25	102/3059 (3.3%)	2.48	219/4115 (5.3%)
30	K	2.33	125/3156 (4.0%)	2.76	232/4261 (5.4%)
31	L	2.28	116/3128 (3.7%)	2.86	221/4201 (5.3%)
32	M	2.57	119/3323 (3.6%)	2.70	232/4478 (5.2%)
33	J	2.63	147/3212 (4.6%)	2.77	251/4316 (5.8%)
All	All	2.17	3504/112094 (3.1%)	2.38	6405/151356 (4.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	9
2	b	0	3
3	c	0	5
4	D	0	1
4	d	0	5
5	e	0	3
6	F	0	1
6	f	0	6
7	G	0	2
7	g	0	12
8	1	0	6
8	h	0	8
9	2	0	4
9	i	0	6
10	3	0	4
10	j	0	4
11	4	0	6
11	k	0	4
12	5	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	l	0	5
13	6	0	9
13	m	0	6
14	7	0	5
14	n	0	12
15	W	0	7
16	V	0	6
17	T	0	10
18	X	0	2
19	Y	0	1
20	Z	0	9
21	N	0	24
22	S	0	18
23	P	0	16
24	Q	0	13
25	R	0	11
26	U	0	6
27	O	0	9
28	H	0	13
29	I	0	9
30	K	0	19
31	L	0	18
32	M	0	13
33	J	0	15
All	All	0	351

All (3504) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	20	ARG	NE-CZ	73.61	2.14	1.33
33	J	211	ILE	C-N	-58.03	0.52	1.33
20	Z	728	LYS	CG-CD	52.64	3.10	1.52
20	Z	728	LYS	CA-CB	35.97	2.14	1.53
20	Z	738	TYR	CZ-OH	35.14	2.11	1.38
20	Z	728	LYS	CA-C	32.48	1.96	1.52
32	M	433	TYR	CG-CD1	31.61	2.05	1.39
32	M	433	TYR	CG-CD2	31.10	2.04	1.39
20	Z	255	LEU	CB-CG	28.96	2.11	1.53
33	J	309	ARG	CA-CB	-28.28	1.07	1.53
30	K	220	THR	C-N	-28.24	0.91	1.33
32	M	433	TYR	CE2-CZ	28.03	2.05	1.38
32	M	433	TYR	CE1-CZ	26.36	2.01	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	212	ARG	C-N	25.44	1.68	1.33
32	M	338	LEU	C-N	25.27	1.69	1.33
32	M	433	TYR	CD2-CE2	23.05	2.07	1.38
32	M	433	TYR	CD1-CE1	22.86	2.07	1.38
20	Z	728	LYS	CB-CG	16.32	2.01	1.52
20	Z	728	LYS	CD-CE	16.10	2.00	1.52
11	k	105	GLY	CA-C	-16.07	1.39	1.52
20	Z	728	LYS	C-N	15.61	1.55	1.33
20	Z	729	GLU	N-CA	14.10	1.64	1.46
18	X	94	ASN	CA-C	-14.04	1.43	1.52
20	Z	253	VAL	CA-CB	13.75	1.63	1.53
31	L	185	GLY	C-N	13.55	1.51	1.33
20	Z	729	GLU	CA-C	13.30	1.68	1.52
11	k	106	GLY	CA-C	-12.96	1.39	1.51
14	n	252	TRP	NE1-CE2	12.30	1.50	1.37
21	N	507	GLU	CA-C	-12.28	1.36	1.52
20	Z	728	LYS	CE-NZ	12.24	1.86	1.49
21	N	836	GLU	CA-C	-12.12	1.40	1.53
32	M	328	ASN	CA-C	-11.33	1.39	1.52
32	M	342	ARG	C-N	-11.18	1.18	1.33
31	L	331	ASP	CA-C	-11.18	1.37	1.52
32	M	303	ARG	NE-CZ	11.17	1.45	1.33
33	J	317	PRO	CA-CB	10.96	1.64	1.53
12	5	124	ALA	CA-C	-10.93	1.39	1.52
30	K	294	ARG	NE-CZ	10.71	1.44	1.33
5	E	20	ARG	CD-NE	10.69	1.61	1.46
3	c	5	ARG	NE-CZ	10.66	1.44	1.33
25	R	43	ARG	NE-CZ	10.65	1.44	1.33
33	J	5	VAL	CA-CB	-10.65	1.42	1.54
15	W	19	GLY	CA-C	-10.58	1.43	1.51
13	m	11	ASN	CA-C	-10.56	1.44	1.52
14	7	76	ILE	CA-C	-10.47	1.44	1.53
9	i	142	ILE	N-CA	-10.42	1.33	1.46
6	f	71	GLY	N-CA	-10.34	1.35	1.45
8	1	111	TYR	N-CA	-10.21	1.33	1.46
22	S	80	VAL	CA-C	-10.17	1.41	1.52
6	f	182	ILE	CA-C	-10.15	1.40	1.52
21	N	84	ALA	N-CA	-10.14	1.32	1.46
24	Q	309	ARG	NE-CZ	10.11	1.44	1.33
18	X	99	PHE	CA-C	-10.09	1.40	1.52
20	Z	255	LEU	CG-CD1	-10.07	1.19	1.52
10	3	34	LEU	C-N	10.06	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	225	VAL	CA-CB	10.04	1.66	1.54
3	c	63	THR	CA-CB	-9.96	1.45	1.53
3	c	77	VAL	CA-C	9.95	1.64	1.52
21	N	916	LEU	N-CA	-9.83	1.33	1.45
15	W	96	LEU	CA-C	-9.82	1.39	1.52
14	n	172	SER	CA-C	-9.79	1.39	1.52
33	J	123	HIS	CA-C	-9.75	1.44	1.52
28	H	245	GLY	CA-C	-9.74	1.44	1.52
4	d	97	ARG	CD-NE	9.63	1.59	1.46
3	c	68	LYS	CA-C	-9.63	1.41	1.52
27	O	45	LEU	C-N	9.61	1.46	1.33
14	n	225	SER	CA-C	-9.58	1.40	1.52
14	n	198	ILE	CA-C	-9.58	1.44	1.52
10	j	49	VAL	C-N	9.56	1.46	1.33
11	4	61	GLN	CA-C	-9.56	1.40	1.52
28	H	273	ARG	NE-CZ	9.54	1.43	1.33
28	H	57	LYS	N-CA	-9.54	1.34	1.46
22	S	334	HIS	ND1-CE1	9.53	1.42	1.32
24	Q	340	ASP	CA-C	-9.49	1.40	1.52
31	L	188	GLU	N-CA	-9.47	1.34	1.46
30	K	360	MET	CA-C	-9.44	1.42	1.52
24	Q	62	GLY	N-CA	-9.44	1.32	1.45
2	b	42	GLY	CA-C	-9.39	1.42	1.51
30	K	383	ILE	CA-C	9.33	1.65	1.52
1	a	228	ALA	CA-C	-9.30	1.41	1.52
1	a	25	LEU	CA-C	-9.28	1.43	1.53
7	g	123	HIS	ND1-CE1	9.27	1.41	1.32
5	e	188	HIS	ND1-CE1	9.27	1.41	1.32
13	m	97	ALA	C-N	9.26	1.45	1.33
24	Q	202	ARG	CD-NE	9.25	1.59	1.46
14	7	129	LEU	CA-C	9.25	1.64	1.52
23	P	96	MET	CA-C	-9.23	1.40	1.52
31	L	323	ILE	CA-C	-9.22	1.41	1.52
17	T	161	TRP	N-CA	-9.22	1.35	1.46
21	N	235	ALA	CA-C	-9.13	1.40	1.52
10	j	139	SER	CA-C	-9.10	1.41	1.52
16	V	234	GLU	N-CA	-9.08	1.35	1.46
32	M	34	ALA	N-CA	-9.06	1.35	1.46
23	P	349	ASN	N-CA	-9.04	1.35	1.46
2	b	146	SER	CA-C	-9.02	1.41	1.52
16	V	285	ASP	N-CA	-8.99	1.35	1.46
22	S	271	ARG	CD-NE	8.96	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	191	HIS	ND1-CE1	8.95	1.41	1.32
21	N	344	THR	CA-C	-8.94	1.41	1.52
24	Q	162	LEU	CA-C	-8.92	1.41	1.52
16	V	106	GLY	C-N	8.89	1.44	1.33
33	J	194	GLY	C-N	-8.88	1.22	1.33
20	Z	254	PRO	N-CA	-8.87	1.37	1.47
13	m	215	VAL	CA-CB	-8.87	1.43	1.54
23	P	198	VAL	N-CA	-8.86	1.36	1.46
10	3	67	PHE	C-N	8.82	1.45	1.33
2	b	100	ILE	N-CA	8.78	1.54	1.46
3	c	63	THR	C-N	8.76	1.45	1.33
23	P	3	ARG	NE-CZ	8.75	1.42	1.33
21	N	31	VAL	CA-C	-8.74	1.42	1.53
3	c	139	GLY	CA-C	8.73	1.61	1.51
11	k	94	SER	CA-CB	8.73	1.67	1.53
28	H	223	GLU	CA-CB	8.73	1.67	1.53
8	1	137	GLY	CA-C	-8.71	1.42	1.52
33	J	45	GLU	CA-C	-8.71	1.41	1.52
5	e	132	ARG	CD-NE	8.71	1.58	1.46
9	i	192	ILE	C-N	8.68	1.45	1.33
10	3	128	GLY	CA-C	-8.67	1.39	1.51
7	g	132	PHE	CA-CB	8.66	1.66	1.53
11	4	146	HIS	ND1-CE1	8.66	1.41	1.32
27	O	318	HIS	CA-C	-8.66	1.44	1.53
30	K	163	GLU	C-N	8.65	1.44	1.33
21	N	526	TYR	C-N	8.64	1.42	1.33
21	N	572	LEU	N-CA	-8.64	1.35	1.46
28	H	236	ALA	N-CA	-8.62	1.36	1.46
9	2	107	SER	CA-CB	8.61	1.67	1.53
26	U	75	ASN	C-N	8.59	1.45	1.34
21	N	761	ILE	CA-C	-8.59	1.41	1.52
5	e	219	LEU	CA-C	-8.59	1.42	1.52
15	W	18	ASN	C-N	8.59	1.38	1.33
4	d	6	ARG	CD-NE	8.57	1.58	1.46
1	a	144	VAL	N-CA	-8.56	1.36	1.46
24	Q	65	TYR	C-N	8.53	1.44	1.34
12	l	278	GLU	CA-CB	8.51	1.66	1.53
9	i	59	ASN	C-N	8.49	1.44	1.33
5	e	50	VAL	CA-C	-8.49	1.42	1.52
24	Q	13	ARG	CA-CB	8.48	1.66	1.53
24	Q	126	LYS	N-CA	-8.48	1.35	1.46
27	O	226	LYS	CA-C	-8.47	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	411	ASN	CA-C	-8.47	1.42	1.53
32	M	42	ARG	NE-CZ	8.47	1.42	1.33
33	J	15	HIS	N-CA	-8.47	1.36	1.46
27	O	254	LEU	C-N	8.46	1.44	1.33
1	a	188	LYS	C-N	8.45	1.45	1.33
12	5	89	VAL	N-CA	-8.44	1.36	1.46
23	P	272	PRO	CA-CB	8.44	1.65	1.53
9	i	48	ARG	NE-CZ	8.44	1.42	1.33
27	O	310	PHE	CA-CB	8.42	1.66	1.53
14	n	214	MET	C-N	8.41	1.45	1.33
10	3	147	PHE	C-N	8.41	1.44	1.33
29	I	279	VAL	CA-C	-8.40	1.42	1.52
10	3	168	SER	N-CA	-8.38	1.36	1.46
12	l	219	TYR	C-N	8.37	1.40	1.33
26	U	57	GLU	CA-C	-8.37	1.42	1.52
30	K	167	PRO	C-N	-8.36	1.21	1.33
31	L	140	LEU	CA-C	-8.35	1.42	1.52
21	N	394	ARG	NE-CZ	8.35	1.42	1.33
2	b	132	VAL	CA-C	-8.34	1.42	1.52
12	5	272	PHE	CA-CB	8.34	1.66	1.53
19	Y	12	SER	CA-CB	8.34	1.66	1.53
31	L	408	ASP	CA-C	-8.34	1.41	1.52
28	H	444	LEU	CA-C	-8.32	1.42	1.52
23	P	381	SER	N-CA	-8.31	1.36	1.46
29	I	64	ARG	NE-CZ	8.29	1.42	1.33
31	L	220	LEU	CA-C	-8.29	1.42	1.52
18	X	73	THR	CA-C	-8.29	1.41	1.53
16	V	204	HIS	ND1-CE1	8.28	1.40	1.32
10	j	51	LEU	C-N	8.28	1.39	1.33
9	2	126	TYR	CA-C	-8.27	1.43	1.53
33	J	201	ALA	CA-C	-8.26	1.42	1.52
30	K	45	SER	CA-C	-8.26	1.42	1.52
7	g	222	SER	C-N	8.25	1.48	1.33
27	O	342	ASP	CA-C	-8.25	1.42	1.52
5	e	149	ALA	CA-CB	8.24	1.65	1.53
20	Z	738	TYR	CA-CB	8.24	1.66	1.53
29	I	367	SER	CA-CB	8.24	1.66	1.53
1	a	43	LEU	CA-C	-8.23	1.42	1.52
10	3	202	MET	CA-C	-8.22	1.42	1.52
2	b	128	ARG	CA-CB	8.22	1.64	1.54
22	S	158	PHE	C-N	8.21	1.45	1.33
9	2	142	ILE	CA-C	-8.20	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	18	ARG	NE-CZ	8.19	1.42	1.33
7	g	94	GLU	CA-C	-8.19	1.42	1.52
14	7	163	VAL	N-CA	-8.18	1.37	1.46
12	l	196	ARG	CA-C	-8.18	1.46	1.53
9	i	225	ARG	NE-CZ	8.18	1.42	1.33
14	n	228	PHE	CA-C	-8.18	1.42	1.52
33	J	128	ASN	C-N	8.17	1.44	1.33
2	b	228	PRO	N-CA	-8.17	1.41	1.47
10	3	92	SER	CA-CB	8.17	1.66	1.53
11	4	89	ALA	CA-C	-8.17	1.42	1.52
20	Z	248	TYR	CA-C	-8.17	1.42	1.52
17	T	124	SER	CA-CB	8.16	1.66	1.53
22	S	221	ALA	C-N	8.16	1.45	1.34
30	K	40	LEU	CA-C	-8.16	1.41	1.52
22	S	68	LEU	CA-C	-8.14	1.43	1.53
30	K	169	VAL	C-N	8.14	1.40	1.33
30	K	349	ARG	NE-CZ	8.14	1.42	1.33
13	m	162	VAL	CA-CB	-8.13	1.46	1.55
25	R	103	CYS	C-O	-8.11	1.14	1.24
32	M	110	ASN	CA-CB	8.11	1.67	1.53
2	b	102	GLY	CA-C	-8.10	1.43	1.51
8	h	109	ALA	N-CA	-8.10	1.35	1.45
21	N	643	PRO	C-N	8.09	1.45	1.33
3	c	143	ARG	NE-CZ	8.09	1.42	1.33
29	I	313	LEU	CA-CB	8.08	1.66	1.53
2	b	4	ARG	CA-C	-8.08	1.42	1.52
29	I	365	HIS	ND1-CE1	8.08	1.40	1.32
25	R	27	SER	CA-C	-8.08	1.42	1.52
29	I	422	ARG	NE-CZ	8.08	1.42	1.33
32	M	268	ALA	C-N	8.08	1.45	1.33
32	M	47	GLU	CA-C	-8.07	1.42	1.52
9	i	143	HIS	CA-C	-8.07	1.42	1.52
32	M	217	GLY	CA-C	8.06	1.60	1.51
2	b	144	GLY	CA-C	-8.06	1.44	1.52
3	c	119	LYS	C-O	-8.06	1.14	1.24
4	d	46	CYS	CA-C	-8.06	1.42	1.52
9	2	207	MET	C-N	8.04	1.44	1.33
13	m	45	SER	CA-C	-8.04	1.42	1.52
26	U	67	PHE	CA-C	-8.04	1.43	1.52
15	W	68	GLU	CA-C	-8.04	1.42	1.52
11	k	6	GLY	CA-C	-8.03	1.44	1.51
1	a	91	ARG	CD-NE	8.02	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	O	172	TYR	N-CA	-8.02	1.35	1.46
15	W	12	ASN	CA-C	-8.02	1.43	1.52
32	M	413	GLU	CA-C	-8.02	1.41	1.52
10	j	52	GLY	CA-C	-8.00	1.46	1.52
27	O	58	ARG	CD-NE	8.00	1.57	1.46
27	O	97	LYS	N-CA	-8.00	1.36	1.46
10	3	98	ARG	NE-CZ	7.99	1.41	1.33
9	i	216	LEU	CA-C	-7.99	1.45	1.53
10	3	40	PHE	CA-C	-7.99	1.42	1.52
30	K	330	ARG	CD-NE	7.98	1.57	1.46
32	M	174	GLU	N-CA	-7.97	1.36	1.46
33	J	138	MET	N-CA	-7.97	1.36	1.46
12	l	109	VAL	CA-C	-7.97	1.43	1.52
29	I	154	MET	CA-CB	7.97	1.64	1.53
30	K	214	PRO	CA-C	7.96	1.56	1.51
16	V	252	SER	C-N	7.96	1.44	1.33
21	N	200	SER	CA-C	-7.96	1.41	1.52
13	6	92	LEU	CA-C	-7.96	1.43	1.52
6	f	39	ARG	NE-CZ	7.96	1.41	1.33
9	i	160	SER	C-N	7.95	1.44	1.33
10	j	116	SER	C-N	7.95	1.42	1.33
33	J	238	ARG	NE-CZ	7.94	1.41	1.33
2	b	45	ILE	N-CA	-7.94	1.36	1.46
9	2	195	ASP	N-CA	-7.93	1.36	1.46
24	Q	426	LEU	CA-C	-7.93	1.42	1.52
3	c	134	SER	CA-C	7.93	1.62	1.52
23	P	293	LEU	CA-C	-7.93	1.42	1.52
9	2	198	SER	CA-C	-7.93	1.43	1.52
26	U	102	SER	CA-C	-7.93	1.41	1.52
13	6	161	GLN	C-N	7.92	1.41	1.33
10	3	37	SER	CA-C	-7.92	1.42	1.52
21	N	585	ARG	NE-CZ	7.92	1.41	1.33
21	N	869	ASP	CA-C	-7.92	1.42	1.52
16	V	254	ARG	C-N	7.92	1.43	1.33
31	L	130	GLY	N-CA	-7.91	1.37	1.44
11	k	27	VAL	CA-CB	-7.91	1.46	1.54
11	4	4	ILE	CA-C	-7.91	1.43	1.52
8	1	141	THR	CA-C	-7.90	1.42	1.52
22	S	67	GLU	N-CA	-7.90	1.35	1.46
9	i	104	ARG	CA-C	-7.90	1.43	1.52
31	L	242	ASN	CA-CB	7.88	1.66	1.53
8	h	25	ALA	CA-C	-7.88	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	290	ARG	NE-CZ	7.88	1.41	1.33
10	3	28	ARG	CD-NE	7.88	1.57	1.46
21	N	622	ALA	CA-C	-7.87	1.42	1.52
10	j	32	GLN	CA-C	-7.87	1.46	1.53
21	N	873	ARG	C-N	7.86	1.43	1.33
33	J	224	GLY	N-CA	-7.86	1.38	1.45
11	k	43	LEU	N-CA	-7.86	1.35	1.45
21	N	79	VAL	C-N	7.86	1.44	1.33
1	a	73	PHE	N-CA	-7.85	1.36	1.46
15	W	44	ASN	CA-C	-7.85	1.43	1.52
32	M	79	VAL	CA-CB	7.85	1.64	1.54
21	N	510	HIS	ND1-CE1	7.84	1.40	1.32
32	M	28	GLN	N-CA	-7.84	1.36	1.46
22	S	196	ARG	CZ-NH1	7.84	1.43	1.32
3	c	151	SER	CA-C	-7.83	1.43	1.52
9	i	51	GLN	CA-C	-7.82	1.43	1.52
24	Q	24	GLU	C-N	7.82	1.44	1.33
25	R	70	TYR	CA-C	7.81	1.63	1.52
10	3	107	PRO	C-O	-7.80	1.15	1.23
33	J	80	SER	C-N	7.80	1.44	1.33
5	e	155	LEU	CA-C	-7.80	1.43	1.52
17	T	215	LYS	N-CA	-7.80	1.36	1.46
13	m	202	ARG	CD-NE	7.79	1.57	1.46
10	j	95	LEU	C-N	7.79	1.44	1.33
21	N	631	GLY	C-N	7.77	1.43	1.33
29	I	92	GLU	CA-C	-7.77	1.43	1.52
29	I	356	SER	C-N	7.76	1.43	1.33
29	I	113	ILE	N-CA	-7.76	1.36	1.46
30	K	116	MET	N-CA	-7.75	1.36	1.46
26	U	40	ASP	N-CA	7.74	1.55	1.45
33	J	87	LYS	CA-CB	7.74	1.63	1.53
21	N	873	ARG	CD-NE	7.74	1.57	1.46
2	b	140	ASP	CA-C	-7.74	1.43	1.52
23	P	313	ILE	CA-C	-7.72	1.45	1.52
31	L	309	LEU	CA-CB	7.72	1.65	1.53
2	b	199	SER	CA-C	-7.72	1.42	1.52
27	O	160	LYS	C-N	7.72	1.44	1.33
28	H	289	ARG	NE-CZ	7.72	1.41	1.33
29	I	117	HIS	ND1-CE1	7.71	1.40	1.32
5	e	114	GLN	CA-CB	7.71	1.65	1.53
27	O	315	LYS	CA-C	-7.71	1.42	1.52
33	J	145	SER	CA-C	-7.71	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	402	ILE	CA-C	-7.70	1.43	1.52
32	M	342	ARG	CA-C	-7.69	1.43	1.52
14	n	142	PRO	CA-C	-7.69	1.45	1.53
26	U	124	ASP	CA-CB	7.68	1.64	1.53
24	Q	130	ARG	CD-NE	7.67	1.56	1.46
30	K	246	TYR	CA-C	-7.67	1.45	1.53
33	J	341	ILE	CA-C	-7.67	1.43	1.52
17	T	34	LEU	C-N	7.66	1.43	1.33
32	M	248	ALA	N-CA	-7.65	1.37	1.46
23	P	207	THR	CA-CB	7.65	1.66	1.53
31	L	153	LEU	CA-C	-7.64	1.44	1.53
28	H	299	ARG	NE-CZ	7.64	1.41	1.33
5	e	171	ALA	N-CA	-7.63	1.36	1.46
33	J	344	ARG	CD-NE	7.63	1.56	1.46
26	U	137	TYR	CA-C	-7.62	1.43	1.52
26	U	143	VAL	CA-C	7.62	1.61	1.52
21	N	350	LYS	CA-C	-7.62	1.42	1.52
21	N	853	ASP	CA-C	-7.62	1.43	1.52
22	S	389	LYS	C-N	7.62	1.44	1.33
23	P	23	LYS	N-CA	-7.62	1.37	1.46
14	n	247	VAL	CA-C	-7.61	1.44	1.52
27	O	195	TYR	CA-CB	7.61	1.65	1.53
25	R	398	ALA	CA-C	-7.61	1.42	1.52
26	U	226	LEU	N-CA	-7.61	1.36	1.46
28	H	349	ILE	CA-CB	-7.60	1.45	1.54
30	K	234	PHE	C-N	7.59	1.43	1.33
33	J	214	SER	CA-C	-7.59	1.43	1.52
9	2	71	TRP	CA-C	-7.58	1.43	1.52
9	2	184	ALA	N-CA	-7.57	1.37	1.46
7	g	165	THR	C-N	7.56	1.43	1.32
25	R	178	GLY	N-CA	-7.56	1.36	1.45
2	b	190	HIS	ND1-CE1	7.55	1.40	1.32
24	Q	8	LEU	CA-CB	7.55	1.65	1.53
23	P	191	GLY	C-N	7.54	1.43	1.33
10	j	72	ASN	CA-C	-7.54	1.42	1.52
6	f	6	TYR	CA-C	-7.54	1.42	1.52
21	N	732	GLY	CA-C	-7.54	1.43	1.51
28	H	293	GLU	CA-C	-7.53	1.43	1.52
1	a	53	VAL	CA-C	-7.52	1.43	1.52
6	f	185	ASN	C-N	7.52	1.43	1.34
26	U	238	ASN	CA-C	-7.52	1.43	1.52
32	M	353	SER	CA-C	-7.52	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	178	SER	CA-C	-7.52	1.43	1.52
1	a	56	GLN	CA-C	-7.51	1.43	1.52
25	R	416	LYS	C-N	7.51	1.44	1.33
1	a	143	PHE	CA-C	-7.51	1.43	1.52
24	Q	18	LYS	C-N	7.51	1.43	1.33
31	L	88	TYR	CA-CB	7.50	1.65	1.53
31	L	212	ILE	CA-C	-7.50	1.44	1.52
11	4	181	VAL	CA-CB	-7.50	1.45	1.54
4	d	236	ILE	CA-C	-7.50	1.43	1.52
12	5	141	HIS	ND1-CE1	7.50	1.40	1.32
16	V	190	HIS	ND1-CE1	7.50	1.40	1.32
30	K	70	ASP	CA-C	-7.50	1.43	1.52
14	7	140	MET	CA-C	-7.50	1.43	1.52
15	W	90	ALA	CA-C	-7.49	1.43	1.52
21	N	899	ASN	CA-C	-7.49	1.43	1.52
28	H	184	GLU	CA-C	-7.49	1.45	1.52
27	O	109	LEU	N-CA	-7.49	1.37	1.46
13	6	42	SER	C-N	7.49	1.42	1.33
4	d	29	ARG	NE-CZ	7.48	1.41	1.33
30	K	115	GLY	CA-C	-7.48	1.41	1.51
31	L	315	PHE	CA-C	-7.48	1.42	1.52
21	N	607	GLN	CA-C	-7.47	1.43	1.52
2	b	230	ASP	CA-C	-7.47	1.43	1.52
28	H	399	GLU	C-N	7.47	1.43	1.33
7	g	210	LYS	CA-C	-7.46	1.43	1.52
33	J	330	ILE	CA-C	-7.46	1.43	1.53
2	b	183	LEU	N-CA	-7.46	1.36	1.45
27	O	373	TRP	CA-CB	7.46	1.65	1.53
29	I	164	ALA	C-N	7.46	1.41	1.33
22	S	377	TYR	CA-CB	7.45	1.65	1.53
11	4	5	LEU	CA-C	-7.45	1.43	1.52
15	W	7	VAL	CA-C	-7.45	1.43	1.52
11	4	17	SER	C-N	7.44	1.43	1.33
16	V	117	TRP	CA-C	-7.44	1.43	1.52
25	R	69	GLU	CA-CB	7.44	1.65	1.53
6	f	48	ALA	N-CA	-7.44	1.36	1.46
21	N	826	GLU	C-N	7.43	1.43	1.33
16	V	20	ARG	NE-CZ	7.43	1.41	1.33
25	R	372	ILE	CA-CB	-7.42	1.48	1.53
7	g	55	THR	C-N	7.41	1.43	1.33
7	g	122	ALA	N-CA	-7.41	1.36	1.46
17	T	132	HIS	ND1-CE1	7.41	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	267	VAL	C-N	7.41	1.43	1.33
26	U	287	ALA	C-N	7.41	1.43	1.33
7	g	146	ALA	CA-C	-7.40	1.43	1.52
28	H	156	VAL	C-N	7.40	1.42	1.33
29	I	358	LYS	C-N	7.40	1.43	1.33
11	k	88	LEU	C-N	7.39	1.43	1.33
19	Y	47	GLU	CA-CB	7.39	1.63	1.53
12	5	174	THR	CA-C	7.39	1.61	1.52
28	H	76	LEU	N-CA	-7.39	1.35	1.45
11	4	191	GLN	CA-C	-7.38	1.44	1.52
4	d	72	VAL	CA-C	-7.38	1.43	1.52
28	H	424	THR	CA-C	-7.38	1.43	1.52
22	S	183	LEU	C-N	7.37	1.43	1.34
31	L	299	ARG	NE-CZ	7.37	1.41	1.33
18	X	89	LEU	CA-C	-7.37	1.44	1.52
22	S	259	TYR	CA-C	7.37	1.61	1.53
23	P	243	GLU	C-N	7.37	1.43	1.33
31	L	83	ASP	CA-CB	7.37	1.64	1.53
5	e	93	ARG	NE-CZ	7.36	1.41	1.33
14	7	215	ARG	CD-NE	7.36	1.56	1.46
4	d	82	SER	C-N	7.36	1.43	1.33
6	f	51	ARG	CA-C	-7.36	1.43	1.52
14	n	231	ALA	CA-C	-7.36	1.43	1.52
29	I	76	VAL	CA-CB	-7.36	1.45	1.54
5	e	102	TYR	CA-CB	7.35	1.65	1.53
26	U	220	PRO	C-N	7.35	1.42	1.33
25	R	334	ARG	CD-NE	7.35	1.56	1.46
33	J	270	ARG	NE-CZ	7.35	1.41	1.33
13	6	34	ASP	CA-CB	7.34	1.65	1.53
8	1	152	ARG	CD-NE	7.34	1.56	1.46
6	f	82	ARG	CD-NE	7.34	1.56	1.46
31	L	161	ARG	CD-NE	7.34	1.56	1.46
13	6	46	ARG	CA-C	-7.34	1.43	1.52
22	S	351	ALA	CA-C	-7.34	1.43	1.52
22	S	191	HIS	CD2-NE2	7.33	1.46	1.37
23	P	282	HIS	CA-C	-7.32	1.42	1.52
2	b	221	LEU	CA-CB	7.32	1.64	1.53
14	n	194	ARG	NE-CZ	7.32	1.41	1.33
21	N	74	GLU	CA-C	-7.32	1.46	1.53
6	f	200	SER	C-N	7.32	1.44	1.33
16	V	259	LYS	C-N	7.31	1.43	1.33
11	k	143	LEU	N-CA	-7.31	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	358	LYS	C-N	7.31	1.43	1.33
18	X	37	PRO	C-N	7.30	1.44	1.33
27	O	6	GLU	C-N	7.30	1.42	1.33
31	L	161	ARG	NE-CZ	7.30	1.41	1.33
8	h	109	ALA	CA-C	-7.29	1.43	1.52
30	K	255	ARG	NE-CZ	7.29	1.41	1.33
13	6	42	SER	CA-C	-7.29	1.43	1.52
9	i	130	ALA	CA-C	-7.28	1.43	1.52
12	l	81	PHE	CA-C	-7.28	1.43	1.52
21	N	129	ILE	C-N	7.28	1.43	1.33
21	N	28	ILE	CA-CB	-7.28	1.45	1.54
29	I	368	LYS	CA-C	-7.27	1.43	1.52
32	M	144	ASP	CA-C	-7.27	1.43	1.52
21	N	464	GLU	CA-CB	7.27	1.64	1.53
22	S	471	LEU	CA-C	-7.27	1.43	1.52
18	X	52	PRO	N-CA	-7.26	1.38	1.47
31	L	409	HIS	CA-C	-7.26	1.43	1.52
21	N	556	ALA	CA-C	-7.26	1.43	1.52
25	R	294	ILE	C-O	-7.26	1.15	1.24
21	N	885	ILE	CA-C	-7.25	1.43	1.52
11	4	38	LEU	CA-C	-7.25	1.44	1.52
32	M	136	ASP	CA-C	-7.25	1.44	1.53
9	i	31	THR	N-CA	-7.25	1.37	1.46
9	2	55	VAL	CA-C	-7.25	1.43	1.52
23	P	263	HIS	CE1-NE2	-7.25	1.25	1.32
9	i	48	ARG	CD-NE	7.25	1.56	1.46
13	m	111	PHE	N-CA	-7.25	1.39	1.46
10	j	34	LEU	CA-C	-7.25	1.43	1.52
22	S	51	ARG	CD-NE	7.24	1.56	1.46
32	M	381	ARG	NE-CZ	7.24	1.41	1.33
21	N	79	VAL	CA-C	-7.24	1.43	1.52
22	S	193	THR	C-N	7.24	1.43	1.33
31	L	130	GLY	CA-C	-7.24	1.43	1.52
28	H	313	ALA	N-CA	-7.23	1.36	1.45
10	j	75	LYS	CA-C	-7.23	1.43	1.52
3	c	92	ARG	CZ-NH2	7.22	1.42	1.33
23	P	440	HIS	ND1-CE1	7.22	1.39	1.32
16	V	269	ARG	CD-NE	7.22	1.56	1.46
7	g	236	LEU	CA-C	-7.22	1.43	1.52
29	I	159	VAL	N-CA	-7.22	1.37	1.46
4	d	118	GLN	CA-C	-7.21	1.43	1.52
13	m	62	ALA	N-CA	-7.21	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	43	ILE	C-N	7.21	1.42	1.33
26	U	45	THR	CA-C	-7.21	1.44	1.52
28	H	218	ILE	CA-CB	-7.21	1.45	1.54
33	J	43	ARG	NE-CZ	7.20	1.41	1.33
7	g	52	LYS	CA-C	-7.20	1.44	1.52
10	j	99	ARG	NE-CZ	7.20	1.41	1.33
24	Q	47	ASP	N-CA	7.20	1.55	1.46
25	R	41	GLU	N-CA	-7.20	1.37	1.46
24	Q	425	GLN	C-N	7.19	1.43	1.33
6	f	142	ALA	CA-C	-7.18	1.43	1.52
30	K	330	ARG	NE-CZ	7.18	1.41	1.33
21	N	409	GLY	N-CA	-7.18	1.36	1.45
12	l	232	GLY	CA-C	-7.17	1.44	1.52
10	3	68	ARG	N-CA	-7.16	1.37	1.46
15	W	113	PHE	CA-CB	7.16	1.64	1.53
26	U	176	ARG	CZ-NH2	7.16	1.42	1.33
32	M	281	ASP	N-CA	-7.16	1.37	1.46
30	K	256	ASP	CA-C	-7.16	1.42	1.52
28	H	82	TRP	CA-CB	7.16	1.64	1.53
33	J	160	ILE	C-N	7.15	1.43	1.33
23	P	69	ARG	NE-CZ	7.15	1.41	1.33
21	N	673	PRO	CA-C	-7.15	1.40	1.52
1	a	120	ARG	NE-CZ	7.15	1.41	1.33
29	I	204	HIS	ND1-CE1	7.15	1.39	1.32
28	H	392	HIS	ND1-CE1	7.15	1.39	1.32
6	f	101	ARG	CZ-NH2	7.14	1.42	1.33
23	P	63	VAL	C-N	7.14	1.43	1.33
22	S	271	ARG	NE-CZ	7.14	1.41	1.33
31	L	78	ARG	NE-CZ	7.14	1.41	1.33
25	R	328	PHE	CA-C	-7.14	1.43	1.52
11	k	53	THR	CA-C	-7.13	1.43	1.52
16	V	229	ASP	N-CA	-7.13	1.37	1.46
23	P	58	VAL	C-N	7.13	1.43	1.33
28	H	329	VAL	C-N	7.13	1.44	1.33
13	6	30	VAL	N-CA	-7.13	1.37	1.46
4	d	58	ARG	CD-NE	7.13	1.56	1.46
30	K	77	ARG	CA-C	-7.13	1.43	1.52
4	d	133	THR	CA-C	7.13	1.61	1.52
33	J	87	LYS	C-N	7.13	1.41	1.33
30	K	52	LYS	N-CA	-7.12	1.37	1.46
12	l	185	PRO	C-N	7.12	1.42	1.33
9	2	178	GLU	CA-C	-7.12	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	166	LYS	C-N	7.12	1.42	1.33
11	k	160	LEU	CA-C	-7.11	1.43	1.52
14	n	232	ILE	C-N	7.11	1.42	1.33
3	c	142	ASP	C-N	7.11	1.43	1.33
8	h	186	VAL	N-CA	-7.11	1.38	1.46
13	m	167	GLN	CA-C	-7.11	1.44	1.52
26	U	187	SER	N-CA	-7.11	1.37	1.46
14	n	185	ASN	CA-CB	7.11	1.62	1.53
13	6	177	LYS	CA-C	-7.10	1.43	1.53
25	R	192	GLU	N-CA	-7.09	1.37	1.46
25	R	254	SER	N-CA	-7.09	1.37	1.46
33	J	386	VAL	C-N	7.09	1.42	1.33
28	H	174	VAL	C-N	7.09	1.38	1.33
15	W	41	ARG	CD-NE	7.09	1.56	1.46
9	i	229	GLN	CA-CB	7.08	1.65	1.53
18	X	92	SER	CA-CB	7.08	1.64	1.53
33	J	34	ILE	C-O	-7.08	1.15	1.24
12	l	227	ASP	CA-C	-7.08	1.43	1.52
13	6	221	ARG	CD-NE	7.08	1.56	1.46
21	N	226	ASN	C-N	7.07	1.43	1.33
30	K	142	HIS	ND1-CE1	7.07	1.39	1.32
31	L	125	PRO	C-N	7.07	1.42	1.33
15	W	25	ARG	CD-NE	7.07	1.56	1.46
21	N	178	SER	CA-CB	7.07	1.65	1.53
29	I	77	SER	N-CA	-7.07	1.37	1.46
25	R	82	ASP	CA-C	-7.07	1.44	1.52
9	2	214	GLU	CA-C	-7.06	1.43	1.52
28	H	385	ARG	CZ-NH1	7.06	1.42	1.32
11	4	23	ARG	CA-C	-7.06	1.44	1.52
21	N	256	GLN	CA-C	-7.06	1.43	1.52
21	N	692	GLU	CA-CB	7.06	1.65	1.53
14	7	231	ALA	CA-C	-7.06	1.44	1.52
28	H	147	ILE	CA-C	7.05	1.58	1.52
28	H	322	GLY	C-N	7.05	1.43	1.33
19	Y	76	GLU	CA-C	7.05	1.61	1.52
33	J	22	TYR	CA-CB	7.05	1.64	1.53
12	5	176	ILE	CA-C	-7.05	1.44	1.52
16	V	229	ASP	CA-C	-7.05	1.43	1.52
21	N	112	GLU	CA-C	-7.05	1.43	1.52
3	c	120	GLN	C-N	7.05	1.43	1.33
25	R	336	LYS	N-CA	-7.05	1.37	1.46
5	e	169	ALA	CA-C	-7.04	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	515	ARG	CD-NE	7.04	1.56	1.46
11	4	182	LYS	CA-C	-7.04	1.43	1.52
2	b	76	SER	CA-C	-7.03	1.44	1.52
15	W	158	ILE	CA-C	-7.03	1.43	1.52
26	U	113	TYR	CA-CB	7.03	1.64	1.54
27	O	370	LEU	C-N	7.03	1.42	1.33
6	f	25	ALA	C-N	7.03	1.44	1.33
25	R	206	ARG	NE-CZ	7.02	1.40	1.33
16	V	143	PRO	C-N	7.02	1.40	1.33
22	S	95	PHE	CA-CB	7.02	1.64	1.53
28	H	233	GLU	CA-C	-7.02	1.43	1.52
31	L	95	ILE	C-N	7.01	1.43	1.33
29	I	61	ARG	CD-NE	7.01	1.56	1.46
8	l	181	VAL	CA-C	-7.01	1.45	1.52
29	I	407	ARG	CD-NE	7.01	1.56	1.46
9	i	46	ASP	CA-CB	7.00	1.64	1.53
13	m	46	ARG	NE-CZ	7.00	1.40	1.33
13	m	212	ILE	CA-C	-7.00	1.43	1.52
23	P	7	ILE	CA-C	-7.00	1.44	1.52
27	O	318	HIS	C-N	7.00	1.41	1.33
10	j	186	VAL	C-N	7.00	1.42	1.33
21	N	309	ILE	N-CA	-7.00	1.38	1.46
2	b	240	SER	CA-C	-7.00	1.43	1.52
26	U	194	LEU	C-N	7.00	1.43	1.33
30	K	260	LEU	CA-C	-7.00	1.43	1.52
17	T	160	ALA	CA-C	-7.00	1.43	1.52
21	N	916	LEU	CA-C	-7.00	1.44	1.52
14	n	146	ALA	N-CA	-7.00	1.37	1.46
11	4	126	VAL	CA-C	-6.99	1.43	1.52
11	k	74	GLU	CA-CB	6.99	1.63	1.53
27	O	325	GLU	CA-CB	6.99	1.64	1.53
27	O	375	ASP	C-N	6.99	1.43	1.33
28	H	119	ASN	CA-C	-6.99	1.44	1.52
4	d	159	TRP	CA-C	-6.99	1.44	1.52
24	Q	238	TYR	CZ-OH	6.99	1.52	1.38
10	3	122	ALA	CA-C	-6.98	1.44	1.52
24	Q	150	GLN	CA-CB	6.98	1.64	1.53
7	g	239	ALA	N-CA	-6.98	1.37	1.46
22	S	476	LEU	N-CA	-6.98	1.38	1.46
29	I	151	HIS	CB-CG	6.98	1.59	1.50
21	N	918	GLU	N-CA	-6.98	1.37	1.46
27	O	366	MET	CA-CB	6.98	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	198	ARG	CA-C	-6.97	1.44	1.52
24	Q	186	HIS	CB-CG	-6.97	1.40	1.50
28	H	330	GLN	CA-CB	6.97	1.65	1.53
9	i	206	VAL	N-CA	-6.97	1.38	1.46
21	N	365	PHE	CA-CB	6.97	1.64	1.53
24	Q	261	VAL	CA-CB	-6.97	1.45	1.54
30	K	262	ARG	NE-CZ	6.97	1.40	1.33
26	U	35	GLY	N-CA	-6.97	1.38	1.45
11	k	179	VAL	CA-C	-6.97	1.44	1.52
30	K	158	ILE	CA-CB	6.97	1.62	1.54
27	O	350	ILE	CA-C	-6.97	1.43	1.52
8	l	129	HIS	ND1-CE1	6.96	1.39	1.32
31	L	75	LYS	C-N	6.96	1.43	1.33
3	c	213	PHE	CA-C	-6.96	1.43	1.52
21	N	781	ALA	CA-C	-6.96	1.43	1.52
33	J	15	HIS	ND1-CE1	6.96	1.39	1.32
5	e	53	ARG	NE-CZ	6.96	1.40	1.33
6	f	28	ALA	C-N	6.96	1.42	1.33
28	H	53	GLU	N-CA	-6.96	1.37	1.46
1	a	68	THR	CA-C	-6.95	1.44	1.53
4	d	111	ARG	CD-NE	6.95	1.55	1.46
27	O	76	LEU	CA-C	6.94	1.61	1.52
15	W	173	THR	CA-C	-6.94	1.44	1.52
17	T	42	PRO	CA-C	-6.93	1.45	1.52
24	Q	187	LYS	CA-C	-6.93	1.43	1.52
9	i	64	HIS	ND1-CE1	6.93	1.39	1.32
11	k	119	ILE	CA-C	-6.93	1.43	1.52
17	T	63	GLU	C-N	6.93	1.41	1.33
3	c	228	LYS	CA-C	-6.92	1.44	1.52
33	J	373	ARG	CA-CB	6.92	1.64	1.53
29	I	66	LYS	C-N	6.92	1.43	1.33
32	M	321	VAL	C-N	6.92	1.43	1.33
9	i	129	VAL	CA-C	-6.92	1.44	1.52
16	V	60	ASP	CA-C	-6.92	1.43	1.52
27	O	328	VAL	C-N	6.92	1.43	1.33
17	T	52	LEU	N-CA	-6.92	1.38	1.46
25	R	50	VAL	CA-CB	-6.92	1.44	1.54
7	g	61	PRO	C-N	6.91	1.42	1.33
12	l	181	ARG	CD-NE	6.91	1.55	1.46
23	P	355	GLU	N-CA	-6.91	1.38	1.46
23	P	428	THR	C-N	6.91	1.42	1.33
25	R	343	GLU	CA-C	-6.91	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	44	ALA	N-CA	-6.91	1.38	1.46
24	Q	410	ASP	N-CA	6.90	1.55	1.46
28	H	86	GLY	CA-C	-6.90	1.43	1.52
14	7	195	GLU	CA-CB	6.90	1.62	1.52
14	7	74	ARG	NE-CZ	6.90	1.40	1.33
14	n	243	LYS	N-CA	-6.89	1.37	1.45
22	S	481	TYR	C-N	6.89	1.42	1.34
32	M	299	ARG	CZ-NH2	6.89	1.42	1.33
12	l	87	ILE	CA-C	-6.89	1.43	1.52
17	T	188	GLU	CA-C	-6.88	1.44	1.52
8	1	133	TYR	CA-C	-6.88	1.44	1.52
21	N	748	PHE	C-N	6.87	1.43	1.33
25	R	397	ASN	CA-CB	6.87	1.64	1.53
21	N	859	ASN	CA-C	-6.87	1.44	1.52
10	3	154	TYR	C-N	6.87	1.43	1.33
4	d	111	ARG	NE-CZ	6.87	1.40	1.33
6	f	156	LEU	CA-C	6.87	1.62	1.53
21	N	749	LEU	C-N	6.87	1.43	1.34
14	7	225	SER	CA-C	-6.87	1.45	1.53
28	H	126	ASN	CA-C	-6.86	1.45	1.52
11	k	23	ARG	NE-CZ	6.86	1.40	1.33
31	L	82	ARG	NE-CZ	6.86	1.40	1.33
18	X	85	ARG	NE-CZ	6.86	1.40	1.33
21	N	197	VAL	CA-CB	6.86	1.61	1.53
13	6	109	ARG	CD-NE	6.86	1.55	1.46
23	P	146	ILE	CA-CB	-6.86	1.45	1.54
10	j	129	CYS	CA-C	-6.85	1.44	1.52
10	3	60	VAL	N-CA	6.85	1.54	1.46
32	M	18	LEU	CA-C	-6.85	1.44	1.53
28	H	215	LYS	CA-C	-6.85	1.44	1.52
33	J	195	LYS	C-N	-6.85	1.25	1.33
27	O	228	TYR	C-O	-6.84	1.16	1.24
5	e	174	SER	N-CA	-6.84	1.38	1.46
32	M	140	LEU	CA-CB	6.84	1.61	1.52
9	2	167	LEU	CA-C	-6.84	1.43	1.52
22	S	326	ASP	CA-CB	6.84	1.64	1.53
30	K	206	PRO	C-N	6.84	1.43	1.33
26	U	35	GLY	CA-C	-6.84	1.45	1.52
22	S	472	HIS	ND1-CE1	6.83	1.39	1.32
11	4	136	SER	CA-C	-6.83	1.44	1.52
24	Q	270	ILE	CA-C	6.83	1.61	1.52
33	J	339	ARG	NE-CZ	6.83	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	68	VAL	CA-C	-6.83	1.45	1.52
32	M	198	VAL	CA-C	-6.83	1.44	1.52
8	h	65	ALA	CA-C	-6.82	1.43	1.52
9	2	34	GLY	C-N	6.82	1.42	1.33
28	H	434	ARG	CZ-NH1	6.82	1.42	1.32
30	K	174	VAL	CA-C	-6.82	1.44	1.52
17	T	95	LYS	C-N	6.82	1.41	1.33
1	a	205	PHE	C-O	-6.81	1.16	1.24
15	W	88	ALA	N-CA	-6.81	1.38	1.46
25	R	412	THR	N-CA	-6.81	1.38	1.46
11	4	172	MET	CA-C	-6.81	1.44	1.53
21	N	35	LEU	C-N	6.81	1.42	1.33
22	S	433	GLU	N-CA	-6.81	1.37	1.46
23	P	40	LEU	N-CA	-6.81	1.38	1.46
27	O	147	ARG	CZ-NH1	6.81	1.42	1.32
2	b	209	ILE	CA-C	-6.81	1.44	1.52
15	W	43	SER	CA-C	-6.81	1.43	1.52
13	m	179	PRO	C-N	6.80	1.42	1.33
24	Q	314	PHE	N-CA	-6.80	1.38	1.46
14	n	193	ASP	CA-C	-6.80	1.43	1.52
12	5	92	ASP	C-O	6.80	1.30	1.23
12	l	82	ARG	N-CA	-6.80	1.37	1.45
29	I	298	GLY	C-N	6.80	1.42	1.33
18	X	119	LYS	N-CA	-6.79	1.38	1.46
17	T	94	HIS	N-CA	-6.79	1.37	1.46
23	P	193	TYR	CA-C	-6.79	1.43	1.52
33	J	156	GLN	CA-CB	6.79	1.63	1.53
8	1	26	ASP	CA-C	6.78	1.60	1.52
11	4	47	ALA	N-CA	-6.78	1.38	1.46
4	d	58	ARG	NE-CZ	6.78	1.40	1.33
12	5	82	ARG	CD-NE	6.78	1.55	1.46
25	R	365	ASP	N-CA	-6.78	1.38	1.46
8	1	171	ALA	N-CA	-6.78	1.38	1.46
25	R	305	PHE	CA-CB	6.78	1.62	1.53
29	I	250	SER	CA-C	-6.78	1.43	1.52
33	J	276	LEU	N-CA	-6.78	1.37	1.46
28	H	273	ARG	CA-C	-6.77	1.44	1.52
30	K	142	HIS	CB-CG	6.77	1.59	1.50
21	N	807	THR	CA-C	-6.77	1.44	1.52
7	g	27	ALA	C-N	6.77	1.41	1.34
12	l	212	TYR	CA-CB	6.77	1.64	1.53
21	N	867	LYS	C-N	6.77	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	313	ASP	CA-CB	6.77	1.64	1.53
12	5	263	HIS	N-CA	-6.77	1.38	1.46
17	T	221	ALA	C-N	6.76	1.43	1.33
29	I	81	ILE	CA-CB	-6.76	1.46	1.54
9	i	196	LEU	N-CA	-6.76	1.37	1.46
10	3	100	PHE	N-CA	-6.76	1.37	1.46
17	T	235	PHE	N-CA	-6.76	1.37	1.46
21	N	679	ASN	CA-C	-6.76	1.44	1.52
33	J	209	LYS	N-CA	-6.76	1.38	1.46
31	L	234	ALA	CA-C	-6.75	1.45	1.52
17	T	257	THR	CA-C	6.75	1.61	1.52
2	b	66	LEU	CA-C	-6.75	1.44	1.52
12	l	245	TYR	C-N	6.75	1.43	1.33
14	7	42	THR	C-N	6.75	1.43	1.33
16	V	129	PHE	CA-CB	6.74	1.64	1.53
29	I	380	LEU	CA-C	-6.74	1.44	1.52
5	e	242	GLU	C-N	6.74	1.43	1.33
21	N	878	GLN	C-N	6.74	1.43	1.34
9	i	128	ILE	C-N	6.74	1.42	1.33
24	Q	255	TYR	C-N	6.74	1.42	1.33
24	Q	328	ASP	CA-C	-6.74	1.44	1.52
10	j	155	GLU	CA-C	-6.73	1.47	1.52
14	n	131	THR	C-N	6.73	1.42	1.33
14	7	159	PHE	C-N	6.73	1.42	1.33
23	P	9	ALA	CA-C	-6.73	1.44	1.52
2	b	246	ARG	CA-CB	6.73	1.64	1.53
12	5	275	VAL	CA-C	-6.73	1.42	1.52
23	P	127	GLU	N-CA	6.73	1.54	1.46
9	2	102	GLU	C-N	6.73	1.42	1.33
14	7	220	ARG	CD-NE	6.73	1.55	1.46
15	W	179	ARG	NE-CZ	6.73	1.40	1.33
16	V	231	GLU	CA-CB	6.73	1.63	1.53
25	R	331	ARG	CA-C	-6.73	1.44	1.52
4	d	228	GLU	N-CA	-6.72	1.38	1.46
14	n	98	ARG	CZ-NH1	6.72	1.42	1.32
9	2	107	SER	CA-C	-6.72	1.44	1.52
26	U	127	GLN	N-CA	-6.72	1.36	1.46
30	K	350	ARG	NE-CZ	6.72	1.40	1.33
30	K	307	ASP	CA-C	-6.72	1.43	1.52
17	T	37	ASN	CA-C	-6.72	1.43	1.52
9	i	86	GLN	C-N	6.72	1.43	1.33
8	h	42	LYS	CA-C	-6.71	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	184	PRO	N-CD	-6.71	1.38	1.47
25	R	209	ARG	NE-CZ	6.71	1.40	1.33
1	a	200	GLU	CA-C	6.71	1.61	1.52
29	I	94	LYS	CA-C	-6.71	1.44	1.52
16	V	146	SER	N-CA	-6.70	1.37	1.46
20	Z	255	LEU	CA-CB	6.70	1.64	1.53
26	U	196	SER	C-N	6.70	1.43	1.33
29	I	175	LYS	C-N	6.70	1.42	1.33
5	e	139	GLY	N-CA	-6.70	1.35	1.45
13	m	30	VAL	C-N	6.70	1.42	1.33
25	R	262	GLU	N-CA	-6.70	1.37	1.45
12	5	196	ARG	CZ-NH1	6.70	1.42	1.32
22	S	142	VAL	CA-C	6.70	1.61	1.52
6	f	19	LEU	CA-C	-6.70	1.44	1.52
16	V	91	MET	N-CA	-6.70	1.38	1.46
2	b	46	ALA	C-N	6.69	1.41	1.33
2	b	179	TRP	CA-CB	6.69	1.64	1.53
11	4	98	TYR	CA-C	-6.69	1.44	1.52
14	n	218	TYR	CA-C	-6.69	1.44	1.52
28	H	318	ARG	N-CA	-6.69	1.37	1.46
30	K	146	LEU	N-CA	-6.68	1.38	1.46
33	J	48	ARG	CA-CB	6.68	1.64	1.53
12	l	198	LYS	CA-C	-6.68	1.43	1.53
21	N	52	ASP	N-CA	-6.68	1.37	1.45
32	M	133	GLY	C-O	-6.68	1.16	1.24
4	d	148	TYR	CA-C	6.68	1.60	1.52
25	R	128	LEU	N-CA	-6.68	1.37	1.46
21	N	184	LYS	C-O	6.67	1.31	1.24
32	M	59	LEU	N-CA	-6.67	1.38	1.46
24	Q	179	LEU	CB-CG	6.67	1.66	1.53
27	O	53	LYS	C-N	6.67	1.42	1.33
29	I	100	ARG	CA-CB	6.67	1.62	1.53
16	V	55	GLY	N-CA	6.67	1.51	1.45
22	S	265	SER	CA-C	-6.67	1.44	1.52
3	c	172	ALA	CA-C	-6.67	1.44	1.52
9	i	239	THR	CA-C	-6.67	1.44	1.52
28	H	305	ILE	C-N	6.67	1.42	1.33
22	S	441	GLY	N-CA	-6.66	1.35	1.45
26	U	225	ILE	C-N	6.66	1.42	1.34
3	c	229	ILE	CA-C	-6.66	1.44	1.52
18	X	83	SER	N-CA	-6.66	1.37	1.45
21	N	694	LEU	CA-C	-6.66	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	91	THR	N-CA	-6.66	1.38	1.46
24	Q	427	PHE	N-CA	-6.65	1.38	1.46
9	2	65	ARG	NE-CZ	6.65	1.40	1.33
15	W	32	SER	C-N	6.65	1.42	1.33
27	O	201	PRO	C-N	6.65	1.42	1.33
21	N	307	LYS	CA-C	-6.65	1.44	1.52
3	c	206	LEU	N-CA	-6.64	1.38	1.46
10	3	185	ALA	CA-C	-6.64	1.43	1.52
10	j	56	LEU	N-CA	-6.64	1.37	1.46
12	l	111	GLU	CA-CB	6.64	1.61	1.52
14	n	174	THR	CA-CB	6.64	1.65	1.53
7	g	120	VAL	C-O	6.64	1.32	1.24
7	g	204	HIS	ND1-CE1	6.64	1.39	1.32
14	7	144	TRP	C-N	6.64	1.41	1.33
23	P	346	ILE	C-N	6.64	1.43	1.33
8	1	13	MET	N-CA	-6.63	1.38	1.46
21	N	58	ARG	NE-CZ	6.63	1.40	1.33
33	J	56	ARG	CD-NE	6.63	1.55	1.46
17	T	133	ILE	N-CA	-6.63	1.40	1.46
33	J	116	ARG	CD-NE	6.63	1.55	1.46
23	P	3	ARG	CZ-NH2	6.63	1.42	1.33
3	c	78	ALA	N-CA	-6.62	1.38	1.46
21	N	830	LYS	CA-C	-6.62	1.44	1.52
15	W	133	LYS	CA-CB	6.62	1.64	1.53
14	n	125	ILE	C-N	6.62	1.42	1.33
29	I	228	GLY	C-N	-6.62	1.24	1.33
6	f	115	LYS	N-CA	-6.62	1.38	1.46
24	Q	297	ASP	N-CA	-6.62	1.38	1.46
21	N	762	ARG	CD-NE	6.62	1.55	1.46
29	I	167	MET	C-N	6.62	1.42	1.33
13	6	148	GLY	CA-C	-6.61	1.43	1.51
27	O	320	PRO	CA-CB	6.61	1.63	1.53
23	P	6	PRO	CA-CB	-6.61	1.44	1.53
2	b	236	ARG	NE-CZ	6.61	1.40	1.33
15	W	173	THR	CA-CB	6.61	1.62	1.53
22	S	235	ASN	N-CA	-6.60	1.38	1.46
17	T	60	ARG	CD-NE	6.60	1.55	1.46
18	X	117	LYS	CA-CB	6.60	1.61	1.52
25	R	176	ARG	NE-CZ	6.60	1.40	1.33
11	k	185	ASP	CA-C	-6.60	1.44	1.52
23	P	52	LEU	CA-CB	6.60	1.63	1.53
27	O	260	VAL	C-N	6.60	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	345	ARG	CD-NE	6.60	1.55	1.46
31	L	298	ASP	CA-C	-6.60	1.44	1.52
8	h	158	GLU	CA-C	-6.59	1.44	1.52
25	R	383	ARG	CD-NE	6.59	1.55	1.46
22	S	101	LYS	N-CA	-6.59	1.38	1.46
21	N	576	VAL	CA-C	-6.59	1.44	1.52
4	d	254	HIS	CD2-NE2	6.59	1.45	1.37
28	H	320	ASP	CA-C	-6.59	1.44	1.52
17	T	130	ASP	C-N	6.59	1.42	1.33
24	Q	142	ALA	C-N	6.59	1.42	1.33
6	f	43	HIS	ND1-CE1	6.59	1.39	1.32
21	N	873	ARG	NE-CZ	6.58	1.40	1.33
30	K	145	ALA	C-O	-6.58	1.16	1.23
31	L	153	LEU	CA-CB	6.58	1.63	1.53
6	f	133	LEU	CA-C	-6.58	1.44	1.52
29	I	269	LYS	CA-C	6.58	1.61	1.52
3	c	52	VAL	CA-C	-6.58	1.44	1.52
23	P	327	LEU	CA-CB	6.58	1.63	1.53
25	R	262	GLU	C-N	6.58	1.42	1.33
13	6	75	ARG	NE-CZ	6.58	1.40	1.33
21	N	45	ASP	CA-CB	6.58	1.63	1.53
12	l	254	HIS	C-N	6.58	1.41	1.33
10	3	21	VAL	CA-C	-6.58	1.46	1.52
31	L	132	ARG	CZ-NH2	6.58	1.42	1.33
13	6	146	ALA	C-N	-6.57	1.25	1.33
21	N	695	ALA	N-CA	6.57	1.54	1.46
10	3	188	TYR	C-N	6.57	1.42	1.33
14	7	175	LEU	C-N	6.57	1.41	1.33
8	1	183	ARG	NE-CZ	6.57	1.40	1.33
29	I	61	ARG	CZ-NH2	6.57	1.42	1.33
14	7	35	GLN	CA-CB	6.57	1.65	1.53
33	J	187	LEU	C-O	-6.57	1.16	1.24
13	6	41	TYR	C-N	6.57	1.42	1.33
15	W	40	LYS	N-CA	-6.57	1.38	1.46
22	S	371	LEU	CA-C	6.57	1.61	1.52
29	I	129	TYR	CA-CB	6.57	1.62	1.53
12	l	84	GLN	C-N	6.56	1.43	1.33
11	4	8	ARG	CA-CB	6.56	1.62	1.53
10	j	139	SER	C-N	6.56	1.41	1.33
4	d	220	ASP	C-N	6.56	1.41	1.33
13	m	87	HIS	ND1-CE1	6.56	1.39	1.32
28	H	381	ASP	CA-C	-6.56	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	59	GLU	CA-CB	-6.55	1.43	1.53
13	6	117	THR	CA-C	-6.55	1.45	1.52
4	d	149	GLN	C-N	6.55	1.43	1.33
23	P	315	GLN	CA-C	-6.55	1.44	1.52
11	k	102	VAL	CA-C	-6.55	1.44	1.52
18	X	120	GLU	N-CA	-6.55	1.38	1.46
18	X	29	VAL	N-CA	-6.55	1.38	1.46
3	c	225	VAL	N-CA	-6.55	1.39	1.46
17	T	94	HIS	CA-CB	6.55	1.62	1.53
23	P	425	HIS	ND1-CE1	6.54	1.39	1.32
14	7	190	LYS	N-CA	-6.54	1.38	1.46
21	N	23	TYR	CA-C	-6.54	1.44	1.52
27	O	379	LYS	CA-C	-6.54	1.44	1.52
13	6	193	ARG	NE-CZ	6.54	1.40	1.33
13	m	165	LYS	CA-C	-6.54	1.44	1.52
25	R	102	LEU	CA-C	-6.54	1.44	1.52
33	J	177	LEU	CA-C	-6.54	1.44	1.52
10	j	159	GLU	CA-C	-6.53	1.46	1.53
24	Q	171	LYS	C-N	6.53	1.42	1.34
33	J	258	VAL	CA-C	-6.53	1.44	1.52
15	W	24	THR	C-N	6.53	1.43	1.33
31	L	186	LEU	N-CA	-6.53	1.36	1.46
10	j	156	PRO	CA-CB	-6.53	1.45	1.53
16	V	269	ARG	NE-CZ	6.53	1.40	1.33
30	K	117	SER	CA-CB	6.53	1.62	1.53
11	4	164	CYS	CA-CB	6.53	1.63	1.53
30	K	94	LEU	CA-C	-6.53	1.44	1.52
25	R	240	SER	C-N	6.53	1.39	1.33
32	M	116	ALA	CA-C	-6.53	1.44	1.52
17	T	264	MET	C-N	6.52	1.42	1.33
24	Q	130	ARG	NE-CZ	6.52	1.40	1.33
5	e	36	THR	CA-C	-6.52	1.44	1.52
7	g	16	SER	CA-CB	6.52	1.64	1.53
12	l	229	LEU	CB-CG	6.52	1.66	1.53
25	R	136	ASN	CA-C	-6.52	1.43	1.52
13	6	125	ASP	N-CA	-6.51	1.37	1.46
33	J	171	PRO	C-N	-6.51	1.25	1.33
11	k	38	LEU	CA-C	6.51	1.61	1.52
11	4	103	LEU	CA-CB	6.51	1.62	1.53
15	W	41	ARG	NE-CZ	6.51	1.40	1.33
22	S	57	LEU	CA-C	-6.51	1.44	1.52
30	K	412	ALA	CA-C	-6.51	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	159	THR	N-CA	-6.51	1.38	1.46
8	h	38	ARG	CZ-NH2	6.51	1.42	1.33
25	R	88	LEU	C-N	6.51	1.42	1.33
30	K	225	ALA	CA-C	-6.51	1.44	1.52
8	l	166	HIS	CA-CB	6.51	1.64	1.53
22	S	451	ILE	N-CA	-6.51	1.38	1.46
24	Q	389	VAL	C-N	6.51	1.42	1.33
9	i	82	GLU	CA-CB	-6.50	1.43	1.53
19	Y	15	ASP	CA-CB	6.50	1.63	1.53
3	c	121	GLY	CA-C	-6.50	1.44	1.52
5	e	118	ASP	N-CA	6.49	1.54	1.46
14	7	252	TRP	N-CA	-6.49	1.39	1.46
23	P	201	ARG	CD-NE	6.49	1.55	1.46
7	g	227	LEU	CA-C	-6.49	1.45	1.52
13	6	87	HIS	C-N	6.49	1.42	1.33
13	6	215	VAL	CA-CB	-6.49	1.46	1.54
2	b	61	LEU	CA-C	-6.49	1.44	1.52
8	l	27	SER	C-N	6.49	1.42	1.33
16	V	47	MET	CA-C	-6.49	1.44	1.52
22	S	247	VAL	N-CA	-6.49	1.38	1.46
29	I	79	SER	CA-CB	6.49	1.63	1.53
11	4	46	PHE	N-CA	-6.49	1.37	1.45
30	K	103	ILE	CA-CB	-6.49	1.45	1.54
10	3	125	ASP	CA-C	-6.48	1.44	1.52
3	c	9	ARG	NE-CZ	6.48	1.40	1.33
28	H	181	TYR	C-N	6.48	1.42	1.33
14	n	263	THR	N-CA	-6.48	1.38	1.46
11	4	82	SER	N-CA	-6.48	1.38	1.46
21	N	332	VAL	C-N	6.48	1.42	1.33
29	I	151	HIS	CA-CB	6.48	1.63	1.53
17	T	114	LEU	CA-CB	6.48	1.64	1.53
10	3	35	GLY	CA-C	-6.48	1.45	1.52
24	Q	389	VAL	CA-C	-6.48	1.44	1.52
9	i	65	ARG	NE-CZ	6.48	1.40	1.33
18	X	32	GLU	CA-C	-6.48	1.44	1.52
2	b	99	ARG	NE-CZ	6.47	1.40	1.33
10	3	203	ARG	CD-NE	6.47	1.55	1.46
16	V	154	ASP	N-CA	-6.47	1.37	1.45
24	Q	156	ALA	N-CA	-6.47	1.38	1.46
30	K	128	ARG	CZ-NH1	6.47	1.41	1.32
1	a	120	ARG	N-CA	-6.46	1.38	1.46
24	Q	404	ASN	N-CA	-6.46	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	78	ILE	CA-CB	-6.46	1.45	1.54
33	J	181	GLN	CA-C	-6.46	1.46	1.52
32	M	26	SER	CA-C	-6.46	1.44	1.52
1	a	21	PRO	N-CA	-6.46	1.39	1.47
21	N	881	TYR	C-N	6.46	1.41	1.33
24	Q	299	MET	C-O	-6.46	1.16	1.24
23	P	275	ASN	N-CA	-6.46	1.37	1.46
20	Z	254	PRO	CA-C	-6.45	1.45	1.52
27	O	47	LYS	C-N	6.45	1.42	1.33
9	2	64	HIS	CD2-NE2	6.45	1.45	1.37
28	H	252	PRO	CA-C	-6.45	1.45	1.52
32	M	410	VAL	N-CA	-6.45	1.38	1.46
33	J	231	ARG	NE-CZ	6.45	1.40	1.33
33	J	29	GLU	CA-C	-6.45	1.44	1.52
11	k	96	ARG	C-N	6.44	1.42	1.33
4	d	96	HIS	ND1-CE1	6.44	1.39	1.32
6	f	202	ARG	C-N	6.44	1.42	1.33
17	T	186	ARG	NE-CZ	6.44	1.40	1.33
33	J	371	ARG	NE-CZ	6.44	1.40	1.33
13	m	71	ALA	CA-CB	6.43	1.63	1.53
28	H	69	VAL	C-N	6.43	1.42	1.33
22	S	196	ARG	N-CA	-6.43	1.38	1.46
28	H	213	GLY	N-CA	-6.43	1.38	1.45
24	Q	299	MET	CA-C	-6.43	1.44	1.52
31	L	420	ARG	C-N	6.43	1.42	1.33
8	h	103	THR	N-CA	-6.43	1.38	1.46
12	l	261	ILE	CA-CB	-6.43	1.46	1.54
22	S	176	LEU	CA-C	6.42	1.61	1.52
12	l	83	PHE	C-N	6.42	1.42	1.34
14	n	219	TYR	CA-CB	6.42	1.63	1.53
12	5	175	MET	CA-C	-6.42	1.45	1.52
13	6	145	ARG	CD-NE	6.42	1.55	1.46
17	T	251	HIS	N-CA	-6.42	1.37	1.46
28	H	231	SER	N-CA	-6.42	1.40	1.46
31	L	417	LYS	N-CA	-6.42	1.38	1.46
4	d	172	ARG	CD-NE	6.41	1.55	1.46
21	N	51	ASP	C-N	6.41	1.41	1.33
31	L	54	ASN	CA-CB	6.41	1.63	1.53
27	O	288	ARG	NE-CZ	6.41	1.40	1.33
21	N	375	HIS	N-CA	-6.41	1.38	1.46
29	I	141	LEU	CA-C	-6.41	1.44	1.53
3	c	156	ASN	N-CA	-6.41	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	51	TRP	CD2-CE3	-6.40	1.30	1.40
4	d	194	LEU	N-CA	-6.40	1.38	1.46
8	l	110	GLY	CA-C	-6.40	1.44	1.51
14	n	74	ARG	NE-CZ	6.40	1.40	1.33
32	M	93	ASP	C-N	6.40	1.42	1.33
14	n	194	ARG	CD-NE	6.40	1.55	1.46
1	a	193	HIS	ND1-CE1	6.39	1.39	1.32
12	l	255	VAL	CA-C	-6.39	1.45	1.52
21	N	555	ILE	CA-C	-6.39	1.44	1.52
32	M	420	SER	C-N	6.39	1.43	1.33
22	S	164	ILE	CA-CB	6.39	1.57	1.54
28	H	378	SER	CA-CB	6.39	1.63	1.53
27	O	8	ASP	CA-CB	6.39	1.63	1.53
5	e	228	PHE	N-CA	-6.39	1.38	1.46
12	5	234	ARG	N-CA	-6.39	1.38	1.46
33	J	345	LYS	C-N	6.39	1.41	1.33
21	N	336	ASN	CA-C	-6.38	1.44	1.52
28	H	289	ARG	CZ-NH1	6.38	1.41	1.32
8	l	127	SER	CA-C	-6.38	1.44	1.52
6	f	110	HIS	C-N	6.38	1.42	1.33
29	I	175	LYS	N-CA	-6.38	1.37	1.45
6	f	51	ARG	CA-CB	6.38	1.64	1.53
11	4	7	ILE	C-O	-6.37	1.17	1.24
12	5	261	ILE	CA-C	-6.37	1.45	1.52
22	S	282	ILE	N-CA	-6.37	1.38	1.46
29	I	363	GLY	C-N	6.37	1.42	1.33
30	K	172	ALA	CA-C	-6.37	1.44	1.52
33	J	71	TYR	CA-CB	6.37	1.64	1.53
26	U	72	TYR	CA-C	-6.37	1.44	1.52
26	U	175	LEU	CA-CB	6.37	1.60	1.52
32	M	21	GLU	C-N	6.37	1.42	1.33
13	6	43	ILE	CA-C	-6.37	1.45	1.52
22	S	159	ASN	CA-CB	6.37	1.63	1.53
27	O	278	PRO	N-CA	-6.37	1.43	1.47
1	a	79	ILE	CA-C	-6.36	1.44	1.52
9	2	236	ARG	NE-CZ	6.36	1.40	1.33
21	N	350	LYS	C-N	6.36	1.42	1.33
10	j	59	ASP	N-CA	-6.36	1.37	1.46
1	a	175	GLN	CD-NE2	6.36	1.46	1.33
9	i	33	VAL	CA-C	-6.36	1.44	1.52
17	T	38	ASN	CA-C	-6.36	1.44	1.52
6	f	18	ARG	NE-CZ	6.36	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1	53	CYS	N-CA	-6.36	1.38	1.46
8	1	141	THR	N-CA	-6.36	1.38	1.46
12	l	139	ARG	CZ-NH1	6.35	1.41	1.32
12	l	243	ASP	CA-C	-6.35	1.45	1.52
33	J	391	ASN	CA-C	-6.35	1.44	1.52
16	V	284	ALA	N-CA	-6.35	1.38	1.46
10	3	188	TYR	CA-C	6.35	1.60	1.52
12	5	189	TYR	N-CA	-6.34	1.38	1.46
21	N	198	THR	CA-C	-6.34	1.44	1.52
9	i	54	ILE	CA-CB	6.34	1.62	1.54
32	M	193	LEU	CA-C	6.34	1.60	1.52
33	J	257	ARG	NE-CZ	6.34	1.40	1.33
15	W	170	HIS	ND1-CE1	6.34	1.38	1.32
21	N	162	ARG	NE-CZ	6.34	1.40	1.33
33	J	324	ARG	CD-NE	6.34	1.55	1.46
29	I	97	GLU	C-N	6.33	1.42	1.33
29	I	316	PHE	CA-CB	6.33	1.61	1.52
14	n	224	SER	N-CA	-6.33	1.38	1.46
21	N	758	VAL	C-N	6.33	1.41	1.33
14	7	72	VAL	C-N	6.33	1.42	1.33
22	S	431	VAL	CA-C	-6.33	1.45	1.52
17	T	88	TYR	CA-CB	6.33	1.63	1.53
25	R	231	LEU	CA-CB	6.33	1.63	1.53
27	O	270	ILE	CA-C	-6.33	1.44	1.52
28	H	323	ALA	C-N	6.33	1.41	1.33
29	I	64	ARG	CZ-NH1	6.33	1.41	1.32
4	d	203	VAL	C-N	6.32	1.42	1.33
21	N	518	ALA	C-N	6.32	1.41	1.33
12	l	160	ASN	CA-CB	6.32	1.63	1.53
8	1	60	ASP	CA-C	-6.32	1.44	1.52
26	U	276	ILE	CA-C	-6.32	1.44	1.52
10	j	120	PHE	CA-C	-6.32	1.45	1.52
11	4	27	VAL	C-N	6.32	1.41	1.33
27	O	87	LYS	CA-C	-6.32	1.44	1.52
26	U	169	ILE	N-CA	-6.32	1.39	1.46
12	l	192	SER	CA-C	-6.31	1.44	1.52
24	Q	233	LYS	N-CA	-6.31	1.38	1.46
29	I	363	GLY	CA-C	-6.31	1.44	1.52
32	M	381	ARG	CD-NE	6.31	1.55	1.46
2	b	197	LYS	N-CA	-6.31	1.38	1.46
8	h	45	ARG	CD-NE	6.31	1.55	1.46
22	S	270	ALA	CA-C	-6.31	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	238	GLN	CA-C	-6.31	1.44	1.52
4	d	254	HIS	ND1-CE1	6.31	1.38	1.32
8	h	21	VAL	CA-C	-6.31	1.44	1.52
24	Q	259	CYS	N-CA	6.30	1.54	1.46
14	7	189	ARG	NE-CZ	6.30	1.40	1.33
3	c	37	GLY	N-CA	-6.30	1.39	1.45
5	e	215	ASN	CA-CB	6.30	1.63	1.53
16	V	137	VAL	CA-C	-6.30	1.44	1.52
30	K	43	VAL	CA-C	-6.30	1.45	1.52
31	L	57	LEU	CA-C	-6.30	1.44	1.52
33	J	84	VAL	N-CA	-6.30	1.39	1.46
32	M	212	ILE	N-CA	-6.30	1.37	1.46
31	L	368	VAL	CA-C	-6.29	1.45	1.53
5	e	28	LEU	N-CA	-6.29	1.38	1.46
6	f	6	TYR	CA-CB	6.29	1.64	1.53
9	2	101	ARG	NE-CZ	6.29	1.40	1.33
21	N	214	LEU	CA-C	6.29	1.60	1.52
24	Q	88	PHE	N-CA	-6.29	1.38	1.46
5	e	13	SER	C-O	-6.29	1.19	1.23
28	H	229	LEU	C-N	6.29	1.42	1.33
15	W	40	LYS	CA-C	-6.29	1.44	1.52
33	J	231	ARG	CZ-NH1	6.29	1.41	1.32
20	Z	249	MET	N-CA	-6.29	1.38	1.46
10	3	65	GLU	CA-C	-6.28	1.44	1.52
33	J	55	VAL	CA-C	-6.28	1.44	1.52
7	g	204	HIS	CB-CG	6.28	1.58	1.50
9	2	158	SER	CA-CB	6.28	1.63	1.53
28	H	136	ALA	CA-C	-6.28	1.44	1.52
28	H	270	THR	C-N	6.28	1.42	1.33
17	T	187	ASP	C-N	6.28	1.42	1.33
26	U	278	ILE	CA-C	-6.28	1.45	1.52
27	O	382	LYS	C-N	6.28	1.42	1.33
8	h	38	ARG	CZ-NH1	6.28	1.41	1.32
8	1	67	ILE	CA-C	-6.27	1.44	1.52
28	H	230	LEU	CA-CB	6.27	1.63	1.53
30	K	264	ASN	CA-CB	6.27	1.61	1.53
6	f	131	GLY	CA-C	-6.27	1.43	1.51
17	T	185	ILE	CA-CB	6.27	1.61	1.54
28	H	55	ASP	CA-C	6.27	1.60	1.52
22	S	29	ASP	N-CA	-6.27	1.38	1.46
13	m	53	ASP	N-CA	-6.27	1.38	1.46
11	4	41	HIS	ND1-CE1	6.27	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	95	ALA	CA-C	-6.27	1.45	1.52
21	N	375	HIS	CA-C	-6.27	1.43	1.52
12	l	79	LEU	CA-C	-6.26	1.45	1.52
13	6	60	MET	C-N	6.26	1.42	1.33
28	H	266	ARG	N-CA	-6.26	1.38	1.46
11	k	108	ASP	CA-CB	6.26	1.61	1.53
28	H	367	ARG	CD-NE	6.26	1.55	1.46
30	K	226	VAL	CA-C	-6.26	1.44	1.52
25	R	227	ALA	C-N	6.26	1.42	1.33
4	d	59	ILE	N-CA	-6.26	1.39	1.46
25	R	51	LEU	C-N	6.25	1.42	1.33
29	I	247	ILE	CA-C	-6.25	1.45	1.52
7	g	14	VAL	C-N	-6.25	1.25	1.33
22	S	236	LEU	C-N	6.25	1.41	1.33
23	P	395	ARG	C-N	6.25	1.41	1.33
1	a	99	ALA	CA-CB	6.25	1.63	1.53
10	3	100	PHE	C-N	6.25	1.42	1.33
21	N	651	PHE	CA-C	-6.25	1.44	1.52
30	K	423	LYS	C-O	-6.25	1.16	1.24
25	R	246	TYR	C-N	6.25	1.41	1.33
4	d	199	LEU	CA-CB	6.24	1.63	1.53
12	5	266	HIS	CA-C	-6.24	1.45	1.52
4	d	119	ARG	CA-CB	6.24	1.63	1.53
16	V	277	LYS	CA-CB	6.24	1.63	1.53
18	X	106	SER	C-N	6.24	1.38	1.33
25	R	250	ALA	C-N	6.24	1.41	1.33
28	H	382	LEU	CA-C	-6.24	1.44	1.52
2	b	130	PHE	CA-C	-6.24	1.44	1.52
11	4	182	LYS	N-CA	-6.24	1.38	1.46
14	7	100	LEU	C-O	-6.24	1.16	1.24
15	W	100	HIS	C-N	6.23	1.41	1.33
22	S	239	ARG	CD-NE	6.23	1.54	1.46
27	O	50	ASP	N-CA	-6.23	1.38	1.46
29	I	225	PRO	CA-C	-6.23	1.44	1.52
28	H	64	LYS	CA-C	-6.23	1.44	1.52
1	a	69	VAL	CA-CB	6.23	1.61	1.54
24	Q	14	LEU	N-CA	-6.22	1.38	1.46
24	Q	87	GLN	N-CA	-6.22	1.38	1.46
27	O	15	ARG	CD-NE	6.22	1.54	1.46
28	H	223	GLU	N-CA	-6.22	1.38	1.46
12	l	247	GLY	C-O	-6.22	1.20	1.24
11	4	67	TYR	N-CA	-6.22	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	56	GLU	CA-C	-6.22	1.44	1.52
28	H	190	ARG	CD-NE	-6.22	1.37	1.46
30	K	233	ALA	C-O	-6.22	1.16	1.23
12	l	241	HIS	CA-C	-6.22	1.45	1.52
14	n	231	ALA	N-CA	-6.22	1.38	1.45
9	2	69	LYS	CA-C	-6.22	1.44	1.52
21	N	528	ARG	C-N	6.22	1.41	1.33
24	Q	374	GLU	CA-CB	6.22	1.63	1.53
29	I	301	GLU	CA-CB	6.22	1.63	1.53
22	S	302	HIS	ND1-CE1	6.22	1.38	1.32
1	a	144	VAL	CA-C	-6.22	1.45	1.52
30	K	152	PRO	N-CD	-6.22	1.39	1.47
1	a	108	TYR	CA-C	-6.21	1.44	1.52
2	b	8	SER	C-N	6.21	1.41	1.33
9	i	69	LYS	N-CA	-6.21	1.37	1.46
10	j	89	GLN	CA-CB	-6.21	1.43	1.53
14	7	243	LYS	C-N	6.21	1.42	1.33
29	I	69	LEU	C-N	6.21	1.42	1.33
31	L	141	LYS	C-N	6.21	1.41	1.33
32	M	184	GLY	C-N	6.21	1.42	1.33
13	6	179	PRO	CA-C	-6.21	1.47	1.53
33	J	54	LYS	C-N	6.21	1.41	1.33
21	N	705	ILE	C-N	6.21	1.42	1.33
23	P	364	ARG	N-CA	-6.21	1.39	1.46
26	U	42	ASN	CA-C	-6.21	1.44	1.52
3	c	58	GLU	CA-CB	6.21	1.60	1.53
22	S	63	LEU	CA-CB	6.21	1.62	1.53
25	R	27	SER	CA-CB	6.21	1.62	1.53
23	P	228	SER	N-CA	-6.21	1.38	1.46
24	Q	103	LYS	C-N	6.21	1.42	1.33
31	L	202	LYS	CA-C	-6.21	1.45	1.52
4	d	18	PHE	CA-C	-6.20	1.44	1.52
24	Q	350	ILE	CA-CB	6.20	1.62	1.54
29	I	93	LYS	N-CA	-6.20	1.38	1.46
10	3	135	ASP	CA-C	-6.20	1.44	1.52
17	T	244	ASP	C-N	6.20	1.42	1.33
13	m	103	HIS	ND1-CE1	6.20	1.38	1.32
12	5	185	PRO	C-O	6.20	1.30	1.23
25	R	105	LYS	CA-CB	6.20	1.62	1.53
31	L	57	LEU	CA-CB	6.20	1.63	1.53
31	L	354	GLU	CA-CB	6.20	1.62	1.53
12	l	168	ALA	C-N	6.20	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	913	PRO	CA-C	-6.20	1.45	1.52
12	l	94	ARG	CZ-NH1	6.20	1.41	1.32
9	2	229	GLN	C-N	6.19	1.41	1.33
1	a	24	ARG	CD-NE	6.19	1.54	1.46
4	d	202	VAL	C-N	6.19	1.41	1.33
10	j	203	ARG	N-CA	-6.19	1.38	1.46
21	N	736	PHE	CA-CB	6.19	1.62	1.53
23	P	175	GLU	CA-C	-6.19	1.44	1.52
19	Y	59	ILE	C-O	-6.19	1.17	1.24
31	L	74	LEU	CA-C	-6.19	1.45	1.52
7	g	18	ASP	N-CA	-6.19	1.38	1.46
8	h	155	MET	C-N	6.19	1.41	1.33
32	M	409	SER	CA-C	-6.19	1.45	1.52
33	J	49	ASN	C-N	6.19	1.42	1.33
22	S	118	PHE	CA-C	-6.19	1.44	1.52
12	5	241	HIS	C-N	6.18	1.42	1.33
16	V	81	GLU	C-N	6.18	1.42	1.33
32	M	236	ALA	CA-C	6.18	1.60	1.52
5	e	136	ARG	NE-CZ	6.18	1.39	1.33
8	h	167	SER	N-CA	-6.18	1.38	1.46
8	h	194	ARG	CD-NE	6.18	1.54	1.46
18	X	48	PHE	C-N	6.18	1.42	1.33
19	Y	83	ARG	CD-NE	6.18	1.54	1.46
33	J	395	GLU	CA-C	-6.18	1.44	1.52
4	d	166	ARG	C-N	6.18	1.42	1.33
31	L	349	ILE	CA-C	-6.18	1.47	1.53
10	j	203	ARG	NE-CZ	6.17	1.39	1.33
29	I	157	VAL	C-N	6.17	1.40	1.33
11	4	116	LEU	CA-C	-6.17	1.45	1.52
27	O	29	PHE	C-N	6.17	1.41	1.33
6	f	72	LEU	CA-C	6.17	1.60	1.52
28	H	433	ALA	N-CA	6.17	1.54	1.46
8	l	131	LEU	CB-CG	6.17	1.65	1.53
17	T	217	THR	CA-C	6.17	1.60	1.52
29	I	195	LYS	CA-C	-6.17	1.44	1.52
4	d	106	VAL	CA-C	-6.17	1.44	1.52
21	N	48	ALA	C-N	6.17	1.42	1.34
19	Y	87	GLU	CA-C	-6.17	1.44	1.52
30	K	290	ARG	N-CA	6.16	1.53	1.46
31	L	203	ASN	CA-CB	6.16	1.61	1.53
15	W	101	ARG	NE-CZ	6.16	1.39	1.33
22	S	238	LEU	C-N	6.16	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	270	VAL	CA-CB	-6.16	1.46	1.54
26	U	213	LYS	C-N	6.16	1.41	1.33
31	L	409	HIS	ND1-CE1	6.16	1.38	1.32
7	g	35	THR	CA-C	-6.16	1.44	1.52
9	i	122	HIS	CD2-NE2	6.16	1.44	1.37
33	J	18	GLY	N-CA	-6.16	1.38	1.45
23	P	220	TYR	CA-CB	6.16	1.62	1.53
29	I	344	ILE	CA-C	-6.16	1.45	1.52
5	e	208	MET	CA-CB	6.16	1.62	1.53
12	5	94	ARG	NE-CZ	6.16	1.39	1.33
22	S	136	CYS	N-CA	-6.16	1.38	1.46
31	L	85	GLU	N-CA	-6.16	1.38	1.46
33	J	306	ARG	CZ-NH1	6.16	1.41	1.32
14	n	83	VAL	C-N	6.15	1.41	1.33
27	O	283	HIS	CG-ND1	6.15	1.45	1.38
22	S	384	ARG	NE-CZ	6.15	1.39	1.33
28	H	90	ARG	NE-CZ	6.15	1.39	1.33
13	m	91	LYS	C-N	6.15	1.42	1.33
30	K	251	PRO	CA-C	-6.15	1.42	1.52
24	Q	75	ARG	CD-NE	6.15	1.54	1.46
27	O	227	ILE	CA-CB	6.15	1.61	1.54
32	M	45	ARG	CD-NE	6.15	1.54	1.46
10	j	184	GLY	CA-C	-6.14	1.45	1.52
33	J	196	THR	CA-C	6.14	1.60	1.52
16	V	171	ARG	NE-CZ	6.14	1.39	1.33
30	K	333	ARG	NE-CZ	6.14	1.39	1.33
9	i	172	LYS	CA-C	-6.14	1.45	1.52
21	N	349	ILE	CA-CB	6.14	1.61	1.54
29	I	408	ARG	NE-CZ	6.14	1.39	1.33
32	M	277	ILE	N-CA	-6.14	1.38	1.46
14	n	111	ASN	C-N	-6.14	1.27	1.34
21	N	618	ARG	CA-CB	6.13	1.63	1.53
23	P	104	LEU	N-CA	6.13	1.53	1.46
23	P	355	GLU	CA-C	-6.13	1.45	1.52
27	O	355	PRO	N-CA	-6.13	1.40	1.47
21	N	398	ARG	CA-CB	6.13	1.63	1.53
5	e	152	GLY	CA-C	-6.13	1.41	1.52
7	g	53	LEU	N-CA	-6.13	1.38	1.46
19	Y	26	LYS	CA-C	-6.13	1.45	1.52
24	Q	341	THR	C-N	6.13	1.42	1.34
32	M	216	LYS	C-O	-6.12	1.16	1.24
9	i	154	LEU	C-N	6.12	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	217	ARG	NE-CZ	6.12	1.39	1.33
21	N	373	VAL	C-N	6.12	1.41	1.33
24	Q	12	ARG	CZ-NH1	6.12	1.41	1.32
32	M	54	GLU	C-N	6.12	1.42	1.33
9	i	155	SER	C-N	6.12	1.41	1.33
29	I	368	LYS	N-CA	-6.12	1.38	1.46
10	j	79	GLU	N-CA	6.12	1.55	1.46
11	k	85	ARG	CZ-NH1	6.12	1.41	1.32
17	T	123	HIS	CB-CG	-6.12	1.41	1.50
27	O	128	LEU	N-CA	6.12	1.53	1.46
5	e	31	ILE	CA-CB	6.12	1.61	1.54
12	l	99	ASN	C-O	-6.12	1.15	1.24
31	L	145	ARG	NE-CZ	6.12	1.39	1.33
28	H	327	ASN	N-CA	-6.12	1.38	1.46
9	i	229	GLN	C-N	6.11	1.41	1.33
21	N	532	ALA	CA-C	-6.11	1.44	1.52
8	h	108	VAL	CA-C	-6.11	1.44	1.52
11	4	180	ILE	CA-C	-6.11	1.45	1.52
16	V	58	VAL	CA-C	6.11	1.58	1.52
4	d	231	GLN	CA-C	-6.11	1.44	1.52
12	5	107	LYS	CA-CB	6.11	1.61	1.53
16	V	159	ILE	CA-C	-6.11	1.45	1.52
17	T	151	TRP	NE1-CE2	-6.11	1.30	1.37
11	4	96	ARG	CA-C	-6.11	1.44	1.52
8	h	166	HIS	ND1-CE1	6.10	1.38	1.32
23	P	150	GLU	CA-CB	6.10	1.62	1.53
29	I	148	LEU	CA-CB	6.10	1.62	1.53
30	K	254	VAL	CA-C	-6.10	1.44	1.52
31	L	214	PRO	CA-C	-6.10	1.46	1.52
9	2	48	ARG	NE-CZ	6.10	1.39	1.33
27	O	188	PHE	CA-CB	6.10	1.62	1.53
31	L	325	MET	N-CA	-6.10	1.38	1.46
9	2	142	ILE	C-N	6.10	1.41	1.33
21	N	737	SER	CA-CB	6.10	1.63	1.53
22	S	476	LEU	CA-C	-6.10	1.45	1.52
30	K	346	ARG	N-CA	-6.10	1.39	1.46
16	V	25	GLU	CA-C	-6.10	1.45	1.52
14	n	141	ASN	CA-CB	6.09	1.61	1.53
9	2	253	GLN	C-N	6.09	1.42	1.33
12	5	273	TRP	NE1-CE2	6.09	1.44	1.37
32	M	251	LEU	C-N	6.09	1.41	1.33
12	l	204	VAL	CA-C	6.09	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	346	ARG	NE-CZ	6.09	1.39	1.33
2	b	165	GLY	C-O	-6.09	1.17	1.23
18	X	83	SER	CA-C	-6.09	1.45	1.52
5	e	234	GLU	CA-C	-6.09	1.44	1.52
6	f	32	GLY	C-O	-6.09	1.18	1.23
9	2	114	GLN	CA-C	-6.09	1.45	1.52
3	c	44	ILE	N-CA	-6.08	1.39	1.46
16	V	217	HIS	CA-C	-6.08	1.44	1.52
22	S	234	ILE	CA-C	-6.08	1.45	1.52
24	Q	65	TYR	CA-C	-6.08	1.44	1.52
7	g	138	PHE	CA-C	-6.08	1.45	1.52
17	T	224	ARG	NE-CZ	6.08	1.39	1.33
5	e	230	ILE	CA-CB	6.07	1.61	1.54
7	g	207	ASN	CA-CB	6.07	1.61	1.53
12	l	115	PHE	C-N	6.07	1.41	1.33
24	Q	313	ASP	N-CA	-6.07	1.38	1.46
28	H	311	ILE	CA-CB	-6.07	1.46	1.54
6	f	163	ALA	CA-C	-6.07	1.44	1.52
7	g	123	HIS	CA-C	-6.07	1.44	1.52
14	7	57	ALA	CA-C	-6.07	1.45	1.52
25	R	336	LYS	C-N	6.07	1.41	1.33
5	e	248	ALA	CA-C	-6.07	1.44	1.52
4	d	71	VAL	CA-CB	6.07	1.62	1.54
14	n	184	ALA	CA-CB	6.07	1.62	1.53
25	R	403	LEU	C-N	6.07	1.41	1.33
14	7	111	ASN	CA-CB	6.07	1.56	1.52
27	O	218	SER	CA-C	-6.07	1.45	1.52
27	O	315	LYS	C-N	6.07	1.42	1.33
3	c	146	TYR	N-CA	-6.06	1.38	1.46
10	3	80	ARG	NE-CZ	6.06	1.39	1.33
3	c	5	ARG	CD-NE	6.06	1.54	1.46
22	S	366	LYS	CA-C	-6.06	1.45	1.52
25	R	259	PHE	CA-CB	6.06	1.62	1.53
26	U	78	GLU	CA-C	-6.06	1.45	1.52
23	P	250	ILE	N-CA	-6.06	1.39	1.46
14	n	106	GLU	N-CA	6.06	1.53	1.46
9	2	175	LEU	CA-C	-6.05	1.45	1.52
13	6	99	ARG	NE-CZ	6.05	1.39	1.33
31	L	205	GLU	C-N	6.05	1.41	1.33
33	J	336	ASN	CA-C	-6.05	1.45	1.52
10	3	46	TYR	CA-C	6.05	1.59	1.53
31	L	430	GLY	C-N	6.05	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	95	ILE	CA-CB	6.05	1.61	1.54
22	S	200	GLU	N-CA	-6.05	1.38	1.46
29	I	170	VAL	C-N	6.05	1.42	1.33
32	M	392	LYS	C-N	6.05	1.41	1.33
8	h	204	GLN	C-N	6.05	1.41	1.33
14	n	113	LEU	N-CA	6.05	1.53	1.46
17	T	229	VAL	CA-C	-6.05	1.45	1.52
28	H	101	ARG	CA-CB	6.05	1.64	1.53
3	c	14	SER	CA-CB	6.04	1.62	1.53
26	U	123	VAL	CA-CB	6.04	1.61	1.53
30	K	185	ARG	NE-CZ	6.04	1.39	1.33
13	6	157	PHE	CA-CB	6.04	1.63	1.53
2	b	246	ARG	NE-CZ	6.04	1.39	1.33
6	f	132	LEU	CA-C	-6.04	1.45	1.52
10	3	188	TYR	CA-CB	6.04	1.61	1.53
28	H	101	ARG	NE-CZ	6.04	1.39	1.33
8	1	62	GLN	N-CA	-6.04	1.39	1.46
21	N	398	ARG	CD-NE	6.04	1.54	1.46
29	I	212	GLY	CA-C	-6.04	1.43	1.51
5	e	73	HIS	CG-CD2	6.04	1.42	1.35
22	S	161	LYS	N-CA	-6.04	1.39	1.46
23	P	300	VAL	C-O	-6.04	1.17	1.24
26	U	223	HIS	ND1-CE1	6.04	1.38	1.32
30	K	362	LEU	CA-C	-6.04	1.45	1.52
9	2	122	HIS	C-N	6.03	1.41	1.33
13	6	80	VAL	CA-CB	-6.03	1.47	1.54
33	J	125	VAL	C-N	6.03	1.42	1.33
22	S	317	HIS	ND1-CE1	6.03	1.38	1.32
3	c	92	ARG	CZ-NH1	6.03	1.41	1.32
13	6	48	GLU	C-N	6.03	1.41	1.33
14	7	81	ASN	N-CA	-6.03	1.40	1.46
22	S	244	ASN	C-N	6.03	1.41	1.33
21	N	148	SER	CA-C	-6.03	1.44	1.52
2	b	41	ASN	C-N	6.03	1.40	1.32
13	6	190	LYS	C-N	6.03	1.41	1.33
21	N	138	GLU	CA-C	-6.03	1.44	1.52
32	M	368	MET	C-N	6.03	1.41	1.33
13	m	145	ARG	N-CA	-6.02	1.38	1.46
14	n	125	ILE	CA-C	-6.02	1.45	1.52
11	4	58	GLU	CA-C	-6.02	1.44	1.52
11	4	70	ARG	CD-NE	6.02	1.54	1.46
18	X	50	TRP	CA-C	-6.02	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	82	SER	N-CA	-6.02	1.39	1.46
31	L	399	GLY	CA-C	-6.02	1.43	1.51
9	i	244	GLU	N-CA	-6.02	1.38	1.46
8	1	110	GLY	C-N	6.02	1.41	1.33
16	V	194	ARG	CA-C	-6.02	1.44	1.52
10	j	193	ASP	CA-CB	6.01	1.63	1.53
26	U	275	VAL	N-CA	-6.01	1.38	1.46
27	O	222	LEU	CA-C	6.01	1.60	1.52
12	l	83	PHE	CA-C	-6.01	1.45	1.52
32	M	390	GLN	C-N	6.01	1.42	1.33
1	a	151	GLY	C-N	-6.01	1.26	1.33
9	i	173	GLN	CA-CB	6.01	1.62	1.53
12	5	112	ILE	N-CA	-6.01	1.39	1.46
17	T	237	ASN	C-N	6.01	1.41	1.33
24	Q	22	GLU	C-N	6.01	1.42	1.34
27	O	95	SER	CA-C	-6.01	1.45	1.52
8	h	95	CYS	CA-CB	6.01	1.63	1.53
14	7	128	TYR	CA-C	6.01	1.60	1.52
22	S	375	ASP	CA-C	6.01	1.60	1.53
29	I	308	GLU	CA-C	-6.01	1.45	1.52
32	M	293	SER	CA-CB	6.01	1.63	1.53
21	N	839	ARG	NE-CZ	6.01	1.39	1.33
22	S	484	ASP	C-O	-6.01	1.17	1.24
14	n	215	ARG	C-N	6.01	1.41	1.33
15	W	77	HIS	ND1-CE1	6.01	1.38	1.32
23	P	316	LYS	N-CA	6.01	1.53	1.46
26	U	214	VAL	C-N	6.01	1.40	1.33
2	b	4	ARG	CZ-NH2	6.00	1.41	1.33
4	d	224	LEU	N-CA	-6.00	1.38	1.46
12	5	263	HIS	ND1-CE1	6.00	1.38	1.32
29	I	132	ILE	CA-CB	-6.00	1.46	1.54
4	d	178	ASN	CA-C	-6.00	1.44	1.52
17	T	136	LEU	CA-C	-6.00	1.44	1.52
22	S	121	VAL	CA-C	6.00	1.60	1.52
28	H	238	LEU	C-N	6.00	1.42	1.33
4	d	122	GLN	C-N	6.00	1.41	1.33
24	Q	117	VAL	C-N	6.00	1.41	1.33
27	O	306	ARG	N-CA	-6.00	1.39	1.46
31	L	410	ILE	CA-C	-6.00	1.45	1.52
31	L	62	ARG	NE-CZ	6.00	1.39	1.33
7	g	155	GLY	C-N	6.00	1.42	1.33
13	6	146	ALA	N-CA	-6.00	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	152	ASN	C-N	-5.99	1.26	1.34
7	g	177	GLU	C-N	5.99	1.42	1.34
21	N	705	ILE	N-CA	-5.99	1.39	1.46
9	i	181	ILE	C-O	5.99	1.31	1.24
11	k	85	ARG	NE-CZ	5.99	1.39	1.33
25	R	360	SER	CA-CB	5.99	1.62	1.53
30	K	227	ALA	CA-C	-5.99	1.44	1.52
18	X	67	ILE	N-CA	-5.99	1.39	1.46
7	g	80	GLY	C-O	-5.99	1.20	1.24
8	1	201	GLU	CA-C	-5.99	1.45	1.52
9	2	181	ILE	CA-CB	5.99	1.62	1.54
14	7	108	ALA	C-N	5.99	1.42	1.33
21	N	58	ARG	N-CA	-5.99	1.39	1.46
29	I	278	ILE	CA-C	-5.99	1.45	1.52
25	R	154	LEU	CA-C	-5.98	1.44	1.52
23	P	183	GLN	CA-CB	5.98	1.62	1.53
31	L	345	ARG	N-CA	-5.98	1.38	1.46
5	e	157	HIS	CA-C	-5.98	1.45	1.52
7	g	77	VAL	C-N	5.98	1.42	1.33
21	N	423	LEU	N-CA	-5.98	1.38	1.46
8	h	152	ARG	CD-NE	5.98	1.54	1.46
18	X	27	ILE	CA-C	-5.98	1.48	1.53
21	N	9	LEU	C-N	5.98	1.42	1.34
24	Q	413	LEU	CA-C	-5.98	1.45	1.52
8	1	17	PHE	N-CA	-5.98	1.39	1.46
13	6	151	ALA	CA-C	-5.98	1.45	1.52
28	H	244	LYS	N-CA	-5.98	1.38	1.46
4	d	6	ARG	CA-CB	5.98	1.61	1.53
3	c	180	TYR	CA-CB	5.97	1.62	1.53
31	L	69	ARG	CD-NE	5.97	1.54	1.46
33	J	297	LEU	CA-C	5.97	1.60	1.52
24	Q	67	THR	C-N	5.97	1.41	1.33
27	O	283	HIS	CB-CG	5.97	1.58	1.50
6	f	15	PRO	C-N	5.97	1.41	1.33
21	N	586	ALA	C-N	5.97	1.42	1.34
12	5	144	ARG	NE-CZ	5.96	1.39	1.33
16	V	71	MET	CA-CB	5.96	1.63	1.52
13	m	33	GLY	CA-C	-5.96	1.45	1.51
18	X	96	ARG	CD-NE	5.96	1.54	1.46
25	R	271	ILE	C-O	5.96	1.31	1.24
30	K	36	ASN	N-CA	5.96	1.53	1.46
31	L	145	ARG	CD-NE	5.96	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	308	LEU	C-N	5.96	1.41	1.33
31	L	305	LEU	N-CA	-5.96	1.39	1.46
1	a	52	VAL	N-CA	-5.96	1.39	1.46
7	G	22	PHE	CA-C	5.96	1.59	1.52
10	3	187	VAL	CA-CB	-5.96	1.46	1.54
26	U	149	SER	CA-CB	5.96	1.61	1.53
27	O	186	ASN	CA-C	-5.96	1.45	1.52
31	L	342	ARG	CD-NE	5.96	1.54	1.46
33	J	231	ARG	N-CA	-5.96	1.39	1.46
10	3	152	SER	CA-C	-5.96	1.45	1.52
13	6	47	TYR	CA-CB	5.96	1.63	1.53
5	e	80	GLY	N-CA	-5.95	1.36	1.45
9	i	219	TYR	N-CA	-5.95	1.39	1.46
9	2	166	VAL	CA-CB	-5.95	1.47	1.54
11	4	50	ALA	CA-C	-5.95	1.45	1.52
12	5	232	GLY	C-N	5.95	1.41	1.33
13	m	37	ASN	CG-ND2	5.95	1.45	1.33
9	2	64	HIS	N-CA	-5.95	1.38	1.45
10	3	166	THR	CB-OG1	-5.95	1.34	1.43
5	e	248	ALA	C-N	5.95	1.41	1.33
14	7	228	PHE	N-CA	-5.95	1.38	1.45
21	N	650	ASP	CA-C	-5.95	1.44	1.52
23	P	420	ASP	C-N	5.95	1.42	1.33
25	R	209	ARG	CD-NE	5.95	1.54	1.46
28	H	357	ARG	NE-CZ	5.95	1.39	1.33
8	1	146	TYR	C-N	5.95	1.41	1.33
17	T	111	LEU	N-CA	-5.95	1.39	1.46
24	Q	117	VAL	CA-C	5.95	1.60	1.52
1	a	75	ILE	CA-CB	5.95	1.62	1.54
9	2	240	ALA	CA-CB	5.95	1.61	1.53
15	W	153	LEU	N-CA	-5.95	1.38	1.46
21	N	872	THR	CA-CB	-5.95	1.43	1.53
13	m	145	ARG	NE-CZ	5.94	1.39	1.33
10	3	108	VAL	N-CA	-5.94	1.39	1.46
13	6	204	ILE	N-CA	-5.94	1.38	1.46
32	M	179	THR	N-CA	-5.94	1.38	1.46
4	d	38	GLY	CA-C	-5.94	1.44	1.51
24	Q	199	THR	CA-C	5.94	1.60	1.52
24	Q	294	ARG	CZ-NH2	5.94	1.41	1.33
25	R	277	LEU	CA-C	-5.94	1.45	1.52
30	K	84	GLU	C-N	5.94	1.41	1.33
33	J	364	GLU	CA-CB	5.94	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	387	ASN	C-N	5.94	1.41	1.33
32	M	382	SER	CA-C	-5.94	1.45	1.52
29	I	300	ARG	CD-NE	5.94	1.54	1.46
13	6	185	VAL	CA-CB	-5.94	1.47	1.54
33	J	78	ILE	N-CA	-5.94	1.39	1.46
13	6	81	LYS	N-CA	-5.93	1.39	1.46
21	N	894	ARG	CD-NE	5.93	1.54	1.46
16	V	159	ILE	N-CA	-5.93	1.39	1.46
12	l	149	ILE	C-N	5.93	1.41	1.33
22	S	168	LEU	CB-CG	5.93	1.65	1.53
24	Q	363	SER	C-N	5.93	1.41	1.33
21	N	42	GLU	N-CA	-5.93	1.39	1.46
12	l	166	LYS	C-N	5.93	1.40	1.33
15	W	59	PRO	C-N	5.93	1.42	1.33
17	T	186	ARG	CD-NE	5.93	1.54	1.46
22	S	59	ASP	C-N	5.93	1.41	1.33
4	d	216	LYS	CA-CB	5.92	1.62	1.53
22	S	444	GLU	CA-C	-5.92	1.45	1.52
16	V	40	HIS	ND1-CE1	5.92	1.38	1.32
25	R	197	MET	N-CA	5.92	1.53	1.46
29	I	151	HIS	N-CA	-5.92	1.39	1.46
8	l	194	ARG	C-N	5.92	1.41	1.33
21	N	103	SER	C-N	5.92	1.42	1.33
25	R	109	LYS	C-O	-5.92	1.17	1.24
31	L	72	ASP	CA-C	-5.92	1.45	1.52
11	k	147	HIS	N-CA	-5.92	1.38	1.45
10	3	43	ILE	CA-C	-5.91	1.45	1.52
10	3	115	LYS	CA-C	-5.91	1.45	1.52
21	N	305	ASN	CA-CB	5.91	1.62	1.53
21	N	683	LEU	CA-CB	5.91	1.62	1.53
23	P	359	ARG	CZ-NH2	5.91	1.41	1.33
25	R	148	ASP	CA-C	-5.91	1.45	1.52
14	n	223	ARG	CD-NE	5.91	1.54	1.46
6	f	8	GLY	C-N	-5.91	1.26	1.33
10	j	107	PRO	N-CA	-5.91	1.40	1.46
12	5	94	ARG	CA-CB	5.91	1.61	1.53
33	J	110	SER	N-CA	-5.91	1.37	1.46
5	e	147	HIS	ND1-CE1	5.90	1.38	1.32
13	m	99	ARG	CZ-NH1	5.90	1.41	1.32
9	2	170	HIS	CA-C	-5.90	1.44	1.52
13	6	80	VAL	C-N	5.90	1.41	1.33
18	X	86	ILE	CA-C	-5.90	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	357	ARG	CD-NE	5.90	1.54	1.46
25	R	67	CYS	CA-CB	5.90	1.62	1.53
31	L	82	ARG	CD-NE	5.90	1.54	1.46
4	d	20	VAL	CA-CB	-5.90	1.46	1.54
7	g	81	LEU	CA-C	-5.90	1.45	1.52
13	6	18	GLY	CA-C	-5.90	1.45	1.52
21	N	510	HIS	CG-CD2	5.90	1.42	1.35
8	h	31	THR	C-O	-5.90	1.17	1.24
14	n	35	GLN	CA-CB	5.90	1.63	1.53
15	W	2	VAL	CA-CB	-5.90	1.47	1.54
25	R	207	ARG	NE-CZ	5.90	1.39	1.33
6	f	104	ALA	CA-C	-5.89	1.45	1.52
8	1	183	ARG	CA-C	-5.89	1.45	1.52
26	U	210	TYR	N-CA	-5.89	1.39	1.46
30	K	187	ALA	N-CA	-5.89	1.39	1.46
15	W	181	LEU	N-CA	-5.89	1.39	1.46
21	N	605	ILE	C-N	5.89	1.41	1.33
23	P	47	ARG	NE-CZ	5.89	1.39	1.33
30	K	239	GLY	N-CA	5.89	1.53	1.45
30	K	255	ARG	CA-C	-5.89	1.44	1.52
8	1	176	GLY	CA-C	5.89	1.61	1.51
11	k	93	ARG	NE-CZ	5.89	1.39	1.33
24	Q	310	SER	N-CA	-5.89	1.39	1.46
25	R	246	TYR	CA-C	-5.89	1.44	1.52
27	O	322	ASP	CA-C	-5.89	1.45	1.52
27	O	346	GLU	CA-C	-5.89	1.45	1.53
32	M	366	ARG	C-N	5.89	1.41	1.33
33	J	306	ARG	NE-CZ	5.89	1.39	1.33
16	V	190	HIS	CG-ND1	-5.89	1.31	1.38
24	Q	73	LYS	C-N	5.89	1.41	1.33
25	R	220	ALA	C-O	-5.89	1.16	1.24
14	n	154	SER	CA-C	5.89	1.60	1.52
21	N	216	ASN	C-N	5.89	1.42	1.33
3	c	239	LEU	C-N	5.88	1.41	1.33
21	N	16	ASN	CA-C	-5.88	1.45	1.52
21	N	910	PRO	N-CA	-5.88	1.40	1.47
9	2	229	GLN	N-CA	-5.88	1.38	1.46
10	j	110	ALA	CA-C	-5.88	1.45	1.52
12	l	262	TYR	N-CA	-5.88	1.38	1.46
29	I	94	LYS	CA-CB	5.88	1.62	1.53
21	N	864	LYS	N-CA	-5.88	1.39	1.46
27	O	175	ASN	CA-C	-5.88	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I	119	ILE	N-CA	-5.88	1.39	1.46
11	k	3	ILE	CA-CB	5.88	1.62	1.54
13	6	98	ALA	N-CA	5.88	1.53	1.46
27	O	151	ASP	N-CA	-5.88	1.39	1.46
9	i	145	HIS	CE1-NE2	-5.88	1.26	1.32
21	N	502	PHE	CA-CB	5.87	1.62	1.53
30	K	141	ARG	CZ-NH1	5.87	1.41	1.32
33	J	87	LYS	CA-C	-5.87	1.45	1.52
3	c	96	GLN	CA-C	-5.87	1.44	1.52
9	2	212	ASP	C-N	5.87	1.41	1.33
22	S	358	LYS	CA-C	-5.87	1.45	1.52
29	I	357	THR	CA-C	-5.87	1.45	1.52
31	L	430	GLY	N-CA	5.87	1.51	1.45
30	K	349	ARG	CZ-NH2	5.87	1.41	1.33
14	7	36	GLN	CD-NE2	5.87	1.45	1.33
25	R	235	LEU	CA-C	-5.87	1.45	1.52
30	K	368	LEU	CA-C	-5.87	1.44	1.52
26	U	36	VAL	CA-CB	-5.87	1.46	1.54
30	K	133	PRO	N-CA	-5.87	1.40	1.47
14	n	98	ARG	C-N	5.86	1.42	1.34
14	7	38	ILE	C-N	5.86	1.41	1.33
22	S	406	ASP	CA-C	-5.86	1.45	1.52
28	H	89	GLN	CA-C	-5.86	1.44	1.52
33	J	272	MET	CA-CB	5.86	1.62	1.53
23	P	165	VAL	CA-CB	-5.86	1.46	1.54
25	R	302	ALA	C-N	5.86	1.42	1.33
32	M	24	ASN	CA-C	-5.86	1.45	1.52
4	d	109	LEU	C-N	5.86	1.41	1.33
31	L	90	LYS	N-CA	-5.86	1.39	1.46
16	V	31	SER	N-CA	-5.86	1.39	1.46
17	T	118	ASN	N-CA	-5.86	1.39	1.46
24	Q	106	GLN	C-N	5.86	1.40	1.33
30	K	107	THR	CA-CB	-5.86	1.43	1.53
11	k	93	ARG	CD-NE	5.85	1.54	1.46
22	S	425	ARG	CZ-NH2	5.85	1.41	1.33
24	Q	66	VAL	CA-CB	5.85	1.61	1.54
13	6	143	GLN	C-N	5.85	1.41	1.33
26	U	143	VAL	CA-CB	5.85	1.60	1.54
12	5	178	GLY	N-CA	-5.85	1.39	1.45
13	6	203	HIS	N-CA	-5.85	1.38	1.46
33	J	110	SER	CA-CB	5.85	1.62	1.53
22	S	179	ILE	CA-CB	5.85	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	212	TYR	CA-CB	5.85	1.64	1.53
13	6	228	LYS	CA-CB	-5.85	1.44	1.53
26	U	177	ASP	C-N	5.85	1.40	1.34
11	4	107	TYR	CA-CB	5.84	1.61	1.53
13	6	202	ARG	NE-CZ	5.84	1.39	1.33
19	Y	50	LYS	CA-CB	5.84	1.63	1.53
21	N	161	TYR	CA-CB	5.84	1.62	1.53
32	M	42	ARG	C-N	5.84	1.41	1.33
12	l	196	ARG	NE-CZ	5.84	1.39	1.33
21	N	674	GLN	C-N	5.84	1.41	1.33
12	l	239	ALA	C-O	-5.84	1.17	1.24
16	V	165	ILE	N-CA	-5.84	1.39	1.46
21	N	570	ARG	CA-C	-5.84	1.45	1.52
21	N	616	HIS	ND1-CE1	5.84	1.38	1.32
30	K	205	PRO	N-CD	5.84	1.55	1.47
33	J	339	ARG	CD-NE	5.84	1.54	1.46
13	m	84	HIS	CG-CD2	5.83	1.42	1.35
24	Q	75	ARG	NE-CZ	5.83	1.39	1.33
25	R	198	ILE	N-CA	-5.83	1.39	1.46
30	K	393	ARG	NE-CZ	5.83	1.39	1.33
32	M	30	LEU	CA-C	-5.83	1.45	1.52
32	M	233	ARG	CD-NE	5.83	1.54	1.46
16	V	138	ALA	C-N	5.83	1.41	1.33
14	n	36	GLN	CD-NE2	5.83	1.45	1.33
11	4	15	LEU	CA-CB	5.83	1.63	1.53
28	H	216	ASP	C-N	5.83	1.42	1.34
31	L	161	ARG	CA-C	-5.83	1.45	1.52
11	4	85	ARG	CD-NE	5.83	1.54	1.46
16	V	162	GLY	CA-C	5.83	1.59	1.52
23	P	348	HIS	ND1-CE1	5.83	1.38	1.32
26	U	185	GLY	C-N	5.83	1.41	1.33
11	4	21	VAL	N-CA	-5.82	1.39	1.46
22	S	466	LYS	CA-CB	5.82	1.62	1.53
24	Q	107	VAL	CA-C	-5.82	1.46	1.52
24	Q	399	VAL	CA-C	-5.82	1.45	1.52
1	a	216	THR	CA-C	-5.82	1.45	1.52
3	c	196	THR	C-O	-5.82	1.17	1.24
14	7	56	ALA	CA-C	-5.82	1.45	1.52
17	T	199	PHE	CG-CD2	5.82	1.51	1.38
4	d	87	GLU	CA-CB	5.82	1.62	1.53
21	N	110	VAL	C-N	5.82	1.40	1.33
24	Q	240	PHE	C-N	5.82	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	O	277	ILE	CA-C	-5.82	1.47	1.52
3	c	94	HIS	N-CA	-5.82	1.39	1.46
32	M	92	GLU	CA-CB	5.82	1.62	1.53
4	d	106	VAL	N-CA	-5.81	1.39	1.46
9	2	236	ARG	CZ-NH1	5.81	1.40	1.32
21	N	124	TYR	C-N	5.81	1.41	1.33
23	P	239	GLN	CA-C	-5.81	1.45	1.52
24	Q	75	ARG	C-N	5.81	1.41	1.33
28	H	173	ARG	NE-CZ	5.81	1.39	1.33
7	g	241	ASP	C-N	5.81	1.40	1.33
14	n	110	ASP	CA-CB	5.81	1.63	1.53
14	n	245	LEU	CA-CB	5.81	1.62	1.53
16	V	92	MET	SD-CE	5.81	1.94	1.79
22	S	22	GLU	CA-C	-5.81	1.45	1.52
22	S	62	SER	CA-CB	5.81	1.62	1.53
16	V	116	CYS	C-N	5.81	1.40	1.33
2	b	25	LEU	CA-CB	5.80	1.62	1.53
5	e	188	HIS	CE1-NE2	-5.80	1.26	1.32
6	f	219	ASP	CA-CB	5.80	1.62	1.53
12	l	223	LEU	CA-C	-5.80	1.45	1.52
1	a	249	ALA	C-N	5.80	1.42	1.34
2	b	47	THR	CA-C	5.80	1.59	1.52
5	e	86	ARG	NE-CZ	5.80	1.39	1.33
9	i	213	ALA	CA-C	-5.80	1.45	1.52
21	N	417	ARG	CD-NE	5.80	1.54	1.46
30	K	77	ARG	NE-CZ	5.80	1.39	1.33
9	i	207	MET	N-CA	-5.80	1.39	1.46
22	S	97	THR	C-N	5.80	1.41	1.33
2	b	175	LEU	CA-CB	5.80	1.63	1.53
25	R	176	ARG	C-N	5.80	1.41	1.34
25	R	335	ARG	CD-NE	5.80	1.54	1.46
26	U	2	SER	N-CA	-5.80	1.38	1.46
27	O	16	MET	CA-C	-5.80	1.45	1.52
33	J	68	PRO	CA-C	-5.80	1.46	1.52
3	c	15	PRO	CA-C	-5.80	1.44	1.52
4	d	145	PRO	C-N	5.80	1.41	1.33
31	L	339	ARG	NE-CZ	5.80	1.39	1.33
19	Y	55	THR	CA-C	5.79	1.60	1.52
10	3	168	SER	CA-C	-5.79	1.45	1.52
10	3	198	ARG	NE-CZ	5.79	1.39	1.33
22	S	362	SER	N-CA	-5.79	1.39	1.46
27	O	280	LEU	N-CA	-5.79	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	135	HIS	C-N	5.79	1.41	1.33
21	N	374	ILE	CA-CB	-5.79	1.47	1.54
21	N	887	ASP	N-CA	5.79	1.53	1.46
21	N	463	TYR	CA-CB	5.79	1.62	1.53
22	S	39	ASN	C-N	5.79	1.41	1.33
4	d	135	ILE	CA-C	-5.79	1.45	1.52
5	e	136	ARG	N-CA	-5.79	1.40	1.45
12	l	185	PRO	CA-C	-5.79	1.45	1.52
21	N	455	MET	CA-C	-5.79	1.45	1.53
14	n	44	VAL	CA-C	-5.78	1.45	1.52
17	T	224	ARG	CZ-NH1	5.78	1.40	1.32
8	1	12	ILE	CA-C	-5.78	1.45	1.52
30	K	298	GLU	N-CA	-5.78	1.39	1.46
31	L	302	GLN	N-CA	-5.78	1.39	1.46
8	h	205	LEU	CA-CB	5.78	1.65	1.53
13	m	220	VAL	C-N	5.78	1.41	1.33
11	k	170	LYS	N-CA	-5.78	1.39	1.46
11	4	192	VAL	CA-C	-5.78	1.45	1.52
16	V	61	TYR	C-N	5.78	1.41	1.33
21	N	146	LYS	C-N	5.78	1.41	1.33
22	S	122	ASN	CA-C	5.78	1.60	1.52
32	M	238	GLN	CA-CB	5.78	1.62	1.53
7	g	239	ALA	C-N	5.78	1.41	1.33
9	2	122	HIS	ND1-CE1	5.78	1.38	1.32
27	O	12	SER	CA-CB	5.78	1.62	1.53
8	1	21	VAL	CA-C	-5.78	1.45	1.52
15	W	86	HIS	CA-CB	5.78	1.62	1.53
26	U	295	LYS	CA-CB	5.78	1.62	1.53
28	H	226	GLU	CA-C	-5.78	1.45	1.52
31	L	197	ILE	N-CA	-5.78	1.39	1.46
31	L	409	HIS	N-CA	-5.78	1.39	1.46
11	k	157	GLY	C-N	5.77	1.41	1.33
28	H	313	ALA	CA-C	-5.77	1.45	1.52
4	d	179	TYR	CA-C	-5.77	1.45	1.52
5	e	157	HIS	CD2-NE2	-5.77	1.31	1.37
9	i	52	GLY	C-N	-5.77	1.28	1.33
21	N	731	VAL	N-CA	-5.77	1.39	1.46
29	I	319	ARG	CZ-NH1	5.77	1.40	1.32
13	6	225	TYR	N-CA	-5.77	1.38	1.46
28	H	336	LEU	CA-CB	5.77	1.62	1.53
8	1	17	PHE	CA-CB	5.77	1.62	1.53
14	7	135	GLN	C-N	5.77	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	174	THR	CA-C	-5.77	1.45	1.52
26	U	176	ARG	NE-CZ	5.77	1.39	1.33
30	K	147	VAL	CA-C	-5.77	1.44	1.52
32	M	359	GLN	CA-C	-5.77	1.45	1.52
27	O	175	ASN	C-N	5.77	1.41	1.33
6	f	110	HIS	ND1-CE1	5.76	1.38	1.32
7	g	23	GLN	CA-CB	5.76	1.62	1.53
16	V	298	ALA	CA-C	-5.76	1.45	1.52
22	S	449	LEU	CA-C	-5.76	1.48	1.53
4	d	185	PRO	CA-CB	5.76	1.61	1.53
17	T	182	LYS	C-N	5.76	1.41	1.33
23	P	292	LYS	CA-C	5.76	1.60	1.52
4	d	67	ILE	CA-C	-5.76	1.45	1.52
6	f	121	GLN	CA-C	-5.76	1.45	1.52
11	4	191	GLN	C-N	5.76	1.42	1.33
8	h	106	ILE	CA-CB	-5.76	1.47	1.54
14	7	95	HIS	CE1-NE2	-5.76	1.26	1.32
14	7	224	SER	C-N	5.76	1.38	1.33
21	N	116	GLN	C-N	5.76	1.41	1.33
26	U	100	ARG	NE-CZ	5.76	1.39	1.33
27	O	350	ILE	CA-CB	5.76	1.62	1.54
11	4	43	LEU	CA-C	-5.75	1.45	1.52
32	M	125	GLN	CA-CB	5.75	1.65	1.54
14	n	96	ILE	CB-CG1	5.75	1.65	1.53
32	M	166	ARG	CD-NE	5.75	1.54	1.46
33	J	123	HIS	CA-CB	5.75	1.60	1.53
2	b	184	GLU	N-CA	-5.75	1.38	1.45
14	n	136	ARG	NE-CZ	5.75	1.39	1.33
30	K	39	ALA	CA-C	-5.75	1.45	1.52
21	N	551	GLY	CA-C	-5.75	1.44	1.51
28	H	352	MET	CA-C	-5.75	1.46	1.52
6	f	84	LEU	CA-CB	5.75	1.62	1.53
8	h	23	LEU	CA-C	-5.75	1.46	1.52
10	j	132	GLU	CA-CB	5.75	1.62	1.53
11	k	149	ARG	NE-CZ	5.75	1.39	1.33
31	L	384	ASP	N-CA	5.75	1.53	1.45
8	h	68	VAL	CA-CB	5.74	1.61	1.54
16	V	269	ARG	C-N	5.74	1.41	1.33
1	a	39	ASN	CA-C	-5.74	1.43	1.52
1	a	57	LYS	CA-C	-5.74	1.45	1.52
28	H	62	ARG	NE-CZ	5.74	1.39	1.33
8	1	99	LYS	CA-C	-5.74	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	45	ALA	N-CA	-5.74	1.39	1.46
10	j	68	ARG	CD-NE	5.74	1.54	1.46
7	g	109	ILE	C-N	5.74	1.41	1.33
16	V	98	THR	C-N	5.74	1.41	1.33
28	H	332	THR	CA-C	5.74	1.60	1.52
8	h	41	ASP	CA-C	-5.73	1.45	1.52
14	7	212	ASN	N-CA	-5.73	1.39	1.46
7	g	30	ALA	C-N	5.73	1.40	1.33
12	5	254	HIS	ND1-CE1	5.73	1.38	1.32
33	J	289	LYS	C-O	-5.73	1.17	1.23
9	2	41	VAL	N-CA	-5.73	1.39	1.46
10	3	178	ASP	CA-C	5.73	1.59	1.52
32	M	384	ASP	CA-C	-5.73	1.45	1.52
3	c	40	ALA	CA-C	-5.72	1.45	1.53
32	M	169	ALA	CA-C	-5.72	1.45	1.52
13	m	126	GLY	CA-C	5.72	1.60	1.51
27	O	331	ALA	CA-C	-5.72	1.45	1.52
29	I	176	SER	CA-C	-5.72	1.47	1.53
13	6	20	ILE	CA-C	-5.72	1.46	1.52
23	P	215	SER	N-CA	-5.72	1.39	1.46
31	L	160	PRO	C-N	5.72	1.41	1.33
9	2	79	ALA	CA-C	-5.72	1.44	1.52
24	Q	357	VAL	C-N	5.72	1.41	1.33
32	M	257	GLY	C-N	5.72	1.41	1.33
8	h	183	ARG	NE-CZ	5.72	1.39	1.33
2	b	115	ALA	N-CA	-5.72	1.38	1.46
28	H	401	GLY	C-N	5.72	1.40	1.33
29	I	325	ILE	CA-CB	-5.71	1.46	1.54
2	b	53	SER	CA-CB	5.71	1.62	1.54
3	c	47	ALA	CA-C	-5.71	1.45	1.52
5	e	230	ILE	N-CA	-5.71	1.39	1.46
9	2	246	ILE	CA-C	-5.71	1.46	1.52
30	K	77	ARG	CD-NE	5.71	1.54	1.46
9	2	223	ASN	N-CA	-5.71	1.39	1.46
11	4	23	ARG	NE-CZ	5.71	1.39	1.33
21	N	104	LYS	CA-C	-5.71	1.45	1.52
23	P	197	THR	N-CA	-5.71	1.39	1.46
24	Q	234	THR	N-CA	5.71	1.53	1.46
5	e	231	TYR	C-N	5.71	1.41	1.33
12	5	255	VAL	CA-C	-5.71	1.46	1.52
13	6	107	GLY	N-CA	-5.71	1.38	1.45
4	d	215	VAL	CA-C	-5.71	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	247	GLU	CA-CB	5.71	1.62	1.53
12	5	90	ALA	C-N	5.71	1.41	1.33
21	N	734	VAL	C-O	-5.71	1.17	1.24
27	O	369	ARG	CZ-NH1	5.71	1.40	1.32
33	J	167	PRO	CA-CB	5.71	1.61	1.53
21	N	915	ALA	CA-C	-5.71	1.45	1.53
22	S	116	ALA	CA-CB	5.70	1.61	1.53
30	K	285	GLN	CA-C	-5.70	1.45	1.52
12	l	139	ARG	CZ-NH2	5.70	1.40	1.33
13	6	212	ILE	N-CA	-5.70	1.39	1.46
6	f	144	LEU	CA-CB	5.70	1.62	1.53
9	2	52	GLY	C-N	-5.70	1.27	1.34
13	6	41	TYR	N-CA	5.70	1.52	1.46
16	V	44	GLY	N-CA	-5.70	1.36	1.45
21	N	385	VAL	CA-CB	-5.70	1.46	1.54
27	O	359	SER	CA-CB	5.70	1.62	1.53
8	h	55	SER	CA-C	-5.70	1.45	1.52
9	i	146	GLY	CA-C	-5.70	1.44	1.51
10	3	154	TYR	N-CA	-5.70	1.38	1.46
21	N	51	ASP	CA-CB	5.70	1.62	1.53
27	O	269	LEU	CA-C	-5.70	1.45	1.52
3	c	143	ARG	CZ-NH1	5.70	1.40	1.32
33	J	233	LEU	CA-CB	5.70	1.62	1.53
13	6	33	GLY	CA-C	-5.70	1.44	1.51
13	6	187	GLU	CA-CB	5.69	1.62	1.53
15	W	195	GLY	C-N	5.69	1.41	1.33
31	L	209	ARG	CD-NE	5.69	1.54	1.46
1	a	92	ASN	CA-CB	5.69	1.62	1.53
3	c	39	MET	N-CA	-5.69	1.39	1.46
9	i	34	GLY	N-CA	-5.69	1.37	1.45
10	j	27	LEU	CA-CB	-5.69	1.45	1.53
21	N	321	LEU	CA-C	-5.69	1.45	1.52
23	P	401	ASN	CA-C	-5.69	1.45	1.53
25	R	203	ASP	CA-C	-5.69	1.45	1.52
8	h	43	LEU	N-CA	-5.69	1.39	1.46
21	N	437	GLU	CA-C	-5.69	1.45	1.52
26	U	252	HIS	ND1-CE1	5.69	1.38	1.32
2	b	196	LEU	C-N	5.69	1.41	1.33
12	5	143	LEU	N-CA	-5.69	1.39	1.46
12	5	282	PHE	CA-CB	5.69	1.62	1.53
9	2	225	ARG	NE-CZ	5.69	1.39	1.33
24	Q	127	ARG	C-N	5.69	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	144	ARG	N-CA	-5.69	1.39	1.46
21	N	398	ARG	CZ-NH2	5.68	1.40	1.33
26	U	130	VAL	C-N	5.68	1.41	1.33
26	U	246	GLU	CA-C	-5.68	1.45	1.52
2	b	246	ARG	C-N	5.68	1.41	1.33
13	m	190	LYS	CA-C	-5.68	1.45	1.52
25	R	275	GLU	CA-C	-5.68	1.45	1.52
31	L	409	HIS	CG-ND1	-5.68	1.32	1.38
33	J	40	ASN	CA-CB	5.68	1.62	1.53
2	b	240	SER	C-N	5.68	1.41	1.33
22	S	337	ASN	CA-CB	5.68	1.62	1.53
27	O	151	ASP	CA-CB	5.68	1.62	1.53
28	H	294	LEU	C-N	5.68	1.41	1.33
8	h	106	ILE	C-N	5.68	1.40	1.33
10	3	151	GLU	CA-C	-5.68	1.45	1.52
14	7	77	PRO	N-CA	-5.68	1.40	1.47
6	f	51	ARG	NE-CZ	5.68	1.39	1.33
11	4	12	SER	CA-C	-5.68	1.45	1.52
21	N	747	HIS	C-N	5.68	1.41	1.33
10	j	90	LEU	N-CA	-5.68	1.39	1.46
17	T	123	HIS	C-O	-5.68	1.17	1.24
29	I	83	LYS	CA-CB	5.68	1.60	1.53
33	J	43	ARG	CZ-NH2	5.68	1.40	1.33
27	O	150	LEU	C-N	5.67	1.41	1.33
17	T	19	ASP	CA-C	5.67	1.59	1.52
28	H	187	LEU	CA-C	-5.67	1.45	1.52
16	V	296	LEU	N-CA	-5.67	1.39	1.46
32	M	397	GLU	N-CA	-5.67	1.38	1.46
27	O	314	SER	C-N	5.67	1.41	1.33
15	W	141	ILE	N-CA	-5.67	1.39	1.46
17	T	23	CYS	CA-CB	5.67	1.62	1.53
25	R	248	SER	CA-C	5.67	1.60	1.52
26	U	80	CYS	CA-CB	5.67	1.62	1.53
31	L	166	LEU	CA-CB	5.67	1.62	1.53
32	M	350	PRO	C-N	5.67	1.41	1.33
4	d	217	PRO	CA-CB	-5.67	1.45	1.53
22	S	351	ALA	C-N	5.67	1.41	1.33
27	O	348	VAL	CA-CB	5.67	1.61	1.54
9	i	146	GLY	C-N	5.67	1.41	1.33
30	K	401	VAL	CA-C	-5.67	1.45	1.52
17	T	193	THR	CA-C	-5.66	1.44	1.52
19	Y	16	LEU	CA-C	-5.66	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	604	ARG	CD-NE	5.66	1.54	1.46
24	Q	80	HIS	CG-ND1	-5.66	1.32	1.38
31	L	357	ARG	NE-CZ	5.66	1.39	1.33
3	c	72	LYS	CA-C	-5.66	1.45	1.52
23	P	26	SER	C-N	5.66	1.41	1.33
15	W	138	ALA	CA-C	-5.66	1.46	1.52
25	R	208	ASN	CA-CB	5.66	1.62	1.53
12	5	150	SER	C-N	5.66	1.41	1.33
14	7	191	VAL	N-CA	-5.66	1.39	1.46
25	R	282	THR	CA-CB	5.66	1.63	1.53
14	n	242	LYS	N-CA	-5.66	1.39	1.46
11	k	184	VAL	CA-CB	-5.65	1.47	1.54
6	f	177	ASP	C-N	5.65	1.41	1.33
13	m	99	ARG	CZ-NH2	5.65	1.40	1.33
13	m	193	ARG	NE-CZ	5.65	1.39	1.33
9	2	234	PHE	C-N	-5.65	1.26	1.33
10	3	159	GLU	CA-C	-5.65	1.45	1.52
22	S	413	LEU	CA-C	-5.65	1.45	1.52
23	P	127	GLU	CA-C	-5.65	1.45	1.52
24	Q	400	TYR	N-CA	-5.65	1.39	1.46
28	H	405	GLU	CA-CB	5.65	1.63	1.53
33	J	202	VAL	CA-CB	-5.65	1.47	1.54
1	a	95	LEU	C-N	5.65	1.41	1.33
6	f	176	LEU	N-CA	-5.65	1.39	1.46
25	R	261	LEU	N-CA	-5.65	1.39	1.46
21	N	528	ARG	CZ-NH1	5.65	1.40	1.32
23	P	127	GLU	C-N	5.65	1.41	1.33
7	g	77	VAL	CA-C	-5.65	1.45	1.52
21	N	290	LEU	N-CA	-5.65	1.38	1.46
12	l	121	ALA	N-CA	-5.65	1.39	1.46
24	Q	381	ILE	CA-CB	-5.65	1.47	1.54
13	m	92	LEU	N-CA	-5.64	1.39	1.46
13	6	214	ILE	CA-CB	-5.64	1.47	1.54
12	l	219	TYR	CA-CB	5.64	1.61	1.53
14	n	162	TYR	CA-C	-5.64	1.45	1.52
8	1	93	GLU	CA-C	5.64	1.60	1.52
21	N	697	PHE	CA-C	-5.64	1.45	1.52
28	H	193	PRO	N-CA	5.64	1.54	1.47
32	M	233	ARG	C-N	5.64	1.41	1.33
21	N	183	VAL	C-N	5.64	1.41	1.33
21	N	800	ALA	C-N	5.64	1.41	1.33
1	a	162	TYR	C-O	-5.64	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	143	HIS	CE1-NE2	-5.64	1.26	1.32
21	N	515	ARG	NE-CZ	5.64	1.39	1.33
11	4	143	LEU	CA-C	-5.63	1.45	1.52
12	l	144	ARG	CD-NE	5.63	1.54	1.46
33	J	404	PHE	C-O	-5.63	1.17	1.24
3	c	49	GLU	C-N	5.63	1.40	1.33
12	l	266	HIS	ND1-CE1	5.63	1.38	1.32
21	N	924	LYS	CA-CB	5.63	1.62	1.53
22	S	199	GLU	N-CA	-5.63	1.39	1.46
27	O	238	ILE	CA-C	5.63	1.59	1.52
29	I	128	TYR	CA-C	-5.63	1.45	1.52
9	i	185	SER	CA-CB	5.63	1.62	1.53
13	m	36	ARG	CD-NE	5.63	1.54	1.46
27	O	214	ALA	CA-C	-5.63	1.45	1.52
10	3	156	PRO	CA-C	-5.63	1.46	1.52
24	Q	388	GLY	N-CA	-5.63	1.37	1.45
5	e	122	ARG	CZ-NH2	5.63	1.40	1.33
11	4	32	ASP	C-N	5.63	1.41	1.33
32	M	46	SER	CA-CB	5.63	1.62	1.53
33	J	138	MET	C-N	5.63	1.41	1.33
33	J	212	ARG	NE-CZ	5.63	1.39	1.33
17	T	134	LYS	CA-C	-5.62	1.45	1.52
24	Q	145	HIS	C-N	5.62	1.41	1.34
1	a	208	THR	N-CA	5.62	1.53	1.46
17	T	207	ALA	CA-C	5.62	1.59	1.52
27	O	77	SER	C-N	5.62	1.41	1.33
32	M	411	LYS	CA-C	-5.62	1.45	1.53
5	e	52	LYS	C-N	5.62	1.41	1.33
12	5	99	ASN	CG-ND2	5.62	1.45	1.33
30	K	149	ILE	C-N	5.62	1.42	1.33
32	M	383	THR	CA-C	5.62	1.60	1.52
12	l	128	GLN	C-N	5.62	1.41	1.33
32	M	379	LEU	C-N	5.62	1.41	1.33
8	1	185	VAL	CA-C	-5.62	1.45	1.52
13	6	46	ARG	CD-NE	5.62	1.54	1.46
22	S	341	SER	C-N	5.62	1.40	1.33
33	J	123	HIS	N-CA	-5.62	1.41	1.46
12	l	82	ARG	CZ-NH1	5.61	1.40	1.32
21	N	853	ASP	C-N	5.61	1.40	1.33
28	H	440	GLU	CA-CB	5.61	1.62	1.53
4	d	193	LYS	CA-C	-5.61	1.44	1.52
8	h	140	SER	N-CA	-5.61	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	95	ALA	C-O	-5.61	1.16	1.23
22	S	127	THR	CB-OG1	-5.61	1.34	1.43
4	d	238	GLN	CA-C	-5.61	1.45	1.52
21	N	874	ILE	N-CA	-5.61	1.38	1.46
17	T	43	ASP	CA-CB	5.61	1.61	1.53
9	2	31	THR	C-N	5.61	1.40	1.33
21	N	28	ILE	CA-C	-5.61	1.45	1.52
21	N	491	GLY	C-N	5.61	1.41	1.33
31	L	165	PRO	C-N	5.61	1.41	1.33
3	c	220	ALA	C-N	5.61	1.41	1.33
6	f	141	GLY	C-N	5.61	1.41	1.33
24	Q	164	GLU	CA-CB	5.61	1.62	1.53
24	Q	168	LEU	N-CA	-5.61	1.39	1.46
32	M	266	ALA	N-CA	-5.61	1.39	1.46
33	J	306	ARG	CD-NE	5.61	1.54	1.46
9	i	47	THR	N-CA	-5.60	1.38	1.46
14	n	197	ASP	N-CA	-5.60	1.38	1.46
21	N	372	GLY	CA-C	5.60	1.59	1.51
9	2	82	GLU	CA-CB	5.60	1.62	1.53
10	3	80	ARG	CA-C	-5.60	1.45	1.52
13	6	92	LEU	N-CA	-5.60	1.38	1.46
29	I	265	ARG	C-N	5.60	1.41	1.33
31	L	88	TYR	N-CA	-5.60	1.39	1.46
7	g	205	GLU	CA-CB	5.60	1.61	1.53
21	N	100	THR	CA-C	-5.60	1.45	1.52
27	O	188	PHE	C-N	5.60	1.41	1.33
32	M	327	THR	CA-C	-5.60	1.45	1.52
10	j	126	LEU	CA-CB	5.60	1.62	1.53
23	P	414	GLU	N-CA	-5.60	1.39	1.46
28	H	238	LEU	CA-C	5.60	1.60	1.52
17	T	113	LEU	C-N	5.60	1.41	1.34
3	c	183	ASP	N-CA	-5.59	1.39	1.46
13	6	153	LEU	CA-CB	5.59	1.62	1.53
16	V	243	SER	C-N	5.59	1.41	1.34
21	N	582	ASP	N-CA	5.59	1.53	1.46
21	N	909	GLU	C-O	-5.59	1.19	1.24
33	J	162	GLU	CA-C	-5.59	1.45	1.52
33	J	204	HIS	CD2-NE2	5.59	1.44	1.37
29	I	335	ASP	N-CA	-5.59	1.38	1.45
13	m	170	PRO	CA-C	5.59	1.59	1.52
14	7	183	MET	CA-C	-5.59	1.49	1.52
27	O	133	ILE	C-N	5.59	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	137	VAL	C-N	5.59	1.41	1.33
7	g	190	ARG	CZ-NH1	5.59	1.40	1.32
8	h	83	SER	CA-CB	5.59	1.61	1.53
21	N	282	TYR	C-N	5.59	1.41	1.33
33	J	319	PRO	N-CA	-5.59	1.40	1.46
4	d	194	LEU	CA-CB	5.58	1.62	1.53
13	6	16	ASN	N-CA	-5.58	1.40	1.46
25	R	159	SER	CA-CB	5.58	1.62	1.53
11	4	124	THR	C-N	5.58	1.41	1.33
30	K	297	ILE	CA-CB	5.58	1.60	1.54
33	J	234	PHE	C-N	5.58	1.41	1.33
33	J	243	SER	C-N	5.58	1.40	1.33
1	a	205	PHE	C-N	5.58	1.41	1.33
18	X	10	PHE	CA-C	-5.58	1.45	1.52
24	Q	300	LYS	C-N	5.58	1.41	1.33
33	J	40	ASN	N-CA	5.58	1.53	1.46
26	U	220	PRO	CA-CB	5.58	1.61	1.53
4	d	53	LYS	CA-CB	5.58	1.62	1.53
7	g	12	ASN	N-CA	-5.58	1.41	1.46
10	j	19	ASP	C-N	5.58	1.40	1.33
11	k	84	VAL	CA-C	-5.58	1.45	1.52
21	N	107	GLU	N-CA	-5.58	1.39	1.46
29	I	126	PRO	CA-C	5.58	1.60	1.52
10	j	98	ARG	CA-CB	5.57	1.60	1.52
10	j	204	GLN	CA-C	-5.57	1.45	1.52
23	P	74	ASP	CA-C	-5.57	1.45	1.52
29	I	159	VAL	CA-CB	-5.57	1.49	1.55
33	J	73	GLY	N-CA	-5.57	1.37	1.45
11	k	31	SER	N-CA	-5.57	1.41	1.46
14	7	100	LEU	C-N	5.57	1.41	1.33
22	S	382	ARG	C-N	5.57	1.42	1.33
6	f	83	VAL	C-N	5.57	1.42	1.33
6	f	209	ASP	N-CA	-5.57	1.39	1.46
28	H	99	VAL	N-CA	-5.57	1.39	1.46
2	b	122	THR	CA-C	-5.57	1.44	1.52
4	d	131	VAL	CA-C	-5.57	1.45	1.52
21	N	880	ARG	CD-NE	5.57	1.54	1.46
28	H	199	THR	C-N	5.57	1.40	1.33
1	a	154	ILE	CA-C	-5.57	1.45	1.52
7	g	116	LEU	C-N	5.57	1.41	1.33
7	g	187	LEU	C-N	5.57	1.40	1.33
31	L	345	ARG	CZ-NH2	5.57	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	219	LEU	CA-CB	5.56	1.61	1.53
29	I	134	SER	CA-C	-5.56	1.45	1.52
5	e	141	ALA	C-N	5.56	1.41	1.33
13	m	40	ASP	CA-CB	5.56	1.63	1.52
8	l	126	GLY	C-N	5.56	1.41	1.33
12	5	286	ILE	N-CA	-5.56	1.40	1.46
21	N	228	VAL	CA-CB	5.56	1.60	1.54
21	N	390	LEU	CA-C	-5.56	1.45	1.53
24	Q	115	ILE	N-CA	-5.56	1.39	1.46
28	H	134	THR	C-N	5.56	1.41	1.33
28	H	187	LEU	N-CA	-5.56	1.39	1.45
28	H	415	THR	CA-C	-5.56	1.45	1.53
1	a	220	LYS	N-CA	-5.56	1.38	1.46
7	g	123	HIS	CG-ND1	-5.56	1.32	1.38
2	b	134	LEU	CA-C	-5.56	1.46	1.52
9	2	213	ALA	CA-C	-5.56	1.45	1.52
13	6	205	GLN	C-N	5.56	1.40	1.33
27	O	286	PHE	CA-CB	5.56	1.62	1.53
23	P	357	TYR	CA-C	-5.56	1.46	1.52
5	e	73	HIS	ND1-CE1	5.55	1.38	1.32
14	7	174	THR	C-N	5.55	1.40	1.33
23	P	113	ASN	N-CA	-5.55	1.39	1.46
26	U	222	ASN	CA-CB	5.55	1.61	1.53
13	m	160	ASN	N-CA	-5.55	1.39	1.46
21	N	310	ASP	N-CA	-5.55	1.40	1.46
28	H	357	ARG	C-O	-5.55	1.18	1.24
30	K	252	ARG	N-CA	-5.55	1.39	1.46
2	b	7	PHE	CA-CB	5.55	1.62	1.53
9	2	179	GLU	C-N	5.55	1.41	1.33
21	N	411	ILE	CA-CB	5.55	1.60	1.54
21	N	908	ARG	CA-C	-5.55	1.45	1.52
9	2	75	ALA	CA-CB	5.55	1.61	1.53
14	7	149	VAL	CA-C	-5.55	1.45	1.52
25	R	201	GLY	N-CA	5.55	1.53	1.45
28	H	266	ARG	CD-NE	5.55	1.54	1.46
29	I	299	GLU	C-O	-5.55	1.16	1.24
22	S	87	SER	N-CA	-5.55	1.39	1.46
30	K	223	VAL	CA-C	5.55	1.60	1.52
11	4	131	GLY	C-O	-5.54	1.18	1.23
23	P	189	LEU	N-CA	-5.54	1.39	1.46
29	I	435	LEU	C-N	5.54	1.41	1.33
32	M	86	MET	CA-C	-5.54	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	7	ILE	CB-CG1	5.54	1.64	1.53
23	P	193	TYR	N-CA	-5.54	1.38	1.46
25	R	217	HIS	CE1-NE2	-5.54	1.27	1.32
32	M	219	LEU	CA-C	-5.54	1.45	1.52
33	J	123	HIS	ND1-CE1	5.54	1.38	1.32
23	P	362	LEU	CA-C	-5.54	1.45	1.52
33	J	255	SER	N-CA	-5.54	1.38	1.46
15	W	101	ARG	CZ-NH1	5.54	1.40	1.32
1	a	212	ASP	N-CA	-5.54	1.39	1.46
17	T	29	PRO	CA-CB	-5.54	1.45	1.53
24	Q	361	HIS	CA-C	-5.54	1.45	1.52
25	R	136	ASN	CA-CB	5.54	1.62	1.53
33	J	251	ASP	CA-C	-5.54	1.45	1.52
9	i	201	ASN	C-N	5.53	1.40	1.33
12	5	181	ARG	NE-CZ	5.53	1.39	1.33
21	N	744	PRO	N-CA	-5.53	1.40	1.47
9	i	230	LYS	CA-C	-5.53	1.45	1.52
4	d	172	ARG	C-N	5.53	1.41	1.33
18	X	122	TYR	CA-CB	5.53	1.62	1.53
30	K	370	SER	CA-C	-5.53	1.45	1.52
6	f	155	GLU	CA-C	-5.53	1.46	1.52
10	j	169	GLN	N-CA	5.53	1.52	1.46
15	W	140	ASP	N-CA	-5.53	1.39	1.46
33	J	383	GLU	CA-CB	5.53	1.61	1.53
2	b	200	VAL	C-N	5.53	1.41	1.33
14	7	44	VAL	CA-C	-5.53	1.45	1.52
14	7	194	ARG	C-N	5.53	1.40	1.33
26	U	256	ASN	CA-CB	5.53	1.61	1.53
33	J	306	ARG	C-N	5.53	1.40	1.33
2	b	74	VAL	CA-C	5.52	1.58	1.52
14	7	231	ALA	C-N	5.52	1.40	1.33
21	N	43	LEU	C-O	-5.52	1.19	1.24
25	R	93	LYS	CA-CB	5.52	1.60	1.53
11	k	120	ASP	CA-CB	5.52	1.61	1.53
32	M	360	ILE	CA-CB	-5.52	1.47	1.54
7	g	78	TYR	N-CA	-5.52	1.38	1.45
13	6	36	ARG	CD-NE	5.52	1.53	1.46
12	l	139	ARG	CD-NE	5.52	1.53	1.46
21	N	871	MET	C-N	5.52	1.41	1.33
9	i	251	ASP	CA-CB	5.52	1.62	1.53
8	1	90	VAL	N-CA	-5.52	1.39	1.46
27	O	262	ASP	CA-CB	5.52	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	219	LYS	CA-CB	5.52	1.61	1.53
21	N	624	ALA	C-O	-5.52	1.17	1.24
23	P	268	LEU	CA-C	-5.52	1.45	1.52
33	J	201	ALA	C-O	-5.52	1.17	1.24
21	N	58	ARG	CD-NE	5.51	1.53	1.46
22	S	281	ALA	CA-CB	5.51	1.61	1.53
33	J	45	GLU	CA-CB	5.51	1.62	1.53
9	i	163	ALA	N-CA	-5.51	1.39	1.46
21	N	766	GLN	CA-C	-5.51	1.47	1.53
8	h	112	ASP	CA-CB	5.51	1.62	1.53
22	S	323	LEU	C-N	5.51	1.41	1.33
32	M	160	PRO	C-N	5.51	1.41	1.33
21	N	383	LYS	N-CA	-5.51	1.39	1.46
24	Q	369	ASP	CA-C	5.51	1.59	1.52
26	U	283	ARG	CZ-NH2	5.51	1.40	1.33
26	U	291	LEU	N-CA	-5.51	1.39	1.46
29	I	150	HIS	C-N	5.51	1.40	1.33
28	H	311	ILE	CB-CG1	5.51	1.64	1.53
9	i	204	VAL	CA-CB	-5.51	1.45	1.55
21	N	711	ARG	NE-CZ	5.51	1.39	1.33
32	M	368	MET	CA-C	-5.51	1.46	1.53
9	i	236	ARG	NE-CZ	5.50	1.39	1.33
8	l	168	LEU	N-CA	-5.50	1.38	1.46
8	h	82	PRO	CA-C	5.50	1.58	1.53
10	j	42	LYS	N-CA	-5.50	1.38	1.46
9	2	247	VAL	C-O	-5.50	1.18	1.24
13	6	116	HIS	ND1-CE1	5.50	1.38	1.32
22	S	239	ARG	CZ-NH2	5.50	1.40	1.33
30	K	39	ALA	N-CA	-5.50	1.38	1.45
30	K	226	VAL	CA-CB	-5.50	1.47	1.54
2	b	117	ILE	CA-C	5.50	1.59	1.52
15	W	185	ILE	CA-C	-5.50	1.46	1.52
5	e	108	ASN	CA-CB	5.50	1.62	1.53
14	n	140	MET	CA-C	-5.50	1.45	1.52
17	T	140	SER	C-O	-5.50	1.17	1.24
22	S	119	TYR	CZ-OH	5.50	1.49	1.38
22	S	451	ILE	CA-CB	-5.50	1.47	1.54
26	U	181	GLN	CA-C	-5.50	1.46	1.52
2	b	106	PRO	C-N	5.50	1.42	1.33
2	b	128	ARG	CZ-NH1	5.50	1.40	1.32
10	3	60	VAL	C-N	5.50	1.42	1.33
21	N	87	ASP	CA-C	-5.50	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	10	ASP	N-CA	-5.50	1.39	1.46
21	N	918	GLU	CA-C	5.50	1.59	1.52
26	U	285	ILE	CA-C	5.50	1.59	1.52
5	e	189	SER	CA-CB	5.49	1.61	1.53
9	i	127	LEU	N-CA	-5.49	1.39	1.46
8	l	56	GLY	C-N	5.49	1.40	1.33
17	T	126	LEU	C-N	5.49	1.41	1.33
13	m	220	VAL	N-CA	-5.49	1.39	1.46
21	N	352	ASN	N-CA	-5.49	1.40	1.46
29	I	247	ILE	C-N	5.49	1.40	1.33
31	L	53	HIS	CE1-NE2	-5.49	1.27	1.32
13	m	203	HIS	CG-CD2	5.49	1.41	1.35
11	4	19	LYS	C-N	5.49	1.41	1.33
25	R	339	ALA	C-O	-5.49	1.17	1.24
30	K	292	VAL	CA-CB	-5.49	1.47	1.54
6	f	66	CYS	CA-C	-5.49	1.45	1.52
27	O	28	GLN	C-N	5.49	1.41	1.33
33	J	117	SER	N-CA	-5.49	1.38	1.46
6	f	105	VAL	CA-C	-5.49	1.46	1.52
14	7	81	ASN	CA-C	-5.49	1.46	1.53
14	n	148	ILE	CA-CB	-5.49	1.47	1.54
24	Q	370	THR	C-O	-5.49	1.17	1.24
30	K	372	ILE	C-N	5.49	1.40	1.33
17	T	208	LEU	C-N	5.48	1.41	1.33
23	P	214	GLU	N-CA	-5.48	1.39	1.46
16	V	95	LEU	C-N	5.48	1.41	1.34
23	P	417	HIS	CG-ND1	5.48	1.44	1.38
24	Q	129	LYS	C-N	5.48	1.41	1.33
33	J	329	ARG	NE-CZ	5.48	1.39	1.33
24	Q	302	VAL	C-O	-5.48	1.17	1.24
27	O	364	THR	CA-C	-5.48	1.45	1.52
30	K	222	LEU	CA-CB	5.48	1.61	1.53
31	L	160	PRO	CA-C	5.48	1.58	1.52
9	i	65	ARG	C-N	5.48	1.40	1.33
24	Q	260	GLN	CA-C	-5.48	1.45	1.52
14	n	136	ARG	CD-NE	5.48	1.53	1.46
8	l	103	THR	N-CA	5.48	1.52	1.45
11	4	3	ILE	CA-CB	5.48	1.60	1.53
24	Q	47	ASP	CA-CB	5.48	1.62	1.53
24	Q	396	TRP	NE1-CE2	-5.48	1.31	1.37
24	Q	212	THR	CA-C	-5.48	1.45	1.52
32	M	330	VAL	CA-CB	5.48	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	185	ASN	N-CA	-5.47	1.41	1.46
11	4	22	THR	CA-CB	-5.47	1.45	1.53
21	N	64	ILE	CA-C	5.47	1.59	1.52
21	N	791	ALA	C-N	5.47	1.41	1.33
25	R	117	ILE	C-O	-5.47	1.18	1.24
9	i	126	TYR	CB-CG	-5.47	1.39	1.51
21	N	417	ARG	NE-CZ	5.47	1.39	1.33
27	O	72	LYS	C-N	5.47	1.40	1.33
8	h	198	TYR	CA-CB	5.47	1.61	1.53
21	N	400	ILE	N-CA	-5.47	1.39	1.46
31	L	92	GLU	N-CA	-5.47	1.39	1.46
1	a	221	ASN	CA-CB	5.47	1.61	1.53
14	n	61	GLY	N-CA	-5.47	1.37	1.45
12	5	234	ARG	CZ-NH1	5.47	1.40	1.32
12	5	235	SER	C-N	5.47	1.40	1.33
23	P	272	PRO	N-CA	-5.47	1.40	1.47
25	R	376	GLN	N-CA	-5.47	1.39	1.46
16	V	190	HIS	CG-CD2	5.47	1.41	1.35
29	I	125	MET	N-CA	-5.47	1.41	1.46
1	a	14	ARG	CZ-NH1	5.47	1.40	1.32
5	e	135	SER	C-N	5.47	1.39	1.33
13	m	170	PRO	C-N	5.46	1.41	1.33
21	N	444	HIS	N-CA	5.46	1.52	1.46
21	N	849	THR	CA-C	-5.46	1.46	1.53
22	S	19	HIS	CA-CB	5.46	1.61	1.53
5	e	91	HIS	CG-CD2	-5.46	1.29	1.35
8	h	144	TYR	CA-C	-5.46	1.45	1.52
27	O	58	ARG	C-N	5.46	1.41	1.33
12	5	227	ASP	CA-C	5.46	1.59	1.52
4	d	125	GLY	C-N	5.46	1.40	1.33
21	N	805	SER	C-N	5.46	1.41	1.33
1	a	170	ALA	C-N	5.46	1.40	1.33
11	4	78	GLN	C-N	5.46	1.41	1.33
11	4	188	GLY	CA-C	-5.46	1.44	1.51
14	7	233	ILE	CA-C	-5.46	1.45	1.52
21	N	794	LYS	CA-C	-5.46	1.45	1.52
22	S	131	THR	C-N	5.46	1.40	1.33
24	Q	143	THR	N-CA	-5.46	1.39	1.46
30	K	158	ILE	CA-C	5.46	1.58	1.52
14	n	96	ILE	CA-C	-5.46	1.44	1.52
11	4	159	ASP	C-N	5.46	1.41	1.33
2	b	236	ARG	N-CA	-5.46	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	264	ARG	CZ-NH2	5.46	1.40	1.33
8	1	166	HIS	ND1-CE1	5.45	1.38	1.32
17	T	71	GLN	C-N	5.45	1.41	1.33
32	M	262	LEU	C-N	5.45	1.40	1.33
8	1	47	HIS	CA-C	-5.45	1.46	1.52
9	2	127	LEU	N-CA	-5.45	1.39	1.45
13	6	74	LYS	CA-C	-5.45	1.45	1.52
21	N	681	ASN	C-N	5.45	1.41	1.33
4	d	19	GLN	C-N	5.45	1.40	1.33
21	N	90	ASP	C-N	5.45	1.40	1.33
21	N	119	LYS	C-O	-5.45	1.17	1.24
25	R	386	GLY	CA-C	5.45	1.59	1.51
9	i	213	ALA	C-N	5.45	1.41	1.33
22	S	217	PHE	N-CA	-5.45	1.39	1.46
31	L	70	TYR	N-CA	-5.45	1.39	1.46
33	J	334	LYS	N-CA	-5.45	1.39	1.46
2	b	14	PRO	C-O	-5.44	1.17	1.24
13	6	221	ARG	CZ-NH2	5.44	1.40	1.33
23	P	363	LEU	CA-CB	5.44	1.61	1.53
27	O	115	ARG	CD-NE	5.44	1.53	1.46
32	M	345	ARG	CZ-NH2	5.44	1.40	1.33
33	J	283	GLU	C-N	5.44	1.41	1.33
13	m	84	HIS	ND1-CE1	5.44	1.38	1.32
25	R	93	LYS	C-N	5.44	1.40	1.33
28	H	352	MET	SD-CE	5.44	1.93	1.79
31	L	242	ASN	CA-C	-5.44	1.46	1.52
13	6	116	HIS	CA-C	-5.44	1.46	1.52
26	U	180	ASP	CA-C	-5.44	1.45	1.52
28	H	103	THR	CA-CB	-5.44	1.46	1.54
28	H	178	ARG	NE-CZ	5.44	1.39	1.33
11	k	124	THR	C-N	5.44	1.41	1.33
16	V	73	GLN	CA-C	5.44	1.59	1.52
33	J	79	VAL	N-CA	-5.44	1.39	1.46
6	f	69	HIS	N-CA	-5.44	1.42	1.47
8	h	62	GLN	CA-C	-5.44	1.45	1.52
9	i	128	ILE	N-CA	-5.44	1.39	1.46
13	6	96	SER	N-CA	-5.44	1.39	1.46
13	6	180	LEU	C-N	5.44	1.40	1.33
25	R	223	ASN	N-CA	-5.44	1.39	1.46
31	L	346	LYS	C-N	5.44	1.40	1.33
31	L	372	GLY	CA-C	-5.44	1.44	1.51
32	M	130	PRO	CA-C	-5.44	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	261	LYS	CA-CB	5.44	1.61	1.53
5	e	176	SER	C-N	5.43	1.41	1.33
8	h	134	ALA	N-CA	-5.43	1.39	1.45
9	2	241	VAL	C-N	5.43	1.41	1.33
21	N	349	ILE	C-N	5.43	1.41	1.33
3	c	65	LYS	CA-C	5.43	1.60	1.52
8	h	197	PHE	CA-C	-5.43	1.46	1.52
9	i	167	LEU	C-N	5.43	1.41	1.33
23	P	180	ILE	CA-C	5.43	1.59	1.52
23	P	201	ARG	CZ-NH1	5.43	1.40	1.32
24	Q	295	GLY	CA-C	-5.43	1.44	1.51
9	i	170	HIS	C-O	-5.43	1.17	1.24
25	R	308	LEU	CA-C	-5.43	1.45	1.52
26	U	281	LEU	CA-CB	5.43	1.61	1.53
30	K	237	VAL	C-N	5.43	1.40	1.33
24	Q	99	THR	CA-C	-5.43	1.45	1.52
30	K	347	ARG	NE-CZ	5.43	1.39	1.33
1	a	24	ARG	CZ-NH1	5.43	1.40	1.32
13	6	89	ASP	CA-C	-5.43	1.45	1.52
15	W	46	GLU	N-CA	-5.43	1.38	1.46
3	c	20	TYR	CG-CD1	5.42	1.50	1.39
5	e	161	SER	CA-CB	5.42	1.61	1.53
8	1	69	GLN	CA-C	-5.42	1.45	1.52
22	S	347	HIS	N-CA	5.42	1.52	1.46
29	I	267	ILE	CB-CG1	5.42	1.64	1.53
31	L	286	ILE	CA-C	-5.42	1.47	1.53
21	N	41	ASN	N-CA	-5.42	1.39	1.46
4	d	94	GLN	N-CA	-5.42	1.39	1.46
8	1	134	ALA	CA-C	-5.42	1.46	1.52
33	J	381	ASP	CA-CB	5.42	1.61	1.53
33	J	15	HIS	CA-CB	5.42	1.61	1.53
4	d	195	THR	C-N	5.42	1.40	1.33
5	e	18	GLU	N-CA	-5.42	1.39	1.46
13	m	95	ASN	CA-CB	5.42	1.61	1.53
14	7	174	THR	N-CA	-5.42	1.39	1.45
17	T	156	SER	CA-C	-5.42	1.46	1.53
22	S	179	ILE	N-CA	-5.42	1.39	1.46
24	Q	298	ALA	N-CA	-5.42	1.39	1.46
1	a	76	SER	CA-CB	5.42	1.62	1.53
4	d	70	HIS	CA-C	5.42	1.58	1.52
15	W	141	ILE	CA-C	-5.42	1.45	1.52
29	I	325	ILE	CA-C	-5.42	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	396	THR	C-O	-5.42	1.17	1.24
13	m	202	ARG	NE-CZ	5.42	1.39	1.33
3	c	230	PHE	C-O	-5.41	1.17	1.23
24	Q	353	PRO	C-N	5.41	1.40	1.33
9	i	202	VAL	C-N	5.41	1.40	1.33
21	N	787	MET	CA-C	-5.41	1.45	1.53
23	P	116	ILE	N-CA	5.41	1.52	1.46
7	g	229	LYS	N-CA	-5.41	1.38	1.46
8	h	167	SER	CA-CB	5.41	1.61	1.53
9	i	122	HIS	ND1-CE1	5.41	1.38	1.32
24	Q	301	ALA	CA-C	-5.41	1.45	1.52
25	R	383	ARG	NE-CZ	5.41	1.39	1.33
32	M	342	ARG	CD-NE	5.41	1.53	1.46
3	c	18	ARG	CA-C	-5.41	1.45	1.52
12	5	170	LEU	CA-CB	5.41	1.61	1.53
31	L	289	ARG	CD-NE	5.41	1.53	1.46
16	V	40	HIS	C-N	5.41	1.40	1.33
31	L	369	LYS	CA-C	-5.41	1.46	1.52
12	l	144	ARG	CZ-NH2	5.41	1.40	1.33
30	K	355	THR	CA-C	-5.41	1.45	1.52
8	h	144	TYR	N-CA	-5.40	1.40	1.46
33	J	205	HIS	C-N	5.40	1.41	1.33
12	l	127	CYS	C-N	5.40	1.40	1.33
10	3	130	ILE	N-CA	-5.40	1.40	1.46
15	W	23	ARG	NE-CZ	5.40	1.39	1.33
22	S	196	ARG	C-N	5.40	1.41	1.33
28	H	370	ARG	CD-NE	5.40	1.53	1.46
1	a	107	LYS	CA-CB	5.40	1.63	1.53
6	f	62	LYS	CA-C	-5.40	1.45	1.52
1	a	246	VAL	CA-CB	-5.40	1.46	1.54
2	b	16	GLY	CA-C	-5.40	1.44	1.52
3	c	128	LEU	N-CA	-5.40	1.39	1.46
16	V	241	THR	C-N	5.40	1.41	1.34
22	S	282	ILE	CA-C	-5.40	1.45	1.52
29	I	291	ARG	CZ-NH1	5.40	1.40	1.32
33	J	238	ARG	CZ-NH2	5.40	1.40	1.33
9	i	75	ALA	C-N	5.40	1.41	1.33
22	S	222	SER	C-N	5.40	1.41	1.33
24	Q	379	GLN	CA-C	-5.40	1.45	1.52
4	d	135	ILE	CA-CB	-5.40	1.47	1.54
16	V	204	HIS	CA-C	-5.40	1.46	1.52
8	1	166	HIS	N-CA	-5.39	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	312	PRO	CA-C	5.39	1.59	1.52
21	N	418	ASP	N-CA	-5.39	1.39	1.46
21	N	564	ASN	CG-ND2	5.39	1.44	1.33
23	P	364	ARG	CA-C	-5.39	1.46	1.52
27	O	171	PHE	CA-C	-5.39	1.45	1.52
11	k	81	SER	N-CA	-5.39	1.39	1.46
14	7	197	ASP	CA-CB	5.39	1.62	1.53
27	O	170	SER	CA-C	-5.39	1.45	1.52
3	c	37	GLY	CA-C	-5.39	1.47	1.51
10	j	198	ARG	NE-CZ	5.39	1.39	1.33
14	7	116	ALA	C-N	5.39	1.40	1.33
16	V	157	ARG	NE-CZ	5.39	1.39	1.33
21	N	713	VAL	N-CA	-5.39	1.40	1.46
17	T	200	LEU	C-O	-5.39	1.17	1.24
21	N	255	ALA	N-CA	-5.39	1.39	1.46
21	N	584	ARG	CZ-NH1	5.39	1.40	1.32
6	f	5	ASN	CA-CB	5.39	1.61	1.54
6	f	119	ASN	C-O	-5.39	1.17	1.24
8	1	169	SER	CA-CB	5.39	1.61	1.53
28	H	292	ARG	CZ-NH1	5.39	1.40	1.32
7	g	193	VAL	C-O	-5.38	1.17	1.24
14	n	55	ILE	C-N	5.38	1.40	1.33
13	6	211	GLU	CA-CB	5.38	1.61	1.53
16	V	213	LEU	CA-C	-5.38	1.45	1.52
32	M	85	VAL	C-N	5.38	1.40	1.33
1	a	51	THR	CA-C	-5.38	1.46	1.52
1	a	57	LYS	CA-CB	5.38	1.67	1.54
2	b	184	GLU	CA-CB	5.38	1.62	1.53
6	f	187	ASP	CA-C	-5.38	1.45	1.52
7	g	92	GLY	C-N	5.38	1.41	1.33
15	W	41	ARG	CA-CB	5.38	1.61	1.53
31	L	67	HIS	ND1-CE1	5.38	1.38	1.32
21	N	61	ALA	N-CA	-5.38	1.39	1.46
26	U	121	LEU	CA-CB	5.38	1.61	1.53
33	J	7	SER	CA-C	5.38	1.59	1.52
28	H	424	THR	C-N	5.38	1.41	1.33
9	i	101	ARG	CA-C	-5.38	1.46	1.52
12	l	139	ARG	C-N	5.38	1.41	1.33
13	m	46	ARG	N-CA	-5.38	1.39	1.46
14	n	69	PHE	C-N	5.38	1.41	1.33
16	V	70	ALA	N-CA	-5.38	1.39	1.46
22	S	393	ARG	CD-NE	5.38	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	84	GLU	CA-C	-5.38	1.45	1.52
33	J	197	LEU	N-CA	-5.38	1.39	1.46
33	J	274	GLU	N-CA	-5.38	1.40	1.46
28	H	373	ARG	CD-NE	5.38	1.53	1.46
29	I	64	ARG	CA-C	-5.38	1.46	1.52
1	a	29	GLU	CA-C	-5.37	1.45	1.52
14	n	217	LEU	CA-CB	5.37	1.61	1.53
21	N	914	VAL	CA-C	-5.37	1.46	1.52
24	Q	121	SER	C-N	5.37	1.40	1.33
26	U	105	LYS	N-CA	-5.37	1.39	1.46
10	j	90	LEU	CA-C	-5.37	1.46	1.52
13	m	128	GLY	CA-C	-5.37	1.47	1.52
13	6	83	TYR	CA-C	5.37	1.59	1.52
2	b	181	ASP	N-CA	5.37	1.52	1.46
8	h	56	GLY	CA-C	-5.37	1.46	1.52
11	k	165	VAL	CA-C	-5.37	1.46	1.52
10	3	27	LEU	CA-C	-5.37	1.45	1.52
12	5	244	ALA	C-N	5.37	1.41	1.33
6	f	51	ARG	CZ-NH1	5.37	1.40	1.32
15	W	18	ASN	CG-ND2	5.37	1.44	1.33
24	Q	22	GLU	CA-C	-5.37	1.45	1.52
8	h	34	TYR	C-N	-5.37	1.27	1.33
16	V	107	TRP	CA-C	-5.37	1.45	1.52
21	N	335	ALA	CA-C	-5.37	1.46	1.52
21	N	831	GLU	CA-CB	5.37	1.61	1.53
23	P	164	GLN	N-CA	5.37	1.53	1.46
26	U	128	GLN	CA-C	-5.37	1.45	1.52
8	h	114	LYS	N-CA	-5.36	1.39	1.45
9	2	168	GLU	C-N	5.36	1.41	1.33
23	P	277	GLN	N-CA	-5.36	1.39	1.46
33	J	95	ILE	C-N	5.36	1.40	1.33
18	X	38	ASN	CA-CB	5.36	1.62	1.53
30	K	259	ARG	CZ-NH2	5.36	1.40	1.33
3	c	68	LYS	N-CA	-5.36	1.39	1.46
6	f	13	PHE	C-N	5.36	1.40	1.33
6	f	87	TYR	CA-CB	5.36	1.61	1.53
13	m	186	GLU	CA-C	-5.36	1.46	1.52
8	1	29	THR	N-CA	-5.36	1.40	1.46
18	X	59	ARG	CZ-NH1	5.36	1.40	1.32
21	N	573	HIS	C-O	-5.36	1.17	1.24
29	I	88	LYS	N-CA	5.36	1.52	1.46
12	5	241	HIS	N-CA	-5.36	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	178	LYS	C-N	5.36	1.40	1.33
21	N	742	TRP	NE1-CE2	5.36	1.43	1.37
1	a	150	LEU	CA-CB	5.36	1.62	1.53
14	n	215	ARG	CA-C	-5.36	1.45	1.52
17	T	258	ASN	C-N	5.36	1.40	1.34
22	S	410	LYS	CA-C	-5.36	1.45	1.52
25	R	334	ARG	NE-CZ	5.36	1.39	1.33
29	I	404	LEU	CB-CG	5.36	1.64	1.53
6	f	68	GLU	N-CA	-5.36	1.39	1.46
14	7	150	ALA	N-CA	5.36	1.52	1.46
28	H	98	GLN	N-CA	-5.36	1.39	1.46
23	P	344	ARG	CD-NE	5.35	1.53	1.46
2	b	161	ALA	CA-CB	5.35	1.62	1.53
3	c	137	TYR	N-CA	-5.35	1.39	1.46
14	n	133	MET	C-N	5.35	1.40	1.33
8	1	18	LYS	N-CA	5.35	1.52	1.46
22	S	488	GLN	N-CA	-5.35	1.39	1.46
8	h	66	ASP	CA-CB	5.35	1.61	1.53
32	M	84	GLU	CA-C	-5.35	1.46	1.52
33	J	208	CYS	CA-C	5.35	1.59	1.52
7	g	91	ARG	CZ-NH1	5.35	1.40	1.32
12	l	84	GLN	CA-C	-5.35	1.45	1.52
14	n	198	ILE	N-CA	-5.35	1.40	1.46
8	1	141	THR	C-N	5.35	1.41	1.33
8	1	195	LEU	C-N	5.35	1.40	1.33
12	5	194	GLY	C-N	5.35	1.41	1.33
21	N	500	ASP	CA-CB	-5.35	1.45	1.53
25	R	166	ALA	C-N	5.35	1.41	1.33
28	H	132	GLN	C-O	-5.35	1.17	1.24
33	J	361	VAL	N-CA	5.35	1.52	1.46
5	e	227	GLY	CA-C	-5.35	1.46	1.52
14	7	104	VAL	CA-C	-5.35	1.45	1.52
25	R	383	ARG	CZ-NH1	5.34	1.40	1.32
29	I	61	ARG	CZ-NH1	5.34	1.40	1.32
30	K	281	ARG	CA-C	-5.34	1.46	1.52
7	g	126	TYR	CA-C	-5.34	1.46	1.52
9	2	241	VAL	N-CA	5.34	1.52	1.46
21	N	788	TYR	C-N	5.34	1.41	1.33
26	U	68	LEU	C-N	5.34	1.41	1.33
7	g	33	ASN	CA-C	-5.34	1.45	1.52
9	2	93	GLU	CA-CB	5.34	1.61	1.53
9	2	143	HIS	CB-CG	5.34	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	X	30	GLN	N-CA	-5.34	1.39	1.46
29	I	153	THR	N-CA	-5.34	1.40	1.46
3	c	94	HIS	CE1-NE2	-5.34	1.27	1.32
4	d	160	SER	CA-C	-5.34	1.45	1.52
5	e	99	HIS	ND1-CE1	5.34	1.37	1.32
10	j	68	ARG	N-CA	-5.34	1.39	1.46
8	l	104	ALA	C-N	5.34	1.41	1.33
24	Q	104	PHE	C-N	5.34	1.41	1.33
7	g	237	GLN	C-N	5.34	1.41	1.33
14	7	80	ASP	N-CA	5.33	1.53	1.46
23	P	103	TYR	CA-CB	5.33	1.61	1.53
7	g	202	LEU	C-N	5.33	1.41	1.33
10	3	172	LEU	C-N	5.33	1.41	1.33
10	3	181	SER	C-N	5.33	1.41	1.33
27	O	219	ILE	N-CA	-5.33	1.40	1.46
23	P	36	LEU	CA-CB	5.33	1.61	1.53
10	j	36	VAL	CA-CB	-5.33	1.48	1.54
10	j	105	VAL	C-N	5.33	1.41	1.33
11	k	167	GLU	N-CA	-5.33	1.40	1.46
21	N	784	TYR	C-N	5.33	1.40	1.33
25	R	336	LYS	C-O	5.33	1.30	1.24
29	I	371	LEU	CA-C	-5.33	1.46	1.53
14	n	129	LEU	N-CA	-5.33	1.40	1.46
12	5	116	LEU	CA-C	-5.33	1.45	1.52
1	a	231	ASP	C-N	5.32	1.40	1.33
7	g	160	TYR	N-CA	-5.32	1.39	1.46
24	Q	345	SER	CA-C	-5.32	1.46	1.52
27	O	221	ALA	C-N	5.32	1.41	1.33
32	M	102	GLN	CA-C	-5.32	1.46	1.52
33	J	177	LEU	C-N	5.32	1.41	1.33
21	N	497	ALA	CA-CB	-5.32	1.44	1.53
25	R	290	SER	CA-C	-5.32	1.45	1.52
31	L	293	GLU	N-CA	-5.32	1.38	1.45
8	h	185	VAL	CA-C	-5.32	1.46	1.52
10	3	68	ARG	NE-CZ	5.32	1.39	1.33
21	N	524	ILE	CA-C	-5.32	1.46	1.52
23	P	365	LEU	C-N	5.32	1.40	1.33
25	R	329	PHE	CA-CB	5.32	1.61	1.53
27	O	309	SER	CA-C	-5.32	1.46	1.53
31	L	324	ILE	N-CA	-5.32	1.40	1.46
1	a	244	ARG	C-N	5.32	1.41	1.33
3	c	198	SER	CA-C	-5.32	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	80	VAL	C-N	5.32	1.41	1.33
10	3	98	ARG	CD-NE	5.32	1.53	1.46
18	X	106	SER	CA-C	-5.32	1.45	1.52
22	S	245	GLY	N-CA	-5.32	1.37	1.45
32	M	124	ARG	C-N	5.32	1.40	1.33
32	M	314	GLY	CA-C	-5.32	1.44	1.51
33	J	309	ARG	CD-NE	5.32	1.53	1.46
10	j	187	VAL	CA-C	-5.32	1.46	1.52
12	5	198	LYS	C-N	5.32	1.39	1.33
12	5	225	VAL	C-N	5.32	1.41	1.33
30	K	169	VAL	CA-CB	-5.32	1.47	1.54
2	b	128	ARG	CD-NE	5.31	1.53	1.46
3	c	160	TRP	CZ2-CH2	5.31	1.47	1.37
12	l	285	VAL	C-N	5.31	1.40	1.33
27	O	363	ILE	CA-C	-5.31	1.46	1.52
11	k	54	VAL	N-CA	-5.31	1.40	1.46
13	m	208	ASP	N-CA	5.31	1.53	1.46
32	M	425	ARG	CD-NE	5.31	1.53	1.46
5	e	72	ARG	CZ-NH2	5.31	1.40	1.33
6	f	70	MET	CA-CB	5.31	1.62	1.53
19	Y	83	ARG	CZ-NH1	5.31	1.40	1.32
22	S	265	SER	N-CA	-5.31	1.39	1.45
27	O	283	HIS	CA-C	-5.31	1.45	1.52
27	O	346	GLU	C-N	5.31	1.40	1.33
21	N	546	LEU	N-CA	-5.31	1.40	1.46
28	H	432	ARG	NE-CZ	5.31	1.38	1.33
31	L	412	PRO	CA-CB	5.31	1.61	1.53
14	7	210	ILE	CB-CG1	5.30	1.64	1.53
18	X	72	GLU	N-CA	-5.30	1.38	1.46
23	P	247	THR	CB-OG1	-5.30	1.35	1.43
10	3	99	ARG	N-CA	-5.30	1.39	1.46
20	Z	154	ILE	CA-C	-5.30	1.46	1.52
1	a	168	ALA	N-CA	-5.30	1.40	1.46
3	c	210	ARG	NE-CZ	5.30	1.38	1.33
9	i	65	ARG	CD-NE	5.30	1.53	1.46
28	H	223	GLU	C-N	5.30	1.40	1.33
32	M	248	ALA	CA-CB	5.30	1.61	1.54
13	6	100	ASN	CA-C	-5.30	1.45	1.52
31	L	393	ASN	CG-ND2	5.30	1.44	1.33
13	6	109	ARG	CA-C	-5.30	1.46	1.52
21	N	234	ASP	C-O	-5.30	1.17	1.24
23	P	152	LYS	CA-CB	5.30	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	119	ARG	CA-C	-5.29	1.45	1.52
10	j	158	LEU	N-CA	-5.29	1.39	1.46
25	R	223	ASN	CA-C	-5.29	1.46	1.52
28	H	200	VAL	CA-C	5.29	1.58	1.52
8	h	137	GLY	C-O	-5.29	1.16	1.23
16	V	22	ASP	CA-CB	5.29	1.61	1.53
26	U	83	ILE	C-O	-5.29	1.18	1.24
3	c	65	LYS	N-CA	-5.29	1.39	1.46
28	H	390	ARG	CD-NE	5.29	1.53	1.46
2	b	16	GLY	C-N	5.29	1.41	1.33
16	V	29	ILE	C-N	5.29	1.40	1.33
21	N	587	ALA	C-O	-5.29	1.17	1.24
25	R	401	HIS	CE1-NE2	-5.29	1.27	1.32
31	L	357	ARG	CD-NE	5.29	1.53	1.46
8	h	165	LYS	CA-C	-5.29	1.46	1.52
16	V	135	ARG	C-N	5.29	1.40	1.33
25	R	98	LEU	C-N	5.29	1.40	1.33
25	R	324	ARG	CD-NE	5.29	1.53	1.46
26	U	60	GLU	CA-CB	5.29	1.62	1.53
28	H	409	ARG	CA-C	-5.29	1.46	1.52
29	I	286	ALA	C-N	5.29	1.40	1.33
2	b	247	LEU	C-O	5.29	1.30	1.24
27	O	166	ARG	CZ-NH2	5.29	1.40	1.33
29	I	264	CYS	C-O	-5.29	1.18	1.24
16	V	252	SER	C-O	-5.28	1.18	1.24
22	S	160	ARG	NE-CZ	5.28	1.38	1.33
24	Q	221	MET	CA-CB	5.28	1.61	1.53
26	U	26	GLN	C-N	5.28	1.40	1.33
26	U	231	ASP	C-N	5.28	1.40	1.33
11	k	29	LYS	N-CA	-5.28	1.39	1.46
14	7	161	ARG	CD-NE	5.28	1.53	1.46
16	V	27	VAL	N-CA	-5.28	1.40	1.46
21	N	577	SER	CA-C	-5.28	1.45	1.52
22	S	314	ASN	N-CA	5.28	1.52	1.46
30	K	396	ARG	CA-C	-5.28	1.46	1.52
6	f	112	LEU	C-N	5.28	1.40	1.33
26	U	116	ASN	CA-CB	5.28	1.62	1.53
8	1	25	ALA	CA-C	-5.28	1.46	1.52
9	2	150	VAL	C-O	-5.28	1.17	1.23
16	V	269	ARG	CZ-NH2	5.28	1.40	1.33
23	P	325	ASP	CA-CB	5.28	1.60	1.53
33	J	72	VAL	CA-CB	5.28	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	90	PRO	C-N	5.28	1.37	1.33
33	J	322	ALA	CA-C	5.28	1.59	1.52
21	N	775	CYS	C-N	5.27	1.41	1.33
6	f	110	HIS	CG-ND1	-5.27	1.32	1.38
10	3	198	ARG	CZ-NH2	5.27	1.40	1.33
23	P	62	ILE	CA-CB	5.27	1.60	1.54
11	k	126	VAL	C-N	5.27	1.41	1.33
10	3	183	TRP	CA-C	-5.27	1.46	1.52
27	O	330	ARG	NE-CZ	5.27	1.38	1.33
11	k	16	ALA	C-N	5.27	1.40	1.33
21	N	628	ALA	CA-C	-5.27	1.46	1.52
27	O	108	GLU	CA-CB	5.27	1.61	1.53
31	L	195	GLU	N-CA	-5.27	1.39	1.46
5	e	132	ARG	NE-CZ	5.27	1.38	1.33
10	3	68	ARG	CZ-NH1	5.27	1.40	1.32
21	N	302	PHE	C-O	-5.27	1.18	1.24
25	R	227	ALA	N-CA	-5.27	1.40	1.46
26	U	70	HIS	CD2-NE2	5.27	1.43	1.37
26	U	233	PHE	C-N	5.27	1.40	1.33
11	k	101	ASN	CA-C	-5.27	1.46	1.52
10	3	153	LEU	C-N	5.27	1.40	1.33
14	7	108	ALA	CA-C	5.27	1.60	1.52
26	U	248	ASP	C-N	5.27	1.40	1.33
30	K	399	ARG	CD-NE	5.27	1.53	1.46
22	S	78	VAL	CA-CB	-5.26	1.48	1.54
24	Q	88	PHE	C-N	5.26	1.40	1.33
2	b	117	ILE	N-CA	-5.26	1.40	1.46
4	d	210	ILE	CA-CB	-5.26	1.47	1.54
28	H	97	LEU	CA-C	-5.26	1.46	1.52
30	K	215	PRO	N-CA	-5.26	1.40	1.47
8	1	204	GLN	CA-C	-5.26	1.46	1.52
25	R	313	ALA	CA-CB	5.26	1.61	1.53
26	U	100	ARG	N-CA	-5.26	1.39	1.45
27	O	169	ASN	CA-C	-5.26	1.45	1.52
30	K	336	ARG	NE-CZ	5.26	1.38	1.33
4	d	77	GLY	CA-C	-5.26	1.45	1.52
9	i	107	SER	CA-C	5.26	1.59	1.52
21	N	906	ARG	N-CA	-5.26	1.39	1.46
25	R	114	ASN	CA-C	-5.26	1.46	1.52
31	L	190	ILE	C-N	5.26	1.40	1.33
1	a	137	LEU	N-CA	5.26	1.52	1.46
14	n	104	VAL	C-O	-5.26	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	127	ILE	CA-C	-5.26	1.46	1.52
22	S	135	ASN	CA-C	-5.26	1.46	1.52
28	H	241	ASP	N-CA	-5.26	1.38	1.45
3	c	107	PRO	N-CD	-5.26	1.40	1.47
22	S	216	LYS	CA-C	-5.26	1.46	1.52
31	L	107	GLU	CA-C	-5.26	1.46	1.52
11	4	14	ILE	C-O	-5.25	1.18	1.24
14	7	55	ILE	CA-CB	-5.25	1.47	1.54
15	W	29	GLN	N-CA	-5.25	1.39	1.46
19	Y	50	LYS	CA-C	-5.25	1.46	1.52
21	N	338	PHE	N-CA	-5.25	1.39	1.46
26	U	94	HIS	C-N	-5.25	1.26	1.34
28	H	119	ASN	CG-ND2	5.25	1.44	1.33
1	a	152	PRO	N-CA	-5.25	1.41	1.47
5	e	236	THR	N-CA	-5.25	1.40	1.46
9	i	205	CYS	C-N	5.25	1.40	1.33
15	W	109	ARG	CA-C	-5.25	1.46	1.52
16	V	180	LEU	CA-C	-5.25	1.46	1.52
18	X	94	ASN	N-CA	-5.25	1.40	1.46
9	i	114	GLN	N-CA	5.25	1.52	1.46
12	5	158	LEU	C-N	5.25	1.40	1.33
16	V	217	HIS	ND1-CE1	5.25	1.37	1.32
33	J	221	LYS	C-N	5.25	1.41	1.33
5	e	136	ARG	CD-NE	5.25	1.53	1.46
14	n	82	THR	CA-C	-5.25	1.46	1.52
3	c	44	ILE	CA-C	-5.25	1.46	1.52
4	d	160	SER	N-CA	-5.25	1.39	1.46
15	W	157	PHE	CA-C	-5.25	1.46	1.52
21	N	9	LEU	CB-CG	5.25	1.64	1.53
26	U	248	ASP	N-CA	5.25	1.53	1.46
4	d	235	GLN	CA-CB	-5.25	1.45	1.53
6	f	110	HIS	CA-CB	5.25	1.61	1.53
8	h	11	SER	N-CA	-5.25	1.40	1.46
12	l	138	CYS	C-N	5.25	1.41	1.33
13	6	221	ARG	N-CA	5.25	1.52	1.46
17	T	143	SER	CA-CB	5.25	1.62	1.53
26	U	260	ASN	N-CA	5.25	1.52	1.46
12	5	162	VAL	CA-CB	5.25	1.60	1.54
15	W	27	GLU	C-N	5.25	1.41	1.33
16	V	39	LYS	C-N	5.25	1.41	1.33
5	e	63	SER	C-N	5.24	1.40	1.33
11	4	171	ARG	CZ-NH2	5.24	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	114	TYR	CA-C	-5.24	1.46	1.52
22	S	156	VAL	N-CA	5.24	1.52	1.46
11	4	29	LYS	C-O	-5.24	1.17	1.24
11	4	177	LYS	CA-C	-5.24	1.46	1.53
14	7	193	ASP	CA-C	-5.24	1.46	1.52
16	V	65	VAL	N-CA	-5.24	1.40	1.46
21	N	896	PHE	CA-CB	5.24	1.61	1.53
23	P	27	LEU	C-O	-5.24	1.17	1.24
32	M	70	LYS	CA-CB	5.24	1.61	1.53
26	U	176	ARG	CD-NE	5.24	1.53	1.46
26	U	235	LEU	CA-C	-5.24	1.46	1.52
32	M	250	GLN	CD-NE2	5.24	1.44	1.33
4	d	225	SER	N-CA	-5.24	1.38	1.45
13	6	122	LEU	C-N	5.24	1.41	1.33
16	V	261	LEU	C-N	5.24	1.41	1.33
21	N	775	CYS	C-O	5.24	1.29	1.23
21	N	790	GLU	C-O	-5.24	1.17	1.24
11	k	108	ASP	C-O	-5.24	1.17	1.24
15	W	119	SER	C-N	5.24	1.40	1.33
30	K	113	THR	N-CA	-5.24	1.39	1.46
2	b	6	SER	CA-C	-5.24	1.46	1.52
32	M	33	ARG	CZ-NH1	5.24	1.40	1.32
21	N	424	LYS	N-CA	-5.23	1.39	1.46
22	S	358	LYS	CA-CB	5.23	1.61	1.53
33	J	48	ARG	CA-C	-5.23	1.46	1.52
27	O	279	ILE	C-N	5.23	1.41	1.33
28	H	281	GLN	C-N	5.23	1.41	1.33
4	d	181	ARG	N-CA	-5.23	1.39	1.46
26	U	82	LYS	CA-CB	5.23	1.61	1.53
32	M	69	ILE	C-N	5.23	1.40	1.33
17	T	68	ALA	CA-C	-5.23	1.46	1.52
19	Y	16	LEU	C-N	5.23	1.41	1.33
21	N	262	VAL	N-CA	5.23	1.52	1.46
21	N	543	ASP	CA-C	-5.23	1.45	1.52
22	S	484	ASP	C-N	5.23	1.41	1.33
25	R	49	PHE	CA-CB	5.23	1.61	1.53
28	H	404	TRP	NE1-CE2	-5.23	1.31	1.37
1	a	212	ASP	C-N	5.23	1.41	1.33
6	f	152	ASN	C-N	5.23	1.40	1.33
13	m	152	SER	CA-C	-5.23	1.45	1.52
33	J	333	ARG	CA-CB	5.23	1.61	1.53
4	d	246	GLN	C-N	5.22	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	225	TYR	N-CA	-5.22	1.39	1.46
12	5	125	ALA	CA-C	-5.22	1.46	1.52
21	N	567	ALA	CA-C	-5.22	1.46	1.52
27	O	115	ARG	CA-CB	5.22	1.61	1.53
31	L	77	ARG	NE-CZ	5.22	1.38	1.33
3	c	39	MET	CA-CB	5.22	1.60	1.53
7	g	118	GLN	N-CA	-5.22	1.40	1.46
10	j	79	GLU	C-N	5.22	1.40	1.33
22	S	115	PRO	CA-C	-5.22	1.47	1.52
22	S	174	ARG	CD-NE	5.22	1.53	1.46
24	Q	339	TYR	C-O	-5.22	1.18	1.24
2	b	167	GLY	CA-C	5.22	1.59	1.51
9	i	101	ARG	CD-NE	5.22	1.53	1.46
11	4	41	HIS	CD2-NE2	5.22	1.43	1.37
31	L	392	ARG	CA-C	-5.22	1.46	1.52
6	f	43	HIS	CA-C	-5.22	1.46	1.52
7	g	170	GLN	N-CA	5.22	1.52	1.46
9	i	34	GLY	C-N	5.22	1.40	1.33
13	m	57	ASN	CA-C	-5.22	1.45	1.52
11	4	29	LYS	N-CA	-5.22	1.39	1.46
17	T	222	LEU	CA-C	-5.22	1.46	1.52
21	N	85	ALA	CA-C	-5.22	1.46	1.52
21	N	669	GLU	N-CA	-5.22	1.39	1.46
14	7	151	GLY	N-CA	-5.22	1.37	1.45
1	a	122	ALA	CA-C	-5.22	1.45	1.52
3	c	74	ALA	N-CA	5.22	1.52	1.45
5	e	158	ALA	CA-C	-5.22	1.46	1.52
11	k	30	ASP	C-O	-5.22	1.19	1.24
11	k	155	GLU	CA-C	5.22	1.59	1.52
14	n	101	LYS	C-N	5.22	1.41	1.33
21	N	52	ASP	CA-CB	5.22	1.61	1.53
21	N	608	LEU	CA-C	-5.22	1.45	1.52
23	P	398	LYS	CA-C	-5.22	1.46	1.53
31	L	359	GLU	C-N	5.22	1.40	1.33
1	a	168	ALA	CA-C	-5.21	1.46	1.52
10	j	80	ARG	CZ-NH1	5.21	1.40	1.32
8	1	83	SER	CA-CB	5.21	1.61	1.53
14	7	122	PRO	N-CD	-5.21	1.40	1.47
17	T	210	PHE	C-N	5.21	1.40	1.33
23	P	163	LEU	N-CA	-5.21	1.40	1.46
25	R	286	LEU	C-N	5.21	1.41	1.33
25	R	286	LEU	N-CA	-5.21	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	136	SER	CA-C	-5.21	1.46	1.52
8	l	59	ALA	CA-C	-5.21	1.46	1.52
23	P	138	ARG	NE-CZ	5.21	1.38	1.33
24	Q	431	SER	C-N	5.21	1.39	1.34
7	g	58	LEU	C-N	5.21	1.40	1.33
13	m	222	LYS	N-CA	-5.21	1.40	1.46
11	4	31	SER	C-N	5.21	1.40	1.33
21	N	91	ILE	CA-CB	-5.21	1.47	1.54
21	N	639	ASP	N-CA	5.21	1.52	1.46
22	S	424	SER	C-N	5.21	1.40	1.33
4	d	119	ARG	CZ-NH2	5.21	1.40	1.33
13	m	193	ARG	CD-NE	5.21	1.53	1.46
21	N	584	ARG	NE-CZ	5.21	1.38	1.33
21	N	675	VAL	CA-CB	5.21	1.60	1.54
24	Q	111	LEU	C-O	5.21	1.30	1.24
27	O	262	ASP	C-N	5.21	1.40	1.33
12	5	134	LEU	C-N	5.21	1.40	1.33
22	S	399	TYR	CA-C	-5.21	1.46	1.52
6	f	203	ASP	CA-CB	5.20	1.62	1.53
33	J	78	ILE	C-N	5.20	1.40	1.33
8	h	76	THR	CA-C	-5.20	1.46	1.52
28	H	244	LYS	CA-CB	5.20	1.63	1.54
9	i	87	LEU	C-N	5.20	1.39	1.33
19	Y	37	ASP	N-CA	-5.20	1.40	1.46
17	T	191	LYS	CA-C	-5.20	1.46	1.52
22	S	112	ASN	C-N	5.20	1.41	1.33
23	P	3	ARG	C-N	5.20	1.41	1.33
24	Q	58	ILE	N-CA	-5.20	1.40	1.46
24	Q	316	THR	CA-C	5.20	1.59	1.52
28	H	63	ILE	CA-C	-5.20	1.46	1.52
4	d	197	ARG	NE-CZ	5.20	1.38	1.33
17	T	107	SER	C-N	5.20	1.41	1.33
32	M	21	GLU	CA-C	-5.20	1.45	1.52
33	J	116	ARG	NE-CZ	5.20	1.38	1.33
4	d	83	ARG	CZ-NH1	5.20	1.40	1.32
25	R	392	ARG	NE-CZ	5.20	1.38	1.33
29	I	285	ASP	C-N	5.20	1.41	1.33
13	m	121	GLY	CA-C	-5.19	1.44	1.51
21	N	166	ILE	CA-C	5.19	1.59	1.52
2	b	162	THR	C-N	5.19	1.40	1.33
4	d	161	ALA	C-N	5.19	1.40	1.33
20	Z	727	GLU	C-N	5.19	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	30	LEU	CA-CB	5.19	1.61	1.53
10	j	114	SER	CA-CB	5.19	1.61	1.53
12	5	150	SER	N-CA	-5.19	1.39	1.45
14	7	198	ILE	CA-CB	-5.19	1.50	1.53
16	V	197	TYR	C-O	-5.19	1.17	1.23
16	V	236	SER	N-CA	-5.19	1.40	1.46
24	Q	153	ASP	C-N	5.19	1.40	1.33
33	J	337	LEU	CB-CG	5.19	1.63	1.53
13	6	207	GLY	CA-C	-5.19	1.46	1.51
1	a	232	LYS	N-CA	-5.19	1.39	1.46
15	W	25	ARG	NE-CZ	5.19	1.38	1.33
24	Q	51	ARG	CA-CB	5.19	1.62	1.52
16	V	279	HIS	CE1-NE2	5.19	1.37	1.32
30	K	170	THR	CA-C	-5.19	1.48	1.53
2	b	204	PHE	N-CA	-5.18	1.41	1.46
11	k	58	GLU	CA-CB	5.18	1.61	1.53
26	U	87	GLU	CA-C	-5.18	1.46	1.52
27	O	147	ARG	C-N	-5.18	1.26	1.33
28	H	435	ARG	NE-CZ	5.18	1.38	1.33
22	S	101	LYS	C-N	5.18	1.41	1.33
23	P	299	LEU	CA-CB	5.18	1.61	1.53
3	c	112	VAL	N-CA	-5.18	1.40	1.46
26	U	2	SER	CA-CB	5.18	1.62	1.53
33	J	119	SER	C-O	-5.18	1.17	1.24
10	3	133	ALA	CA-C	-5.18	1.46	1.52
23	P	157	ALA	N-CA	-5.18	1.40	1.46
31	L	409	HIS	CE1-NE2	-5.18	1.27	1.32
16	V	194	ARG	C-N	5.18	1.41	1.33
21	N	418	ASP	CA-C	-5.18	1.46	1.52
31	L	127	TYR	C-N	5.18	1.40	1.33
33	J	245	ILE	C-N	5.18	1.39	1.33
9	i	195	ASP	CA-C	-5.18	1.46	1.52
10	j	138	VAL	N-CA	-5.18	1.40	1.46
13	6	72	LEU	C-N	5.18	1.40	1.33
13	6	205	GLN	CA-C	-5.18	1.45	1.52
24	Q	201	ALA	C-N	5.18	1.40	1.33
28	H	418	GLU	C-O	-5.18	1.17	1.24
31	L	261	ARG	CD-NE	5.18	1.53	1.46
13	6	127	LYS	N-CA	-5.17	1.39	1.45
17	T	135	ASN	C-N	5.17	1.41	1.33
14	7	198	ILE	CA-C	5.17	1.56	1.52
25	R	176	ARG	CZ-NH2	5.17	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	115	GLU	N-CA	-5.17	1.40	1.46
32	M	371	ASP	CA-C	-5.17	1.46	1.52
33	J	165	GLU	N-CA	-5.17	1.40	1.46
1	a	211	ILE	CA-C	-5.17	1.46	1.52
21	N	232	LEU	CA-C	-5.17	1.45	1.52
10	3	105	VAL	CA-CB	-5.17	1.48	1.54
21	N	921	ARG	CZ-NH2	5.17	1.40	1.33
7	g	219	CYS	CA-C	-5.17	1.46	1.52
24	Q	146	TYR	C-N	5.17	1.41	1.33
27	O	59	LEU	C-N	5.17	1.41	1.33
4	d	29	ARG	N-CA	-5.17	1.39	1.46
4	d	92	GLU	C-N	5.17	1.41	1.33
8	1	90	VAL	CA-C	-5.17	1.46	1.52
9	2	133	ASP	CA-CB	5.17	1.61	1.53
23	P	193	TYR	CZ-OH	5.17	1.48	1.38
24	Q	338	LEU	N-CA	-5.17	1.40	1.46
32	M	432	PHE	CA-CB	5.17	1.62	1.53
4	d	240	LYS	C-N	5.17	1.40	1.33
14	n	141	ASN	C-N	5.17	1.39	1.33
28	H	242	PRO	CA-C	5.17	1.56	1.52
30	K	79	LEU	N-CA	5.17	1.52	1.46
32	M	284	ASP	C-O	5.17	1.31	1.24
11	k	76	SER	CA-CB	5.16	1.61	1.53
12	5	149	ILE	CA-CB	5.16	1.60	1.54
14	7	234	ASP	CA-CB	5.16	1.61	1.53
22	S	365	THR	C-N	5.16	1.40	1.33
23	P	323	ASN	N-CA	-5.16	1.39	1.46
26	U	197	LEU	N-CA	-5.16	1.40	1.46
2	b	12	PHE	N-CA	-5.16	1.39	1.46
6	f	137	TYR	CA-CB	5.16	1.61	1.53
22	S	111	ARG	NE-CZ	5.16	1.38	1.33
22	S	480	ARG	NE-CZ	5.16	1.38	1.33
30	K	336	ARG	CD-NE	5.16	1.53	1.46
8	h	129	HIS	CD2-NE2	5.16	1.43	1.37
8	h	185	VAL	CA-CB	5.16	1.61	1.54
14	n	132	VAL	C-O	5.16	1.29	1.24
17	T	52	LEU	CA-C	5.16	1.59	1.52
19	Y	36	GLU	CA-C	5.16	1.59	1.52
33	J	25	GLN	C-N	5.16	1.40	1.33
11	k	27	VAL	CA-C	5.16	1.59	1.52
14	n	220	ARG	CZ-NH2	5.16	1.40	1.33
16	V	70	ALA	CA-C	-5.16	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	400	ILE	CA-C	-5.16	1.46	1.52
25	R	40	ILE	CA-C	-5.16	1.45	1.52
25	R	159	SER	C-N	5.16	1.40	1.33
32	M	362	GLN	C-O	-5.16	1.18	1.24
1	a	189	SER	CA-CB	5.15	1.61	1.53
3	c	186	VAL	CA-CB	5.15	1.60	1.54
13	6	155	MET	CA-C	-5.15	1.46	1.52
9	2	156	LEU	N-CA	-5.15	1.39	1.46
14	7	137	ARG	CZ-NH1	5.15	1.40	1.32
17	T	243	ALA	CA-CB	5.15	1.61	1.53
23	P	331	GLY	N-CA	5.15	1.52	1.45
21	N	801	THR	C-N	5.15	1.40	1.33
22	S	155	LEU	C-N	5.15	1.40	1.33
27	O	195	TYR	CZ-OH	5.15	1.48	1.38
10	j	26	ASP	CA-CB	5.15	1.60	1.53
30	K	336	ARG	C-O	5.15	1.30	1.24
11	4	41	HIS	CG-CD2	5.15	1.41	1.35
2	b	31	GLY	CA-C	-5.15	1.45	1.51
2	b	95	THR	N-CA	5.15	1.52	1.46
27	O	111	SER	C-N	5.15	1.41	1.33
4	d	141	ARG	CZ-NH1	5.14	1.40	1.32
7	g	239	ALA	CA-CB	5.14	1.61	1.53
14	n	131	THR	CA-C	5.14	1.59	1.52
9	2	62	LYS	CA-C	-5.14	1.45	1.52
19	Y	81	LEU	N-CA	-5.14	1.40	1.46
21	N	436	ASP	N-CA	-5.14	1.39	1.46
22	S	225	HIS	ND1-CE1	5.14	1.37	1.32
22	S	441	GLY	CA-C	-5.14	1.44	1.51
6	f	87	TYR	C-N	5.14	1.41	1.33
24	Q	315	ASN	CA-C	-5.14	1.46	1.52
25	R	422	ARG	CD-NE	5.14	1.53	1.46
3	c	15	PRO	C-N	5.14	1.41	1.33
9	i	122	HIS	CG-ND1	5.14	1.44	1.38
14	n	163	VAL	CA-C	5.14	1.58	1.52
20	Z	154	ILE	CA-CB	-5.14	1.48	1.54
21	N	531	LEU	CA-CB	5.14	1.62	1.53
1	a	64	LEU	N-CA	-5.14	1.39	1.46
3	c	29	ILE	N-CA	-5.14	1.39	1.46
6	f	26	LEU	C-N	5.14	1.41	1.33
10	3	193	ASP	C-N	5.14	1.39	1.33
22	S	205	ASN	CA-CB	5.14	1.61	1.53
24	Q	238	TYR	N-CA	-5.14	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	274	MET	CA-CB	5.14	1.61	1.53
27	O	90	LYS	CA-CB	5.14	1.61	1.53
27	O	197	SER	C-O	-5.14	1.18	1.24
28	H	447	VAL	CA-CB	-5.14	1.48	1.54
1	a	185	HIS	ND1-CE1	5.14	1.37	1.32
21	N	807	THR	C-O	-5.14	1.18	1.24
28	H	206	VAL	CA-C	-5.14	1.46	1.52
28	H	211	VAL	C-N	5.14	1.41	1.33
1	a	181	ASN	CA-C	-5.13	1.46	1.52
12	l	159	SER	CA-CB	5.13	1.61	1.53
12	l	168	ALA	N-CA	-5.13	1.38	1.46
8	1	45	ARG	C-N	5.13	1.38	1.33
32	M	186	LEU	CA-C	-5.13	1.46	1.53
32	M	399	GLY	C-N	5.13	1.41	1.33
11	k	45	SER	CA-C	-5.13	1.46	1.52
15	W	67	ALA	N-CA	-5.13	1.40	1.46
24	Q	44	ALA	CA-C	-5.13	1.45	1.52
33	J	181	GLN	N-CA	-5.13	1.41	1.45
33	J	324	ARG	C-N	5.13	1.41	1.33
1	a	55	SER	CA-C	5.13	1.58	1.52
5	e	23	GLN	CA-C	-5.13	1.45	1.52
5	e	80	GLY	CA-C	-5.13	1.44	1.51
10	3	149	MET	CA-C	-5.13	1.46	1.52
12	5	268	VAL	CA-CB	-5.13	1.47	1.54
16	V	23	THR	CB-OG1	-5.13	1.35	1.43
22	S	178	LEU	N-CA	5.13	1.52	1.46
22	S	465	ILE	CA-C	-5.13	1.46	1.52
27	O	207	LEU	CA-C	5.13	1.59	1.52
14	n	245	LEU	C-O	5.13	1.30	1.23
21	N	821	LYS	CA-CB	5.13	1.61	1.53
22	S	322	LEU	CA-C	-5.13	1.45	1.52
23	P	12	ASP	CA-C	5.13	1.59	1.52
26	U	98	LYS	C-O	5.13	1.30	1.24
27	O	259	THR	C-N	5.13	1.40	1.34
9	i	134	PRO	N-CD	5.13	1.54	1.47
25	R	391	ASN	CA-C	-5.13	1.47	1.53
22	S	86	SER	N-CA	-5.12	1.40	1.46
30	K	259	ARG	CA-C	-5.12	1.46	1.52
1	a	14	ARG	NE-CZ	5.12	1.38	1.33
8	1	38	ARG	CA-C	-5.12	1.45	1.52
26	U	54	LEU	CA-CB	5.12	1.60	1.54
27	O	371	VAL	CA-C	-5.12	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	81	LEU	CA-C	-5.12	1.45	1.52
29	I	403	ALA	N-CA	-5.12	1.39	1.46
1	a	30	TYR	CA-C	5.12	1.59	1.52
4	d	32	CYS	CA-C	-5.12	1.46	1.52
15	W	122	ARG	CD-NE	5.12	1.53	1.46
15	W	141	ILE	C-O	5.12	1.29	1.24
22	S	101	LYS	CA-CB	5.12	1.61	1.53
24	Q	14	LEU	C-O	-5.12	1.17	1.24
28	H	373	ARG	CA-C	-5.12	1.46	1.52
30	K	181	LYS	N-CA	-5.12	1.40	1.46
4	d	197	ARG	C-N	5.12	1.40	1.33
12	l	181	ARG	NE-CZ	5.12	1.38	1.33
27	O	324	VAL	CA-C	-5.12	1.46	1.52
11	k	60	ILE	C-N	5.12	1.40	1.33
8	1	189	ALA	C-O	-5.12	1.17	1.24
32	M	328	ASN	C-N	5.12	1.40	1.33
33	J	243	SER	CA-CB	5.12	1.64	1.53
10	3	12	VAL	N-CA	-5.12	1.40	1.46
10	3	198	ARG	C-N	5.12	1.40	1.33
28	H	177	ASP	C-N	5.12	1.40	1.34
3	c	222	ASP	CA-CB	5.12	1.60	1.53
14	7	139	LYS	CA-CB	5.12	1.61	1.53
17	T	109	TYR	C-O	-5.12	1.18	1.24
19	Y	31	GLU	CA-C	-5.12	1.46	1.52
23	P	267	PHE	CA-C	-5.12	1.45	1.52
25	R	299	SER	CA-C	-5.12	1.46	1.52
31	L	359	GLU	CA-CB	5.12	1.61	1.53
4	d	43	VAL	CA-C	5.11	1.58	1.52
7	g	25	GLU	CA-C	-5.11	1.46	1.52
21	N	25	LEU	N-CA	-5.11	1.40	1.46
32	M	377	GLN	CA-CB	5.11	1.61	1.53
9	i	252	ILE	N-CA	-5.11	1.40	1.46
29	I	407	ARG	CA-C	-5.11	1.48	1.53
7	g	190	ARG	C-N	5.11	1.41	1.34
9	2	179	GLU	CA-C	-5.11	1.46	1.52
16	V	104	VAL	CA-C	-5.11	1.46	1.52
16	V	161	THR	CB-OG1	-5.11	1.35	1.43
17	T	165	GLN	CA-C	-5.11	1.45	1.52
25	R	226	GLU	C-N	5.11	1.40	1.33
25	R	372	ILE	CA-C	5.11	1.56	1.52
30	K	203	ILE	CA-C	-5.11	1.46	1.52
1	a	17	THR	N-CA	-5.11	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	270	ILE	C-N	5.11	1.41	1.33
18	X	75	TRP	N-CA	-5.11	1.40	1.46
20	Z	726	GLU	CA-C	5.11	1.59	1.52
24	Q	252	HIS	ND1-CE1	5.11	1.37	1.32
32	M	50	ARG	C-O	-5.11	1.18	1.24
33	J	12	LEU	CA-C	-5.11	1.45	1.52
33	J	112	ARG	CA-C	-5.11	1.46	1.52
33	J	387	GLY	C-N	5.11	1.40	1.33
21	N	455	MET	CG-SD	5.11	1.93	1.80
21	N	569	LYS	CA-C	5.11	1.59	1.52
25	R	60	ALA	C-O	-5.11	1.19	1.24
28	H	214	CYS	C-O	-5.11	1.17	1.24
7	g	242	PHE	CA-C	5.10	1.59	1.52
24	Q	321	TYR	N-CA	5.10	1.52	1.46
26	U	174	LEU	C-N	5.10	1.40	1.33
21	N	156	ILE	CA-C	-5.10	1.44	1.52
27	O	285	SER	CA-CB	5.10	1.61	1.53
28	H	116	THR	CA-C	5.10	1.59	1.52
28	H	396	MET	CA-C	-5.10	1.46	1.52
29	I	142	GLU	N-CA	-5.10	1.39	1.46
13	m	173	ASN	N-CA	-5.10	1.39	1.46
12	5	142	GLU	CA-C	-5.10	1.46	1.52
14	7	172	SER	CA-C	5.10	1.58	1.52
2	b	225	THR	C-O	5.10	1.30	1.23
6	f	101	ARG	CZ-NH1	5.10	1.39	1.32
7	g	20	ARG	NE-CZ	5.10	1.38	1.33
30	K	155	ASP	CA-C	-5.10	1.46	1.53
33	J	24	GLU	C-N	5.10	1.40	1.33
33	J	215	GLY	CA-C	-5.10	1.46	1.52
9	i	115	HIS	ND1-CE1	5.10	1.37	1.32
27	O	83	LEU	CA-C	5.10	1.59	1.52
28	H	152	ILE	C-O	-5.10	1.18	1.24
7	g	221	LEU	CA-C	-5.09	1.46	1.52
8	h	13	MET	C-N	5.09	1.40	1.33
10	j	64	ASN	CA-C	5.09	1.59	1.52
14	n	133	MET	N-CA	5.09	1.52	1.46
12	5	264	GLY	C-N	5.09	1.40	1.33
24	Q	237	SER	CA-C	-5.09	1.45	1.52
25	R	34	THR	CA-CB	-5.09	1.45	1.53
28	H	173	ARG	CD-NE	5.09	1.53	1.46
31	L	289	ARG	CZ-NH1	5.09	1.39	1.32
12	l	286	ILE	CA-CB	-5.09	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	162	LYS	CA-C	-5.09	1.46	1.52
30	K	398	ASN	CA-CB	5.09	1.60	1.53
5	e	105	GLU	C-N	5.09	1.40	1.33
12	l	76	THR	C-N	5.09	1.40	1.33
12	l	261	ILE	CB-CG1	5.09	1.63	1.53
13	m	25	GLY	C-N	5.09	1.41	1.33
14	n	193	ASP	C-O	-5.09	1.17	1.23
21	N	119	LYS	CA-C	5.09	1.59	1.52
30	K	364	PRO	C-N	5.09	1.40	1.33
1	a	128	TYR	N-CA	5.09	1.52	1.46
2	b	238	LEU	CA-C	-5.09	1.46	1.52
5	e	238	GLU	CA-C	-5.09	1.46	1.52
6	f	82	ARG	CZ-NH1	5.09	1.39	1.32
11	4	163	LEU	N-CA	5.09	1.52	1.46
12	5	197	LEU	CA-C	-5.09	1.46	1.52
21	N	597	ARG	NE-CZ	5.09	1.38	1.33
22	S	382	ARG	NE-CZ	5.09	1.38	1.33
30	K	247	LEU	CA-CB	5.09	1.60	1.53
30	K	281	ARG	N-CA	-5.09	1.40	1.46
32	M	385	GLU	C-N	5.09	1.40	1.33
17	T	180	ILE	C-N	5.09	1.41	1.33
24	Q	72	ASP	CA-CB	5.09	1.61	1.53
33	J	176	SER	N-CA	-5.09	1.40	1.46
3	c	238	ILE	CB-CG1	5.09	1.63	1.53
11	4	190	ARG	CZ-NH1	5.09	1.39	1.32
14	7	199	PRO	N-CA	-5.09	1.41	1.47
16	V	214	MET	C-N	5.09	1.40	1.33
21	N	459	ASN	CA-CB	5.09	1.60	1.53
28	H	297	MET	CA-C	-5.09	1.46	1.52
14	7	215	ARG	NE-CZ	5.08	1.38	1.33
21	N	237	LEU	C-N	5.08	1.40	1.33
31	L	81	ILE	C-N	5.08	1.40	1.33
33	J	52	ASN	C-N	5.08	1.40	1.33
5	e	226	ASP	CA-C	5.08	1.59	1.52
8	1	34	TYR	CA-CB	5.08	1.60	1.53
14	7	98	ARG	CD-NE	5.08	1.53	1.46
21	N	286	LEU	CA-C	-5.08	1.46	1.52
21	N	391	PRO	C-N	5.08	1.40	1.33
21	N	410	LEU	CA-CB	5.08	1.61	1.53
25	R	281	SER	CA-CB	5.08	1.59	1.53
30	K	44	ASN	C-N	5.08	1.40	1.33
2	b	116	LYS	C-N	5.08	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	23	ILE	CA-C	-5.08	1.46	1.52
15	W	134	LYS	CA-CB	5.08	1.61	1.53
15	W	150	ASN	CG-ND2	5.08	1.44	1.33
24	Q	148	LYS	C-O	-5.08	1.17	1.24
27	O	40	GLN	CA-CB	-5.08	1.45	1.53
28	H	333	MET	CA-C	-5.08	1.46	1.52
33	J	34	ILE	C-N	5.08	1.40	1.33
11	k	23	ARG	CA-C	5.08	1.58	1.52
9	2	30	THR	N-CA	5.08	1.55	1.46
15	W	154	LEU	N-CA	-5.08	1.40	1.46
21	N	901	GLY	C-N	5.08	1.39	1.33
24	Q	160	ASP	C-N	5.08	1.40	1.33
1	a	193	HIS	CA-CB	5.08	1.62	1.53
9	i	41	VAL	CA-C	-5.08	1.46	1.52
12	l	148	ARG	CD-NE	5.08	1.53	1.46
14	n	161	ARG	CA-C	-5.08	1.46	1.52
10	3	97	GLU	CA-C	-5.08	1.46	1.52
12	5	260	TRP	C-N	5.08	1.39	1.33
17	T	253	GLU	CA-CB	5.08	1.61	1.53
32	M	205	ASP	C-N	5.08	1.40	1.33
32	M	389	ALA	C-N	5.08	1.40	1.33
33	J	349	LYS	C-N	5.08	1.39	1.33
13	m	210	LEU	CA-C	-5.08	1.46	1.52
23	P	223	LEU	C-N	5.08	1.41	1.34
31	L	103	GLN	CA-C	-5.08	1.46	1.52
33	J	53	ASP	N-CA	-5.08	1.40	1.46
8	1	186	VAL	CA-C	-5.08	1.46	1.52
17	T	252	GLU	C-N	5.08	1.40	1.33
22	S	138	MET	CA-C	5.08	1.59	1.52
25	R	234	SER	C-N	5.08	1.40	1.33
28	H	175	GLY	CA-C	-5.08	1.48	1.52
6	f	89	ARG	CA-C	5.07	1.59	1.52
9	i	241	VAL	CA-C	-5.07	1.46	1.52
23	P	94	GLN	CA-C	-5.07	1.45	1.52
24	Q	404	ASN	CA-CB	5.07	1.61	1.53
30	K	225	ALA	CA-CB	5.07	1.61	1.53
2	b	41	ASN	CA-CB	5.07	1.62	1.53
6	f	157	TYR	CA-C	-5.07	1.46	1.52
14	n	142	PRO	N-CA	-5.07	1.42	1.46
14	7	74	ARG	CZ-NH2	5.07	1.40	1.33
17	T	92	ASN	CA-CB	5.07	1.61	1.53
24	Q	248	ASN	CA-CB	5.07	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	241	GLN	CA-C	-5.07	1.46	1.52
21	N	579	SER	C-N	5.07	1.40	1.33
27	O	147	ARG	CZ-NH2	5.07	1.40	1.33
1	a	243	GLU	CA-C	-5.07	1.46	1.52
13	6	12	PRO	C-N	5.07	1.40	1.33
1	a	166	TYR	CA-C	-5.07	1.46	1.52
7	g	133	GLY	N-CA	-5.07	1.38	1.45
25	R	272	ASP	CA-CB	5.07	1.60	1.53
28	H	116	THR	C-N	5.07	1.41	1.33
16	V	119	SER	CA-C	5.07	1.59	1.53
30	K	278	ALA	CA-C	-5.07	1.46	1.52
10	3	143	SER	CA-CB	5.06	1.61	1.53
15	W	119	SER	CA-CB	5.06	1.60	1.53
33	J	356	ALA	CA-CB	5.06	1.61	1.53
1	a	210	MET	C-N	5.06	1.40	1.33
4	d	221	ILE	CA-C	-5.06	1.46	1.52
7	g	141	VAL	C-N	5.06	1.37	1.33
7	g	185	GLU	CA-CB	5.06	1.61	1.53
10	3	101	GLY	N-CA	5.06	1.51	1.44
12	5	184	GLY	N-CA	-5.06	1.37	1.44
15	W	17	ARG	CA-C	-5.06	1.46	1.52
31	L	328	ASN	N-CA	-5.06	1.39	1.46
2	b	107	THR	N-CA	-5.06	1.39	1.46
2	b	218	ASN	C-O	-5.06	1.21	1.25
17	T	53	ASN	C-N	5.06	1.41	1.34
21	N	818	LYS	N-CA	-5.06	1.40	1.46
22	S	393	ARG	CZ-NH1	5.06	1.39	1.32
24	Q	132	PHE	CA-C	-5.06	1.46	1.52
29	I	437	LEU	CA-CB	5.06	1.63	1.53
12	5	154	ALA	C-O	-5.06	1.18	1.24
13	6	101	ILE	CA-CB	-5.06	1.48	1.54
26	U	155	LEU	N-CA	-5.06	1.39	1.46
4	d	235	GLN	C-N	-5.06	1.27	1.33
7	g	182	HIS	CA-CB	5.06	1.61	1.53
9	i	78	ALA	C-O	5.06	1.30	1.24
8	1	114	LYS	N-CA	5.06	1.52	1.46
13	6	119	ILE	CA-C	-5.06	1.45	1.53
14	7	203	VAL	C-O	-5.06	1.18	1.24
24	Q	222	SER	CA-CB	5.06	1.61	1.53
28	H	374	LYS	CA-C	-5.06	1.46	1.52
29	I	115	ASP	CA-CB	5.06	1.62	1.53
21	N	895	LYS	C-N	5.06	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	375	LYS	C-N	5.06	1.40	1.33
29	I	264	CYS	C-N	5.06	1.40	1.33
13	m	176	VAL	C-N	5.05	1.40	1.33
16	V	219	GLU	C-N	5.05	1.40	1.33
23	P	306	ASN	CA-CB	5.05	1.60	1.53
26	U	133	PRO	C-N	5.05	1.40	1.33
30	K	121	ARG	NE-CZ	5.05	1.38	1.33
32	M	256	ILE	CA-C	-5.05	1.46	1.52
23	P	204	LEU	C-N	5.05	1.41	1.33
29	I	314	ASP	CG-OD2	5.05	1.34	1.25
8	1	154	ASN	CA-CB	-5.05	1.46	1.53
9	2	46	ASP	CA-C	-5.05	1.46	1.52
17	T	183	SER	C-N	5.05	1.40	1.33
25	R	262	GLU	CA-C	-5.05	1.46	1.53
28	H	419	LEU	C-N	5.05	1.40	1.33
2	b	234	ARG	CD-NE	5.05	1.53	1.46
3	c	39	MET	C-N	5.05	1.40	1.33
4	d	76	SER	CA-C	-5.05	1.46	1.52
10	j	96	TYR	CZ-OH	5.05	1.48	1.38
12	l	242	ARG	CD-NE	5.05	1.53	1.46
14	n	161	ARG	CD-NE	5.05	1.53	1.46
15	W	10	ILE	CA-CB	5.05	1.59	1.54
17	T	85	LEU	CA-CB	5.05	1.61	1.53
21	N	465	ALA	CA-C	5.05	1.59	1.52
27	O	282	GLN	CA-C	-5.05	1.45	1.52
33	J	42	ARG	CZ-NH2	5.05	1.40	1.33
17	T	17	ASN	CA-C	-5.05	1.46	1.52
21	N	538	LYS	C-N	5.05	1.40	1.33
22	S	64	ARG	N-CA	5.05	1.52	1.46
24	Q	62	GLY	CA-C	5.05	1.58	1.51
24	Q	353	PRO	N-CD	-5.05	1.40	1.47
27	O	330	ARG	CZ-NH2	5.05	1.40	1.33
8	h	46	VAL	C-N	5.05	1.40	1.33
13	6	13	TYR	N-CA	-5.05	1.39	1.45
21	N	305	ASN	CA-C	-5.05	1.46	1.52
21	N	510	HIS	N-CA	5.05	1.52	1.46
22	S	226	ASP	CA-C	-5.05	1.46	1.52
27	O	196	LEU	CA-C	-5.05	1.46	1.52
28	H	340	LEU	CA-CB	5.05	1.60	1.53
30	K	77	ARG	CZ-NH1	5.05	1.39	1.32
22	S	483	GLU	CA-C	-5.04	1.46	1.52
28	H	144	LYS	CA-C	-5.04	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	81	ALA	C-N	5.04	1.40	1.33
9	i	112	LEU	C-N	5.04	1.40	1.33
24	Q	50	ARG	NE-CZ	5.04	1.38	1.33
30	K	48	TYR	CA-C	-5.04	1.46	1.52
30	K	84	GLU	CA-CB	5.04	1.61	1.53
2	b	213	ILE	C-O	5.04	1.29	1.24
8	h	38	ARG	CA-C	-5.04	1.46	1.52
10	j	26	ASP	N-CA	-5.04	1.39	1.45
12	l	259	GLY	C-O	-5.04	1.17	1.23
16	V	243	SER	N-CA	-5.04	1.40	1.46
21	N	680	LYS	CA-C	-5.04	1.46	1.52
21	N	747	HIS	ND1-CE1	5.04	1.37	1.32
23	P	56	LYS	C-O	-5.04	1.18	1.24
23	P	123	ARG	CZ-NH2	5.04	1.40	1.33
29	I	123	PRO	C-N	5.04	1.40	1.33
30	K	129	GLU	C-N	5.04	1.40	1.33
8	h	119	VAL	N-CA	-5.04	1.40	1.46
28	H	197	MET	CA-CB	5.04	1.61	1.53
3	c	206	LEU	CA-C	-5.04	1.46	1.52
5	e	235	LYS	CA-C	-5.04	1.46	1.52
13	m	193	ARG	CZ-NH2	5.04	1.40	1.33
9	2	126	TYR	CG-CD1	5.04	1.50	1.39
21	N	602	VAL	C-N	5.04	1.40	1.33
24	Q	70	ALA	CA-CB	5.04	1.59	1.52
31	L	182	GLY	C-N	5.04	1.38	1.33
33	J	371	ARG	N-CA	-5.04	1.40	1.46
12	5	218	ASN	CA-C	-5.04	1.45	1.52
22	S	248	ASP	CA-CB	5.04	1.61	1.53
25	R	309	LEU	N-CA	-5.04	1.40	1.46
7	g	108	PRO	CA-C	-5.04	1.46	1.52
11	k	63	ASN	C-N	5.04	1.40	1.33
8	1	194	ARG	CZ-NH1	5.04	1.39	1.32
23	P	113	ASN	CA-CB	5.04	1.61	1.53
23	P	211	PRO	C-N	5.04	1.40	1.33
27	O	36	LYS	CB-CG	5.04	1.67	1.52
30	K	133	PRO	CA-CB	-5.04	1.46	1.53
14	7	236	ASN	CA-C	-5.03	1.45	1.52
30	K	74	HIS	ND1-CE1	5.03	1.37	1.32
31	L	228	LYS	N-CA	-5.03	1.40	1.46
31	L	261	ARG	CZ-NH1	5.03	1.39	1.32
8	1	24	GLY	N-CA	-5.03	1.40	1.45
14	7	46	SER	N-CA	-5.03	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	156	LYS	CA-CB	5.03	1.61	1.53
1	a	144	VAL	C-N	5.03	1.39	1.33
7	g	86	ARG	NE-CZ	5.03	1.38	1.33
22	S	245	GLY	C-N	5.03	1.41	1.33
9	i	171	TRP	NE1-CE2	5.03	1.43	1.37
13	6	87	HIS	CD2-NE2	5.03	1.43	1.37
15	W	122	ARG	CA-C	-5.03	1.46	1.52
27	O	35	GLU	C-N	5.03	1.40	1.33
28	H	113	ASP	CA-CB	5.03	1.61	1.53
2	b	71	ILE	C-N	5.03	1.40	1.33
13	6	145	ARG	NE-CZ	5.03	1.38	1.33
15	W	112	ALA	CA-C	-5.03	1.46	1.52
16	V	175	SER	CA-CB	5.03	1.61	1.53
33	J	351	ASN	C-N	5.03	1.39	1.33
3	c	158	THR	N-CA	-5.02	1.39	1.46
9	2	247	VAL	N-CA	-5.02	1.40	1.46
17	T	12	SER	C-O	-5.02	1.18	1.24
21	N	503	THR	CA-CB	5.02	1.61	1.53
23	P	380	ILE	C-N	5.02	1.40	1.33
15	W	77	HIS	CB-CG	5.02	1.57	1.50
15	W	149	GLN	C-N	5.02	1.40	1.33
16	V	147	VAL	N-CA	-5.02	1.40	1.46
8	h	14	ALA	CA-C	-5.02	1.46	1.52
10	j	56	LEU	CA-CB	5.02	1.61	1.53
3	c	120	GLN	CA-CB	5.02	1.61	1.53
13	m	188	VAL	CA-CB	5.02	1.60	1.54
14	7	130	ALA	CA-C	5.02	1.59	1.52
16	V	80	VAL	N-CA	-5.02	1.40	1.46
16	V	212	MET	C-N	5.02	1.40	1.33
23	P	337	HIS	CG-CD2	5.02	1.41	1.35
24	Q	377	LEU	N-CA	-5.02	1.39	1.46
26	U	182	ALA	N-CA	-5.02	1.39	1.46
10	j	39	LYS	N-CA	5.02	1.52	1.46
23	P	143	LEU	CA-C	-5.02	1.45	1.52
27	O	137	TYR	N-CA	-5.02	1.40	1.46
28	H	71	GLU	C-N	5.02	1.40	1.33
30	K	236	ARG	NE-CZ	5.02	1.38	1.33
17	T	8	THR	C-N	5.02	1.41	1.33
30	K	142	HIS	CA-C	-5.02	1.46	1.52
30	K	335	ASP	CA-CB	5.01	1.61	1.53
3	c	172	ALA	CA-CB	5.01	1.61	1.53
15	W	124	GLU	C-O	5.01	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	708	ALA	C-N	5.01	1.40	1.33
23	P	379	TYR	C-O	-5.01	1.17	1.24
3	c	43	GLY	CA-C	-5.01	1.47	1.52
10	j	203	ARG	CA-C	-5.01	1.46	1.52
13	m	60	MET	C-O	-5.01	1.18	1.23
13	m	193	ARG	CA-C	-5.01	1.46	1.52
9	2	100	SER	CA-C	-5.01	1.46	1.53
14	7	98	ARG	CZ-NH1	5.01	1.39	1.32
22	S	464	ARG	NE-CZ	5.01	1.38	1.33
24	Q	292	GLN	N-CA	-5.01	1.40	1.46
25	R	204	TRP	N-CA	-5.01	1.39	1.46
27	O	387	ARG	NE-CZ	5.01	1.38	1.33
29	I	306	MET	CA-C	-5.01	1.46	1.52
3	c	241	LYS	C-N	5.01	1.41	1.33
21	N	141	ILE	CA-CB	-5.01	1.48	1.54
21	N	339	MET	C-N	5.01	1.40	1.33
24	Q	265	MET	N-CA	-5.01	1.40	1.46
6	f	184	GLY	CA-C	-5.01	1.44	1.51
10	j	112	ILE	CA-C	-5.01	1.46	1.52
9	2	95	HIS	CA-C	5.01	1.59	1.52
16	V	138	ALA	N-CA	5.01	1.52	1.46
16	V	205	LYS	C-N	5.01	1.40	1.33
21	N	482	ALA	CA-C	-5.01	1.46	1.52
22	S	393	ARG	NE-CZ	5.01	1.38	1.33
22	S	491	GLU	CA-C	-5.01	1.46	1.52
29	I	100	ARG	CZ-NH2	5.01	1.40	1.33
32	M	164	ASP	CA-CB	5.01	1.61	1.53
3	c	148	LEU	C-N	5.00	1.39	1.33
4	d	16	HIS	N-CA	-5.00	1.38	1.46
8	h	144	TYR	CA-CB	5.00	1.61	1.53
14	7	254	PHE	CA-C	-5.00	1.46	1.52
29	I	408	ARG	CD-NE	5.00	1.53	1.46
7	g	15	PHE	CA-CB	5.00	1.62	1.53
13	6	55	GLY	N-CA	-5.00	1.39	1.45
22	S	104	VAL	C-O	-5.00	1.20	1.24
22	S	384	ARG	CZ-NH1	5.00	1.39	1.32
11	k	70	ARG	C-N	5.00	1.40	1.33
11	4	142	SER	C-N	5.00	1.41	1.33
13	6	158	LEU	CA-C	-5.00	1.45	1.52
21	N	300	ASN	CA-C	-5.00	1.46	1.52
21	N	903	VAL	CA-C	-5.00	1.46	1.52
23	P	154	ASP	N-CA	5.00	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	308	LEU	CA-CB	5.00	1.61	1.53
26	U	189	ARG	CZ-NH2	5.00	1.40	1.33
27	O	372	GLU	CA-C	-5.00	1.46	1.52
30	K	73	ARG	C-N	5.00	1.40	1.33
32	M	81	ASN	C-N	5.00	1.39	1.33

All (6405) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L	185	GLY	O-C-N	-86.19	16.00	122.87
33	J	211	ILE	O-C-N	-64.49	47.31	122.12
30	K	167	PRO	O-C-N	-55.87	47.21	122.64
32	M	338	LEU	O-C-N	-39.48	69.00	122.30
20	Z	728	LYS	CG-CD-CE	-38.20	23.45	111.30
32	M	342	ARG	CA-C-N	-35.76	53.25	121.54
32	M	342	ARG	C-N-CA	-35.76	53.25	121.54
7	g	22	PHE	O-C-N	34.99	169.25	122.36
7	g	22	PHE	CA-C-O	-33.96	80.86	119.24
7	G	22	PHE	CA-C-O	-33.29	81.38	119.67
7	G	22	PHE	O-C-N	30.59	168.02	122.13
20	Z	253	VAL	N-CA-CB	25.95	126.85	110.50
30	K	167	PRO	CA-C-N	24.73	163.35	122.54
30	K	167	PRO	C-N-CA	24.73	163.35	122.54
33	J	212	ARG	O-C-N	23.90	154.37	122.59
20	Z	728	LYS	CA-CB-CG	22.48	159.06	114.10
30	K	220	THR	O-C-N	-20.60	94.72	122.33
5	E	20	ARG	CD-NE-CZ	18.87	150.82	124.40
33	J	309	ARG	CB-CA-C	-18.57	76.72	110.70
5	E	20	ARG	NH1-CZ-NH2	-18.53	95.22	119.30
30	K	220	THR	CA-C-N	18.10	154.82	121.52
30	K	220	THR	C-N-CA	18.10	154.82	121.52
20	Z	730	ALA	N-CA-C	17.77	130.65	111.28
33	J	309	ARG	N-CA-CB	17.59	136.40	110.20
29	I	228	GLY	O-C-N	-16.06	103.66	122.45
32	M	342	ARG	O-C-N	-16.00	102.83	122.19
20	Z	726	GLU	N-CA-C	15.60	130.43	111.40
20	Z	252	CYS	CA-C-N	15.57	130.05	120.24
20	Z	252	CYS	C-N-CA	15.57	130.05	120.24
20	Z	254	PRO	CA-C-N	14.82	149.84	121.54
20	Z	254	PRO	C-N-CA	14.82	149.84	121.54
7	g	109	ILE	N-CA-CB	14.56	119.67	110.50
20	Z	255	LEU	CD1-CG-CD2	-13.86	80.30	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	20	ARG	NE-CZ-NH2	13.82	131.64	119.20
30	K	195	ALA	CA-C-N	13.28	138.07	120.28
30	K	195	ALA	C-N-CA	13.28	138.07	120.28
5	e	136	ARG	O-C-N	-13.15	113.30	121.71
20	Z	729	GLU	N-CA-CB	12.91	129.12	110.40
20	Z	251	ALA	N-CA-C	12.84	125.36	111.36
31	L	186	LEU	N-CA-C	-12.82	93.55	111.24
20	Z	153	TYR	CA-C-N	12.56	137.67	120.46
20	Z	153	TYR	C-N-CA	12.56	137.67	120.46
20	Z	728	LYS	CB-CA-C	12.55	135.39	110.42
14	7	197	ASP	CA-C-N	12.41	128.06	120.24
14	7	197	ASP	C-N-CA	12.41	128.06	120.24
13	6	164	PHE	CA-CB-CG	-12.33	101.47	113.80
7	g	48	PHE	CA-CB-CG	-12.22	101.58	113.80
20	Z	253	VAL	N-CA-C	-12.09	95.09	112.61
8	h	141	THR	N-CA-C	-12.06	98.97	112.72
32	M	338	LEU	CA-C-N	12.02	144.50	121.54
32	M	338	LEU	C-N-CA	12.02	144.50	121.54
20	Z	729	GLU	CB-CA-C	-11.98	90.77	109.34
30	K	107	THR	CA-C-N	11.87	132.74	122.17
30	K	107	THR	C-N-CA	11.87	132.74	122.17
14	7	190	LYS	CA-C-N	11.63	135.44	120.56
14	7	190	LYS	C-N-CA	11.63	135.44	120.56
5	E	20	ARG	NE-CZ-NH1	11.63	133.13	121.50
11	4	145	ASP	CA-CB-CG	11.62	124.22	112.60
18	X	69	ILE	CA-C-O	-11.56	111.52	119.38
21	N	548	ARG	CA-C-N	11.49	135.37	120.44
21	N	548	ARG	C-N-CA	11.49	135.37	120.44
20	Z	728	LYS	O-C-N	-11.48	107.31	122.59
23	P	337	HIS	N-CA-C	-11.37	99.89	113.88
28	H	184	GLU	N-CA-C	-11.31	96.96	112.12
14	7	145	ASN	CA-CB-CG	11.27	123.87	112.60
25	R	214	TYR	CA-C-N	11.17	132.61	119.99
25	R	214	TYR	C-N-CA	11.17	132.61	119.99
11	k	101	ASN	CA-CB-CG	-11.09	101.51	112.60
5	e	151	ASP	CA-C-N	11.06	131.71	121.31
5	e	151	ASP	C-N-CA	11.06	131.71	121.31
21	N	494	LYS	CA-C-O	-11.06	108.67	119.51
17	T	174	PHE	CA-CB-CG	-11.03	102.77	113.80
18	X	102	GLN	N-CA-C	-10.99	96.87	110.61
20	Z	248	TYR	N-CA-CB	10.97	126.39	110.16
32	M	222	GLY	CA-C-N	10.95	131.66	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	M	222	GLY	C-N-CA	10.95	131.66	120.38
29	I	165	ASP	O-C-N	-10.94	114.71	121.71
31	L	187	THR	CA-C-N	10.83	135.21	120.38
31	L	187	THR	C-N-CA	10.83	135.21	120.38
30	K	286	THR	N-CA-C	-10.81	94.18	108.34
14	n	197	ASP	CA-C-N	10.79	127.03	120.24
14	n	197	ASP	C-N-CA	10.79	127.03	120.24
27	O	54	SER	N-CA-C	-10.74	99.70	113.12
28	H	326	ASP	CA-CB-CG	-10.71	101.89	112.60
16	V	147	VAL	N-CA-C	-10.69	103.14	112.12
27	O	279	ILE	N-CA-C	-10.65	100.29	111.58
22	S	205	ASN	CA-CB-CG	-10.64	101.96	112.60
30	K	218	GLY	CA-C-N	-10.63	101.24	121.54
30	K	218	GLY	C-N-CA	-10.63	101.24	121.54
20	Z	729	GLU	CA-C-N	10.63	134.52	120.28
20	Z	729	GLU	C-N-CA	10.63	134.52	120.28
23	P	387	GLY	CA-C-N	10.62	134.15	120.56
23	P	387	GLY	C-N-CA	10.62	134.15	120.56
23	P	113	ASN	CA-CB-CG	-10.59	102.01	112.60
28	H	148	ASN	CA-CB-CG	-10.56	102.03	112.60
27	O	311	GLU	CA-C-N	10.47	134.06	120.44
27	O	311	GLU	C-N-CA	10.47	134.06	120.44
30	K	214	PRO	CA-C-O	-10.44	113.38	120.90
22	S	122	ASN	CA-CB-CG	-10.44	102.16	112.60
14	n	175	LEU	CA-C-O	10.42	133.36	120.54
13	m	196	PHE	CA-CB-CG	-10.41	103.39	113.80
25	R	76	GLN	N-CA-C	-10.40	101.15	114.04
23	P	313	ILE	N-CA-C	-10.39	103.48	111.90
11	4	151	ASP	CA-CB-CG	10.38	122.98	112.60
24	Q	335	PHE	CA-CB-CG	10.37	124.17	113.80
29	I	255	LYS	N-CA-C	-10.36	100.12	113.17
20	Z	916	LEU	N-CA-C	-10.33	101.44	114.56
20	Z	247	GLN	CB-CA-C	10.33	130.50	110.67
20	Z	729	GLU	N-CA-C	10.31	126.54	113.55
31	L	185	GLY	CA-C-N	10.31	137.84	122.68
31	L	185	GLY	C-N-CA	10.31	137.84	122.68
16	V	35	LEU	CA-C-N	10.31	134.93	120.29
16	V	35	LEU	C-N-CA	10.31	134.93	120.29
7	g	195	GLN	CA-C-O	10.25	130.42	119.14
26	U	233	PHE	CA-CB-CG	-10.25	103.55	113.80
23	P	326	ASP	CA-CB-CG	-10.24	102.36	112.60
6	f	13	PHE	CA-C-N	10.23	140.12	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	13	PHE	C-N-CA	10.23	140.12	121.70
25	R	120	LEU	N-CA-C	-10.20	99.73	112.88
16	V	101	ASP	CA-CB-CG	10.19	122.79	112.60
18	X	117	LYS	CA-C-N	10.19	134.10	120.65
18	X	117	LYS	C-N-CA	10.19	134.10	120.65
31	L	200	PRO	N-CA-CB	10.16	112.91	103.46
10	3	38	ASN	N-CA-C	-10.14	97.22	112.54
14	n	184	ALA	CA-C-N	10.13	135.96	120.97
14	n	184	ALA	C-N-CA	10.13	135.96	120.97
3	c	81	THR	CA-C-N	10.07	133.54	120.44
3	c	81	THR	C-N-CA	10.07	133.54	120.44
21	N	242	PHE	CA-CB-CG	-10.06	103.74	113.80
22	S	78	VAL	CA-C-N	10.04	133.74	120.28
22	S	78	VAL	C-N-CA	10.04	133.74	120.28
15	W	184	ASN	CA-CB-CG	-10.02	102.58	112.60
20	Z	253	VAL	CB-CA-C	-10.02	103.73	114.35
24	Q	206	ASN	N-CA-C	-10.02	100.44	111.36
30	K	213	GLY	CA-C-N	10.01	126.97	119.66
30	K	213	GLY	C-N-CA	10.01	126.97	119.66
28	H	442	ASP	CA-CB-CG	-10.00	102.60	112.60
29	I	287	ILE	N-CA-C	-9.97	101.15	110.82
20	Z	918	ASP	CA-CB-CG	-9.89	102.71	112.60
31	L	234	ALA	N-CA-C	-9.86	100.09	112.72
1	a	85	GLY	CA-C-N	9.86	130.48	119.93
1	a	85	GLY	C-N-CA	9.86	130.48	119.93
9	2	122	HIS	CA-CB-CG	-9.86	103.94	113.80
27	O	65	PHE	CA-CB-CG	-9.86	103.94	113.80
31	L	164	ASP	CA-C-N	9.85	129.60	119.56
31	L	164	ASP	C-N-CA	9.85	129.60	119.56
22	S	117	SER	N-CA-C	-9.85	102.34	114.75
22	S	309	PHE	CA-CB-CG	-9.78	104.02	113.80
8	h	90	VAL	O-C-N	-9.77	111.74	121.90
30	K	78	GLU	CA-C-N	9.75	133.34	120.28
30	K	78	GLU	C-N-CA	9.75	133.34	120.28
21	N	692	GLU	CA-C-N	9.74	130.79	119.98
21	N	692	GLU	C-N-CA	9.74	130.79	119.98
33	J	317	PRO	O-C-N	9.74	125.79	121.31
1	a	143	PHE	CA-CB-CG	-9.72	104.08	113.80
21	N	451	GLY	O-C-N	9.70	131.50	122.19
13	m	52	PHE	CA-CB-CG	-9.69	104.11	113.80
33	J	190	PRO	O-C-N	-9.68	116.86	121.31
13	m	106	TYR	CA-C-N	9.64	130.65	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	106	TYR	C-N-CA	9.64	130.65	119.94
3	c	89	ASN	CA-CB-CG	-9.63	102.97	112.60
20	Z	738	TYR	CD1-CE1-CZ	9.62	136.91	119.60
13	m	68	ASP	CA-C-N	9.62	130.85	119.99
13	m	68	ASP	C-N-CA	9.62	130.85	119.99
24	Q	359	ILE	CA-C-N	9.59	133.48	120.54
24	Q	359	ILE	C-N-CA	9.59	133.48	120.54
27	O	245	ASP	CA-CB-CG	-9.57	103.03	112.60
21	N	719	ASN	CA-CB-CG	-9.55	103.05	112.60
23	P	243	GLU	CA-C-N	9.55	133.98	120.42
23	P	243	GLU	C-N-CA	9.55	133.98	120.42
4	d	172	ARG	CA-C-N	9.54	133.06	120.28
4	d	172	ARG	C-N-CA	9.54	133.06	120.28
32	M	33	ARG	NE-CZ-NH2	9.53	127.78	119.20
12	l	284	ASN	N-CA-C	-9.53	100.87	111.07
24	Q	48	ASP	CA-C-N	9.51	135.11	120.75
24	Q	48	ASP	C-N-CA	9.51	135.11	120.75
22	S	132	ALA	N-CA-C	9.45	122.55	111.02
10	3	50	PHE	CA-CB-CG	-9.43	104.37	113.80
4	d	227	GLU	CA-C-N	9.42	132.69	120.44
4	d	227	GLU	C-N-CA	9.42	132.69	120.44
31	L	254	LYS	CA-C-N	9.42	134.80	121.24
31	L	254	LYS	C-N-CA	9.42	134.80	121.24
24	Q	214	THR	O-C-N	9.41	132.09	122.12
7	g	109	ILE	CB-CA-C	-9.41	104.38	114.35
20	Z	738	TYR	CB-CG-CD2	9.40	134.91	120.80
9	2	232	TYR	N-CA-C	-9.40	99.16	110.44
22	S	475	TYR	CA-C-N	9.37	132.62	120.44
22	S	475	TYR	C-N-CA	9.37	132.62	120.44
1	a	130	GLN	N-CA-C	-9.36	102.37	113.88
21	N	99	GLU	N-CA-C	-9.35	102.06	112.72
30	K	419	ASN	CA-CB-CG	-9.35	103.25	112.60
32	M	74	GLN	CA-C-N	9.35	133.39	120.39
32	M	74	GLN	C-N-CA	9.35	133.39	120.39
11	k	54	VAL	CA-C-N	9.35	132.59	120.44
11	k	54	VAL	C-N-CA	9.35	132.59	120.44
17	T	110	LEU	CA-C-O	-9.33	110.53	120.42
21	N	41	ASN	N-CA-C	-9.33	101.45	113.12
20	Z	255	LEU	CA-CB-CG	9.33	148.96	116.30
22	S	184	TRP	CB-CG-CD2	-9.32	113.75	126.80
32	M	38	ASP	N-CA-CB	9.31	123.94	110.16
13	m	172	THR	N-CA-C	-9.29	102.08	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	284	ASN	N-CA-C	-9.28	101.52	113.12
8	h	56	GLY	N-CA-C	-9.28	99.81	112.52
13	6	34	ASP	CA-CB-CG	9.27	121.87	112.60
28	H	257	THR	CA-C-N	9.27	132.70	120.28
28	H	257	THR	C-N-CA	9.27	132.70	120.28
14	7	149	VAL	N-CA-C	-9.25	95.16	108.11
16	V	142	ASP	N-CA-C	-9.25	97.55	110.31
26	U	77	ASN	N-CA-C	9.25	121.36	111.28
16	V	190	HIS	CA-CB-CG	9.23	123.03	113.80
17	T	252	GLU	N-CA-C	-9.23	102.15	113.97
32	M	426	LYS	N-CA-C	-9.21	99.78	112.30
3	c	42	ASP	N-CA-C	-9.20	98.65	113.19
14	n	92	ASP	CA-CB-CG	-9.20	103.40	112.60
19	Y	85	LYS	CA-C-N	9.20	132.61	120.28
19	Y	85	LYS	C-N-CA	9.20	132.61	120.28
23	P	121	THR	N-CA-C	9.20	121.39	111.36
21	N	16	ASN	CA-CB-CG	-9.18	103.42	112.60
30	K	284	ALA	CA-C-N	9.16	132.35	120.44
30	K	284	ALA	C-N-CA	9.16	132.35	120.44
25	R	59	MET	N-CA-C	-9.16	102.22	112.57
22	S	373	LYS	O-C-N	9.15	131.82	122.12
24	Q	280	ASN	N-CA-C	9.15	121.25	111.28
27	O	10	ILE	CA-C-N	9.15	132.54	120.28
27	O	10	ILE	C-N-CA	9.15	132.54	120.28
13	6	78	ASN	CA-CB-CG	9.15	121.75	112.60
20	Z	785	VAL	CA-C-N	9.14	132.53	120.28
20	Z	785	VAL	C-N-CA	9.14	132.53	120.28
13	m	44	ASN	OD1-CG-ND2	9.11	131.71	122.60
9	2	122	HIS	CE1-NE2-CD2	-9.11	99.89	109.00
7	g	139	GLY	O-C-N	-9.11	113.15	123.62
25	R	129	GLU	N-CA-C	9.11	121.28	111.36
25	R	319	CYS	CA-C-N	9.10	132.48	120.28
25	R	319	CYS	C-N-CA	9.10	132.48	120.28
11	4	54	VAL	N-CA-C	-9.09	101.87	110.42
29	I	156	ILE	CB-CA-C	-9.06	101.47	111.35
8	1	23	LEU	CA-C-O	-9.06	110.92	121.16
21	N	109	TYR	CA-C-N	9.05	132.15	120.56
21	N	109	TYR	C-N-CA	9.05	132.15	120.56
18	X	119	LYS	CA-C-N	9.03	132.18	120.44
18	X	119	LYS	C-N-CA	9.03	132.18	120.44
14	n	257	ASP	CA-CB-CG	-9.02	103.58	112.60
30	K	258	PHE	CA-CB-CG	-9.02	104.78	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	340	PHE	CA-CB-CG	-9.02	104.78	113.80
19	Y	66	ASP	N-CA-C	-9.02	102.00	113.72
21	N	731	VAL	CA-C-N	9.02	130.18	119.99
21	N	731	VAL	C-N-CA	9.02	130.18	119.99
5	e	150	ASP	CA-CB-CG	-9.00	103.60	112.60
19	Y	72	ASP	CA-CB-CG	-8.99	103.61	112.60
24	Q	84	TYR	CA-C-N	8.95	132.28	120.28
24	Q	84	TYR	C-N-CA	8.95	132.28	120.28
21	N	614	ASN	OD1-CG-ND2	-8.94	113.66	122.60
31	L	203	ASN	CA-CB-CG	-8.94	103.66	112.60
17	T	118	ASN	CA-C-N	8.94	132.98	120.29
17	T	118	ASN	C-N-CA	8.94	132.98	120.29
13	6	25	GLY	N-CA-C	-8.92	99.84	112.60
30	K	218	GLY	O-C-N	-8.92	111.01	122.34
25	R	372	ILE	O-C-N	-8.91	113.74	120.07
20	Z	727	GLU	CA-C-N	8.91	138.56	121.54
20	Z	727	GLU	C-N-CA	8.91	138.56	121.54
9	2	64	HIS	CE1-NE2-CD2	-8.90	100.10	109.00
21	N	8	PRO	CA-C-N	8.90	132.54	120.44
21	N	8	PRO	C-N-CA	8.90	132.54	120.44
23	P	78	GLN	CA-C-N	8.90	132.55	120.54
23	P	78	GLN	C-N-CA	8.90	132.55	120.54
10	3	171	LEU	CA-C-N	8.89	132.55	120.54
10	3	171	LEU	C-N-CA	8.89	132.55	120.54
14	7	72	VAL	N-CA-CB	8.89	121.14	111.00
33	J	78	ILE	N-CA-C	-8.87	95.70	108.48
33	J	5	VAL	N-CA-C	-8.85	104.41	112.90
26	U	206	ASP	CA-CB-CG	-8.84	103.76	112.60
28	H	319	PHE	CA-C-N	8.83	132.11	120.28
28	H	319	PHE	C-N-CA	8.83	132.11	120.28
13	6	105	LEU	CA-C-N	8.82	132.98	120.28
13	6	105	LEU	C-N-CA	8.82	132.98	120.28
24	Q	336	ASN	N-CA-CB	8.81	122.85	110.07
33	J	310	ILE	N-CA-C	-8.81	94.88	107.75
1	a	79	ILE	CA-C-N	8.80	132.19	122.16
1	a	79	ILE	C-N-CA	8.80	132.19	122.16
4	d	102	ASP	CA-CB-CG	8.80	121.40	112.60
22	S	191	HIS	CA-C-N	8.80	132.78	120.29
22	S	191	HIS	C-N-CA	8.80	132.78	120.29
24	Q	252	HIS	CA-CB-CG	8.79	122.59	113.80
28	H	272	ILE	N-CA-C	-8.79	94.76	107.77
20	Z	843	ASP	CA-CB-CG	-8.78	103.82	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	23	GLN	N-CA-C	8.77	120.83	111.28
13	m	215	VAL	N-CA-C	-8.76	95.85	108.11
17	T	137	GLU	N-CA-C	-8.76	103.72	114.75
29	I	119	ILE	N-CA-C	-8.75	95.92	108.17
2	b	42	GLY	CA-C-O	-8.75	112.76	121.86
21	N	416	GLY	CA-C-O	8.74	127.84	120.76
27	O	97	LYS	N-CA-C	8.74	120.89	111.36
32	M	198	VAL	CB-CA-C	-8.73	100.35	112.14
21	N	675	VAL	N-CA-C	8.73	119.52	110.62
30	K	141	ARG	NE-CZ-NH2	8.73	127.06	119.20
20	Z	735	GLU	N-CA-CB	8.72	123.66	110.22
28	H	56	LEU	CA-C-O	-8.72	111.30	120.55
8	h	161	VAL	N-CA-C	8.72	119.52	110.62
6	f	5	ASN	CA-CB-CG	-8.71	103.89	112.60
20	Z	738	TYR	OH-CZ-CE2	8.71	146.03	119.90
33	J	342	ASN	CA-C-N	8.71	132.82	120.28
33	J	342	ASN	C-N-CA	8.71	132.82	120.28
21	N	38	GLU	CB-CG-CD	-8.71	97.80	112.60
17	T	16	GLU	CA-C-N	8.70	131.94	120.28
17	T	16	GLU	C-N-CA	8.70	131.94	120.28
23	P	184	MET	CA-C-N	8.70	132.64	120.29
23	P	184	MET	C-N-CA	8.70	132.64	120.29
11	4	55	GLN	CA-C-O	-8.69	111.20	120.42
12	5	258	ASP	N-CA-C	-8.69	102.45	113.23
30	K	425	ASP	CA-CB-CG	8.69	121.29	112.60
3	c	216	ILE	N-CA-C	-8.68	94.85	107.78
28	H	187	LEU	O-C-N	-8.68	113.97	121.35
33	J	332	SER	CA-C-O	-8.68	110.30	120.10
21	N	721	ASP	N-CA-C	-8.67	102.70	113.28
24	Q	87	GLN	CA-C-N	8.67	131.90	120.28
24	Q	87	GLN	C-N-CA	8.67	131.90	120.28
2	b	220	ASP	CA-CB-CG	8.67	121.27	112.60
20	Z	255	LEU	N-CA-CB	8.66	125.14	110.49
11	4	195	PHE	CA-CB-CG	-8.66	105.14	113.80
16	V	133	ASN	OD1-CG-ND2	8.66	131.26	122.60
23	P	45	LYS	N-CA-C	-8.66	97.54	108.45
25	R	383	ARG	CA-C-N	8.65	131.28	120.72
25	R	383	ARG	C-N-CA	8.65	131.28	120.72
23	P	417	HIS	CA-CB-CG	8.65	122.45	113.80
27	O	179	PHE	CA-CB-CG	-8.64	105.16	113.80
28	H	95	HIS	CA-CB-CG	8.64	122.44	113.80
11	4	76	SER	CA-C-N	8.63	128.77	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	4	76	SER	C-N-CA	8.63	128.77	119.28
28	H	359	ASN	CA-CB-CG	-8.63	103.97	112.60
11	k	153	THR	N-CA-C	-8.63	96.28	109.14
22	S	253	PHE	CA-CB-CG	-8.63	105.17	113.80
10	3	44	PHE	CA-CB-CG	-8.62	105.18	113.80
3	c	152	ASN	O-C-N	-8.62	114.00	121.32
24	Q	139	ILE	N-CA-C	-8.62	102.02	110.72
9	i	133	ASP	CA-CB-CG	8.61	121.21	112.60
21	N	604	ARG	CA-C-N	8.61	131.58	120.56
21	N	604	ARG	C-N-CA	8.61	131.58	120.56
3	c	19	LEU	CA-C-N	8.60	132.15	120.54
3	c	19	LEU	C-N-CA	8.60	132.15	120.54
14	n	35	GLN	CA-C-N	8.60	134.53	122.06
14	n	35	GLN	C-N-CA	8.60	134.53	122.06
20	Z	258	PRO	N-CA-C	8.60	121.19	110.70
13	m	202	ARG	NE-CZ-NH2	-8.59	111.47	119.20
30	K	235	ILE	CA-C-N	8.59	136.77	122.76
30	K	235	ILE	C-N-CA	8.59	136.77	122.76
26	U	14	VAL	CB-CA-C	-8.59	100.98	111.97
23	P	274	GLY	N-CA-C	-8.58	102.09	112.48
25	R	208	ASN	CA-C-O	8.58	129.52	120.42
13	6	155	MET	O-C-N	-8.57	113.61	120.38
21	N	354	PRO	CA-C-N	8.55	132.44	120.29
21	N	354	PRO	C-N-CA	8.55	132.44	120.29
28	H	174	VAL	CA-C-N	8.55	130.33	122.20
28	H	174	VAL	C-N-CA	8.55	130.33	122.20
9	2	163	ALA	CA-C-N	8.55	131.74	120.28
9	2	163	ALA	C-N-CA	8.55	131.74	120.28
8	h	19	ASP	O-C-N	-8.54	111.84	122.35
22	S	349	THR	N-CA-C	-8.54	101.97	111.28
28	H	164	SER	CA-C-O	-8.54	112.91	120.60
6	f	210	ASN	N-CA-C	-8.54	103.45	114.04
10	3	68	ARG	CA-C-N	8.52	131.52	120.44
10	3	68	ARG	C-N-CA	8.52	131.52	120.44
20	Z	214	HIS	N-CA-C	8.52	120.65	111.36
20	Z	250	VAL	CA-C-N	8.51	132.38	120.29
20	Z	250	VAL	C-N-CA	8.51	132.38	120.29
32	M	261	LYS	N-CA-C	8.51	120.55	111.28
29	I	345	ASP	CA-C-N	8.50	132.78	120.71
29	I	345	ASP	C-N-CA	8.50	132.78	120.71
4	d	228	GLU	CA-C-N	8.49	132.50	120.53
4	d	228	GLU	C-N-CA	8.49	132.50	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	211	GLU	CA-C-O	-8.49	111.16	120.33
28	H	305	ILE	N-CA-C	-8.49	95.89	108.45
18	X	100	TRP	N-CA-C	-8.49	94.17	108.26
22	S	317	HIS	CA-CB-CG	8.48	122.28	113.80
3	c	11	THR	N-CA-C	-8.47	101.95	112.88
5	e	70	ILE	N-CA-C	-8.46	103.58	111.45
22	S	139	HIS	CE1-NE2-CD2	-8.46	100.54	109.00
33	J	16	GLU	CA-C-N	8.45	132.45	120.28
33	J	16	GLU	C-N-CA	8.45	132.45	120.28
24	Q	249	LEU	CA-C-N	8.45	132.70	120.71
24	Q	249	LEU	C-N-CA	8.45	132.70	120.71
32	M	175	LYS	N-CA-C	-8.44	97.57	110.32
24	Q	270	ILE	O-C-N	8.44	130.06	121.87
26	U	118	PRO	N-CA-CB	8.44	111.18	103.33
31	L	368	VAL	N-CA-C	8.44	119.74	110.21
17	T	253	GLU	O-C-N	8.42	131.19	122.09
11	k	9	VAL	N-CA-CB	-8.42	102.47	112.07
22	S	115	PRO	N-CA-C	-8.42	102.69	114.98
13	6	56	ASP	CA-CB-CG	-8.42	104.18	112.60
13	6	83	TYR	N-CA-C	-8.42	102.05	111.14
9	i	149	ASP	CA-CB-CG	-8.41	104.19	112.60
27	O	83	LEU	CA-C-N	8.41	131.88	120.44
27	O	83	LEU	C-N-CA	8.41	131.88	120.44
6	f	112	LEU	CA-C-N	8.41	131.37	120.44
6	f	112	LEU	C-N-CA	8.41	131.37	120.44
14	7	128	TYR	O-C-N	8.40	130.83	122.09
14	n	76	ILE	CA-C-N	8.40	129.06	119.99
14	n	76	ILE	C-N-CA	8.40	129.06	119.99
13	m	71	ALA	N-CA-C	8.40	120.44	111.28
11	4	28	LEU	N-CA-C	-8.39	101.52	112.68
33	J	361	VAL	CB-CA-C	-8.39	100.64	112.22
25	R	325	HIS	CA-CB-CG	-8.39	105.41	113.80
28	H	366	LEU	CA-C-O	-8.39	110.32	119.97
9	i	252	ILE	CA-C-O	8.39	131.67	121.02
20	Z	614	VAL	N-CA-C	-8.37	102.70	111.58
26	U	292	ILE	CA-C-N	8.37	133.03	120.31
26	U	292	ILE	C-N-CA	8.37	133.03	120.31
9	i	85	THR	N-CA-C	8.37	120.40	111.28
20	Z	206	ASP	N-CA-C	8.36	120.31	111.03
22	S	287	SER	CA-C-O	8.36	129.60	120.82
33	J	359	LYS	CA-C-N	8.36	130.59	120.14
33	J	359	LYS	C-N-CA	8.36	130.59	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	112	ASP	N-CA-C	8.36	121.14	111.11
12	5	193	ASP	N-CA-C	-8.35	103.11	113.38
16	V	111	HIS	CA-CB-CG	8.35	122.15	113.80
16	V	68	VAL	O-C-N	-8.34	113.69	122.95
33	J	393	ASN	CA-CB-CG	-8.33	104.27	112.60
3	c	114	ARG	CA-C-N	8.33	131.44	120.28
3	c	114	ARG	C-N-CA	8.33	131.44	120.28
28	H	448	ASP	N-CA-C	8.33	120.36	111.28
24	Q	91	SER	N-CA-C	-8.33	102.14	112.88
12	5	104	GLN	N-CA-C	-8.32	102.90	113.72
1	a	219	SER	N-CA-C	-8.32	97.97	109.95
8	h	190	ALA	N-CA-C	8.32	120.35	111.28
33	J	251	ASP	N-CA-CB	8.32	124.55	110.49
21	N	408	LEU	CA-C-O	-8.30	111.62	120.42
32	M	352	PRO	CA-C-O	-8.30	111.94	121.56
5	e	51	GLU	N-CA-C	-8.29	95.22	108.73
11	k	5	LEU	CA-C-N	8.29	127.99	121.61
11	k	5	LEU	C-N-CA	8.29	127.99	121.61
31	L	422	VAL	CA-C-O	-8.28	112.07	120.85
2	b	168	SER	CA-C-N	8.28	131.80	120.46
2	b	168	SER	C-N-CA	8.28	131.80	120.46
29	I	187	LEU	CA-C-N	8.28	131.20	120.44
29	I	187	LEU	C-N-CA	8.28	131.20	120.44
28	H	450	VAL	N-CA-C	8.28	119.08	110.72
14	n	141	ASN	CA-C-N	8.27	129.79	120.85
14	n	141	ASN	C-N-CA	8.27	129.79	120.85
30	K	322	ASP	CA-CB-CG	8.27	120.87	112.60
15	W	107	HIS	CA-CB-CG	-8.26	105.55	113.80
14	7	136	ARG	N-CA-C	-8.24	102.68	112.89
16	V	138	ALA	N-CA-C	-8.24	94.84	108.76
25	R	382	ASP	CA-CB-CG	-8.23	104.36	112.60
29	I	387	LEU	N-CA-CB	8.23	124.13	111.46
1	a	147	ASP	N-CA-C	-8.22	98.11	109.95
11	4	77	PRO	CA-C-N	8.22	131.13	120.44
11	4	77	PRO	C-N-CA	8.22	131.13	120.44
24	Q	276	ASP	CA-CB-CG	-8.22	104.38	112.60
1	a	124	LEU	CA-C-O	-8.22	111.84	120.55
22	S	202	ASN	OD1-CG-ND2	8.21	130.81	122.60
12	l	115	PHE	CA-CB-CG	-8.20	105.60	113.80
33	J	237	ALA	CA-C-N	8.20	131.26	120.28
33	J	237	ALA	C-N-CA	8.20	131.26	120.28
19	Y	87	GLU	N-CA-C	8.19	120.21	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	127	LYS	CA-C-N	8.19	127.88	120.10
13	6	127	LYS	C-N-CA	8.19	127.88	120.10
23	P	158	ASP	CA-CB-CG	8.18	120.78	112.60
19	Y	87	GLU	CA-C-O	8.18	129.22	120.55
23	P	425	HIS	CA-CB-CG	8.17	121.97	113.80
17	T	74	ASN	CA-C-N	8.17	131.23	120.28
17	T	74	ASN	C-N-CA	8.17	131.23	120.28
9	2	122	HIS	CG-CD2-NE2	8.16	115.36	107.20
21	N	17	GLN	N-CA-C	-8.16	93.41	110.80
22	S	184	TRP	CB-CG-CD1	8.16	139.14	126.90
22	S	488	GLN	CA-C-N	8.16	134.93	121.39
22	S	488	GLN	C-N-CA	8.16	134.93	121.39
29	I	431	ASN	N-CA-C	-8.15	102.89	112.92
14	n	259	LYS	N-CA-C	-8.14	97.62	109.18
20	Z	206	ASP	CA-CB-CG	-8.14	104.46	112.60
22	S	333	PHE	N-CA-C	8.14	120.23	111.36
27	O	298	GLU	CA-C-O	-8.13	112.32	120.70
20	Z	213	LYS	N-CA-CB	-8.13	98.13	110.16
24	Q	309	ARG	N-CA-CB	8.13	124.23	110.49
12	5	272	PHE	CA-CB-CG	-8.12	105.68	113.80
12	l	227	ASP	CA-CB-CG	8.12	120.72	112.60
21	N	27	SER	CA-C-N	8.12	131.58	120.46
21	N	27	SER	C-N-CA	8.12	131.58	120.46
27	O	193	LEU	CA-C-N	8.12	131.82	120.29
27	O	193	LEU	C-N-CA	8.12	131.82	120.29
32	M	151	ASP	CA-CB-CG	-8.12	104.48	112.60
29	I	350	PHE	CA-CB-CG	-8.11	105.69	113.80
17	T	19	ASP	CA-CB-CG	8.11	120.71	112.60
25	R	146	ASP	N-CA-C	-8.10	93.60	108.02
3	c	61	THR	N-CA-C	-8.10	101.09	113.89
2	b	208	THR	N-CA-C	-8.10	104.28	114.56
13	6	198	SER	N-CA-C	-8.10	102.54	111.36
27	O	236	HIS	CA-C-N	8.09	128.55	119.32
27	O	236	HIS	C-N-CA	8.09	128.55	119.32
12	5	148	ARG	CA-C-N	8.09	132.50	120.69
12	5	148	ARG	C-N-CA	8.09	132.50	120.69
20	Z	738	TYR	CE1-CZ-CE2	-8.09	104.12	120.30
11	4	112	ASN	CA-CB-CG	-8.09	104.51	112.60
31	L	91	THR	N-CA-CB	8.09	122.13	110.16
33	J	54	LYS	N-CA-C	8.09	119.72	111.07
6	f	78	ALA	CA-C-O	-8.08	109.09	120.16
7	g	165	THR	N-CA-C	-8.07	96.44	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	124	LEU	CA-C-N	8.07	131.09	120.28
1	a	124	LEU	C-N-CA	8.07	131.09	120.28
10	j	176	ASP	CA-CB-CG	-8.06	104.54	112.60
33	J	83	LYS	N-CA-C	-8.06	97.07	109.24
7	g	149	TYR	CB-CG-CD1	-8.05	108.72	120.80
12	5	163	TYR	CA-C-N	8.05	131.07	120.28
12	5	163	TYR	C-N-CA	8.05	131.07	120.28
5	e	84	ASP	CA-CB-CG	-8.05	104.55	112.60
22	S	179	ILE	CB-CA-C	-8.05	101.45	112.24
1	a	151	GLY	CA-C-N	8.05	128.54	119.93
1	a	151	GLY	C-N-CA	8.05	128.54	119.93
29	I	94	LYS	N-CA-C	8.05	119.68	111.07
14	n	68	ARG	N-CA-C	-8.03	103.61	113.41
12	5	125	ALA	CA-C-N	8.03	132.52	120.31
12	5	125	ALA	C-N-CA	8.03	132.52	120.31
22	S	199	GLU	CA-C-O	8.04	128.90	120.30
6	f	186	PRO	CA-C-N	8.03	131.04	120.28
6	f	186	PRO	C-N-CA	8.03	131.04	120.28
23	P	144	VAL	CA-C-N	8.03	131.04	120.28
23	P	144	VAL	C-N-CA	8.03	131.04	120.28
9	2	247	VAL	N-CA-C	-8.03	96.45	108.17
16	V	181	ASN	CB-CG-ND2	8.03	128.44	116.40
17	T	110	LEU	CA-C-N	8.03	131.38	120.38
17	T	110	LEU	C-N-CA	8.03	131.38	120.38
30	K	191	PRO	CA-C-N	8.02	131.68	120.29
30	K	191	PRO	C-N-CA	8.02	131.68	120.29
1	a	231	ASP	CA-CB-CG	-8.01	104.59	112.60
8	h	50	ILE	CA-C-O	8.01	128.16	120.31
25	R	94	PHE	N-CA-C	8.01	120.66	110.33
24	Q	397	LEU	N-CA-C	-8.00	95.23	108.76
7	g	144	ASN	CA-CB-CG	-8.00	104.60	112.60
31	L	290	ARG	NE-CZ-NH1	-8.00	113.50	121.50
33	J	306	ARG	CA-C-O	-7.99	111.99	120.70
13	6	143	GLN	N-CA-C	-7.99	104.42	114.56
29	I	335	ASP	O-C-N	-7.99	115.24	121.47
32	M	42	ARG	NE-CZ-NH2	-7.98	112.02	119.20
3	c	100	LYS	O-C-N	-7.97	113.06	122.15
8	1	156	SER	CA-C-N	7.97	130.97	120.28
8	1	156	SER	C-N-CA	7.97	130.97	120.28
28	H	293	GLU	N-CA-C	7.97	119.75	111.14
11	k	64	ILE	CA-C-N	7.97	132.42	120.31
11	k	64	ILE	C-N-CA	7.97	132.42	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	230	ASP	CA-CB-CG	7.96	120.56	112.60
20	Z	728	LYS	CD-CE-NZ	7.96	137.38	111.90
10	3	173	ASN	CA-CB-CG	-7.96	104.64	112.60
15	W	174	VAL	N-CA-C	-7.96	96.66	108.12
15	W	180	LEU	CA-C-N	7.95	130.93	120.28
15	W	180	LEU	C-N-CA	7.95	130.93	120.28
20	Z	248	TYR	N-CA-C	-7.95	102.70	111.36
24	Q	372	GLN	O-C-N	7.95	130.25	122.07
29	I	416	PHE	CA-CB-CG	-7.94	105.86	113.80
27	O	199	LEU	CA-C-N	7.94	132.75	120.60
27	O	199	LEU	C-N-CA	7.94	132.75	120.60
20	Z	255	LEU	CB-CG-CD2	7.94	134.51	110.70
3	c	186	VAL	CA-C-N	7.93	130.75	120.44
3	c	186	VAL	C-N-CA	7.93	130.75	120.44
12	l	183	GLU	CB-CG-CD	-7.93	99.12	112.60
9	i	238	THR	N-CA-C	-7.93	103.06	112.89
12	5	164	GLN	CA-C-O	-7.93	112.15	120.55
8	1	140	SER	CA-C-N	7.92	130.74	120.44
8	1	140	SER	C-N-CA	7.92	130.74	120.44
21	N	547	LEU	CA-C-O	-7.92	110.86	119.97
12	5	233	LYS	CA-C-N	7.92	130.90	120.28
12	5	233	LYS	C-N-CA	7.92	130.90	120.28
10	j	137	ILE	N-CA-C	-7.92	96.61	108.17
27	O	148	ASP	CA-C-N	7.90	131.51	120.29
27	O	148	ASP	C-N-CA	7.90	131.51	120.29
30	K	255	ARG	N-CA-C	7.90	121.86	111.75
21	N	767	ALA	CA-C-O	-7.90	112.47	121.40
24	Q	401	GLU	N-CA-C	-7.90	102.15	113.21
13	m	103	HIS	CB-CG-CD2	-7.89	120.94	131.20
30	K	354	GLY	CA-C-N	7.89	130.85	120.28
30	K	354	GLY	C-N-CA	7.89	130.85	120.28
20	Z	727	GLU	N-CA-C	7.88	127.59	110.80
14	7	246	GLN	OE1-CD-NE2	7.88	130.48	122.60
14	n	145	ASN	CA-CB-CG	-7.88	104.72	112.60
23	P	380	ILE	N-CA-C	-7.88	102.76	110.72
25	R	217	HIS	ND1-CE1-NE2	7.88	116.28	108.40
27	O	236	HIS	CA-C-O	-7.88	110.99	120.05
32	M	349	PHE	CA-CB-CG	-7.87	105.93	113.80
31	L	62	ARG	CA-C-N	7.87	130.83	120.28
31	L	62	ARG	C-N-CA	7.87	130.83	120.28
25	R	63	TYR	CA-C-N	7.87	130.83	120.28
25	R	63	TYR	C-N-CA	7.87	130.83	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	69	GLY	N-CA-C	-7.87	105.02	115.32
13	m	163	ASN	CA-CB-CG	-7.86	104.74	112.60
29	I	344	ILE	N-CA-C	-7.86	105.53	113.47
12	5	227	ASP	CA-C-N	7.86	131.45	120.29
12	5	227	ASP	C-N-CA	7.86	131.45	120.29
21	N	135	SER	CA-C-N	7.86	130.46	120.56
21	N	135	SER	C-N-CA	7.86	130.46	120.56
15	W	115	CYS	N-CA-C	-7.85	103.53	113.43
30	K	377	SER	CB-CA-C	-7.85	99.03	109.16
23	P	140	THR	N-CA-C	-7.85	102.72	111.28
10	3	11	ILE	O-C-N	-7.84	114.33	123.04
23	P	336	HIS	ND1-CE1-NE2	7.84	116.24	108.40
5	e	9	ASP	N-CA-C	-7.84	102.73	114.64
7	g	207	ASN	N-CA-C	-7.84	101.16	110.41
29	I	208	TYR	CA-C-N	7.83	130.62	120.44
29	I	208	TYR	C-N-CA	7.83	130.62	120.44
12	5	188	TYR	N-CA-C	-7.83	97.12	109.50
21	N	767	ALA	CA-C-N	-7.83	116.95	122.59
21	N	767	ALA	C-N-CA	-7.83	116.95	122.59
16	V	184	ASN	OD1-CG-ND2	7.83	130.43	122.60
23	P	117	SER	CA-C-O	-7.83	112.12	120.42
4	d	230	ASN	N-CA-CB	7.82	121.61	110.12
9	i	69	LYS	N-CA-C	-7.82	102.82	113.30
20	Z	951	GLN	N-CA-CB	7.82	124.09	111.74
30	K	306	PHE	N-CA-CB	7.82	123.70	110.49
4	d	230	ASN	CB-CA-C	-7.81	97.82	110.79
8	1	78	GLN	N-CA-C	-7.81	102.72	112.72
23	P	238	ALA	CA-C-N	7.81	130.74	120.28
23	P	238	ALA	C-N-CA	7.81	130.74	120.28
24	Q	163	ARG	N-CA-C	7.81	119.57	111.14
2	b	35	LEU	CA-C-O	-7.80	113.10	121.45
12	5	231	LEU	CA-C-N	7.80	128.60	119.94
12	5	231	LEU	C-N-CA	7.80	128.60	119.94
31	L	78	ARG	NE-CZ-NH1	-7.80	113.70	121.50
30	K	234	PHE	CA-CB-CG	7.80	121.60	113.80
17	T	259	ILE	CA-C-N	7.80	131.49	120.42
17	T	259	ILE	C-N-CA	7.80	131.49	120.42
31	L	55	LYS	N-CA-C	7.79	119.85	111.36
9	i	148	THR	CA-CB-OG1	7.79	121.28	109.60
20	Z	728	LYS	N-CA-C	-7.79	94.21	110.80
21	N	545	SER	CA-C-N	7.79	130.56	120.44
21	N	545	SER	C-N-CA	7.79	130.56	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	736	LEU	N-CA-CB	-7.79	98.68	110.12
24	Q	365	ILE	N-CA-CB	-7.79	100.60	110.57
13	m	134	ASP	N-CA-C	-7.78	99.93	110.36
28	H	128	ASN	CA-CB-CG	7.78	120.38	112.60
21	N	654	GLN	CA-C-N	7.78	130.70	120.28
21	N	654	GLN	C-N-CA	7.78	130.70	120.28
23	P	223	LEU	N-CA-CB	7.78	121.67	110.16
27	O	40	GLN	OE1-CD-NE2	-7.78	114.82	122.60
29	I	151	HIS	N-CA-C	7.78	120.44	111.11
16	V	161	THR	N-CA-C	7.77	119.75	111.28
7	g	80	GLY	N-CA-C	-7.77	103.13	111.21
6	f	104	ALA	CA-C-N	7.77	130.35	120.56
6	f	104	ALA	C-N-CA	7.77	130.35	120.56
21	N	731	VAL	CA-C-O	-7.77	112.61	120.85
12	5	99	ASN	OD1-CG-ND2	7.77	130.37	122.60
2	b	166	LYS	N-CA-C	7.76	122.33	113.01
30	K	373	ILE	CA-C-N	7.76	131.31	120.29
30	K	373	ILE	C-N-CA	7.76	131.31	120.29
11	k	146	HIS	CB-CG-CD2	-7.75	121.12	131.20
27	O	355	PRO	CA-C-O	-7.75	112.87	121.32
28	H	169	GLU	CA-C-N	7.75	131.79	120.95
28	H	169	GLU	C-N-CA	7.75	131.79	120.95
9	2	102	GLU	O-C-N	-7.75	113.01	121.53
15	W	47	ASN	CA-C-O	7.75	129.83	121.16
27	O	122	HIS	CA-CB-CG	-7.75	106.06	113.80
6	F	13	PHE	CA-C-N	7.74	135.64	121.70
6	F	13	PHE	C-N-CA	7.74	135.64	121.70
21	N	661	SER	CA-C-O	-7.74	111.07	119.97
14	n	194	ARG	CA-C-N	7.74	132.98	120.60
14	n	194	ARG	C-N-CA	7.74	132.98	120.60
22	S	206	GLN	OE1-CD-NE2	7.74	130.34	122.60
23	P	333	ALA	N-CA-C	-7.73	103.57	113.16
21	N	254	SER	N-CA-C	7.73	119.78	111.36
32	M	193	LEU	CA-C-N	7.73	130.29	120.56
32	M	193	LEU	C-N-CA	7.73	130.29	120.56
21	N	352	ASN	CA-CB-CG	-7.72	104.88	112.60
8	h	81	THR	O-C-N	-7.72	113.78	121.27
25	R	136	ASN	CA-CB-CG	-7.72	104.88	112.60
28	H	281	GLN	N-CA-CB	7.72	121.91	110.49
23	P	55	SER	CA-C-N	7.71	131.24	120.29
23	P	55	SER	C-N-CA	7.71	131.24	120.29
11	4	107	TYR	CA-C-O	7.71	128.71	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	244	GLU	O-C-N	7.71	130.93	122.15
12	5	168	ALA	N-CA-C	-7.70	103.91	113.38
32	M	163	PHE	CA-CB-CG	-7.70	106.10	113.80
10	j	172	LEU	N-CA-CB	7.70	121.18	110.01
26	U	284	SER	CA-C-N	7.70	131.01	120.46
26	U	284	SER	C-N-CA	7.70	131.01	120.46
22	S	110	LEU	N-CA-C	-7.70	96.84	108.46
4	d	112	TYR	CA-C-O	-7.69	112.78	120.70
25	R	116	LYS	O-C-N	-7.69	114.15	122.07
22	S	164	ILE	N-CA-CB	7.68	116.44	110.45
22	S	440	ASP	CA-CB-CG	-7.68	104.92	112.60
8	h	169	SER	N-CA-CB	7.68	121.15	110.01
11	4	117	TYR	CA-CB-CG	-7.68	100.07	113.90
27	O	240	GLU	N-CA-C	7.68	119.29	111.07
24	Q	54	GLN	CA-C-N	7.68	130.57	120.28
24	Q	54	GLN	C-N-CA	7.68	130.57	120.28
12	l	141	HIS	CA-C-N	7.67	131.19	120.29
12	l	141	HIS	C-N-CA	7.67	131.19	120.29
16	V	233	LYS	CA-C-O	7.67	128.76	120.24
25	R	266	LEU	CA-C-O	7.67	128.87	120.82
33	J	15	HIS	CA-CB-CG	7.67	121.47	113.80
21	N	743	PHE	CA-C-O	-7.66	111.22	118.73
16	V	159	ILE	O-C-N	-7.66	115.33	123.14
22	S	357	LEU	CA-C-N	7.66	131.16	120.29
22	S	357	LEU	C-N-CA	7.66	131.16	120.29
30	K	245	LYS	N-CA-C	-7.66	101.89	112.30
30	K	174	VAL	CA-C-N	7.66	136.42	121.41
30	K	174	VAL	C-N-CA	7.66	136.42	121.41
4	d	34	VAL	N-CA-C	-7.65	97.46	108.48
27	O	191	THR	CA-C-O	-7.65	112.31	120.42
31	L	195	GLU	CA-C-O	-7.65	112.31	120.42
25	R	357	PHE	CA-CB-CG	-7.65	106.15	113.80
22	S	389	LYS	O-C-N	7.64	129.94	122.07
31	L	320	GLN	CA-C-N	7.64	135.89	122.67
31	L	320	GLN	C-N-CA	7.64	135.89	122.67
22	S	208	ILE	CB-CA-C	-7.64	102.01	112.02
32	M	328	ASN	N-CA-C	-7.64	102.52	112.68
21	N	230	VAL	N-CA-C	7.64	118.41	110.62
32	M	72	ASN	CA-C-O	-7.63	112.46	120.55
19	Y	32	ASP	CA-CB-CG	-7.63	104.97	112.60
21	N	347	SER	N-CA-C	7.63	119.60	111.28
33	J	277	ASN	CA-C-N	7.63	131.91	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	J	277	ASN	C-N-CA	7.63	131.91	120.31
2	b	194	LEU	CA-C-N	7.63	131.12	120.29
2	b	194	LEU	C-N-CA	7.63	131.12	120.29
2	b	80	PRO	N-CA-CB	7.63	111.95	103.26
16	V	300	VAL	CB-CA-C	7.63	122.75	112.22
22	S	74	LEU	CA-C-N	7.63	130.50	120.28
22	S	74	LEU	C-N-CA	7.63	130.50	120.28
29	I	265	ARG	CA-C-N	7.62	130.50	120.28
29	I	265	ARG	C-N-CA	7.62	130.50	120.28
18	X	58	GLY	CA-C-N	7.62	132.75	122.84
18	X	58	GLY	C-N-CA	7.62	132.75	122.84
33	J	15	HIS	CE1-NE2-CD2	-7.62	101.38	109.00
27	O	342	ASP	CA-CB-CG	-7.62	104.98	112.60
13	6	40	ASP	CA-CB-CG	-7.62	104.98	112.60
18	X	22	ARG	N-CA-CB	7.61	123.36	110.49
17	T	100	ASP	CA-C-N	7.61	133.43	120.72
17	T	100	ASP	C-N-CA	7.61	133.43	120.72
14	7	212	ASN	CA-C-N	7.61	130.33	120.44
14	7	212	ASN	C-N-CA	7.61	130.33	120.44
21	N	912	GLU	CA-C-N	7.61	128.80	119.98
21	N	912	GLU	C-N-CA	7.61	128.80	119.98
33	J	131	ASP	CA-C-N	7.60	127.25	119.19
33	J	131	ASP	C-N-CA	7.60	127.25	119.19
16	V	109	HIS	CA-CB-CG	7.60	121.40	113.80
32	M	108	LEU	N-CA-C	-7.60	103.37	114.39
8	1	118	GLU	CA-C-O	-7.60	112.48	120.99
17	T	97	SER	N-CA-CB	7.59	123.31	110.49
13	m	143	GLN	N-CA-C	-7.58	104.18	113.50
27	O	26	PHE	CA-CB-CG	-7.58	106.22	113.80
26	U	234	ASN	CA-CB-CG	7.58	120.18	112.60
1	a	177	GLU	CA-C-O	-7.58	112.39	120.42
9	i	203	ASP	N-CA-C	-7.58	98.40	110.14
30	K	76	LYS	N-CA-C	-7.57	103.10	111.36
9	2	145	HIS	N-CA-C	-7.57	104.19	113.50
18	X	90	VAL	N-CA-C	-7.57	97.43	108.71
33	J	260	GLY	CA-C-N	7.57	136.00	121.54
33	J	260	GLY	C-N-CA	7.57	136.00	121.54
32	M	149	ASN	CA-CB-CG	-7.57	105.03	112.60
1	a	211	ILE	N-CA-C	-7.56	103.08	110.72
7	g	39	GLY	CA-C-N	7.56	132.95	123.12
7	g	39	GLY	C-N-CA	7.56	132.95	123.12
21	N	657	MET	CA-C-O	7.56	128.56	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	20	PHE	CA-CB-CG	-7.55	106.25	113.80
5	E	15	PHE	CA-C-N	7.55	135.30	121.70
5	E	15	PHE	C-N-CA	7.55	135.30	121.70
21	N	17	GLN	CA-C-N	7.55	130.26	120.44
21	N	17	GLN	C-N-CA	7.55	130.26	120.44
15	W	69	PHE	CA-C-O	7.55	128.67	119.38
28	H	62	ARG	NE-CZ-NH2	-7.55	112.40	119.20
32	M	214	ALA	CA-C-N	7.55	129.28	119.84
32	M	214	ALA	C-N-CA	7.55	129.28	119.84
12	l	142	GLU	N-CA-C	-7.55	103.13	111.36
21	N	177	ASP	N-CA-C	-7.55	102.98	111.14
9	i	59	ASN	OD1-CG-ND2	-7.55	115.05	122.60
21	N	883	SER	CA-C-N	7.55	131.52	120.95
21	N	883	SER	C-N-CA	7.55	131.52	120.95
25	R	328	PHE	CA-CB-CG	-7.55	106.25	113.80
25	R	399	GLN	CA-C-N	7.55	130.40	120.28
25	R	399	GLN	C-N-CA	7.55	130.40	120.28
33	J	306	ARG	N-CA-C	7.55	120.50	110.08
14	n	111	ASN	CA-CB-CG	-7.54	105.06	112.60
16	V	145	GLN	O-C-N	7.54	132.60	122.49
14	n	220	ARG	NE-CZ-NH1	7.54	129.04	121.50
22	S	69	LEU	N-CA-CB	7.54	123.23	110.49
14	n	36	GLN	CA-C-N	7.54	128.00	119.93
14	n	36	GLN	C-N-CA	7.54	128.00	119.93
12	l	195	THR	CA-CB-OG1	7.53	120.90	109.60
11	4	62	ALA	N-CA-C	7.53	119.13	111.07
21	N	860	LYS	N-CA-C	-7.53	102.06	112.30
27	O	73	ILE	N-CA-C	-7.53	97.46	108.23
17	T	42	PRO	CA-C-N	7.53	132.81	122.34
17	T	42	PRO	C-N-CA	7.53	132.81	122.34
28	H	274	VAL	N-CA-C	-7.53	97.24	108.46
20	Z	255	LEU	CB-CA-C	7.53	125.40	110.42
9	i	226	GLU	N-CA-CB	7.53	121.01	110.17
9	i	95	HIS	ND1-CE1-NE2	7.52	115.92	108.40
21	N	639	ASP	CA-CB-CG	-7.52	105.08	112.60
28	H	204	PRO	N-CA-C	-7.52	96.98	112.47
7	g	242	PHE	CA-CB-CG	-7.52	106.28	113.80
27	O	217	LEU	CA-C-N	7.52	130.21	120.44
27	O	217	LEU	C-N-CA	7.52	130.21	120.44
26	U	143	VAL	N-CA-CB	7.51	119.37	110.95
32	M	406	GLY	N-CA-C	-7.51	104.37	115.72
21	N	249	ASN	CA-CB-CG	-7.51	105.09	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	123	HIS	CE1-NE2-CD2	-7.51	101.49	109.00
9	i	95	HIS	CE1-NE2-CD2	-7.51	101.49	109.00
17	T	150	ARG	CA-C-N	7.51	133.42	120.58
17	T	150	ARG	C-N-CA	7.51	133.42	120.58
25	R	91	TRP	N-CA-C	-7.51	103.24	113.30
21	N	184	LYS	CA-C-N	7.51	131.08	120.42
21	N	184	LYS	C-N-CA	7.51	131.08	120.42
7	g	79	SER	CA-C-N	7.50	130.36	122.63
7	g	79	SER	C-N-CA	7.50	130.36	122.63
20	Z	946	THR	N-CA-C	-7.50	96.29	108.52
24	Q	20	TYR	CA-C-N	7.50	130.34	120.28
24	Q	20	TYR	C-N-CA	7.50	130.34	120.28
3	c	91	ALA	CA-C-N	7.50	130.19	120.44
3	c	91	ALA	C-N-CA	7.50	130.19	120.44
13	6	224	PHE	N-CA-C	-7.50	96.67	108.90
22	S	303	ASN	CA-CB-CG	-7.50	105.10	112.60
1	a	209	HIS	CE1-NE2-CD2	-7.50	101.50	109.00
30	K	233	ALA	CB-CA-C	-7.50	96.37	109.64
16	V	186	GLN	CA-C-N	7.50	130.32	120.28
16	V	186	GLN	C-N-CA	7.50	130.32	120.28
26	U	267	VAL	N-CA-C	-7.49	103.15	110.72
24	Q	328	ASP	CA-C-N	7.49	130.32	120.28
24	Q	328	ASP	C-N-CA	7.49	130.32	120.28
25	R	29	LYS	CA-C-N	7.49	130.32	120.28
25	R	29	LYS	C-N-CA	7.49	130.32	120.28
18	X	107	GLY	N-CA-C	-7.49	103.91	111.85
29	I	253	ILE	N-CA-CB	7.49	119.97	110.99
30	K	306	PHE	N-CA-C	-7.49	94.86	110.80
17	T	133	ILE	N-CA-C	-7.48	105.91	113.47
24	Q	171	LYS	CA-C-N	7.48	127.12	119.19
24	Q	171	LYS	C-N-CA	7.48	127.12	119.19
14	7	109	TYR	N-CA-CB	7.48	121.23	109.71
17	T	118	ASN	CB-CA-C	-7.48	99.65	111.17
24	Q	404	ASN	N-CA-C	-7.48	103.23	112.88
33	J	298	ASP	N-CA-C	-7.47	102.06	112.45
1	a	148	GLU	N-CA-C	-7.47	102.70	112.41
30	K	190	LEU	N-CA-CB	7.47	119.24	110.42
33	J	257	ARG	CA-C-N	7.47	130.69	120.46
33	J	257	ARG	C-N-CA	7.47	130.69	120.46
23	P	198	VAL	CA-C-O	-7.47	113.25	121.17
30	K	140	HIS	N-CA-CB	7.46	120.92	110.17
9	2	252	ILE	CA-C-N	7.46	131.72	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	252	ILE	C-N-CA	7.46	131.72	121.05
26	U	70	HIS	CE1-NE2-CD2	-7.46	101.54	109.00
12	l	170	LEU	N-CA-C	-7.46	97.74	109.07
21	N	672	ASN	CA-CB-CG	-7.46	105.14	112.60
25	R	216	ILE	CB-CA-C	-7.45	101.94	112.22
22	S	215	MET	CA-C-N	7.45	130.12	120.44
22	S	215	MET	C-N-CA	7.45	130.12	120.44
21	N	191	THR	CA-C-N	7.45	130.12	120.44
21	N	191	THR	C-N-CA	7.45	130.12	120.44
4	d	70	HIS	CE1-NE2-CD2	-7.45	101.56	109.00
17	T	186	ARG	CA-C-N	7.45	130.56	120.44
17	T	186	ARG	C-N-CA	7.45	130.56	120.44
20	Z	249	MET	CA-C-O	-7.44	112.53	120.42
26	U	303	GLU	N-CA-C	7.44	119.03	111.07
13	m	169	GLU	N-CA-C	-7.44	100.39	109.83
23	P	137	ALA	CA-C-N	7.44	130.11	120.44
23	P	137	ALA	C-N-CA	7.44	130.11	120.44
10	j	126	LEU	CA-C-N	7.44	131.37	120.74
10	j	126	LEU	C-N-CA	7.44	131.37	120.74
21	N	297	ASP	CA-C-N	7.43	130.24	120.28
21	N	297	ASP	C-N-CA	7.43	130.24	120.28
21	N	800	ALA	N-CA-C	7.43	119.38	111.28
24	Q	208	ILE	N-CA-C	-7.43	105.11	112.17
31	L	305	LEU	CA-C-N	7.43	131.60	120.31
31	L	305	LEU	C-N-CA	7.43	131.60	120.31
7	g	206	ASP	N-CA-C	-7.43	102.15	113.89
8	1	203	GLU	CA-C-N	7.43	130.54	120.44
8	1	203	GLU	C-N-CA	7.43	130.54	120.44
17	T	245	TYR	N-CA-CB	7.43	121.04	110.12
10	j	199	TYR	O-C-N	7.42	131.62	122.86
12	5	198	LYS	N-CA-CB	7.42	121.57	110.29
17	T	254	ASP	CA-C-N	7.42	130.54	120.44
17	T	254	ASP	C-N-CA	7.42	130.54	120.44
21	N	210	SER	CA-C-N	7.42	130.23	120.28
21	N	210	SER	C-N-CA	7.42	130.23	120.28
9	i	114	GLN	CA-C-N	7.42	130.09	120.44
9	i	114	GLN	C-N-CA	7.42	130.09	120.44
14	n	78	VAL	CA-C-O	7.42	128.30	120.51
10	3	36	VAL	N-CA-C	-7.42	104.55	111.45
9	2	62	LYS	CA-C-O	-7.42	112.75	120.32
1	a	209	HIS	ND1-CE1-NE2	7.42	115.82	108.40
11	4	34	LYS	CA-C-O	7.42	127.89	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	140	HIS	CB-CG-CD2	-7.42	121.56	131.20
4	d	123	SER	O-C-N	-7.42	114.33	122.79
33	J	310	ILE	CA-C-N	7.42	131.36	120.90
33	J	310	ILE	C-N-CA	7.42	131.36	120.90
8	h	197	PHE	CA-CB-CG	-7.42	106.39	113.80
9	2	67	SER	CA-C-O	-7.41	113.68	120.50
25	R	38	VAL	CA-C-N	7.41	131.24	120.71
25	R	38	VAL	C-N-CA	7.41	131.24	120.71
14	7	198	ILE	CB-CA-C	-7.41	106.49	114.35
24	Q	178	HIS	CE1-NE2-CD2	-7.41	101.59	109.00
4	d	80	ALA	CA-C-N	7.41	131.57	120.31
4	d	80	ALA	C-N-CA	7.41	131.57	120.31
17	T	176	SER	N-CA-C	-7.41	103.70	112.89
31	L	208	GLN	CA-C-N	7.41	130.07	120.44
31	L	208	GLN	C-N-CA	7.41	130.07	120.44
23	P	288	ASN	CA-CB-CG	-7.41	105.19	112.60
5	e	71	ASP	N-CA-C	-7.41	98.38	108.38
8	h	14	ALA	N-CA-C	-7.41	97.36	108.99
21	N	118	THR	CA-C-O	-7.41	111.45	119.97
16	V	153	ILE	N-CA-C	-7.40	96.75	107.78
21	N	682	PHE	CB-CA-C	-7.40	98.27	110.85
24	Q	287	THR	N-CA-CB	7.40	121.37	110.56
3	c	22	VAL	N-CA-C	-7.40	103.25	110.72
27	O	74	ASN	CA-C-N	7.39	130.79	120.29
27	O	74	ASN	C-N-CA	7.39	130.79	120.29
23	P	130	ILE	CA-C-N	7.39	133.06	120.72
23	P	130	ILE	C-N-CA	7.39	133.06	120.72
12	5	212	TYR	N-CA-CB	7.39	120.95	109.94
29	I	294	SER	N-CA-C	-7.39	102.01	113.02
28	H	401	GLY	N-CA-C	-7.39	104.86	115.64
9	i	165	ALA	CA-C-N	7.38	130.01	120.56
9	i	165	ALA	C-N-CA	7.38	130.01	120.56
33	J	211	ILE	N-CA-C	-7.38	102.96	113.07
3	c	240	VAL	CA-C-N	7.38	130.04	120.44
3	c	240	VAL	C-N-CA	7.38	130.04	120.44
31	L	429	GLU	CA-C-N	7.38	127.01	119.92
31	L	429	GLU	C-N-CA	7.38	127.01	119.92
3	c	191	GLU	CA-C-O	7.38	128.24	120.42
28	H	187	LEU	CA-C-N	7.38	127.98	120.38
28	H	187	LEU	C-N-CA	7.38	127.98	120.38
21	N	533	ASP	CA-C-N	7.38	130.03	120.44
21	N	533	ASP	C-N-CA	7.38	130.03	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	150	LYS	CA-C-O	7.38	129.03	120.32
9	i	88	ILE	CA-C-N	7.38	128.13	119.94
9	i	88	ILE	C-N-CA	7.38	128.13	119.94
2	b	78	MET	CA-C-N	7.37	133.45	121.87
2	b	78	MET	C-N-CA	7.37	133.45	121.87
7	g	157	TYR	O-C-N	-7.37	114.85	123.25
7	g	228	HIS	CE1-NE2-CD2	-7.37	101.63	109.00
30	K	282	PHE	CA-CB-CG	-7.37	106.43	113.80
3	c	186	VAL	N-CA-C	7.37	118.14	110.62
27	O	293	LEU	CA-C-N	7.37	130.75	120.29
27	O	293	LEU	C-N-CA	7.37	130.75	120.29
3	c	128	LEU	N-CA-CB	7.37	120.87	110.04
12	l	208	GLN	OE1-CD-NE2	-7.37	115.23	122.60
3	c	3	SER	N-CA-C	-7.36	104.16	113.43
28	H	211	VAL	N-CA-CB	7.36	119.82	110.99
26	U	21	HIS	CA-C-N	7.36	130.74	120.29
26	U	21	HIS	C-N-CA	7.36	130.74	120.29
31	L	179	THR	CA-C-N	7.36	133.00	120.72
31	L	179	THR	C-N-CA	7.36	133.00	120.72
20	Z	728	LYS	CB-CG-CD	7.35	128.21	111.30
25	R	105	LYS	CA-C-N	7.35	130.47	120.54
25	R	105	LYS	C-N-CA	7.35	130.47	120.54
28	H	300	THR	CB-CA-C	-7.35	99.34	110.88
14	n	74	ARG	N-CA-CB	7.35	121.46	110.65
25	R	149	ASN	N-CA-C	-7.35	103.78	112.89
28	H	232	PRO	CA-C-N	7.35	130.13	120.28
28	H	232	PRO	C-N-CA	7.35	130.13	120.28
32	M	164	ASP	CA-C-N	7.35	130.86	120.28
32	M	164	ASP	C-N-CA	7.35	130.86	120.28
2	b	104	TYR	CB-CA-C	7.35	119.23	108.87
21	N	129	ILE	N-CA-C	-7.34	97.67	108.54
31	L	195	GLU	CA-C-N	7.34	129.96	120.56
31	L	195	GLU	C-N-CA	7.34	129.96	120.56
6	f	113	CYS	N-CA-C	-7.34	103.21	111.07
22	S	330	LEU	CA-C-N	7.34	130.85	120.28
22	S	330	LEU	C-N-CA	7.34	130.85	120.28
33	J	382	PHE	CA-C-N	7.34	130.12	120.28
33	J	382	PHE	C-N-CA	7.34	130.12	120.28
12	l	141	HIS	CB-CG-CD2	-7.34	121.66	131.20
4	d	20	VAL	N-CA-C	-7.34	103.80	111.58
17	T	265	ASP	CA-C-N	7.34	130.11	120.28
17	T	265	ASP	C-N-CA	7.34	130.11	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	290	THR	N-CA-C	-7.34	105.51	114.75
30	K	268	ILE	N-CA-C	-7.33	96.91	107.77
21	N	584	ARG	O-C-N	7.33	129.62	122.07
28	H	102	CYS	CA-C-N	7.33	133.75	122.24
28	H	102	CYS	C-N-CA	7.33	133.75	122.24
15	W	31	ASP	CA-C-O	-7.33	112.78	120.55
22	S	23	LYS	N-CA-CB	7.33	121.00	110.16
21	N	645	THR	O-C-N	7.33	130.50	122.15
31	L	320	GLN	N-CA-C	-7.33	101.45	111.56
4	d	240	LYS	CA-C-N	7.32	129.96	120.44
4	d	240	LYS	C-N-CA	7.32	129.96	120.44
2	b	224	TYR	CA-C-O	-7.32	113.40	121.23
11	4	185	ASP	CA-CB-CG	-7.32	105.28	112.60
11	k	183	ILE	O-C-N	-7.32	115.68	123.14
25	R	115	GLU	CA-C-N	7.31	129.95	120.44
25	R	115	GLU	C-N-CA	7.31	129.95	120.44
7	g	237	GLN	OE1-CD-NE2	7.31	129.91	122.60
16	V	90	LYS	O-C-N	7.31	129.87	122.12
12	l	283	ASN	CA-C-N	7.31	129.94	120.44
12	l	283	ASN	C-N-CA	7.31	129.94	120.44
25	R	92	ILE	CA-C-N	7.31	132.32	121.72
25	R	92	ILE	C-N-CA	7.31	132.32	121.72
1	a	175	GLN	CA-C-N	7.30	130.07	120.28
1	a	175	GLN	C-N-CA	7.30	130.07	120.28
9	i	82	GLU	CA-C-N	7.30	130.07	120.28
9	i	82	GLU	C-N-CA	7.30	130.07	120.28
15	W	15	TYR	N-CA-C	-7.30	104.62	113.97
28	H	386	ALA	CA-C-N	7.30	130.38	120.44
28	H	386	ALA	C-N-CA	7.30	130.38	120.44
8	h	179	GLY	CA-C-O	-7.30	115.87	120.91
12	5	116	LEU	CA-C-N	7.30	133.90	122.94
12	5	116	LEU	C-N-CA	7.30	133.90	122.94
22	S	478	SER	CA-C-N	7.30	129.93	120.44
22	S	478	SER	C-N-CA	7.30	129.93	120.44
25	R	20	ARG	CA-C-N	7.30	127.44	120.43
25	R	20	ARG	C-N-CA	7.30	127.44	120.43
4	d	242	GLU	N-CA-C	7.30	119.23	111.28
25	R	45	GLU	CA-C-N	7.30	130.06	120.28
25	R	45	GLU	C-N-CA	7.30	130.06	120.28
27	O	292	CYS	CA-C-N	7.30	130.06	120.28
27	O	292	CYS	C-N-CA	7.30	130.06	120.28
14	7	111	ASN	CB-CA-C	-7.29	104.65	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	100	ASP	CA-CB-CG	-7.29	105.31	112.60
30	K	80	LYS	CA-C-O	7.29	128.14	120.42
10	3	124	PHE	CA-CB-CG	-7.28	106.52	113.80
31	L	239	ILE	CB-CA-C	-7.28	102.48	112.24
23	P	148	LYS	N-CA-C	7.28	120.08	111.71
33	J	9	ASN	N-CA-CB	7.28	122.79	110.49
4	d	65	SER	O-C-N	-7.28	114.80	123.31
14	7	128	TYR	CA-C-N	7.28	129.90	120.44
14	7	128	TYR	C-N-CA	7.28	129.90	120.44
17	T	134	LYS	N-CA-C	7.28	118.86	111.07
5	e	53	ARG	NE-CZ-NH1	7.27	128.77	121.50
17	T	170	ASN	CA-CB-CG	7.27	119.87	112.60
6	f	45	VAL	N-CA-C	-7.27	98.75	108.35
11	4	96	ARG	CA-C-N	7.27	127.03	119.76
11	4	96	ARG	C-N-CA	7.27	127.03	119.76
23	P	364	ARG	N-CA-C	7.27	118.85	111.07
10	j	89	GLN	CA-C-N	7.27	129.89	120.44
10	j	89	GLN	C-N-CA	7.27	129.89	120.44
21	N	398	ARG	CA-C-N	7.27	130.02	120.28
21	N	398	ARG	C-N-CA	7.27	130.02	120.28
10	j	118	LYS	CA-C-N	7.26	127.31	119.90
10	j	118	LYS	C-N-CA	7.26	127.31	119.90
9	2	149	ASP	CA-C-O	7.26	129.96	121.46
28	H	97	LEU	N-CA-C	-7.26	96.68	108.52
24	Q	255	TYR	O-C-N	7.26	130.42	122.15
22	S	366	LYS	N-CA-C	7.25	118.98	111.14
33	J	316	PHE	CA-C-N	7.25	124.96	119.66
33	J	316	PHE	C-N-CA	7.25	124.96	119.66
11	4	190	ARG	NE-CZ-NH2	-7.25	112.67	119.20
14	7	72	VAL	CA-C-N	7.25	131.01	120.71
14	7	72	VAL	C-N-CA	7.25	131.01	120.71
19	Y	20	LYS	N-CA-C	7.25	119.18	111.28
22	S	233	LEU	CA-C-N	7.25	129.70	120.56
22	S	233	LEU	C-N-CA	7.25	129.70	120.56
33	J	317	PRO	CA-C-O	-7.25	115.68	120.90
16	V	174	THR	CA-C-O	7.25	129.25	120.92
25	R	377	LEU	CA-C-N	7.25	133.07	122.63
25	R	377	LEU	C-N-CA	7.25	133.07	122.63
15	W	79	THR	N-CA-CB	7.25	120.69	110.04
24	Q	411	SER	CA-C-N	7.25	131.32	120.31
24	Q	411	SER	C-N-CA	7.25	131.32	120.31
8	1	138	SER	N-CA-C	-7.24	104.57	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	129	HIS	CE1-NE2-CD2	-7.24	101.76	109.00
23	P	63	VAL	CA-C-N	7.24	130.57	120.29
23	P	63	VAL	C-N-CA	7.24	130.57	120.29
13	6	90	LYS	N-CA-C	-7.24	96.53	108.76
22	S	458	GLN	OE1-CD-NE2	7.24	129.84	122.60
25	R	82	ASP	CA-C-N	7.24	131.02	120.82
25	R	82	ASP	C-N-CA	7.24	131.02	120.82
2	b	190	HIS	ND1-CE1-NE2	7.23	115.63	108.40
6	f	203	ASP	N-CA-CB	7.23	122.72	110.49
29	I	413	ALA	CA-C-N	7.23	129.97	120.28
29	I	413	ALA	C-N-CA	7.23	129.97	120.28
29	I	329	ASN	OD1-CG-ND2	-7.23	115.37	122.60
5	e	31	ILE	N-CA-C	-7.23	103.24	113.07
5	e	118	ASP	N-CA-CB	7.23	121.48	110.28
31	L	374	PHE	CA-CB-CG	-7.23	106.57	113.80
18	X	27	ILE	N-CA-C	-7.23	99.87	107.60
9	2	252	ILE	N-CA-C	-7.23	97.44	107.99
12	l	218	ASN	N-CA-C	-7.22	102.75	112.94
28	H	382	LEU	N-CA-C	7.22	118.80	111.07
22	S	45	THR	N-CA-C	7.22	119.89	110.43
23	P	235	LEU	CA-C-N	7.22	129.96	120.28
23	P	235	LEU	C-N-CA	7.22	129.96	120.28
29	I	321	ASP	N-CA-C	-7.22	103.67	114.64
2	b	133	SER	N-CA-C	-7.21	97.64	109.40
14	n	136	ARG	NE-CZ-NH1	7.21	128.71	121.50
7	g	109	ILE	O-C-N	-7.21	114.95	120.07
33	J	344	ARG	N-CA-CB	7.21	121.40	110.30
10	3	83	GLU	CA-C-O	-7.21	112.88	120.23
13	6	57	ASN	CA-CB-CG	-7.20	105.40	112.60
13	m	178	LYS	CA-C-O	-7.20	113.35	119.76
22	S	388	ILE	N-CA-CB	7.20	119.78	110.57
28	H	426	ALA	CA-C-N	7.20	128.09	120.03
28	H	426	ALA	C-N-CA	7.20	128.09	120.03
26	U	162	GLU	N-CA-C	-7.20	106.42	114.62
28	H	128	ASN	CA-C-O	7.20	127.61	118.54
26	U	246	GLU	CB-CG-CD	-7.19	100.37	112.60
32	M	19	ASP	CA-CB-CG	-7.19	105.41	112.60
22	S	195	ALA	CA-C-O	-7.19	112.80	120.42
33	J	208	CYS	N-CA-C	-7.19	98.25	108.96
5	e	101	LEU	CA-C-O	-7.19	113.30	120.70
26	U	16	LEU	CA-C-O	-7.18	112.80	120.42
27	O	305	ILE	CA-CB-CG2	-7.18	98.29	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	M	171	GLU	CA-C-N	7.18	134.89	121.97
32	M	171	GLU	C-N-CA	7.18	134.89	121.97
14	7	211	VAL	O-C-N	7.18	129.12	121.94
6	f	80	ASP	CA-C-N	7.18	131.22	120.31
6	f	80	ASP	C-N-CA	7.18	131.22	120.31
27	O	216	ASP	CA-CB-CG	-7.18	105.42	112.60
11	4	131	GLY	CA-C-O	7.17	129.24	121.56
21	N	552	ALA	N-CA-CB	7.17	121.40	110.28
4	d	143	ASP	N-CA-C	-7.17	101.45	112.99
18	X	78	ILE	CA-CB-CG1	7.17	122.59	110.40
19	Y	69	VAL	CA-C-O	-7.17	111.55	121.51
30	K	342	SER	CA-C-N	7.17	129.88	120.28
30	K	342	SER	C-N-CA	7.17	129.88	120.28
6	f	47	VAL	CA-C-O	-7.16	113.29	120.31
17	T	73	PHE	CA-CB-CG	-7.16	106.64	113.80
27	O	106	PHE	CA-CB-CG	-7.16	106.64	113.80
21	N	745	LEU	N-CA-C	-7.16	103.00	114.09
12	5	200	ASP	N-CA-C	-7.16	105.47	114.56
24	Q	279	LYS	N-CA-CB	7.16	120.64	110.12
29	I	215	PRO	CA-C-N	7.15	128.78	119.84
29	I	215	PRO	C-N-CA	7.15	128.78	119.84
10	3	100	PHE	CA-CB-CG	-7.15	106.65	113.80
23	P	19	GLU	N-CA-C	-7.15	103.22	112.23
32	M	97	SER	N-CA-C	-7.15	104.56	113.28
8	h	22	ILE	N-CA-C	-7.15	98.19	108.48
32	M	71	ASN	CA-C-N	7.15	129.86	120.28
32	M	71	ASN	C-N-CA	7.15	129.86	120.28
29	I	190	GLN	CA-C-N	7.14	132.02	120.30
29	I	190	GLN	C-N-CA	7.14	132.02	120.30
32	M	192	GLU	CA-C-O	-7.14	112.98	120.55
15	W	12	ASN	N-CA-CB	7.14	121.94	110.65
29	I	127	ASP	CA-CB-CG	-7.14	105.46	112.60
24	Q	244	GLU	CA-C-O	-7.14	112.85	120.42
19	Y	44	ALA	N-CA-CB	7.14	122.55	110.49
10	3	11	ILE	CA-C-O	7.13	129.16	121.67
12	5	241	HIS	ND1-CE1-NE2	7.13	115.53	108.40
23	P	342	GLN	CB-CG-CD	-7.13	100.47	112.60
12	5	192	SER	N-CA-C	7.13	125.99	110.80
17	T	149	ASP	CA-C-N	7.13	130.54	120.28
17	T	149	ASP	C-N-CA	7.13	130.54	120.28
21	N	636	SER	CA-C-N	7.13	129.83	120.28
21	N	636	SER	C-N-CA	7.13	129.83	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	743	PHE	CA-CB-CG	-7.13	106.67	113.80
23	P	47	ARG	CA-C-N	7.13	129.83	120.28
23	P	47	ARG	C-N-CA	7.13	129.83	120.28
29	I	151	HIS	CG-CD2-NE2	7.12	114.32	107.20
32	M	68	LYS	CA-C-N	7.12	130.54	120.42
32	M	68	LYS	C-N-CA	7.12	130.54	120.42
33	J	232	GLU	CA-C-N	7.12	129.82	120.28
33	J	232	GLU	C-N-CA	7.12	129.82	120.28
1	a	203	VAL	CB-CA-C	-7.12	102.39	112.22
27	O	28	GLN	CA-C-N	7.12	129.82	120.28
27	O	28	GLN	C-N-CA	7.12	129.82	120.28
24	Q	345	SER	O-C-N	7.12	130.26	122.15
27	O	23	HIS	CA-C-O	-7.12	111.78	118.33
29	I	151	HIS	CE1-NE2-CD2	-7.12	101.88	109.00
29	I	293	ASP	N-CA-C	-7.12	98.35	108.96
21	N	605	ILE	N-CA-C	-7.12	103.84	110.53
21	N	127	ASP	CA-C-O	7.11	127.57	119.18
32	M	145	LEU	N-CA-CB	7.11	120.45	109.85
23	P	56	LYS	N-CA-C	-7.11	103.61	111.36
33	J	261	SER	N-CA-CB	7.11	122.50	110.49
3	c	79	GLY	N-CA-C	-7.11	101.19	110.29
9	i	226	GLU	CA-C-O	7.11	129.30	121.56
21	N	445	GLY	CA-C-N	7.11	129.68	120.44
21	N	445	GLY	C-N-CA	7.11	129.68	120.44
30	K	332	GLY	N-CA-C	-7.11	104.65	114.67
27	O	36	LYS	N-CA-CB	7.10	122.50	110.49
31	L	329	ARG	O-C-N	-7.10	114.56	121.38
32	M	330	VAL	N-CA-C	-7.10	105.69	113.43
8	1	47	HIS	N-CA-CB	7.10	122.56	111.56
11	4	175	ASP	N-CA-C	-7.10	98.80	109.94
21	N	97	PHE	CA-CB-CG	-7.10	106.70	113.80
6	f	93	ASN	CA-C-N	7.09	130.50	120.28
6	f	93	ASN	C-N-CA	7.09	130.50	120.28
12	5	161	LEU	CA-C-O	7.09	127.94	120.42
32	M	248	ALA	CA-C-O	-7.09	111.10	117.98
16	V	281	SER	N-CA-C	7.09	118.80	111.14
28	H	364	ALA	CA-C-N	7.09	130.36	120.29
28	H	364	ALA	C-N-CA	7.09	130.36	120.29
10	j	173	ASN	N-CA-C	7.09	119.01	111.28
2	B	100	ILE	N-CA-C	-7.09	106.17	112.12
32	M	57	VAL	CA-C-N	7.09	129.78	120.28
32	M	57	VAL	C-N-CA	7.09	129.78	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	204	HIS	ND1-CE1-NE2	7.09	115.49	108.40
22	S	57	LEU	CA-C-N	7.09	130.11	120.54
22	S	57	LEU	C-N-CA	7.09	130.11	120.54
5	e	223	THR	N-CA-C	-7.08	98.31	109.50
25	R	233	ASP	N-CA-CB	7.08	120.65	110.16
3	c	124	GLN	N-CA-C	7.08	119.08	111.36
21	N	659	ALA	CA-C-N	7.08	130.10	120.54
21	N	659	ALA	C-N-CA	7.08	130.10	120.54
22	S	412	ASN	CA-CB-CG	7.08	119.68	112.60
3	c	207	THR	CA-C-N	7.08	129.77	120.28
3	c	207	THR	C-N-CA	7.08	129.77	120.28
17	T	258	ASN	CA-CB-CG	-7.08	105.52	112.60
17	T	158	GLN	N-CA-C	7.08	118.64	111.07
23	P	329	PHE	CA-CB-CG	-7.08	106.72	113.80
5	e	15	PHE	CA-C-N	7.07	134.43	121.70
5	e	15	PHE	C-N-CA	7.07	134.43	121.70
6	f	43	HIS	CE1-NE2-CD2	-7.07	101.93	109.00
22	S	233	LEU	N-CA-C	-7.07	103.65	111.36
16	V	275	ASP	O-C-N	-7.07	115.01	121.30
22	S	240	ASP	CA-CB-CG	-7.07	105.53	112.60
24	Q	42	ALA	N-CA-C	-7.07	101.61	112.99
22	S	106	GLY	N-CA-C	-7.06	105.47	115.43
30	K	342	SER	N-CA-C	-7.06	103.90	114.64
2	b	221	LEU	CA-C-N	7.06	131.04	120.31
2	b	221	LEU	C-N-CA	7.06	131.04	120.31
22	S	321	GLN	CA-C-O	-7.06	112.94	120.42
15	W	93	ILE	CA-C-N	7.06	129.74	120.28
15	W	93	ILE	C-N-CA	7.06	129.74	120.28
20	Z	248	TYR	CB-CA-C	-7.06	98.85	110.85
30	K	245	LYS	CB-CA-C	-7.06	99.28	110.85
29	I	160	LEU	N-CA-C	-7.06	105.86	114.75
30	K	240	SER	N-CA-C	-7.05	104.41	113.16
8	l	195	LEU	CA-C-O	7.05	129.69	121.44
21	N	120	ASP	CA-C-N	7.05	129.73	120.28
21	N	120	ASP	C-N-CA	7.05	129.73	120.28
27	O	354	GLN	CA-C-N	7.05	127.48	119.93
27	O	354	GLN	C-N-CA	7.05	127.48	119.93
17	T	239	SER	N-CA-CB	7.05	120.23	110.01
27	O	130	ASP	N-CA-CB	7.05	120.59	110.16
23	P	83	SER	O-C-N	-7.05	114.81	122.07
8	h	91	PHE	CA-C-N	7.05	129.60	120.44
8	h	91	PHE	C-N-CA	7.05	129.60	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	73	ASN	CA-CB-CG	-7.05	105.55	112.60
11	k	149	ARG	O-C-N	-7.04	113.22	121.32
9	2	167	LEU	N-CA-C	7.04	119.56	111.11
29	I	380	LEU	N-CA-CB	7.04	120.58	110.16
31	L	59	GLN	OE1-CD-NE2	7.04	129.64	122.60
28	H	362	ASP	CA-CB-CG	7.04	119.64	112.60
12	l	283	ASN	CB-CG-ND2	7.04	126.96	116.40
24	Q	220	LEU	CA-C-N	7.04	129.71	120.28
24	Q	220	LEU	C-N-CA	7.04	129.71	120.28
30	K	373	ILE	CA-C-O	7.04	128.27	120.95
29	I	172	LYS	CA-C-O	7.04	128.93	121.19
17	T	33	GLU	CA-C-O	7.03	128.03	119.31
23	P	325	ASP	CA-CB-CG	7.03	119.63	112.60
26	U	31	LYS	N-CA-C	-7.03	99.52	110.42
3	c	13	PHE	CA-CB-CG	7.03	120.83	113.80
9	2	122	HIS	ND1-CE1-NE2	7.03	115.43	108.40
16	V	158	LEU	N-CA-C	7.03	120.42	110.23
28	H	85	MET	CA-C-N	7.03	128.93	120.14
28	H	85	MET	C-N-CA	7.03	128.93	120.14
17	T	54	ASP	CA-C-N	7.03	129.70	120.28
17	T	54	ASP	C-N-CA	7.03	129.70	120.28
20	Z	630	LYS	CA-C-N	7.03	127.90	120.03
20	Z	630	LYS	C-N-CA	7.03	127.90	120.03
7	g	13	SER	N-CA-C	-7.03	104.36	114.12
12	l	231	LEU	N-CA-C	-7.03	103.70	111.36
28	H	422	VAL	CA-C-O	-7.03	113.74	121.05
29	I	168	VAL	CA-C-N	7.03	129.57	120.44
29	I	168	VAL	C-N-CA	7.03	129.57	120.44
14	n	141	ASN	CA-C-O	-7.02	111.89	120.74
15	W	38	GLN	O-C-N	-7.02	114.14	122.15
22	S	143	GLN	N-CA-CB	7.02	120.55	110.16
29	I	159	VAL	CB-CA-C	7.02	121.56	111.80
24	Q	76	GLU	N-CA-C	7.02	118.93	111.28
29	I	264	CYS	CB-CA-C	-7.02	99.14	110.79
21	N	263	SER	CA-C-N	7.01	130.25	120.29
21	N	263	SER	C-N-CA	7.01	130.25	120.29
14	7	107	ASN	CA-CB-CG	7.01	119.61	112.60
31	L	145	ARG	N-CA-CB	7.01	120.28	109.97
18	X	53	THR	N-CA-C	-7.01	105.66	114.56
9	i	38	ASN	OD1-CG-ND2	7.01	129.61	122.60
22	S	475	TYR	N-CA-CB	7.00	120.17	110.01
24	Q	147	GLN	O-C-N	-7.00	112.79	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	91	TRP	CA-C-N	7.00	133.12	122.69
25	R	91	TRP	C-N-CA	7.00	133.12	122.69
27	O	162	SER	CA-C-O	7.00	128.09	120.32
27	O	171	PHE	CB-CG-CD1	-7.00	108.79	120.70
9	i	225	ARG	NE-CZ-NH2	-7.00	112.90	119.20
8	l	195	LEU	O-C-N	-7.00	114.05	123.15
5	e	216	ASN	CA-CB-CG	7.00	119.60	112.60
15	W	39	ALA	CA-C-O	7.00	127.97	120.55
29	I	347	LYS	N-CA-C	-7.00	97.80	109.07
7	g	126	TYR	O-C-N	-7.00	114.32	123.21
12	l	180	THR	N-CA-CB	7.00	121.63	110.85
27	O	263	PHE	CA-CB-CG	-7.00	106.80	113.80
26	U	94	HIS	CE1-NE2-CD2	-7.00	102.00	109.00
29	I	100	ARG	NE-CZ-NH1	-7.00	114.50	121.50
14	n	102	ASP	CA-CB-CG	-6.99	105.61	112.60
26	U	110	PHE	CA-C-O	6.99	128.28	119.12
21	N	422	TYR	O-C-N	6.99	129.27	122.07
22	S	77	THR	CA-C-N	6.99	129.37	120.56
22	S	77	THR	C-N-CA	6.99	129.37	120.56
15	W	62	LEU	N-CA-CB	6.99	120.81	110.33
29	I	150	HIS	CE1-NE2-CD2	-6.99	102.01	109.00
27	O	326	HIS	CA-C-N	6.99	129.64	120.28
27	O	326	HIS	C-N-CA	6.99	129.64	120.28
32	M	341	GLY	CA-C-O	6.99	126.78	119.02
21	N	74	GLU	CA-C-N	6.99	130.34	120.28
21	N	74	GLU	C-N-CA	6.99	130.34	120.28
29	I	325	ILE	N-CA-CB	6.99	121.32	111.82
33	J	195	LYS	N-CA-C	6.99	119.78	111.33
30	K	311	ASN	CA-CB-CG	-6.98	105.62	112.60
21	N	251	GLU	CA-C-N	6.98	127.85	120.03
21	N	251	GLU	C-N-CA	6.98	127.85	120.03
27	O	141	ASN	OD1-CG-ND2	6.98	129.58	122.60
24	Q	313	ASP	N-CA-C	6.98	118.97	111.36
25	R	318	PRO	O-C-N	6.98	131.22	122.22
29	I	75	PHE	CA-C-N	6.98	130.33	120.42
29	I	75	PHE	C-N-CA	6.98	130.33	120.42
17	T	26	LEU	N-CA-C	-6.97	104.77	113.28
25	R	73	ASN	OD1-CG-ND2	6.97	129.57	122.60
27	O	341	ILE	N-CA-C	-6.97	97.57	107.75
22	S	85	SER	CA-C-O	6.97	127.95	119.38
32	M	412	HIS	CA-CB-CG	6.97	120.77	113.80
7	g	23	GLN	O-C-N	-6.97	114.73	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	87	HIS	ND1-CE1-NE2	6.97	115.37	108.40
9	2	128	ILE	N-CA-C	-6.97	97.58	107.75
14	n	40	THR	CA-C-N	6.97	131.63	121.67
14	n	40	THR	C-N-CA	6.97	131.63	121.67
30	K	344	ARG	N-CA-C	6.97	122.14	109.32
29	I	78	ASN	CA-CB-CG	-6.96	105.64	112.60
9	2	117	PHE	CA-CB-CG	-6.96	106.84	113.80
21	N	310	ASP	CA-CB-CG	6.96	119.56	112.60
4	d	239	GLU	CA-C-N	6.96	129.49	120.44
4	d	239	GLU	C-N-CA	6.96	129.49	120.44
32	M	44	PHE	N-CA-CB	6.96	120.35	110.12
1	a	29	GLU	CA-C-N	6.96	130.29	120.28
1	a	29	GLU	C-N-CA	6.96	130.29	120.28
13	6	204	ILE	CB-CA-C	-6.96	102.58	111.20
21	N	815	LYS	CA-C-N	6.96	130.88	120.31
21	N	815	LYS	C-N-CA	6.96	130.88	120.31
9	2	143	HIS	CG-CD2-NE2	6.95	114.15	107.20
21	N	357	GLY	CA-C-N	6.95	132.50	120.68
21	N	357	GLY	C-N-CA	6.95	132.50	120.68
30	K	402	ILE	N-CA-CB	6.95	119.33	110.99
13	m	162	VAL	N-CA-C	-6.95	105.07	111.67
13	m	200	THR	N-CA-C	-6.95	103.78	111.36
2	b	194	LEU	N-CA-C	-6.95	103.79	111.36
4	d	167	ASN	CA-C-N	6.95	130.87	120.31
4	d	167	ASN	C-N-CA	6.95	130.87	120.31
20	Z	253	VAL	CA-CB-CG2	6.95	122.21	110.40
21	N	763	GLY	N-CA-C	-6.94	104.14	115.46
28	H	309	ASP	CA-C-O	-6.94	113.31	121.16
27	O	71	ASP	CA-CB-CG	6.94	119.54	112.60
2	b	67	LEU	N-CA-C	-6.94	103.45	112.68
8	1	69	GLN	O-C-N	-6.94	114.76	122.12
17	T	50	ILE	O-C-N	-6.94	114.68	121.83
8	h	69	GLN	CA-C-N	6.94	129.46	120.44
8	h	69	GLN	C-N-CA	6.94	129.46	120.44
16	V	210	THR	CA-C-N	6.94	129.58	120.28
16	V	210	THR	C-N-CA	6.94	129.58	120.28
21	N	408	LEU	O-C-N	6.94	130.06	122.15
33	J	312	ARG	N-CA-CB	6.94	122.21	110.49
22	S	484	ASP	O-C-N	6.94	129.21	122.07
18	X	67	ILE	CA-C-O	-6.93	113.08	121.54
25	R	96	GLN	CA-C-N	6.93	129.57	120.28
25	R	96	GLN	C-N-CA	6.93	129.57	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	J	14	THR	CA-C-N	6.93	129.57	120.28
33	J	14	THR	C-N-CA	6.93	129.57	120.28
9	2	172	LYS	N-CA-C	-6.93	98.78	109.24
19	Y	83	ARG	N-CA-CB	6.93	120.41	110.16
24	Q	168	LEU	N-CA-C	-6.93	102.10	111.87
31	L	70	TYR	CA-C-O	-6.93	113.08	120.42
23	P	119	ILE	CB-CA-C	-6.92	102.79	112.14
12	l	127	CYS	N-CA-C	6.92	118.62	111.14
27	O	174	THR	N-CA-CB	6.92	120.30	110.12
32	M	203	ARG	NE-CZ-NH2	6.92	125.43	119.20
20	Z	213	LYS	CA-C-N	6.92	130.12	120.29
20	Z	213	LYS	C-N-CA	6.92	130.12	120.29
24	Q	176	ASP	CA-CB-CG	6.92	119.52	112.60
27	O	345	ASN	CA-CB-CG	-6.92	105.68	112.60
16	V	140	VAL	CB-CA-C	-6.92	100.95	110.77
22	S	305	LYS	N-CA-C	-6.92	104.46	113.17
20	Z	734	ASP	N-CA-C	6.91	118.90	111.36
25	R	81	HIS	ND1-CE1-NE2	6.91	115.31	108.40
25	R	92	ILE	N-CA-C	-6.91	106.26	112.90
32	M	124	ARG	CA-C-O	-6.91	113.17	121.40
7	g	50	VAL	CA-C-N	6.91	130.63	120.95
7	g	50	VAL	C-N-CA	6.91	130.63	120.95
33	J	71	TYR	CA-CB-CG	-6.91	101.46	113.90
21	N	340	HIS	CE1-NE2-CD2	-6.91	102.09	109.00
21	N	818	LYS	CA-C-N	6.91	129.54	120.28
21	N	818	LYS	C-N-CA	6.91	129.54	120.28
9	i	223	ASN	CA-CB-CG	-6.90	105.70	112.60
27	O	151	ASP	N-CA-C	6.90	118.80	111.28
19	Y	25	ASN	CA-C-N	6.90	129.82	120.44
19	Y	25	ASN	C-N-CA	6.90	129.82	120.44
23	P	319	GLU	N-CA-CB	6.90	118.56	110.42
33	J	287	ASN	CA-CB-CG	6.90	119.50	112.60
12	l	193	ASP	CA-CB-CG	6.90	119.50	112.60
21	N	96	GLN	O-C-N	6.90	130.76	122.27
16	V	21	ASP	CA-CB-CG	-6.90	105.70	112.60
26	U	70	HIS	ND1-CE1-NE2	6.90	115.30	108.40
32	M	369	THR	CA-C-O	-6.90	113.60	121.19
13	m	166	ASN	OD1-CG-ND2	-6.90	115.70	122.60
17	T	218	GLU	CA-C-O	-6.90	112.58	120.24
4	d	247	ASP	N-CA-C	-6.89	103.21	111.69
9	i	212	ASP	CA-CB-CG	6.89	119.50	112.60
23	P	357	TYR	CA-C-N	6.89	130.79	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	357	TYR	C-N-CA	6.89	130.79	120.31
8	1	64	ILE	CA-C-O	-6.89	113.33	120.71
21	N	653	ARG	O-C-N	6.89	129.17	122.07
16	V	212	MET	CG-SD-CE	-6.89	85.74	100.90
14	n	201	THR	N-CA-C	-6.89	98.55	109.23
14	7	186	PRO	CA-C-N	6.89	129.51	120.28
14	7	186	PRO	C-N-CA	6.89	129.51	120.28
29	I	432	LEU	CA-C-O	6.89	127.89	120.24
14	7	63	TYR	CA-C-O	6.89	126.31	119.08
21	N	765	ASP	N-CA-C	-6.89	106.07	114.75
12	l	179	TYR	CB-CG-CD2	-6.89	110.47	120.80
11	4	81	SER	CA-C-O	6.89	127.89	119.97
13	6	213	LEU	N-CA-CB	6.89	121.38	110.57
15	W	126	ILE	N-CA-C	-6.89	103.77	110.72
24	Q	104	PHE	CA-C-N	6.89	130.07	120.29
24	Q	104	PHE	C-N-CA	6.89	130.07	120.29
20	Z	793	PHE	CA-CB-CG	-6.88	106.92	113.80
24	Q	227	CYS	CA-C-O	6.88	127.72	120.42
32	M	423	GLN	CA-C-N	6.88	130.77	120.31
32	M	423	GLN	C-N-CA	6.88	130.77	120.31
33	J	368	TYR	CA-C-N	6.88	129.50	120.28
33	J	368	TYR	C-N-CA	6.88	129.50	120.28
23	P	317	THR	O-C-N	6.88	130.00	122.15
22	S	185	PHE	CA-C-N	6.88	130.06	120.29
22	S	185	PHE	C-N-CA	6.88	130.06	120.29
8	1	64	ILE	N-CA-C	-6.88	103.50	111.00
21	N	36	TRP	CA-C-N	6.88	129.83	120.54
21	N	36	TRP	C-N-CA	6.88	129.83	120.54
21	N	181	GLU	CB-CG-CD	-6.88	100.91	112.60
12	l	105	THR	N-CA-C	-6.88	103.24	112.94
14	7	206	ALA	CA-C-O	-6.88	113.26	120.55
21	N	408	LEU	CA-C-N	6.88	127.56	120.00
21	N	408	LEU	C-N-CA	6.88	127.56	120.00
23	P	78	GLN	N-CA-CB	6.87	119.97	110.01
8	1	112	ASP	N-CA-C	-6.87	99.00	109.85
27	O	136	THR	CA-C-N	6.87	130.17	120.28
27	O	136	THR	C-N-CA	6.87	130.17	120.28
32	M	372	ASP	N-CA-C	-6.87	104.71	113.23
3	c	59	GLN	N-CA-C	-6.87	103.48	112.41
3	c	90	THR	CA-C-N	6.87	130.04	120.29
3	c	90	THR	C-N-CA	6.87	130.04	120.29
5	e	223	THR	CA-C-N	6.87	129.48	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	223	THR	C-N-CA	6.87	129.48	120.28
30	K	302	GLN	CA-C-N	6.87	130.40	120.38
30	K	302	GLN	C-N-CA	6.87	130.40	120.38
16	V	179	LEU	N-CA-C	-6.86	98.07	109.46
15	W	170	HIS	CE1-NE2-CD2	-6.86	102.14	109.00
21	N	354	PRO	N-CA-CB	6.86	110.79	103.52
26	U	152	LYS	N-CA-C	-6.86	98.03	109.07
29	I	192	GLN	CA-C-O	6.86	128.03	119.59
30	K	293	GLN	CA-C-N	6.85	129.46	120.28
30	K	293	GLN	C-N-CA	6.85	129.46	120.28
21	N	811	LYS	N-CA-C	6.85	119.33	111.11
25	R	34	THR	CA-C-N	6.85	130.59	120.87
25	R	34	THR	C-N-CA	6.85	130.59	120.87
28	H	392	HIS	ND1-CE1-NE2	6.85	115.25	108.40
29	I	248	VAL	N-CA-C	-6.85	98.59	108.17
30	K	41	SER	CA-C-N	6.85	129.45	120.28
30	K	41	SER	C-N-CA	6.85	129.45	120.28
21	N	45	ASP	CA-CB-CG	-6.84	105.75	112.60
12	5	241	HIS	CE1-NE2-CD2	-6.84	102.16	109.00
16	V	230	TYR	CA-C-N	6.84	129.45	120.28
16	V	230	TYR	C-N-CA	6.84	129.45	120.28
28	H	121	ASN	N-CA-CB	6.84	120.29	110.16
28	H	440	GLU	N-CA-CB	6.84	120.95	110.14
7	g	100	LYS	N-CA-C	6.84	119.57	111.71
21	N	69	TYR	CA-C-O	-6.84	113.66	120.70
23	P	178	GLN	N-CA-C	6.84	118.39	111.07
26	U	21	HIS	O-C-N	-6.84	114.22	122.22
31	L	62	ARG	N-CA-CB	6.84	120.28	110.16
3	c	25	ALA	CA-C-O	-6.83	113.31	120.55
6	f	99	PHE	CA-CB-CG	-6.83	106.97	113.80
27	O	345	ASN	N-CA-C	-6.83	104.83	113.72
16	V	132	LEU	CA-C-O	6.83	127.66	120.42
19	Y	86	ARG	N-CA-CB	6.83	120.17	110.12
4	d	60	THR	CA-C-N	6.83	127.21	119.83
4	d	60	THR	C-N-CA	6.83	127.21	119.83
14	n	207	GLU	CA-C-N	6.83	129.32	120.44
14	n	207	GLU	C-N-CA	6.83	129.32	120.44
1	a	232	LYS	CA-C-N	6.83	133.79	122.73
1	a	232	LYS	C-N-CA	6.83	133.79	122.73
9	2	115	HIS	CA-CB-CG	-6.83	106.97	113.80
31	L	362	LYS	N-CA-C	6.83	118.72	111.28
10	3	52	GLY	CA-C-O	-6.83	114.25	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	M	346	LYS	N-CA-C	-6.83	95.87	108.02
8	1	69	GLN	CA-C-O	6.83	127.79	120.55
8	1	98	ASN	OD1-CG-ND2	6.83	129.43	122.60
26	U	270	ASN	CA-CB-CG	-6.83	105.77	112.60
33	J	33	LYS	O-C-N	6.83	129.35	122.12
24	Q	13	ARG	CA-C-N	6.82	130.10	120.28
24	Q	13	ARG	C-N-CA	6.82	130.10	120.28
26	U	98	LYS	CA-C-N	6.82	131.18	121.42
26	U	98	LYS	C-N-CA	6.82	131.18	121.42
31	L	310	THR	N-CA-C	6.82	118.80	111.36
33	J	375	ILE	N-CA-C	6.82	116.94	110.53
14	n	162	TYR	CA-CB-CG	6.82	126.18	113.90
24	Q	402	THR	CA-C-N	6.82	126.78	119.76
24	Q	402	THR	C-N-CA	6.82	126.78	119.76
28	H	99	VAL	CA-C-N	6.82	133.51	122.53
28	H	99	VAL	C-N-CA	6.82	133.51	122.53
28	H	443	PHE	CA-CB-CG	-6.82	106.98	113.80
25	R	179	PHE	CA-C-N	6.82	129.30	120.44
25	R	179	PHE	C-N-CA	6.82	129.30	120.44
30	K	106	ASN	CA-CB-CG	-6.82	105.78	112.60
8	1	116	LYS	CA-C-N	6.82	126.81	120.34
8	1	116	LYS	C-N-CA	6.82	126.81	120.34
13	6	220	VAL	N-CA-C	-6.82	97.80	107.75
9	i	145	HIS	ND1-CE1-NE2	6.81	115.21	108.40
10	j	195	VAL	CA-CB-CG2	-6.81	98.82	110.40
13	6	24	ALA	CB-CA-C	-6.81	98.04	109.48
31	L	387	ASN	CA-CB-CG	-6.81	105.79	112.60
4	d	60	THR	CA-C-O	-6.81	112.99	119.80
9	2	59	ASN	CA-CB-CG	-6.81	105.79	112.60
23	P	198	VAL	CA-C-N	6.81	129.41	120.28
23	P	198	VAL	C-N-CA	6.81	129.41	120.28
16	V	71	MET	N-CA-C	-6.81	101.21	109.72
14	7	240	THR	N-CA-C	-6.80	95.94	107.99
29	I	268	PHE	CA-CB-CG	-6.80	107.00	113.80
6	f	195	GLU	CA-C-N	6.80	129.39	120.28
6	f	195	GLU	C-N-CA	6.80	129.39	120.28
32	M	176	PRO	O-C-N	6.80	131.82	122.64
24	Q	245	SER	O-C-N	6.80	129.07	122.07
31	L	152	THR	CA-C-N	6.80	132.42	122.63
31	L	152	THR	C-N-CA	6.80	132.42	122.63
22	S	314	ASN	CB-CA-C	-6.79	99.51	110.79
22	S	346	TYR	N-CA-C	-6.79	103.96	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	154	LEU	CA-C-N	6.79	127.47	120.00
25	R	154	LEU	C-N-CA	6.79	127.47	120.00
25	R	341	LEU	CA-C-N	6.79	130.63	120.31
25	R	341	LEU	C-N-CA	6.79	130.63	120.31
4	d	252	SER	CA-C-N	6.79	129.26	120.44
4	d	252	SER	C-N-CA	6.79	129.26	120.44
21	N	875	LEU	CA-C-O	-6.79	113.31	120.23
30	K	153	ASP	CA-C-O	6.79	127.96	120.63
24	Q	170	ASP	CA-C-N	6.78	130.12	120.49
24	Q	170	ASP	C-N-CA	6.78	130.12	120.49
3	c	44	ILE	N-CA-CB	6.78	122.56	111.58
22	S	91	ASN	CA-C-O	6.78	127.61	120.42
14	7	36	GLN	CA-C-O	-6.78	112.78	119.69
21	N	178	SER	CA-C-N	6.78	129.25	120.44
21	N	178	SER	C-N-CA	6.78	129.25	120.44
24	Q	184	VAL	CA-C-O	-6.77	113.67	120.85
27	O	312	ASP	N-CA-CB	6.77	119.83	110.01
14	7	121	GLU	CA-C-N	6.77	126.73	119.28
14	7	121	GLU	C-N-CA	6.77	126.73	119.28
22	S	112	ASN	CA-CB-CG	-6.77	105.83	112.60
33	J	205	HIS	ND1-CE1-NE2	6.77	115.17	108.40
23	P	337	HIS	CA-C-N	6.77	129.90	120.29
23	P	337	HIS	C-N-CA	6.77	129.90	120.29
13	6	26	GLU	N-CA-C	-6.76	103.40	112.94
2	b	191	ILE	CA-C-N	6.76	129.34	120.28
2	b	191	ILE	C-N-CA	6.76	129.34	120.28
28	H	111	GLU	N-CA-C	-6.76	104.67	113.12
9	2	181	ILE	CA-C-N	6.76	129.63	120.44
9	2	181	ILE	C-N-CA	6.76	129.63	120.44
32	M	44	PHE	CA-C-O	-6.76	113.39	120.55
23	P	336	HIS	CE1-NE2-CD2	-6.76	102.24	109.00
31	L	150	ILE	N-CA-C	-6.75	102.39	111.44
21	N	340	HIS	ND1-CE1-NE2	6.75	115.15	108.40
11	k	95	ARG	N-CA-C	-6.75	103.92	111.28
23	P	170	SER	O-C-N	-6.74	113.30	122.33
22	S	415	SER	CA-C-N	6.74	129.20	120.44
22	S	415	SER	C-N-CA	6.74	129.20	120.44
28	H	398	VAL	CA-C-N	6.74	130.44	120.87
28	H	398	VAL	C-N-CA	6.74	130.44	120.87
33	J	172	GLU	CA-C-O	-6.74	113.28	120.42
8	h	171	ALA	CA-C-N	6.74	129.69	120.46
8	h	171	ALA	C-N-CA	6.74	129.69	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	M	72	ASN	O-C-N	6.74	129.26	122.12
8	h	162	ASP	N-CA-C	-6.74	103.74	112.23
2	b	63	LYS	CA-C-N	6.74	131.96	123.14
2	b	63	LYS	C-N-CA	6.74	131.96	123.14
9	2	148	THR	O-C-N	6.74	131.19	123.31
23	P	352	VAL	N-CA-CB	6.74	118.43	110.55
5	e	248	ALA	N-CA-C	-6.73	105.10	113.38
30	K	325	ASP	CA-CB-CG	6.73	119.33	112.60
1	a	148	GLU	CA-C-N	6.73	133.15	122.11
1	a	148	GLU	C-N-CA	6.73	133.15	122.11
7	g	219	CYS	N-CA-CB	6.73	121.07	110.84
1	a	152	PRO	N-CA-CB	6.73	109.25	103.19
7	g	116	LEU	CB-CA-C	-6.73	99.62	110.79
21	N	528	ARG	N-CA-CB	6.73	120.54	110.65
24	Q	293	SER	CA-C-N	6.73	129.97	120.28
24	Q	293	SER	C-N-CA	6.73	129.97	120.28
10	3	53	ILE	N-CA-C	-6.72	99.48	108.35
11	4	37	GLN	N-CA-CB	6.72	119.98	109.83
7	g	183	HIS	O-C-N	6.72	127.44	121.32
16	V	142	ASP	CB-CA-C	6.72	118.02	108.68
27	O	353	VAL	N-CA-CB	6.72	120.38	111.64
33	J	205	HIS	CA-C-N	6.72	129.29	120.28
33	J	205	HIS	C-N-CA	6.72	129.29	120.28
6	f	69	HIS	N-CA-C	-6.72	103.80	113.21
17	T	105	LEU	N-CA-C	6.72	118.68	111.36
23	P	429	ILE	CA-C-N	6.72	128.54	120.14
23	P	429	ILE	C-N-CA	6.72	128.54	120.14
24	Q	412	ALA	N-CA-CB	6.72	120.70	110.28
28	H	57	LYS	CA-C-N	6.72	129.28	120.28
28	H	57	LYS	C-N-CA	6.72	129.28	120.28
28	H	140	ASP	O-C-N	6.72	131.53	122.59
3	c	82	ALA	CA-C-N	6.72	129.83	120.29
3	c	82	ALA	C-N-CA	6.72	129.83	120.29
7	g	123	HIS	CG-CD2-NE2	6.72	113.92	107.20
1	a	110	TYR	CA-C-N	6.71	130.24	120.71
1	a	110	TYR	C-N-CA	6.71	130.24	120.71
33	J	185	VAL	N-CA-CB	6.71	122.45	111.58
16	V	37	MET	N-CA-CB	6.71	120.09	110.16
16	V	304	ALA	N-CA-C	6.71	118.38	111.14
17	T	41	ILE	CA-C-O	-6.71	112.88	121.13
9	2	64	HIS	CG-CD2-NE2	6.71	113.91	107.20
8	h	153	GLU	CA-C-N	6.70	134.34	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	153	GLU	C-N-CA	6.70	134.34	121.54
21	N	258	ALA	CA-C-N	6.70	130.50	120.31
21	N	258	ALA	C-N-CA	6.70	130.50	120.31
25	R	120	LEU	O-C-N	-6.70	114.27	122.25
22	S	318	CYS	CA-C-N	6.70	129.26	120.28
22	S	318	CYS	C-N-CA	6.70	129.26	120.28
13	m	82	TRP	CB-CG-CD2	-6.70	117.42	126.80
10	3	89	GLN	CA-C-N	6.70	129.26	120.28
10	3	89	GLN	C-N-CA	6.70	129.26	120.28
17	T	50	ILE	CA-C-O	6.70	127.95	120.85
7	g	216	ILE	N-CA-C	-6.70	99.51	108.35
22	S	387	VAL	N-CA-C	6.70	117.45	110.62
11	k	88	LEU	CA-C-N	6.69	129.14	120.44
11	k	88	LEU	C-N-CA	6.69	129.14	120.44
16	V	250	GLN	CA-C-N	6.69	130.49	120.31
16	V	250	GLN	C-N-CA	6.69	130.49	120.31
21	N	882	ILE	N-CA-CB	6.69	118.54	110.31
2	b	148	TYR	CA-C-N	6.69	132.20	122.77
2	b	148	TYR	C-N-CA	6.69	132.20	122.77
12	5	122	GLY	CA-C-N	6.69	126.34	119.92
12	5	122	GLY	C-N-CA	6.69	126.34	119.92
4	d	63	LYS	CA-C-N	6.68	132.93	122.70
4	d	63	LYS	C-N-CA	6.68	132.93	122.70
4	d	112	TYR	O-C-N	6.68	129.31	122.09
10	j	114	SER	N-CA-C	-6.68	103.58	113.61
10	3	48	HIS	ND1-CE1-NE2	6.68	115.08	108.40
23	P	194	SER	CA-C-N	6.68	129.78	120.29
23	P	194	SER	C-N-CA	6.68	129.78	120.29
14	7	139	LYS	N-CA-CB	6.68	120.05	110.16
14	7	174	THR	CA-CB-OG1	6.68	119.62	109.60
11	k	31	SER	N-CA-C	-6.68	102.48	113.50
10	3	159	GLU	N-CA-C	-6.68	101.41	110.36
21	N	521	LEU	CA-C-N	6.68	129.56	120.54
21	N	521	LEU	C-N-CA	6.68	129.56	120.54
21	N	598	ASP	N-CA-C	-6.68	99.63	109.11
10	3	137	ILE	N-CA-C	-6.68	98.51	108.46
21	N	640	VAL	N-CA-C	6.68	117.46	110.72
22	S	387	VAL	CA-C-N	6.68	129.11	120.56
22	S	387	VAL	C-N-CA	6.68	129.11	120.56
27	O	86	LEU	N-CA-C	6.68	121.44	113.16
32	M	199	LEU	O-C-N	-6.68	114.54	120.48
17	T	111	LEU	CA-C-O	6.67	127.84	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	M	268	ALA	CA-C-N	6.67	129.77	120.29
32	M	268	ALA	C-N-CA	6.67	129.77	120.29
33	J	61	GLU	CA-C-N	6.67	129.22	120.28
33	J	61	GLU	C-N-CA	6.67	129.22	120.28
20	Z	861	THR	N-CA-C	-6.67	107.02	114.62
21	N	654	GLN	OE1-CD-NE2	-6.67	115.93	122.60
21	N	888	ASP	CA-C-N	6.67	129.76	120.29
21	N	888	ASP	C-N-CA	6.67	129.76	120.29
30	K	58	TYR	CB-CG-CD2	-6.67	110.79	120.80
33	J	306	ARG	CA-C-N	6.67	127.03	119.83
33	J	306	ARG	C-N-CA	6.67	127.03	119.83
21	N	407	GLY	CA-C-N	6.67	129.76	120.29
21	N	407	GLY	C-N-CA	6.67	129.76	120.29
2	b	143	ASN	CB-CG-ND2	6.67	126.40	116.40
13	m	144	CYS	CA-C-O	-6.67	112.34	120.54
15	W	153	LEU	CA-C-N	6.67	129.21	120.28
15	W	153	LEU	C-N-CA	6.67	129.21	120.28
23	P	195	GLN	OE1-CD-NE2	6.67	129.27	122.60
32	M	134	LEU	N-CA-C	6.67	119.11	111.11
11	4	52	ASP	CA-C-N	6.67	129.21	120.28
11	4	52	ASP	C-N-CA	6.67	129.21	120.28
17	T	111	LEU	CA-C-N	6.67	129.21	120.28
17	T	111	LEU	C-N-CA	6.67	129.21	120.28
20	Z	733	VAL	CB-CA-C	-6.67	103.44	111.97
20	Z	152	GLU	N-CA-C	6.66	118.62	111.36
33	J	15	HIS	CA-C-N	6.66	129.21	120.28
33	J	15	HIS	C-N-CA	6.66	129.21	120.28
4	d	86	ILE	CB-CA-C	-6.66	103.03	112.22
32	M	278	ILE	N-CA-CB	6.66	117.98	110.72
10	3	148	GLY	CA-C-N	6.66	129.49	120.44
10	3	148	GLY	C-N-CA	6.66	129.49	120.44
20	Z	738	TYR	CB-CG-CD1	-6.66	110.81	120.80
1	a	13	ASP	N-CA-C	-6.66	104.38	113.30
14	n	207	GLU	CB-CA-C	-6.66	99.69	110.74
12	5	154	ALA	CA-C-N	6.66	129.09	120.44
12	5	154	ALA	C-N-CA	6.66	129.09	120.44
9	i	171	TRP	N-CA-C	6.66	124.97	110.80
28	H	56	LEU	O-C-N	6.66	129.18	122.12
8	1	185	VAL	N-CA-C	-6.65	98.54	108.12
30	K	294	ARG	NE-CZ-NH2	-6.65	113.21	119.20
30	K	345	ASP	N-CA-C	-6.65	98.61	108.79
27	O	326	HIS	CA-CB-CG	6.65	120.45	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	118	LYS	CA-C-O	-6.65	114.21	119.66
28	H	439	THR	CA-C-N	6.65	130.08	120.38
28	H	439	THR	C-N-CA	6.65	130.08	120.38
1	a	178	ILE	N-CA-C	-6.64	104.02	110.72
16	V	216	LEU	N-CA-C	-6.64	102.58	110.41
25	R	92	ILE	O-C-N	-6.64	116.12	122.16
25	R	297	TYR	N-CA-C	6.64	118.17	111.07
3	c	236	LYS	CA-C-O	-6.63	113.52	120.55
20	Z	952	SER	N-CA-C	-6.63	98.58	108.99
21	N	525	ASN	CA-C-N	6.63	130.13	120.71
21	N	525	ASN	C-N-CA	6.63	130.13	120.71
23	P	119	ILE	N-CA-C	6.63	117.39	110.62
33	J	138	MET	CA-C-O	-6.63	113.52	120.55
2	b	18	LEU	N-CA-CB	6.63	121.18	110.77
16	V	226	LYS	N-CA-CB	6.63	119.83	109.69
20	Z	950	THR	N-CA-C	6.63	120.98	113.02
29	I	68	HIS	CE1-NE2-CD2	-6.63	102.37	109.00
10	j	174	ALA	CA-C-O	6.63	127.45	120.42
26	U	161	ILE	N-CA-C	-6.63	98.83	108.71
10	3	35	GLY	CA-C-O	-6.63	115.39	120.76
18	X	123	ASN	CA-CB-CG	-6.63	105.97	112.60
6	f	130	VAL	CA-C-O	6.62	128.19	121.63
30	K	205	PRO	CA-C-N	6.62	128.12	119.84
30	K	205	PRO	C-N-CA	6.62	128.12	119.84
8	h	90	VAL	CA-C-N	6.62	129.15	120.28
8	h	90	VAL	C-N-CA	6.62	129.15	120.28
13	m	179	PRO	CA-C-N	6.62	130.75	120.75
13	m	179	PRO	C-N-CA	6.62	130.75	120.75
27	O	75	GLN	OE1-CD-NE2	6.62	129.22	122.60
10	j	145	GLN	CA-C-N	6.62	129.47	120.54
10	j	145	GLN	C-N-CA	6.62	129.47	120.54
15	W	26	PHE	N-CA-C	6.62	118.57	111.36
17	T	20	TYR	N-CA-C	-6.62	105.78	114.31
25	R	104	LYS	CA-C-N	6.62	129.04	120.44
25	R	104	LYS	C-N-CA	6.62	129.04	120.44
30	K	422	ASP	CA-C-N	6.62	129.15	120.28
30	K	422	ASP	C-N-CA	6.62	129.15	120.28
6	f	143	HIS	CA-CB-CG	-6.61	107.19	113.80
24	Q	270	ILE	CB-CA-C	6.61	121.07	112.14
25	R	81	HIS	CE1-NE2-CD2	-6.61	102.39	109.00
29	I	269	LYS	CA-C-N	6.61	129.52	120.46
29	I	269	LYS	C-N-CA	6.61	129.52	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	153	ASP	CA-C-N	6.61	130.10	120.71
30	K	153	ASP	C-N-CA	6.61	130.10	120.71
15	W	94	ALA	CA-C-N	6.61	129.68	120.29
15	W	94	ALA	C-N-CA	6.61	129.68	120.29
14	7	183	MET	O-C-N	6.61	129.36	121.76
24	Q	400	TYR	N-CA-C	-6.61	98.20	109.24
32	M	157	ASP	CA-CB-CG	6.61	119.21	112.60
12	l	266	HIS	ND1-CE1-NE2	6.61	115.01	108.40
1	a	123	ASN	N-CA-C	-6.61	103.56	111.69
32	M	144	ASP	N-CA-C	-6.61	98.49	109.46
7	g	123	HIS	CA-CB-CG	-6.61	107.19	113.80
14	n	185	ASN	CA-C-O	-6.61	112.55	118.63
17	T	21	ALA	CA-C-N	6.61	129.79	120.28
17	T	21	ALA	C-N-CA	6.61	129.79	120.28
17	T	69	SER	O-C-N	6.61	130.39	122.27
20	Z	780	MET	CA-C-N	6.61	127.31	119.98
20	Z	780	MET	C-N-CA	6.61	127.31	119.98
16	V	148	LYS	N-CA-C	6.60	118.27	111.14
20	Z	247	GLN	CA-CB-CG	6.60	127.30	114.10
6	f	39	ARG	O-C-N	-6.60	115.12	123.24
25	R	238	PHE	N-CA-C	-6.60	98.22	109.24
10	j	43	ILE	CA-C-N	6.60	132.92	122.36
10	j	43	ILE	C-N-CA	6.60	132.92	122.36
12	l	241	HIS	CE1-NE2-CD2	-6.60	102.40	109.00
13	6	87	HIS	CE1-NE2-CD2	-6.60	102.40	109.00
9	i	147	SER	N-CA-C	-6.60	98.88	109.96
22	S	75	CYS	N-CA-C	-6.60	104.09	111.28
7	g	66	LYS	N-CA-CB	6.59	120.95	110.73
21	N	877	GLN	O-C-N	6.59	129.11	122.12
22	S	48	LEU	N-CA-C	6.59	118.13	111.07
6	f	170	THR	CA-C-O	6.59	127.41	120.42
11	k	76	SER	CA-C-N	6.59	126.37	119.05
11	k	76	SER	C-N-CA	6.59	126.37	119.05
32	M	364	HIS	CA-CB-CG	-6.59	107.21	113.80
6	f	28	ALA	CA-C-N	6.59	131.63	120.29
6	f	28	ALA	C-N-CA	6.59	131.63	120.29
9	2	138	HIS	CE1-NE2-CD2	-6.59	102.41	109.00
16	V	274	GLN	N-CA-C	-6.59	102.38	111.28
26	U	227	GLY	O-C-N	6.59	128.58	122.19
15	W	20	ASP	CA-CB-CG	-6.59	106.01	112.60
30	K	372	ILE	O-C-N	6.59	128.62	121.83
4	d	179	TYR	N-CA-C	-6.59	97.33	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	W	38	GLN	CA-C-N	6.58	129.10	120.28
15	W	38	GLN	C-N-CA	6.58	129.10	120.28
20	Z	151	HIS	N-CA-C	-6.58	105.78	113.88
20	Z	245	VAL	N-CA-C	6.58	116.74	110.42
22	S	133	GLU	CA-C-N	6.58	129.77	120.42
22	S	133	GLU	C-N-CA	6.58	129.77	120.42
30	K	295	ILE	N-CA-C	-6.58	104.10	110.42
13	m	80	VAL	N-CA-C	-6.58	104.34	110.53
23	P	210	ASN	CA-C-O	-6.58	113.57	120.87
30	K	140	HIS	CB-CG-ND1	6.58	132.57	122.70
33	J	322	ALA	N-CA-C	-6.58	104.19	111.36
5	E	16	SER	N-CA-CB	6.58	121.68	110.50
30	K	50	LYS	CA-C-N	6.58	129.63	120.29
30	K	50	LYS	C-N-CA	6.58	129.63	120.29
33	J	260	GLY	N-CA-C	-6.58	101.44	111.24
21	N	436	ASP	N-CA-CB	6.58	121.28	110.69
3	c	60	ASP	N-CA-C	-6.58	103.50	113.89
7	g	126	TYR	CA-C-O	6.58	127.68	120.71
26	U	50	ASN	CA-CB-CG	6.58	119.17	112.60
27	O	236	HIS	CG-CD2-NE2	6.58	113.78	107.20
1	A	85	GLY	CA-C-N	6.57	126.61	119.90
1	A	85	GLY	C-N-CA	6.57	126.61	119.90
23	P	110	LEU	CA-C-N	6.57	130.68	120.82
23	P	110	LEU	C-N-CA	6.57	130.68	120.82
15	W	170	HIS	CG-CD2-NE2	6.57	113.77	107.20
16	V	124	ASN	OD1-CG-ND2	-6.57	116.03	122.60
22	S	268	LEU	N-CA-CB	6.57	119.89	110.16
31	L	428	LEU	O-C-N	-6.57	114.66	122.15
9	2	102	GLU	CA-C-O	6.57	127.86	120.70
22	S	375	ASP	CA-CB-CG	-6.57	106.03	112.60
28	H	105	ILE	O-C-N	-6.57	114.94	122.62
30	K	397	LYS	N-CA-C	-6.57	104.75	112.89
9	i	174	ASP	CA-C-O	-6.57	113.82	122.03
25	R	283	THR	N-CA-C	-6.57	98.28	109.24
28	H	74	THR	N-CA-C	-6.57	100.76	110.48
23	P	138	ARG	O-C-N	-6.56	115.31	122.07
23	P	335	LYS	N-CA-C	-6.56	104.21	111.82
6	f	196	ALA	O-C-N	6.56	129.07	122.12
14	7	152	VAL	N-CA-C	-6.56	98.75	108.45
8	1	163	PHE	CA-C-O	-6.56	113.53	120.55
21	N	914	VAL	CA-C-O	-6.56	113.33	120.67
9	2	64	HIS	ND1-CE1-NE2	6.55	114.95	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	62	TYR	N-CA-CB	6.55	119.75	110.12
18	X	95	GLU	N-CA-C	-6.55	104.43	112.88
24	Q	207	SER	N-CA-C	6.55	119.48	110.24
31	L	186	LEU	CA-C-N	6.55	128.96	120.44
31	L	186	LEU	C-N-CA	6.55	128.96	120.44
21	N	735	MET	CG-SD-CE	-6.55	86.49	100.90
31	L	206	ILE	CA-C-N	6.55	129.59	120.29
31	L	206	ILE	C-N-CA	6.55	129.59	120.29
27	O	357	ILE	O-C-N	6.55	129.57	122.63
33	J	46	ALA	CA-C-N	6.55	129.05	120.28
33	J	46	ALA	C-N-CA	6.55	129.05	120.28
12	l	254	HIS	CE1-NE2-CD2	-6.54	102.45	109.00
14	n	106	GLU	CA-C-O	6.54	127.36	120.42
14	n	212	ASN	CA-CB-CG	-6.54	106.06	112.60
15	W	5	ALA	CA-C-O	6.54	127.65	120.71
4	d	254	HIS	CE1-NE2-CD2	-6.54	102.46	109.00
31	L	342	ARG	N-CA-C	-6.54	104.48	114.16
5	e	205	LYS	CA-C-N	6.54	129.58	120.29
5	e	205	LYS	C-N-CA	6.54	129.58	120.29
12	l	139	ARG	NE-CZ-NH2	6.54	125.09	119.20
32	M	28	GLN	CB-CG-CD	-6.54	101.48	112.60
4	d	246	GLN	CG-CD-OE1	6.54	133.88	120.80
24	Q	198	LEU	CA-C-N	6.54	129.58	120.29
24	Q	198	LEU	C-N-CA	6.54	129.58	120.29
23	P	229	LEU	CA-C-N	6.53	129.69	120.28
23	P	229	LEU	C-N-CA	6.53	129.69	120.28
2	b	88	LYS	CA-C-N	6.53	129.57	120.29
2	b	88	LYS	C-N-CA	6.53	129.57	120.29
28	H	62	ARG	N-CA-C	6.53	118.40	111.28
7	g	82	ILE	CA-C-N	6.53	126.30	119.05
7	g	82	ILE	C-N-CA	6.53	126.30	119.05
17	T	71	GLN	OE1-CD-NE2	-6.53	116.07	122.60
24	Q	5	GLY	CA-C-N	6.53	129.32	120.44
24	Q	5	GLY	C-N-CA	6.53	129.32	120.44
25	R	310	GLU	N-CA-CB	6.53	119.71	110.12
31	L	124	GLY	CA-C-N	6.53	126.44	119.85
31	L	124	GLY	C-N-CA	6.53	126.44	119.85
14	n	185	ASN	CA-C-N	6.53	128.00	119.84
14	n	185	ASN	C-N-CA	6.53	128.00	119.84
32	M	125	GLN	N-CA-C	-6.53	99.39	109.24
21	N	494	LYS	CA-C-N	6.52	126.23	119.64
21	N	494	LYS	C-N-CA	6.52	126.23	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	379	LYS	CA-C-N	6.52	129.56	120.29
27	O	379	LYS	C-N-CA	6.52	129.56	120.29
2	b	200	VAL	N-CA-C	-6.52	98.81	108.85
11	k	169	GLU	O-C-N	-6.52	114.72	122.15
23	P	136	ARG	NE-CZ-NH1	6.52	128.02	121.50
16	V	167	ASN	OD1-CG-ND2	-6.52	116.08	122.60
17	T	169	GLN	N-CA-C	-6.51	104.91	112.92
26	U	15	LEU	CB-CA-C	-6.51	99.78	110.85
30	K	377	SER	N-CA-C	-6.51	106.54	114.75
31	L	292	SER	N-CA-CB	6.51	121.50	110.49
21	N	444	HIS	ND1-CE1-NE2	6.51	114.91	108.40
30	K	321	ALA	CA-C-O	6.51	127.07	119.32
4	d	173	GLU	CA-C-N	6.51	129.00	120.28
4	d	173	GLU	C-N-CA	6.51	129.00	120.28
21	N	118	THR	CA-C-N	6.51	129.53	120.29
21	N	118	THR	C-N-CA	6.51	129.53	120.29
31	L	203	ASN	CA-C-O	-6.51	112.66	120.54
27	O	81	TYR	CB-CG-CD2	-6.51	111.04	120.80
3	c	166	GLY	N-CA-C	6.50	119.45	111.45
13	6	30	VAL	N-CA-C	-6.50	98.68	108.17
8	h	169	SER	CA-C-O	-6.50	113.99	120.82
23	P	211	PRO	CA-C-N	6.50	129.52	120.29
23	P	211	PRO	C-N-CA	6.50	129.52	120.29
24	Q	172	PRO	N-CA-C	-6.50	105.05	113.57
25	R	339	ALA	CA-C-N	6.50	129.28	120.44
25	R	339	ALA	C-N-CA	6.50	129.28	120.44
27	O	166	ARG	CA-C-N	6.50	128.75	120.56
27	O	166	ARG	C-N-CA	6.50	128.75	120.56
28	H	236	ALA	CA-C-N	6.50	129.52	120.29
28	H	236	ALA	C-N-CA	6.50	129.52	120.29
22	S	56	SER	CA-C-N	6.50	129.31	120.54
22	S	56	SER	C-N-CA	6.50	129.31	120.54
12	l	249	SER	N-CA-CB	6.50	121.82	111.56
17	T	123	HIS	O-C-N	6.50	129.56	122.15
27	O	70	TYR	N-CA-CB	6.50	121.47	110.49
21	N	474	SER	CA-C-O	-6.49	113.89	121.16
29	I	344	ILE	CA-C-O	6.49	124.82	118.98
18	X	75	TRP	CD2-CE2-CZ2	-6.49	115.91	122.40
20	Z	154	ILE	N-CA-CB	-6.49	101.71	110.54
28	H	80	HIS	CG-CD2-NE2	6.49	113.69	107.20
33	J	15	HIS	CG-CD2-NE2	6.49	113.69	107.20
13	m	82	TRP	CD2-CE2-CZ2	-6.49	115.91	122.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	4	42	THR	N-CA-C	-6.49	97.20	108.69
15	W	157	PHE	CA-C-N	6.49	129.35	120.46
15	W	157	PHE	C-N-CA	6.49	129.35	120.46
22	S	125	LYS	CA-C-N	6.49	131.34	122.19
22	S	125	LYS	C-N-CA	6.49	131.34	122.19
1	a	37	GLN	N-CA-C	-6.48	104.61	113.30
1	a	51	THR	N-CA-C	-6.48	97.21	108.69
10	3	38	ASN	OD1-CG-ND2	6.48	129.08	122.60
28	H	451	ILE	CB-CA-C	6.48	120.23	111.87
9	i	145	HIS	CE1-NE2-CD2	-6.48	102.52	109.00
11	k	31	SER	CA-C-O	-6.48	111.71	118.65
22	S	173	LEU	CA-C-N	6.48	129.29	120.54
22	S	173	LEU	C-N-CA	6.48	129.29	120.54
29	I	87	LYS	CA-C-N	6.48	129.29	120.54
29	I	87	LYS	C-N-CA	6.48	129.29	120.54
12	l	226	GLU	N-CA-C	-6.48	104.14	111.14
5	e	27	SER	CA-C-N	6.48	130.16	120.31
5	e	27	SER	C-N-CA	6.48	130.16	120.31
11	4	66	LEU	CA-C-N	6.48	128.86	120.44
11	4	66	LEU	C-N-CA	6.48	128.86	120.44
22	S	139	HIS	ND1-CE1-NE2	6.48	114.88	108.40
25	R	141	TYR	CA-C-N	6.48	128.96	120.28
25	R	141	TYR	C-N-CA	6.48	128.96	120.28
30	K	281	ARG	NE-CZ-NH2	-6.48	113.37	119.20
7	g	239	ALA	CA-C-N	6.47	128.72	120.56
7	g	239	ALA	C-N-CA	6.47	128.72	120.56
21	N	191	THR	CA-C-O	6.47	127.41	120.55
33	J	203	ALA	CA-C-N	6.47	128.86	120.44
33	J	203	ALA	C-N-CA	6.47	128.86	120.44
23	P	440	HIS	CB-CG-ND1	6.47	132.41	122.70
7	g	66	LYS	N-CA-C	-6.47	104.54	112.88
17	T	245	TYR	CB-CA-C	-6.47	100.05	110.79
22	S	186	TYR	N-CA-CB	6.47	119.73	110.16
21	N	462	VAL	N-CA-C	-6.47	104.45	110.53
4	d	118	GLN	CA-C-N	6.46	128.94	120.28
4	d	118	GLN	C-N-CA	6.46	128.94	120.28
15	W	128	LEU	N-CA-CB	6.46	120.94	110.40
16	V	208	LYS	N-CA-C	-6.46	103.46	112.45
9	i	43	ILE	CB-CA-C	6.46	119.76	110.33
24	Q	110	SER	N-CA-CB	6.46	121.41	110.49
31	L	56	ALA	CB-CA-C	-6.46	100.73	110.88
14	n	205	VAL	CA-C-N	6.46	128.84	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	n	205	VAL	C-N-CA	6.46	128.84	120.44
8	l	163	PHE	O-C-N	6.46	129.99	122.17
23	P	71	LYS	CA-C-N	6.46	129.46	120.29
23	P	71	LYS	C-N-CA	6.46	129.46	120.29
12	l	239	ALA	CA-C-N	6.46	128.83	120.44
12	l	239	ALA	C-N-CA	6.46	128.83	120.44
22	S	244	ASN	CA-CB-CG	-6.46	106.14	112.60
28	H	357	ARG	N-CA-C	-6.46	99.57	109.64
29	I	304	ARG	CA-C-N	6.46	128.93	120.28
29	I	304	ARG	C-N-CA	6.46	128.93	120.28
31	L	53	HIS	N-CA-C	-6.46	105.22	113.23
16	V	184	ASN	CA-CB-CG	-6.45	106.15	112.60
24	Q	51	ARG	CA-C-N	6.45	129.57	120.28
24	Q	51	ARG	C-N-CA	6.45	129.57	120.28
31	L	394	CYS	CA-C-N	6.45	129.45	120.29
31	L	394	CYS	C-N-CA	6.45	129.45	120.29
24	Q	283	ASN	CA-CB-CG	-6.45	106.15	112.60
25	R	416	LYS	CB-CA-C	-6.45	100.71	110.90
9	2	192	ILE	CB-CA-C	-6.45	103.32	112.22
13	6	134	ASP	CA-CB-CG	6.45	119.05	112.60
16	V	187	ALA	CA-C-N	6.45	129.75	120.79
16	V	187	ALA	C-N-CA	6.45	129.75	120.79
27	O	115	ARG	CA-C-N	6.45	129.21	120.44
27	O	115	ARG	C-N-CA	6.45	129.21	120.44
12	l	144	ARG	NE-CZ-NH1	-6.45	115.05	121.50
23	P	318	TYR	CB-CG-CD2	-6.45	111.13	120.80
33	J	249	GLU	N-CA-CB	6.45	119.78	110.37
23	P	364	ARG	CA-C-N	6.44	128.91	120.28
23	P	364	ARG	C-N-CA	6.44	128.91	120.28
15	W	74	ALA	CA-C-N	6.44	128.40	120.22
15	W	74	ALA	C-N-CA	6.44	128.40	120.22
17	T	222	LEU	CA-C-N	6.44	128.91	120.28
17	T	222	LEU	C-N-CA	6.44	128.91	120.28
26	U	203	LYS	CA-C-N	6.44	128.91	120.28
26	U	203	LYS	C-N-CA	6.44	128.91	120.28
11	4	190	ARG	NH1-CZ-NH2	6.44	127.67	119.30
13	6	94	ILE	N-CA-CB	6.44	120.24	110.58
22	S	163	VAL	CA-C-N	6.44	125.48	120.33
22	S	163	VAL	C-N-CA	6.44	125.48	120.33
10	j	52	GLY	O-C-N	-6.44	118.65	123.61
6	F	210	ASN	N-CA-C	-6.44	106.00	114.31
23	P	139	VAL	CA-C-N	6.44	128.91	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	139	VAL	C-N-CA	6.44	128.91	120.28
12	l	161	LEU	CA-C-N	6.43	129.60	120.53
12	l	161	LEU	C-N-CA	6.43	129.60	120.53
21	N	132	LYS	CA-C-O	-6.43	113.60	120.42
27	O	218	SER	CB-CA-C	-6.43	100.78	110.88
29	I	125	MET	CA-C-N	6.43	127.88	119.84
29	I	125	MET	C-N-CA	6.43	127.88	119.84
31	L	418	ALA	CB-CA-C	-6.43	99.91	110.85
18	X	85	ARG	CD-NE-CZ	-6.43	115.40	124.40
17	T	135	ASN	N-CA-C	-6.43	103.03	113.19
32	M	331	ASP	CA-CB-CG	6.43	119.03	112.60
30	K	198	TYR	N-CA-C	6.43	119.28	111.82
2	b	181	ASP	CA-CB-CG	-6.43	106.17	112.60
14	7	169	THR	O-C-N	-6.43	115.89	123.41
21	N	24	ALA	CA-C-O	-6.43	113.74	120.55
23	P	325	ASP	N-CA-CB	6.43	120.35	109.87
21	N	390	LEU	CA-C-O	-6.42	113.80	120.87
13	6	160	ASN	N-CA-C	-6.42	105.48	113.38
32	M	25	LEU	CA-C-N	6.42	133.80	121.54
32	M	25	LEU	C-N-CA	6.42	133.80	121.54
4	d	105	THR	CA-C-N	6.42	129.54	120.42
4	d	105	THR	C-N-CA	6.42	129.54	120.42
29	I	67	ASP	CA-CB-CG	-6.42	106.18	112.60
13	6	62	ALA	N-CA-C	-6.42	96.79	108.02
23	P	416	SER	N-CA-CB	6.42	120.23	110.28
33	J	333	ARG	NE-CZ-NH1	-6.42	115.08	121.50
24	Q	145	HIS	CA-CB-CG	-6.42	107.39	113.80
7	g	204	HIS	N-CA-C	-6.41	105.41	112.72
12	l	140	LEU	CA-C-O	6.41	127.22	120.42
11	4	67	TYR	CA-CB-CG	-6.41	102.36	113.90
21	N	311	ILE	CA-C-O	6.41	127.17	120.25
27	O	145	LYS	CA-C-N	6.41	128.87	120.28
27	O	145	LYS	C-N-CA	6.41	128.87	120.28
23	P	165	VAL	N-CA-C	-6.41	104.25	110.72
22	S	227	ASN	OD1-CG-ND2	6.41	129.01	122.60
24	Q	1	MET	CA-C-N	6.41	129.15	120.44
24	Q	1	MET	C-N-CA	6.41	129.15	120.44
32	M	377	GLN	CB-CG-CD	6.41	123.49	112.60
33	J	144	ASP	CA-C-N	6.41	130.42	120.75
33	J	144	ASP	C-N-CA	6.41	130.42	120.75
14	n	122	PRO	CA-C-N	6.40	129.50	120.28
14	n	122	PRO	C-N-CA	6.40	129.50	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	35	ILE	CA-C-N	6.40	129.38	120.29
17	T	35	ILE	C-N-CA	6.40	129.38	120.29
9	2	143	HIS	CE1-NE2-CD2	-6.40	102.60	109.00
28	H	235	PHE	CA-C-N	6.40	128.76	120.44
28	H	235	PHE	C-N-CA	6.40	128.76	120.44
31	L	66	GLU	N-CA-C	6.40	118.26	111.28
31	L	81	ILE	N-CA-CB	6.40	119.24	110.54
13	m	90	LYS	N-CA-CB	6.40	119.56	109.71
12	5	202	PHE	CA-CB-CG	-6.40	107.40	113.80
3	c	202	ASP	CA-CB-CG	6.40	119.00	112.60
13	6	52	PHE	N-CA-C	-6.40	99.27	109.76
30	K	69	LYS	CA-C-N	6.40	129.38	120.29
30	K	69	LYS	C-N-CA	6.40	129.38	120.29
31	L	55	LYS	CA-C-N	6.40	128.76	120.44
31	L	55	LYS	C-N-CA	6.40	128.76	120.44
32	M	405	ASN	CA-C-O	6.40	127.33	119.97
33	J	276	LEU	CA-C-N	6.40	128.85	120.28
33	J	276	LEU	C-N-CA	6.40	128.85	120.28
14	n	245	LEU	N-CA-CB	6.40	119.38	110.17
22	S	146	LEU	CA-C-N	6.40	128.75	120.44
22	S	146	LEU	C-N-CA	6.40	128.75	120.44
13	6	140	GLU	N-CA-C	-6.39	98.95	108.99
32	M	180	TYR	CB-CG-CD2	6.39	130.39	120.80
30	K	104	ASP	N-CA-C	-6.39	97.19	110.80
3	c	31	HIS	ND1-CE1-NE2	6.39	114.79	108.40
24	Q	89	ALA	N-CA-C	6.39	120.18	111.17
7	g	10	LEU	N-CA-C	-6.39	104.40	111.36
27	O	80	LYS	O-C-N	-6.39	115.35	122.12
28	H	242	PRO	CA-C-O	-6.39	111.30	120.56
9	i	149	ASP	N-CA-C	-6.39	99.62	109.52
24	Q	53	GLU	CA-C-N	6.39	129.48	120.28
24	Q	53	GLU	C-N-CA	6.39	129.48	120.28
30	K	214	PRO	O-C-N	6.39	124.25	121.31
14	n	83	VAL	CA-C-O	6.39	127.10	120.39
10	3	67	PHE	CA-C-N	6.39	128.84	120.28
10	3	67	PHE	C-N-CA	6.39	128.84	120.28
14	7	221	ASP	CA-CB-CG	-6.38	106.22	112.60
25	R	64	LYS	O-C-N	6.38	128.89	122.12
5	e	245	GLU	N-CA-C	-6.38	105.50	113.28
29	I	68	HIS	CG-CD2-NE2	6.38	113.58	107.20
17	T	162	ASP	CA-C-N	6.38	128.73	120.44
17	T	162	ASP	C-N-CA	6.38	128.73	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	185	HIS	CE1-NE2-CD2	-6.38	102.62	109.00
21	N	417	ARG	N-CA-C	-6.38	105.13	113.17
32	M	247	ALA	CA-C-N	6.38	127.65	120.06
32	M	247	ALA	C-N-CA	6.38	127.65	120.06
14	n	197	ASP	CA-C-O	6.38	126.81	119.35
12	5	141	HIS	ND1-CE1-NE2	6.38	114.78	108.40
24	Q	30	LEU	CA-C-N	6.38	128.73	120.44
24	Q	30	LEU	C-N-CA	6.38	128.73	120.44
28	H	377	PHE	N-CA-CB	6.38	119.83	109.95
27	O	387	ARG	N-CA-C	-6.38	100.13	110.20
24	Q	105	GLU	N-CA-CB	6.37	119.59	110.16
28	H	132	GLN	CB-CG-CD	-6.37	101.76	112.60
3	c	194	LEU	CA-C-N	6.37	128.82	120.28
3	c	194	LEU	C-N-CA	6.37	128.82	120.28
5	e	188	HIS	N-CA-C	-6.37	99.95	108.74
16	V	290	ASN	CA-CB-CG	-6.37	106.23	112.60
30	K	227	ALA	CA-C-N	6.37	128.72	120.44
30	K	227	ALA	C-N-CA	6.37	128.72	120.44
6	f	85	SER	CA-C-N	6.37	128.81	120.28
6	f	85	SER	C-N-CA	6.37	128.81	120.28
8	l	108	VAL	N-CA-C	-6.37	99.19	108.11
8	h	177	SER	CA-C-O	6.37	126.80	119.35
29	I	137	ASP	N-CA-C	-6.37	100.78	109.95
32	M	235	CYS	CB-CA-C	-6.37	100.03	110.85
9	i	64	HIS	CE1-NE2-CD2	-6.37	102.64	109.00
13	6	50	LYS	N-CA-C	-6.37	104.67	112.88
22	S	47	THR	CA-CB-OG1	6.37	119.15	109.60
14	n	136	ARG	NE-CZ-NH2	-6.36	113.47	119.20
21	N	79	VAL	N-CA-C	6.36	117.11	110.62
21	N	735	MET	CA-C-N	6.36	128.71	120.44
21	N	735	MET	C-N-CA	6.36	128.71	120.44
8	h	91	PHE	CB-CA-C	-6.36	100.23	110.79
22	S	328	PRO	CA-C-O	-6.36	114.18	121.56
33	J	59	LYS	N-CA-C	6.36	119.02	111.71
13	6	161	GLN	OE1-CD-NE2	6.36	128.96	122.60
31	L	415	LEU	N-CA-C	6.36	118.29	111.36
1	a	88	PRO	CA-C-N	6.36	129.97	120.31
1	a	88	PRO	C-N-CA	6.36	129.97	120.31
29	I	356	SER	CA-C-N	6.36	128.70	120.44
29	I	356	SER	C-N-CA	6.36	128.70	120.44
4	d	119	ARG	NE-CZ-NH2	-6.36	113.48	119.20
9	i	145	HIS	CG-CD2-NE2	6.36	113.56	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	147	HIS	CB-CG-CD2	6.36	139.46	131.20
22	S	371	LEU	CA-C-N	6.36	128.80	120.28
22	S	371	LEU	C-N-CA	6.36	128.80	120.28
12	l	139	ARG	N-CA-CB	6.35	119.56	110.16
21	N	426	ILE	CA-C-N	6.35	128.69	120.56
21	N	426	ILE	C-N-CA	6.35	128.69	120.56
3	c	22	VAL	CA-C-N	6.35	128.70	120.44
3	c	22	VAL	C-N-CA	6.35	128.70	120.44
4	d	102	ASP	CA-C-N	6.35	127.78	119.84
4	d	102	ASP	C-N-CA	6.35	127.78	119.84
18	X	111	LEU	CA-C-N	6.35	129.89	120.87
18	X	111	LEU	C-N-CA	6.35	129.89	120.87
21	N	778	LYS	CA-C-N	6.35	133.97	121.58
21	N	778	LYS	C-N-CA	6.35	133.97	121.58
24	Q	152	LYS	N-CA-C	-6.35	104.27	111.07
22	S	460	VAL	CA-C-N	6.35	129.43	120.28
22	S	460	VAL	C-N-CA	6.35	129.43	120.28
1	a	117	LEU	N-CA-C	-6.35	104.44	111.36
20	Z	735	GLU	CB-CA-C	-6.35	98.88	110.63
22	S	307	LEU	N-CA-C	6.35	118.20	111.28
32	M	277	ILE	N-CA-C	-6.35	98.59	107.80
15	W	109	ARG	NE-CZ-NH1	6.35	127.85	121.50
17	T	44	LEU	CA-C-O	-6.35	113.11	120.98
21	N	827	GLU	CB-CG-CD	-6.35	101.81	112.60
24	Q	6	SER	N-CA-CB	6.35	119.27	110.07
15	W	164	PRO	N-CA-C	6.35	120.80	111.03
23	P	359	ARG	CD-NE-CZ	-6.34	115.52	124.40
31	L	149	ASP	CA-CB-CG	-6.34	106.26	112.60
17	T	28	PRO	CB-CA-C	6.34	118.66	110.92
13	6	103	HIS	N-CA-CB	6.34	119.55	110.16
9	2	32	ILE	N-CA-C	-6.34	98.92	108.17
8	h	113	ASP	N-CA-C	-6.33	104.81	113.30
27	O	268	SER	CA-C-O	-6.33	114.17	120.70
5	e	49	GLY	N-CA-C	-6.33	101.06	111.38
5	e	77	ALA	CA-C-O	-6.33	113.29	120.32
22	S	78	VAL	O-C-N	-6.33	115.70	121.91
26	U	77	ASN	CA-C-N	6.33	129.28	120.29
26	U	77	ASN	C-N-CA	6.33	129.28	120.29
27	O	216	ASP	CA-C-N	6.33	128.67	120.44
27	O	216	ASP	C-N-CA	6.33	128.67	120.44
13	m	135	PRO	O-C-N	6.33	130.39	122.22
14	n	244	ASN	OD1-CG-ND2	-6.33	116.27	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	W	60	ARG	NE-CZ-NH2	6.33	124.90	119.20
15	W	82	GLU	N-CA-C	-6.33	98.09	108.41
24	Q	340	ASP	CA-CB-CG	-6.33	106.27	112.60
13	m	16	ASN	OD1-CG-ND2	-6.33	116.27	122.60
13	6	88	ASN	N-CA-C	6.33	120.12	111.39
16	V	47	MET	O-C-N	-6.33	116.65	123.42
30	K	171	TYR	CA-C-N	6.33	129.05	120.44
30	K	171	TYR	C-N-CA	6.33	129.05	120.44
32	M	391	LEU	CA-C-N	6.33	128.76	120.28
32	M	391	LEU	C-N-CA	6.33	128.76	120.28
26	U	215	ILE	CA-C-O	-6.33	112.95	118.96
28	H	162	ARG	N-CA-C	-6.33	103.19	113.19
12	l	118	GLY	N-CA-C	-6.33	101.44	111.18
14	7	209	ALA	CA-C-N	6.33	128.66	120.56
14	7	209	ALA	C-N-CA	6.33	128.66	120.56
17	T	127	GLN	N-CA-CB	6.33	119.42	110.12
29	I	327	ALA	CB-CA-C	-6.33	98.85	109.48
32	M	334	ASP	CA-C-O	-6.33	113.59	120.17
1	a	126	GLN	OE1-CD-NE2	6.32	128.92	122.60
4	d	220	ASP	CA-CB-CG	-6.32	106.28	112.60
12	l	255	VAL	CB-CA-C	6.32	118.48	111.08
25	R	277	LEU	O-C-N	6.32	129.36	122.15
30	K	281	ARG	CA-C-O	6.32	127.19	120.36
10	j	73	LEU	O-C-N	6.32	128.82	122.12
21	N	375	HIS	CE1-NE2-CD2	-6.32	102.68	109.00
9	i	195	ASP	CA-CB-CG	6.32	118.92	112.60
24	Q	211	PRO	CA-C-N	6.32	129.38	120.28
24	Q	211	PRO	C-N-CA	6.32	129.38	120.28
2	b	221	LEU	CA-C-O	6.32	127.04	119.59
5	e	190	SER	CA-C-N	6.32	130.10	120.82
5	e	190	SER	C-N-CA	6.32	130.10	120.82
11	k	146	HIS	CB-CG-ND1	6.32	132.17	122.70
10	3	41	GLU	N-CA-C	-6.32	100.35	110.14
16	V	32	ILE	N-CA-CB	6.32	119.13	110.54
26	U	131	GLY	N-CA-C	-6.32	98.21	113.18
32	M	404	ARG	CA-C-N	6.32	129.91	120.31
32	M	404	ARG	C-N-CA	6.32	129.91	120.31
21	N	130	ASP	CA-CB-CG	-6.31	106.29	112.60
28	H	65	GLU	CA-C-N	6.31	129.25	120.29
28	H	65	GLU	C-N-CA	6.31	129.25	120.29
28	H	403	ARG	CA-C-N	6.31	129.25	120.29
28	H	403	ARG	C-N-CA	6.31	129.25	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	144	ASN	N-CA-C	-6.31	105.52	113.72
11	k	59	TYR	CA-C-N	6.31	129.38	120.42
11	k	59	TYR	C-N-CA	6.31	129.38	120.42
13	6	203	HIS	CB-CG-CD2	6.31	139.40	131.20
8	h	38	ARG	NE-CZ-NH2	6.31	124.88	119.20
10	j	152	SER	N-CA-C	-6.31	104.40	111.28
8	l	164	ILE	CA-C-O	-6.31	114.39	120.95
17	T	151	TRP	N-CA-C	-6.31	103.93	111.69
19	Y	41	ASP	CA-C-O	6.31	127.20	120.70
21	N	425	ASN	N-CA-CB	6.31	119.50	110.16
6	f	188	GLU	CA-C-O	6.31	127.22	119.97
10	j	144	ASP	CA-C-N	6.31	128.64	120.44
10	j	144	ASP	C-N-CA	6.31	128.64	120.44
12	l	251	ASN	OD1-CG-ND2	6.31	128.91	122.60
14	7	76	ILE	N-CA-C	-6.31	100.85	107.60
14	7	219	TYR	CB-CA-C	-6.31	100.94	110.90
25	R	193	ALA	CA-C-O	6.31	127.22	119.97
14	n	148	ILE	N-CA-C	-6.31	99.40	108.48
27	O	250	TRP	N-CA-CB	6.30	119.49	110.16
28	H	63	ILE	N-CA-C	6.30	117.05	110.62
16	V	277	LYS	CA-C-N	6.30	128.72	120.28
16	V	277	LYS	C-N-CA	6.30	128.72	120.28
25	R	365	ASP	CA-C-N	6.30	129.24	120.29
25	R	365	ASP	C-N-CA	6.30	129.24	120.29
25	R	384	VAL	CA-C-N	6.30	129.24	120.29
25	R	384	VAL	C-N-CA	6.30	129.24	120.29
11	4	81	SER	O-C-N	-6.30	114.52	122.27
16	V	45	VAL	O-C-N	-6.30	114.14	121.07
27	O	170	SER	CA-C-N	6.30	129.23	120.29
27	O	170	SER	C-N-CA	6.30	129.23	120.29
17	T	161	TRP	CA-C-N	6.29	128.72	120.28
17	T	161	TRP	C-N-CA	6.29	128.72	120.28
5	e	204	LEU	CA-C-N	6.29	129.23	120.29
5	e	204	LEU	C-N-CA	6.29	129.23	120.29
13	m	180	LEU	CA-C-N	6.29	129.65	120.71
13	m	180	LEU	C-N-CA	6.29	129.65	120.71
16	V	27	VAL	N-CA-CB	6.29	118.17	111.00
31	L	229	THR	CA-C-N	6.29	129.34	120.28
31	L	229	THR	C-N-CA	6.29	129.34	120.28
6	f	98	VAL	CA-C-O	-6.29	114.08	120.69
21	N	146	LYS	N-CA-CB	6.29	120.03	110.28
25	R	387	ILE	CA-CB-CG1	6.29	121.09	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	311	ASN	OD1-CG-ND2	6.29	128.89	122.60
30	K	395	VAL	CA-CB-CG2	-6.29	99.71	110.40
33	J	377	VAL	N-CA-C	-6.29	100.70	109.45
29	I	63	GLU	CB-CG-CD	-6.29	101.91	112.60
21	N	411	ILE	CB-CA-C	-6.29	103.92	111.97
26	U	285	ILE	N-CA-CB	6.29	119.09	110.54
27	O	183	ASN	O-C-N	-6.29	114.23	122.59
8	1	107	ILE	N-CA-C	-6.29	99.37	108.17
21	N	637	ALA	O-C-N	6.29	128.78	122.12
23	P	407	ASN	OD1-CG-ND2	6.29	128.88	122.60
13	m	108	LYS	CA-C-N	6.28	132.41	122.11
13	m	108	LYS	C-N-CA	6.28	132.41	122.11
22	S	19	HIS	O-C-N	6.28	128.54	122.07
14	n	93	MET	O-C-N	6.28	128.54	122.07
24	Q	53	GLU	N-CA-C	6.28	118.12	111.28
2	b	128	ARG	N-CA-C	-6.28	98.17	109.09
9	i	225	ARG	NE-CZ-NH1	6.28	127.78	121.50
15	W	25	ARG	CD-NE-CZ	-6.28	115.61	124.40
16	V	213	LEU	N-CA-C	6.28	118.12	111.28
21	N	355	TRP	CE2-CD2-CE3	6.28	125.08	118.80
32	M	170	MET	CB-CA-C	-6.28	101.03	110.88
16	V	257	GLU	N-CA-C	-6.28	97.43	110.80
28	H	58	ASP	CA-C-O	-6.28	113.90	120.55
17	T	160	ALA	CA-C-N	6.27	128.97	120.44
17	T	160	ALA	C-N-CA	6.27	128.97	120.44
21	N	228	VAL	CB-CA-C	-6.27	103.94	111.97
21	N	316	LYS	CB-CA-C	-6.27	100.19	110.85
26	U	134	THR	N-CA-C	-6.27	98.40	109.06
17	T	54	ASP	CA-CB-CG	-6.27	106.33	112.60
6	f	106	GLU	N-CA-CB	6.27	119.10	110.01
9	2	145	HIS	CA-CB-CG	-6.27	107.53	113.80
10	3	130	ILE	CA-CB-CG2	-6.27	99.84	110.50
25	R	300	ASP	CA-CB-CG	-6.27	106.33	112.60
2	b	3	ASP	CA-CB-CG	-6.27	106.33	112.60
2	b	189	ILE	N-CA-CB	6.27	117.88	110.55
10	j	127	ILE	CA-C-N	6.27	133.69	121.41
10	j	127	ILE	C-N-CA	6.27	133.69	121.41
17	T	230	ASN	OD1-CG-ND2	-6.27	116.33	122.60
7	g	112	PHE	N-CA-C	-6.26	104.53	111.36
18	X	82	LYS	CA-C-O	6.26	127.36	119.78
21	N	286	LEU	CA-C-N	6.26	128.58	120.44
21	N	286	LEU	C-N-CA	6.26	128.58	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I	392	ILE	N-CA-C	-6.26	104.23	110.62
29	I	117	HIS	CG-CD2-NE2	6.26	113.46	107.20
23	P	166	GLU	CA-C-O	-6.26	111.56	120.51
5	e	188	HIS	CE1-NE2-CD2	-6.26	102.74	109.00
12	5	272	PHE	CA-C-O	6.26	127.39	120.82
13	6	87	HIS	CA-C-N	6.26	131.25	122.36
13	6	87	HIS	C-N-CA	6.26	131.25	122.36
21	N	36	TRP	N-CA-CB	6.26	119.32	110.12
1	a	169	THR	O-C-N	-6.26	116.72	123.42
12	l	205	GLY	N-CA-C	-6.26	101.51	110.46
23	P	18	LYS	N-CA-C	-6.26	105.80	113.50
10	j	12	VAL	N-CA-C	-6.26	99.14	108.46
24	Q	28	LEU	CA-C-O	6.26	127.18	120.55
20	Z	257	PRO	CA-C-N	6.25	126.82	120.38
20	Z	257	PRO	C-N-CA	6.25	126.82	120.38
23	P	107	SER	CA-C-N	6.25	132.79	121.97
23	P	107	SER	C-N-CA	6.25	132.79	121.97
10	j	13	VAL	CB-CA-C	6.25	119.90	110.90
22	S	217	PHE	CA-C-N	6.25	129.17	120.29
22	S	217	PHE	C-N-CA	6.25	129.17	120.29
27	O	38	TRP	CD2-CE2-CZ2	-6.25	116.15	122.40
27	O	164	PRO	CA-C-N	6.25	129.28	120.28
27	O	164	PRO	C-N-CA	6.25	129.28	120.28
21	N	32	VAL	N-CA-C	6.25	116.42	110.42
22	S	403	SER	CA-C-N	6.25	129.81	120.31
22	S	403	SER	C-N-CA	6.25	129.81	120.31
27	O	142	ASP	O-C-N	-6.25	114.39	122.83
21	N	421	ASP	CA-C-N	6.25	128.56	120.44
21	N	421	ASP	C-N-CA	6.25	128.56	120.44
29	I	335	ASP	CA-C-N	6.25	125.87	119.56
29	I	335	ASP	C-N-CA	6.25	125.87	119.56
30	K	108	GLY	N-CA-C	-6.25	102.55	111.42
33	J	316	PHE	N-CA-CB	6.25	119.13	110.01
12	l	255	VAL	N-CA-CB	6.25	117.95	110.95
21	N	511	GLY	CA-C-N	6.25	129.16	120.29
21	N	511	GLY	C-N-CA	6.25	129.16	120.29
24	Q	95	LYS	CA-C-N	6.25	128.43	120.56
24	Q	95	LYS	C-N-CA	6.25	128.43	120.56
22	S	108	ALA	O-C-N	-6.25	114.28	122.59
1	a	240	ASN	CA-CB-CG	-6.24	106.36	112.60
12	l	221	TRP	N-CA-C	-6.24	106.26	114.31
23	P	155	GLU	CB-CA-C	-6.24	101.04	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	J	302	PRO	CB-CA-C	-6.24	102.99	112.11
23	P	8	LYS	CA-C-O	-6.24	114.27	120.70
20	Z	948	TRP	N-CA-C	-6.24	104.58	111.82
23	P	365	LEU	CA-C-N	6.24	128.55	120.44
23	P	365	LEU	C-N-CA	6.24	128.55	120.44
33	J	288	ILE	O-C-N	-6.24	116.58	123.20
14	n	129	LEU	N-CA-CB	6.24	119.06	110.01
21	N	684	SER	CA-C-N	6.24	129.28	120.42
21	N	684	SER	C-N-CA	6.24	129.28	120.42
23	P	36	LEU	CA-C-N	6.24	128.64	120.28
23	P	36	LEU	C-N-CA	6.24	128.64	120.28
25	R	23	ASN	CA-CB-CG	6.24	118.84	112.60
25	R	139	GLU	N-CA-CB	6.24	119.11	110.07
33	J	137	MET	CA-C-N	6.24	128.64	120.28
33	J	137	MET	C-N-CA	6.24	128.64	120.28
32	M	397	GLU	CA-C-N	6.24	129.15	120.29
32	M	397	GLU	C-N-CA	6.24	129.15	120.29
6	F	233	TYR	N-CA-C	-6.24	106.89	114.75
11	4	39	SER	CA-C-O	-6.24	114.64	120.94
31	L	90	LYS	CA-C-N	6.24	129.14	120.29
31	L	90	LYS	C-N-CA	6.24	129.14	120.29
33	J	380	GLU	CA-C-N	6.23	129.14	120.29
33	J	380	GLU	C-N-CA	6.23	129.14	120.29
9	2	217	ARG	CD-NE-CZ	-6.23	115.67	124.40
23	P	37	ASP	N-CA-CB	6.23	119.28	110.12
27	O	332	ILE	CA-C-O	6.23	127.43	120.95
5	e	22	PHE	N-CA-CB	6.23	119.95	110.42
6	f	23	GLU	CB-CA-C	-6.23	100.26	110.85
14	7	226	ARG	NE-CZ-NH1	-6.23	115.27	121.50
32	M	302	GLN	CA-C-N	6.23	128.63	120.28
32	M	302	GLN	C-N-CA	6.23	128.63	120.28
21	N	329	HIS	CG-CD2-NE2	6.23	113.43	107.20
22	S	378	GLN	CA-C-N	6.23	129.14	120.29
22	S	378	GLN	C-N-CA	6.23	129.14	120.29
23	P	79	LEU	CA-C-N	6.23	128.63	120.28
23	P	79	LEU	C-N-CA	6.23	128.63	120.28
25	R	367	ASP	CA-CB-CG	-6.23	106.37	112.60
27	O	310	PHE	CA-C-O	-6.23	113.82	120.42
29	I	203	THR	N-CA-C	6.23	118.15	111.36
6	f	51	ARG	CA-CB-CG	6.22	126.55	114.10
8	h	68	VAL	CA-C-N	6.22	128.62	120.28
8	h	68	VAL	C-N-CA	6.22	128.62	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	190	HIS	CA-C-N	6.22	126.89	119.98
16	V	190	HIS	C-N-CA	6.22	126.89	119.98
17	T	269	SER	CA-C-N	6.22	129.26	120.42
17	T	269	SER	C-N-CA	6.22	129.26	120.42
25	R	230	LEU	CB-CA-C	-6.22	101.06	110.90
32	M	126	THR	N-CA-CB	6.22	121.14	110.68
24	Q	152	LYS	CA-C-N	6.22	128.53	120.44
24	Q	152	LYS	C-N-CA	6.22	128.53	120.44
26	U	19	LEU	CA-C-N	6.22	128.53	120.44
26	U	19	LEU	C-N-CA	6.22	128.53	120.44
2	b	178	ARG	N-CA-C	-6.22	105.85	113.50
4	d	51	THR	CA-C-N	6.22	129.67	120.90
4	d	51	THR	C-N-CA	6.22	129.67	120.90
19	Y	30	GLU	CA-C-N	6.22	133.42	121.54
19	Y	30	GLU	C-N-CA	6.22	133.42	121.54
26	U	48	VAL	N-CA-CB	6.22	118.96	111.31
30	K	283	ASP	N-CA-C	-6.22	99.87	109.14
10	j	85	GLU	CA-C-N	6.22	129.12	120.29
10	j	85	GLU	C-N-CA	6.22	129.12	120.29
28	H	364	ALA	O-C-N	6.22	128.71	122.12
29	I	196	GLU	CB-CG-CD	-6.22	102.03	112.60
10	j	83	GLU	CA-C-O	-6.22	114.24	120.64
29	I	420	LYS	N-CA-CB	6.22	119.26	110.12
32	M	331	ASP	CA-C-N	6.22	128.47	120.70
32	M	331	ASP	C-N-CA	6.22	128.47	120.70
32	M	400	MET	CG-SD-CE	-6.22	87.22	100.90
31	L	133	ASN	O-C-N	6.21	129.24	122.15
12	5	175	MET	N-CA-CB	6.21	120.55	110.42
3	c	128	LEU	CA-C-O	-6.21	114.97	121.55
4	d	37	LYS	CA-C-N	6.21	130.99	122.04
4	d	37	LYS	C-N-CA	6.21	130.99	122.04
24	Q	180	LEU	O-C-N	6.21	129.91	122.27
27	O	52	ALA	N-CA-C	-6.21	101.18	110.06
32	M	195	GLU	CB-CG-CD	-6.21	102.04	112.60
33	J	190	PRO	N-CA-CB	6.21	106.67	103.19
13	6	195	SER	N-CA-C	6.21	118.05	111.28
19	Y	11	GLN	CB-CG-CD	-6.21	102.04	112.60
25	R	382	ASP	CA-C-N	6.21	131.20	120.58
25	R	382	ASP	C-N-CA	6.21	131.20	120.58
8	1	115	ASN	O-C-N	6.21	129.00	122.23
26	U	165	GLU	O-C-N	-6.21	115.08	122.15
27	O	275	SER	CA-C-O	-6.21	113.35	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	50	LYS	N-CA-C	6.21	118.04	111.28
11	k	92	ILE	CA-C-N	6.20	131.19	120.58
11	k	92	ILE	C-N-CA	6.20	131.19	120.58
27	O	175	ASN	OD1-CG-ND2	6.20	128.80	122.60
28	H	237	THR	N-CA-C	-6.20	104.60	111.36
7	g	135	SER	O-C-N	6.20	131.29	123.23
13	m	114	TYR	N-CA-C	-6.20	102.94	110.88
14	7	208	GLU	CA-C-O	-6.20	114.31	120.82
27	O	221	ALA	CB-CA-C	-6.20	100.31	110.85
31	L	146	VAL	CB-CA-C	-6.20	99.83	110.30
31	L	191	ARG	CA-CB-CG	6.20	126.50	114.10
31	L	360	ILE	N-CA-C	6.20	116.94	110.62
24	Q	336	ASN	CA-CB-CG	-6.20	106.41	112.60
30	K	58	TYR	N-CA-CB	6.20	119.88	110.28
33	J	13	GLU	CA-C-N	6.20	129.09	120.29
33	J	13	GLU	C-N-CA	6.20	129.09	120.29
29	I	420	LYS	O-C-N	6.19	128.69	122.12
5	e	95	ALA	CA-C-N	6.19	128.58	120.28
5	e	95	ALA	C-N-CA	6.19	128.58	120.28
8	1	72	LEU	N-CA-C	-6.19	105.88	113.50
8	1	100	ASP	N-CA-C	-6.19	105.03	112.59
16	V	185	ILE	N-CA-C	-6.19	96.46	109.34
24	Q	364	LYS	CA-C-N	6.19	128.48	120.56
24	Q	364	LYS	C-N-CA	6.19	128.48	120.56
12	l	227	ASP	CA-C-N	6.19	129.72	120.31
12	l	227	ASP	C-N-CA	6.19	129.72	120.31
9	2	170	HIS	CE1-NE2-CD2	-6.19	102.81	109.00
21	N	474	SER	CA-C-N	6.19	128.48	120.44
21	N	474	SER	C-N-CA	6.19	128.48	120.44
26	U	298	ASN	CA-C-N	6.19	128.57	120.28
26	U	298	ASN	C-N-CA	6.19	128.57	120.28
20	Z	947	GLY	CA-C-N	6.18	129.71	120.31
20	Z	947	GLY	C-N-CA	6.18	129.71	120.31
21	N	79	VAL	CB-CA-C	6.18	120.49	112.14
31	L	391	ILE	N-CA-C	6.18	116.97	110.72
16	V	220	GLN	CA-C-O	6.18	127.10	120.55
23	P	155	GLU	CA-C-N	6.18	128.56	120.28
23	P	155	GLU	C-N-CA	6.18	128.56	120.28
2	b	228	PRO	N-CA-C	-6.18	106.77	114.68
10	j	73	LEU	CA-C-N	6.18	129.07	120.29
10	j	73	LEU	C-N-CA	6.18	129.07	120.29
8	1	143	ILE	CA-C-N	6.18	128.85	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	143	ILE	C-N-CA	6.18	128.85	120.38
24	Q	332	ARG	NE-CZ-NH2	6.18	124.76	119.20
17	T	48	ASN	N-CA-CB	6.18	121.62	111.62
23	P	226	LYS	CA-C-N	6.18	128.34	120.56
23	P	226	LYS	C-N-CA	6.18	128.34	120.56
13	m	202	ARG	NH1-CZ-NH2	6.17	127.33	119.30
14	7	95	HIS	ND1-CE1-NE2	6.17	114.58	108.40
22	S	397	LEU	CA-C-O	-6.17	113.88	120.42
22	S	467	PHE	CA-CB-CG	6.17	119.97	113.80
25	R	129	GLU	CA-C-N	6.17	128.55	120.28
25	R	129	GLU	C-N-CA	6.17	128.55	120.28
31	L	430	GLY	O-C-N	-6.17	116.82	122.93
33	J	25	GLN	CA-C-N	6.17	128.55	120.28
33	J	25	GLN	C-N-CA	6.17	128.55	120.28
17	T	250	MET	N-CA-C	-6.17	104.39	112.41
28	H	214	CYS	N-CA-C	-6.17	99.34	109.40
11	4	70	ARG	CB-CA-C	-6.17	101.19	110.88
2	b	79	GLY	CA-C-N	6.17	126.35	119.32
2	b	79	GLY	C-N-CA	6.17	126.35	119.32
21	N	621	THR	O-C-N	-6.17	115.72	122.07
32	M	23	LEU	CA-C-O	-6.17	113.88	120.42
32	M	196	ALA	N-CA-C	6.17	118.08	111.36
8	h	129	HIS	N-CA-C	-6.17	97.38	108.48
11	4	163	LEU	CB-CA-C	-6.17	101.16	110.90
14	7	87	SER	O-C-N	-6.17	115.71	123.17
21	N	333	SER	N-CA-CB	6.17	119.01	110.07
10	j	72	ASN	CB-CA-C	6.17	120.67	110.81
10	3	22	ALA	CA-C-O	-6.17	112.96	120.54
21	N	273	LEU	N-CA-C	6.17	118.97	111.82
27	O	59	LEU	CA-C-O	-6.17	114.02	120.55
27	O	64	ASN	CB-CG-ND2	-6.17	107.15	116.40
8	h	95	CYS	CA-C-N	6.16	129.04	120.29
8	h	95	CYS	C-N-CA	6.16	129.04	120.29
21	N	169	ALA	CA-C-N	6.16	129.04	120.29
21	N	169	ALA	C-N-CA	6.16	129.04	120.29
29	I	102	ASN	O-C-N	-6.16	115.77	122.06
27	O	203	THR	O-C-N	-6.16	116.31	123.27
9	i	150	VAL	CA-C-O	6.16	126.89	120.36
27	O	356	ARG	NE-CZ-NH1	-6.16	115.34	121.50
29	I	326	MET	CB-CA-C	-6.16	100.82	110.74
24	Q	354	PHE	O-C-N	-6.16	115.16	123.10
25	R	327	ASP	CA-C-N	6.16	128.53	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	327	ASP	C-N-CA	6.16	128.53	120.28
22	S	440	ASP	N-CA-CB	6.16	119.86	110.44
29	I	81	ILE	O-C-N	-6.16	115.60	121.94
3	c	235	ILE	N-CA-C	-6.16	104.50	110.72
5	e	158	ALA	N-CA-CB	6.16	121.54	110.83
11	4	19	LYS	CA-C-O	6.16	126.17	119.15
28	H	370	ARG	NE-CZ-NH2	-6.16	113.66	119.20
9	i	234	PHE	CA-CB-CG	-6.15	107.65	113.80
27	O	327	LEU	O-C-N	6.15	128.64	122.12
29	I	232	LEU	O-C-N	6.15	128.64	122.12
9	i	75	ALA	N-CA-C	-6.15	100.06	109.41
5	e	15	PHE	O-C-N	-6.15	115.98	123.30
14	n	234	ASP	N-CA-C	-6.15	100.17	109.95
10	3	19	ASP	CA-CB-CG	-6.15	106.45	112.60
15	W	99	LYS	O-C-N	6.15	128.73	122.09
23	P	249	ALA	CA-C-N	6.15	129.15	120.42
23	P	249	ALA	C-N-CA	6.15	129.15	120.42
21	N	585	ARG	CA-C-N	6.15	129.02	120.29
21	N	585	ARG	C-N-CA	6.15	129.02	120.29
21	N	660	LEU	CA-C-N	6.15	129.65	120.31
21	N	660	LEU	C-N-CA	6.15	129.65	120.31
31	L	232	ALA	CA-C-O	6.15	127.07	120.55
15	W	91	LEU	N-CA-CB	6.15	119.16	110.12
30	K	196	ASP	CA-C-N	6.15	128.51	120.28
30	K	196	ASP	C-N-CA	6.15	128.51	120.28
15	W	121	SER	CA-C-O	-6.14	114.86	121.56
21	N	464	GLU	N-CA-C	6.14	117.98	111.28
23	P	320	PRO	N-CA-C	-6.14	107.61	114.92
1	a	64	LEU	O-C-N	-6.14	116.00	123.19
1	a	139	VAL	CA-C-N	6.14	130.76	122.90
1	a	139	VAL	C-N-CA	6.14	130.76	122.90
10	j	134	LYS	N-CA-C	-6.14	103.48	111.71
18	X	38	ASN	CA-CB-CG	-6.14	106.46	112.60
24	Q	382	LEU	CA-C-O	-6.14	112.91	119.97
3	c	33	GLY	CA-C-N	6.14	129.48	120.82
3	c	33	GLY	C-N-CA	6.14	129.48	120.82
13	m	47	TYR	N-CA-C	-6.14	98.27	108.34
12	5	141	HIS	CE1-NE2-CD2	-6.14	102.86	109.00
29	I	90	GLU	CA-C-N	6.14	128.51	120.28
29	I	90	GLU	C-N-CA	6.14	128.51	120.28
5	e	20	ARG	NE-CZ-NH2	6.14	124.72	119.20
21	N	21	LYS	CA-C-N	6.14	128.42	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	21	LYS	C-N-CA	6.14	128.42	120.44
25	R	380	VAL	CA-C-N	6.14	131.26	123.10
25	R	380	VAL	C-N-CA	6.14	131.26	123.10
27	O	228	TYR	CA-CB-CG	-6.14	102.85	113.90
20	Z	718	ASP	CA-C-N	6.14	126.92	119.99
20	Z	718	ASP	C-N-CA	6.14	126.92	119.99
23	P	153	ILE	O-C-N	6.14	127.82	121.87
2	b	160	LYS	N-CA-C	-6.13	106.12	113.97
20	Z	85	VAL	CA-C-O	-6.13	111.73	119.95
21	N	89	PHE	CA-CB-CG	-6.13	107.67	113.80
30	K	355	THR	CA-C-N	6.13	129.13	120.42
30	K	355	THR	C-N-CA	6.13	129.13	120.42
7	g	49	ALA	CA-C-O	6.13	127.86	120.99
8	h	195	LEU	N-CA-CB	6.13	122.22	111.55
30	K	396	ARG	N-CA-C	6.13	117.96	111.28
32	M	65	ASN	CA-CB-CG	-6.13	106.47	112.60
6	f	110	HIS	CE1-NE2-CD2	-6.13	102.87	109.00
21	N	901	GLY	CA-C-N	6.13	130.38	121.80
21	N	901	GLY	C-N-CA	6.13	130.38	121.80
30	K	236	ARG	CB-CA-C	6.13	120.28	111.82
6	f	182	ILE	N-CA-CB	6.13	118.38	111.21
15	W	40	LYS	CA-C-N	6.12	128.49	120.28
15	W	40	LYS	C-N-CA	6.12	128.49	120.28
16	V	181	ASN	CA-CB-CG	-6.12	106.47	112.60
33	J	75	VAL	CA-CB-CG2	-6.12	99.99	110.40
11	4	162	LYS	CA-C-N	6.12	128.77	120.44
11	4	162	LYS	C-N-CA	6.12	128.77	120.44
21	N	318	LYS	CA-C-N	6.12	128.77	120.44
21	N	318	LYS	C-N-CA	6.12	128.77	120.44
2	b	182	GLU	CB-CG-CD	-6.12	102.19	112.60
22	S	297	ILE	CB-CA-C	-6.12	103.77	112.22
24	Q	99	THR	O-C-N	-6.12	115.63	122.12
12	l	122	GLY	N-CA-C	-6.12	104.14	112.52
23	P	346	ILE	CA-C-O	-6.12	113.64	120.25
33	J	294	THR	CA-C-O	-6.12	114.72	121.33
22	S	434	ALA	N-CA-C	-6.12	100.49	109.18
24	Q	309	ARG	NE-CZ-NH1	-6.12	115.38	121.50
26	U	126	LYS	N-CA-C	-6.12	105.85	113.38
3	c	227	GLN	CG-CD-NE2	6.12	125.57	116.40
6	f	34	VAL	CA-C-O	-6.12	114.19	121.28
24	Q	87	GLN	CA-C-O	-6.12	114.07	120.55
24	Q	273	ASN	CA-CB-CG	6.12	118.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	J	38	THR	N-CA-C	6.12	117.94	111.28
8	h	198	TYR	CA-C-N	6.11	125.51	118.85
8	h	198	TYR	C-N-CA	6.11	125.51	118.85
12	l	283	ASN	OD1-CG-ND2	-6.11	116.49	122.60
9	2	211	LYS	CA-CB-CG	6.11	126.32	114.10
22	S	347	HIS	CA-C-N	6.11	128.47	120.28
22	S	347	HIS	C-N-CA	6.11	128.47	120.28
13	m	50	LYS	N-CA-C	-6.11	103.42	113.50
15	W	170	HIS	ND1-CE1-NE2	6.11	114.51	108.40
30	K	77	ARG	NE-CZ-NH2	-6.11	113.70	119.20
9	i	43	ILE	N-CA-C	-6.11	99.32	108.12
22	S	263	ASP	N-CA-CB	6.11	121.36	110.79
24	Q	193	LYS	N-CA-C	-6.11	105.66	113.23
24	Q	308	ASN	OD1-CG-ND2	6.11	128.71	122.60
26	U	81	LYS	N-CA-CB	6.11	119.62	110.22
27	O	203	THR	N-CA-CB	6.11	120.38	110.43
33	J	166	LEU	CA-C-N	6.11	126.00	119.28
33	J	166	LEU	C-N-CA	6.11	126.00	119.28
13	m	118	ILE	N-CA-CB	6.10	120.43	111.52
14	n	164	ASN	CA-C-N	6.10	128.46	120.28
14	n	164	ASN	C-N-CA	6.10	128.46	120.28
12	5	82	ARG	CA-C-N	6.10	131.26	122.23
12	5	82	ARG	C-N-CA	6.10	131.26	122.23
21	N	7	ALA	CA-C-N	6.10	125.82	119.05
21	N	7	ALA	C-N-CA	6.10	125.82	119.05
8	l	71	HIS	ND1-CE1-NE2	6.10	114.50	108.40
31	L	304	THR	CA-C-O	6.10	126.89	120.42
31	L	357	ARG	CA-C-N	6.10	128.45	120.28
31	L	357	ARG	C-N-CA	6.10	128.45	120.28
17	T	106	ILE	CA-C-N	6.10	128.45	120.28
17	T	106	ILE	C-N-CA	6.10	128.45	120.28
21	N	584	ARG	N-CA-C	6.10	117.59	111.07
23	P	246	GLN	OE1-CD-NE2	6.10	128.70	122.60
33	J	153	LEU	N-CA-CB	6.10	121.29	111.65
1	a	183	GLU	CA-C-N	6.10	128.45	120.28
1	a	183	GLU	C-N-CA	6.10	128.45	120.28
13	m	172	THR	CA-C-N	6.09	131.32	122.36
13	m	172	THR	C-N-CA	6.09	131.32	122.36
20	Z	24	THR	CA-C-O	-6.09	111.81	120.16
21	N	222	TYR	CA-C-N	6.09	128.45	120.28
21	N	222	TYR	C-N-CA	6.09	128.45	120.28
22	S	358	LYS	CA-C-O	6.09	126.88	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	318	TYR	CB-CG-CD1	6.09	129.94	120.80
5	e	73	HIS	CA-CB-CG	6.09	119.89	113.80
5	e	156	PHE	CA-CB-CG	-6.09	107.71	113.80
13	m	136	VAL	CA-CB-CG1	-6.09	100.04	110.40
8	l	60	ASP	CA-CB-CG	-6.09	106.51	112.60
11	4	152	MET	CG-SD-CE	-6.09	87.50	100.90
23	P	431	HIS	N-CA-CB	6.09	119.18	110.16
29	I	370	ASN	CA-CB-CG	-6.09	106.51	112.60
31	L	392	ARG	CG-CD-NE	-6.09	98.60	112.00
15	W	157	PHE	CA-CB-CG	-6.09	107.71	113.80
21	N	713	VAL	CA-CB-CG2	6.09	120.75	110.40
2	b	94	HIS	ND1-CE1-NE2	6.09	114.49	108.40
7	g	9	ASP	CA-CB-CG	-6.09	106.51	112.60
13	m	57	ASN	CA-CB-CG	-6.09	106.51	112.60
14	7	39	VAL	N-CA-C	-6.09	99.59	108.11
21	N	448	LEU	CA-C-N	6.09	126.74	119.98
21	N	448	LEU	C-N-CA	6.09	126.74	119.98
24	Q	227	CYS	CA-C-N	6.09	129.56	120.31
24	Q	227	CYS	C-N-CA	6.09	129.56	120.31
33	J	244	ILE	CB-CA-C	-6.09	101.62	110.63
21	N	283	ASP	O-C-N	-6.08	115.03	121.30
21	N	498	ILE	N-CA-C	-6.08	104.57	110.72
3	c	236	LYS	O-C-N	6.08	128.57	122.12
9	2	138	HIS	ND1-CE1-NE2	6.08	114.48	108.40
23	P	38	GLN	N-CA-C	6.08	118.71	111.71
26	U	146	ASP	N-CA-CB	6.08	120.77	110.49
29	I	308	GLU	N-CA-C	-6.08	104.73	111.36
30	K	308	GLN	N-CA-CB	6.08	120.77	110.49
10	3	150	CYS	O-C-N	-6.08	115.81	122.07
25	R	89	ASN	CA-CB-CG	-6.08	106.52	112.60
14	n	170	TYR	CB-CG-CD1	-6.08	111.68	120.80
6	f	5	ASN	OD1-CG-ND2	6.08	128.68	122.60
13	6	48	GLU	O-C-N	-6.08	114.33	121.32
33	J	396	THR	N-CA-C	-6.08	105.86	113.28
23	P	20	GLU	N-CA-C	-6.08	105.44	112.92
11	4	120	ASP	CA-CB-CG	-6.08	106.52	112.60
27	O	322	ASP	CA-CB-CG	-6.08	106.52	112.60
27	O	352	TRP	CA-C-O	6.08	128.01	120.54
31	L	295	THR	CA-C-O	-6.08	114.78	121.89
20	Z	413	ASP	CA-C-N	6.07	126.72	119.98
20	Z	413	ASP	C-N-CA	6.07	126.72	119.98
21	N	388	PRO	CA-C-O	-6.07	111.25	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	459	GLN	N-CA-CB	-6.07	101.17	110.16
23	P	311	TRP	CA-C-O	-6.07	112.45	118.34
27	O	105	GLN	CA-C-O	6.07	126.86	120.42
32	M	378	GLU	CA-C-N	6.07	128.91	120.29
32	M	378	GLU	C-N-CA	6.07	128.91	120.29
28	H	388	ILE	CA-C-N	6.07	128.42	120.28
28	H	388	ILE	C-N-CA	6.07	128.42	120.28
9	i	87	LEU	CA-C-O	6.07	126.86	120.42
14	n	216	VAL	CA-CB-CG1	6.07	120.72	110.40
20	Z	353	VAL	N-CA-CB	6.07	114.32	110.50
25	R	378	ASN	OD1-CG-ND2	6.07	128.67	122.60
6	f	14	SER	CA-C-N	6.07	125.77	119.82
6	f	14	SER	C-N-CA	6.07	125.77	119.82
7	g	228	HIS	CG-CD2-NE2	6.07	113.27	107.20
10	j	166	THR	CA-C-O	-6.07	114.06	120.55
17	T	123	HIS	CE1-NE2-CD2	-6.07	102.93	109.00
24	Q	142	ALA	CA-C-N	6.07	128.33	120.44
24	Q	142	ALA	C-N-CA	6.07	128.33	120.44
3	c	14	SER	N-CA-CB	6.07	116.34	109.49
15	W	152	GLU	O-C-N	6.07	130.27	123.05
28	H	80	HIS	CE1-NE2-CD2	-6.07	102.94	109.00
7	g	157	TYR	CA-C-O	6.06	127.88	121.33
21	N	535	LEU	CA-C-N	6.06	129.03	120.42
21	N	535	LEU	C-N-CA	6.06	129.03	120.42
31	L	277	ILE	N-CA-C	-6.06	99.62	108.11
14	n	168	VAL	CA-CB-CG1	6.06	120.70	110.40
9	2	31	THR	N-CA-C	-6.06	100.09	109.24
24	Q	29	SER	CA-C-O	6.06	126.84	120.42
31	L	361	PHE	O-C-N	6.06	128.54	122.12
17	T	272	ASN	CA-CB-CG	6.06	118.66	112.60
21	N	819	LYS	CA-C-O	-6.06	114.13	120.55
22	S	466	LYS	CA-C-N	6.06	128.32	120.44
22	S	466	LYS	C-N-CA	6.06	128.32	120.44
24	Q	386	PHE	CA-CB-CG	6.06	119.86	113.80
33	J	102	ILE	O-C-N	6.06	129.78	123.05
2	b	78	MET	O-C-N	-6.06	116.10	123.19
12	5	206	SER	N-CA-C	-6.06	104.76	111.36
15	W	47	ASN	OD1-CG-ND2	-6.06	116.54	122.60
21	N	51	ASP	CA-CB-CG	-6.06	106.54	112.60
21	N	570	ARG	CA-C-N	6.06	128.89	120.29
21	N	570	ARG	C-N-CA	6.06	128.89	120.29
25	R	107	GLU	CA-C-O	-6.06	114.42	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	204	HIS	CE1-NE2-CD2	-6.05	102.94	109.00
9	2	247	VAL	N-CA-CB	6.05	121.39	111.58
30	K	79	LEU	N-CA-C	-6.05	104.68	111.28
21	N	515	ARG	CA-C-N	6.05	127.70	120.14
21	N	515	ARG	C-N-CA	6.05	127.70	120.14
21	N	352	ASN	N-CA-CB	6.05	118.71	110.42
22	S	452	TYR	CA-C-N	6.05	130.82	120.72
22	S	452	TYR	C-N-CA	6.05	130.82	120.72
27	O	59	LEU	N-CA-CB	6.05	119.01	110.12
9	i	202	VAL	N-CA-CB	6.05	119.50	111.64
22	S	374	ASP	CA-CB-CG	-6.05	106.55	112.60
26	U	125	VAL	N-CA-C	-6.05	107.09	112.90
29	I	205	PRO	CA-C-N	6.05	128.66	120.38
29	I	205	PRO	C-N-CA	6.05	128.66	120.38
22	S	63	LEU	CA-C-N	6.04	128.38	120.28
22	S	63	LEU	C-N-CA	6.04	128.38	120.28
33	J	171	PRO	CA-C-N	6.04	128.87	120.29
33	J	171	PRO	C-N-CA	6.04	128.87	120.29
25	R	180	PHE	CA-CB-CG	6.04	119.84	113.80
33	J	284	THR	CA-C-N	6.04	133.08	121.54
33	J	284	THR	C-N-CA	6.04	133.08	121.54
7	g	64	ASN	N-CA-C	-6.04	99.15	109.24
11	k	183	ILE	CA-CB-CG2	-6.04	100.23	110.50
22	S	68	LEU	O-C-N	6.04	129.83	122.58
30	K	285	GLN	OE1-CD-NE2	-6.04	116.56	122.60
14	7	41	GLY	O-C-N	-6.04	118.34	123.60
6	f	187	ASP	CB-CA-C	-6.04	100.77	110.79
17	T	146	ILE	CA-C-N	6.04	128.37	120.28
17	T	146	ILE	C-N-CA	6.04	128.37	120.28
23	P	111	ASP	CA-CB-CG	-6.04	106.56	112.60
9	2	184	ALA	CA-C-O	6.04	127.16	120.82
33	J	204	HIS	CE1-NE2-CD2	-6.04	102.96	109.00
3	c	129	ARG	CA-C-N	6.04	127.39	119.84
3	c	129	ARG	C-N-CA	6.04	127.39	119.84
5	e	26	TYR	CA-C-N	6.04	128.37	120.28
5	e	26	TYR	C-N-CA	6.04	128.37	120.28
10	3	175	ALA	O-C-N	-6.04	115.27	122.15
21	N	522	ALA	CA-C-N	6.04	128.65	120.38
21	N	522	ALA	C-N-CA	6.04	128.65	120.38
28	H	420	ARG	CA-C-N	6.04	128.28	120.44
28	H	420	ARG	C-N-CA	6.04	128.28	120.44
9	i	236	ARG	NE-CZ-NH1	-6.03	115.47	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	W	35	PHE	CA-CB-CG	6.03	119.83	113.80
19	Y	86	ARG	NE-CZ-NH2	-6.03	113.77	119.20
27	O	326	HIS	ND1-CE1-NE2	6.03	114.43	108.40
15	W	118	ILE	CA-CB-CG1	6.03	120.65	110.40
24	Q	138	SER	CA-C-N	6.03	128.98	120.42
24	Q	138	SER	C-N-CA	6.03	128.98	120.42
25	R	325	HIS	CB-CG-CD2	-6.03	123.36	131.20
31	L	260	ALA	CA-C-N	6.03	128.36	120.28
31	L	260	ALA	C-N-CA	6.03	128.36	120.28
12	5	95	ALA	CA-C-O	6.03	126.84	120.33
16	V	50	MET	CA-C-O	6.03	128.57	121.58
33	J	12	LEU	CA-C-N	6.03	128.96	120.28
33	J	12	LEU	C-N-CA	6.03	128.96	120.28
33	J	201	ALA	N-CA-C	6.03	117.65	111.14
18	X	108	ASN	CA-C-N	6.03	130.50	120.86
18	X	108	ASN	C-N-CA	6.03	130.50	120.86
30	K	66	ASP	CA-C-N	6.03	128.35	120.28
30	K	66	ASP	C-N-CA	6.03	128.35	120.28
24	Q	78	ILE	CA-C-N	6.02	125.72	119.82
24	Q	78	ILE	C-N-CA	6.02	125.72	119.82
25	R	360	SER	CA-C-N	6.02	128.15	120.56
25	R	360	SER	C-N-CA	6.02	128.15	120.56
29	I	234	LYS	CA-C-N	6.02	129.16	120.79
29	I	234	LYS	C-N-CA	6.02	129.16	120.79
23	P	420	ASP	CA-CB-CG	-6.02	106.58	112.60
32	M	360	ILE	CA-C-N	6.02	128.35	120.28
32	M	360	ILE	C-N-CA	6.02	128.35	120.28
10	j	91	VAL	N-CA-CB	6.02	119.61	110.58
14	7	257	ASP	CA-CB-CG	-6.02	106.58	112.60
5	e	99	HIS	CA-C-N	6.02	130.91	120.68
5	e	99	HIS	C-N-CA	6.02	130.91	120.68
23	P	123	ARG	NE-CZ-NH1	6.02	127.52	121.50
27	O	140	LYS	CA-C-N	6.02	133.04	121.54
27	O	140	LYS	C-N-CA	6.02	133.04	121.54
28	H	253	GLY	CA-C-N	6.02	133.32	121.58
28	H	253	GLY	C-N-CA	6.02	133.32	121.58
17	T	260	ILE	N-CA-C	-6.02	104.64	110.72
23	P	440	HIS	CB-CG-CD2	-6.02	123.38	131.20
32	M	154	LEU	O-C-N	-6.02	116.37	123.41
4	d	246	GLN	N-CA-C	-6.02	105.94	113.28
31	L	270	ALA	CA-C-O	-6.02	114.04	120.42
4	d	31	THR	CA-C-N	6.01	131.25	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	31	THR	C-N-CA	6.01	131.25	122.77
13	m	165	LYS	O-C-N	-6.01	116.21	123.13
20	Z	207	ILE	N-CA-C	-6.01	105.82	113.22
21	N	362	TRP	CZ3-CH2-CZ2	-6.01	113.68	121.50
30	K	228	ASN	CA-C-N	6.01	133.25	122.06
30	K	228	ASN	C-N-CA	6.01	133.25	122.06
26	U	192	ASN	CA-CB-CG	6.01	118.61	112.60
27	O	57	LEU	N-CA-C	-6.01	105.70	113.16
2	b	43	VAL	N-CA-C	-6.01	99.07	108.81
9	i	180	ALA	N-CA-CB	6.01	118.96	110.12
2	b	18	LEU	N-CA-C	-6.01	98.49	108.34
21	N	110	VAL	N-CA-C	-6.01	104.88	110.53
5	e	22	PHE	CA-C-N	6.01	128.93	120.28
5	e	22	PHE	C-N-CA	6.01	128.93	120.28
7	g	246	GLU	CA-C-O	-6.01	114.05	120.42
29	I	219	VAL	N-CA-CB	6.01	119.88	111.05
14	n	184	ALA	N-CA-C	6.01	117.91	111.36
10	3	101	GLY	CA-C-N	6.01	125.98	120.03
10	3	101	GLY	C-N-CA	6.01	125.98	120.03
13	6	70	ASP	N-CA-C	-6.01	106.11	113.50
24	Q	22	GLU	CA-C-O	-6.01	114.05	120.42
29	I	94	LYS	CA-C-O	-6.01	114.51	120.82
33	J	227	SER	N-CA-C	-6.01	105.26	112.59
16	V	159	ILE	CA-C-N	6.00	130.26	121.31
16	V	159	ILE	C-N-CA	6.00	130.26	121.31
32	M	293	SER	CA-C-N	6.00	133.01	121.54
32	M	293	SER	C-N-CA	6.00	133.01	121.54
9	i	170	HIS	CE1-NE2-CD2	-6.00	103.00	109.00
26	U	295	LYS	CA-C-N	6.00	128.94	120.42
26	U	295	LYS	C-N-CA	6.00	128.94	120.42
27	O	86	LEU	CA-C-N	6.00	130.85	120.58
27	O	86	LEU	C-N-CA	6.00	130.85	120.58
31	L	107	GLU	CA-C-O	-6.00	114.27	120.99
1	A	130	GLN	N-CA-C	-6.00	104.70	112.68
16	V	255	ILE	O-C-N	6.00	128.17	122.05
22	S	46	LEU	N-CA-C	-6.00	104.61	112.41
14	n	104	VAL	N-CA-C	-6.00	104.50	110.62
24	Q	105	GLU	CA-C-N	6.00	128.32	120.28
24	Q	105	GLU	C-N-CA	6.00	128.32	120.28
26	U	298	ASN	N-CA-CB	6.00	119.04	110.16
31	L	77	ARG	CA-C-N	6.00	128.24	120.44
31	L	77	ARG	C-N-CA	6.00	128.24	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	187	VAL	CA-C-O	6.00	126.84	120.48
8	1	62	GLN	CA-C-N	6.00	128.31	120.28
8	1	62	GLN	C-N-CA	6.00	128.31	120.28
21	N	57	ASP	CA-CB-CG	-6.00	106.60	112.60
26	U	25	THR	CA-CB-OG1	6.00	118.59	109.60
29	I	107	GLY	CA-C-O	-6.00	114.77	121.31
8	1	71	HIS	CE1-NE2-CD2	-6.00	103.00	109.00
28	H	385	ARG	CA-C-N	6.00	128.31	120.28
28	H	385	ARG	C-N-CA	6.00	128.31	120.28
3	c	171	ALA	CB-CA-C	-5.99	100.66	110.85
7	g	173	LYS	O-C-N	5.99	129.23	122.22
12	l	266	HIS	CA-CB-CG	-5.99	107.81	113.80
21	N	732	GLY	O-C-N	-5.99	116.20	122.13
24	Q	205	ALA	CA-C-N	5.99	128.80	120.29
24	Q	205	ALA	C-N-CA	5.99	128.80	120.29
30	K	198	TYR	O-C-N	5.99	129.64	122.27
15	W	107	HIS	CB-CG-CD2	-5.99	123.41	131.20
24	Q	243	PHE	CA-CB-CG	-5.99	107.81	113.80
25	R	192	GLU	N-CA-CB	5.99	119.03	110.16
25	R	217	HIS	CB-CG-ND1	5.99	131.69	122.70
32	M	355	ASP	CA-CB-CG	-5.99	106.61	112.60
12	5	268	VAL	N-CA-C	-5.99	103.42	111.44
19	Y	74	THR	CA-C-N	5.99	128.79	120.29
19	Y	74	THR	C-N-CA	5.99	128.79	120.29
29	I	137	ASP	N-CA-CB	5.99	119.70	110.60
13	6	43	ILE	N-CA-CB	5.99	117.66	110.95
18	X	11	ARG	NE-CZ-NH2	5.99	124.59	119.20
26	U	156	HIS	CE1-NE2-CD2	-5.99	103.01	109.00
12	5	92	ASP	CA-CB-CG	5.99	118.59	112.60
23	P	83	SER	N-CA-CB	5.99	118.69	110.01
31	L	255	TYR	N-CA-C	-5.99	100.79	109.59
17	T	161	TRP	CA-CB-CG	5.98	124.97	113.60
29	I	291	ARG	NE-CZ-NH2	5.98	124.59	119.20
27	O	212	GLN	CA-C-O	5.98	126.76	120.42
32	M	413	GLU	CA-C-N	5.98	128.30	120.28
32	M	413	GLU	C-N-CA	5.98	128.30	120.28
33	J	385	ALA	CA-C-O	-5.98	114.21	120.55
3	c	133	VAL	O-C-N	-5.98	116.18	123.00
5	e	177	GLU	N-CA-C	5.98	117.60	111.14
11	4	156	GLU	CA-C-O	5.98	126.85	119.97
12	5	277	GLU	CA-C-N	5.98	128.57	120.44
12	5	277	GLU	C-N-CA	5.98	128.57	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	681	ASN	CA-CB-CG	-5.98	106.62	112.60
25	R	90	GLU	N-CA-C	-5.98	104.17	112.30
7	g	29	LYS	CA-C-N	5.98	128.78	120.29
7	g	29	LYS	C-N-CA	5.98	128.78	120.29
31	L	311	GLN	OE1-CD-NE2	-5.98	116.62	122.60
2	b	229	THR	N-CA-C	-5.98	106.03	113.38
18	X	69	ILE	N-CA-C	-5.98	101.38	107.89
27	O	58	ARG	NE-CZ-NH1	-5.98	115.52	121.50
28	H	398	VAL	CA-C-O	5.98	127.72	121.44
16	V	142	ASP	CA-CB-CG	-5.98	106.62	112.60
22	S	184	TRP	N-CA-C	5.98	118.58	111.71
14	n	93	MET	CA-C-N	5.97	128.29	120.28
14	n	93	MET	C-N-CA	5.97	128.29	120.28
23	P	293	LEU	N-CA-CB	5.97	119.08	110.06
32	M	104	GLY	CA-C-N	5.97	132.95	121.54
32	M	104	GLY	C-N-CA	5.97	132.95	121.54
4	d	24	LEU	O-C-N	5.97	128.96	122.15
7	g	149	TYR	CB-CG-CD2	5.97	129.76	120.80
12	5	201	ILE	N-CA-CB	5.97	121.15	111.36
21	N	765	ASP	CA-C-N	5.97	131.23	122.63
21	N	765	ASP	C-N-CA	5.97	131.23	122.63
23	P	197	THR	O-C-N	-5.97	114.47	122.23
29	I	77	SER	N-CA-C	5.97	118.58	111.71
29	I	361	ILE	N-CA-C	-5.97	104.69	110.72
24	Q	320	GLN	CA-C-O	5.97	126.28	119.18
25	R	77	SER	CA-C-O	-5.97	114.71	120.92
7	g	209	GLU	N-CA-C	-5.97	106.04	113.38
11	k	95	ARG	NE-CZ-NH2	5.97	124.57	119.20
33	J	150	VAL	N-CA-CB	5.97	117.81	111.00
2	B	219	PRO	N-CA-C	-5.97	107.82	114.92
2	b	14	PRO	N-CA-CB	5.97	109.84	103.52
19	Y	36	GLU	N-CA-CB	5.97	118.96	110.67
33	J	346	VAL	O-C-N	5.97	127.76	121.91
21	N	106	ILE	CA-C-N	5.96	129.38	120.31
21	N	106	ILE	C-N-CA	5.96	129.38	120.31
12	l	125	ALA	CA-C-N	5.96	128.19	120.44
12	l	125	ALA	C-N-CA	5.96	128.19	120.44
8	1	154	ASN	CA-CB-CG	-5.96	106.64	112.60
17	T	134	LYS	O-C-N	5.96	128.21	122.07
12	l	210	PHE	CA-CB-CG	-5.96	107.84	113.80
14	n	187	LEU	CA-C-N	5.96	128.27	120.28
14	n	187	LEU	C-N-CA	5.96	128.27	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	622	ALA	CA-C-N	5.96	128.27	120.28
21	N	622	ALA	C-N-CA	5.96	128.27	120.28
26	U	153	THR	CA-CB-OG1	5.96	118.54	109.60
31	L	67	HIS	O-C-N	5.96	128.95	122.15
6	f	216	VAL	N-CA-C	-5.96	100.48	108.35
6	f	219	ASP	N-CA-C	-5.96	104.67	113.61
10	j	101	GLY	O-C-N	-5.96	115.81	121.77
21	N	256	GLN	CA-C-N	5.96	128.63	120.46
21	N	256	GLN	C-N-CA	5.96	128.63	120.46
10	j	169	GLN	O-C-N	-5.96	115.93	122.07
30	K	42	ASN	CA-C-O	-5.96	114.23	120.55
33	J	205	HIS	CE1-NE2-CD2	-5.96	103.04	109.00
12	l	266	HIS	CE1-NE2-CD2	-5.96	103.04	109.00
16	V	109	HIS	CE1-NE2-CD2	-5.96	103.04	109.00
21	N	213	PHE	CA-CB-CG	-5.96	107.84	113.80
23	P	198	VAL	CB-CA-C	-5.96	104.34	111.97
30	K	360	MET	N-CA-CB	5.96	119.07	110.37
8	h	47	HIS	N-CA-CB	5.96	120.55	110.49
26	U	272	GLU	CA-C-N	5.96	128.26	120.28
26	U	272	GLU	C-N-CA	5.96	128.26	120.28
6	f	179	PHE	N-CA-C	5.95	118.73	111.82
7	g	157	TYR	N-CA-C	-5.95	100.02	109.07
31	L	414	ASP	CA-C-O	-5.95	114.24	120.55
16	V	290	ASN	O-C-N	5.95	128.94	122.15
17	T	8	THR	O-C-N	5.95	130.41	122.43
20	Z	210	TYR	CA-C-N	5.95	128.25	120.28
20	Z	210	TYR	C-N-CA	5.95	128.25	120.28
26	U	19	LEU	N-CA-CB	5.95	118.64	110.01
29	I	236	VAL	N-CA-C	5.95	117.40	110.62
24	Q	29	SER	N-CA-C	5.95	117.84	111.36
25	R	398	ALA	CA-C-N	5.95	128.74	120.29
25	R	398	ALA	C-N-CA	5.95	128.74	120.29
33	J	382	PHE	CA-C-O	-5.95	114.57	120.70
9	2	124	GLY	CA-C-N	5.95	129.28	120.95
9	2	124	GLY	C-N-CA	5.95	129.28	120.95
13	6	142	GLU	CB-CG-CD	-5.95	102.49	112.60
8	1	47	HIS	N-CA-C	-5.95	99.69	108.79
21	N	695	ALA	CA-C-N	5.95	128.73	120.29
21	N	695	ALA	C-N-CA	5.95	128.73	120.29
22	S	61	SER	CA-C-N	5.95	128.53	120.44
22	S	61	SER	C-N-CA	5.95	128.53	120.44
24	Q	364	LYS	O-C-N	-5.95	115.94	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	264	ASP	CB-CA-C	-5.95	100.74	110.85
32	M	431	SER	N-CA-CB	5.95	120.54	110.49
17	T	132	HIS	CE1-NE2-CD2	-5.94	103.06	109.00
6	F	14	SER	N-CA-CB	5.94	120.60	110.50
22	S	347	HIS	ND1-CE1-NE2	5.94	114.34	108.40
31	L	418	ALA	N-CA-C	5.94	117.84	111.36
33	J	385	ALA	N-CA-C	5.94	117.76	111.28
6	f	187	ASP	N-CA-CB	5.94	118.85	110.12
11	4	190	ARG	O-C-N	5.94	130.91	123.19
21	N	910	PRO	N-CD-CG	5.94	112.11	103.20
32	M	43	ILE	CA-C-N	5.94	128.24	120.28
32	M	43	ILE	C-N-CA	5.94	128.24	120.28
12	l	179	TYR	CB-CG-CD1	5.94	129.71	120.80
3	c	6	TYR	CA-C-N	5.94	129.14	120.71
3	c	6	TYR	C-N-CA	5.94	129.14	120.71
22	S	373	LYS	CB-CA-C	-5.94	100.94	110.79
23	P	104	LEU	O-C-N	5.94	128.41	122.12
29	I	348	ILE	CB-CA-C	-5.94	103.00	111.31
2	b	181	ASP	CB-CA-C	-5.94	100.59	110.68
2	b	247	LEU	N-CA-CB	5.93	118.94	110.16
6	f	36	VAL	N-CA-C	-5.93	99.57	108.12
16	V	181	ASN	N-CA-CB	5.93	120.44	110.77
22	S	228	GLU	N-CA-C	-5.93	104.89	111.36
31	L	369	LYS	N-CA-C	-5.93	100.03	109.76
14	7	232	ILE	N-CA-CB	5.93	119.32	111.25
19	Y	83	ARG	NE-CZ-NH1	5.93	127.43	121.50
22	S	431	VAL	CA-C-N	5.93	130.49	120.29
22	S	431	VAL	C-N-CA	5.93	130.49	120.29
30	K	90	GLN	N-CA-CB	5.93	118.84	110.12
7	g	186	GLY	CA-C-O	-5.93	116.42	122.59
10	j	55	GLY	CA-C-N	5.93	132.87	121.54
10	j	55	GLY	C-N-CA	5.93	132.87	121.54
2	B	30	GLN	N-CA-C	-5.93	106.59	113.88
8	1	68	VAL	CA-C-N	5.93	128.23	120.28
8	1	68	VAL	C-N-CA	5.93	128.23	120.28
14	7	166	LEU	O-C-N	5.93	128.40	122.12
22	S	192	GLU	CA-C-O	5.93	126.70	120.42
25	R	309	LEU	N-CA-CB	5.93	118.61	110.01
1	a	62	LYS	N-CA-C	-5.93	104.94	111.82
8	h	164	ILE	CA-C-N	5.93	128.15	120.44
8	h	164	ILE	C-N-CA	5.93	128.15	120.44
25	R	215	GLY	O-C-N	5.93	128.00	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	H	135	ASP	CA-CB-CG	-5.93	106.67	112.60
30	K	106	ASN	N-CA-CB	5.93	120.76	110.98
9	i	225	ARG	CA-C-N	5.92	130.24	120.94
9	i	225	ARG	C-N-CA	5.92	130.24	120.94
9	2	170	HIS	ND1-CE1-NE2	5.92	114.32	108.40
21	N	103	SER	O-C-N	5.92	128.40	122.12
22	S	112	ASN	CA-C-N	5.92	132.86	121.54
22	S	112	ASN	C-N-CA	5.92	132.86	121.54
22	S	292	TYR	N-CA-C	5.92	117.82	111.36
1	a	113	PRO	CA-C-N	5.92	128.70	120.29
1	a	113	PRO	C-N-CA	5.92	128.70	120.29
14	n	75	LEU	N-CA-C	-5.92	100.84	110.20
18	X	36	LYS	CB-CG-CD	5.92	124.92	111.30
7	g	23	GLN	CA-C-O	5.92	126.83	120.55
26	U	287	ALA	CA-C-N	5.92	128.21	120.28
26	U	287	ALA	C-N-CA	5.92	128.21	120.28
25	R	331	ARG	CA-C-N	5.92	128.21	120.28
25	R	331	ARG	C-N-CA	5.92	128.21	120.28
32	M	251	LEU	CA-C-O	-5.92	113.17	119.97
33	J	356	ALA	N-CA-C	5.92	118.52	111.71
11	4	151	ASP	CA-C-N	5.92	129.27	120.87
11	4	151	ASP	C-N-CA	5.92	129.27	120.87
20	Z	917	ASN	CA-C-N	5.92	130.70	120.58
20	Z	917	ASN	C-N-CA	5.92	130.70	120.58
23	P	381	SER	N-CA-CB	5.92	118.92	110.16
26	U	69	ASP	CA-CB-CG	5.92	118.52	112.60
28	H	452	SER	CA-C-N	5.92	126.51	119.94
28	H	452	SER	C-N-CA	5.92	126.51	119.94
30	K	333	ARG	N-CA-C	-5.92	105.15	112.90
30	K	334	LEU	N-CA-CB	5.92	120.49	110.49
13	m	141	ARG	NE-CZ-NH1	-5.91	115.59	121.50
33	J	19	ILE	CA-C-N	5.91	128.18	120.26
33	J	19	ILE	C-N-CA	5.91	128.18	120.26
12	5	134	LEU	O-C-N	-5.91	115.00	122.27
8	h	95	CYS	N-CA-C	-5.91	104.96	111.82
21	N	7	ALA	O-C-N	-5.91	115.22	120.48
21	N	579	SER	N-CA-C	-5.91	105.38	112.59
30	K	347	ARG	NE-CZ-NH2	-5.91	113.88	119.20
33	J	47	GLN	N-CA-C	-5.91	104.84	111.28
9	i	216	LEU	CB-CA-C	5.91	120.76	111.72
20	Z	340	LEU	N-CA-C	-5.91	104.82	112.68
30	K	125	THR	CA-CB-OG1	5.91	118.46	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	128	ARG	N-CA-C	-5.91	105.66	112.92
32	M	84	GLU	N-CA-C	-5.91	99.98	108.60
33	J	137	MET	O-C-N	5.91	128.38	122.12
5	e	103	TYR	O-C-N	-5.90	115.67	121.93
30	K	277	ILE	N-CA-C	-5.90	105.96	113.22
11	k	102	VAL	O-C-N	-5.90	116.78	123.10
22	S	100	HIS	CE1-NE2-CD2	-5.90	103.10	109.00
24	Q	419	LEU	CA-C-N	5.90	128.11	120.44
24	Q	419	LEU	C-N-CA	5.90	128.11	120.44
25	R	333	MET	N-CA-CB	5.90	118.90	110.16
31	L	81	ILE	CA-C-N	5.90	128.47	120.44
31	L	81	ILE	C-N-CA	5.90	128.47	120.44
10	3	174	ALA	N-CA-CB	-5.90	101.43	110.16
24	Q	100	LEU	CA-C-N	5.90	128.00	120.56
24	Q	100	LEU	C-N-CA	5.90	128.00	120.56
29	I	396	CYS	CA-C-O	-5.90	114.30	120.55
30	K	335	ASP	CA-C-O	5.90	126.81	120.55
31	L	432	ILE	N-CA-CB	5.90	120.97	111.23
3	c	127	GLY	N-CA-C	-5.90	107.51	115.36
26	U	86	LYS	CA-C-N	5.90	130.51	122.19
26	U	86	LYS	C-N-CA	5.90	130.51	122.19
28	H	161	GLU	N-CA-C	-5.90	105.39	113.30
6	f	43	HIS	ND1-CE1-NE2	5.90	114.30	108.40
12	l	101	VAL	O-C-N	5.90	130.08	122.77
8	1	75	TYR	CA-C-N	5.90	130.71	120.68
8	1	75	TYR	C-N-CA	5.90	130.71	120.68
9	2	215	TYR	CA-C-N	5.90	131.01	122.16
9	2	215	TYR	C-N-CA	5.90	131.01	122.16
4	d	75	PHE	CA-CB-CG	-5.90	107.90	113.80
33	J	291	ILE	CA-CB-CG1	5.90	120.42	110.40
17	T	213	ASN	N-CA-C	-5.89	99.74	108.99
28	H	120	ASN	CA-C-O	-5.89	113.44	120.10
29	I	266	GLN	CA-C-N	5.89	127.99	120.56
29	I	266	GLN	C-N-CA	5.89	127.99	120.56
32	M	65	ASN	CA-C-O	5.89	126.80	120.55
33	J	15	HIS	ND1-CE1-NE2	5.89	114.29	108.40
13	m	150	ALA	CA-C-N	5.89	129.27	120.31
13	m	150	ALA	C-N-CA	5.89	129.27	120.31
5	E	238	GLU	CA-C-N	5.89	128.18	120.28
5	E	238	GLU	C-N-CA	5.89	128.18	120.28
15	W	19	GLY	O-C-N	-5.89	119.64	123.35
21	N	177	ASP	N-CA-CB	5.89	118.61	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	795	GLU	CB-CA-C	-5.89	100.83	110.85
23	P	132	VAL	CA-C-N	5.89	128.66	120.29
23	P	132	VAL	C-N-CA	5.89	128.66	120.29
27	O	177	GLN	CA-C-N	5.89	128.10	120.44
27	O	177	GLN	C-N-CA	5.89	128.10	120.44
5	e	35	SER	CA-C-O	5.89	126.48	120.24
33	J	388	LYS	CB-CG-CD	5.89	124.85	111.30
11	4	133	HIS	ND1-CE1-NE2	5.89	114.29	108.40
17	T	102	LYS	N-CA-CB	-5.89	101.16	109.94
22	S	52	TYR	CA-C-O	-5.89	114.18	120.42
25	R	274	PRO	N-CA-C	-5.89	106.50	113.86
27	O	95	SER	CA-C-N	5.89	128.65	120.29
27	O	95	SER	C-N-CA	5.89	128.65	120.29
30	K	88	ARG	NE-CZ-NH2	-5.89	113.90	119.20
30	K	221	MET	N-CA-C	-5.89	105.19	112.90
1	a	14	ARG	CB-CA-C	-5.89	100.51	110.64
30	K	256	ASP	CA-CB-CG	-5.89	106.71	112.60
10	3	32	GLN	N-CA-CB	5.89	120.44	110.49
23	P	228	SER	N-CA-C	5.89	118.65	111.82
29	I	150	HIS	ND1-CE1-NE2	5.89	114.29	108.40
10	3	142	ALA	CB-CA-C	5.88	118.99	111.40
17	T	79	GLU	CB-CG-CD	-5.88	102.60	112.60
3	c	189	ALA	CA-C-N	5.88	128.77	120.42
3	c	189	ALA	C-N-CA	5.88	128.77	120.42
14	n	254	PHE	N-CA-C	-5.88	106.07	113.72
12	5	161	LEU	O-C-N	-5.88	115.44	122.15
16	V	89	ALA	O-C-N	5.88	128.86	122.15
21	N	630	ALA	CB-CA-C	-5.88	101.03	110.79
21	N	888	ASP	CA-CB-CG	-5.88	106.72	112.60
32	M	227	GLY	CA-C-O	-5.88	112.48	119.01
22	S	206	GLN	CA-C-N	5.88	128.16	120.28
22	S	206	GLN	C-N-CA	5.88	128.16	120.28
32	M	281	ASP	CA-C-N	5.88	131.10	122.63
32	M	281	ASP	C-N-CA	5.88	131.10	122.63
2	b	128	ARG	NE-CZ-NH2	5.88	124.49	119.20
9	i	209	ILE	CA-C-O	5.88	127.95	121.13
24	Q	264	TYR	N-CA-C	5.88	118.64	111.82
33	J	330	ILE	CA-C-O	-5.88	113.75	119.92
6	f	164	ARG	CA-C-N	5.88	129.24	120.31
6	f	164	ARG	C-N-CA	5.88	129.24	120.31
9	2	104	ARG	CA-C-N	5.88	128.76	120.42
9	2	104	ARG	C-N-CA	5.88	128.76	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	276	LYS	CA-C-N	5.88	128.08	120.44
12	l	276	LYS	C-N-CA	5.88	128.08	120.44
29	I	144	GLY	CA-C-N	5.88	132.12	122.07
29	I	144	GLY	C-N-CA	5.88	132.12	122.07
10	3	66	MET	CA-C-N	5.87	128.63	120.29
10	3	66	MET	C-N-CA	5.87	128.63	120.29
14	7	72	VAL	O-C-N	-5.87	115.78	122.94
26	U	12	PRO	N-CA-C	-5.87	106.34	114.27
27	O	233	LEU	N-CA-CB	5.87	119.27	110.22
21	N	617	VAL	N-CA-CB	5.87	117.42	110.55
12	5	266	HIS	O-C-N	-5.87	116.31	123.30
6	f	166	GLN	CA-C-N	5.87	127.67	120.22
6	f	166	GLN	C-N-CA	5.87	127.67	120.22
14	n	96	ILE	N-CA-C	-5.87	106.00	113.22
16	V	186	GLN	CB-CA-C	-5.87	108.81	115.79
22	S	138	MET	CA-C-N	5.87	128.73	120.28
22	S	138	MET	C-N-CA	5.87	128.73	120.28
23	P	162	GLU	N-CA-C	5.87	117.68	111.28
30	K	227	ALA	O-C-N	5.87	129.49	122.27
8	1	164	ILE	CA-C-N	5.87	128.07	120.44
8	1	164	ILE	C-N-CA	5.87	128.07	120.44
20	Z	455	ILE	CA-C-N	5.87	126.62	119.99
20	Z	455	ILE	C-N-CA	5.87	126.62	119.99
27	O	238	ILE	N-CA-C	5.87	117.31	110.62
28	H	202	GLU	CA-C-O	-5.87	112.12	120.51
6	f	231	ALA	CA-C-N	5.87	128.62	120.29
6	f	231	ALA	C-N-CA	5.87	128.62	120.29
10	3	17	GLY	N-CA-C	-5.87	99.28	113.18
31	L	101	ILE	CB-CA-C	5.87	120.91	111.29
2	b	99	ARG	N-CA-C	-5.86	106.10	113.72
12	l	190	VAL	N-CA-C	-5.86	100.03	108.53
22	S	338	MET	N-CA-C	-5.86	103.60	111.87
24	Q	246	TYR	CA-C-O	-5.86	113.23	119.97
31	L	195	GLU	O-C-N	5.86	128.84	122.15
15	W	24	THR	N-CA-C	-5.86	100.86	109.18
29	I	204	HIS	CE1-NE2-CD2	-5.86	103.14	109.00
2	b	5	TYR	CA-C-O	-5.86	115.32	122.64
6	f	130	VAL	CA-C-N	5.86	132.90	121.41
6	f	130	VAL	C-N-CA	5.86	132.90	121.41
24	Q	350	ILE	CB-CA-C	-5.86	104.39	112.24
6	f	14	SER	N-CA-CB	5.86	120.46	110.50
12	5	212	TYR	CB-CA-C	-5.86	101.44	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	42	SER	CA-C-O	-5.86	114.05	120.43
24	Q	109	ASP	CA-CB-CG	-5.86	106.74	112.60
33	J	330	ILE	CA-CB-CG1	5.86	120.36	110.40
14	n	95	HIS	CB-CG-CD2	-5.86	123.59	131.20
16	V	38	LEU	CA-C-N	5.86	128.05	120.44
16	V	38	LEU	C-N-CA	5.86	128.05	120.44
21	N	422	TYR	CA-C-O	-5.86	114.67	120.82
24	Q	22	GLU	O-C-N	5.86	128.83	122.15
24	Q	101	ILE	CA-C-N	5.86	128.05	120.44
24	Q	101	ILE	C-N-CA	5.86	128.05	120.44
28	H	314	VAL	N-CA-CB	5.86	120.89	111.23
23	P	322	LEU	N-CA-C	-5.85	106.68	113.88
7	g	121	GLN	OE1-CD-NE2	-5.85	116.75	122.60
14	n	219	TYR	CA-C-O	-5.85	114.86	121.00
13	6	125	ASP	N-CA-C	-5.85	106.18	113.38
17	T	123	HIS	ND1-CE1-NE2	5.85	114.25	108.40
25	R	406	GLN	N-CA-C	5.85	117.74	111.36
32	M	359	GLN	OE1-CD-NE2	5.85	128.45	122.60
1	a	235	THR	N-CA-C	-5.85	100.65	109.95
32	M	334	ASP	CA-CB-CG	5.85	118.45	112.60
33	J	252	SER	N-CA-C	-5.85	98.34	110.80
7	g	239	ALA	CB-CA-C	-5.85	100.91	110.85
13	6	193	ARG	NE-CZ-NH1	-5.85	115.65	121.50
23	P	239	GLN	CB-CG-CD	-5.85	102.66	112.60
28	H	293	GLU	CA-C-N	5.85	129.20	120.31
28	H	293	GLU	C-N-CA	5.85	129.20	120.31
11	k	128	LEU	N-CA-CB	5.85	121.11	111.17
21	N	177	ASP	CB-CA-C	-5.84	101.67	110.90
31	L	317	ASN	CA-CB-CG	-5.84	106.75	112.60
22	S	273	PHE	CB-CG-CD2	-5.84	110.77	120.70
7	g	166	GLY	O-C-N	-5.84	117.30	122.85
8	h	60	ASP	CB-CA-C	-5.84	99.46	110.67
11	4	84	VAL	CA-C-O	-5.84	114.66	120.85
19	Y	40	ILE	CA-C-N	5.84	128.39	120.44
19	Y	40	ILE	C-N-CA	5.84	128.39	120.44
27	O	116	ASN	CB-CG-OD1	-5.84	109.12	120.80
13	6	75	ARG	CA-C-N	5.84	128.58	120.29
13	6	75	ARG	C-N-CA	5.84	128.58	120.29
22	S	235	ASN	OD1-CG-ND2	-5.84	116.76	122.60
26	U	279	SER	CA-C-N	5.84	128.69	120.28
26	U	279	SER	C-N-CA	5.84	128.69	120.28
17	T	173	GLU	CA-C-O	5.84	125.21	119.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	44	SER	CA-C-N	5.84	128.58	120.29
27	O	44	SER	C-N-CA	5.84	128.58	120.29
28	H	350	LYS	CB-CA-C	5.84	119.37	109.50
3	c	134	SER	N-CA-C	-5.84	98.90	108.76
4	d	108	TYR	N-CA-CB	5.84	118.70	110.12
10	j	149	MET	CA-C-N	5.84	128.10	120.28
10	j	149	MET	C-N-CA	5.84	128.10	120.28
13	m	35	THR	N-CA-C	-5.84	105.82	113.17
16	V	56	GLU	N-CA-C	-5.84	98.77	108.75
23	P	386	GLN	N-CA-C	-5.84	105.92	113.16
14	n	63	TYR	CA-C-O	5.83	128.85	120.51
10	3	162	ASP	CA-CB-CG	5.83	118.44	112.60
21	N	100	THR	CA-CB-OG1	5.83	118.35	109.60
29	I	240	THR	O-C-N	5.83	128.31	122.12
13	m	67	ALA	CA-C-O	-5.83	114.37	120.55
12	5	128	GLN	CA-C-O	-5.83	114.66	120.90
13	6	89	ASP	CA-CB-CG	-5.83	106.77	112.60
21	N	55	PHE	O-C-N	5.83	129.92	123.33
21	N	293	LEU	O-C-N	-5.83	114.61	121.32
25	R	116	LYS	CA-C-N	5.83	127.91	120.56
25	R	116	LYS	C-N-CA	5.83	127.91	120.56
25	R	240	SER	N-CA-C	-5.83	104.33	113.02
30	K	331	PRO	CA-C-O	-5.83	114.80	121.56
32	M	417	GLU	CA-C-N	5.83	127.43	120.14
32	M	417	GLU	C-N-CA	5.83	127.43	120.14
25	R	217	HIS	CB-CG-CD2	-5.83	123.62	131.20
6	f	143	HIS	ND1-CE1-NE2	5.83	114.23	108.40
8	1	186	VAL	N-CA-C	-5.83	98.74	107.37
9	2	205	CYS	N-CA-C	-5.83	98.78	108.34
23	P	169	GLY	CA-C-N	5.83	130.59	120.68
23	P	169	GLY	C-N-CA	5.83	130.59	120.68
28	H	400	ARG	N-CA-CB	5.83	119.72	110.57
30	K	179	MET	N-CA-C	5.83	117.63	111.28
8	h	112	ASP	N-CA-CB	5.83	119.31	110.45
10	3	88	THR	CA-C-O	-5.83	114.70	120.82
21	N	117	TYR	O-C-N	5.83	128.79	122.15
7	g	163	ALA	N-CA-CB	5.83	121.83	111.69
23	P	116	ILE	CB-CA-C	5.83	120.26	112.22
33	J	64	LEU	CA-C-O	-5.83	114.37	120.55
33	J	96	VAL	N-CA-C	5.83	116.75	108.42
6	f	115	LYS	CA-C-O	5.82	126.59	120.42
9	i	230	LYS	N-CA-CB	5.82	120.38	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	7	100	LEU	O-C-N	-5.82	115.51	122.15
16	V	202	ASP	N-CA-C	-5.82	100.21	109.59
27	O	377	VAL	CA-C-N	5.82	128.56	120.29
27	O	377	VAL	C-N-CA	5.82	128.56	120.29
29	I	174	ASP	CA-CB-CG	-5.82	106.78	112.60
30	K	91	SER	CA-C-N	5.82	132.90	122.13
30	K	91	SER	C-N-CA	5.82	132.90	122.13
3	c	84	ALA	CA-C-N	5.82	128.66	120.28
3	c	84	ALA	C-N-CA	5.82	128.66	120.28
12	5	182	LYS	N-CA-C	-5.82	103.99	113.19
21	N	747	HIS	CE1-NE2-CD2	-5.82	103.18	109.00
25	R	230	LEU	CA-C-N	5.82	130.58	120.68
25	R	230	LEU	C-N-CA	5.82	130.58	120.68
29	I	55	CYS	N-CA-C	-5.82	104.53	111.69
29	I	325	ILE	N-CA-C	-5.82	99.15	107.77
31	L	70	TYR	O-C-N	5.82	128.79	122.15
14	n	212	ASN	N-CA-C	5.82	117.62	111.28
8	1	111	TYR	N-CA-C	-5.82	99.70	109.07
11	4	126	VAL	CA-C-N	5.82	129.14	120.87
11	4	126	VAL	C-N-CA	5.82	129.14	120.87
12	5	279	GLU	CA-C-O	5.82	126.69	120.70
21	N	610	SER	N-CA-CB	5.82	118.87	110.20
26	U	94	HIS	ND1-CE1-NE2	5.82	114.22	108.40
26	U	252	HIS	CA-CB-CG	5.82	119.62	113.80
23	P	49	ALA	N-CA-C	5.82	117.62	111.28
25	R	54	ILE	N-CA-CB	5.82	117.36	110.55
3	c	16	GLU	CA-C-N	5.82	130.33	120.91
3	c	16	GLU	C-N-CA	5.82	130.33	120.91
3	c	168	ASN	O-C-N	5.82	129.56	122.58
13	m	223	GLU	N-CA-CB	5.82	119.90	110.77
16	V	223	SER	N-CA-C	5.82	119.48	112.38
22	S	44	THR	N-CA-CB	5.82	120.32	110.49
13	m	158	LEU	CA-C-N	5.82	129.15	120.31
13	m	158	LEU	C-N-CA	5.82	129.15	120.31
9	2	42	VAL	CB-CA-C	5.82	119.78	110.82
33	J	404	PHE	O-C-N	-5.82	116.52	123.27
15	W	73	LEU	CB-CA-C	-5.81	101.14	110.79
21	N	327	LEU	CA-C-N	5.81	128.54	120.29
21	N	327	LEU	C-N-CA	5.81	128.54	120.29
27	O	19	ASP	CA-CB-CG	-5.81	106.79	112.60
2	b	120	GLU	N-CA-C	-5.81	106.05	113.02
10	j	106	GLY	CA-C-O	-5.81	113.21	121.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	250	VAL	CA-C-O	5.81	126.44	120.39
12	l	255	VAL	N-CA-C	-5.81	99.94	108.54
12	5	274	LYS	CB-CA-C	-5.81	101.72	110.90
21	N	368	THR	N-CA-CB	5.81	118.76	110.16
23	P	383	LEU	CA-C-N	5.81	129.83	120.82
23	P	383	LEU	C-N-CA	5.81	129.83	120.82
33	J	345	LYS	CA-C-N	5.81	127.88	120.56
33	J	345	LYS	C-N-CA	5.81	127.88	120.56
33	J	404	PHE	CA-C-O	5.81	126.52	120.30
20	Z	470	ALA	CA-C-N	5.81	128.38	120.54
20	Z	470	ALA	C-N-CA	5.81	128.38	120.54
25	R	130	GLN	OE1-CD-NE2	-5.81	116.79	122.60
27	O	299	THR	N-CA-CB	5.81	118.76	110.16
16	V	71	MET	CA-C-O	-5.81	114.90	119.66
22	S	339	GLN	N-CA-CB	5.81	120.03	110.39
23	P	183	GLN	CA-C-N	5.81	128.06	120.28
23	P	183	GLN	C-N-CA	5.81	128.06	120.28
30	K	224	LYS	CA-C-N	5.81	128.34	120.44
30	K	224	LYS	C-N-CA	5.81	128.34	120.44
33	J	76	ILE	N-CA-C	-5.81	106.05	111.45
7	g	189	ALA	CA-C-N	5.81	128.54	120.29
7	g	189	ALA	C-N-CA	5.81	128.54	120.29
8	h	75	TYR	N-CA-C	-5.81	105.03	111.36
12	l	206	SER	N-CA-C	-5.81	106.24	113.38
13	6	29	ALA	N-CA-C	-5.81	99.91	108.79
14	7	55	ILE	N-CA-C	-5.81	99.81	108.46
17	T	118	ASN	CA-CB-CG	-5.81	106.79	112.60
26	U	135	ASP	N-CA-CB	5.81	121.51	111.00
24	Q	356	CYS	CA-C-N	5.81	128.88	120.98
24	Q	356	CYS	C-N-CA	5.81	128.88	120.98
26	U	226	LEU	CA-C-N	5.81	126.39	120.00
26	U	226	LEU	C-N-CA	5.81	126.39	120.00
32	M	186	LEU	CA-C-N	5.81	128.06	120.28
32	M	186	LEU	C-N-CA	5.81	128.06	120.28
33	J	213	VAL	N-CA-C	-5.80	97.27	109.34
10	j	17	GLY	CA-C-N	5.80	131.36	122.77
10	j	17	GLY	C-N-CA	5.80	131.36	122.77
13	m	189	ILE	N-CA-C	5.80	115.99	110.42
30	K	415	VAL	N-CA-CB	5.80	120.81	111.23
31	L	221	TYR	N-CA-CB	5.80	122.31	111.52
10	3	146	LEU	O-C-N	-5.80	116.06	122.09
22	S	173	LEU	N-CA-C	-5.80	101.43	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	369	GLN	CA-C-N	5.80	127.98	120.44
22	S	369	GLN	C-N-CA	5.80	127.98	120.44
24	Q	249	LEU	N-CA-C	-5.80	102.72	110.55
3	c	187	ASP	O-C-N	-5.80	116.10	122.07
5	e	87	SER	N-CA-C	-5.80	105.04	111.36
14	7	94	GLN	N-CA-C	5.80	118.38	111.71
6	f	107	ARG	NE-CZ-NH2	-5.80	113.98	119.20
17	T	58	THR	CA-C-N	5.80	128.05	120.28
17	T	58	THR	C-N-CA	5.80	128.05	120.28
25	R	347	THR	O-C-N	-5.80	116.64	123.25
27	O	63	ASP	CA-C-N	5.79	127.97	120.44
27	O	63	ASP	C-N-CA	5.79	127.97	120.44
33	J	48	ARG	NE-CZ-NH1	5.79	127.30	121.50
8	h	60	ASP	N-CA-CB	5.79	119.26	110.28
9	i	254	GLU	O-C-N	-5.79	115.97	122.75
13	m	109	ARG	N-CA-C	-5.79	106.55	113.97
16	V	201	ILE	N-CA-CB	5.79	117.94	110.99
23	P	348	HIS	ND1-CE1-NE2	5.79	114.19	108.40
23	P	407	ASN	CA-C-N	5.79	128.36	120.54
23	P	407	ASN	C-N-CA	5.79	128.36	120.54
24	Q	195	LYS	O-C-N	5.79	128.26	122.12
2	b	23	TYR	CB-CG-CD1	5.79	129.49	120.80
14	n	51	ASN	CA-C-O	-5.79	112.35	119.18
15	W	22	PRO	CA-C-N	5.79	132.12	121.70
15	W	22	PRO	C-N-CA	5.79	132.12	121.70
24	Q	83	GLU	N-CA-C	-5.79	105.05	111.36
17	T	34	LEU	N-CA-C	-5.79	105.48	112.54
21	N	774	ASN	N-CA-CB	5.79	119.71	110.16
23	P	143	LEU	CA-C-O	-5.79	112.13	119.31
24	Q	67	THR	CA-C-N	5.79	132.12	121.70
24	Q	67	THR	C-N-CA	5.79	132.12	121.70
16	V	189	ILE	N-CA-C	5.79	116.56	110.72
13	m	60	MET	CG-SD-CE	-5.79	88.17	100.90
14	7	34	THR	CA-CB-CG2	5.79	120.33	110.50
28	H	438	ALA	N-CA-CB	5.79	119.59	110.56
32	M	357	ARG	CG-CD-NE	-5.79	99.27	112.00
1	a	224	GLU	N-CA-C	-5.78	98.18	108.13
12	5	115	PHE	CA-CB-CG	-5.78	108.02	113.80
20	Z	432	GLY	CA-C-N	5.78	128.82	120.38
20	Z	432	GLY	C-N-CA	5.78	128.82	120.38
22	S	280	ASN	CA-C-N	5.78	128.03	120.28
22	S	280	ASN	C-N-CA	5.78	128.03	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	H	112	SER	CA-C-N	5.78	128.03	120.28
28	H	112	SER	C-N-CA	5.78	128.03	120.28
4	d	26	ALA	CA-C-N	5.78	130.24	120.29
4	d	26	ALA	C-N-CA	5.78	130.24	120.29
13	6	198	SER	N-CA-CB	5.78	118.72	110.16
15	W	25	ARG	NE-CZ-NH2	5.78	124.40	119.20
21	N	613	HIS	CA-CB-CG	5.78	119.58	113.80
23	P	254	GLU	CA-C-N	5.78	128.50	120.29
23	P	254	GLU	C-N-CA	5.78	128.50	120.29
25	R	74	ASN	CA-CB-CG	-5.78	106.82	112.60
27	O	226	LYS	CA-C-O	5.78	125.64	119.34
32	M	258	GLU	CA-C-N	5.78	127.56	120.22
32	M	258	GLU	C-N-CA	5.78	127.56	120.22
32	M	361	LEU	O-C-N	5.78	128.25	122.12
16	V	273	ARG	CG-CD-NE	-5.78	99.29	112.00
25	R	84	LYS	N-CA-C	-5.78	100.63	109.41
28	H	87	ASP	CB-CA-C	-5.78	101.20	110.79
8	h	193	GLU	CA-C-N	5.78	130.34	122.19
8	h	193	GLU	C-N-CA	5.78	130.34	122.19
14	7	87	SER	N-CA-CB	5.78	121.74	111.69
29	I	207	LEU	CA-C-O	5.78	126.67	120.55
33	J	156	GLN	CA-C-N	5.78	127.95	120.56
33	J	156	GLN	C-N-CA	5.78	127.95	120.56
7	g	234	ASP	CA-C-N	5.77	128.02	120.28
7	g	234	ASP	C-N-CA	5.77	128.02	120.28
18	X	98	PHE	CA-CB-CG	5.77	119.57	113.80
31	L	391	ILE	O-C-N	5.77	127.78	121.83
9	i	106	VAL	N-CA-C	5.77	118.26	111.05
11	4	173	PRO	N-CA-C	-5.77	106.48	114.27
13	6	214	ILE	CA-CB-CG1	-5.77	100.59	110.40
17	T	255	GLN	CA-C-O	5.77	126.65	120.70
23	P	39	LEU	CA-C-O	5.77	126.61	119.97
24	Q	408	THR	CA-CB-OG1	5.77	118.26	109.60
8	1	118	GLU	N-CA-CB	5.77	122.25	111.52
24	Q	245	SER	N-CA-C	5.77	117.25	111.07
33	J	139	VAL	N-CA-C	5.77	115.95	110.53
14	n	257	ASP	N-CA-C	-5.77	106.41	113.50
22	S	335	GLN	CB-CA-C	-5.77	99.62	110.01
23	P	86	HIS	CB-CG-ND1	5.77	131.35	122.70
24	Q	87	GLN	O-C-N	5.77	128.24	122.12
25	R	57	GLU	N-CA-C	-5.77	105.90	113.17
15	W	124	GLU	CB-CA-C	-5.77	101.22	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	X	86	ILE	N-CA-C	-5.77	98.73	107.73
23	P	290	LEU	CA-C-O	-5.77	113.58	120.10
26	U	62	ASN	N-CA-C	-5.77	98.89	108.75
27	O	69	PHE	CA-CB-CG	-5.77	108.03	113.80
32	M	15	ASP	CA-C-O	5.77	128.76	120.51
13	m	85	PHE	CB-CG-CD2	-5.77	110.90	120.70
13	m	138	SER	N-CA-CB	5.77	120.23	110.49
22	S	337	ASN	N-CA-C	-5.77	106.47	112.93
33	J	85	LEU	CA-C-O	-5.77	114.08	120.60
8	l	18	LYS	N-CA-C	5.76	118.31	111.33
28	H	86	GLY	CA-C-N	5.76	128.00	120.28
28	H	86	GLY	C-N-CA	5.76	128.00	120.28
28	H	185	LEU	CA-C-N	5.76	126.09	119.92
28	H	185	LEU	C-N-CA	5.76	126.09	119.92
32	M	53	HIS	CA-C-N	5.76	128.28	120.44
32	M	53	HIS	C-N-CA	5.76	128.28	120.44
8	h	38	ARG	NH1-CZ-NH2	-5.76	111.81	119.30
22	S	309	PHE	CA-C-N	5.76	127.93	120.44
22	S	309	PHE	C-N-CA	5.76	127.93	120.44
24	Q	413	LEU	CA-C-N	5.76	128.00	120.28
24	Q	413	LEU	C-N-CA	5.76	128.00	120.28
32	M	401	ILE	CB-CA-C	-5.76	104.27	112.22
4	d	79	ASN	CA-C-N	5.76	128.28	120.44
4	d	79	ASN	C-N-CA	5.76	128.28	120.44
4	d	131	VAL	CA-C-O	-5.76	114.15	120.43
4	d	222	VAL	O-C-N	5.76	129.16	123.00
6	f	85	SER	N-CA-C	5.76	117.56	111.28
17	T	200	LEU	CA-C-O	-5.76	113.81	120.03
21	N	377	GLY	CA-C-O	-5.76	114.05	122.06
21	N	759	ILE	CA-CB-CG2	-5.76	100.71	110.50
28	H	118	ASP	N-CA-CB	5.76	119.80	110.41
11	4	58	GLU	N-CA-C	-5.76	105.75	112.89
12	5	140	LEU	N-CA-C	-5.76	105.92	113.17
19	Y	43	TRP	CA-C-N	5.76	132.54	121.54
19	Y	43	TRP	C-N-CA	5.76	132.54	121.54
21	N	566	SER	CA-C-N	5.76	128.27	120.44
21	N	566	SER	C-N-CA	5.76	128.27	120.44
22	S	287	SER	O-C-N	-5.76	116.14	122.07
4	d	149	GLN	OE1-CD-NE2	5.76	128.36	122.60
7	g	91	ARG	O-C-N	-5.76	116.02	122.12
9	i	102	GLU	CB-CA-C	-5.76	100.58	109.62
12	l	164	GLN	N-CA-C	5.76	117.36	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	130	GLN	CG-CD-NE2	5.76	125.03	116.40
28	H	400	ARG	N-CA-C	-5.76	99.80	109.07
2	b	179	TRP	CA-CB-CG	5.75	124.53	113.60
15	W	12	ASN	CA-CB-CG	-5.75	106.84	112.60
29	I	431	ASN	N-CA-CB	5.75	118.96	110.56
4	d	216	LYS	CA-C-O	-5.75	113.56	120.41
11	4	153	THR	N-CA-C	-5.75	101.48	110.17
24	Q	277	ASP	N-CA-C	-5.75	106.30	113.38
26	U	215	ILE	O-C-N	5.75	128.06	122.25
27	O	110	ASP	N-CA-C	-5.75	106.22	113.18
2	b	188	ALA	CA-C-N	5.75	127.81	120.56
2	b	188	ALA	C-N-CA	5.75	127.81	120.56
30	K	353	PHE	N-CA-CB	5.75	118.57	110.12
10	j	8	ASN	CA-CB-CG	5.75	118.35	112.60
11	4	84	VAL	CA-C-N	5.75	127.98	120.28
11	4	84	VAL	C-N-CA	5.75	127.98	120.28
14	n	211	VAL	CA-C-N	5.75	127.98	120.28
14	n	211	VAL	C-N-CA	5.75	127.98	120.28
15	W	121	SER	CA-C-N	5.75	127.91	120.44
15	W	121	SER	C-N-CA	5.75	127.91	120.44
30	K	66	ASP	CA-CB-CG	-5.75	106.85	112.60
31	L	192	GLU	CB-CA-C	-5.75	101.08	110.85
8	h	19	ASP	CA-CB-CG	-5.75	106.86	112.60
10	j	44	PHE	CA-CB-CG	-5.75	108.06	113.80
13	m	107	GLY	N-CA-C	-5.75	105.84	112.50
8	h	140	SER	N-CA-C	-5.74	104.68	112.26
21	N	381	GLU	CA-C-N	5.74	126.32	120.00
21	N	381	GLU	C-N-CA	5.74	126.32	120.00
29	I	121	THR	CA-CB-CG2	5.74	120.26	110.50
29	I	213	ILE	CA-C-N	5.74	128.37	120.39
29	I	213	ILE	C-N-CA	5.74	128.37	120.39
12	l	230	TYR	CA-C-N	5.74	128.44	120.29
12	l	230	TYR	C-N-CA	5.74	128.44	120.29
11	k	10	GLN	OE1-CD-NE2	5.74	128.34	122.60
9	2	219	TYR	CA-C-O	5.74	126.64	120.55
17	T	195	LEU	N-CA-C	-5.74	105.94	113.17
31	L	254	LYS	CA-CB-CG	5.74	125.58	114.10
31	L	395	ALA	N-CA-CB	-5.74	101.67	110.16
23	P	419	VAL	CB-CA-C	-5.74	104.30	112.22
27	O	215	TYR	CA-C-N	5.74	127.97	120.28
27	O	215	TYR	C-N-CA	5.74	127.97	120.28
29	I	309	LEU	N-CA-C	5.74	117.61	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	W	22	PRO	CA-C-O	-5.74	114.67	121.67
28	H	404	TRP	CA-C-N	5.74	130.30	120.72
28	H	404	TRP	C-N-CA	5.74	130.30	120.72
29	I	376	ASN	CA-C-N	5.74	127.97	120.28
29	I	376	ASN	C-N-CA	5.74	127.97	120.28
4	d	91	VAL	CA-C-N	5.74	128.54	120.28
4	d	91	VAL	C-N-CA	5.74	128.54	120.28
14	7	34	THR	CA-CB-OG1	-5.74	101.00	109.60
25	R	354	ALA	CA-C-N	5.73	128.43	120.29
25	R	354	ALA	C-N-CA	5.73	128.43	120.29
25	R	414	LEU	CA-C-N	5.73	127.89	120.44
25	R	414	LEU	C-N-CA	5.73	127.89	120.44
4	d	95	SER	N-CA-C	-5.73	104.64	111.69
6	f	224	ILE	CA-C-O	5.73	126.56	120.48
12	5	92	ASP	N-CA-CB	5.73	118.19	109.94
26	U	156	HIS	CA-C-O	-5.73	114.22	120.81
30	K	71	GLU	CA-C-N	5.73	128.43	120.29
30	K	71	GLU	C-N-CA	5.73	128.43	120.29
1	a	214	LEU	N-CA-C	-5.73	106.33	113.38
14	n	133	MET	O-C-N	5.73	128.05	122.09
14	7	211	VAL	CA-C-O	-5.73	115.31	121.27
16	V	91	MET	N-CA-C	5.73	117.20	111.07
21	N	167	GLU	O-C-N	5.73	128.19	122.12
21	N	609	LEU	N-CA-C	-5.73	106.12	113.23
21	N	921	ARG	N-CA-C	5.73	118.30	111.71
24	Q	35	SER	CA-C-O	5.73	126.50	120.42
25	R	81	HIS	CA-C-O	-5.73	114.57	120.99
26	U	172	GLU	O-C-N	5.73	128.68	122.15
26	U	283	ARG	N-CA-CB	5.73	119.04	110.22
7	g	87	HIS	CE1-NE2-CD2	-5.73	103.27	109.00
9	i	128	ILE	N-CA-C	-5.73	100.33	108.58
24	Q	416	VAL	CA-C-N	5.73	126.46	119.99
24	Q	416	VAL	C-N-CA	5.73	126.46	119.99
29	I	307	LEU	N-CA-C	5.73	117.52	111.28
6	f	43	HIS	CG-CD2-NE2	5.73	112.93	107.20
13	6	12	PRO	N-CA-CB	5.73	106.64	101.83
21	N	762	ARG	N-CA-CB	5.73	118.39	109.97
23	P	128	ASN	O-C-N	-5.73	116.19	122.84
26	U	37	ILE	N-CA-CB	5.73	120.83	111.44
27	O	373	TRP	CE2-CD2-CE3	5.73	124.53	118.80
21	N	541	ALA	CA-C-O	-5.73	111.78	119.11
32	M	411	LYS	N-CA-C	-5.73	101.99	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	161	LYS	N-CA-C	-5.72	106.84	113.88
9	2	236	ARG	NE-CZ-NH2	-5.72	114.05	119.20
21	N	784	TYR	CA-C-O	5.72	125.57	120.02
27	O	164	PRO	CA-C-O	-5.72	114.92	121.56
28	H	100	ALA	N-CA-CB	-5.72	101.75	111.31
30	K	226	VAL	CA-C-N	5.72	129.01	120.31
30	K	226	VAL	C-N-CA	5.72	129.01	120.31
32	M	320	ARG	CA-C-O	5.72	125.35	119.05
6	f	70	MET	O-C-N	-5.72	116.96	123.48
24	Q	241	GLU	CA-C-N	5.72	128.52	120.28
24	Q	241	GLU	C-N-CA	5.72	128.52	120.28
24	Q	343	LEU	CA-C-O	-5.72	114.36	120.42
32	M	26	SER	CA-C-N	5.72	127.95	120.28
32	M	26	SER	C-N-CA	5.72	127.95	120.28
6	f	116	ALA	CA-C-N	5.72	127.95	120.28
6	f	116	ALA	C-N-CA	5.72	127.95	120.28
11	4	59	TYR	N-CA-C	-5.72	105.12	111.36
9	2	196	LEU	O-C-N	5.72	129.16	122.24
23	P	131	PHE	CA-C-N	5.72	128.59	120.53
23	P	131	PHE	C-N-CA	5.72	128.59	120.53
24	Q	281	ILE	CA-C-O	-5.72	114.59	120.71
25	R	349	SER	CA-C-N	5.72	127.94	120.28
25	R	349	SER	C-N-CA	5.72	127.94	120.28
28	H	375	VAL	CA-CB-CG1	5.72	120.12	110.40
1	a	15	HIS	CA-CB-CG	5.72	119.52	113.80
10	j	168	SER	N-CA-C	-5.72	104.95	111.07
13	m	96	SER	CA-C-N	5.72	128.26	120.54
13	m	96	SER	C-N-CA	5.72	128.26	120.54
9	2	143	HIS	ND1-CE1-NE2	5.72	114.12	108.40
14	7	192	VAL	N-CA-C	-5.72	99.26	107.78
22	S	44	THR	CA-C-N	5.72	130.53	120.87
22	S	44	THR	C-N-CA	5.72	130.53	120.87
3	c	80	LEU	CA-C-N	5.72	130.36	120.58
3	c	80	LEU	C-N-CA	5.72	130.36	120.58
9	2	73	ALA	N-CA-C	-5.72	100.66	109.52
10	3	107	PRO	CB-CA-C	-5.72	103.61	111.21
14	7	106	GLU	CB-CA-C	-5.72	101.30	110.79
21	N	383	LYS	O-C-N	5.72	128.67	122.15
27	O	326	HIS	CE1-NE2-CD2	-5.72	103.28	109.00
32	M	375	ASN	CA-C-N	5.72	129.00	120.31
32	M	375	ASN	C-N-CA	5.72	129.00	120.31
9	i	239	THR	N-CA-C	-5.71	99.87	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	145	HIS	CE1-NE2-CD2	-5.71	103.28	109.00
11	4	7	ILE	N-CA-C	-5.71	99.27	107.78
12	5	270	GLU	N-CA-CB	5.71	118.90	110.33
21	N	637	ALA	CA-C-N	5.71	128.29	120.46
21	N	637	ALA	C-N-CA	5.71	128.29	120.46
28	H	148	ASN	CA-C-O	5.71	126.30	120.24
31	L	353	ASN	CA-C-O	-5.71	115.57	122.03
22	S	444	GLU	CA-C-N	5.71	128.87	120.82
22	S	444	GLU	C-N-CA	5.71	128.87	120.82
27	O	251	LEU	N-CA-C	5.71	117.51	111.28
1	a	207	ILE	N-CA-CB	5.71	118.31	110.54
21	N	57	ASP	N-CA-C	-5.71	106.21	112.72
33	J	374	ARG	CA-C-N	5.71	127.87	120.56
33	J	374	ARG	C-N-CA	5.71	127.87	120.56
14	7	214	MET	CA-C-N	5.71	127.86	120.44
14	7	214	MET	C-N-CA	5.71	127.86	120.44
25	R	48	GLU	CA-C-N	5.71	127.86	120.44
25	R	48	GLU	C-N-CA	5.71	127.86	120.44
31	L	302	GLN	CA-C-N	5.71	128.40	120.29
31	L	302	GLN	C-N-CA	5.71	128.40	120.29
4	D	117	GLN	CA-C-N	5.71	127.93	120.28
4	D	117	GLN	C-N-CA	5.71	127.93	120.28
22	S	33	GLU	CA-C-N	5.71	127.93	120.28
22	S	33	GLU	C-N-CA	5.71	127.93	120.28
24	Q	80	HIS	CE1-NE2-CD2	-5.71	103.29	109.00
31	L	388	GLY	CA-C-N	5.71	127.93	120.28
31	L	388	GLY	C-N-CA	5.71	127.93	120.28
32	M	38	ASP	CB-CA-C	-5.71	101.15	110.85
31	L	416	MET	N-CA-C	5.71	117.50	111.28
12	l	160	ASN	CA-C-N	5.70	128.39	120.29
12	l	160	ASN	C-N-CA	5.70	128.39	120.29
21	N	24	ALA	N-CA-CB	5.70	118.50	110.12
29	I	282	ASP	N-CA-C	-5.70	99.99	109.46
32	M	425	ARG	NE-CZ-NH1	-5.70	115.80	121.50
15	W	99	LYS	CA-C-N	5.70	130.79	122.41
15	W	99	LYS	C-N-CA	5.70	130.79	122.41
21	N	702	ALA	CA-C-O	-5.70	114.51	120.55
22	S	347	HIS	CB-CG-CD2	-5.70	123.79	131.20
27	O	185	PHE	CA-C-N	5.70	128.19	120.44
27	O	185	PHE	C-N-CA	5.70	128.19	120.44
4	d	47	GLU	CA-C-N	5.70	130.59	122.72
4	d	47	GLU	C-N-CA	5.70	130.59	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	210	ASN	N-CA-CB	5.70	119.25	110.81
16	V	255	ILE	N-CA-C	5.70	116.98	111.91
17	T	132	HIS	CG-CD2-NE2	5.70	112.90	107.20
18	X	113	GLU	CA-C-N	5.70	134.25	121.76
18	X	113	GLU	C-N-CA	5.70	134.25	121.76
20	Z	64	TYR	N-CA-C	-5.70	106.25	113.43
25	R	358	GLY	O-C-N	-5.70	115.29	122.70
5	e	65	GLU	CA-C-N	5.70	131.73	122.67
5	e	65	GLU	C-N-CA	5.70	131.73	122.67
22	S	52	TYR	CA-C-N	5.70	128.27	120.46
22	S	52	TYR	C-N-CA	5.70	128.27	120.46
24	Q	92	LYS	CA-C-N	5.70	127.92	120.28
24	Q	92	LYS	C-N-CA	5.70	127.92	120.28
26	U	264	ALA	N-CA-C	-5.70	105.15	111.36
28	H	384	GLY	CA-C-N	5.70	130.37	120.68
28	H	384	GLY	C-N-CA	5.70	130.37	120.68
21	N	430	ASN	OD1-CG-ND2	-5.70	116.90	122.60
31	L	76	GLN	N-CA-C	5.70	117.49	111.28
11	k	84	VAL	CA-C-N	5.70	127.91	120.28
11	k	84	VAL	C-N-CA	5.70	127.91	120.28
11	4	186	LYS	CA-C-N	5.70	130.36	120.68
11	4	186	LYS	C-N-CA	5.70	130.36	120.68
16	V	279	HIS	CE1-NE2-CD2	-5.70	103.31	109.00
19	Y	2	SER	N-CA-C	-5.70	100.64	109.24
21	N	245	LEU	N-CA-C	-5.70	105.99	113.17
22	S	77	THR	N-CA-C	5.70	117.16	111.07
27	O	40	GLN	CG-CD-NE2	5.70	124.94	116.40
7	g	98	SER	CA-C-O	-5.69	114.52	120.55
10	3	151	GLU	N-CA-C	5.69	117.56	111.36
14	7	124	TYR	CB-CG-CD2	-5.69	112.26	120.80
25	R	66	LEU	N-CA-C	5.69	117.48	111.28
2	b	37	ILE	CA-C-O	5.69	126.36	120.39
24	Q	158	ILE	N-CA-C	-5.69	104.97	110.72
25	R	325	HIS	CB-CG-ND1	5.69	131.24	122.70
27	O	8	ASP	CA-CB-CG	5.69	118.29	112.60
24	Q	37	GLN	OE1-CD-NE2	-5.69	116.91	122.60
25	R	246	TYR	N-CA-C	-5.69	105.06	112.23
25	R	401	HIS	CE1-NE2-CD2	-5.69	103.31	109.00
28	H	387	ASN	CA-CB-CG	-5.69	106.91	112.60
2	b	183	LEU	N-CA-C	-5.68	100.07	108.99
6	f	206	LEU	CA-C-O	5.68	126.63	120.32
27	O	275	SER	O-C-N	5.68	129.62	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	67	SER	N-CA-C	-5.68	101.60	108.14
13	m	191	LEU	CA-C-N	5.68	127.93	120.60
13	m	191	LEU	C-N-CA	5.68	127.93	120.60
20	Z	208	VAL	CA-C-O	-5.68	114.88	118.69
21	N	638	ILE	N-CA-C	-5.68	104.82	110.62
26	U	285	ILE	CB-CA-C	-5.68	104.47	112.14
31	L	292	SER	CA-C-O	5.68	128.64	120.51
10	3	59	ASP	CA-C-N	5.68	127.80	120.70
10	3	59	ASP	C-N-CA	5.68	127.80	120.70
16	V	190	HIS	CA-C-O	-5.68	114.53	120.55
17	T	124	SER	CB-CA-C	-5.68	101.19	110.85
3	c	109	GLU	N-CA-C	5.68	117.47	111.28
4	d	17	ILE	CA-C-N	5.68	128.16	120.38
4	d	17	ILE	C-N-CA	5.68	128.16	120.38
13	m	163	ASN	CA-C-N	5.68	131.03	122.68
13	m	163	ASN	C-N-CA	5.68	131.03	122.68
10	3	69	TYR	CA-C-N	5.68	128.36	120.29
10	3	69	TYR	C-N-CA	5.68	128.36	120.29
11	4	52	ASP	CA-CB-CG	-5.68	106.92	112.60
16	V	245	VAL	CB-CA-C	-5.68	104.38	112.22
17	T	62	LEU	N-CA-C	-5.68	104.99	111.07
27	O	68	LYS	N-CA-C	-5.68	106.16	114.39
33	J	198	LEU	O-C-N	5.68	128.63	122.15
12	l	116	LEU	N-CA-CB	5.68	120.14	110.71
27	O	135	ARG	NE-CZ-NH2	-5.68	114.09	119.20
5	e	20	ARG	N-CA-CB	5.68	121.57	111.69
12	l	135	GLY	N-CA-C	-5.68	107.62	114.66
14	7	126	PHE	CA-C-N	5.68	127.89	120.28
14	7	126	PHE	C-N-CA	5.68	127.89	120.28
21	N	503	THR	N-CA-CB	5.68	118.56	110.16
22	S	246	GLU	CA-C-N	5.68	128.48	120.42
22	S	246	GLU	C-N-CA	5.68	128.48	120.42
23	P	140	THR	CA-C-N	5.68	128.45	120.28
23	P	140	THR	C-N-CA	5.68	128.45	120.28
26	U	171	VAL	N-CA-C	-5.68	104.99	110.72
5	e	220	SER	N-CA-C	-5.67	99.79	108.76
6	f	69	HIS	CE1-NE2-CD2	-5.67	103.33	109.00
10	j	52	GLY	CA-C-O	-5.67	115.97	120.91
12	l	127	CYS	CA-C-N	5.67	127.82	120.44
12	l	127	CYS	C-N-CA	5.67	127.82	120.44
33	J	108	LYS	N-CA-C	-5.67	101.80	110.14
1	a	232	LYS	CG-CD-CE	5.67	124.35	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	189	ALA	CA-C-N	5.67	128.15	120.44
8	1	189	ALA	C-N-CA	5.67	128.15	120.44
21	N	163	LEU	CA-C-N	5.67	127.88	120.28
21	N	163	LEU	C-N-CA	5.67	127.88	120.28
21	N	584	ARG	CG-CD-NE	-5.67	99.52	112.00
24	Q	361	HIS	N-CA-CB	5.67	118.46	110.12
24	Q	372	GLN	CA-C-O	-5.67	114.87	120.82
21	N	167	GLU	N-CA-CB	5.67	118.45	110.12
24	Q	404	ASN	OD1-CG-ND2	5.67	128.27	122.60
29	I	131	SER	CA-C-N	5.67	129.68	122.37
29	I	131	SER	C-N-CA	5.67	129.68	122.37
30	K	220	THR	CA-CB-OG1	5.67	118.10	109.60
2	b	218	ASN	CA-CB-CG	5.67	118.27	112.60
9	i	58	LYS	CA-C-N	5.67	130.01	121.40
9	i	58	LYS	C-N-CA	5.67	130.01	121.40
9	i	159	GLY	CA-C-N	5.67	129.32	120.82
9	i	159	GLY	C-N-CA	5.67	129.32	120.82
9	2	59	ASN	CA-C-N	5.67	132.36	121.54
9	2	59	ASN	C-N-CA	5.67	132.36	121.54
14	7	248	GLU	CA-C-N	5.67	130.17	122.07
14	7	248	GLU	C-N-CA	5.67	130.17	122.07
16	V	229	ASP	N-CA-CB	5.67	118.30	109.97
20	Z	786	SER	N-CA-CB	-5.67	101.79	110.12
25	R	89	ASN	OD1-CG-ND2	-5.67	116.93	122.60
31	L	389	ALA	N-CA-CB	5.67	118.45	110.12
25	R	210	TYR	CA-C-O	-5.67	114.87	120.82
28	H	207	THR	CA-CB-OG1	5.66	118.09	109.60
30	K	307	ASP	CA-C-N	5.66	132.36	121.54
30	K	307	ASP	C-N-CA	5.66	132.36	121.54
31	L	166	LEU	N-CA-C	-5.66	105.19	111.36
32	M	278	ILE	N-CA-C	-5.66	100.42	108.58
23	P	399	ILE	CA-C-O	5.66	127.19	121.64
25	R	355	SER	CA-C-N	5.66	128.14	120.44
25	R	355	SER	C-N-CA	5.66	128.14	120.44
33	J	337	LEU	CA-C-N	5.66	129.14	120.82
33	J	337	LEU	C-N-CA	5.66	129.14	120.82
23	P	211	PRO	N-CA-C	-5.66	107.27	114.35
27	O	342	ASP	N-CA-CB	5.66	119.59	110.65
1	a	109	GLY	O-C-N	5.66	129.34	122.32
9	i	132	VAL	N-CA-C	-5.66	99.61	108.95
21	N	239	LEU	O-C-N	5.66	128.12	122.12
21	N	793	GLY	CA-C-N	5.66	128.33	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	793	GLY	C-N-CA	5.66	128.33	120.29
22	S	47	THR	CA-C-N	5.66	127.80	120.44
22	S	47	THR	C-N-CA	5.66	127.80	120.44
25	R	401	HIS	ND1-CE1-NE2	5.66	114.06	108.40
29	I	230	THR	CA-CB-OG1	5.66	118.09	109.60
1	a	105	ARG	CD-NE-CZ	-5.66	116.48	124.40
10	j	28	ARG	CB-CA-C	-5.66	100.77	110.22
31	L	64	LEU	CB-CA-C	-5.66	101.40	110.79
15	W	193	GLU	CB-CG-CD	-5.66	102.99	112.60
22	S	180	ASN	CA-CB-CG	5.66	118.25	112.60
23	P	76	ASN	CA-C-N	5.66	127.86	120.28
23	P	76	ASN	C-N-CA	5.66	127.86	120.28
24	Q	329	GLU	N-CA-CB	5.66	118.43	110.12
26	U	273	LEU	CA-C-O	-5.65	114.56	120.55
31	L	217	GLY	CA-C-N	5.65	130.85	122.71
31	L	217	GLY	C-N-CA	5.65	130.85	122.71
1	a	101	ALA	CA-C-N	5.65	127.85	120.28
1	a	101	ALA	C-N-CA	5.65	127.85	120.28
6	f	4	ASN	CA-CB-CG	5.65	118.25	112.60
14	7	216	VAL	N-CA-C	-5.65	105.01	110.72
31	L	107	GLU	O-C-N	5.65	129.72	123.33
1	a	140	ILE	N-CA-CB	5.65	117.82	111.21
2	b	152	PRO	CA-C-N	5.65	127.85	120.28
2	b	152	PRO	C-N-CA	5.65	127.85	120.28
12	5	118	GLY	CA-C-O	-5.65	116.53	120.94
29	I	365	HIS	CA-C-N	5.65	130.16	120.72
29	I	365	HIS	C-N-CA	5.65	130.16	120.72
31	L	91	THR	CA-C-N	5.65	128.90	120.31
31	L	91	THR	C-N-CA	5.65	128.90	120.31
3	c	100	LYS	CA-C-O	5.65	126.41	120.42
4	d	158	SER	O-C-N	5.65	129.26	122.94
8	1	177	SER	N-CA-C	-5.65	106.16	113.16
8	1	187	LEU	CA-C-O	-5.65	114.11	120.32
11	4	73	TYR	N-CA-C	-5.65	99.22	108.76
22	S	424	SER	CB-CA-C	-5.65	102.02	110.88
26	U	251	ASN	CA-CB-CG	-5.65	106.95	112.60
27	O	371	VAL	N-CA-C	-5.65	105.02	110.72
30	K	200	GLN	CA-C-N	5.65	128.20	120.46
30	K	200	GLN	C-N-CA	5.65	128.20	120.46
33	J	269	GLN	CA-C-N	5.65	127.85	120.28
33	J	269	GLN	C-N-CA	5.65	127.85	120.28
12	l	275	VAL	CA-CB-CG2	-5.64	100.81	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	413	LEU	CA-C-O	5.64	128.13	121.36
16	V	38	LEU	CA-C-O	-5.64	114.57	120.55
21	N	760	GLY	O-C-N	5.64	129.93	122.76
22	S	259	TYR	O-C-N	-5.64	116.75	121.38
25	R	357	PHE	N-CA-CB	5.64	119.03	110.28
14	n	95	HIS	CA-C-O	5.64	125.89	119.18
25	R	418	GLY	CA-C-N	5.64	127.77	120.44
25	R	418	GLY	C-N-CA	5.64	127.77	120.44
6	f	50	LYS	CB-CA-C	-5.64	99.96	109.83
12	l	141	HIS	CE1-NE2-CD2	-5.64	103.36	109.00
13	m	14	GLY	N-CA-C	-5.64	101.86	111.27
12	5	239	ALA	CA-C-O	5.64	126.53	120.55
17	T	9	LYS	CA-C-N	5.64	130.22	120.58
17	T	9	LYS	C-N-CA	5.64	130.22	120.58
33	J	378	THR	CA-C-N	5.64	128.30	120.29
33	J	378	THR	C-N-CA	5.64	128.30	120.29
1	a	102	ALA	CA-C-N	5.64	128.29	120.29
1	a	102	ALA	C-N-CA	5.64	128.29	120.29
21	N	704	GLY	CA-C-O	-5.64	114.94	120.75
26	U	294	ASN	CA-C-N	5.64	127.83	120.28
26	U	294	ASN	C-N-CA	5.64	127.83	120.28
31	L	116	LYS	O-C-N	-5.64	116.48	123.36
33	J	253	ILE	O-C-N	-5.64	116.71	122.23
14	7	72	VAL	CA-CB-CG1	5.63	119.98	110.40
22	S	319	CYS	CA-C-N	5.63	129.54	120.30
22	S	319	CYS	C-N-CA	5.63	129.54	120.30
25	R	321	TYR	CB-CG-CD1	5.63	129.25	120.80
26	U	18	ALA	CA-C-N	5.63	127.76	120.44
26	U	18	ALA	C-N-CA	5.63	127.76	120.44
9	i	200	SER	CA-C-N	5.63	129.26	120.75
9	i	200	SER	C-N-CA	5.63	129.26	120.75
11	k	41	HIS	N-CA-C	-5.63	103.92	112.99
9	2	216	LEU	CA-C-N	5.63	128.84	120.95
9	2	216	LEU	C-N-CA	5.63	128.84	120.95
22	S	290	ASN	CA-CB-CG	5.63	118.23	112.60
24	Q	151	TYR	O-C-N	5.63	130.04	122.49
4	d	70	HIS	CG-CD2-NE2	5.63	112.83	107.20
21	N	491	GLY	CA-C-O	-5.63	112.26	119.13
32	M	363	ILE	N-CA-C	-5.63	105.03	110.72
21	N	182	ASN	CA-CB-CG	-5.63	106.97	112.60
22	S	193	THR	CA-C-N	5.63	127.82	120.28
22	S	193	THR	C-N-CA	5.63	127.82	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	390	THR	CA-C-N	5.63	126.19	120.00
22	S	390	THR	C-N-CA	5.63	126.19	120.00
26	U	195	LYS	CA-C-N	5.63	127.82	120.28
26	U	195	LYS	C-N-CA	5.63	127.82	120.28
31	L	118	ILE	N-CA-C	-5.63	100.21	108.54
5	e	221	CYS	CA-C-O	-5.63	115.04	121.68
14	n	39	VAL	N-CA-C	-5.63	100.23	108.11
26	U	20	ASP	CA-C-O	-5.63	114.91	120.82
26	U	275	VAL	CA-CB-CG1	5.63	119.97	110.40
28	H	327	ASN	OD1-CG-ND2	-5.63	116.97	122.60
29	I	230	THR	O-C-N	-5.63	114.69	122.46
32	M	223	PRO	CA-C-N	5.63	126.88	119.84
32	M	223	PRO	C-N-CA	5.63	126.88	119.84
33	J	317	PRO	N-CA-C	5.63	115.87	110.47
1	a	36	ASN	N-CA-C	-5.63	105.62	112.88
12	l	241	HIS	CA-CB-CG	5.63	119.43	113.80
16	V	80	VAL	CA-C-N	5.63	131.38	122.60
16	V	80	VAL	C-N-CA	5.63	131.38	122.60
25	R	109	LYS	N-CA-C	5.63	117.22	111.14
28	H	348	ASN	N-CA-CB	5.63	120.00	110.49
29	I	174	ASP	N-CA-C	-5.63	105.00	113.89
26	U	220	PRO	CA-C-O	-5.62	115.21	121.23
2	b	18	LEU	CA-C-O	5.62	126.20	120.24
4	d	245	GLU	N-CA-C	5.62	118.18	111.71
8	h	74	LEU	CA-C-N	5.62	128.28	120.29
8	h	74	LEU	C-N-CA	5.62	128.28	120.29
25	R	314	ASN	N-CA-CB	-5.62	103.42	110.90
10	3	97	GLU	CB-CA-C	-5.62	101.46	110.79
13	6	95	ASN	CB-CA-C	-5.62	101.46	110.79
17	T	209	LEU	N-CA-C	-5.62	106.09	113.17
24	Q	386	PHE	CA-C-N	5.62	132.28	121.54
24	Q	386	PHE	C-N-CA	5.62	132.28	121.54
29	I	113	ILE	N-CA-C	-5.62	100.38	108.53
16	V	47	MET	CA-C-O	5.62	127.24	121.23
2	b	59	GLU	N-CA-C	-5.62	105.63	112.88
7	g	59	LEU	CB-CA-C	-5.62	99.56	109.62
10	j	137	ILE	N-CA-CB	5.62	120.68	111.58
11	4	20	ALA	CA-C-N	5.62	130.50	123.14
11	4	20	ALA	C-N-CA	5.62	130.50	123.14
17	T	170	ASN	CA-C-N	5.62	132.09	121.97
17	T	170	ASN	C-N-CA	5.62	132.09	121.97
23	P	203	ILE	N-CA-C	-5.62	101.64	109.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	100	ASN	CA-C-O	-5.62	114.92	120.82
25	R	307	TYR	O-C-N	5.62	128.08	122.12
29	I	349	LEU	N-CA-C	5.62	117.81	108.20
32	M	109	ASP	CA-CB-CG	5.62	118.22	112.60
21	N	244	LYS	N-CA-C	-5.62	105.30	111.82
21	N	425	ASN	CB-CA-C	-5.62	101.30	110.85
22	S	68	LEU	CA-C-O	-5.62	115.08	121.65
33	J	146	THR	N-CA-C	-5.62	100.99	108.74
9	i	209	ILE	N-CA-C	5.62	116.95	109.37
14	n	121	GLU	O-C-N	5.62	126.12	121.35
9	2	43	ILE	CA-C-O	-5.62	114.58	120.76
14	7	261	TYR	CA-C-N	5.62	131.81	121.70
14	7	261	TYR	C-N-CA	5.62	131.81	121.70
7	g	185	GLU	CA-C-N	5.61	128.81	121.85
7	g	185	GLU	C-N-CA	5.61	128.81	121.85
14	n	210	ILE	CA-C-N	5.61	127.84	120.60
14	n	210	ILE	C-N-CA	5.61	127.84	120.60
23	P	139	VAL	CA-C-O	-5.61	114.41	120.47
24	Q	243	PHE	CA-C-N	5.61	128.26	120.29
24	Q	243	PHE	C-N-CA	5.61	128.26	120.29
23	P	173	MET	CA-C-N	5.61	127.80	120.28
23	P	173	MET	C-N-CA	5.61	127.80	120.28
27	O	53	LYS	CA-C-N	5.61	133.31	122.53
27	O	53	LYS	C-N-CA	5.61	133.31	122.53
10	j	146	LEU	N-CA-CB	5.61	118.30	109.94
23	P	266	TYR	CB-CG-CD2	-5.61	112.38	120.80
30	K	339	GLU	O-C-N	-5.61	116.83	123.22
6	f	220	THR	CA-C-O	-5.61	112.72	119.67
14	n	98	ARG	CA-C-N	5.61	128.84	120.31
14	n	98	ARG	C-N-CA	5.61	128.84	120.31
11	4	100	VAL	CA-C-N	5.61	130.74	123.00
11	4	100	VAL	C-N-CA	5.61	130.74	123.00
21	N	675	VAL	CB-CA-C	-5.61	104.57	112.14
23	P	86	HIS	CB-CG-CD2	-5.61	123.91	131.20
23	P	115	ARG	N-CA-C	-5.61	105.08	111.14
10	j	57	ALA	CA-C-N	5.61	127.79	120.28
10	j	57	ALA	C-N-CA	5.61	127.79	120.28
12	l	238	ALA	CA-C-O	5.61	126.36	120.42
9	2	62	LYS	O-C-N	5.61	129.16	122.21
23	P	282	HIS	CB-CG-CD2	-5.61	123.91	131.20
24	Q	92	LYS	N-CA-C	-5.61	106.48	113.38
30	K	421	VAL	CA-C-N	5.61	127.80	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	421	VAL	C-N-CA	5.61	127.80	120.28
11	k	93	ARG	N-CA-C	-5.61	104.79	111.69
6	F	230	VAL	N-CA-C	-5.61	107.52	112.90
13	6	220	VAL	CA-C-N	-5.61	115.09	122.99
13	6	220	VAL	C-N-CA	-5.61	115.09	122.99
26	U	247	ILE	CA-CB-CG1	5.61	119.93	110.40
28	H	222	ARG	N-CA-CB	5.61	118.36	110.12
29	I	217	LYS	CA-C-N	5.61	130.08	121.45
29	I	217	LYS	C-N-CA	5.61	130.08	121.45
2	b	38	LYS	CB-CA-C	5.60	119.58	110.22
13	m	103	HIS	CB-CG-ND1	5.60	131.10	122.70
13	m	156	PRO	N-CA-C	-5.60	106.39	114.18
21	N	240	GLN	CB-CA-C	-5.60	101.49	110.79
24	Q	106	GLN	O-C-N	-5.60	116.18	122.12
26	U	245	ASP	CA-C-N	5.60	127.79	120.28
26	U	245	ASP	C-N-CA	5.60	127.79	120.28
31	L	216	LYS	N-CA-CB	5.60	121.94	111.52
32	M	339	ARG	CA-CB-CG	5.60	125.30	114.10
16	V	267	LYS	CA-C-O	5.60	126.49	120.55
17	T	82	PHE	N-CA-CB	5.60	118.45	110.16
2	b	89	SER	CA-C-O	-5.60	114.48	120.42
13	6	102	GLN	O-C-N	5.60	128.06	122.12
17	T	87	PRO	N-CA-C	5.60	120.92	114.03
20	Z	739	ALA	N-CA-C	5.60	117.38	111.28
21	N	319	SER	N-CA-CB	5.60	118.19	110.07
21	N	819	LYS	CB-CA-C	-5.60	101.49	110.79
23	P	440	HIS	CG-CD2-NE2	5.60	112.80	107.20
24	Q	210	CYS	N-CA-C	-5.60	102.56	110.29
29	I	57	LEU	CA-C-O	-5.60	114.48	120.42
3	c	232	PRO	N-CA-CB	5.60	108.84	103.52
7	g	40	ILE	N-CA-C	-5.60	99.69	107.80
23	P	161	CYS	CA-C-O	5.60	126.35	120.42
30	K	89	ILE	CA-C-N	5.60	127.78	120.28
30	K	89	ILE	C-N-CA	5.60	127.78	120.28
31	L	82	ARG	N-CA-CB	5.60	118.19	110.07
32	M	281	ASP	N-CA-CB	5.60	119.70	110.69
16	V	217	HIS	N-CA-CB	5.60	119.95	110.49
30	K	214	PRO	N-CA-C	5.60	115.84	110.47
11	4	80	VAL	CA-CB-CG1	5.59	119.91	110.40
16	V	291	ASN	OD1-CG-ND2	-5.59	117.01	122.60
17	T	124	SER	CA-C-N	5.59	127.71	120.44
17	T	124	SER	C-N-CA	5.59	127.71	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	868	VAL	N-CA-CB	5.59	119.13	111.41
33	J	181	GLN	CA-C-O	-5.59	115.35	120.50
4	d	132	SER	N-CA-C	-5.59	100.28	109.40
15	W	142	ILE	CA-C-O	-5.59	114.49	120.59
1	a	37	GLN	CB-CA-C	-5.59	100.72	110.17
12	l	133	TRP	CE2-CD2-CE3	5.59	124.39	118.80
10	3	24	ALA	CA-C-O	-5.59	114.57	121.06
16	V	49	VAL	N-CA-CB	5.59	122.38	111.92
21	N	575	ALA	N-CA-CB	5.59	118.34	110.12
25	R	25	GLU	CA-C-N	5.59	127.72	120.56
25	R	25	GLU	C-N-CA	5.59	127.72	120.56
3	c	205	ALA	CB-CA-C	-5.59	100.72	111.78
16	V	279	HIS	CA-C-O	-5.59	114.50	120.42
19	Y	57	THR	N-CA-C	-5.59	106.59	113.41
24	Q	251	THR	N-CA-CB	5.59	119.75	110.47
9	2	59	ASN	O-C-N	5.59	130.09	123.33
21	N	902	VAL	CB-CA-C	-5.59	104.54	111.08
28	H	423	CYS	CA-C-N	5.59	127.77	120.28
28	H	423	CYS	C-N-CA	5.59	127.77	120.28
31	L	153	LEU	CA-C-N	5.59	130.65	122.77
31	L	153	LEU	C-N-CA	5.59	130.65	122.77
12	l	219	TYR	CA-CB-CG	-5.58	103.85	113.90
4	d	80	ALA	N-CA-C	-5.58	105.11	111.14
14	7	213	ALA	CA-C-O	-5.58	114.96	120.82
16	V	124	ASN	CA-C-N	5.58	127.76	120.28
16	V	124	ASN	C-N-CA	5.58	127.76	120.28
23	P	289	ASN	CA-C-O	5.58	126.39	119.97
27	O	341	ILE	N-CA-CB	5.58	118.90	111.64
1	a	35	THR	N-CA-C	-5.58	106.24	113.16
14	7	182	HIS	CE1-NE2-CD2	-5.58	103.42	109.00
15	W	118	ILE	O-C-N	5.58	128.54	122.57
21	N	92	ASP	CA-C-O	5.58	126.23	119.31
21	N	572	LEU	N-CA-CB	5.58	118.42	110.16
23	P	239	GLN	CA-C-O	-5.58	114.63	120.55
10	j	103	TYR	N-CA-CB	5.58	118.17	109.97
33	J	336	ASN	CA-C-O	-5.58	114.23	120.54
14	n	90	ILE	CA-C-O	5.58	126.28	120.25
15	W	151	THR	O-C-N	-5.58	116.81	123.06
33	J	336	ASN	CB-CA-C	-5.58	100.65	109.80
12	l	149	ILE	O-C-N	5.58	129.30	122.83
27	O	356	ARG	NE-CZ-NH2	5.58	124.22	119.20
31	L	223	PRO	N-CA-C	5.58	117.50	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	73	GLU	N-CA-CB	5.58	118.09	110.01
13	6	157	PHE	CA-CB-CG	-5.58	108.22	113.80
21	N	797	GLU	CA-C-N	5.58	128.02	120.38
21	N	797	GLU	C-N-CA	5.58	128.02	120.38
7	g	33	ASN	N-CA-C	-5.57	105.83	113.30
11	k	96	ARG	N-CA-CB	5.57	117.25	110.17
23	P	61	LYS	CA-C-O	5.57	126.67	120.82
24	Q	80	HIS	ND1-CE1-NE2	5.57	113.97	108.40
32	M	299	ARG	NE-CZ-NH1	5.57	127.07	121.50
32	M	102	GLN	CB-CG-CD	-5.57	103.13	112.60
2	b	68	THR	CA-C-O	-5.57	115.37	120.50
10	3	97	GLU	N-CA-C	5.57	117.35	111.28
15	W	89	THR	N-CA-C	-5.57	105.29	111.36
24	Q	360	SER	O-C-N	5.57	127.88	122.09
3	c	188	ASP	CA-CB-CG	5.57	118.17	112.60
9	2	158	SER	CA-C-N	5.57	132.33	121.41
9	2	158	SER	C-N-CA	5.57	132.33	121.41
28	H	372	ASP	O-C-N	-5.57	115.45	122.19
13	m	163	ASN	O-C-N	5.57	129.30	122.34
23	P	143	LEU	N-CA-C	-5.57	105.99	112.89
3	c	130	PRO	N-CA-CB	5.57	109.09	103.25
32	M	239	THR	N-CA-CB	5.57	119.47	110.40
33	J	49	ASN	CA-C-N	5.57	127.74	120.28
33	J	49	ASN	C-N-CA	5.57	127.74	120.28
6	f	183	ASP	CA-CB-CG	-5.56	107.04	112.60
11	k	73	TYR	N-CA-C	-5.56	98.95	110.80
14	n	77	PRO	CA-C-N	5.56	130.29	123.17
14	n	77	PRO	C-N-CA	5.56	130.29	123.17
12	5	133	TRP	N-CA-C	-5.56	105.99	112.89
20	Z	729	GLU	CA-CB-CG	-5.56	102.97	114.10
27	O	305	ILE	CA-CB-CG1	5.56	119.86	110.40
2	b	34	SER	O-C-N	-5.56	117.05	123.33
13	m	40	ASP	CB-CA-C	-5.56	110.18	116.63
13	6	108	LYS	N-CA-C	-5.56	98.29	108.02
33	J	196	THR	CB-CA-C	-5.56	101.56	110.79
13	6	12	PRO	N-CA-C	-5.56	107.56	114.68
19	Y	5	VAL	CA-C-N	5.56	128.76	120.31
19	Y	5	VAL	C-N-CA	5.56	128.76	120.31
20	Z	841	GLU	N-CA-C	-5.56	100.34	109.40
21	N	353	LEU	CA-C-N	5.56	125.08	119.19
21	N	353	LEU	C-N-CA	5.56	125.08	119.19
30	K	352	ILE	CA-C-N	5.56	127.73	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	352	ILE	C-N-CA	5.56	127.73	120.28
31	L	246	SER	CA-C-O	5.56	123.93	119.59
31	L	306	MET	CA-C-N	5.56	128.18	120.29
31	L	306	MET	C-N-CA	5.56	128.18	120.29
21	N	815	LYS	CB-CA-C	-5.56	101.92	110.81
26	U	157	LEU	CA-C-N	5.56	125.88	119.93
26	U	157	LEU	C-N-CA	5.56	125.88	119.93
26	U	257	ILE	N-CA-C	-5.56	104.94	111.00
31	L	286	ILE	CA-C-N	-5.56	115.41	122.19
31	L	286	ILE	C-N-CA	-5.56	115.41	122.19
5	e	92	ALA	CA-C-O	-5.56	114.66	120.55
10	j	199	TYR	CA-C-O	-5.56	115.50	121.56
25	R	393	PRO	CA-C-O	-5.56	115.28	121.23
29	I	408	ARG	CA-CB-CG	5.56	125.21	114.10
32	M	63	LYS	CA-C-N	5.56	127.66	120.44
32	M	63	LYS	C-N-CA	5.56	127.66	120.44
4	d	182	LYS	O-C-N	5.55	128.89	122.17
7	g	34	GLY	CA-C-N	5.55	129.66	120.94
7	g	34	GLY	C-N-CA	5.55	129.66	120.94
23	P	428	THR	N-CA-C	5.55	117.33	111.28
31	L	123	SER	O-C-N	5.55	127.79	122.07
31	L	132	ARG	N-CA-C	-5.55	103.05	110.55
6	f	155	GLU	N-CA-C	-5.55	99.85	108.90
3	c	49	GLU	CA-C-O	-5.55	114.38	120.43
10	j	73	LEU	N-CA-C	5.55	117.33	111.28
12	l	217	SER	CA-C-O	5.55	126.19	119.31
28	H	434	ARG	NE-CZ-NH2	5.55	124.20	119.20
30	K	236	ARG	CB-CG-CD	5.55	124.07	111.30
6	f	41	ASN	CA-CB-CG	5.55	118.15	112.60
13	6	183	LEU	CA-C-N	5.55	131.28	122.62
13	6	183	LEU	C-N-CA	5.55	131.28	122.62
23	P	257	TRP	CA-CB-CG	5.55	124.14	113.60
27	O	153	LEU	CA-C-N	5.55	127.72	120.28
27	O	153	LEU	C-N-CA	5.55	127.72	120.28
29	I	132	ILE	N-CA-C	-5.55	100.59	108.58
32	M	173	ASP	N-CA-C	-5.55	103.67	110.61
4	d	110	THR	N-CA-CB	5.55	118.11	110.07
16	V	84	ASP	N-CA-C	-5.55	100.67	109.76
22	S	151	GLU	CA-C-O	5.55	128.38	121.89
7	g	57	LYS	N-CA-C	-5.54	106.52	113.28
22	S	368	LYS	CA-C-N	5.54	127.98	120.44
22	S	368	LYS	C-N-CA	5.54	127.98	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L	313	ASP	O-C-N	-5.54	116.50	123.27
1	a	124	LEU	O-C-N	5.54	128.00	122.12
8	1	60	ASP	N-CA-C	-5.54	105.32	111.36
12	5	254	HIS	ND1-CE1-NE2	5.54	113.94	108.40
14	7	34	THR	CA-C-N	5.54	131.66	121.85
14	7	34	THR	C-N-CA	5.54	131.66	121.85
25	R	275	GLU	CA-C-N	5.54	128.74	120.31
25	R	275	GLU	C-N-CA	5.54	128.74	120.31
26	U	262	GLN	N-CA-C	-5.54	105.32	111.36
29	I	193	GLU	N-CA-C	-5.54	106.45	113.43
30	K	109	ILE	O-C-N	5.54	129.19	123.20
30	K	330	ARG	O-C-N	-5.54	114.94	121.32
2	b	36	GLY	N-CA-C	-5.54	100.05	113.18
24	Q	146	TYR	CA-C-O	5.54	126.34	119.97
25	R	239	THR	O-C-N	-5.54	116.70	123.30
27	O	266	PHE	N-CA-CB	5.54	118.27	110.12
29	I	403	ALA	N-CA-C	-5.54	105.25	112.23
22	S	351	ALA	CA-C-N	5.54	128.28	120.42
22	S	351	ALA	C-N-CA	5.54	128.28	120.42
30	K	57	GLU	CA-C-N	5.54	128.73	120.31
30	K	57	GLU	C-N-CA	5.54	128.73	120.31
30	K	163	GLU	CA-C-N	5.54	128.49	120.79
30	K	163	GLU	C-N-CA	5.54	128.49	120.79
31	L	289	ARG	CA-C-N	5.54	132.12	121.54
31	L	289	ARG	C-N-CA	5.54	132.12	121.54
2	b	227	ILE	O-C-N	-5.54	114.79	121.10
26	U	66	TRP	N-CA-C	-5.54	100.52	108.60
1	a	22	GLU	N-CA-C	-5.54	105.88	113.30
5	e	233	ASN	OD1-CG-ND2	-5.54	117.06	122.60
13	m	168	TYR	CA-C-N	5.54	128.35	120.49
13	m	168	TYR	C-N-CA	5.54	128.35	120.49
11	4	133	HIS	CE1-NE2-CD2	-5.54	103.47	109.00
13	6	115	VAL	CB-CA-C	-5.54	102.63	110.82
21	N	302	PHE	CA-C-O	-5.54	114.98	120.90
28	H	365	LEU	N-CA-C	5.54	117.39	111.36
31	L	154	THR	CA-C-O	5.54	126.11	120.24
2	b	213	ILE	CA-CB-CG1	5.53	119.81	110.40
4	d	56	ASP	N-CA-C	-5.53	100.16	108.96
8	h	51	TRP	CA-C-O	-5.53	114.86	121.56
28	H	454	TYR	CA-C-N	5.53	127.69	120.28
28	H	454	TYR	C-N-CA	5.53	127.69	120.28
32	M	256	ILE	N-CA-C	5.53	116.26	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	145	HIS	ND1-CE1-NE2	5.53	113.93	108.40
16	V	284	ALA	CB-CA-C	-5.53	101.61	110.79
17	T	246	GLU	O-C-N	5.53	127.98	122.12
4	d	118	GLN	CB-CG-CD	-5.53	103.20	112.60
15	W	47	ASN	CB-CG-OD1	5.53	131.86	120.80
17	T	28	PRO	CA-C-N	5.53	125.19	119.05
17	T	28	PRO	C-N-CA	5.53	125.19	119.05
21	N	782	PHE	N-CA-C	-5.53	105.75	112.88
8	h	56	GLY	O-C-N	-5.53	117.60	122.85
1	a	53	VAL	CB-CA-C	5.53	117.64	110.12
12	l	141	HIS	CB-CG-ND1	5.53	130.99	122.70
14	7	39	VAL	N-CA-CB	5.53	119.04	111.41
14	7	189	ARG	CA-C-N	5.53	127.96	120.44
14	7	189	ARG	C-N-CA	5.53	127.96	120.44
17	T	84	GLN	O-C-N	5.53	128.45	122.15
19	Y	22	GLU	N-CA-C	5.53	117.39	111.36
20	Z	915	ALA	N-CA-C	-5.53	103.81	110.44
21	N	9	LEU	N-CA-C	-5.53	105.17	111.14
22	S	395	ILE	CA-C-O	-5.53	115.20	120.95
5	e	40	ILE	N-CA-CB	5.53	118.82	111.64
3	C	207	THR	CA-C-N	5.53	127.69	120.28
3	C	207	THR	C-N-CA	5.53	127.69	120.28
15	W	47	ASN	O-C-N	-5.53	116.15	122.89
16	V	206	THR	N-CA-C	-5.53	101.73	109.69
19	Y	58	ASN	N-CA-CB	5.53	119.83	110.49
21	N	24	ALA	CA-C-N	5.53	127.69	120.28
21	N	24	ALA	C-N-CA	5.53	127.69	120.28
21	N	565	ASN	CA-C-O	5.53	126.28	120.42
30	K	79	LEU	CA-C-N	5.53	128.14	120.29
30	K	79	LEU	C-N-CA	5.53	128.14	120.29
32	M	52	SER	CA-C-O	5.53	126.41	120.55
33	J	180	ALA	CA-C-N	5.53	133.00	123.11
33	J	180	ALA	C-N-CA	5.53	133.00	123.11
21	N	411	ILE	N-CA-C	-5.52	105.12	110.42
32	M	304	THR	O-C-N	-5.52	114.84	122.46
13	6	130	VAL	N-CA-CB	5.52	119.58	111.52
20	Z	919	GLU	N-CA-C	-5.52	105.26	111.28
27	O	128	LEU	CA-C-O	5.52	126.28	120.42
28	H	370	ARG	NE-CZ-NH1	5.52	127.02	121.50
32	M	351	LEU	CA-C-N	5.52	125.47	119.78
32	M	351	LEU	C-N-CA	5.52	125.47	119.78
32	M	413	GLU	CA-C-O	5.52	126.34	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	69	VAL	N-CA-C	5.52	116.82	109.37
14	7	186	PRO	O-C-N	5.52	128.59	122.24
1	a	190	LYS	N-CA-CB	5.52	119.82	110.49
9	i	153	TYR	N-CA-CB	5.52	119.87	110.71
15	W	152	GLU	CA-C-N	5.52	130.80	121.14
15	W	152	GLU	C-N-CA	5.52	130.80	121.14
17	T	107	SER	CB-CA-C	-5.52	101.63	110.79
21	N	373	VAL	CA-C-N	5.52	128.02	120.46
21	N	373	VAL	C-N-CA	5.52	128.02	120.46
24	Q	83	GLU	CA-C-N	5.52	128.23	120.28
24	Q	83	GLU	C-N-CA	5.52	128.23	120.28
32	M	324	LEU	N-CA-C	-5.52	100.89	109.72
6	f	16	THR	CA-CB-CG2	-5.52	101.12	110.50
9	2	170	HIS	CA-CB-CG	-5.52	108.28	113.80
4	d	209	ASN	CA-CB-CG	5.52	118.12	112.60
8	1	46	VAL	N-CA-C	-5.52	107.90	113.47
17	T	219	LYS	CB-CA-C	-5.52	101.63	110.79
22	S	46	LEU	CB-CA-C	-5.52	102.08	111.02
25	R	142	ALA	CA-C-N	5.52	127.67	120.28
25	R	142	ALA	C-N-CA	5.52	127.67	120.28
30	K	338	ILE	CA-C-N	5.52	129.97	122.19
30	K	338	ILE	C-N-CA	5.52	129.97	122.19
16	V	240	ALA	N-CA-C	5.51	117.29	111.28
21	N	215	MET	CA-C-O	5.51	126.39	120.55
23	P	199	LEU	CA-C-O	-5.51	114.70	120.55
25	R	304	TYR	CA-C-O	5.51	126.27	120.42
30	K	381	ALA	CA-C-O	-5.51	114.57	120.42
31	L	345	ARG	N-CA-CB	5.51	119.23	110.57
11	k	167	GLU	CA-C-N	5.51	127.67	120.28
11	k	167	GLU	C-N-CA	5.51	127.67	120.28
17	T	136	LEU	N-CA-C	-5.51	106.55	113.72
23	P	30	ASN	CA-C-O	-5.51	115.02	120.70
25	R	187	VAL	CA-CB-CG1	5.51	119.77	110.40
29	I	386	ASP	CA-CB-CG	-5.51	107.09	112.60
30	K	74	HIS	CE1-NE2-CD2	-5.51	103.49	109.00
10	j	13	VAL	N-CA-C	-5.51	100.39	108.99
9	2	214	GLU	CA-C-O	-5.51	114.56	120.46
21	N	690	HIS	CG-CD2-NE2	5.51	112.71	107.20
24	Q	408	THR	N-CA-CB	5.51	118.32	110.16
29	I	73	GLU	N-CA-C	-5.51	105.43	111.82
31	L	421	LYS	CA-C-N	5.51	128.25	120.42
31	L	421	LYS	C-N-CA	5.51	128.25	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	M	381	ARG	NE-CZ-NH1	-5.51	115.99	121.50
28	H	425	GLU	CA-C-O	5.51	126.37	120.70
3	c	31	HIS	CA-C-N	5.51	128.53	120.71
3	c	31	HIS	C-N-CA	5.51	128.53	120.71
9	2	252	ILE	N-CA-CB	5.51	117.65	111.21
17	T	121	LYS	CA-C-N	5.51	127.60	120.44
17	T	121	LYS	C-N-CA	5.51	127.60	120.44
21	N	302	PHE	CA-C-N	5.51	127.66	120.28
21	N	302	PHE	C-N-CA	5.51	127.66	120.28
21	N	756	THR	CA-CB-OG1	5.51	117.86	109.60
24	Q	372	GLN	CA-C-N	5.51	127.50	120.56
24	Q	372	GLN	C-N-CA	5.51	127.50	120.56
27	O	363	ILE	CA-C-N	5.51	128.11	120.29
27	O	363	ILE	C-N-CA	5.51	128.11	120.29
33	J	110	SER	N-CA-C	5.50	119.29	112.24
5	e	52	LYS	O-C-N	5.50	128.42	122.15
9	2	91	ASN	OD1-CG-ND2	-5.50	117.10	122.60
10	3	180	LEU	O-C-N	-5.50	115.58	122.35
23	P	66	LEU	CA-C-O	-5.50	115.17	122.44
3	c	208	TYR	N-CA-CB	5.50	118.21	110.12
4	d	12	SER	N-CA-CB	5.50	117.69	109.88
5	e	196	ALA	CA-C-N	5.50	127.59	120.44
5	e	196	ALA	C-N-CA	5.50	127.59	120.44
14	n	171	SER	N-CA-C	-5.50	101.16	109.85
14	n	187	LEU	N-CA-C	-5.50	105.20	111.14
21	N	162	ARG	N-CA-C	-5.50	100.27	109.24
29	I	195	LYS	N-CA-C	5.50	118.04	111.71
9	i	86	GLN	CA-C-N	5.50	128.10	120.29
9	i	86	GLN	C-N-CA	5.50	128.10	120.29
21	N	467	LYS	N-CA-C	-5.50	105.44	111.82
13	m	190	LYS	CA-C-O	-5.50	115.02	120.90
16	V	176	ASN	N-CA-C	-5.50	101.15	108.74
31	L	330	PRO	N-CA-C	-5.50	107.48	114.35
33	J	263	GLY	CA-C-N	5.50	127.27	120.34
33	J	263	GLY	C-N-CA	5.50	127.27	120.34
14	n	91	SER	CA-C-N	5.50	128.66	120.31
14	n	91	SER	C-N-CA	5.50	128.66	120.31
10	3	14	ALA	N-CA-CB	5.50	120.97	111.13
20	Z	285	ALA	CA-C-N	5.50	127.99	120.46
20	Z	285	ALA	C-N-CA	5.50	127.99	120.46
21	N	594	VAL	N-CA-CB	5.50	118.01	110.54
21	N	882	ILE	N-CA-C	-5.50	102.43	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	56	THR	CA-C-N	5.50	127.64	120.28
24	Q	56	THR	C-N-CA	5.50	127.64	120.28
24	Q	242	SER	CA-C-N	5.50	127.64	120.28
24	Q	242	SER	C-N-CA	5.50	127.64	120.28
29	I	122	SER	CA-C-N	5.50	125.17	119.56
29	I	122	SER	C-N-CA	5.50	125.17	119.56
14	n	85	GLY	N-CA-C	-5.50	102.30	110.71
7	g	61	PRO	N-CA-CB	5.49	108.66	102.67
13	m	149	ALA	CA-C-O	5.49	126.43	120.55
7	G	137	ILE	N-CA-C	-5.49	99.64	107.77
20	Z	444	GLU	CA-C-N	5.49	125.16	119.56
20	Z	444	GLU	C-N-CA	5.49	125.16	119.56
10	3	122	ALA	CA-C-O	-5.49	115.35	121.23
20	Z	727	GLU	O-C-N	5.49	129.90	122.59
33	J	274	GLU	CA-C-O	5.49	126.36	120.70
13	m	38	ILE	CA-C-O	5.49	127.07	121.63
21	N	630	ALA	CA-C-N	5.49	127.00	120.14
21	N	630	ALA	C-N-CA	5.49	127.00	120.14
23	P	196	ALA	N-CA-C	5.49	118.02	111.71
24	Q	287	THR	N-CA-C	-5.49	106.17	112.92
31	L	136	ASP	CA-CB-CG	-5.49	107.11	112.60
13	6	55	GLY	O-C-N	5.49	127.57	122.47
31	L	118	ILE	CB-CA-C	5.49	117.50	111.08
11	k	20	ALA	CA-C-N	5.49	131.10	122.70
11	k	20	ALA	C-N-CA	5.49	131.10	122.70
28	H	79	SER	CA-C-N	5.49	128.65	120.31
28	H	79	SER	C-N-CA	5.49	128.65	120.31
31	L	349	ILE	CB-CA-C	-5.49	104.54	110.85
32	M	102	GLN	CA-C-O	5.49	124.99	118.79
5	e	100	ASN	N-CA-C	-5.49	105.32	112.23
9	i	93	GLU	O-C-N	5.49	128.40	122.15
13	m	73	VAL	CA-C-N	5.49	127.57	120.44
13	m	73	VAL	C-N-CA	5.49	127.57	120.44
11	4	108	ASP	CA-CB-CG	5.49	118.09	112.60
19	Y	21	ASN	CA-CB-CG	5.49	118.08	112.60
24	Q	360	SER	CA-C-O	-5.49	115.03	120.90
28	H	394	LYS	CA-C-O	-5.49	114.74	120.55
32	M	332	VAL	CA-C-N	5.49	128.64	120.90
32	M	332	VAL	C-N-CA	5.49	128.64	120.90
32	M	362	GLN	CA-C-N	5.49	128.21	120.42
32	M	362	GLN	C-N-CA	5.49	128.21	120.42
3	c	176	LEU	CA-C-O	-5.48	114.61	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	244	MET	CA-C-O	-5.48	113.90	120.10
2	b	100	ILE	CB-CA-C	5.48	116.02	110.65
11	k	146	HIS	CE1-NE2-CD2	-5.48	103.52	109.00
8	1	152	ARG	NE-CZ-NH1	5.48	126.98	121.50
11	4	54	VAL	CA-CB-CG1	-5.48	101.08	110.40
21	N	483	LEU	CB-CA-C	-5.48	101.69	110.79
28	H	80	HIS	ND1-CE1-NE2	5.48	113.88	108.40
29	I	179	GLU	CB-CG-CD	-5.48	103.28	112.60
32	M	223	PRO	N-CA-CB	5.48	108.40	103.08
2	b	190	HIS	CA-C-O	-5.48	113.67	119.97
16	V	60	ASP	O-C-N	5.48	128.20	122.23
22	S	302	HIS	O-C-N	-5.48	116.22	123.13
9	2	121	GLY	CA-C-N	5.48	129.95	120.58
9	2	121	GLY	C-N-CA	5.48	129.95	120.58
30	K	151	PRO	CA-C-N	5.48	125.09	119.56
30	K	151	PRO	C-N-CA	5.48	125.09	119.56
10	j	70	LYS	CA-C-N	5.48	127.62	120.28
10	j	70	LYS	C-N-CA	5.48	127.62	120.28
17	T	234	TYR	CA-C-N	5.48	129.87	120.72
17	T	234	TYR	C-N-CA	5.48	129.87	120.72
20	Z	254	PRO	N-CA-C	5.48	122.48	111.69
24	Q	6	SER	N-CA-C	-5.48	105.22	111.14
29	I	284	ILE	CA-C-N	5.48	129.36	120.60
29	I	284	ILE	C-N-CA	5.48	129.36	120.60
2	b	37	ILE	CA-C-N	5.48	129.69	122.30
2	b	37	ILE	C-N-CA	5.48	129.69	122.30
2	b	70	ASP	CA-CB-CG	-5.48	107.12	112.60
1	a	28	VAL	CA-CB-CG2	-5.47	101.09	110.40
17	T	74	ASN	N-CA-CB	5.47	119.50	110.69
20	Z	212	LEU	CA-C-N	5.47	128.06	120.29
20	Z	212	LEU	C-N-CA	5.47	128.06	120.29
21	N	614	ASN	CB-CG-OD1	5.47	131.75	120.80
21	N	922	GLN	CB-CG-CD	-5.47	103.29	112.60
32	M	141	LYS	CA-C-N	5.47	126.68	119.84
32	M	141	LYS	C-N-CA	5.47	126.68	119.84
4	d	177	LYS	N-CA-CB	5.47	118.98	110.44
6	f	5	ASN	N-CA-C	-5.47	106.51	114.12
11	k	149	ARG	NE-CZ-NH2	-5.47	114.28	119.20
21	N	228	VAL	N-CA-C	5.47	115.67	110.42
22	S	132	ALA	CA-C-N	5.47	129.98	120.68
22	S	132	ALA	C-N-CA	5.47	129.98	120.68
23	P	197	THR	CA-C-N	5.47	127.45	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	197	THR	C-N-CA	5.47	127.45	120.56
11	4	191	GLN	N-CA-C	-5.47	100.78	109.59
13	6	129	ALA	N-CA-CB	5.47	119.79	110.71
13	6	204	ILE	N-CA-CB	5.47	119.32	112.26
26	U	260	ASN	CA-C-O	5.47	126.22	120.42
29	I	241	SER	CA-C-O	5.47	128.33	120.51
33	J	317	PRO	N-CD-CG	5.47	111.41	103.20
4	d	235	GLN	CA-C-N	5.47	128.19	120.42
4	d	235	GLN	C-N-CA	5.47	128.19	120.42
21	N	97	PHE	N-CA-C	-5.47	106.28	113.17
24	Q	148	LYS	CA-C-N	5.47	131.99	121.54
24	Q	148	LYS	C-N-CA	5.47	131.99	121.54
25	R	259	PHE	CB-CG-CD2	5.47	130.00	120.70
26	U	55	PRO	CA-C-O	-5.47	115.38	121.23
31	L	58	ASN	CA-CB-CG	-5.47	107.13	112.60
31	L	282	GLU	CA-C-N	5.47	129.88	121.19
31	L	282	GLU	C-N-CA	5.47	129.88	121.19
8	1	157	LYS	N-CA-CB	-5.47	102.08	110.12
13	6	31	LEU	N-CA-CB	5.47	119.18	110.65
18	X	128	VAL	CA-C-N	5.47	129.74	120.88
18	X	128	VAL	C-N-CA	5.47	129.74	120.88
24	Q	352	GLU	CA-C-O	-5.47	113.37	118.73
27	O	117	ASN	OD1-CG-ND2	-5.47	117.13	122.60
7	g	23	GLN	CA-C-N	5.47	129.29	120.55
7	g	23	GLN	C-N-CA	5.47	129.29	120.55
7	g	99	PHE	CA-C-N	5.47	128.15	120.28
7	g	99	PHE	C-N-CA	5.47	128.15	120.28
9	i	205	CYS	N-CA-CB	5.47	119.79	110.71
9	2	248	ASN	OD1-CG-ND2	-5.47	117.13	122.60
19	Y	16	LEU	N-CA-C	-5.47	101.00	109.14
24	Q	115	ILE	O-C-N	5.47	127.17	121.87
10	j	97	GLU	N-CA-C	5.46	116.92	111.07
12	l	188	TYR	CA-CB-CG	-5.46	104.06	113.90
9	2	243	LYS	N-CA-C	-5.46	100.41	107.73
12	5	221	TRP	CG-CD2-CE3	-5.46	128.44	133.90
21	N	296	CYS	N-CA-C	-5.46	105.24	111.14
23	P	153	ILE	CA-C-O	-5.46	115.27	120.95
25	R	170	VAL	CA-CB-CG2	-5.46	101.11	110.40
32	M	209	ASP	CB-CA-C	-5.46	101.72	110.79
14	7	72	VAL	N-CA-C	-5.46	99.88	108.23
20	Z	524	ALA	CA-C-N	5.46	129.42	120.63
20	Z	524	ALA	C-N-CA	5.46	129.42	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	312	PRO	N-CA-C	-5.46	107.52	114.35
27	O	200	GLU	CA-C-N	5.46	125.08	119.56
27	O	200	GLU	C-N-CA	5.46	125.08	119.56
29	I	422	ARG	NH1-CZ-NH2	5.46	126.40	119.30
4	d	30	GLY	CA-C-N	5.46	131.97	121.54
4	d	30	GLY	C-N-CA	5.46	131.97	121.54
4	d	246	GLN	CG-CD-NE2	-5.46	108.21	116.40
1	a	40	ILE	CB-CA-C	-5.46	104.14	110.91
1	a	248	ILE	CB-CA-C	-5.46	104.69	112.22
3	c	244	ILE	CB-CA-C	-5.46	105.06	111.94
10	j	4	PRO	N-CA-C	-5.46	107.32	114.03
13	6	10	PHE	N-CA-C	-5.46	99.53	108.76
21	N	520	GLY	O-C-N	5.46	127.43	122.19
21	N	657	MET	O-C-N	-5.46	116.33	122.12
24	Q	385	ILE	CA-C-O	5.46	123.89	118.98
10	3	23	ILE	O-C-N	-5.46	117.30	123.03
21	N	173	LYS	CA-C-O	5.46	126.25	119.97
25	R	78	ASP	N-CA-C	-5.46	101.01	108.38
32	M	15	ASP	O-C-N	-5.46	115.33	122.59
33	J	299	ILE	N-CA-C	-5.46	106.51	113.22
2	b	87	ASP	CA-C-N	5.46	127.59	120.28
2	b	87	ASP	C-N-CA	5.46	127.59	120.28
9	2	247	VAL	O-C-N	-5.46	117.18	123.07
16	V	38	LEU	O-C-N	5.46	127.90	122.12
1	a	182	LEU	N-CA-CB	5.45	118.23	110.16
8	1	23	LEU	O-C-N	5.45	130.03	123.16
9	2	104	ARG	N-CA-CB	5.45	118.74	110.45
12	5	193	ASP	CA-CB-CG	-5.45	107.15	112.60
25	R	27	SER	N-CA-C	5.45	117.22	111.28
25	R	362	ALA	N-CA-C	5.45	117.22	111.28
1	a	49	ASP	CA-C-O	5.45	128.31	120.51
1	a	123	ASN	OD1-CG-ND2	-5.45	117.15	122.60
12	5	232	GLY	CA-C-O	-5.45	115.11	121.00
15	W	164	PRO	O-C-N	5.45	129.28	123.01
16	V	278	LYS	CA-C-N	5.45	128.03	120.29
16	V	278	LYS	C-N-CA	5.45	128.03	120.29
16	V	279	HIS	O-C-N	5.45	128.36	122.15
21	N	839	ARG	CG-CD-NE	-5.45	100.01	112.00
22	S	318	CYS	CA-C-O	-5.45	114.77	120.55
23	P	22	PRO	CA-C-N	5.45	127.90	120.54
23	P	22	PRO	C-N-CA	5.45	127.90	120.54
3	c	23	GLU	O-C-N	-5.45	116.46	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	273	TRP	CA-C-N	5.45	128.03	120.29
12	l	273	TRP	C-N-CA	5.45	128.03	120.29
8	1	61	THR	CA-C-O	-5.45	114.65	120.42
15	W	86	HIS	O-C-N	5.45	130.22	123.14
6	f	20	PHE	CA-C-N	5.45	128.59	120.31
6	f	20	PHE	C-N-CA	5.45	128.59	120.31
17	T	151	TRP	CD2-CE2-CZ2	-5.45	116.95	122.40
18	X	61	LEU	N-CA-CB	5.45	119.69	110.49
21	N	879	SER	CA-C-N	5.45	127.58	120.28
21	N	879	SER	C-N-CA	5.45	127.58	120.28
30	K	312	VAL	CA-C-N	5.45	128.50	120.82
30	K	312	VAL	C-N-CA	5.45	128.50	120.82
30	K	330	ARG	CA-C-N	5.45	125.39	119.78
30	K	330	ARG	C-N-CA	5.45	125.39	119.78
9	2	128	ILE	N-CA-CB	5.44	118.72	111.64
27	O	82	LEU	O-C-N	5.44	128.36	122.15
31	L	72	ASP	CA-CB-CG	-5.44	107.16	112.60
31	L	364	HIS	CG-CD2-NE2	5.44	112.64	107.20
8	h	12	ILE	O-C-N	-5.44	117.19	123.07
14	7	155	ASN	N-CA-C	-5.44	105.90	112.54
15	W	8	LEU	N-CA-CB	5.44	118.56	110.29
21	N	857	TYR	CA-CB-CG	-5.44	104.10	113.90
28	H	231	SER	O-C-N	5.44	125.36	121.12
14	n	118	GLU	CA-C-O	-5.44	113.53	119.95
12	5	164	GLN	O-C-N	5.44	127.89	122.12
16	V	28	TYR	CB-CA-C	-5.44	102.17	111.31
23	P	115	ARG	NE-CZ-NH2	5.44	124.10	119.20
24	Q	109	ASP	N-CA-C	-5.44	104.90	112.30
24	Q	113	ASP	N-CA-CB	5.44	118.12	110.12
30	K	177	LEU	N-CA-C	5.44	119.08	111.74
31	L	249	SER	N-CA-C	-5.44	106.64	113.28
12	l	82	ARG	NE-CZ-NH1	-5.44	116.06	121.50
12	l	265	ASN	CA-C-O	5.44	126.23	120.36
28	H	189	PRO	CA-C-N	5.44	131.93	121.54
28	H	189	PRO	C-N-CA	5.44	131.93	121.54
16	V	287	THR	N-CA-C	5.44	117.29	111.36
26	U	241	THR	N-CA-CB	5.44	117.60	109.88
28	H	283	TYR	CA-C-O	-5.44	115.11	120.98
28	H	288	ALA	N-CA-CB	5.44	118.11	110.12
31	L	364	HIS	CE1-NE2-CD2	-5.44	103.56	109.00
32	M	323	VAL	N-CA-C	-5.44	99.72	107.77
33	J	401	ALA	N-CA-CB	5.44	118.63	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	714	THR	N-CA-C	-5.44	101.04	109.14
14	n	89	ASP	CA-C-O	5.43	127.25	121.05
21	N	147	ALA	CA-C-N	5.43	131.92	121.54
21	N	147	ALA	C-N-CA	5.43	131.92	121.54
22	S	223	LEU	O-C-N	5.43	127.88	122.12
24	Q	267	LEU	CA-C-N	5.43	127.56	120.28
24	Q	267	LEU	C-N-CA	5.43	127.56	120.28
25	R	82	ASP	N-CA-CB	5.43	119.13	110.16
28	H	241	ASP	CA-CB-CG	-5.43	107.17	112.60
29	I	118	ALA	CA-C-N	5.43	129.93	123.19
29	I	118	ALA	C-N-CA	5.43	129.93	123.19
5	e	15	PHE	N-CA-C	-5.43	100.04	108.90
5	e	16	SER	N-CA-CB	5.43	119.73	110.50
6	f	6	TYR	N-CA-CB	5.43	119.67	110.49
22	S	188	TYR	CA-C-N	5.43	128.00	120.29
22	S	188	TYR	C-N-CA	5.43	128.00	120.29
25	R	183	ASP	CA-CB-CG	-5.43	107.17	112.60
28	H	359	ASN	CB-CA-C	-5.43	101.98	110.94
30	K	336	ARG	CA-CB-CG	5.43	124.97	114.10
2	b	3	ASP	N-CA-C	-5.43	101.31	109.95
6	f	124	GLY	N-CA-C	-5.43	107.61	115.27
9	i	251	ASP	N-CA-C	-5.43	102.42	110.46
31	L	308	LEU	CA-C-O	5.43	126.71	120.90
3	c	113	ARG	NH1-CZ-NH2	-5.43	112.24	119.30
4	d	250	LYS	CA-C-N	5.43	127.55	120.28
4	d	250	LYS	C-N-CA	5.43	127.55	120.28
11	4	98	TYR	N-CA-C	-5.43	99.67	108.52
18	X	59	ARG	N-CA-C	-5.43	98.92	108.20
21	N	384	LYS	N-CA-C	5.43	117.28	111.36
30	K	356	ILE	CA-C-N	5.43	128.10	120.28
30	K	356	ILE	C-N-CA	5.43	128.10	120.28
32	M	173	ASP	N-CA-CB	5.43	119.25	111.65
13	6	150	ALA	CA-C-N	5.43	127.50	120.44
13	6	150	ALA	C-N-CA	5.43	127.50	120.44
20	Z	743	ILE	CA-C-N	5.43	127.55	120.28
20	Z	743	ILE	C-N-CA	5.43	127.55	120.28
22	S	90	LYS	N-CA-C	5.43	117.20	111.28
3	c	245	THR	CA-CB-OG1	5.43	117.74	109.60
12	5	206	SER	N-CA-CB	5.43	118.19	110.16
22	S	235	ASN	CB-CG-ND2	5.43	124.54	116.40
23	P	141	LYS	N-CA-C	5.43	117.95	111.71
23	P	342	GLN	CB-CA-C	-5.43	102.36	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	338	LYS	N-CA-C	-5.43	100.82	109.07
28	H	263	VAL	CA-C-N	5.43	127.55	120.28
28	H	263	VAL	C-N-CA	5.43	127.55	120.28
32	M	399	GLY	CA-C-N	5.43	129.91	120.68
32	M	399	GLY	C-N-CA	5.43	129.91	120.68
33	J	282	PHE	N-CA-C	-5.43	106.83	113.50
16	V	20	ARG	CA-C-N	5.42	127.55	120.28
16	V	20	ARG	C-N-CA	5.42	127.55	120.28
23	P	117	SER	O-C-N	5.42	128.33	122.15
24	Q	348	CYS	CB-CA-C	-5.42	102.36	110.88
31	L	149	ASP	CA-C-N	5.42	129.62	120.29
31	L	149	ASP	C-N-CA	5.42	129.62	120.29
16	V	195	HIS	CA-CB-CG	-5.42	108.38	113.80
31	L	125	PRO	N-CA-CB	5.42	108.37	103.33
15	W	7	VAL	N-CA-C	-5.42	99.94	107.80
21	N	174	LEU	N-CA-CB	5.42	118.07	109.51
28	H	90	ARG	CA-C-N	5.42	128.09	120.28
28	H	90	ARG	C-N-CA	5.42	128.09	120.28
10	j	150	CYS	N-CA-C	5.42	117.19	111.28
14	7	83	VAL	N-CA-C	-5.42	100.68	108.48
16	V	242	LYS	CA-C-N	5.42	127.48	120.44
16	V	242	LYS	C-N-CA	5.42	127.48	120.44
20	Z	237	VAL	CA-C-N	5.42	128.95	120.82
20	Z	237	VAL	C-N-CA	5.42	128.95	120.82
21	N	199	ASN	N-CA-C	-5.42	100.41	109.24
21	N	513	ILE	N-CA-C	5.42	116.19	110.72
24	Q	319	LYS	N-CA-CB	5.42	117.87	110.01
3	C	120	GLN	CA-C-N	5.42	126.91	120.14
3	C	120	GLN	C-N-CA	5.42	126.91	120.14
14	7	43	SER	CA-C-N	5.42	130.51	122.71
14	7	43	SER	C-N-CA	5.42	130.51	122.71
18	X	86	ILE	CA-C-O	5.42	127.36	120.75
26	U	171	VAL	CA-C-N	5.42	127.98	120.29
26	U	171	VAL	C-N-CA	5.42	127.98	120.29
9	2	187	ALA	N-CA-C	5.42	117.26	111.36
16	V	86	VAL	N-CA-CB	5.42	117.50	110.57
30	K	364	PRO	CA-C-N	5.42	131.05	122.60
30	K	364	PRO	C-N-CA	5.42	131.05	122.60
1	a	112	MET	O-C-N	-5.41	116.48	121.30
24	Q	328	ASP	N-CA-CB	5.41	119.05	110.55
28	H	216	ASP	O-C-N	5.41	128.32	122.15
11	k	153	THR	CA-C-N	5.41	127.97	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	153	THR	C-N-CA	5.41	127.97	120.29
28	H	299	ARG	N-CA-CB	5.41	118.08	110.12
11	4	53	THR	CA-C-N	5.41	127.32	120.72
11	4	53	THR	C-N-CA	5.41	127.32	120.72
22	S	372	LEU	N-CA-C	-5.41	105.38	111.28
29	I	125	MET	CA-C-O	-5.41	113.43	118.73
32	M	110	ASN	CA-C-O	-5.41	112.77	120.51
33	J	122	LEU	N-CA-C	5.41	117.52	110.43
10	3	134	LYS	CB-CA-C	-5.41	103.74	112.07
16	V	137	VAL	O-C-N	5.41	128.61	122.98
31	L	214	PRO	CA-C-N	5.41	125.83	119.99
31	L	214	PRO	C-N-CA	5.41	125.83	119.99
6	f	30	LYS	N-CA-CB	5.41	118.07	110.12
10	j	49	VAL	O-C-N	5.41	128.66	123.14
12	l	226	GLU	CB-CA-C	-5.41	102.36	110.90
10	3	49	VAL	CA-C-N	5.41	131.05	122.94
10	3	49	VAL	C-N-CA	5.41	131.05	122.94
11	4	30	ASP	CB-CA-C	-5.41	101.06	110.09
14	7	94	GLN	CB-CG-CD	-5.41	103.41	112.60
21	N	444	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
25	R	373	PRO	O-C-N	5.41	129.92	122.35
13	m	24	ALA	CA-C-N	5.41	128.21	121.83
13	m	24	ALA	C-N-CA	5.41	128.21	121.83
8	1	90	VAL	CA-C-N	5.41	128.30	120.79
8	1	90	VAL	C-N-CA	5.41	128.30	120.79
8	1	197	PHE	CA-CB-CG	-5.41	108.39	113.80
13	6	214	ILE	N-CA-C	-5.41	100.69	108.53
19	Y	78	LYS	CA-C-N	5.41	127.47	120.44
19	Y	78	LYS	C-N-CA	5.41	127.47	120.44
20	Z	738	TYR	CA-CB-CG	5.41	123.63	113.90
33	J	393	ASN	N-CA-C	-5.41	106.62	113.43
19	Y	84	TYR	CA-C-N	5.40	127.52	120.28
19	Y	84	TYR	C-N-CA	5.40	127.52	120.28
5	e	236	THR	CA-C-O	-5.40	114.82	120.55
14	7	107	ASN	OD1-CG-ND2	-5.40	117.20	122.60
17	T	241	GLU	O-C-N	5.40	127.85	122.12
20	Z	361	HIS	CA-C-N	5.40	128.06	120.28
20	Z	361	HIS	C-N-CA	5.40	128.06	120.28
23	P	74	ASP	CA-CB-CG	-5.40	107.20	112.60
23	P	214	GLU	N-CA-C	5.40	117.87	111.33
25	R	50	VAL	CA-C-N	5.40	127.96	120.29
25	R	50	VAL	C-N-CA	5.40	127.96	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	232	VAL	CA-C-N	5.40	127.96	120.29
25	R	232	VAL	C-N-CA	5.40	127.96	120.29
27	O	269	LEU	O-C-N	-5.40	116.50	122.07
33	J	247	MET	N-CA-C	-5.40	100.30	108.67
33	J	332	SER	CA-C-N	5.40	127.96	120.29
33	J	332	SER	C-N-CA	5.40	127.96	120.29
1	a	177	GLU	CB-CG-CD	-5.40	103.42	112.60
9	i	201	ASN	N-CA-CB	5.40	117.98	110.04
13	m	74	LYS	O-C-N	5.40	127.63	122.07
13	m	82	TRP	CB-CG-CD1	5.40	135.00	126.90
14	n	106	GLU	O-C-N	-5.40	115.99	122.15
8	l	124	LEU	N-CA-C	5.40	119.87	113.28
21	N	814	ALA	N-CA-C	5.40	117.92	111.71
28	H	67	ALA	N-CA-C	-5.40	106.64	113.18
29	I	261	PRO	N-CA-C	5.40	120.64	113.57
31	L	340	PRO	CA-C-O	-5.40	115.45	121.23
8	h	17	PHE	CA-C-N	5.40	127.51	120.28
8	h	17	PHE	C-N-CA	5.40	127.51	120.28
11	k	177	LYS	O-C-N	5.40	129.65	122.41
14	7	221	ASP	O-C-N	5.40	129.96	123.16
22	S	400	LYS	N-CA-C	-5.40	106.37	113.12
25	R	42	GLN	OE1-CD-NE2	5.40	128.00	122.60
29	I	341	PRO	N-CA-C	5.40	121.64	113.81
29	I	381	VAL	CA-C-O	-5.40	114.64	120.47
8	h	23	LEU	N-CA-C	-5.40	101.37	109.95
10	j	143	SER	N-CA-CB	5.40	118.65	110.28
21	N	581	ASP	CA-C-N	5.40	127.95	120.29
21	N	581	ASP	C-N-CA	5.40	127.95	120.29
23	P	379	TYR	N-CA-C	5.40	118.08	111.82
4	d	7	ALA	N-CA-C	5.40	118.30	110.42
12	5	232	GLY	N-CA-C	-5.40	106.24	112.50
14	7	128	TYR	CA-C-O	-5.40	115.13	120.90
16	V	39	LYS	CG-CD-CE	5.40	123.71	111.30
17	T	65	GLY	CA-C-O	-5.40	114.94	120.66
21	N	755	PRO	O-C-N	5.40	129.57	123.10
22	S	352	VAL	CA-C-O	-5.39	115.13	120.85
26	U	69	ASP	CA-C-N	5.39	127.95	120.29
26	U	69	ASP	C-N-CA	5.39	127.95	120.29
27	O	391	ILE	O-C-N	-5.39	117.33	123.10
33	J	265	ASP	CA-C-O	-5.39	114.70	120.42
1	a	135	ARG	NE-CZ-NH2	-5.39	114.35	119.20
3	c	32	ALA	N-CA-C	5.39	118.05	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	51	ARG	CA-C-N	5.39	132.91	122.07
6	f	51	ARG	C-N-CA	5.39	132.91	122.07
16	V	169	GLU	CA-C-O	-5.39	113.67	118.63
20	Z	213	LYS	CA-CB-CG	5.39	124.88	114.10
27	O	149	LEU	CB-CA-C	-5.39	101.68	110.85
28	H	389	PHE	CA-C-N	5.39	127.77	120.38
28	H	389	PHE	C-N-CA	5.39	127.77	120.38
33	J	127	GLU	N-CA-C	-5.39	106.01	112.59
33	J	275	LEU	N-CA-C	5.39	120.27	111.37
16	V	95	LEU	CA-C-O	5.39	126.17	119.97
21	N	81	TYR	CA-C-O	-5.39	112.62	119.31
22	S	244	ASN	N-CA-CB	5.39	118.85	110.44
22	S	394	ILE	CA-C-N	5.39	127.84	120.46
22	S	394	ILE	C-N-CA	5.39	127.84	120.46
5	e	115	SER	CA-C-O	-5.39	114.84	120.55
7	g	197	ALA	N-CA-CB	5.39	118.14	110.16
16	V	165	ILE	N-CA-CB	-5.39	103.67	110.57
26	U	173	HIS	ND1-CE1-NE2	5.39	113.79	108.40
28	H	156	VAL	N-CA-CB	5.39	116.59	110.72
30	K	121	ARG	CA-C-O	-5.39	115.12	121.16
30	K	404	GLN	CA-C-O	5.39	126.01	119.11
4	d	165	GLY	CA-C-N	5.39	128.49	120.95
4	d	165	GLY	C-N-CA	5.39	128.49	120.95
12	l	223	LEU	CA-C-N	5.39	130.77	120.97
12	l	223	LEU	C-N-CA	5.39	130.77	120.97
15	W	132	LEU	N-CA-CB	5.39	117.82	110.01
15	W	163	ASN	N-CA-C	-5.39	97.91	109.81
21	N	58	ARG	N-CA-CB	-5.39	102.20	110.12
25	R	24	TYR	N-CA-CB	5.39	118.59	110.30
27	O	327	LEU	CB-CA-C	-5.39	101.85	110.79
28	H	375	VAL	CA-C-O	5.39	126.30	120.43
30	K	196	ASP	CA-C-O	-5.39	114.84	120.55
10	j	193	ASP	CA-CB-CG	5.38	117.98	112.60
21	N	789	GLU	O-C-N	5.38	129.61	123.31
31	L	339	ARG	CA-C-O	-5.38	115.09	120.64
32	M	144	ASP	CB-CA-C	5.38	118.63	109.80
25	R	252	TYR	CA-C-N	5.38	127.93	120.29
25	R	252	TYR	C-N-CA	5.38	127.93	120.29
28	H	127	SER	CA-C-O	-5.38	115.52	121.33
32	M	286	ILE	CA-CB-CG2	-5.38	101.35	110.50
6	f	191	LYS	CB-CA-C	-5.38	100.67	110.63
8	h	115	ASN	CA-CB-CG	5.38	117.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	H	141	GLU	CB-CG-CD	-5.38	103.45	112.60
29	I	385	ASP	CA-C-N	5.38	129.96	121.56
29	I	385	ASP	C-N-CA	5.38	129.96	121.56
33	J	301	ASP	CA-CB-CG	-5.38	107.22	112.60
3	c	56	LEU	O-C-N	-5.38	115.73	122.35
20	Z	253	VAL	CG1-CB-CG2	-5.38	98.96	110.80
21	N	124	TYR	CA-C-O	5.38	126.00	119.11
28	H	131	GLN	N-CA-C	-5.38	106.76	113.38
2	b	94	HIS	CE1-NE2-CD2	-5.38	103.62	109.00
10	3	40	PHE	CA-CB-CG	5.38	119.18	113.80
24	Q	362	ILE	CA-C-N	5.38	127.93	120.29
24	Q	362	ILE	C-N-CA	5.38	127.93	120.29
27	O	200	GLU	CB-CA-C	-5.38	100.64	109.46
31	L	399	GLY	CA-C-O	5.38	125.84	119.50
11	4	162	LYS	N-CA-C	5.38	117.14	111.28
29	I	398	GLU	CA-C-N	5.38	128.02	120.28
29	I	398	GLU	C-N-CA	5.38	128.02	120.28
6	f	6	TYR	CA-C-N	5.38	131.41	122.54
6	f	6	TYR	C-N-CA	5.38	131.41	122.54
10	3	197	LYS	N-CA-C	-5.38	100.42	109.07
33	J	332	SER	O-C-N	5.38	128.51	122.22
2	b	130	PHE	O-C-N	-5.37	116.32	122.93
6	f	46	LEU	CA-C-O	-5.37	114.90	120.70
11	k	59	TYR	CB-CG-CD1	-5.37	112.74	120.80
11	k	97	PRO	CA-C-N	-5.37	115.41	122.99
11	k	97	PRO	C-N-CA	-5.37	115.41	122.99
12	5	196	ARG	N-CA-C	-5.37	99.18	108.69
21	N	410	LEU	CD1-CG-CD2	-5.37	98.98	110.80
22	S	83	PRO	N-CA-C	-5.37	101.40	112.47
24	Q	311	LEU	CA-C-N	5.37	127.79	120.54
24	Q	311	LEU	C-N-CA	5.37	127.79	120.54
33	J	35	ARG	N-CA-C	-5.37	105.50	111.36
11	k	172	MET	CG-SD-CE	-5.37	89.08	100.90
13	m	120	ALA	N-CA-C	-5.37	100.57	108.79
13	m	194	ASP	CB-CA-C	-5.37	101.87	110.79
17	T	245	TYR	CA-C-O	-5.37	114.86	120.55
21	N	74	GLU	CB-CG-CD	-5.37	103.47	112.60
25	R	88	LEU	CA-C-N	-5.37	115.14	122.93
25	R	88	LEU	C-N-CA	-5.37	115.14	122.93
31	L	175	GLN	OE1-CD-NE2	5.37	127.97	122.60
3	c	176	LEU	N-CA-CB	5.37	118.11	110.16
13	m	82	TRP	CE2-CD2-CE3	5.37	124.17	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	129	ALA	CA-C-O	5.37	127.46	120.21
18	X	10	PHE	CA-CB-CG	-5.37	108.43	113.80
22	S	424	SER	N-CA-CB	5.37	117.80	110.01
25	R	347	THR	CA-C-O	5.37	127.13	121.33
33	J	362	CYS	O-C-N	5.37	127.89	122.09
2	b	44	VAL	N-CA-C	-5.37	100.75	108.48
3	c	179	ASP	CA-CB-CG	-5.37	107.23	112.60
8	h	192	VAL	N-CA-CB	5.37	118.97	112.10
25	R	68	GLU	N-CA-C	5.37	116.81	111.07
33	J	286	LYS	CA-C-O	5.37	127.18	121.11
9	i	122	HIS	ND1-CE1-NE2	5.37	113.77	108.40
12	5	128	GLN	CA-C-N	5.37	127.73	120.65
12	5	128	GLN	C-N-CA	5.37	127.73	120.65
24	Q	405	GLN	N-CA-CB	5.37	119.72	111.46
30	K	265	ALA	N-CA-C	5.37	117.30	109.84
31	L	168	TYR	CA-C-N	5.37	127.47	120.28
31	L	168	TYR	C-N-CA	5.37	127.47	120.28
7	g	76	CYS	N-CA-C	-5.37	99.19	108.69
12	l	218	ASN	CA-CB-CG	-5.37	107.23	112.60
25	R	122	GLU	N-CA-C	-5.37	103.35	111.56
26	U	20	ASP	O-C-N	5.37	127.60	122.07
27	O	81	TYR	CA-C-N	5.37	127.91	120.29
27	O	81	TYR	C-N-CA	5.37	127.91	120.29
29	I	69	LEU	CA-C-N	5.37	127.47	120.28
29	I	69	LEU	C-N-CA	5.37	127.47	120.28
29	I	175	LYS	N-CA-CB	5.37	118.61	110.45
2	b	176	GLU	CA-C-O	-5.36	114.73	120.42
4	d	46	CYS	N-CA-C	-5.36	100.92	109.23
12	l	191	ASP	CA-C-N	5.36	128.00	120.28
12	l	191	ASP	C-N-CA	5.36	128.00	120.28
12	5	220	LYS	CA-C-O	-5.36	114.99	120.89
15	W	142	ILE	N-CA-CB	5.36	117.48	111.21
16	V	46	PRO	N-CD-CG	5.36	110.23	103.80
23	P	159	ILE	CA-C-N	5.36	128.46	120.31
23	P	159	ILE	C-N-CA	5.36	128.46	120.31
23	P	426	ILE	CA-C-N	5.36	127.91	120.29
23	P	426	ILE	C-N-CA	5.36	127.91	120.29
24	Q	423	VAL	N-CA-CB	5.36	118.62	110.58
27	O	236	HIS	CE1-NE2-CD2	-5.36	103.64	109.00
31	L	194	ARG	NE-CZ-NH1	-5.36	116.14	121.50
32	M	419	ILE	CA-C-O	-5.36	115.37	120.95
9	i	56	ALA	CB-CA-C	-5.36	102.46	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Y	17	THR	CA-C-N	5.36	127.90	120.29
19	Y	17	THR	C-N-CA	5.36	127.90	120.29
20	Z	385	PHE	CA-C-N	5.36	128.94	120.47
20	Z	385	PHE	C-N-CA	5.36	128.94	120.47
23	P	300	VAL	CA-CB-CG1	5.36	119.52	110.40
5	e	168	ASN	OD1-CG-ND2	5.36	127.96	122.60
21	N	607	GLN	CA-C-N	5.36	128.00	120.28
21	N	607	GLN	C-N-CA	5.36	128.00	120.28
22	S	342	LEU	CA-C-N	5.36	126.43	119.78
22	S	342	LEU	C-N-CA	5.36	126.43	119.78
27	O	172	TYR	CA-C-O	-5.36	112.66	119.31
28	H	196	THR	O-C-N	5.36	128.26	122.15
33	J	270	ARG	NE-CZ-NH1	5.36	126.86	121.50
21	N	653	ARG	CA-C-O	-5.36	115.19	120.82
13	m	160	ASN	CA-CB-CG	-5.36	107.24	112.60
21	N	315	ASN	CB-CA-C	-5.36	100.89	110.70
22	S	244	ASN	CB-CA-C	-5.36	98.67	109.55
28	H	437	VAL	N-CA-CB	5.36	119.11	111.82
29	I	138	LYS	CA-C-N	5.36	129.74	120.58
29	I	138	LYS	C-N-CA	5.36	129.74	120.58
32	M	349	PHE	CA-C-N	5.36	125.82	120.52
32	M	349	PHE	C-N-CA	5.36	125.82	120.52
33	J	296	ARG	NH1-CZ-NH2	5.36	126.26	119.30
7	g	52	LYS	CA-C-N	5.36	128.47	120.87
7	g	52	LYS	C-N-CA	5.36	128.47	120.87
21	N	733	LEU	CA-C-O	5.36	125.95	119.31
22	S	488	GLN	OE1-CD-NE2	-5.36	117.25	122.60
24	Q	330	LEU	CA-C-N	5.36	127.46	120.28
24	Q	330	LEU	C-N-CA	5.36	127.46	120.28
28	H	299	ARG	CA-C-N	5.36	127.40	120.44
28	H	299	ARG	C-N-CA	5.36	127.40	120.44
29	I	301	GLU	CA-C-N	5.36	127.51	120.60
29	I	301	GLU	C-N-CA	5.36	127.51	120.60
33	J	57	PHE	CA-C-O	5.36	126.23	120.55
12	l	77	THR	N-CA-C	-5.35	98.84	108.48
4	d	226	SER	N-CA-C	5.35	118.60	111.75
7	g	94	GLU	N-CA-CB	5.35	118.08	110.16
15	W	96	LEU	N-CA-CB	5.35	118.46	110.22
16	V	90	LYS	CA-C-O	-5.35	114.88	120.55
22	S	129	GLU	N-CA-C	5.35	117.55	108.02
25	R	46	ALA	O-C-N	5.35	127.79	122.12
29	I	68	HIS	ND1-CE1-NE2	5.35	113.75	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	118	ILE	CA-C-O	5.35	126.03	120.36
21	N	697	PHE	N-CA-C	5.35	116.80	111.07
23	P	263	HIS	ND1-CE1-NE2	5.35	113.75	108.40
32	M	194	VAL	CB-CA-C	5.35	118.82	111.97
3	c	165	VAL	N-CA-C	-5.35	100.89	108.65
10	j	205	ASP	CA-CB-CG	-5.35	107.25	112.60
9	2	231	SER	N-CA-C	-5.35	101.16	109.72
17	T	190	ALA	N-CA-C	5.35	117.19	111.36
28	H	165	PRO	CA-C-N	5.35	127.45	120.28
28	H	165	PRO	C-N-CA	5.35	127.45	120.28
31	L	394	CYS	N-CA-CB	5.35	117.77	110.01
4	d	139	ASP	CA-C-O	-5.35	115.12	120.63
10	j	108	VAL	N-CA-C	-5.35	100.36	108.17
11	k	136	SER	CA-C-N	5.35	126.02	120.03
11	k	136	SER	C-N-CA	5.35	126.02	120.03
14	n	87	SER	N-CA-C	-5.35	101.28	109.41
10	3	195	VAL	N-CA-CB	5.35	119.09	111.82
1	a	211	ILE	CA-C-O	-5.35	115.18	120.85
8	h	130	LYS	N-CA-C	-5.35	100.98	109.96
12	5	131	GLU	N-CA-C	-5.35	106.81	113.38
2	b	187	ASP	CA-C-N	5.34	127.44	120.28
2	b	187	ASP	C-N-CA	5.34	127.44	120.28
12	l	140	LEU	N-CA-CB	5.34	118.07	110.16
12	l	212	TYR	CB-CA-C	-5.34	102.26	110.81
24	Q	148	LYS	N-CA-C	-5.34	105.90	112.90
25	R	401	HIS	CG-CD2-NE2	5.34	112.55	107.20
31	L	434	TYR	CA-C-O	5.34	126.25	120.32
4	d	233	VAL	CA-C-N	5.34	127.44	120.28
4	d	233	VAL	C-N-CA	5.34	127.44	120.28
8	h	93	GLU	CB-CG-CD	-5.34	103.52	112.60
11	k	7	ILE	N-CA-CB	5.34	121.03	111.63
11	k	98	TYR	N-CA-C	-5.34	100.19	108.90
12	l	231	LEU	CA-C-N	5.34	125.87	119.94
12	l	231	LEU	C-N-CA	5.34	125.87	119.94
22	S	34	LEU	CA-C-N	5.34	128.43	120.31
22	S	34	LEU	C-N-CA	5.34	128.43	120.31
2	b	180	ASN	N-CA-C	-5.34	100.95	109.07
8	1	129	HIS	CA-CB-CG	5.34	119.14	113.80
14	7	145	ASN	CA-C-O	5.34	127.04	121.38
16	V	77	GLY	CA-C-O	-5.34	115.81	122.65
18	X	11	ARG	NH1-CZ-NH2	-5.34	112.36	119.30
18	X	106	SER	N-CA-CB	5.34	119.52	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	227	ASN	CA-CB-CG	-5.34	107.26	112.60
26	U	94	HIS	O-C-N	-5.34	116.87	123.33
26	U	156	HIS	ND1-CE1-NE2	5.34	113.74	108.40
28	H	246	ILE	N-CA-C	-5.34	101.30	108.35
31	L	368	VAL	CB-CA-C	-5.34	105.47	111.45
32	M	396	VAL	CA-C-N	5.34	129.76	120.68
32	M	396	VAL	C-N-CA	5.34	129.76	120.68
4	d	56	ASP	CA-C-O	5.34	126.41	120.43
12	l	276	LYS	CA-C-O	5.34	126.43	120.82
9	2	45	ALA	N-CA-C	-5.34	100.80	108.60
14	7	95	HIS	CE1-NE2-CD2	-5.34	103.66	109.00
21	N	553	PHE	CA-CB-CG	-5.34	108.46	113.80
33	J	49	ASN	CA-C-O	-5.34	114.89	120.55
27	O	206	THR	CA-C-O	5.34	128.08	121.94
12	l	141	HIS	N-CA-C	5.34	117.18	111.36
8	1	31	THR	O-C-N	-5.34	114.88	122.99
10	3	98	ARG	N-CA-CB	5.34	118.04	110.46
23	P	275	ASN	N-CA-C	-5.34	105.91	112.90
25	R	51	LEU	CA-C-O	5.34	126.08	120.42
25	R	228	ALA	N-CA-CB	5.34	117.96	110.12
27	O	187	SER	CA-C-N	5.34	127.38	120.44
27	O	187	SER	C-N-CA	5.34	127.38	120.44
33	J	254	GLY	CA-C-N	5.34	131.98	122.06
33	J	254	GLY	C-N-CA	5.34	131.98	122.06
15	W	27	GLU	N-CA-C	-5.33	106.27	112.89
21	N	765	ASP	CA-CB-CG	5.33	117.94	112.60
22	S	155	LEU	N-CA-C	5.33	117.09	111.28
22	S	251	SER	O-C-N	-5.33	116.47	122.12
12	l	254	HIS	N-CA-CB	5.33	119.17	110.37
9	2	91	ASN	N-CA-C	5.33	117.84	111.71
14	7	151	GLY	O-C-N	-5.33	115.77	122.70
15	W	72	ILE	CA-C-N	5.33	127.43	120.28
15	W	72	ILE	C-N-CA	5.33	127.43	120.28
16	V	129	PHE	CA-C-N	5.33	127.43	120.28
16	V	129	PHE	C-N-CA	5.33	127.43	120.28
26	U	249	VAL	N-CA-C	-5.33	105.33	110.72
32	M	55	ASN	CB-CA-C	-5.33	101.94	110.79
32	M	169	ALA	CA-C-N	5.33	127.37	120.44
32	M	169	ALA	C-N-CA	5.33	127.37	120.44
32	M	329	ARG	CD-NE-CZ	5.33	131.87	124.40
4	d	158	SER	CA-C-O	-5.33	115.43	121.72
11	4	91	SER	N-CA-C	5.33	119.05	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	313	ASP	CA-CB-CG	-5.33	107.27	112.60
26	U	80	CYS	CA-C-N	5.33	127.96	120.28
26	U	80	CYS	C-N-CA	5.33	127.96	120.28
28	H	96	PRO	N-CA-CB	5.33	108.46	102.60
30	K	217	THR	CA-CB-OG1	5.33	117.60	109.60
10	j	173	ASN	CA-C-N	5.33	127.86	120.29
10	j	173	ASN	C-N-CA	5.33	127.86	120.29
21	N	729	SER	N-CA-C	5.33	117.09	111.28
11	4	2	ASP	CA-CB-CG	5.33	117.93	112.60
21	N	432	GLY	N-CA-C	-5.33	100.55	113.18
21	N	756	THR	CA-C-O	5.33	125.89	120.24
23	P	299	LEU	O-C-N	5.33	127.84	122.09
25	R	260	THR	N-CA-CB	5.33	118.20	110.26
25	R	356	ALA	O-C-N	-5.33	116.33	122.09
27	O	301	PHE	CA-CB-CG	-5.33	108.47	113.80
28	H	289	ARG	CA-C-N	5.33	127.42	120.28
28	H	289	ARG	C-N-CA	5.33	127.42	120.28
29	I	370	ASN	CA-C-O	-5.33	114.97	121.36
31	L	207	PHE	CA-CB-CG	-5.33	108.47	113.80
27	O	269	LEU	CA-C-O	5.33	126.41	120.82
13	6	212	ILE	N-CA-CB	-5.33	104.92	110.72
22	S	162	VAL	CB-CA-C	-5.33	105.15	111.97
27	O	82	LEU	CA-C-O	-5.33	114.78	120.42
27	O	131	SER	CA-C-N	5.33	128.40	120.31
27	O	131	SER	C-N-CA	5.33	128.40	120.31
29	I	150	HIS	CA-CB-CG	-5.33	108.47	113.80
31	L	323	ILE	N-CA-C	-5.33	100.53	108.46
2	b	49	LYS	N-CA-CB	5.32	119.37	110.85
21	N	135	SER	N-CA-C	-5.32	105.56	111.36
23	P	271	SER	CA-C-O	-5.32	115.02	119.76
25	R	411	LEU	CA-C-N	5.32	127.41	120.28
25	R	411	LEU	C-N-CA	5.32	127.41	120.28
28	H	155	PHE	CA-CB-CG	-5.32	108.48	113.80
12	l	93	SER	N-CA-C	-5.32	105.76	113.21
13	m	91	LYS	CB-CA-C	5.32	118.55	109.72
14	n	165	LEU	CA-C-N	5.32	127.41	120.28
14	n	165	LEU	C-N-CA	5.32	127.41	120.28
14	n	207	GLU	N-CA-CB	5.32	118.45	109.78
13	6	37	ASN	OD1-CG-ND2	-5.32	117.28	122.60
24	Q	177	VAL	CA-C-N	5.32	127.85	120.29
24	Q	177	VAL	C-N-CA	5.32	127.85	120.29
32	M	29	GLU	N-CA-CB	5.32	118.03	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	M	58	MET	CA-C-N	5.32	127.41	120.28
32	M	58	MET	C-N-CA	5.32	127.41	120.28
8	h	162	ASP	CA-C-N	5.32	127.36	120.44
8	h	162	ASP	C-N-CA	5.32	127.36	120.44
13	6	44	ASN	CB-CA-C	-5.32	102.50	110.90
33	J	36	SER	CB-CA-C	-5.32	101.81	110.85
9	i	41	VAL	O-C-N	-5.32	118.34	122.97
10	3	31	SER	O-C-N	-5.32	117.09	123.31
15	W	188	SER	N-CA-C	-5.32	103.24	110.36
17	T	205	ILE	CA-C-N	5.32	127.35	120.44
17	T	205	ILE	C-N-CA	5.32	127.35	120.44
18	X	14	VAL	CB-CA-C	5.32	118.97	111.63
32	M	131	MET	CG-SD-CE	-5.32	89.20	100.90
33	J	206	THR	N-CA-CB	5.32	117.94	110.12
6	f	221	PRO	N-CD-CG	5.32	111.17	103.20
27	O	285	SER	N-CA-C	5.32	117.07	111.28
28	H	95	HIS	ND1-CE1-NE2	5.32	113.72	108.40
32	M	86	MET	N-CA-C	-5.32	98.56	108.02
17	T	10	SER	O-C-N	5.31	129.14	122.23
21	N	816	LYS	CA-C-N	5.31	127.40	120.28
21	N	816	LYS	C-N-CA	5.31	127.40	120.28
23	P	171	MET	N-CA-CB	5.31	117.82	110.17
29	I	139	GLU	CA-CB-CG	5.31	124.73	114.10
10	3	160	PRO	CA-C-N	5.31	127.83	120.29
10	3	160	PRO	C-N-CA	5.31	127.83	120.29
14	7	141	ASN	N-CA-C	-5.31	95.81	108.40
24	Q	322	GLU	CA-C-N	5.31	128.38	120.31
24	Q	322	GLU	C-N-CA	5.31	128.38	120.31
28	H	116	THR	CA-CB-OG1	5.31	117.57	109.60
33	J	398	ILE	CA-CB-CG2	5.31	119.53	110.50
21	N	300	ASN	N-CA-CB	5.31	118.11	110.20
29	I	251	GLU	O-C-N	-5.31	115.70	122.34
3	c	221	ASN	CA-CB-CG	5.31	117.91	112.60
10	j	181	SER	CA-C-N	5.31	131.81	121.41
10	j	181	SER	C-N-CA	5.31	131.81	121.41
14	7	105	THR	CA-C-N	5.31	127.39	120.28
14	7	105	THR	C-N-CA	5.31	127.39	120.28
17	T	125	GLU	CA-C-N	5.31	127.39	120.28
17	T	125	GLU	C-N-CA	5.31	127.39	120.28
27	O	207	LEU	CA-C-N	5.31	127.39	120.28
27	O	207	LEU	C-N-CA	5.31	127.39	120.28
33	J	179	ILE	CA-CB-CG1	5.31	119.43	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	185	GLU	CA-CB-CG	5.31	124.71	114.10
17	T	126	LEU	N-CA-C	-5.31	105.49	111.28
21	N	597	ARG	N-CA-C	-5.31	105.54	112.23
31	L	414	ASP	N-CA-C	-5.31	105.49	111.28
10	j	32	GLN	CG-CD-OE1	5.31	131.41	120.80
12	l	88	ILE	CA-C-N	5.30	130.09	123.14
12	l	88	ILE	C-N-CA	5.30	130.09	123.14
21	N	676	ALA	CA-C-N	5.30	127.34	120.44
21	N	676	ALA	C-N-CA	5.30	127.34	120.44
24	Q	111	LEU	CB-CA-C	-5.30	101.94	110.74
26	U	75	ASN	CA-C-N	5.30	127.92	120.28
26	U	75	ASN	C-N-CA	5.30	127.92	120.28
29	I	389	GLY	CA-C-N	5.30	127.39	120.28
29	I	389	GLY	C-N-CA	5.30	127.39	120.28
30	K	313	LYS	CA-C-O	-5.30	114.87	120.92
22	S	417	GLN	CA-C-N	5.30	127.33	120.44
22	S	417	GLN	C-N-CA	5.30	127.33	120.44
25	R	306	PRO	CA-C-O	-5.30	111.55	119.34
25	R	318	PRO	N-CD-CG	5.30	111.16	103.20
33	J	301	ASP	N-CA-CB	5.30	117.10	109.78
33	J	378	THR	CA-CB-OG1	5.30	117.56	109.60
4	d	72	VAL	CA-CB-CG1	-5.30	101.39	110.40
11	k	169	GLU	CA-C-O	5.30	126.04	120.42
8	l	155	MET	O-C-N	-5.30	117.00	122.94
20	Z	857	LEU	N-CA-C	-5.30	106.66	113.23
25	R	335	ARG	N-CA-CB	5.30	118.01	110.16
26	U	141	GLU	N-CA-C	-5.30	99.80	108.76
29	I	261	PRO	CB-CA-C	-5.30	104.37	112.11
10	j	142	ALA	N-CA-C	-5.30	105.26	112.26
11	k	128	LEU	CB-CA-C	-5.30	101.23	109.55
13	m	54	CYS	N-CA-CB	5.30	118.44	110.65
13	6	41	TYR	N-CA-C	-5.30	104.82	113.19
16	V	176	ASN	OD1-CG-ND2	-5.30	117.30	122.60
3	c	20	TYR	CB-CA-C	-5.30	102.33	110.81
26	U	228	LYS	CG-CD-CE	5.30	123.49	111.30
14	n	181	ALA	CA-C-N	5.30	129.87	121.18
14	n	181	ALA	C-N-CA	5.30	129.87	121.18
13	6	135	PRO	N-CA-C	5.30	120.72	113.84
22	S	346	TYR	CB-CG-CD1	5.29	128.74	120.80
5	e	97	VAL	CA-C-N	5.29	127.37	120.28
5	e	97	VAL	C-N-CA	5.29	127.37	120.28
28	H	193	PRO	O-C-N	5.29	129.57	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L	300	GLU	CA-C-N	5.29	127.71	120.46
31	L	300	GLU	C-N-CA	5.29	127.71	120.46
9	i	234	PHE	CA-C-N	5.29	125.27	120.03
9	i	234	PHE	C-N-CA	5.29	125.27	120.03
3	C	63	THR	N-CA-C	-5.29	101.63	109.83
23	P	414	GLU	CB-CG-CD	-5.29	103.60	112.60
24	Q	336	ASN	CB-CA-C	-5.29	102.54	110.90
25	R	349	SER	O-C-N	-5.29	117.05	123.03
31	L	144	VAL	CA-C-N	5.29	128.38	120.87
31	L	144	VAL	C-N-CA	5.29	128.38	120.87
33	J	402	LYS	N-CA-C	-5.29	100.68	108.99
9	i	180	ALA	CB-CA-C	-5.29	102.01	110.79
21	N	280	GLN	CA-C-O	5.29	126.03	120.42
23	P	214	GLU	CA-C-N	5.29	127.63	120.44
23	P	214	GLU	C-N-CA	5.29	127.63	120.44
4	d	154	GLY	N-CA-C	-5.29	107.34	116.01
10	j	32	GLN	CG-CD-NE2	-5.29	108.47	116.40
12	5	260	TRP	CA-C-N	5.29	129.75	123.19
12	5	260	TRP	C-N-CA	5.29	129.75	123.19
21	N	498	ILE	CA-C-O	-5.29	115.25	120.85
29	I	240	THR	CA-C-O	-5.29	114.94	120.55
29	I	293	ASP	O-C-N	-5.29	117.02	123.10
33	J	157	ILE	N-CA-CB	5.29	117.34	110.57
3	c	14	SER	CA-C-N	5.29	126.45	119.84
3	c	14	SER	C-N-CA	5.29	126.45	119.84
33	J	244	ILE	CA-CB-CG1	-5.29	101.41	110.40
1	a	238	ALA	CA-C-N	5.29	127.36	120.28
1	a	238	ALA	C-N-CA	5.29	127.36	120.28
6	f	27	GLU	O-C-N	5.29	129.75	122.46
27	O	245	ASP	CA-C-N	5.29	127.36	120.28
27	O	245	ASP	C-N-CA	5.29	127.36	120.28
27	O	389	GLN	CA-C-N	5.29	127.80	120.29
27	O	389	GLN	C-N-CA	5.29	127.80	120.29
1	a	226	GLY	N-CA-C	-5.28	102.21	111.46
12	5	157	ILE	CA-CB-CG2	5.28	119.48	110.50
20	Z	738	TYR	CE1-CZ-OH	-5.28	104.05	119.90
22	S	372	LEU	CA-C-O	-5.28	114.95	120.55
22	S	393	ARG	NE-CZ-NH2	5.28	123.95	119.20
24	Q	189	ARG	NE-CZ-NH1	5.28	126.78	121.50
29	I	237	ALA	CA-C-N	5.28	127.63	120.44
29	I	237	ALA	C-N-CA	5.28	127.63	120.44
30	K	269	ILE	CA-C-O	-5.28	114.88	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	87	ILE	O-C-N	-5.28	115.08	121.10
10	j	23	ILE	N-CA-C	-5.28	100.23	108.95
14	7	99	LEU	N-CA-C	5.28	117.78	111.71
15	W	45	PRO	CB-CA-C	5.28	115.73	109.92
24	Q	140	LYS	CA-C-N	5.28	127.31	120.44
24	Q	140	LYS	C-N-CA	5.28	127.31	120.44
5	e	197	GLU	N-CA-C	5.28	116.72	111.07
9	i	252	ILE	N-CA-CB	-5.28	103.27	110.56
12	l	167	GLY	O-C-N	5.28	128.11	122.41
11	4	157	GLY	CA-C-N	5.28	127.36	120.28
11	4	157	GLY	C-N-CA	5.28	127.36	120.28
16	V	117	TRP	CE2-CD2-CE3	5.28	124.08	118.80
21	N	58	ARG	NE-CZ-NH2	-5.28	114.45	119.20
21	N	724	THR	CA-C-N	5.28	128.35	120.90
21	N	724	THR	C-N-CA	5.28	128.35	120.90
21	N	731	VAL	N-CA-C	-5.28	105.39	110.72
25	R	73	ASN	N-CA-CB	5.28	119.42	110.49
31	L	432	ILE	CA-C-O	5.28	127.38	120.78
4	d	104	VAL	CA-C-O	5.28	127.14	121.97
14	7	252	TRP	N-CA-C	-5.28	105.11	112.03
27	O	95	SER	N-CA-CB	5.28	117.67	110.01
30	K	143	SER	N-CA-C	-5.28	107.01	113.50
30	K	396	ARG	CB-CA-C	-5.28	102.03	110.79
11	4	166	GLN	CA-C-N	5.28	127.35	120.28
11	4	166	GLN	C-N-CA	5.28	127.35	120.28
21	N	715	ILE	N-CA-C	-5.28	100.81	108.36
22	S	19	HIS	CE1-NE2-CD2	-5.28	103.72	109.00
31	L	255	TYR	CA-C-N	5.28	129.63	121.71
31	L	255	TYR	C-N-CA	5.28	129.63	121.71
2	b	139	HIS	ND1-CE1-NE2	5.28	113.67	108.40
6	f	209	ASP	CA-CB-CG	5.28	117.88	112.60
8	h	106	ILE	N-CA-C	-5.28	100.88	108.48
15	W	11	ASP	N-CA-CB	5.28	118.47	109.87
20	Z	298	PHE	CA-C-N	5.28	127.35	120.28
20	Z	298	PHE	C-N-CA	5.28	127.35	120.28
31	L	184	GLY	N-CA-C	-5.28	101.96	111.19
9	2	176	THR	N-CA-CB	5.27	118.44	110.42
11	4	130	TYR	N-CA-CB	5.27	119.58	111.56
12	5	195	THR	O-C-N	5.27	129.36	123.19
2	b	247	LEU	CB-CA-C	-5.27	101.89	110.85
21	N	387	ALA	N-CA-C	5.27	120.73	113.77
23	P	102	GLU	CA-C-N	5.27	127.34	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	102	GLU	C-N-CA	5.27	127.34	120.28
32	M	19	ASP	CA-C-N	5.27	127.34	120.28
32	M	19	ASP	C-N-CA	5.27	127.34	120.28
9	i	52	GLY	CA-C-N	5.27	126.30	120.45
9	i	52	GLY	C-N-CA	5.27	126.30	120.45
16	V	243	SER	CA-C-N	5.27	127.87	120.28
16	V	243	SER	C-N-CA	5.27	127.87	120.28
1	a	25	LEU	CA-C-N	5.27	128.32	120.31
1	a	25	LEU	C-N-CA	5.27	128.32	120.31
3	c	6	TYR	N-CA-C	-5.27	106.53	113.17
10	3	143	SER	O-C-N	-5.27	115.79	122.27
17	T	251	HIS	CE1-NE2-CD2	-5.27	103.73	109.00
20	Z	196	SER	CA-C-N	5.27	127.34	120.28
20	Z	196	SER	C-N-CA	5.27	127.34	120.28
21	N	859	ASN	N-CA-C	-5.27	100.44	109.24
22	S	317	HIS	CE1-NE2-CD2	-5.27	103.73	109.00
26	U	94	HIS	N-CA-C	-5.27	100.10	109.06
11	k	191	GLN	N-CA-C	-5.27	101.53	109.85
21	N	574	VAL	CA-CB-CG2	-5.27	101.45	110.40
22	S	157	GLU	CA-C-N	5.27	127.77	120.29
22	S	157	GLU	C-N-CA	5.27	127.77	120.29
23	P	320	PRO	CA-C-O	-5.27	112.67	118.68
27	O	195	TYR	CA-C-N	5.27	127.77	120.29
27	O	195	TYR	C-N-CA	5.27	127.77	120.29
28	H	386	ALA	N-CA-C	-5.27	105.54	111.28
29	I	136	VAL	CA-CB-CG2	-5.27	101.44	110.40
31	L	244	ILE	N-CA-C	-5.27	98.91	107.28
32	M	304	THR	N-CA-C	-5.27	106.36	112.89
33	J	61	GLU	CB-CG-CD	-5.27	103.64	112.60
32	M	194	VAL	N-CA-C	-5.27	105.36	110.42
4	d	234	THR	N-CA-CB	5.26	117.86	110.12
11	4	140	THR	CA-C-N	5.26	127.59	120.38
11	4	140	THR	C-N-CA	5.26	127.59	120.38
13	6	36	ARG	NH1-CZ-NH2	-5.26	112.46	119.30
23	P	369	LEU	N-CA-C	5.26	118.96	112.54
24	Q	135	HIS	CA-C-O	5.26	125.84	119.31
33	J	207	ASP	N-CA-CB	5.26	119.39	110.49
25	R	276	LEU	N-CA-C	-5.26	105.72	111.82
6	f	45	VAL	N-CA-CB	5.26	119.99	111.36
12	l	222	ASP	CA-CB-CG	5.26	117.86	112.60
14	n	179	PHE	CA-CB-CG	-5.26	108.54	113.80
15	W	58	ASN	CA-C-O	5.26	124.60	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	401	LYS	CB-CA-C	-5.26	102.05	110.79
22	S	271	ARG	CA-C-O	-5.26	115.30	120.82
23	P	262	SER	O-C-N	5.26	127.70	122.12
2	b	235	PHE	CA-C-N	5.26	129.39	121.40
2	b	235	PHE	C-N-CA	5.26	129.39	121.40
3	c	21	GLN	OE1-CD-NE2	-5.26	117.34	122.60
5	e	35	SER	CA-C-N	5.26	131.07	121.97
5	e	35	SER	C-N-CA	5.26	131.07	121.97
8	h	129	HIS	CE1-NE2-CD2	-5.26	103.74	109.00
10	j	196	VAL	CA-C-N	-5.26	115.69	123.05
10	j	196	VAL	C-N-CA	-5.26	115.69	123.05
10	j	203	ARG	N-CA-CB	5.26	118.10	109.95
12	5	145	GLU	CB-CG-CD	-5.26	103.66	112.60
15	W	30	ILE	CA-C-N	5.26	127.33	120.28
15	W	30	ILE	C-N-CA	5.26	127.33	120.28
16	V	92	MET	CA-C-O	-5.26	114.85	120.42
22	S	149	SER	CA-C-O	-5.26	114.84	120.42
28	H	79	SER	N-CA-C	-5.26	106.25	113.30
21	N	358	LYS	N-CA-CB	5.26	118.40	110.30
21	N	742	TRP	CB-CG-CD2	-5.26	119.44	126.80
29	I	185	GLY	N-CA-C	-5.26	101.99	111.19
30	K	345	ASP	O-C-N	5.26	129.05	123.42
32	M	242	THR	CA-C-O	5.26	127.52	121.47
12	l	100	TRP	CA-C-O	5.26	127.59	121.44
10	3	185	ALA	CA-C-O	5.26	126.64	120.75
18	X	72	GLU	N-CA-C	-5.26	107.52	114.04
21	N	729	SER	CA-C-N	5.26	127.88	120.42
21	N	729	SER	C-N-CA	5.26	127.88	120.42
24	Q	382	LEU	CA-C-N	5.26	127.27	120.44
24	Q	382	LEU	C-N-CA	5.26	127.27	120.44
27	O	87	LYS	O-C-N	-5.26	115.40	122.23
27	O	112	LYS	CA-C-O	5.26	126.17	120.55
32	M	40	GLU	CA-C-N	5.26	127.88	120.42
32	M	40	GLU	C-N-CA	5.26	127.88	120.42
13	6	229	ARG	N-CA-C	5.25	117.92	111.82
14	n	114	ALA	N-CA-C	-5.25	106.18	112.59
18	X	29	VAL	N-CA-C	5.25	120.27	109.34
24	Q	135	HIS	ND1-CE1-NE2	5.25	113.65	108.40
27	O	150	LEU	N-CA-C	5.25	117.00	111.28
31	L	92	GLU	O-C-N	-5.25	115.81	122.27
9	2	245	SER	CA-CB-OG	5.25	121.60	111.10
17	T	111	LEU	N-CA-CB	5.25	117.94	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	325	PHE	CA-C-O	-5.25	114.71	120.43
21	N	825	GLU	CA-C-O	-5.25	114.85	120.42
22	S	208	ILE	N-CA-CB	5.25	117.29	110.57
30	K	427	TYR	N-CA-C	-5.25	105.16	112.30
31	L	53	HIS	ND1-CE1-NE2	5.25	113.65	108.40
5	e	238	GLU	CA-C-N	5.25	127.75	120.29
5	e	238	GLU	C-N-CA	5.25	127.75	120.29
12	l	159	SER	O-C-N	5.25	127.69	122.12
27	O	114	GLN	O-C-N	5.25	127.69	122.12
1	a	142	THR	N-CA-C	-5.25	100.62	109.07
3	c	226	TYR	N-CA-CB	5.25	119.18	110.47
23	P	122	ILE	N-CA-CB	5.25	117.68	110.54
14	7	182	HIS	ND1-CE1-NE2	5.25	113.65	108.40
26	U	217	LYS	N-CA-C	-5.25	106.27	113.30
27	O	279	ILE	CA-C-N	5.25	127.74	120.29
27	O	279	ILE	C-N-CA	5.25	127.74	120.29
30	K	424	PHE	CA-C-N	5.25	127.31	120.28
30	K	424	PHE	C-N-CA	5.25	127.31	120.28
7	g	83	PRO	CA-C-N	5.25	127.74	120.29
7	g	83	PRO	C-N-CA	5.25	127.74	120.29
12	l	274	LYS	CA-C-O	-5.25	114.86	120.42
8	l	119	VAL	CA-C-N	5.25	131.04	122.81
8	l	119	VAL	C-N-CA	5.25	131.04	122.81
28	H	368	PRO	N-CA-C	5.25	119.55	111.21
6	f	220	THR	CA-C-N	5.24	126.39	119.84
6	f	220	THR	C-N-CA	5.24	126.39	119.84
7	g	184	PRO	N-CA-CB	5.24	108.59	102.88
14	n	251	LYS	CA-C-N	5.24	129.68	121.08
14	n	251	LYS	C-N-CA	5.24	129.68	121.08
17	T	94	HIS	CA-C-N	5.24	129.57	122.07
17	T	94	HIS	C-N-CA	5.24	129.57	122.07
18	X	61	LEU	CA-C-N	5.24	128.62	120.60
18	X	61	LEU	C-N-CA	5.24	128.62	120.60
24	Q	167	LYS	CA-C-O	5.24	125.83	119.38
25	R	180	PHE	N-CA-C	5.24	116.68	111.07
14	7	157	ASP	CA-CB-CG	-5.24	107.36	112.60
21	N	207	LEU	CA-C-O	-5.24	114.99	120.55
25	R	417	TYR	CB-CG-CD1	-5.24	112.94	120.80
12	5	204	VAL	CA-CB-CG2	-5.24	101.49	110.40
17	T	213	ASN	CB-CG-ND2	-5.24	108.54	116.40
3	c	194	LEU	CA-C-O	-5.24	115.32	120.82
12	l	179	TYR	N-CA-C	-5.24	98.69	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	842	ASN	N-CA-CB	5.24	119.34	110.49
23	P	340	ASP	CA-CB-CG	5.24	117.84	112.60
25	R	256	THR	OG1-CB-CG2	-5.24	98.82	109.30
25	R	415	GLN	N-CA-C	-5.24	105.47	111.07
27	O	111	SER	CA-C-O	5.24	125.97	120.42
24	Q	202	ARG	N-CA-CB	5.24	117.82	110.12
1	a	30	TYR	CB-CG-CD2	-5.24	112.95	120.80
9	2	87	LEU	CB-CA-C	-5.24	102.63	110.90
17	T	68	ALA	CA-C-N	5.24	128.27	120.31
17	T	68	ALA	C-N-CA	5.24	128.27	120.31
17	T	101	LYS	CA-C-N	5.24	127.61	120.54
17	T	101	LYS	C-N-CA	5.24	127.61	120.54
21	N	567	ALA	CA-C-O	5.24	126.09	120.70
21	N	622	ALA	CA-C-O	-5.24	115.00	120.55
21	N	919	THR	N-CA-C	-5.24	103.78	110.53
23	P	170	SER	N-CA-C	-5.24	105.63	112.23
9	2	203	ASP	CA-C-O	-5.23	115.16	120.71
26	U	124	ASP	CA-C-N	5.23	130.49	122.69
26	U	124	ASP	C-N-CA	5.23	130.49	122.69
27	O	335	GLY	CA-C-O	5.23	124.61	118.96
33	J	40	ASN	CA-C-N	5.23	127.85	120.42
33	J	40	ASN	C-N-CA	5.23	127.85	120.42
11	4	103	LEU	CA-C-O	-5.23	114.76	120.36
21	N	240	GLN	N-CA-CB	5.23	117.81	110.12
22	S	320	ILE	CA-CB-CG1	-5.23	101.50	110.40
31	L	292	SER	CB-CA-C	-5.23	100.01	110.42
11	k	73	TYR	CA-C-N	5.23	130.39	121.29
11	k	73	TYR	C-N-CA	5.23	130.39	121.29
14	n	238	GLY	N-CA-C	5.23	121.32	112.22
13	6	193	ARG	CA-C-O	-5.23	115.01	120.55
16	V	101	ASP	N-CA-C	5.23	117.81	110.23
22	S	23	LYS	CB-CA-C	-5.23	101.96	110.85
23	P	356	TYR	CA-C-O	-5.23	113.62	120.00
24	Q	403	PRO	N-CA-C	5.23	119.30	111.14
28	H	128	ASN	CB-CA-C	5.23	116.24	109.28
33	J	51	LEU	N-CA-C	5.23	116.67	111.07
14	7	91	SER	CB-CA-C	-5.23	102.67	110.88
18	X	21	SER	O-C-N	5.23	129.54	122.59
21	N	654	GLN	CG-CD-NE2	5.23	124.24	116.40
24	Q	185	TYR	CA-C-N	5.23	127.54	120.38
24	Q	185	TYR	C-N-CA	5.23	127.54	120.38
14	n	61	GLY	N-CA-C	-5.23	100.79	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	n	118	GLU	CB-CG-CD	5.23	121.48	112.60
11	4	76	SER	O-C-N	-5.23	115.31	121.32
21	N	863	SER	N-CA-C	-5.23	99.66	110.80
22	S	348	LEU	CA-C-N	5.23	127.29	120.28
22	S	348	LEU	C-N-CA	5.23	127.29	120.28
25	R	327	ASP	CA-CB-CG	-5.23	107.37	112.60
27	O	72	LYS	N-CA-C	-5.23	105.57	112.94
32	M	295	LYS	N-CA-C	-5.23	100.88	109.40
33	J	108	LYS	CA-C-O	5.23	128.47	121.78
1	a	20	SER	CA-C-N	5.22	124.94	119.82
1	a	20	SER	C-N-CA	5.22	124.94	119.82
7	g	197	ALA	CA-C-N	5.22	127.28	120.28
7	g	197	ALA	C-N-CA	5.22	127.28	120.28
13	6	10	PHE	CA-CB-CG	-5.22	108.58	113.80
13	6	164	PHE	CA-C-N	5.22	128.27	120.95
13	6	164	PHE	C-N-CA	5.22	128.27	120.95
17	T	122	PHE	N-CA-C	-5.22	105.48	111.07
22	S	31	VAL	CB-CA-C	-5.22	105.09	112.14
22	S	227	ASN	CA-C-N	5.22	127.71	120.29
22	S	227	ASN	C-N-CA	5.22	127.71	120.29
22	S	490	ASN	CA-C-O	-5.22	116.01	121.55
26	U	231	ASP	CA-C-N	5.22	127.62	120.46
26	U	231	ASP	C-N-CA	5.22	127.62	120.46
2	b	219	PRO	N-CA-C	-5.22	107.22	114.27
4	d	235	GLN	OE1-CD-NE2	-5.22	117.38	122.60
9	2	118	LYS	CA-CB-CG	5.22	124.54	114.10
11	4	14	ILE	CA-CB-CG2	-5.22	101.62	110.50
14	7	186	PRO	CA-C-O	-5.22	111.01	119.84
17	T	94	HIS	N-CA-CB	5.22	118.38	109.87
17	T	169	GLN	CG-CD-OE1	-5.22	110.36	120.80
21	N	399	PHE	O-C-N	-5.22	116.58	122.12
30	K	59	GLU	CA-C-N	5.22	127.28	120.28
30	K	59	GLU	C-N-CA	5.22	127.28	120.28
2	b	85	LEU	N-CA-C	5.22	118.81	112.23
5	e	70	ILE	CA-C-O	5.22	127.20	120.83
12	l	100	TRP	O-C-N	-5.22	116.37	123.15
12	l	112	ILE	CA-CB-CG1	5.22	119.27	110.40
20	Z	809	MET	N-CA-CB	-5.22	102.50	110.07
21	N	411	ILE	N-CA-CB	5.22	116.66	110.55
23	P	154	ASP	CA-CB-CG	-5.22	107.38	112.60
2	b	180	ASN	CA-C-N	5.22	127.53	120.38
2	b	180	ASN	C-N-CA	5.22	127.53	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	82	GLU	CA-C-O	-5.22	115.02	120.55
9	2	160	SER	O-C-N	5.22	127.52	122.09
27	O	371	VAL	O-C-N	-5.22	116.46	121.83
3	c	188	ASP	N-CA-C	-5.22	105.49	111.07
11	k	19	LYS	N-CA-CB	5.22	117.64	110.07
11	k	107	TYR	N-CA-C	-5.22	100.23	108.73
12	l	236	ILE	CA-CB-CG2	5.22	119.37	110.50
5	E	13	SER	N-CA-C	-5.22	99.69	110.80
12	5	227	ASP	N-CA-CB	5.22	117.88	110.16
13	6	125	ASP	N-CA-CB	5.22	118.30	110.53
23	P	425	HIS	CB-CA-C	-5.22	102.13	110.79
28	H	88	ARG	NE-CZ-NH2	5.22	123.89	119.20
31	L	251	ILE	N-CA-C	-5.22	107.89	112.90
33	J	307	PRO	N-CA-C	-5.22	103.00	111.03
11	4	166	GLN	OE1-CD-NE2	5.21	127.81	122.60
13	6	77	LYS	CA-C-N	5.21	127.69	120.29
13	6	77	LYS	C-N-CA	5.21	127.69	120.29
21	N	714	THR	O-C-N	-5.21	116.39	122.96
23	P	425	HIS	CE1-NE2-CD2	-5.21	103.79	109.00
28	H	106	ILE	CA-C-N	5.21	128.62	120.75
28	H	106	ILE	C-N-CA	5.21	128.62	120.75
28	H	293	GLU	CB-CG-CD	-5.21	103.73	112.60
33	J	185	VAL	O-C-N	-5.21	117.44	123.07
33	J	210	PHE	CA-CB-CG	-5.21	108.59	113.80
9	i	188	ILE	O-C-N	-5.21	116.81	121.87
12	l	177	CYS	CA-C-N	5.21	127.74	121.38
12	l	177	CYS	C-N-CA	5.21	127.74	121.38
31	L	433	GLU	O-C-N	-5.21	116.40	122.81
12	l	182	LYS	N-CA-C	5.21	119.74	113.17
12	l	284	ASN	O-C-N	5.21	127.44	122.07
10	3	117	GLY	O-C-N	-5.21	116.78	122.41
12	5	189	TYR	N-CA-C	-5.21	98.77	107.99
13	6	186	GLU	CB-CG-CD	-5.21	103.74	112.60
15	W	185	ILE	N-CA-CB	5.21	116.65	110.55
29	I	234	LYS	N-CA-CB	5.21	117.57	110.01
5	e	109	VAL	CA-C-O	5.21	126.10	120.47
16	V	21	ASP	CA-C-N	5.21	129.96	122.40
16	V	21	ASP	C-N-CA	5.21	129.96	122.40
10	3	28	ARG	NE-CZ-NH2	5.21	123.89	119.20
20	Z	735	GLU	CA-C-N	5.21	127.26	120.28
20	Z	735	GLU	C-N-CA	5.21	127.26	120.28
21	N	160	GLY	N-CA-C	-5.21	107.45	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	287	LEU	CA-C-N	5.21	127.26	120.28
21	N	287	LEU	C-N-CA	5.21	127.26	120.28
21	N	758	VAL	N-CA-CB	-5.21	102.53	110.86
23	P	228	SER	N-CA-CB	-5.21	102.21	110.28
24	Q	175	VAL	CA-C-N	5.21	128.23	120.31
24	Q	175	VAL	C-N-CA	5.21	128.23	120.31
24	Q	346	ASN	OD1-CG-ND2	5.21	127.81	122.60
33	J	249	GLU	N-CA-C	-5.21	98.43	107.49
8	h	47	HIS	CE1-NE2-CD2	-5.21	103.79	109.00
12	l	174	THR	CA-C-O	-5.21	115.26	121.56
14	n	164	ASN	OD1-CG-ND2	-5.21	117.39	122.60
11	4	194	ASP	CB-CA-C	-5.21	99.88	109.46
26	U	15	LEU	CA-C-N	5.21	127.68	120.29
26	U	15	LEU	C-N-CA	5.21	127.68	120.29
18	X	25	THR	CA-CB-OG1	5.21	117.41	109.60
18	X	97	TYR	N-CA-C	-5.21	99.85	108.75
23	P	38	GLN	CA-C-N	5.21	128.22	120.31
23	P	38	GLN	C-N-CA	5.21	128.22	120.31
32	M	154	LEU	CA-C-O	5.21	126.94	120.54
1	a	174	LYS	CG-CD-CE	5.20	123.27	111.30
5	e	113	THR	O-C-N	5.20	127.64	122.12
12	l	273	TRP	N-CA-C	5.20	117.86	111.82
14	7	84	VAL	N-CA-C	-5.20	100.25	107.80
21	N	393	SER	CA-C-N	5.20	130.75	122.94
21	N	393	SER	C-N-CA	5.20	130.75	122.94
22	S	470	GLN	CB-CA-C	-5.20	102.00	110.85
28	H	275	ILE	O-C-N	-5.20	117.67	123.03
32	M	146	VAL	CA-C-N	5.20	126.59	120.71
32	M	146	VAL	C-N-CA	5.20	126.59	120.71
33	J	253	ILE	CA-C-O	5.20	124.19	119.20
6	f	84	LEU	N-CA-C	-5.20	105.68	112.23
14	n	62	SER	CA-C-O	-5.20	115.31	121.66
24	Q	255	TYR	CA-C-O	-5.20	114.91	120.42
24	Q	309	ARG	NH1-CZ-NH2	5.20	126.06	119.30
3	c	35	ALA	N-CA-C	-5.20	100.22	109.06
6	f	11	VAL	O-C-N	-5.20	116.07	122.57
9	2	141	SER	CA-C-N	5.20	130.28	122.58
9	2	141	SER	C-N-CA	5.20	130.28	122.58
12	5	159	SER	N-CA-C	5.20	116.64	111.07
22	S	203	SER	N-CA-CB	5.20	117.86	110.16
23	P	33	ASN	N-CA-C	5.20	117.69	111.71
29	I	421	GLU	CA-C-N	5.20	127.51	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I	421	GLU	C-N-CA	5.20	127.51	120.44
30	K	405	SER	CA-C-N	5.20	127.67	120.29
30	K	405	SER	C-N-CA	5.20	127.67	120.29
3	c	111	LEU	CB-CA-C	-5.20	102.01	110.85
4	d	31	THR	CA-CB-OG1	5.20	117.40	109.60
7	g	22	PHE	N-CA-C	5.20	120.27	113.88
10	j	91	VAL	CA-CB-CG2	-5.20	101.56	110.40
12	5	144	ARG	CD-NE-CZ	-5.20	117.12	124.40
13	6	15	ASP	N-CA-C	-5.20	101.36	108.38
16	V	154	ASP	N-CA-C	-5.20	101.17	109.23
28	H	195	VAL	CA-C-N	5.20	127.67	120.29
28	H	195	VAL	C-N-CA	5.20	127.67	120.29
33	J	134	VAL	CA-C-N	5.20	127.67	120.29
33	J	134	VAL	C-N-CA	5.20	127.67	120.29
12	5	254	HIS	CE1-NE2-CD2	-5.20	103.80	109.00
21	N	58	ARG	O-C-N	5.20	127.63	122.12
21	N	561	GLY	N-CA-C	-5.20	107.82	115.30
25	R	172	LEU	CA-C-N	5.20	127.67	120.29
25	R	172	LEU	C-N-CA	5.20	127.67	120.29
26	U	6	GLU	N-CA-CB	5.20	118.34	110.28
32	M	312	LEU	N-CA-C	-5.20	106.34	113.30
3	c	191	GLU	O-C-N	-5.20	116.23	122.15
9	2	136	GLY	CA-C-O	-5.20	117.24	121.76
16	V	222	GLN	CA-C-N	5.20	128.91	120.60
16	V	222	GLN	C-N-CA	5.20	128.91	120.60
19	Y	80	GLU	CA-C-N	5.20	127.24	120.28
19	Y	80	GLU	C-N-CA	5.20	127.24	120.28
20	Z	809	MET	CB-CA-C	-5.20	102.69	110.90
29	I	150	HIS	CG-CD2-NE2	5.20	112.39	107.20
3	c	176	LEU	O-C-N	5.19	128.07	122.15
8	h	167	SER	O-C-N	5.19	128.07	122.15
15	W	132	LEU	CA-C-O	-5.19	115.37	120.82
19	Y	1	MET	N-CA-CB	-5.19	101.67	110.50
20	Z	351	PRO	CA-C-N	5.19	127.66	120.29
20	Z	351	PRO	C-N-CA	5.19	127.66	120.29
21	N	89	PHE	N-CA-C	-5.19	107.11	113.50
21	N	502	PHE	N-CA-C	5.19	116.94	111.28
22	S	280	ASN	OD1-CG-ND2	5.19	127.79	122.60
29	I	147	VAL	CA-C-N	5.19	129.88	122.72
29	I	147	VAL	C-N-CA	5.19	129.88	122.72
30	K	180	GLN	OE1-CD-NE2	5.19	127.79	122.60
3	c	234	GLU	N-CA-C	-5.19	106.79	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	159	ASP	CA-C-N	5.19	127.66	120.29
11	k	159	ASP	C-N-CA	5.19	127.66	120.29
13	m	99	ARG	CB-CG-CD	5.19	123.24	111.30
13	6	102	GLN	CA-C-N	5.19	127.66	120.29
13	6	102	GLN	C-N-CA	5.19	127.66	120.29
13	6	138	SER	N-CA-C	5.19	121.86	110.80
21	N	352	ASN	N-CA-C	-5.19	104.44	111.55
27	O	116	ASN	CB-CG-ND2	5.19	124.19	116.40
33	J	363	THR	CA-C-N	5.19	127.66	120.29
33	J	363	THR	C-N-CA	5.19	127.66	120.29
13	6	139	TYR	N-CA-C	-5.19	101.41	109.24
21	N	659	ALA	CB-CA-C	-5.19	102.18	110.79
23	P	322	LEU	CB-CA-C	-5.19	100.62	109.03
27	O	281	ALA	N-CA-C	5.19	116.94	111.28
29	I	373	GLU	N-CA-C	-5.19	106.91	114.12
33	J	65	LEU	CA-C-N	5.19	127.23	120.28
33	J	65	LEU	C-N-CA	5.19	127.23	120.28
10	j	64	ASN	N-CA-CB	5.19	117.84	110.16
10	j	139	SER	N-CA-CB	5.19	119.60	111.56
22	S	148	ASP	CA-C-N	5.19	127.66	120.29
22	S	148	ASP	C-N-CA	5.19	127.66	120.29
22	S	373	LYS	N-CA-C	5.19	116.93	111.28
23	P	191	GLY	N-CA-C	-5.19	106.57	115.08
24	Q	266	LEU	CA-C-N	5.19	127.49	120.38
24	Q	266	LEU	C-N-CA	5.19	127.49	120.38
32	M	28	GLN	CA-C-N	5.19	127.66	120.29
32	M	28	GLN	C-N-CA	5.19	127.66	120.29
20	Z	531	ALA	CA-C-N	5.19	127.23	120.28
20	Z	531	ALA	C-N-CA	5.19	127.23	120.28
31	L	332	THR	CA-C-O	5.19	125.91	119.79
5	e	151	ASP	N-CA-C	-5.18	108.22	114.75
10	3	77	LYS	CB-CA-C	5.18	119.09	110.90
24	Q	94	VAL	CA-C-N	5.18	127.49	120.44
24	Q	94	VAL	C-N-CA	5.18	127.49	120.44
30	K	388	GLN	CA-CB-CG	5.18	124.47	114.10
33	J	174	PHE	CA-CB-CG	-5.18	108.61	113.80
33	J	231	ARG	NE-CZ-NH1	-5.18	116.32	121.50
9	i	64	HIS	CG-CD2-NE2	5.18	112.38	107.20
11	k	81	SER	CA-C-N	5.18	127.65	120.29
11	k	81	SER	C-N-CA	5.18	127.65	120.29
14	7	209	ALA	CA-C-O	-5.18	115.06	120.55
21	N	169	ALA	CA-C-O	5.18	126.04	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	380	ILE	N-CA-CB	5.18	118.35	110.58
29	I	104	LEU	N-CA-CB	5.18	119.39	110.68
31	L	261	ARG	NE-CZ-NH2	-5.18	114.54	119.20
15	W	29	GLN	CA-C-N	5.18	127.19	120.56
15	W	29	GLN	C-N-CA	5.18	127.19	120.56
19	Y	71	ASP	N-CA-C	-5.18	106.64	113.17
25	R	329	PHE	CB-CA-C	-5.18	102.75	110.88
33	J	15	HIS	O-C-N	5.18	127.61	122.12
9	i	150	VAL	N-CA-C	-5.18	100.66	108.12
10	j	118	LYS	O-C-N	-5.18	115.02	121.70
13	m	100	ASN	OD1-CG-ND2	-5.18	117.42	122.60
11	4	46	PHE	CA-C-O	-5.18	115.05	121.06
21	N	591	LEU	N-CA-C	5.18	116.92	111.28
23	P	329	PHE	CB-CA-C	-5.18	100.11	110.42
28	H	166	THR	CA-C-O	5.18	126.04	120.55
4	d	65	SER	CA-C-N	5.18	128.90	121.50
4	d	65	SER	C-N-CA	5.18	128.90	121.50
28	H	408	SER	N-CA-CB	5.18	118.31	110.28
1	a	108	TYR	CA-C-O	-5.18	112.74	118.69
9	i	226	GLU	O-C-N	-5.18	116.75	122.86
13	m	33	GLY	O-C-N	5.18	128.37	123.56
10	3	193	ASP	N-CA-C	-5.18	107.63	114.31
21	N	338	PHE	N-CA-CB	5.18	118.27	110.30
26	U	256	ASN	O-C-N	5.18	127.61	122.12
29	I	210	GLU	CA-C-N	5.18	127.22	120.28
29	I	210	GLU	C-N-CA	5.18	127.22	120.28
1	a	120	ARG	CA-C-N	5.17	127.64	120.29
1	a	120	ARG	C-N-CA	5.17	127.64	120.29
1	a	185	HIS	CG-CD2-NE2	5.17	112.37	107.20
4	d	12	SER	CA-C-O	-5.17	115.54	120.97
12	l	240	ALA	CA-C-N	5.17	127.17	120.44
12	l	240	ALA	C-N-CA	5.17	127.17	120.44
12	l	255	VAL	CA-CB-CG2	-5.17	101.60	110.40
4	D	8	LEU	N-CA-C	-5.17	105.64	112.94
17	T	125	GLU	CA-C-O	-5.17	115.39	120.82
17	T	260	ILE	CA-C-O	-5.17	115.37	120.85
19	Y	35	PHE	CA-C-O	5.17	124.37	118.47
22	S	232	MET	CA-C-N	5.17	127.64	120.29
22	S	232	MET	C-N-CA	5.17	127.64	120.29
23	P	344	ARG	NE-CZ-NH1	-5.17	116.33	121.50
24	Q	206	ASN	CB-CA-C	5.17	119.65	110.85
27	O	42	SER	N-CA-CB	5.17	117.82	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	182	GLN	N-CA-C	5.17	116.92	111.28
32	M	255	TYR	CA-C-N	5.17	127.55	120.46
32	M	255	TYR	C-N-CA	5.17	127.55	120.46
5	e	231	TYR	CA-C-N	5.17	128.42	120.82
5	e	231	TYR	C-N-CA	5.17	128.42	120.82
11	k	56	PHE	N-CA-C	5.17	118.85	112.54
11	k	194	ASP	N-CA-C	-5.17	100.73	108.96
8	1	52	CYS	N-CA-CB	5.17	119.73	111.56
15	W	178	PRO	CA-C-O	-5.17	115.69	121.23
20	Z	369	PHE	CA-CB-CG	-5.17	108.63	113.80
22	S	352	VAL	CA-CB-CG1	5.17	119.19	110.40
24	Q	108	PRO	O-C-N	5.17	128.62	122.98
28	H	148	ASN	N-CA-C	-5.17	99.86	108.34
32	M	248	ALA	CA-C-N	5.17	124.67	119.19
32	M	248	ALA	C-N-CA	5.17	124.67	119.19
2	b	192	ALA	O-C-N	-5.17	116.64	122.12
10	j	196	VAL	N-CA-CB	5.17	120.78	111.21
12	l	262	TYR	N-CA-C	-5.17	100.81	109.24
17	T	61	ILE	O-C-N	5.17	127.16	121.83
29	I	280	PHE	CA-CB-CG	5.17	118.97	113.80
11	k	31	SER	O-C-N	5.17	127.94	121.84
21	N	585	ARG	CD-NE-CZ	-5.17	117.16	124.40
21	N	626	GLY	CA-C-N	5.17	128.13	120.74
21	N	626	GLY	C-N-CA	5.17	128.13	120.74
7	g	93	ARG	CA-C-N	5.17	127.63	120.29
7	g	93	ARG	C-N-CA	5.17	127.63	120.29
9	i	192	ILE	CB-CA-C	-5.17	105.16	112.14
15	W	13	SER	CA-C-O	5.17	126.88	121.25
17	T	213	ASN	CA-C-N	5.17	127.63	120.29
17	T	213	ASN	C-N-CA	5.17	127.63	120.29
21	N	191	THR	N-CA-C	5.17	116.91	111.28
21	N	208	ARG	NE-CZ-NH1	-5.17	116.33	121.50
23	P	317	THR	CA-C-N	-5.17	114.38	122.65
23	P	317	THR	C-N-CA	-5.17	114.38	122.65
24	Q	379	GLN	N-CA-CB	5.17	117.81	110.16
25	R	129	GLU	CA-C-O	5.17	125.90	120.42
26	U	265	LEU	CA-C-N	5.17	128.16	120.31
26	U	265	LEU	C-N-CA	5.17	128.16	120.31
28	H	205	ASP	CA-C-N	5.17	130.36	122.25
28	H	205	ASP	C-N-CA	5.17	130.36	122.25
31	L	392	ARG	O-C-N	-5.17	116.64	122.12
10	j	21	VAL	N-CA-CB	5.17	119.75	112.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	4	138	PHE	N-CA-CB	5.17	117.71	110.12
14	7	139	LYS	CA-C-O	5.17	125.90	120.42
27	O	144	VAL	CA-C-O	5.17	126.33	120.85
29	I	107	GLY	O-C-N	5.17	128.28	123.73
30	K	281	ARG	NE-CZ-NH1	5.17	126.67	121.50
32	M	67	GLU	CA-C-N	5.17	127.20	120.28
32	M	67	GLU	C-N-CA	5.17	127.20	120.28
33	J	169	LYS	CA-C-O	-5.17	114.51	120.24
26	U	82	LYS	CG-CD-CE	5.17	123.18	111.30
31	L	240	GLY	N-CA-C	-5.17	107.99	115.27
2	b	216	ASP	CA-CB-CG	-5.16	107.44	112.60
3	c	108	VAL	CA-C-N	5.16	127.20	120.28
3	c	108	VAL	C-N-CA	5.16	127.20	120.28
9	2	185	SER	CA-C-N	5.16	127.20	120.28
9	2	185	SER	C-N-CA	5.16	127.20	120.28
11	4	41	HIS	CE1-NE2-CD2	-5.16	103.84	109.00
13	6	68	ASP	CA-C-O	5.16	125.89	120.42
14	7	100	LEU	CA-C-O	5.16	125.89	120.42
16	V	189	ILE	CA-C-N	5.16	127.20	120.28
16	V	189	ILE	C-N-CA	5.16	127.20	120.28
20	Z	191	SER	CA-C-N	5.16	125.68	120.00
20	Z	191	SER	C-N-CA	5.16	125.68	120.00
22	S	19	HIS	CA-C-O	-5.16	115.40	120.82
25	R	81	HIS	CG-CD2-NE2	5.16	112.36	107.20
27	O	170	SER	N-CA-C	5.16	117.81	111.82
33	J	6	THR	CA-C-N	5.16	131.40	121.54
33	J	6	THR	C-N-CA	5.16	131.40	121.54
4	d	231	GLN	CA-C-O	5.16	126.20	120.63
21	N	317	SER	N-CA-C	-5.16	105.55	111.07
33	J	225	GLU	CA-C-N	5.16	131.53	121.41
33	J	225	GLU	C-N-CA	5.16	131.53	121.41
5	e	147	HIS	CE1-NE2-CD2	-5.16	103.84	109.00
14	n	193	ASP	CB-CA-C	-5.16	100.40	109.07
10	3	48	HIS	CB-CG-CD2	-5.16	124.49	131.20
11	4	9	VAL	O-C-N	-5.16	116.12	122.57
13	6	181	LYS	CA-C-O	-5.16	114.77	120.24
24	Q	332	ARG	CA-C-O	-5.16	115.08	120.55
25	R	139	GLU	O-C-N	5.16	127.66	122.09
25	R	307	TYR	CB-CG-CD1	5.16	128.54	120.80
26	U	289	ASP	CA-C-N	5.16	127.19	120.28
26	U	289	ASP	C-N-CA	5.16	127.19	120.28
28	H	98	GLN	N-CA-C	-5.16	102.05	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	H	445	LYS	O-C-N	5.16	128.03	122.15
30	K	155	ASP	CA-CB-CG	-5.16	107.44	112.60
3	c	154	SER	N-CA-C	-5.16	106.67	113.17
7	g	165	THR	O-C-N	-5.16	117.90	123.42
9	i	41	VAL	CB-CA-C	5.16	118.97	111.80
10	j	156	PRO	CA-C-O	-5.16	115.71	121.23
21	N	325	PHE	O-C-N	5.16	129.10	123.27
22	S	283	GLN	CA-C-N	5.16	129.94	122.36
22	S	283	GLN	C-N-CA	5.16	129.94	122.36
25	R	196	SER	O-C-N	5.16	128.03	122.15
30	K	416	LYS	CA-C-N	5.16	128.54	120.75
30	K	416	LYS	C-N-CA	5.16	128.54	120.75
7	g	79	SER	CA-C-O	-5.16	115.08	121.06
17	T	268	ILE	CA-CB-CG2	-5.16	101.73	110.50
25	R	92	ILE	CA-C-O	5.16	124.77	119.35
12	5	249	SER	CA-C-N	5.16	130.41	122.68
12	5	249	SER	C-N-CA	5.16	130.41	122.68
17	T	100	ASP	CA-C-O	5.16	124.49	118.97
22	S	347	HIS	N-CA-C	5.16	116.59	111.07
6	f	103	LEU	N-CA-CB	5.15	119.03	110.63
3	C	161	LYS	N-CA-C	-5.15	107.54	113.88
8	1	118	GLU	O-C-N	5.15	129.16	123.33
9	2	193	TRP	CB-CG-CD2	-5.15	119.58	126.80
16	V	213	LEU	CA-C-N	5.15	127.19	120.28
16	V	213	LEU	C-N-CA	5.15	127.19	120.28
28	H	417	ALA	CA-C-N	5.15	127.70	120.28
28	H	417	ALA	C-N-CA	5.15	127.70	120.28
25	R	214	TYR	CB-CG-CD2	-5.15	113.07	120.80
28	H	113	ASP	O-C-N	5.15	127.58	122.12
33	J	81	ASP	CA-C-N	5.15	131.38	121.54
33	J	81	ASP	C-N-CA	5.15	131.38	121.54
33	J	283	GLU	N-CA-C	-5.15	104.69	112.99
1	a	126	GLN	O-C-N	-5.15	116.28	122.15
3	c	146	TYR	N-CA-CB	5.15	117.52	109.85
4	d	25	GLU	N-CA-C	5.15	117.63	111.71
12	l	122	GLY	CA-C-N	5.15	125.56	120.31
12	l	122	GLY	C-N-CA	5.15	125.56	120.31
13	m	51	VAL	N-CA-C	-5.15	100.47	107.99
22	S	388	ILE	N-CA-C	-5.15	105.69	110.53
27	O	207	LEU	N-CA-C	-5.15	105.75	111.36
21	N	900	ASN	O-C-N	-5.15	116.92	122.79
30	K	221	MET	CA-C-N	5.15	127.44	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	221	MET	C-N-CA	5.15	127.44	120.44
1	a	234	PHE	O-C-N	-5.15	117.38	123.25
8	h	146	TYR	CA-C-N	5.15	127.60	120.29
8	h	146	TYR	C-N-CA	5.15	127.60	120.29
6	F	148	GLN	CA-C-N	5.15	124.81	119.56
6	F	148	GLN	C-N-CA	5.15	124.81	119.56
8	l	110	GLY	CA-C-O	-5.15	115.87	121.48
20	Z	207	ILE	CA-C-N	5.15	124.45	120.33
20	Z	207	ILE	C-N-CA	5.15	124.45	120.33
21	N	668	THR	CA-C-O	-5.15	115.90	121.87
21	N	676	ALA	N-CA-C	5.15	117.29	111.11
23	P	60	ALA	N-CA-C	5.15	116.89	111.28
25	R	178	GLY	CA-C-N	5.15	127.60	120.29
25	R	178	GLY	C-N-CA	5.15	127.60	120.29
25	R	290	SER	N-CA-CB	5.15	117.69	110.12
26	U	136	ALA	CA-C-O	5.15	126.58	120.66
29	I	262	ARG	N-CA-C	-5.15	105.67	111.28
32	M	405	ASN	CB-CA-C	-5.15	100.79	110.67
1	a	116	VAL	CA-C-N	5.15	127.60	120.29
1	a	116	VAL	C-N-CA	5.15	127.60	120.29
2	b	244	ASN	CA-CB-CG	5.15	117.75	112.60
3	c	146	TYR	CA-CB-CG	-5.15	104.64	113.90
9	2	81	THR	N-CA-C	5.15	116.70	111.14
21	N	310	ASP	CA-C-N	5.15	129.14	120.29
21	N	310	ASP	C-N-CA	5.15	129.14	120.29
7	g	181	ASP	CA-C-N	5.14	127.59	120.29
7	g	181	ASP	C-N-CA	5.14	127.59	120.29
9	i	143	HIS	CA-C-O	-5.14	115.19	121.78
23	P	229	LEU	CA-C-O	5.14	125.86	119.79
23	P	369	LEU	CA-C-N	5.14	130.15	122.74
23	P	369	LEU	C-N-CA	5.14	130.15	122.74
23	P	400	VAL	N-CA-CB	5.14	119.03	111.52
26	U	69	ASP	CA-C-O	5.14	125.98	120.32
20	Z	433	LEU	CA-C-N	5.14	127.59	120.29
20	Z	433	LEU	C-N-CA	5.14	127.59	120.29
23	P	294	GLU	N-CA-C	-5.14	107.67	114.31
30	K	63	LEU	N-CA-C	5.14	117.62	111.71
31	L	286	ILE	N-CA-C	-5.14	107.33	111.91
31	L	299	ARG	NE-CZ-NH1	5.14	126.64	121.50
33	J	305	LEU	N-CA-C	5.14	121.75	110.80
1	a	220	LYS	CA-C-O	-5.14	112.53	119.11
15	W	178	PRO	CA-C-N	5.14	131.36	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	W	178	PRO	C-N-CA	5.14	131.36	121.54
22	S	370	LEU	CA-C-N	5.14	127.59	120.29
22	S	370	LEU	C-N-CA	5.14	127.59	120.29
3	c	113	ARG	NE-CZ-NH2	5.14	123.83	119.20
13	m	149	ALA	CA-C-N	5.14	131.40	122.56
13	m	149	ALA	C-N-CA	5.14	131.40	122.56
21	N	438	ASP	CA-C-N	5.14	127.72	120.42
21	N	438	ASP	C-N-CA	5.14	127.72	120.42
29	I	90	GLU	CB-CA-C	-5.14	102.81	110.88
30	K	419	ASN	OD1-CG-ND2	5.14	127.74	122.60
7	g	57	LYS	O-C-N	-5.14	115.11	122.41
11	k	74	GLU	CB-CG-CD	-5.14	103.87	112.60
28	H	60	GLU	N-CA-CB	5.14	117.76	110.16
5	e	188	HIS	CG-CD2-NE2	5.14	112.34	107.20
9	i	170	HIS	CB-CG-ND1	5.14	130.40	122.70
11	4	23	ARG	NE-CZ-NH1	-5.14	116.36	121.50
21	N	509	GLN	CB-CG-CD	5.14	121.33	112.60
25	R	71	LEU	O-C-N	-5.14	116.93	122.79
26	U	106	ILE	CA-C-N	5.14	127.42	120.38
26	U	106	ILE	C-N-CA	5.14	127.42	120.38
26	U	113	TYR	CA-C-O	-5.14	113.25	118.90
29	I	361	ILE	CA-C-N	5.14	127.16	120.28
29	I	361	ILE	C-N-CA	5.14	127.16	120.28
32	M	377	GLN	OE1-CD-NE2	-5.14	117.46	122.60
2	b	26	THR	N-CA-C	-5.13	105.68	111.28
5	e	114	GLN	N-CA-C	5.13	116.88	111.28
12	5	227	ASP	O-C-N	-5.13	116.30	122.15
16	V	269	ARG	N-CA-C	5.13	116.69	111.14
23	P	415	TRP	CA-C-O	5.13	125.99	120.55
24	Q	425	GLN	N-CA-CB	5.13	117.67	110.12
26	U	13	LEU	CA-C-N	5.13	127.03	120.56
26	U	13	LEU	C-N-CA	5.13	127.03	120.56
27	O	10	ILE	N-CA-CB	5.13	118.28	110.58
29	I	94	LYS	O-C-N	5.13	127.36	122.07
31	L	361	PHE	CA-C-O	-5.13	115.11	120.55
15	W	68	GLU	CA-C-O	-5.13	114.53	120.49
22	S	196	ARG	CA-C-N	5.13	127.16	120.28
22	S	196	ARG	C-N-CA	5.13	127.16	120.28
23	P	348	HIS	CE1-NE2-CD2	-5.13	103.87	109.00
2	b	15	SER	N-CA-C	-5.13	103.91	111.81
5	e	201	LEU	CA-C-N	5.13	127.42	120.44
5	e	201	LEU	C-N-CA	5.13	127.42	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	254	GLU	CA-C-O	5.13	127.52	121.87
14	n	82	THR	N-CA-CB	5.13	119.23	110.71
9	2	154	LEU	CA-C-O	-5.13	115.31	121.11
23	P	73	ASP	CA-CB-CG	-5.13	107.47	112.60
27	O	155	LYS	N-CA-C	5.13	116.87	111.28
27	O	241	THR	CA-CB-OG1	5.13	117.30	109.60
29	I	414	GLU	CA-C-N	5.13	127.11	120.44
29	I	414	GLU	C-N-CA	5.13	127.11	120.44
4	d	224	LEU	N-CA-CB	5.13	118.60	110.55
12	l	193	ASP	CB-CA-C	-5.13	101.52	110.09
12	5	134	LEU	CA-C-N	5.13	126.74	120.22
12	5	134	LEU	C-N-CA	5.13	126.74	120.22
21	N	280	GLN	OE1-CD-NE2	5.13	127.73	122.60
7	g	205	GLU	N-CA-C	-5.13	106.33	112.59
6	F	216	VAL	N-CA-C	-5.13	101.58	108.35
9	2	211	LYS	N-CA-CB	5.13	119.93	111.62
11	4	127	GLU	O-C-N	-5.13	116.63	122.89
21	N	317	SER	CA-C-N	5.13	127.11	120.44
21	N	317	SER	C-N-CA	5.13	127.11	120.44
21	N	920	VAL	O-C-N	5.13	126.84	121.87
24	Q	94	VAL	O-C-N	-5.13	116.89	121.87
29	I	58	LYS	N-CA-CB	5.13	117.75	110.16
3	c	26	LEU	CB-CA-C	-5.13	100.83	110.67
7	g	161	LYS	CA-C-O	5.13	124.69	119.05
8	h	107	ILE	CA-C-N	5.13	129.92	123.10
8	h	107	ILE	C-N-CA	5.13	129.92	123.10
21	N	502	PHE	CA-CB-CG	-5.13	108.67	113.80
23	P	259	PRO	CA-C-N	5.13	127.02	120.56
23	P	259	PRO	C-N-CA	5.13	127.02	120.56
31	L	192	GLU	N-CA-C	5.13	116.95	111.36
25	R	270	VAL	CA-C-N	5.12	127.48	120.46
25	R	270	VAL	C-N-CA	5.12	127.48	120.46
1	a	60	PRO	CB-CA-C	-5.12	103.11	111.56
4	d	70	HIS	ND1-CE1-NE2	5.12	113.52	108.40
11	k	9	VAL	N-CA-C	-5.12	102.39	109.46
16	V	77	GLY	CA-C-N	5.12	127.44	120.63
16	V	77	GLY	C-N-CA	5.12	127.44	120.63
24	Q	341	THR	CA-CB-OG1	5.12	117.29	109.60
26	U	275	VAL	CB-CA-C	-5.12	103.96	112.26
29	I	342	GLY	CA-C-N	5.12	129.28	120.72
29	I	342	GLY	C-N-CA	5.12	129.28	120.72
30	K	320	ARG	N-CA-CB	5.12	119.35	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	202	TYR	O-C-N	-5.12	116.50	121.93
15	W	36	ILE	CB-CA-C	-5.12	105.33	112.04
28	H	424	THR	N-CA-CB	5.12	117.65	110.12
31	L	321	THR	N-CA-C	-5.12	102.88	110.46
32	M	21	GLU	CA-C-O	5.12	125.66	119.31
32	M	57	VAL	O-C-N	5.12	127.23	121.90
14	7	186	PRO	N-CA-CB	5.12	109.10	103.26
15	W	135	ASN	CA-CB-CG	5.12	117.72	112.60
16	V	162	GLY	N-CA-C	-5.12	106.53	113.24
22	S	449	LEU	CB-CA-C	-5.12	110.65	116.54
31	L	414	ASP	O-C-N	5.12	127.55	122.12
3	c	83	ASP	N-CA-CB	5.12	117.74	110.16
5	e	187	TRP	N-CA-CB	5.12	118.52	110.23
5	e	188	HIS	ND1-CE1-NE2	5.12	113.52	108.40
21	N	157	ALA	CA-C-N	5.12	127.56	120.29
21	N	157	ALA	C-N-CA	5.12	127.56	120.29
22	S	42	SER	CB-CA-C	-5.12	99.89	109.72
23	P	300	VAL	CA-C-N	5.12	127.56	120.29
23	P	300	VAL	C-N-CA	5.12	127.56	120.29
31	L	400	PHE	N-CA-CB	5.12	117.43	110.01
9	i	250	CYS	CA-C-N	5.12	131.52	122.67
9	i	250	CYS	C-N-CA	5.12	131.52	122.67
14	n	135	GLN	CB-CA-C	-5.12	99.94	110.38
12	5	96	THR	CA-CB-CG2	-5.12	101.80	110.50
14	7	135	GLN	N-CA-C	-5.12	105.88	111.82
20	Z	28	LYS	CA-C-N	5.12	127.09	120.44
20	Z	28	LYS	C-N-CA	5.12	127.09	120.44
22	S	192	GLU	N-CA-C	-5.12	105.78	111.36
31	L	408	ASP	CB-CA-C	-5.12	102.07	110.72
33	J	306	ARG	NE-CZ-NH2	5.12	123.81	119.20
7	g	111	ALA	CA-C-N	5.12	127.55	120.29
7	g	111	ALA	C-N-CA	5.12	127.55	120.29
21	N	526	TYR	CA-C-N	5.12	127.83	120.11
21	N	526	TYR	C-N-CA	5.12	127.83	120.11
21	N	721	ASP	CA-CB-CG	-5.12	107.48	112.60
22	S	198	SER	O-C-N	5.12	129.11	123.33
24	Q	147	GLN	CA-C-N	5.12	130.93	121.52
24	Q	147	GLN	C-N-CA	5.12	130.93	121.52
2	b	18	LEU	CA-C-N	5.11	126.71	120.22
2	b	18	LEU	C-N-CA	5.11	126.71	120.22
2	b	187	ASP	CA-CB-CG	-5.11	107.49	112.60
9	i	67	SER	CA-C-N	5.11	125.40	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	67	SER	C-N-CA	5.11	125.40	119.47
15	W	106	GLN	N-CA-CB	5.11	118.06	110.29
21	N	329	HIS	CE1-NE2-CD2	-5.11	103.89	109.00
25	R	412	THR	CA-C-N	5.11	128.08	120.31
25	R	412	THR	C-N-CA	5.11	128.08	120.31
30	K	110	VAL	CB-CA-C	-5.11	104.18	111.34
31	L	309	LEU	O-C-N	-5.11	116.70	122.12
13	6	84	HIS	CA-CB-CG	-5.11	108.69	113.80
23	P	111	ASP	CA-C-N	5.11	127.13	120.28
23	P	111	ASP	C-N-CA	5.11	127.13	120.28
24	Q	273	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	a	225	VAL	N-CA-C	-5.11	101.12	108.48
3	c	21	GLN	CA-C-O	-5.11	114.09	119.97
8	h	84	THR	CA-C-N	5.11	127.44	120.54
8	h	84	THR	C-N-CA	5.11	127.44	120.54
14	n	223	ARG	NH1-CZ-NH2	5.11	125.94	119.30
13	6	10	PHE	CA-C-O	5.11	125.99	120.32
14	7	164	ASN	CA-C-N	5.11	127.64	120.28
14	7	164	ASN	C-N-CA	5.11	127.64	120.28
31	L	308	LEU	N-CA-CB	5.11	117.56	109.94
14	n	150	ALA	CB-CA-C	-5.11	100.36	109.71
14	n	240	THR	CA-CB-OG1	5.11	117.26	109.60
10	3	67	PHE	CA-C-O	5.11	125.84	120.42
22	S	327	ILE	N-CA-C	-5.11	99.64	107.71
23	P	252	SER	N-CA-C	5.11	116.85	111.28
33	J	85	LEU	N-CA-CB	5.11	118.11	109.94
2	b	234	ARG	NE-CZ-NH2	5.11	123.80	119.20
4	d	234	THR	N-CA-C	-5.11	105.71	111.28
10	j	71	THR	N-CA-CB	5.11	117.63	110.12
21	N	158	LEU	CA-C-N	5.11	127.39	120.44
21	N	158	LEU	C-N-CA	5.11	127.39	120.44
21	N	859	ASN	OD1-CG-ND2	5.11	127.71	122.60
27	O	273	GLN	CA-C-N	5.11	127.67	120.42
27	O	273	GLN	C-N-CA	5.11	127.67	120.42
21	N	123	PHE	CD1-CG-CD2	-5.11	110.94	118.60
22	S	45	THR	CA-C-O	-5.11	116.25	121.87
23	P	98	GLN	O-C-N	-5.11	116.71	122.12
28	H	409	ARG	CB-CA-C	-5.11	102.32	110.79
31	L	88	TYR	O-C-N	5.11	127.97	122.15
13	m	55	GLY	CA-C-O	-5.10	118.16	122.29
13	m	92	LEU	CA-C-N	5.10	128.95	120.94
13	m	92	LEU	C-N-CA	5.10	128.95	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	413	LYS	O-C-N	-5.10	115.99	122.27
26	U	293	GLU	CA-C-N	5.10	127.12	120.28
26	U	293	GLU	C-N-CA	5.10	127.12	120.28
32	M	422	VAL	CA-C-O	5.10	125.98	120.47
5	e	52	LYS	CB-CA-C	-5.10	102.18	110.85
6	f	146	GLU	N-CA-C	-5.10	100.58	108.90
14	n	131	THR	CA-C-O	-5.10	114.10	119.97
14	7	251	LYS	CA-C-O	5.10	125.94	120.38
17	T	19	ASP	N-CA-C	-5.10	100.58	108.90
23	P	183	GLN	OE1-CD-NE2	5.10	127.70	122.60
23	P	311	TRP	O-C-N	-5.10	115.91	120.71
26	U	115	GLN	OE1-CD-NE2	-5.10	117.50	122.60
29	I	227	THR	N-CA-C	-5.10	107.09	113.72
30	K	359	LYS	CA-C-O	-5.10	115.44	120.70
7	g	14	VAL	CA-C-O	-5.10	116.48	121.58
7	g	40	ILE	O-C-N	-5.10	117.13	123.10
26	U	258	SER	N-CA-CB	5.10	117.62	110.12
2	b	241	GLN	CA-C-N	5.10	127.11	120.28
2	b	241	GLN	C-N-CA	5.10	127.11	120.28
7	g	25	GLU	O-C-N	5.10	127.53	122.12
8	1	121	THR	CA-C-O	-5.10	115.14	121.06
13	6	157	PHE	N-CA-C	-5.10	105.42	111.69
17	T	109	TYR	CA-C-N	5.10	127.53	120.29
17	T	109	TYR	C-N-CA	5.10	127.53	120.29
21	N	342	GLY	CA-C-O	-5.10	113.97	119.27
21	N	436	ASP	CB-CA-C	-5.10	100.20	109.38
25	R	345	TYR	CA-C-O	-5.10	115.14	121.11
26	U	130	VAL	N-CA-C	-5.10	105.56	113.16
26	U	237	PRO	N-CA-CB	5.10	107.86	103.27
29	I	256	TYR	O-C-N	-5.10	117.27	123.03
2	b	190	HIS	CE1-NE2-CD2	-5.10	103.90	109.00
9	i	244	GLU	N-CA-C	-5.10	100.73	109.24
10	j	61	THR	CA-C-N	5.10	127.07	120.44
10	j	61	THR	C-N-CA	5.10	127.07	120.44
9	2	107	SER	CA-C-O	-5.10	115.02	120.42
14	7	193	ASP	N-CA-CB	5.10	117.79	110.20
20	Z	218	GLU	CA-C-N	5.10	127.36	120.38
20	Z	218	GLU	C-N-CA	5.10	127.36	120.38
21	N	33	ASP	N-CA-CB	5.10	118.24	110.44
21	N	145	LEU	N-CA-CB	5.10	118.71	110.40
21	N	597	ARG	CD-NE-CZ	-5.10	117.26	124.40
21	N	615	ALA	CA-C-O	5.10	125.82	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	215	VAL	CA-C-N	5.10	127.11	120.28
24	Q	215	VAL	C-N-CA	5.10	127.11	120.28
24	Q	265	MET	CA-C-N	5.10	127.53	120.29
24	Q	265	MET	C-N-CA	5.10	127.53	120.29
30	K	204	ASP	O-C-N	-5.10	115.92	121.53
3	c	96	GLN	CA-C-N	5.10	127.11	120.28
3	c	96	GLN	C-N-CA	5.10	127.11	120.28
3	c	225	VAL	CA-C-N	5.10	130.35	123.11
3	c	225	VAL	C-N-CA	5.10	130.35	123.11
12	l	135	GLY	CA-C-N	5.10	127.37	120.44
12	l	135	GLY	C-N-CA	5.10	127.37	120.44
21	N	598	ASP	CB-CA-C	-5.10	103.92	111.72
22	S	23	LYS	CA-C-N	5.10	127.11	120.28
22	S	23	LYS	C-N-CA	5.10	127.11	120.28
24	Q	111	LEU	N-CA-CB	5.10	118.09	109.78
4	d	5	ASP	N-CA-C	-5.09	99.95	110.80
11	k	38	LEU	CB-CA-C	-5.09	102.23	110.79
9	2	199	GLY	CA-C-O	-5.09	116.63	121.83
15	W	46	GLU	N-CA-C	-5.09	107.11	113.38
25	R	193	ALA	CA-C-N	5.09	126.98	120.56
25	R	193	ALA	C-N-CA	5.09	126.98	120.56
29	I	153	THR	CA-C-N	5.09	128.58	121.24
29	I	153	THR	C-N-CA	5.09	128.58	121.24
30	K	200	GLN	CB-CA-C	-5.09	102.85	110.90
33	J	374	ARG	N-CA-C	-5.09	99.37	108.13
6	f	175	THR	CA-C-N	5.09	127.42	120.54
6	f	175	THR	C-N-CA	5.09	127.42	120.54
7	g	62	GLN	OE1-CD-NE2	5.09	127.69	122.60
12	l	187	ILE	N-CA-CB	5.09	119.79	111.44
9	2	173	GLN	CB-CG-CD	5.09	121.26	112.60
19	Y	74	THR	N-CA-C	5.09	116.52	111.07
29	I	393	GLN	N-CA-C	-5.09	105.81	111.36
8	h	84	THR	N-CA-CB	5.09	117.39	110.01
9	i	190	ALA	CA-C-N	5.09	131.39	121.41
9	i	190	ALA	C-N-CA	5.09	131.39	121.41
8	l	44	THR	N-CA-C	-5.09	100.60	108.90
17	T	232	LYS	CG-CD-CE	5.09	123.01	111.30
22	S	171	TYR	CA-C-N	5.09	131.26	121.54
22	S	171	TYR	C-N-CA	5.09	131.26	121.54
8	h	115	ASN	N-CA-CB	5.09	119.09	110.49
10	j	104	PHE	CB-CG-CD2	5.09	129.35	120.70
10	j	196	VAL	CA-C-O	-5.09	114.92	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	60	THR	N-CA-C	-5.09	106.31	112.88
7	G	82	ILE	CA-C-O	-5.09	115.28	118.69
27	O	68	LYS	CB-CG-CD	5.09	123.00	111.30
27	O	175	ASN	N-CA-CB	5.09	117.69	110.16
28	H	396	MET	CB-CA-C	5.09	117.93	109.53
32	M	405	ASN	N-CA-C	-5.09	105.92	111.82
5	e	26	TYR	N-CA-C	5.09	116.83	111.28
13	6	182	TYR	CB-CA-C	-5.09	101.27	109.72
23	P	400	VAL	CA-C-N	-5.09	115.24	123.23
23	P	400	VAL	C-N-CA	-5.09	115.24	123.23
12	l	150	SER	CA-C-O	-5.09	116.02	121.56
7	G	206	ASP	N-CA-C	-5.09	106.48	113.30
12	5	196	ARG	CG-CD-NE	-5.09	100.81	112.00
13	6	101	ILE	CA-C-O	-5.09	115.66	120.95
22	S	363	THR	CA-CB-OG1	5.09	117.23	109.60
32	M	73	ARG	NE-CZ-NH2	-5.09	114.62	119.20
2	b	64	VAL	O-C-N	5.08	128.75	123.26
10	j	35	GLY	O-C-N	5.08	127.36	122.99
27	O	229	ASN	CA-C-O	-5.08	114.84	120.33
4	d	101	GLU	N-CA-CB	5.08	119.08	110.49
14	n	89	ASP	N-CA-CB	5.08	117.73	110.06
9	2	214	GLU	O-C-N	5.08	129.53	123.13
16	V	69	PHE	CB-CA-C	5.08	120.77	109.94
20	Z	476	ASP	CA-C-N	5.08	127.51	120.29
20	Z	476	ASP	C-N-CA	5.08	127.51	120.29
21	N	56	SER	CA-C-N	5.08	130.91	122.73
21	N	56	SER	C-N-CA	5.08	130.91	122.73
22	S	367	TYR	CB-CG-CD1	-5.08	113.17	120.80
26	U	147	GLY	CA-C-N	5.08	129.83	121.39
26	U	147	GLY	C-N-CA	5.08	129.83	121.39
29	I	67	ASP	N-CA-CB	5.08	117.69	110.16
4	d	122	GLN	CB-CG-CD	-5.08	103.96	112.60
12	l	86	GLY	N-CA-C	-5.08	101.14	113.18
9	2	185	SER	N-CA-CB	5.08	117.68	110.16
10	3	103	TYR	CB-CG-CD1	5.08	128.42	120.80
13	6	46	ARG	N-CA-C	-5.08	107.25	113.50
20	Z	211	PHE	CA-C-N	5.08	127.05	120.44
20	Z	211	PHE	C-N-CA	5.08	127.05	120.44
22	S	432	ILE	N-CA-C	-5.08	104.63	111.44
24	Q	130	ARG	CA-C-N	5.08	128.50	120.47
24	Q	130	ARG	C-N-CA	5.08	128.50	120.47
31	L	409	HIS	CA-C-O	-5.08	114.89	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	32	CYS	O-C-N	-5.08	117.33	123.27
17	T	220	PHE	CA-C-N	5.08	127.09	120.28
17	T	220	PHE	C-N-CA	5.08	127.09	120.28
19	Y	50	LYS	N-CA-C	-5.08	105.45	113.02
22	S	22	GLU	CA-C-N	5.08	127.50	120.29
22	S	22	GLU	C-N-CA	5.08	127.50	120.29
33	J	68	PRO	N-CD-CG	5.08	110.82	103.20
11	k	148	TYR	CA-C-O	-5.08	116.17	121.55
13	m	142	GLU	N-CA-CB	5.08	120.39	111.55
14	7	229	SER	N-CA-C	-5.08	101.12	109.40
20	Z	29	ASP	CA-C-N	5.08	127.40	120.54
20	Z	29	ASP	C-N-CA	5.08	127.40	120.54
20	Z	351	PRO	N-CA-C	-5.08	108.88	114.92
24	Q	208	ILE	CA-C-N	5.08	130.75	122.67
24	Q	208	ILE	C-N-CA	5.08	130.75	122.67
25	R	361	VAL	CA-C-N	5.08	127.08	120.28
25	R	361	VAL	C-N-CA	5.08	127.08	120.28
11	k	136	SER	CB-CA-C	5.08	119.48	110.85
11	k	150	PRO	N-CA-C	-5.08	106.92	113.57
12	l	274	LYS	CA-C-N	5.08	129.02	120.29
12	l	274	LYS	C-N-CA	5.08	129.02	120.29
16	V	250	GLN	N-CA-CB	5.08	117.58	110.12
31	L	72	ASP	O-C-N	5.08	127.30	122.07
33	J	317	PRO	N-CA-CB	5.08	106.03	103.19
10	j	93	SER	CA-C-O	-5.08	115.04	120.42
14	7	150	ALA	N-CA-CB	5.08	120.31	111.13
21	N	304	LEU	N-CA-CB	5.08	117.67	110.16
21	N	590	ALA	O-C-N	5.08	127.94	122.15
28	H	370	ARG	N-CA-C	-5.08	105.45	111.69
1	a	237	SER	CA-C-O	-5.07	116.20	121.99
6	f	178	THR	N-CA-CB	5.07	117.34	109.98
10	j	138	VAL	CA-CB-CG1	-5.07	101.77	110.40
12	l	77	THR	CA-C-N	5.07	130.55	122.74
12	l	77	THR	C-N-CA	5.07	130.55	122.74
11	4	89	ALA	CA-C-N	5.07	127.04	120.44
11	4	89	ALA	C-N-CA	5.07	127.04	120.44
19	Y	12	SER	N-CA-C	5.07	116.81	111.28
23	P	138	ARG	CA-C-O	5.07	126.15	120.82
29	I	234	LYS	N-CA-C	5.07	116.50	111.07
29	I	291	ARG	NE-CZ-NH1	-5.07	116.43	121.50
32	M	44	PHE	CA-CB-CG	5.07	118.87	113.80
32	M	139	LYS	N-CA-C	-5.07	106.26	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	48	PHE	N-CA-CB	5.07	118.89	110.63
13	m	56	ASP	CB-CA-C	5.07	118.93	111.73
11	4	49	GLU	O-C-N	5.07	128.62	122.94
22	S	207	ASN	CA-CB-CG	-5.07	107.53	112.60
26	U	244	ASP	N-CA-C	-5.07	105.83	111.36
32	M	428	LYS	N-CA-C	-5.07	104.56	111.56
12	l	78	THR	CA-C-O	5.07	125.95	120.32
1	A	36	ASN	N-CA-C	-5.07	106.51	113.30
21	N	839	ARG	O-C-N	5.07	130.01	122.81
29	I	409	MET	CG-SD-CE	-5.07	89.75	100.90
31	L	190	ILE	N-CA-C	-5.07	105.60	110.72
31	L	266	MET	CA-C-N	5.07	127.49	120.29
31	L	266	MET	C-N-CA	5.07	127.49	120.29
1	a	25	LEU	CB-CA-C	-5.07	104.03	111.23
2	b	149	GLN	OE1-CD-NE2	5.07	127.67	122.60
4	d	35	GLY	N-CA-C	-5.07	101.17	113.18
9	i	228	LYS	CA-C-N	5.07	127.58	120.28
9	i	228	LYS	C-N-CA	5.07	127.58	120.28
12	5	287	GLY	N-CA-C	-5.07	98.61	113.30
13	6	95	ASN	N-CA-C	5.07	116.80	111.28
14	7	250	MET	CG-SD-CE	-5.07	89.75	100.90
25	R	283	THR	CA-C-O	5.07	126.49	120.66
28	H	120	ASN	CA-CB-CG	5.07	117.67	112.60
28	H	211	VAL	O-C-N	-5.07	117.41	123.03
1	a	230	LYS	N-CA-CB	5.07	117.51	109.71
5	e	36	THR	CA-C-O	-5.07	116.12	120.88
7	g	230	PHE	CA-C-N	5.07	129.31	122.93
7	g	230	PHE	C-N-CA	5.07	129.31	122.93
8	h	70	TYR	CA-C-N	5.07	127.07	120.28
8	h	70	TYR	C-N-CA	5.07	127.07	120.28
9	2	230	LYS	CA-C-O	-5.07	115.68	121.40
12	5	133	TRP	CG-CD2-CE3	-5.07	128.84	133.90
15	W	174	VAL	O-C-N	5.07	128.67	123.20
17	T	164	LEU	O-C-N	5.07	128.15	122.22
20	Z	736	LEU	N-CA-C	-5.07	105.76	111.28
25	R	237	THR	N-CA-C	-5.07	99.00	108.02
31	L	156	MET	CA-C-N	5.07	130.89	121.62
31	L	156	MET	C-N-CA	5.07	130.89	121.62
31	L	214	PRO	CA-C-O	-5.07	113.22	120.56
31	L	307	GLU	CB-CG-CD	5.07	121.21	112.60
2	b	204	PHE	O-C-N	5.06	127.87	122.05
13	m	226	GLU	N-CA-C	-5.06	103.36	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	91	PHE	N-CA-CB	5.06	117.52	109.82
13	6	213	LEU	N-CA-C	-5.06	100.92	109.07
19	Y	56	GLN	CA-C-N	5.06	131.15	122.09
19	Y	56	GLN	C-N-CA	5.06	131.15	122.09
27	O	391	ILE	CA-CB-CG2	-5.06	101.89	110.50
2	b	169	VAL	N-CA-C	5.06	115.78	110.62
5	e	82	THR	O-C-N	-5.06	116.01	122.34
7	g	26	TYR	CB-CA-C	-5.06	102.39	110.79
10	j	198	ARG	CD-NE-CZ	-5.06	117.31	124.40
12	l	271	LEU	CA-C-N	5.06	127.02	120.44
12	l	271	LEU	C-N-CA	5.06	127.02	120.44
13	6	24	ALA	N-CA-CB	5.06	118.87	110.52
14	7	211	VAL	CA-C-N	5.06	127.37	120.54
14	7	211	VAL	C-N-CA	5.06	127.37	120.54
21	N	236	GLY	CA-C-N	5.06	127.57	120.28
21	N	236	GLY	C-N-CA	5.06	127.57	120.28
22	S	91	ASN	OD1-CG-ND2	5.06	127.66	122.60
22	S	100	HIS	ND1-CE1-NE2	5.06	113.46	108.40
24	Q	188	LEU	CA-C-N	5.06	131.72	123.93
24	Q	188	LEU	C-N-CA	5.06	131.72	123.93
24	Q	345	SER	CA-C-O	-5.06	115.05	120.42
25	R	328	PHE	O-C-N	-5.06	116.75	122.12
26	U	288	PHE	CA-CB-CG	-5.06	108.74	113.80
30	K	339	GLU	N-CA-CB	5.06	118.51	110.16
2	b	70	ASP	CA-C-O	5.06	124.47	118.90
7	g	171	SER	O-C-N	5.06	127.92	122.15
10	j	87	PHE	N-CA-C	5.06	116.88	111.36
21	N	767	ALA	O-C-N	5.06	129.29	123.17
22	S	457	PRO	N-CA-C	5.06	120.42	113.84
23	P	210	ASN	CA-C-N	5.06	126.07	120.45
23	P	210	ASN	C-N-CA	5.06	126.07	120.45
5	e	17	PRO	N-CA-CB	5.06	108.17	103.41
12	l	223	LEU	O-C-N	-5.06	117.65	123.42
13	m	156	PRO	CA-C-O	-5.06	112.13	118.86
13	6	175	LYS	O-C-N	5.06	129.54	122.36
19	Y	56	GLN	O-C-N	-5.06	116.23	122.20
21	N	599	TYR	CA-C-O	5.06	125.20	119.18
21	N	661	SER	CB-CA-C	-5.06	100.95	110.67
23	P	99	LYS	CA-C-N	5.06	128.60	120.30
23	P	99	LYS	C-N-CA	5.06	128.60	120.30
23	P	376	THR	CA-C-O	-5.06	115.51	120.82
28	H	131	GLN	CA-C-N	5.06	130.13	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	H	131	GLN	C-N-CA	5.06	130.13	123.05
1	a	62	LYS	CA-CB-CG	-5.06	103.99	114.10
12	l	200	ASP	N-CA-C	-5.06	107.06	113.18
14	n	186	PRO	CA-C-N	5.06	127.32	120.44
14	n	186	PRO	C-N-CA	5.06	127.32	120.44
12	5	164	GLN	N-CA-C	-5.06	105.77	111.28
22	S	164	ILE	CB-CA-C	-5.06	107.38	114.00
24	Q	203	THR	O-C-N	5.06	128.49	122.27
31	L	181	ASP	CA-CB-CG	5.06	117.66	112.60
9	i	176	THR	N-CA-CB	5.06	117.67	110.44
9	2	79	ALA	N-CA-C	5.06	118.71	112.54
18	X	55	LYS	N-CA-CB	5.06	119.37	110.37
24	Q	252	HIS	CB-CA-C	-5.06	102.56	109.28
24	Q	298	ALA	N-CA-CB	5.06	117.55	110.12
27	O	34	GLU	N-CA-C	5.06	116.79	111.28
3	c	28	SER	CA-C-N	5.05	128.93	120.64
3	c	28	SER	C-N-CA	5.05	128.93	120.64
1	A	226	GLY	N-CA-C	-5.05	102.61	111.46
9	2	99	THR	N-CA-C	-5.05	107.28	113.50
13	6	139	TYR	CA-C-O	5.05	127.11	121.40
16	V	40	HIS	CE1-NE2-CD2	-5.05	103.94	109.00
16	V	76	THR	CA-CB-CG2	-5.05	101.91	110.50
19	Y	16	LEU	CA-C-O	5.05	127.17	121.51
26	U	107	ASN	CA-CB-CG	5.05	117.65	112.60
26	U	173	HIS	CB-CA-C	-5.05	102.94	110.88
27	O	150	LEU	CA-C-O	-5.05	115.19	120.55
33	J	219	VAL	N-CA-C	5.05	115.82	110.72
11	k	101	ASN	N-CA-C	-5.05	100.94	109.07
9	2	218	ASN	CA-C-N	5.05	127.05	120.28
9	2	218	ASN	C-N-CA	5.05	127.05	120.28
23	P	327	LEU	N-CA-C	-5.05	105.15	111.92
1	a	199	TRP	CA-C-N	5.05	127.99	120.31
1	a	199	TRP	C-N-CA	5.05	127.99	120.31
12	l	148	ARG	CA-C-N	5.05	130.58	122.50
12	l	148	ARG	C-N-CA	5.05	130.58	122.50
23	P	247	THR	N-CA-CB	5.05	117.46	109.83
24	Q	420	ASN	OD1-CG-ND2	5.05	127.65	122.60
26	U	269	THR	CA-CB-OG1	5.05	117.18	109.60
28	H	455	LYS	CA-C-N	5.05	127.05	120.28
28	H	455	LYS	C-N-CA	5.05	127.05	120.28
30	K	260	LEU	CA-C-N	5.05	127.01	120.44
30	K	260	LEU	C-N-CA	5.05	127.01	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	M	23	LEU	CB-CA-C	-5.05	102.26	110.85
7	g	137	ILE	N-CA-C	-5.05	100.30	107.77
9	i	115	HIS	CE1-NE2-CD2	-5.05	103.95	109.00
2	B	154	GLY	N-CA-C	-5.05	107.73	116.01
11	4	71	GLU	N-CA-C	-5.05	106.53	113.30
18	X	9	LYS	CB-CA-C	-5.05	100.29	109.38
25	R	51	LEU	N-CA-C	-5.05	105.86	111.36
25	R	289	ILE	CA-CB-CG1	5.05	118.98	110.40
30	K	76	LYS	CA-C-O	-5.05	115.07	120.42
30	K	262	ARG	CA-C-O	5.05	126.12	120.82
31	L	299	ARG	NE-CZ-NH2	-5.05	114.66	119.20
13	6	216	THR	N-CA-C	-5.05	101.77	108.74
22	S	343	LEU	CA-C-O	-5.05	113.94	118.79
22	S	361	THR	CB-CA-C	5.05	118.88	110.90
3	c	154	SER	O-C-N	-5.05	116.03	122.34
6	F	66	CYS	N-CA-C	-5.05	107.67	113.88
10	3	105	VAL	N-CA-CB	-5.05	106.80	112.45
12	5	104	GLN	O-C-N	-5.05	116.14	122.35
14	7	182	HIS	CA-CB-CG	5.05	118.85	113.80
14	7	252	TRP	CZ3-CH2-CZ2	-5.05	114.94	121.50
20	Z	719	GLY	CA-C-N	5.05	127.00	120.44
20	Z	719	GLY	C-N-CA	5.05	127.00	120.44
21	N	138	GLU	CB-CA-C	-5.05	99.44	109.99
21	N	307	LYS	O-C-N	-5.05	116.81	122.97
27	O	268	SER	CA-C-N	5.05	127.00	120.44
27	O	268	SER	C-N-CA	5.05	127.00	120.44
28	H	298	ALA	CA-C-N	5.05	127.04	120.28
28	H	298	ALA	C-N-CA	5.05	127.04	120.28
30	K	203	ILE	CA-CB-CG1	5.05	118.98	110.40
31	L	351	LEU	O-C-N	-5.05	115.52	121.32
4	d	189	GLU	N-CA-C	5.04	116.78	111.28
9	i	188	ILE	CA-CB-CG1	5.04	118.98	110.40
10	j	16	THR	N-CA-CB	5.04	118.43	110.56
10	j	162	ASP	CA-C-N	5.04	127.04	120.28
10	j	162	ASP	C-N-CA	5.04	127.04	120.28
15	W	165	GLN	CB-CG-CD	-5.04	104.02	112.60
15	W	175	THR	CA-C-O	-5.04	115.20	120.70
23	P	405	PRO	CA-N-CD	-5.04	104.94	112.00
28	H	227	LEU	N-CA-CB	5.04	118.25	110.43
1	a	206	ALA	CA-C-N	5.04	127.37	120.46
1	a	206	ALA	C-N-CA	5.04	127.37	120.46
3	c	177	GLN	CB-CA-C	-5.04	102.42	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	151	PHE	O-C-N	-5.04	116.70	122.95
13	m	70	ASP	N-CA-CB	5.04	117.32	110.01
9	2	176	THR	CA-C-O	-5.04	115.99	121.89
10	3	101	GLY	CA-C-O	-5.04	114.31	121.52
13	6	170	PRO	CA-C-O	-5.04	115.43	121.48
13	6	173	ASN	N-CA-CB	5.04	119.75	112.13
16	V	109	HIS	ND1-CE1-NE2	5.04	113.44	108.40
23	P	172	GLU	N-CA-C	-5.04	102.60	110.42
23	P	236	GLU	O-C-N	5.04	127.47	122.12
26	U	42	ASN	CA-CB-CG	-5.04	107.56	112.60
27	O	358	ILE	O-C-N	5.04	127.92	123.03
28	H	422	VAL	O-C-N	5.04	126.83	121.89
29	I	120	VAL	CA-CB-CG2	5.04	118.97	110.40
1	a	118	ALA	N-CA-CB	5.04	117.62	110.16
10	j	34	LEU	CB-CA-C	5.04	117.95	109.89
14	7	241	PHE	CB-CG-CD1	5.04	129.27	120.70
17	T	29	PRO	N-CD-CG	5.04	110.76	103.20
20	Z	238	ASP	CA-C-N	5.04	127.35	120.54
20	Z	238	ASP	C-N-CA	5.04	127.35	120.54
21	N	503	THR	O-C-N	5.04	127.90	122.15
22	S	65	ASN	CA-C-O	-5.04	115.20	120.55
22	S	261	HIS	CE1-NE2-CD2	-5.04	103.96	109.00
22	S	484	ASP	CA-C-N	5.04	127.45	120.29
22	S	484	ASP	C-N-CA	5.04	127.45	120.29
30	K	274	VAL	N-CA-CB	5.04	119.55	111.23
13	6	163	ASN	CA-CB-CG	-5.04	107.56	112.60
1	a	30	TYR	N-CA-C	-5.04	105.92	111.71
8	h	41	ASP	CB-CA-C	5.04	118.35	110.19
12	l	168	ALA	N-CA-CB	-5.04	103.05	111.06
14	n	54	ILE	O-C-N	-5.04	117.74	123.03
21	N	498	ILE	O-C-N	5.04	127.02	121.83
23	P	43	GLU	CA-C-N	5.04	130.74	123.13
23	P	43	GLU	C-N-CA	5.04	130.74	123.13
31	L	82	ARG	NE-CZ-NH2	-5.04	114.67	119.20
31	L	264	ARG	O-C-N	-5.04	116.41	122.15
32	M	162	GLU	O-C-N	5.04	128.58	122.94
25	R	155	GLY	N-CA-C	-5.04	106.32	112.77
26	U	190	LEU	N-CA-CB	5.04	117.70	110.20
1	a	31	ALA	CB-CA-C	-5.04	101.00	110.67
6	f	129	GLY	N-CA-C	-5.04	106.93	115.34
9	i	129	VAL	N-CA-C	-5.04	101.06	108.11
8	1	71	HIS	CA-CB-CG	5.04	118.83	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	114	LYS	CG-CD-CE	5.04	122.88	111.30
14	7	47	MET	N-CA-C	-5.04	101.08	108.79
23	P	84	LYS	CB-CA-C	-5.04	102.97	110.88
25	R	203	ASP	CA-CB-CG	-5.04	107.56	112.60
29	I	309	LEU	CA-C-O	-5.04	115.08	120.42
30	K	126	LEU	CA-C-O	-5.04	115.47	121.16
30	K	349	ARG	CA-C-N	5.04	127.53	120.28
30	K	349	ARG	C-N-CA	5.04	127.53	120.28
3	c	70	ASN	N-CA-C	-5.03	101.79	108.74
10	j	45	HIS	ND1-CE1-NE2	5.03	113.43	108.40
10	3	167	ILE	CA-C-N	5.03	127.44	120.29
10	3	167	ILE	C-N-CA	5.03	127.44	120.29
14	7	213	ALA	O-C-N	5.03	127.25	122.07
22	S	261	HIS	N-CA-C	-5.03	105.52	113.02
25	R	199	GLU	N-CA-C	-5.03	107.19	113.38
1	a	130	GLN	CA-C-O	5.03	124.93	119.24
14	n	158	GLN	OE1-CD-NE2	5.03	127.63	122.60
14	n	244	ASN	N-CA-CB	5.03	119.73	112.13
8	1	15	VAL	N-CA-C	-5.03	101.38	108.27
14	7	243	LYS	CA-C-O	5.03	126.14	120.70
22	S	112	ASN	O-C-N	-5.03	117.15	123.04
5	e	136	ARG	CA-C-O	5.03	125.13	120.50
8	h	94	LEU	CA-C-N	5.03	127.96	120.31
8	h	94	LEU	C-N-CA	5.03	127.96	120.31
13	m	217	LYS	CB-CG-CD	5.03	122.87	111.30
9	2	85	THR	CA-C-N	5.03	126.98	120.44
9	2	85	THR	C-N-CA	5.03	126.98	120.44
11	4	171	ARG	NE-CZ-NH1	5.03	126.53	121.50
17	T	200	LEU	O-C-N	5.03	127.22	121.94
21	N	6	ALA	N-CA-C	-5.03	107.14	113.28
21	N	156	ILE	CA-C-O	-5.03	114.82	120.25
24	Q	113	ASP	CA-C-O	-5.03	115.22	120.55
24	Q	334	HIS	CB-CG-CD2	-5.03	124.66	131.20
27	O	373	TRP	CG-CD2-CE3	-5.03	128.87	133.90
29	I	96	LEU	N-CA-CB	-5.03	102.71	110.16
4	d	119	ARG	CB-CA-C	-5.03	102.44	110.79
4	D	77	GLY	N-CA-C	-5.03	106.48	111.56
13	6	132	SER	N-CA-CB	5.03	119.26	110.81
22	S	82	TYR	CA-C-O	-5.03	114.17	119.50
24	Q	338	LEU	CA-C-N	5.03	127.33	120.54
24	Q	338	LEU	C-N-CA	5.03	127.33	120.54
25	R	72	VAL	N-CA-CB	5.03	119.53	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	K	161	MET	N-CA-C	-5.03	106.99	113.23
3	c	141	ASP	CA-CB-CG	5.03	117.63	112.60
5	e	67	ILE	N-CA-C	-5.03	101.13	108.17
14	n	193	ASP	CA-C-N	5.03	130.11	121.87
14	n	193	ASP	C-N-CA	5.03	130.11	121.87
8	l	152	ARG	N-CA-C	-5.03	101.56	109.50
21	N	568	VAL	CA-C-O	-5.03	115.47	121.05
22	S	343	LEU	CA-C-N	5.03	125.30	119.47
22	S	343	LEU	C-N-CA	5.03	125.30	119.47
22	S	481	TYR	N-CA-C	5.03	119.79	113.25
24	Q	275	ILE	N-CA-C	-5.03	108.22	113.10
26	U	274	MET	CG-SD-CE	-5.03	89.84	100.90
33	J	213	VAL	N-CA-CB	5.03	119.53	111.23
1	a	19	PHE	N-CA-CB	5.03	117.36	109.97
1	a	173	PRO	O-C-N	5.03	129.06	122.27
3	c	16	GLU	CB-CA-C	-5.03	99.95	109.95
9	i	153	TYR	CA-C-O	5.03	126.99	120.21
12	5	121	ALA	N-CA-C	-5.03	101.65	109.14
20	Z	224	LEU	CA-C-N	5.03	127.32	120.54
20	Z	224	LEU	C-N-CA	5.03	127.32	120.54
20	Z	623	ARG	CA-C-N	5.03	127.02	120.28
20	Z	623	ARG	C-N-CA	5.03	127.02	120.28
22	S	446	THR	N-CA-C	-5.03	106.57	113.30
23	P	220	TYR	CB-CG-CD2	-5.03	113.26	120.80
33	J	240	HIS	CE1-NE2-CD2	-5.03	103.97	109.00
23	P	414	GLU	CA-C-N	5.02	127.01	120.28
23	P	414	GLU	C-N-CA	5.02	127.01	120.28
6	f	153	VAL	N-CA-CB	5.02	118.08	111.25
15	W	34	GLU	CB-CA-C	-5.02	102.45	110.79
16	V	117	TRP	CG-CD2-CE3	-5.02	128.88	133.90
16	V	280	LEU	CB-CA-C	-5.02	102.45	110.79
19	Y	21	ASN	CA-C-N	5.02	127.42	120.29
19	Y	21	ASN	C-N-CA	5.02	127.42	120.29
21	N	25	LEU	CA-C-O	-5.02	115.23	120.55
21	N	803	VAL	CA-C-N	5.02	127.42	120.29
21	N	803	VAL	C-N-CA	5.02	127.42	120.29
11	4	66	LEU	N-CA-C	-5.02	105.70	111.07
13	6	104	LEU	CA-C-N	5.02	127.28	120.65
13	6	104	LEU	C-N-CA	5.02	127.28	120.65
17	T	214	GLU	N-CA-C	-5.02	105.89	111.36
24	Q	80	HIS	CB-CG-CD2	-5.02	124.67	131.20
25	R	112	GLU	CA-C-N	5.02	127.01	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	112	GLU	C-N-CA	5.02	127.01	120.28
3	c	14	SER	N-CA-C	-5.02	104.36	110.13
14	n	232	ILE	N-CA-C	-5.02	100.89	108.12
8	1	105	GLY	N-CA-C	-5.02	101.28	113.18
20	Z	491	LEU	N-CA-CB	5.02	117.59	110.16
24	Q	194	SER	CA-C-N	5.02	127.01	120.28
24	Q	194	SER	C-N-CA	5.02	127.01	120.28
26	U	141	GLU	CA-C-O	5.02	125.89	120.32
32	M	31	GLN	CB-CG-CD	-5.02	104.07	112.60
32	M	114	GLY	N-CA-C	-5.02	101.28	113.18
32	M	170	MET	N-CA-CB	5.02	117.29	110.01
33	J	200	ARG	CA-C-N	5.02	127.27	120.44
33	J	200	ARG	C-N-CA	5.02	127.27	120.44
14	7	208	GLU	O-C-N	5.02	127.24	122.07
19	Y	39	PRO	CB-CA-C	-5.02	104.73	111.85
29	I	286	ALA	CA-C-O	5.02	125.15	119.18
29	I	365	HIS	ND1-CE1-NE2	5.02	113.42	108.40
29	I	381	VAL	CA-C-N	5.02	127.26	120.44
29	I	381	VAL	C-N-CA	5.02	127.26	120.44
30	K	266	PRO	N-CA-CB	5.02	108.12	102.60
33	J	67	GLU	CA-C-O	-5.02	115.23	120.70
33	J	238	ARG	NE-CZ-NH1	5.02	126.52	121.50
33	J	300	LEU	CA-C-N	5.02	131.71	121.48
33	J	300	LEU	C-N-CA	5.02	131.71	121.48
7	g	93	ARG	CB-CG-CD	5.02	122.84	111.30
10	j	183	TRP	CB-CA-C	5.02	118.85	111.73
25	R	38	VAL	N-CA-C	-5.02	101.19	109.12
5	e	86	ARG	O-C-N	5.01	127.44	122.12
8	h	86	THR	CA-C-O	5.01	126.08	120.82
9	i	93	GLU	N-CA-C	5.01	116.83	111.36
11	k	6	GLY	CA-C-N	5.01	130.35	122.33
11	k	6	GLY	C-N-CA	5.01	130.35	122.33
14	n	79	GLY	O-C-N	-5.01	117.56	123.17
14	7	42	THR	N-CA-CB	5.01	120.04	111.66
19	Y	51	SER	CA-C-O	5.01	124.70	118.43
20	Z	800	SER	CA-C-N	5.01	127.31	120.54
20	Z	800	SER	C-N-CA	5.01	127.31	120.54
21	N	846	ILE	N-CA-C	-5.01	100.35	107.77
26	U	298	ASN	O-C-N	5.01	127.87	122.15
33	J	339	ARG	CB-CG-CD	5.01	122.83	111.30
3	c	143	ARG	NE-CZ-NH2	-5.01	114.69	119.20
23	P	97	ILE	CB-CA-C	5.01	119.14	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	156	ALA	N-CA-CB	5.01	117.49	110.12
24	Q	361	HIS	O-C-N	5.01	127.43	122.12
29	I	92	GLU	O-C-N	-5.01	116.68	122.09
32	M	352	PRO	CB-CA-C	5.01	117.65	111.23
4	d	242	GLU	CB-CA-C	-5.01	102.47	110.79
22	S	54	TRP	CB-CG-CD2	-5.01	119.78	126.80
23	P	263	HIS	CA-C-N	5.01	127.06	120.60
23	P	263	HIS	C-N-CA	5.01	127.06	120.60
25	R	227	ALA	CA-C-O	-5.01	115.54	120.70
25	R	323	ASN	CA-C-N	5.01	127.93	120.31
25	R	323	ASN	C-N-CA	5.01	127.93	120.31
33	J	16	GLU	CA-CB-CG	-5.01	104.08	114.10
13	m	24	ALA	N-CA-CB	5.01	117.71	109.95
15	W	28	ALA	CA-C-N	5.01	129.09	120.72
15	W	28	ALA	C-N-CA	5.01	129.09	120.72
16	V	144	ILE	N-CA-C	-5.01	108.41	113.47
17	T	170	ASN	N-CA-C	-5.01	105.23	113.50
21	N	794	LYS	CB-CA-C	5.01	119.37	110.85
22	S	366	LYS	CB-CA-C	-5.01	102.99	110.90
23	P	164	GLN	CA-C-O	5.01	125.34	119.28
24	Q	75	ARG	CA-C-N	5.01	126.99	120.28
24	Q	75	ARG	C-N-CA	5.01	126.99	120.28
28	H	210	ASP	CA-CB-CG	-5.01	107.59	112.60
28	H	411	CYS	CA-C-N	5.01	126.10	119.84
28	H	411	CYS	C-N-CA	5.01	126.10	119.84
29	I	155	SER	N-CA-C	-5.01	100.84	108.76
32	M	215	PRO	N-CA-CB	5.01	108.51	103.25
6	f	215	ILE	CB-CA-C	-5.01	103.41	110.82
9	2	193	TRP	CB-CG-CD1	5.01	134.41	126.90
13	6	151	ALA	O-C-N	5.01	127.23	122.07
20	Z	738	TYR	N-CA-C	-5.01	105.82	111.28
23	P	282	HIS	CB-CG-ND1	5.01	130.21	122.70
24	Q	391	ASP	CA-CB-CG	-5.01	107.59	112.60
4	d	141	ARG	CA-C-N	5.01	130.37	122.36
4	d	141	ARG	C-N-CA	5.01	130.37	122.36
9	i	251	ASP	CA-CB-CG	-5.01	107.59	112.60
9	2	211	LYS	N-CA-C	-5.01	101.68	109.14
10	3	163	LEU	N-CA-C	-5.01	106.01	111.82
15	W	99	LYS	N-CA-C	5.01	116.55	111.14
21	N	822	GLY	CA-C-N	5.01	124.50	119.19
21	N	822	GLY	C-N-CA	5.01	124.50	119.19
28	H	321	ASP	CA-C-N	5.01	128.06	122.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	H	321	ASP	C-N-CA	5.01	128.06	122.55
30	K	406	ASP	O-C-N	5.01	127.86	122.15
32	M	46	SER	CA-C-O	5.01	125.73	120.42
32	M	320	ARG	NE-CZ-NH2	5.01	123.70	119.20
10	j	3	ASP	CB-CA-C	5.00	116.40	108.84
4	d	108	TYR	CA-C-N	5.00	127.92	120.31
4	d	108	TYR	C-N-CA	5.00	127.92	120.31
9	i	198	SER	N-CA-C	-5.00	101.01	109.07
15	W	151	THR	CA-CB-OG1	5.00	117.11	109.60
17	T	56	MET	CA-C-N	5.00	127.52	120.42
17	T	56	MET	C-N-CA	5.00	127.52	120.42
21	N	716	GLN	O-C-N	5.00	129.07	123.27
24	Q	343	LEU	N-CA-CB	-5.00	102.75	110.16
29	I	89	GLN	CB-CG-CD	-5.00	104.09	112.60
30	K	342	SER	N-CA-CB	5.00	119.02	111.06
2	b	231	LYS	CB-CG-CD	5.00	122.80	111.30
12	l	246	SER	CA-C-N	5.00	127.78	122.63
12	l	246	SER	C-N-CA	5.00	127.78	122.63
14	n	160	LEU	N-CA-CB	5.00	118.70	110.90
10	3	204	GLN	CA-C-N	5.00	130.70	121.70
10	3	204	GLN	C-N-CA	5.00	130.70	121.70
16	V	147	VAL	CB-CA-C	-5.00	106.01	110.91
21	N	411	ILE	CA-C-N	5.00	130.78	122.73
21	N	411	ILE	C-N-CA	5.00	130.78	122.73
24	Q	147	GLN	CA-C-O	5.00	125.51	119.31
25	R	401	HIS	O-C-N	5.00	128.42	122.27
27	O	239	MET	CB-CA-C	5.00	117.47	109.07
28	H	234	ARG	CB-CA-C	-5.00	100.18	110.38
33	J	304	LEU	CA-C-N	5.00	131.09	121.54
33	J	304	LEU	C-N-CA	5.00	131.09	121.54

There are no chirality outliers.

All (351) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	104	ALA	Peptide
8	1	111	TYR	Sidechain
8	1	120	TYR	Sidechain
8	1	133	TYR	Sidechain
8	1	194	ARG	Sidechain
8	1	202	TYR	Sidechain
9	2	153	TYR	Sidechain

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Mol	Chain	Res	Type	Group
9	2	215	TYR	Sidechain
9	2	232	TYR	Sidechain
9	2	236	ARG	Sidechain
10	3	103	TYR	Sidechain
10	3	46	TYR	Sidechain
10	3	74	TYR	Sidechain
10	3	96	TYR	Sidechain
11	4	133	HIS	Sidechain
11	4	135	TYR	Sidechain
11	4	149	ARG	Sidechain
11	4	59	TYR	Sidechain
11	4	73	TYR	Sidechain
11	4	96	ARG	Sidechain
12	5	139	ARG	Sidechain
12	5	144	ARG	Sidechain
12	5	148	ARG	Sidechain
12	5	179	TYR	Sidechain
12	5	189	TYR	Sidechain
12	5	212	TYR	Sidechain
13	6	103	HIS	Sidechain
13	6	139	TYR	Sidechain
13	6	157	PHE	Sidechain
13	6	168	TYR	Sidechain
13	6	221	ARG	Sidechain
13	6	229	ARG	Sidechain,Peptide
13	6	36	ARG	Sidechain
13	6	83	TYR	Sidechain
14	7	128	TYR	Sidechain
14	7	162	TYR	Sidechain
14	7	219	TYR	Sidechain
14	7	261	TYR	Sidechain
14	7	63	TYR	Sidechain
4	D	90	ARG	Sidechain
6	F	18	ARG	Peptide
7	G	13	SER	Peptide
7	G	21	ASN	Peptide
28	H	173	ARG	Sidechain
28	H	181	TYR	Sidechain
28	H	266	ARG	Sidechain
28	H	271	PHE	Sidechain
28	H	292	ARG	Sidechain
28	H	318	ARG	Sidechain

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Mol	Chain	Res	Type	Group
28	H	319	PHE	Sidechain
28	H	344	ASP	Peptide
28	H	385	ARG	Sidechain
28	H	409	ARG	Sidechain
28	H	454	TYR	Sidechain
28	H	62	ARG	Sidechain
28	H	72	SER	Peptide
29	I	127	ASP	Peptide
29	I	135	PHE	Sidechain
29	I	208	TYR	Sidechain
29	I	223	GLY	Peptide
29	I	228	GLY	Mainchain
29	I	265	ARG	Sidechain
29	I	346	ARG	Sidechain
29	I	424	MET	Peptide
29	I	54	ARG	Sidechain
33	J	116	ARG	Sidechain
33	J	211	ILE	Mainchain
33	J	228	ARG	Sidechain
33	J	274	GLU	Peptide
33	J	296	ARG	Sidechain
33	J	309	ARG	Sidechain
33	J	339	ARG	Sidechain
33	J	344	ARG	Sidechain
33	J	368	TYR	Sidechain
33	J	373	ARG	Sidechain
33	J	374	ARG	Sidechain
33	J	56	ARG	Sidechain
33	J	63	ARG	Sidechain
33	J	71	TYR	Sidechain
33	J	94	TYR	Sidechain
30	K	118	TYR	Sidechain
30	K	128	ARG	Sidechain
30	K	167	PRO	Mainchain,Peptide
30	K	174	VAL	Peptide
30	K	176	GLY	Peptide
30	K	218	GLY	Mainchain
30	K	236	ARG	Peptide
30	K	246	TYR	Sidechain
30	K	258	PHE	Sidechain
30	K	259	ARG	Sidechain
30	K	262	ARG	Sidechain

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Mol	Chain	Res	Type	Group
30	K	303	MET	Peptide
30	K	311	ASN	Peptide
30	K	329	LEU	Peptide
30	K	400	TYR	Sidechain
30	K	411	TYR	Sidechain
30	K	58	TYR	Sidechain
30	K	77	ARG	Sidechain
31	L	132	ARG	Sidechain
31	L	137	ARG	Sidechain
31	L	168	TYR	Sidechain
31	L	185	GLY	Mainchain
31	L	194	ARG	Sidechain
31	L	255	TYR	Sidechain
31	L	261	ARG	Sidechain
31	L	269	TYR	Sidechain
31	L	289	ARG	Sidechain
31	L	290	ARG	Sidechain
31	L	321	THR	Peptide
31	L	341	GLY	Peptide
31	L	342	ARG	Peptide
31	L	345	ARG	Sidechain
31	L	350	PRO	Peptide
31	L	392	ARG	Sidechain
31	L	401	PHE	Sidechain
31	L	69	ARG	Sidechain
32	M	166	ARG	Sidechain
32	M	203	ARG	Sidechain
32	M	290	ARG	Sidechain
32	M	311	GLN	Mainchain
32	M	320	ARG	Sidechain
32	M	321	VAL	Peptide
32	M	329	ARG	Sidechain
32	M	339	ARG	Sidechain
32	M	342	ARG	Sidechain,Mainchain
32	M	364	HIS	Sidechain
32	M	425	ARG	Peptide
32	M	50	ARG	Sidechain
21	N	109	TYR	Sidechain
21	N	282	TYR	Sidechain
21	N	299	TYR	Sidechain
21	N	329	HIS	Sidechain
21	N	389	TYR	Sidechain

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Mol	Chain	Res	Type	Group
21	N	394	ARG	Sidechain
21	N	421	ASP	Sidechain
21	N	471	TYR	Sidechain
21	N	515	ARG	Sidechain
21	N	528	ARG	Sidechain
21	N	549	TYR	Sidechain
21	N	593	PHE	Sidechain
21	N	597	ARG	Sidechain
21	N	69	TYR	Sidechain
21	N	762	ARG	Sidechain
21	N	776	TYR	Sidechain
21	N	786	ARG	Sidechain
21	N	788	TYR	Sidechain
21	N	81	TYR	Sidechain
21	N	836	GLU	Peptide
21	N	861	TYR	Sidechain
21	N	866	TYR	Sidechain
21	N	88	ARG	Sidechain
21	N	921	ARG	Sidechain
27	O	115	ARG	Sidechain
27	O	137	TYR	Sidechain
27	O	181	PHE	Sidechain
27	O	189	TYR	Sidechain
27	O	58	ARG	Sidechain
27	O	62	TYR	Sidechain
27	O	69	PHE	Sidechain
27	O	70	TYR	Sidechain
27	O	92	PHE	Sidechain
23	P	110	LEU	Peptide
23	P	13	TYR	Sidechain
23	P	131	PHE	Sidechain
23	P	220	TYR	Sidechain
23	P	232	ARG	Sidechain
23	P	240	TYR	Sidechain
23	P	245	TYR	Sidechain
23	P	267	PHE	Sidechain
23	P	273	TYR	Sidechain
23	P	344	ARG	Sidechain
23	P	351	ARG	Sidechain
23	P	356	TYR	Sidechain
23	P	386	GLN	Peptide
23	P	390	TYR	Sidechain

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Mol	Chain	Res	Type	Group
23	P	402	PHE	Sidechain
23	P	95	TYR	Sidechain
24	Q	116	PHE	Sidechain
24	Q	127	ARG	Sidechain
24	Q	13	ARG	Sidechain
24	Q	146	TYR	Sidechain
24	Q	151	TYR	Sidechain
24	Q	20	TYR	Sidechain
24	Q	255	TYR	Sidechain
24	Q	291	TYR	Sidechain
24	Q	294	ARG	Sidechain
24	Q	306	TYR	Sidechain
24	Q	334	HIS	Sidechain
24	Q	409	TYR	Sidechain
24	Q	75	ARG	Sidechain
25	R	20	ARG	Sidechain
25	R	214	TYR	Sidechain
25	R	252	TYR	Sidechain
25	R	263	ARG	Sidechain
25	R	297	TYR	Sidechain
25	R	334	ARG	Sidechain
25	R	338	TYR	Sidechain
25	R	400	TYR	Sidechain
25	R	43	ARG	Sidechain
25	R	70	TYR	Peptide
25	R	81	HIS	Sidechain
22	S	111	ARG	Sidechain
22	S	186	TYR	Sidechain
22	S	196	ARG	Sidechain
22	S	25	TYR	Sidechain
22	S	273	PHE	Sidechain
22	S	333	PHE	Sidechain
22	S	345	TYR	Sidechain
22	S	346	TYR	Sidechain
22	S	382	ARG	Sidechain
22	S	425	ARG	Sidechain
22	S	442	PHE	Sidechain
22	S	475	TYR	Sidechain
22	S	480	ARG	Sidechain
22	S	51	ARG	Sidechain
22	S	52	TYR	Sidechain
22	S	55	ARG	Sidechain

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Mol	Chain	Res	Type	Group
22	S	82	TYR	Sidechain
22	S	95	PHE	Sidechain
17	T	177	PHE	Sidechain
17	T	20	TYR	Sidechain
17	T	211	PHE	Sidechain
17	T	234	TYR	Sidechain
17	T	251	HIS	Peptide
17	T	72	THR	Peptide
17	T	75	PHE	Sidechain
17	T	81	TYR	Sidechain
17	T	91	SER	Peptide
17	T	96	LEU	Peptide
26	U	176	ARG	Sidechain
26	U	189	ARG	Sidechain
26	U	277	TYR	Sidechain
26	U	283	ARG	Sidechain
26	U	32	ARG	Sidechain
26	U	72	TYR	Sidechain
16	V	110	SER	Peptide
16	V	230	TYR	Sidechain
16	V	251	TYR	Sidechain
16	V	273	ARG	Sidechain
16	V	28	TYR	Sidechain
16	V	42	ARG	Sidechain
15	W	101	ARG	Sidechain
15	W	109	ARG	Sidechain
15	W	179	ARG	Sidechain
15	W	182	TYR	Sidechain
15	W	23	ARG	Sidechain
15	W	25	ARG	Sidechain
15	W	37	PHE	Sidechain
18	X	27	ILE	Peptide
18	X	51	ARG	Sidechain
19	Y	86	ARG	Sidechain
20	Z	210	TYR	Sidechain
20	Z	248	TYR	Sidechain
20	Z	254	PRO	Mainchain
20	Z	269	TYR	Sidechain
20	Z	726	GLU	Mainchain
20	Z	727	GLU	Peptide
20	Z	728	LYS	Mainchain,Peptide
20	Z	738	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	a	105	ARG	Sidechain
1	a	128	TYR	Sidechain
1	a	131	ARG	Sidechain
1	a	143	PHE	Sidechain
1	a	155	TYR	Sidechain
1	a	166	TYR	Sidechain
1	a	218	PHE	Sidechain
1	a	30	TYR	Sidechain
1	a	46	ARG	Sidechain
2	b	234	ARG	Sidechain
2	b	97	TYR	Sidechain
2	b	99	ARG	Sidechain
3	c	13	PHE	Sidechain
3	c	137	TYR	Sidechain
3	c	143	ARG	Sidechain
3	c	144	TYR	Sidechain
3	c	4	ARG	Sidechain
4	d	11	PHE	Sidechain
4	d	127	ARG	Sidechain
4	d	197	ARG	Sidechain
4	d	22	TYR	Sidechain
4	d	254	HIS	Sidechain
5	e	132	ARG	Sidechain
5	e	167	TYR	Sidechain
5	e	231	TYR	Sidechain
6	f	123	TYR	Sidechain
6	f	164	ARG	Sidechain
6	f	18	ARG	Peptide
6	f	225	TYR	Sidechain
6	f	233	TYR	Sidechain
6	f	94	TYR	Sidechain
7	g	115	ARG	Sidechain
7	g	126	TYR	Sidechain
7	g	13	SER	Peptide
7	g	130	ARG	Sidechain
7	g	138	PHE	Sidechain
7	g	190	ARG	Sidechain
7	g	21	ASN	Peptide
7	g	230	PHE	Sidechain
7	g	242	PHE	Sidechain
7	g	78	TYR	Sidechain
7	g	8	TYR	Sidechain

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Mol	Chain	Res	Type	Group
7	g	86	ARG	Sidechain
8	h	111	TYR	Sidechain
8	h	133	TYR	Sidechain
8	h	146	TYR	Sidechain
8	h	34	TYR	Sidechain
8	h	38	ARG	Sidechain
8	h	70	TYR	Sidechain
8	h	75	TYR	Sidechain
8	h	96	TYR	Sidechain
9	i	117	PHE	Sidechain
9	i	153	TYR	Sidechain
9	i	217	ARG	Sidechain
9	i	234	PHE	Sidechain
9	i	236	ARG	Sidechain
9	i	98	TYR	Sidechain
10	j	103	TYR	Sidechain
10	j	124	PHE	Sidechain
10	j	154	TYR	Sidechain
10	j	199	TYR	Sidechain
11	k	130	TYR	Sidechain
11	k	190	ARG	Sidechain
11	k	59	TYR	Sidechain
11	k	67	TYR	Sidechain
12	l	165	TYR	Sidechain
12	l	179	TYR	Sidechain
12	l	189	TYR	Sidechain
12	l	245	TYR	Sidechain
12	l	262	TYR	Sidechain
13	m	114	TYR	Sidechain
13	m	13	TYR	Sidechain
13	m	131	TYR	Sidechain
13	m	168	TYR	Sidechain
13	m	193	ARG	Sidechain
13	m	41	TYR	Sidechain
14	n	117	GLU	Peptide
14	n	124	TYR	Sidechain
14	n	128	TYR	Sidechain
14	n	134	TYR	Sidechain
14	n	136	ARG	Sidechain
14	n	170	TYR	Sidechain
14	n	189	ARG	Sidechain
14	n	194	ARG	Sidechain

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Mol	Chain	Res	Type	Group
14	n	218	TYR	Sidechain
14	n	219	TYR	Sidechain
14	n	63	TYR	Sidechain
14	n	98	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1908	0	1901	0	0
1	a	1908	0	1901	0	0
2	B	1907	0	1917	0	0
2	b	1907	0	1917	2	0
3	C	1905	0	1901	0	0
3	c	1905	0	1901	6	0
4	D	1859	0	1875	0	0
4	d	1982	0	1993	8	0
5	E	1883	0	1851	21	0
5	e	1883	0	1851	10	0
6	F	1773	0	1775	2	0
6	f	1773	0	1775	5	0
7	G	1886	0	1876	1	0
7	g	1886	0	1876	3	0
8	1	1512	0	1478	4	0
8	h	1512	0	1478	3	0
9	2	1720	0	1716	2	0
9	i	1720	0	1716	3	0
10	3	1581	0	1571	2	0
10	j	1581	0	1571	5	0
11	4	1562	0	1569	8	0
11	k	1562	0	1569	4	0
12	5	1644	0	1592	1	0
12	l	1644	0	1592	5	0
13	6	1757	0	1708	8	0
13	m	1757	0	1708	5	0
14	7	1790	0	1790	5	0
14	n	1816	0	1818	4	0
15	W	1535	0	1542	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	V	2274	0	2273	9	0
17	T	2193	0	2161	5	0
18	X	1033	0	1017	2	0
19	Y	731	0	675	1	0
20	Z	7006	0	6932	194	0
21	N	7158	0	7226	49	0
22	S	3895	0	3938	9	0
23	P	3609	0	3694	11	0
24	Q	3499	0	3524	6	0
25	R	3259	0	3263	8	0
26	U	2427	0	2462	11	0
27	O	3186	0	3213	10	0
28	H	3234	0	3250	29	0
29	I	3022	0	3088	180	0
30	K	3113	0	3164	67	0
31	L	3083	0	3155	45	0
32	M	3285	0	3322	38	0
33	J	3171	0	3311	46	0
34	H	27	0	12	14	0
34	M	27	0	12	0	0
35	H	1	0	0	0	0
35	I	1	0	0	0	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	I	31	0	12	10	0
36	J	31	0	12	4	0
36	K	31	0	12	10	0
36	L	31	0	12	13	0
All	All	110420	0	110468	626	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 (626) 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)
30:K:173:ASP:C	30:K:355:THR:HG21	1.30	1.51
30:K:173:ASP:C	30:K:355:THR:CG2	1.80	1.49
33:J:212:ARG:C	33:J:213:VAL:N	1.68	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:M:338:LEU:C	32:M:339:ARG:N	1.69	1.48
32:M:433:TYR:CZ	32:M:433:TYR:CE1	2.01	1.46
32:M:433:TYR:CZ	32:M:433:TYR:CE2	2.05	1.44
32:M:433:TYR:CD1	32:M:433:TYR:CG	2.05	1.44
32:M:433:TYR:CE1	32:M:433:TYR:CD1	2.07	1.43
32:M:433:TYR:CE2	32:M:433:TYR:CD2	2.07	1.42
32:M:433:TYR:CG	32:M:433:TYR:CD2	2.04	1.42
30:K:166:LYS:NZ	30:K:169:VAL:CG1	1.87	1.38
20:Z:728:LYS:CA	20:Z:728:LYS:C	1.96	1.38
20:Z:728:LYS:CB	20:Z:728:LYS:CG	2.01	1.38
20:Z:728:LYS:CE	20:Z:728:LYS:CD	2.00	1.36
20:Z:728:LYS:CE	20:Z:728:LYS:NZ	1.86	1.36
30:K:173:ASP:O	30:K:355:THR:CG2	1.71	1.31
30:K:166:LYS:NZ	30:K:169:VAL:HG11	1.41	1.29
31:L:179:THR:HB	31:L:181:ASP:N	1.38	1.29
20:Z:255:LEU:CB	20:Z:255:LEU:CG	2.11	1.29
20:Z:728:LYS:HE2	29:I:65:ILE:CB	1.64	1.27
30:K:221:MET:CE	36:K:501:ATP:O3'	1.80	1.26
29:I:186:GLY:O	29:I:188:GLU:N	1.66	1.26
20:Z:728:LYS:CA	20:Z:728:LYS:CB	2.14	1.25
30:K:173:ASP:O	30:K:355:THR:HG21	1.12	1.25
20:Z:728:LYS:CD	29:I:65:ILE:H	1.51	1.23
20:Z:728:LYS:HD2	29:I:62:MET:C	1.64	1.23
33:J:211:ILE:HG22	33:J:212:ARG:O	1.05	1.23
20:Z:728:LYS:CD	29:I:62:MET:C	2.11	1.22
33:J:200:ARG:HG2	33:J:212:ARG:NH1	1.52	1.21
32:M:338:LEU:O	32:M:339:ARG:N	1.69	1.20
20:Z:728:LYS:HD2	29:I:63:GLU:N	1.57	1.19
30:K:173:ASP:CA	30:K:355:THR:HG23	1.74	1.18
31:L:179:THR:CB	31:L:181:ASP:N	1.97	1.18
28:H:388:ILE:HG23	34:H:501:ADP:C2	1.78	1.18
31:L:179:THR:OG1	31:L:182:GLY:N	1.77	1.17
20:Z:728:LYS:NZ	20:Z:728:LYS:HG3	1.53	1.17
20:Z:728:LYS:CD	29:I:61:ARG:O	1.92	1.16
30:K:173:ASP:CA	30:K:355:THR:CG2	2.24	1.15
30:K:166:LYS:HZ3	30:K:169:VAL:CG1	1.51	1.13
30:K:221:MET:HE3	36:K:501:ATP:O3'	0.95	1.10
33:J:211:ILE:CG2	33:J:212:ARG:O	1.98	1.10
30:K:166:LYS:HE2	30:K:169:VAL:HB	1.32	1.10
5:E:20:ARG:CZ	5:E:20:ARG:NE	2.14	1.09
5:E:20:ARG:CZ	32:M:433:TYR:CE2	2.35	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:728:LYS:HE2	29:I:65:ILE:HB	1.24	1.09
5:E:20:ARG:CZ	32:M:433:TYR:CG	2.36	1.09
33:J:210:PHE:CE2	33:J:212:ARG:NH1	2.21	1.08
30:K:166:LYS:HZ3	30:K:169:VAL:HG12	1.01	1.08
30:K:218:GLY:HA2	36:K:501:ATP:O1A	1.51	1.07
29:I:184:ILE:HD13	29:I:235:ALA:HB2	1.34	1.07
5:E:20:ARG:CZ	32:M:433:TYR:CZ	2.38	1.07
29:I:186:GLY:O	29:I:188:GLU:HG2	1.52	1.06
5:E:20:ARG:NE	32:M:433:TYR:CD1	2.24	1.06
5:E:20:ARG:NE	32:M:433:TYR:CE1	2.24	1.06
5:E:20:ARG:CZ	32:M:433:TYR:CE1	2.39	1.05
5:E:20:ARG:CZ	32:M:433:TYR:CD1	2.38	1.05
5:E:20:ARG:NE	32:M:433:TYR:CE2	2.25	1.05
5:E:20:ARG:CZ	32:M:433:TYR:CD2	2.39	1.04
33:J:200:ARG:HG2	33:J:212:ARG:HH12	1.05	1.04
29:I:228:GLY:HA2	36:I:501:ATP:O1A	1.57	1.04
5:E:20:ARG:NE	32:M:433:TYR:CG	2.26	1.04
20:Z:728:LYS:CD	29:I:64:ARG:N	2.21	1.04
20:Z:255:LEU:HD23	21:N:816:LYS:HB2	1.37	1.03
5:E:20:ARG:NE	32:M:433:TYR:CD2	2.26	1.03
5:E:20:ARG:NE	32:M:433:TYR:CZ	2.27	1.02
20:Z:738:TYR:CZ	29:I:69:LEU:HB3	1.95	1.02
20:Z:738:TYR:CZ	20:Z:738:TYR:OH	2.11	1.02
30:K:166:LYS:HZ1	30:K:169:VAL:CG1	1.59	1.02
30:K:173:ASP:HA	30:K:355:THR:CG2	1.89	1.02
20:Z:728:LYS:HB3	29:I:62:MET:SD	1.99	1.01
29:I:186:GLY:C	29:I:188:GLU:HG2	1.85	1.01
30:K:173:ASP:HA	30:K:355:THR:HG23	1.43	1.00
28:H:388:ILE:HG23	34:H:501:ADP:N1	1.75	1.00
20:Z:728:LYS:HD3	29:I:64:ARG:N	1.77	0.99
33:J:210:PHE:HE2	33:J:212:ARG:NH1	1.56	0.99
20:Z:728:LYS:CE	29:I:65:ILE:HB	1.93	0.99
33:J:212:ARG:CA	33:J:213:VAL:N	2.26	0.99
29:I:186:GLY:C	29:I:188:GLU:OE1	2.07	0.98
20:Z:728:LYS:CE	29:I:61:ARG:O	2.13	0.97
20:Z:728:LYS:CE	29:I:62:MET:O	2.13	0.97
20:Z:728:LYS:CD	29:I:65:ILE:N	2.28	0.95
20:Z:728:LYS:CG	20:Z:728:LYS:NZ	2.29	0.95
20:Z:728:LYS:CG	29:I:61:ARG:O	2.14	0.95
30:K:173:ASP:C	30:K:355:THR:HG23	1.86	0.95
29:I:184:ILE:HG21	29:I:232:LEU:HD23	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:738:TYR:CZ	29:I:66:LYS:O	2.21	0.94
20:Z:728:LYS:HE3	29:I:61:ARG:O	1.67	0.93
30:K:221:MET:HE3	36:K:501:ATP:HO3'	1.32	0.93
31:L:230:LEU:CD2	36:L:501:ATP:C5	2.51	0.93
30:K:173:ASP:O	30:K:355:THR:HG22	1.68	0.92
29:I:179:GLU:OE1	29:I:184:ILE:HD11	1.68	0.92
29:I:184:ILE:HG21	29:I:232:LEU:CD2	2.00	0.91
20:Z:738:TYR:OH	29:I:69:LEU:HB3	1.71	0.91
30:K:172:ALA:O	30:K:355:THR:HG23	1.70	0.91
30:K:166:LYS:CE	30:K:169:VAL:HB	2.00	0.90
30:K:166:LYS:HZ1	30:K:169:VAL:HG11	0.75	0.89
20:Z:728:LYS:CG	29:I:62:MET:HA	2.04	0.88
31:L:184:GLY:HA3	31:L:363:ILE:HD11	1.55	0.88
29:I:228:GLY:HA2	36:I:501:ATP:PA	2.13	0.87
31:L:179:THR:HB	31:L:181:ASP:CA	2.03	0.87
20:Z:255:LEU:CB	20:Z:255:LEU:HG	2.04	0.87
20:Z:728:LYS:HG3	20:Z:728:LYS:HZ1	1.38	0.87
33:J:210:PHE:HE2	33:J:212:ARG:HH11	1.12	0.87
20:Z:728:LYS:HE2	29:I:65:ILE:CG1	2.05	0.85
30:K:221:MET:HE3	36:K:501:ATP:C3'	2.05	0.85
33:J:211:ILE:C	33:J:212:ARG:O	2.18	0.85
20:Z:255:LEU:CG	21:N:816:LYS:HB3	2.07	0.85
20:Z:728:LYS:HD3	29:I:65:ILE:H	1.40	0.85
20:Z:728:LYS:HD2	29:I:64:ARG:N	1.90	0.84
20:Z:738:TYR:OH	29:I:69:LEU:CB	2.25	0.83
20:Z:255:LEU:HD23	21:N:816:LYS:CB	2.08	0.83
20:Z:738:TYR:OH	29:I:66:LYS:O	1.95	0.82
33:J:200:ARG:CG	33:J:212:ARG:NH1	2.39	0.82
20:Z:255:LEU:CD1	21:N:812:ALA:O	2.27	0.82
20:Z:728:LYS:CD	29:I:61:ARG:C	2.52	0.82
20:Z:738:TYR:CZ	29:I:66:LYS:HA	2.14	0.81
29:I:186:GLY:O	29:I:188:GLU:CG	2.28	0.81
20:Z:255:LEU:CG	29:I:61:ARG:NH1	2.43	0.81
29:I:231:LEU:CD1	36:I:501:ATP:H3'	2.10	0.81
5:E:20:ARG:NH1	32:M:433:TYR:CD2	2.48	0.81
20:Z:728:LYS:CE	29:I:62:MET:HA	2.10	0.81
5:E:20:ARG:NH1	32:M:433:TYR:CE2	2.49	0.81
29:I:186:GLY:C	29:I:188:GLU:CG	2.54	0.81
5:E:20:ARG:NH2	32:M:433:TYR:CE1	2.48	0.81
20:Z:728:LYS:HD3	29:I:64:ARG:CA	2.10	0.80
30:K:219:LYS:HA	30:K:222:LEU:HD12	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:20:ARG:NH2	32:M:433:TYR:CD1	2.49	0.80
20:Z:255:LEU:HD12	21:N:812:ALA:O	1.81	0.80
20:Z:728:LYS:HD3	29:I:65:ILE:N	1.94	0.80
20:Z:728:LYS:CD	29:I:62:MET:O	2.28	0.80
20:Z:728:LYS:CA	29:I:62:MET:HG2	2.12	0.80
20:Z:738:TYR:OH	29:I:66:LYS:C	2.24	0.79
20:Z:255:LEU:CB	21:N:813:ARG:O	2.30	0.79
20:Z:255:LEU:CB	29:I:61:ARG:NH1	2.45	0.79
20:Z:728:LYS:CE	29:I:62:MET:C	2.56	0.78
30:K:175:GLY:HA2	30:K:352:ILE:HA	1.66	0.78
20:Z:255:LEU:HD13	29:I:61:ARG:NH1	1.98	0.77
20:Z:738:TYR:CE2	29:I:66:LYS:HE2	2.18	0.77
30:K:218:GLY:CA	36:K:501:ATP:O1A	2.33	0.76
20:Z:728:LYS:CE	29:I:65:ILE:H	1.98	0.76
30:K:166:LYS:HE2	30:K:169:VAL:CB	2.15	0.76
20:Z:255:LEU:CB	21:N:816:LYS:HB3	2.17	0.75
20:Z:255:LEU:HB2	21:N:813:ARG:O	1.87	0.75
30:K:218:GLY:HA2	36:K:501:ATP:PA	2.27	0.75
20:Z:255:LEU:HD12	21:N:813:ARG:C	2.12	0.75
28:H:388:ILE:CD1	34:H:501:ADP:N6	2.49	0.74
29:I:231:LEU:HD11	36:I:501:ATP:C3'	2.17	0.74
31:L:390:ASP:CG	32:M:340:SER:OG	2.31	0.74
29:I:186:GLY:C	29:I:188:GLU:N	2.45	0.74
20:Z:728:LYS:CD	29:I:64:ARG:H	2.00	0.74
31:L:179:THR:HB	31:L:181:ASP:CB	2.18	0.73
33:J:212:ARG:HG2	33:J:246:PHE:HB3	1.68	0.73
5:E:20:ARG:CD	32:M:433:TYR:CE2	2.71	0.73
20:Z:728:LYS:C	29:I:62:MET:HG2	2.13	0.73
29:I:184:ILE:CD1	29:I:235:ALA:HB2	2.15	0.73
20:Z:735:GLU:HB2	29:I:66:LYS:HZ3	1.53	0.73
31:L:389:ALA:HA	36:L:501:ATP:O4'	1.87	0.73
30:K:173:ASP:HA	30:K:355:THR:HG22	1.70	0.73
20:Z:728:LYS:CE	29:I:62:MET:CA	2.66	0.72
31:L:230:LEU:HD22	36:L:501:ATP:C8	2.24	0.72
29:I:179:GLU:OE1	29:I:184:ILE:CD1	2.38	0.72
30:K:282:PHE:CD2	33:J:299:ILE:HG21	2.25	0.71
31:L:185:GLY:O	31:L:186:LEU:C	2.07	0.70
20:Z:154:ILE:HD13	28:H:43:ALA:HB2	1.74	0.70
5:e:70:ILE:HD12	5:e:74:ILE:HG22	1.72	0.70
20:Z:728:LYS:HE2	29:I:65:ILE:CA	2.21	0.69
29:I:186:GLY:O	29:I:187:LEU:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:728:LYS:HG2	29:I:65:ILE:HG13	1.73	0.69
29:I:231:LEU:HD11	36:I:501:ATP:O3'	1.92	0.69
11:k:183:ILE:HD12	11:k:190:ARG:HE	1.58	0.69
20:Z:738:TYR:HE1	29:I:70:LEU:HB2	1.58	0.68
30:K:218:GLY:C	30:K:220:THR:N	2.52	0.68
33:J:212:ARG:C	33:J:213:VAL:CA	2.63	0.68
20:Z:255:LEU:CG	21:N:813:ARG:O	2.40	0.68
20:Z:738:TYR:CE1	29:I:66:LYS:O	2.47	0.67
29:I:231:LEU:HD12	36:I:501:ATP:H3'	1.74	0.67
20:Z:255:LEU:HG	21:N:813:ARG:O	1.95	0.67
30:K:172:ALA:C	30:K:355:THR:HG23	2.18	0.67
4:d:96:HIS:CD2	4:d:100:LEU:HD12	2.30	0.67
31:L:230:LEU:CD2	36:L:501:ATP:C4	2.78	0.67
20:Z:254:PRO:HA	21:N:813:ARG:HH12	1.60	0.66
20:Z:738:TYR:OH	29:I:65:ILE:O	2.06	0.66
20:Z:255:LEU:CG	21:N:816:LYS:H	2.08	0.66
29:I:221:LEU:HD23	29:I:229:LYS:HB2	1.78	0.66
20:Z:255:LEU:CB	29:I:61:ARG:HH11	2.08	0.66
27:O:196:LEU:HD13	27:O:236:HIS:CD2	2.31	0.66
29:I:228:GLY:CA	36:I:501:ATP:O1A	2.42	0.66
20:Z:611:THR:HA	21:N:813:ARG:HH21	1.61	0.65
20:Z:738:TYR:CD2	29:I:69:LEU:HD23	2.32	0.65
31:L:179:THR:OG1	31:L:181:ASP:C	2.40	0.65
29:I:186:GLY:C	29:I:188:GLU:CD	2.65	0.65
31:L:230:LEU:HD23	36:L:501:ATP:C5	2.31	0.65
5:E:20:ARG:CD	32:M:433:TYR:CD2	2.79	0.65
29:I:231:LEU:HD11	36:I:501:ATP:H3'	1.78	0.64
20:Z:728:LYS:HD2	29:I:63:GLU:C	2.23	0.64
29:I:221:LEU:HD13	29:I:325:ILE:HG23	1.80	0.64
29:I:231:LEU:CD1	36:I:501:ATP:C3'	2.75	0.64
20:Z:728:LYS:C	20:Z:728:LYS:N	2.55	0.64
31:L:185:GLY:O	31:L:187:THR:N	2.31	0.64
33:J:210:PHE:HE2	33:J:212:ARG:CZ	2.09	0.64
20:Z:255:LEU:CD1	29:I:61:ARG:NH1	2.60	0.64
31:L:389:ALA:HB2	36:L:501:ATP:H5'1	1.80	0.64
20:Z:150:GLY:O	20:Z:154:ILE:HD11	1.98	0.63
20:Z:728:LYS:NZ	29:I:62:MET:O	2.31	0.63
20:Z:738:TYR:OH	29:I:69:LEU:N	2.31	0.63
20:Z:256:LEU:HD13	20:Z:261:ASP:HA	1.81	0.63
33:J:210:PHE:CE2	33:J:212:ARG:CZ	2.80	0.63
29:I:186:GLY:C	29:I:187:LEU:N	2.56	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:255:LEU:CG	29:I:61:ARG:HH12	2.10	0.62
30:K:166:LYS:NZ	30:K:169:VAL:HG12	1.75	0.62
30:K:173:ASP:C	30:K:355:THR:HG22	2.08	0.62
20:Z:738:TYR:CE1	29:I:70:LEU:HB2	2.34	0.62
15:W:77:HIS:CD2	32:M:50:ARG:HD3	2.35	0.61
20:Z:728:LYS:CD	29:I:62:MET:CA	2.79	0.61
20:Z:255:LEU:CD2	21:N:816:LYS:CB	2.77	0.61
28:H:388:ILE:HD13	34:H:501:ADP:N6	2.16	0.61
29:I:179:GLU:HB3	29:I:184:ILE:CD1	2.29	0.61
31:L:178:ILE:HD11	31:L:183:ILE:HD11	1.81	0.61
20:Z:728:LYS:HD2	29:I:63:GLU:CA	2.30	0.61
20:Z:738:TYR:CE2	29:I:66:LYS:CE	2.83	0.61
20:Z:255:LEU:CD2	21:N:816:LYS:HB2	2.22	0.61
20:Z:729:GLU:CA	29:I:62:MET:HG3	2.31	0.61
23:P:261:LEU:HA	23:P:264:ILE:HD12	1.82	0.60
29:I:184:ILE:HG21	29:I:232:LEU:HD21	1.81	0.60
31:L:178:ILE:CD1	31:L:183:ILE:HD11	2.29	0.60
20:Z:728:LYS:NZ	29:I:65:ILE:HB	2.16	0.60
16:V:217:HIS:CD2	16:V:218:LYS:H	2.19	0.60
31:L:183:ILE:HD13	31:L:234:ALA:HB2	1.83	0.60
20:Z:251:ALA:O	20:Z:254:PRO:HG2	2.01	0.60
30:K:319:ASN:OD1	36:K:501:ATP:O3G	2.20	0.60
30:K:166:LYS:CE	30:K:169:VAL:CB	2.77	0.60
31:L:184:GLY:HA3	31:L:363:ILE:CD1	2.31	0.60
20:Z:255:LEU:HB3	21:N:813:ARG:HD2	1.83	0.60
31:L:183:ILE:HD13	31:L:234:ALA:CB	2.32	0.60
20:Z:728:LYS:C	29:I:62:MET:CG	2.75	0.59
20:Z:247:GLN:CD	29:I:54:ARG:HH21	2.10	0.59
20:Z:151:HIS:C	20:Z:154:ILE:HD12	2.28	0.59
20:Z:728:LYS:HD3	29:I:64:ARG:C	2.27	0.59
20:Z:255:LEU:HG	21:N:816:LYS:H	1.66	0.59
30:K:173:ASP:N	30:K:355:THR:HG23	2.18	0.59
28:H:388:ILE:HG12	34:H:501:ADP:C6	2.37	0.58
20:Z:249:MET:O	20:Z:253:VAL:HG23	2.03	0.58
20:Z:728:LYS:N	29:I:62:MET:HE2	2.18	0.58
20:Z:728:LYS:HG2	29:I:65:ILE:CG1	2.33	0.58
5:E:20:ARG:HD3	32:M:433:TYR:CD2	2.39	0.58
29:I:184:ILE:HD13	29:I:235:ALA:CB	2.23	0.58
20:Z:255:LEU:CG	21:N:816:LYS:CB	2.81	0.58
30:K:166:LYS:CE	30:K:169:VAL:CG1	2.82	0.57
28:H:388:ILE:HG23	34:H:501:ADP:C6	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:94:HIS:CD2	3:c:114:ARG:HG2	2.40	0.57
30:K:282:PHE:HD2	33:J:299:ILE:HG21	1.70	0.57
20:Z:728:LYS:HD3	29:I:64:ARG:H	1.63	0.57
21:N:7:ALA:HB3	21:N:8:PRO:HD3	1.87	0.57
20:Z:255:LEU:HD12	21:N:813:ARG:CA	2.35	0.56
20:Z:255:LEU:HG	21:N:816:LYS:HB3	1.85	0.56
31:L:183:ILE:HG13	31:L:230:LEU:HG	1.87	0.56
8:1:68:VAL:HG21	8:1:91:PHE:CD2	2.41	0.56
20:Z:728:LYS:HA	29:I:61:ARG:CG	2.35	0.56
20:Z:918:ASP:H	29:I:58:LYS:HZ1	1.54	0.56
29:I:182:SER:HB3	29:I:185:GLY:HA2	1.87	0.56
20:Z:247:GLN:HG2	29:I:54:ARG:HE	1.70	0.56
20:Z:729:GLU:C	29:I:62:MET:HG3	2.30	0.56
20:Z:738:TYR:CE1	29:I:69:LEU:HB3	2.39	0.56
20:Z:738:TYR:CD2	29:I:66:LYS:HE2	2.39	0.56
9:i:37:PHE:CE2	9:i:177:LYS:HA	2.41	0.56
28:H:388:ILE:HG12	34:H:501:ADP:N1	2.21	0.56
33:J:370:LEU:HD12	33:J:373:ARG:HH12	1.69	0.56
20:Z:255:LEU:HD21	21:N:815:LYS:HB2	1.86	0.56
20:Z:738:TYR:CZ	29:I:66:LYS:CA	2.88	0.56
20:Z:738:TYR:CE2	29:I:69:LEU:HD23	2.41	0.56
30:K:172:ALA:O	30:K:355:THR:CG2	2.49	0.56
29:I:182:SER:CB	29:I:185:GLY:HA2	2.35	0.56
30:K:217:THR:C	30:K:219:LYS:H	2.12	0.56
20:Z:728:LYS:HA	29:I:61:ARG:HG2	1.87	0.56
30:K:166:LYS:NZ	30:K:169:VAL:CB	2.66	0.55
33:J:195:LYS:CG	36:J:501:ATP:O1B	2.54	0.55
33:J:200:ARG:HG2	33:J:212:ARG:HH11	1.61	0.55
28:H:388:ILE:CG2	34:H:501:ADP:N1	2.61	0.55
33:J:116:ARG:HG2	33:J:123:HIS:CE1	2.41	0.55
5:e:70:ILE:HD12	5:e:74:ILE:CG2	2.36	0.55
10:j:63:LEU:HD22	10:j:105:VAL:HG21	1.87	0.55
20:Z:728:LYS:CB	29:I:62:MET:HA	2.37	0.55
31:L:180:PHE:C	31:L:181:ASP:HA	2.31	0.55
16:V:217:HIS:CG	16:V:218:LYS:H	2.25	0.55
21:N:380:LEU:HD12	21:N:380:LEU:H	1.72	0.55
27:O:73:ILE:HD11	27:O:78:VAL:HG22	1.88	0.55
20:Z:151:HIS:O	20:Z:154:ILE:HD12	2.07	0.55
20:Z:735:GLU:CD	29:I:66:LYS:HZ1	2.14	0.55
9:i:161:LEU:HD13	14:7:182:HIS:CE1	2.43	0.55
14:7:163:VAL:HG22	14:7:164:ASN:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:U:70:HIS:CD2	26:U:71:ASN:N	2.75	0.55
23:P:59:LEU:O	23:P:63:VAL:HG23	2.08	0.54
20:Z:214:HIS:HA	21:N:819:LYS:NZ	2.21	0.54
20:Z:255:LEU:HD13	29:I:61:ARG:CZ	2.38	0.54
20:Z:255:LEU:CD2	21:N:816:LYS:H	2.20	0.54
20:Z:728:LYS:CG	29:I:61:ARG:C	2.81	0.54
20:Z:255:LEU:H	21:N:813:ARG:NH1	2.06	0.54
20:Z:728:LYS:CB	20:Z:728:LYS:HA	2.30	0.54
20:Z:738:TYR:CZ	29:I:66:LYS:C	2.85	0.54
29:I:186:GLY:N	29:I:188:GLU:OE1	2.40	0.54
31:L:230:LEU:HD21	36:L:501:ATP:C4	2.43	0.54
30:K:173:ASP:CA	30:K:355:THR:HG22	2.26	0.54
32:M:172:VAL:HG13	32:M:242:THR:HB	1.90	0.54
29:I:186:GLY:O	29:I:187:LEU:C	2.48	0.54
21:N:46:ILE:HD13	21:N:64:ILE:HG21	1.89	0.54
30:K:218:GLY:O	30:K:219:LYS:C	2.46	0.53
15:W:51:LEU:HD21	15:W:76:LEU:HD23	1.89	0.53
28:H:90:ARG:HH22	29:I:150:HIS:CD2	2.27	0.53
31:L:180:PHE:HB3	31:L:181:ASP:HA	1.90	0.53
31:L:230:LEU:HD21	36:L:501:ATP:C5	2.37	0.53
33:J:210:PHE:HE2	33:J:212:ARG:HD3	1.72	0.53
29:I:186:GLY:CA	29:I:188:GLU:HG2	2.37	0.53
20:Z:728:LYS:HG3	29:I:65:ILE:HB	1.91	0.53
20:Z:206:ASP:HA	29:I:53:THR:HG21	1.90	0.53
20:Z:728:LYS:HE2	29:I:65:ILE:N	2.24	0.53
32:M:342:ARG:O	32:M:343:LEU:HD23	2.09	0.53
13:m:46:ARG:HE	13:m:229:ARG:HH21	1.57	0.53
20:Z:729:GLU:N	29:I:62:MET:CG	2.72	0.52
33:J:195:LYS:HG2	36:J:501:ATP:O1B	2.09	0.52
20:Z:154:ILE:CD1	28:H:43:ALA:HB2	2.40	0.52
31:L:145:ARG:HG3	31:L:162:GLU:H	1.73	0.52
22:S:156:VAL:HG11	22:S:194:LEU:HD22	1.92	0.52
20:Z:255:LEU:HB3	29:I:61:ARG:HH11	1.75	0.52
20:Z:728:LYS:CB	29:I:61:ARG:HG3	2.40	0.52
29:I:184:ILE:CG2	29:I:232:LEU:HD21	2.39	0.52
30:K:175:GLY:CA	30:K:352:ILE:HA	2.37	0.52
15:W:33:VAL:HG11	15:W:76:LEU:HD21	1.92	0.52
28:H:388:ILE:HG12	34:H:501:ADP:N6	2.25	0.52
20:Z:154:ILE:HG12	28:H:43:ALA:HB3	1.91	0.52
33:J:210:PHE:HE2	33:J:212:ARG:CD	2.22	0.52
17:T:151:TRP:HE1	17:T:163:LEU:HD22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:100:THR:HG22	22:S:223:LEU:HD11	1.91	0.52
5:e:142:LEU:HD23	5:e:158:ALA:HB3	1.91	0.51
29:I:186:GLY:CA	29:I:188:GLU:OE1	2.58	0.51
14:n:255:ALA:HB1	8:1:183:ARG:HH21	1.76	0.51
20:Z:247:GLN:HG3	29:I:58:LYS:HE2	1.92	0.51
20:Z:728:LYS:HD2	29:I:64:ARG:H	1.63	0.51
3:c:17:GLY:O	4:d:26:ALA:HB2	2.11	0.51
30:K:174:VAL:HG12	30:K:175:GLY:N	2.25	0.51
11:k:3:ILE:HD12	11:k:168:LEU:HD13	1.92	0.51
23:P:393:VAL:H	24:Q:354:PHE:HA	1.75	0.51
30:K:171:TYR:OH	30:K:185:ARG:CG	2.36	0.51
20:Z:729:GLU:N	29:I:62:MET:HG3	2.25	0.51
20:Z:728:LYS:CD	29:I:63:GLU:C	2.80	0.51
29:I:346:ARG:HE	29:I:346:ARG:HA	1.75	0.51
14:n:83:VAL:HG23	14:n:233:ILE:HD11	1.92	0.51
24:Q:391:ASP:HB2	24:Q:396:TRP:H	1.76	0.51
20:Z:255:LEU:CB	29:I:61:ARG:HH12	2.24	0.51
31:L:230:LEU:CD2	36:L:501:ATP:N7	2.74	0.51
14:n:250:MET:HB3	14:n:252:TRP:HE1	1.76	0.51
13:6:214:ILE:HG22	13:6:221:ARG:HH21	1.76	0.51
17:T:117:ASN:HD21	17:T:184:ALA:HB1	1.75	0.51
31:L:183:ILE:CD1	31:L:234:ALA:HB2	2.41	0.51
29:I:228:GLY:HA2	36:I:501:ATP:O5'	2.11	0.50
26:U:70:HIS:CD2	26:U:71:ASN:H	2.29	0.50
31:L:170:MET:HB2	31:L:244:ILE:HG23	1.93	0.50
23:P:365:LEU:HD22	23:P:400:VAL:HG11	1.92	0.50
20:Z:254:PRO:HD3	20:Z:727:GLU:O	2.11	0.50
24:Q:129:LYS:HD2	24:Q:130:ARG:H	1.76	0.50
20:Z:738:TYR:CE2	29:I:69:LEU:CD2	2.95	0.50
20:Z:248:TYR:HA	29:I:54:ARG:HH11	1.76	0.50
20:Z:728:LYS:CE	29:I:65:ILE:N	2.70	0.50
22:S:246:GLU:HG2	22:S:249:SER:H	1.77	0.50
31:L:230:LEU:HD22	36:L:501:ATP:C4	2.46	0.50
31:L:179:THR:CB	31:L:181:ASP:CA	2.78	0.50
26:U:17:SER:HB3	26:U:21:HIS:CE1	2.46	0.49
31:L:179:THR:OG1	31:L:181:ASP:N	2.42	0.49
33:J:200:ARG:HE	33:J:212:ARG:NH1	2.09	0.49
7:g:218:TRP:CH2	7:g:235:LEU:HD21	2.47	0.49
33:J:210:PHE:CE2	33:J:212:ARG:CD	2.95	0.49
33:J:331:HIS:CE1	33:J:359:LYS:HD3	2.47	0.49
20:Z:728:LYS:HE2	29:I:65:ILE:HG12	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:H:227:LEU:HD22	28:H:234:ARG:HH22	1.76	0.49
7:g:18:ASP:HB3	7:g:20:ARG:HE	1.77	0.49
30:K:392:LEU:HD23	31:L:345:ARG:HE	1.78	0.49
2:b:16:GLY:HA3	3:c:31:HIS:CE1	2.46	0.49
20:Z:255:LEU:HD22	29:I:61:ARG:NH2	2.27	0.49
20:Z:728:LYS:CB	29:I:62:MET:SD	2.86	0.49
6:f:117:GLN:HE21	7:g:87:HIS:CG	2.29	0.49
12:l:189:TYR:CE1	12:l:204:VAL:HG21	2.47	0.49
20:Z:154:ILE:HG12	28:H:43:ALA:CB	2.43	0.49
23:P:309:MET:HE1	23:P:348:HIS:CD2	2.47	0.49
16:V:185:ILE:HG23	16:V:189:ILE:HG21	1.95	0.49
33:J:195:LYS:HG3	36:J:501:ATP:O1B	2.13	0.49
33:J:210:PHE:CE2	33:J:212:ARG:HD3	2.48	0.48
30:K:217:THR:C	30:K:219:LYS:N	2.69	0.48
20:Z:247:GLN:O	20:Z:251:ALA:HB3	2.12	0.48
30:K:174:VAL:N	30:K:355:THR:HG21	2.10	0.48
22:S:27:GLU:O	22:S:31:VAL:HG23	2.14	0.48
24:Q:31:LEU:HD12	24:Q:61:LEU:HD11	1.95	0.48
15:W:35:PHE:CE2	15:W:186:ALA:HB2	2.48	0.48
20:Z:748:LEU:HD13	29:I:81:ILE:CG2	2.42	0.48
20:Z:748:LEU:HD13	29:I:81:ILE:HG23	1.94	0.48
20:Z:918:ASP:N	29:I:58:LYS:HZ1	2.11	0.48
29:I:345:ASP:CG	29:I:346:ARG:H	2.21	0.48
28:H:403:ARG:HH21	28:H:409:ARG:HH22	1.61	0.48
6:f:45:VAL:HG22	6:f:215:ILE:HG22	1.96	0.48
20:Z:731:GLY:H	29:I:62:MET:HB3	1.79	0.48
32:M:351:LEU:HD22	32:M:351:LEU:H	1.79	0.48
6:f:166:GLN:H	6:f:166:GLN:CD	2.21	0.48
29:I:346:ARG:HE	29:I:347:LYS:H	1.62	0.48
33:J:116:ARG:CG	33:J:123:HIS:CE1	2.97	0.48
9:2:80:ASP:O	9:2:84:VAL:HG22	2.13	0.48
20:Z:736:LEU:HD13	20:Z:765:MET:HG2	1.96	0.48
33:J:195:LYS:HG2	36:J:501:ATP:PB	2.54	0.48
13:6:168:TYR:CD2	13:6:174:GLY:HA2	2.50	0.47
24:Q:236:PHE:CZ	24:Q:281:ILE:HD11	2.49	0.47
4:d:96:HIS:CD2	4:d:100:LEU:CD1	2.97	0.47
33:J:210:PHE:CD2	33:J:212:ARG:NH1	2.76	0.47
20:Z:731:GLY:O	29:I:66:LYS:CD	2.62	0.47
20:Z:904:LEU:HD21	20:Z:950:THR:HG21	1.95	0.47
3:c:163:ILE:HD12	3:c:164:SER:H	1.79	0.47
11:4:147:HIS:HB2	11:4:160:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:30:LYS:HG3	20:Z:37:GLN:HB3	1.97	0.47
20:Z:786:SER:HB3	28:H:76:LEU:CD2	2.45	0.47
21:N:518:ALA:HB1	21:N:550:GLY:HA3	1.96	0.47
21:N:760:GLY:H	21:N:870:ASN:HD21	1.62	0.47
29:I:184:ILE:CG2	29:I:232:LEU:CD2	2.83	0.47
21:N:214:LEU:HD13	21:N:225:LEU:HG	1.96	0.47
23:P:311:TRP:CD2	23:P:342:GLN:HG3	2.50	0.47
25:R:312:TYR:HA	25:R:316:LEU:HD12	1.97	0.47
4:d:117:GLN:HE21	4:d:152:PRO:HA	1.80	0.47
18:X:37:PRO:HA	18:X:46:TRP:CE3	2.49	0.47
20:Z:734:ASP:HB2	29:I:66:LYS:CG	2.45	0.47
11:4:3:ILE:HD11	11:4:172:MET:SD	2.55	0.46
20:Z:728:LYS:CE	29:I:65:ILE:CB	2.56	0.46
22:S:458:GLN:HG3	26:U:252:HIS:CE1	2.49	0.46
14:n:160:LEU:HG	14:n:175:LEU:HD12	1.96	0.46
16:V:237:ASN:HD21	16:V:291:ASN:HD21	1.62	0.46
30:K:235:ILE:HG21	30:K:257:VAL:HG13	1.98	0.46
33:J:212:ARG:CB	33:J:213:VAL:N	2.77	0.46
7:G:72:ARG:HH12	14:7:104:VAL:HG12	1.79	0.46
20:Z:254:PRO:HA	21:N:813:ARG:NH1	2.28	0.46
20:Z:255:LEU:HD22	29:I:61:ARG:NH1	2.31	0.46
32:M:82:VAL:HA	32:M:119:VAL:HG12	1.97	0.46
26:U:30:ASN:HD22	26:U:32:ARG:HH12	1.63	0.46
28:H:147:ILE:C	28:H:147:ILE:HD12	2.40	0.46
30:K:167:PRO:O	30:K:168:ASP:OD1	2.32	0.46
20:Z:738:TYR:HH	29:I:66:LYS:C	2.24	0.46
21:N:67:LYS:HA	21:N:70:TYR:CE2	2.51	0.46
21:N:156:ILE:HD12	21:N:159:GLU:OE1	2.15	0.46
23:P:216:LEU:HD12	23:P:216:LEU:H	1.80	0.46
29:I:182:SER:HA	29:I:185:GLY:CA	2.34	0.46
31:L:351:LEU:HD12	31:L:351:LEU:H	1.81	0.46
30:K:174:VAL:HG12	30:K:175:GLY:H	1.80	0.46
5:e:167:TYR:CE2	6:f:57:SER:HB2	2.51	0.46
20:Z:248:TYR:HA	29:I:54:ARG:NH1	2.30	0.46
20:Z:809:MET:HB3	29:I:276:PRO:HD2	1.98	0.46
23:P:282:HIS:CE1	23:P:304:THR:HG23	2.51	0.46
12:l:201:ILE:HD11	11:4:171:ARG:HH22	1.81	0.46
13:6:51:VAL:HG12	13:6:213:LEU:HD22	1.98	0.46
20:Z:255:LEU:CD2	29:I:61:ARG:NH1	2.78	0.46
29:I:186:GLY:O	29:I:188:GLU:CA	2.60	0.46
4:d:106:VAL:HG13	4:d:135:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:204:ASN:HD22	22:S:438:HIS:CE1	2.34	0.45
21:N:444:HIS:ND1	21:N:480:ALA:HB2	2.32	0.45
22:S:481:TYR:HB3	22:S:482:PRO:HD3	1.97	0.45
32:M:337:LEU:O	32:M:342:ARG:HB3	2.17	0.45
20:Z:728:LYS:HZ3	29:I:65:ILE:HB	1.80	0.45
24:Q:67:THR:HB	24:Q:68:MET:HA	1.98	0.45
33:J:301:ASP:HB3	33:J:302:PRO:HD2	1.99	0.45
29:I:183:ASP:HB3	29:I:184:ILE:HD12	1.97	0.45
31:L:227:GLY:HA2	36:L:501:ATP:O2A	2.16	0.45
4:d:70:HIS:HB3	4:d:219:SER:HA	1.99	0.45
33:J:210:PHE:CE2	33:J:212:ARG:HG3	2.52	0.45
10:j:11:ILE:HG21	10:j:142:ALA:HB3	1.99	0.45
30:K:166:LYS:HB2	30:K:224:LYS:HG3	1.99	0.45
31:L:230:LEU:CD2	36:L:501:ATP:C8	2.99	0.44
16:V:53:MET:HE2	16:V:65:VAL:HG21	1.98	0.44
5:e:214:GLU:CD	5:e:214:GLU:H	2.25	0.44
20:Z:255:LEU:HD22	29:I:61:ARG:CZ	2.47	0.44
10:j:50:PHE:CD1	10:j:190:ILE:HD13	2.52	0.44
20:Z:248:TYR:CG	29:I:54:ARG:NH1	2.86	0.44
20:Z:253:VAL:HB	20:Z:254:PRO:HD3	2.00	0.44
13:6:184:SER:HB2	13:6:187:GLU:HB2	1.98	0.44
14:7:162:TYR:CD1	14:7:170:TYR:CE2	3.06	0.44
25:R:217:HIS:O	25:R:221:VAL:HG23	2.18	0.44
12:l:201:ILE:CD1	11:4:171:ARG:HH22	2.30	0.44
27:O:134:ALA:HB1	27:O:146:ALA:HB1	2.00	0.44
28:H:388:ILE:CG1	34:H:501:ADP:N6	2.80	0.44
33:J:200:ARG:CG	33:J:212:ARG:HH12	1.99	0.44
11:4:172:MET:HE2	11:4:174:MET:HB2	2.00	0.44
20:Z:728:LYS:HE2	29:I:65:ILE:H	1.72	0.44
28:H:388:ILE:CG1	34:H:501:ADP:C6	3.00	0.44
9:i:196:LEU:HD21	13:6:43:ILE:HG12	1.99	0.44
28:H:388:ILE:HD13	34:H:501:ADP:C6	2.53	0.44
20:Z:161:ILE:HG23	20:Z:214:HIS:CE1	2.53	0.44
20:Z:254:PRO:CA	21:N:813:ARG:HH12	2.30	0.44
28:H:282:LYS:HE2	28:H:314:VAL:HG21	1.99	0.44
28:H:324:GLY:HA2	29:I:299:GLU:O	2.17	0.44
30:K:221:MET:HG3	36:K:501:ATP:H3'	2.00	0.44
30:K:282:PHE:HD2	33:J:299:ILE:CG2	2.30	0.44
20:Z:212:LEU:HD11	20:Z:224:LEU:HD22	2.00	0.43
20:Z:739:ALA:HB2	20:Z:764:LEU:CD1	2.48	0.43
6:F:190:ILE:HG23	6:F:213:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:128:ILE:HD12	22:S:128:ILE:O	2.18	0.43
10:j:183:TRP:HE1	12:5:241:HIS:CE1	2.36	0.43
20:Z:253:VAL:HB	20:Z:254:PRO:CD	2.48	0.43
11:k:192:VAL:HG12	11:k:194:ASP:H	1.84	0.43
13:m:214:ILE:HG22	13:m:216:THR:HG23	2.01	0.43
16:V:296:LEU:O	16:V:300:VAL:HG23	2.18	0.43
18:X:78:ILE:HD13	18:X:78:ILE:H	1.83	0.43
21:N:549:TYR:CE2	21:N:586:ALA:HB2	2.53	0.43
33:J:211:ILE:C	33:J:212:ARG:C	2.34	0.43
31:L:180:PHE:C	31:L:181:ASP:CA	2.88	0.43
28:H:388:ILE:CG2	34:H:501:ADP:C6	3.02	0.43
29:I:141:LEU:HD23	29:I:141:LEU:HA	1.91	0.43
30:K:132:LYS:HB2	30:K:133:PRO:HD3	2.00	0.43
8:l:50:ILE:HG12	8:l:110:GLY:HA3	2.00	0.43
15:W:144:PHE:HB3	15:W:174:VAL:HG12	2.01	0.43
20:Z:728:LYS:HD3	29:I:64:ARG:CB	2.49	0.43
20:Z:729:GLU:N	29:I:62:MET:HG2	2.34	0.43
26:U:70:HIS:HD2	26:U:71:ASN:H	1.67	0.43
8:h:68:VAL:HG21	8:h:91:PHE:CD2	2.54	0.43
16:V:218:LYS:HG3	26:U:132:LEU:H	1.84	0.43
25:R:170:VAL:O	25:R:174:ILE:HG13	2.18	0.43
30:K:218:GLY:C	30:K:220:THR:H	2.26	0.43
8:h:174:TRP:CG	8:l:144:TYR:CD1	3.06	0.42
11:4:97:PRO:HB2	11:4:99:GLN:HE21	1.84	0.42
20:Z:255:LEU:CD2	29:I:61:ARG:HH12	2.31	0.42
30:K:218:GLY:C	36:K:501:ATP:O1A	2.62	0.42
20:Z:247:GLN:HB3	29:I:54:ARG:HH21	1.84	0.42
21:N:46:ILE:HA	21:N:49:LEU:HD12	2.01	0.42
25:R:141:TYR:HB3	25:R:150:ALA:HB2	2.01	0.42
30:K:167:PRO:O	30:K:168:ASP:CG	2.62	0.42
6:F:89:ARG:HD2	13:6:85:PHE:CD1	2.54	0.42
13:6:196:PHE:HA	13:6:199:ALA:HB3	2.02	0.42
21:N:43:LEU:HD12	21:N:46:ILE:HD12	2.00	0.42
21:N:828:LYS:HB3	21:N:829:LYS:HG3	2.00	0.42
26:U:34:VAL:HG21	26:U:56:PHE:CZ	2.54	0.42
30:K:174:VAL:CG1	30:K:175:GLY:N	2.82	0.42
33:J:258:VAL:HG13	33:J:305:LEU:HD22	2.02	0.42
17:T:194:GLU:HA	17:T:235:PHE:HB3	2.00	0.42
21:N:109:TYR:CD2	21:N:137:PHE:CD1	3.07	0.42
13:m:188:VAL:O	13:m:192:VAL:HG23	2.19	0.42
20:Z:248:TYR:CA	29:I:54:ARG:NH1	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:H:80:HIS:CE1	29:I:92:GLU:HA	2.55	0.42
31:L:97:ALA:HB1	32:M:132:VAL:HG22	2.02	0.42
11:4:118:GLN:CG	11:4:133:HIS:CE1	3.03	0.42
11:4:118:GLN:HG2	11:4:133:HIS:CE1	2.54	0.42
14:7:163:VAL:HG22	14:7:164:ASN:N	2.33	0.42
20:Z:249:MET:HG3	20:Z:268:ALA:HB2	2.02	0.42
31:L:259:SER:HB2	31:L:304:THR:OG1	2.19	0.42
4:d:8:LEU:H	4:d:125:GLY:H	1.68	0.42
10:3:157:ASN:O	10:3:158:LEU:HD23	2.20	0.42
33:J:279:LEU:HD13	33:J:279:LEU:O	2.20	0.42
3:c:150:THR:OG1	3:c:163:ILE:HG21	2.19	0.42
20:Z:728:LYS:O	29:I:62:MET:HE2	2.18	0.42
27:O:62:TYR:CE2	27:O:82:LEU:HD12	2.55	0.42
27:O:86:LEU:HD22	27:O:95:SER:HA	2.02	0.42
32:M:274:ALA:HA	32:M:275:PRO:C	2.44	0.42
20:Z:738:TYR:CZ	29:I:69:LEU:CB	2.85	0.42
20:Z:738:TYR:OH	29:I:69:LEU:CA	2.68	0.42
33:J:88:VAL:HG12	33:J:90:PRO:HD2	2.02	0.42
3:c:165:VAL:HG12	3:c:166:GLY:H	1.85	0.42
16:V:305:ILE:HG21	26:U:237:PRO:HD2	2.01	0.42
19:Y:80:GLU:HG2	19:Y:83:ARG:HH21	1.84	0.42
28:H:416:GLY:HA3	34:H:501:ADP:C5	2.55	0.42
31:L:105:ILE:HD12	32:M:126:THR:HG22	2.02	0.42
33:J:31:GLU:HA	33:J:34:ILE:HD12	2.02	0.42
23:P:89:LEU:HG	23:P:91:LEU:H	1.85	0.41
27:O:26:PHE:HA	27:O:29:PHE:CD2	2.55	0.41
28:H:362:ASP:HA	28:H:363:PRO:HD3	1.94	0.41
29:I:186:GLY:O	29:I:188:GLU:CB	2.68	0.41
6:f:171:TYR:CG	6:f:196:ALA:HA	2.54	0.41
20:Z:253:VAL:N	20:Z:254:PRO:HD2	2.35	0.41
26:U:268:LYS:HE3	26:U:268:LYS:HA	2.02	0.41
4:d:13:PRO:HA	5:e:26:TYR:CD2	2.55	0.41
11:k:17:SER:HB3	11:k:34:LYS:HB2	2.02	0.41
20:Z:728:LYS:CD	29:I:62:MET:N	2.83	0.41
21:N:688:ASN:HB3	21:N:690:HIS:CD2	2.55	0.41
21:N:809:ARG:HE	29:I:72:GLU:HB2	1.85	0.41
9:2:192:ILE:HG23	9:2:199:GLY:HA2	2.02	0.41
20:Z:728:LYS:O	29:I:62:MET:CE	2.68	0.41
23:P:431:HIS:CD2	26:U:156:HIS:CE1	3.09	0.41
5:e:201:LEU:HB2	5:e:243:LEU:HD22	2.02	0.41
12:l:189:TYR:CD1	12:l:204:VAL:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:3:108:VAL:HG13	10:3:137:ILE:HG21	2.03	0.41
28:H:363:PRO:HA	28:H:366:LEU:HD12	2.02	0.41
25:R:339:ALA:HA	25:R:392:ARG:HH22	1.86	0.41
29:I:182:SER:HA	29:I:185:GLY:HA2	2.00	0.41
30:K:282:PHE:CD2	33:J:299:ILE:CG2	3.01	0.41
30:K:362:LEU:HB3	30:K:407:LEU:HD11	2.01	0.41
5:e:136:ARG:HG3	5:e:136:ARG:HH11	1.86	0.41
5:E:214:GLU:H	5:E:214:GLU:CD	2.29	0.41
16:V:305:ILE:HG23	27:O:373:TRP:CZ2	2.56	0.41
21:N:430:ASN:HD22	21:N:439:VAL:HG13	1.86	0.41
22:S:237:ILE:HG12	22:S:241:PHE:CZ	2.56	0.41
30:K:160:VAL:HA	30:K:236:ARG:HB3	2.02	0.41
30:K:356:ILE:O	30:K:359:LYS:HB2	2.21	0.41
8:h:88:ALA:O	8:h:92:LYS:HB2	2.20	0.41
13:m:35:THR:HB	13:m:48:GLU:H	1.86	0.41
20:Z:248:TYR:N	29:I:54:ARG:NH1	2.68	0.41
20:Z:253:VAL:N	20:Z:254:PRO:CD	2.83	0.41
21:N:483:LEU:HD22	21:N:735:MET:SD	2.61	0.41
25:R:94:PHE:H	25:R:94:PHE:HD1	1.67	0.41
25:R:348:LEU:HB2	25:R:388:VAL:HB	2.01	0.41
29:I:106:ILE:HD12	29:I:106:ILE:HA	1.92	0.41
13:m:82:TRP:HA	13:m:85:PHE:CD2	2.55	0.41
13:6:76:PHE:O	13:6:80:VAL:HG23	2.20	0.41
23:P:421:GLU:O	23:P:425:HIS:CD2	2.74	0.41
28:H:366:LEU:HA	28:H:371:ILE:HD12	2.01	0.41
31:L:178:ILE:CD1	31:L:183:ILE:CD1	2.96	0.41
31:L:390:ASP:OD1	32:M:340:SER:OG	2.38	0.41
33:J:304:LEU:HA	33:J:310:ILE:HD13	2.01	0.41
5:e:40:ILE:HG12	5:e:200:VAL:HG22	2.02	0.41
20:Z:734:ASP:HB2	29:I:66:LYS:HG2	2.03	0.41
12:l:216:ASP:HA	12:l:219:TYR:HB2	2.02	0.40
17:T:97:SER:HB3	17:T:99:SER:H	1.86	0.40
20:Z:24:THR:HB	20:Z:25:PRO:CD	2.51	0.40
21:N:546:LEU:HD22	21:N:546:LEU:H	1.87	0.40
25:R:94:PHE:CD1	25:R:94:PHE:N	2.89	0.40
31:L:111:GLU:H	31:L:142:LYS:HE2	1.85	0.40
20:Z:728:LYS:CA	29:I:62:MET:HE2	2.51	0.40
27:O:193:LEU:HD22	27:O:232:GLU:HG3	2.03	0.40
5:e:85:ALA:HB2	5:e:140:VAL:HG21	2.03	0.40
30:K:329:LEU:HB3	30:K:334:LEU:HD12	2.03	0.40
31:L:230:LEU:HD22	36:L:501:ATP:N9	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:28:VAL:HA	2:b:77:GLY:HA2	2.03	0.40
10:j:51:LEU:HD11	10:j:107:PRO:HB2	2.03	0.40
20:Z:213:LYS:HD2	21:N:816:LYS:HZ2	1.85	0.40
20:Z:214:HIS:HA	21:N:819:LYS:HZ3	1.85	0.40
27:O:67:SER:HA	27:O:105:GLN:HE22	1.86	0.40
27:O:73:ILE:CD1	27:O:78:VAL:HG22	2.51	0.40
33:J:32:LEU:HD22	33:J:32:LEU:HA	1.99	0.40
33:J:388:LYS:HE2	33:J:388:LYS:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/241 (99%)	223 (93%)	16 (7%)	0	100	100
1	a	239/241 (99%)	226 (95%)	11 (5%)	2 (1%)	16	53
2	B	247/249 (99%)	232 (94%)	15 (6%)	0	100	100
2	b	247/249 (99%)	231 (94%)	14 (6%)	2 (1%)	16	53
3	C	242/244 (99%)	232 (96%)	10 (4%)	0	100	100
3	c	242/244 (99%)	230 (95%)	12 (5%)	0	100	100
4	D	235/251 (94%)	222 (94%)	13 (6%)	0	100	100
4	d	249/251 (99%)	229 (92%)	14 (6%)	6 (2%)	4	26
5	E	242/244 (99%)	225 (93%)	11 (4%)	6 (2%)	4	25
5	e	242/244 (99%)	222 (92%)	17 (7%)	3 (1%)	10	43
6	F	229/231 (99%)	219 (96%)	9 (4%)	1 (0%)	30	67
6	f	229/231 (99%)	211 (92%)	13 (6%)	5 (2%)	5	28
7	G	240/242 (99%)	229 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	g	240/242 (99%)	229 (95%)	10 (4%)	1 (0%)	30	67
8	l	194/196 (99%)	185 (95%)	8 (4%)	1 (0%)	24	63
8	h	194/196 (99%)	177 (91%)	12 (6%)	5 (3%)	4	24
9	2	224/226 (99%)	215 (96%)	7 (3%)	2 (1%)	14	50
9	i	224/226 (99%)	206 (92%)	15 (7%)	3 (1%)	9	40
10	3	202/204 (99%)	187 (93%)	14 (7%)	1 (0%)	24	63
10	j	202/204 (99%)	185 (92%)	11 (5%)	6 (3%)	3	22
11	4	193/195 (99%)	183 (95%)	7 (4%)	3 (2%)	7	36
11	k	193/195 (99%)	176 (91%)	13 (7%)	4 (2%)	5	28
12	5	210/212 (99%)	197 (94%)	12 (6%)	1 (0%)	24	63
12	l	210/212 (99%)	195 (93%)	15 (7%)	0	100	100
13	6	220/222 (99%)	204 (93%)	12 (6%)	4 (2%)	6	33
13	m	220/222 (99%)	207 (94%)	10 (4%)	3 (1%)	9	38
14	7	227/232 (98%)	205 (90%)	18 (8%)	4 (2%)	6	33
14	n	230/232 (99%)	214 (93%)	14 (6%)	2 (1%)	14	50
15	W	195/197 (99%)	178 (91%)	11 (6%)	6 (3%)	3	21
16	V	287/289 (99%)	260 (91%)	20 (7%)	7 (2%)	4	26
17	T	264/266 (99%)	248 (94%)	14 (5%)	2 (1%)	16	53
18	X	125/127 (98%)	105 (84%)	15 (12%)	5 (4%)	2	17
19	Y	87/89 (98%)	72 (83%)	10 (12%)	5 (6%)	1	13
20	Z	902/970 (93%)	820 (91%)	59 (6%)	23 (2%)	4	25
21	N	920/922 (100%)	865 (94%)	41 (4%)	14 (2%)	8	38
22	S	473/475 (100%)	445 (94%)	19 (4%)	9 (2%)	6	31
23	P	438/440 (100%)	415 (95%)	16 (4%)	7 (2%)	7	36
24	Q	432/434 (100%)	394 (91%)	26 (6%)	12 (3%)	4	23
25	R	403/405 (100%)	388 (96%)	10 (2%)	5 (1%)	10	43
26	U	302/304 (99%)	288 (95%)	13 (4%)	1 (0%)	36	71
27	O	386/388 (100%)	371 (96%)	10 (3%)	5 (1%)	9	40
28	H	415/417 (100%)	364 (88%)	39 (9%)	12 (3%)	3	23
29	I	379/385 (98%)	353 (93%)	18 (5%)	8 (2%)	5	28
30	K	392/394 (100%)	353 (90%)	28 (7%)	11 (3%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	L	384/388 (99%)	360 (94%)	18 (5%)	6 (2%)	7	36
32	M	419/421 (100%)	376 (90%)	30 (7%)	13 (3%)	3	21
33	J	403/405 (100%)	362 (90%)	22 (6%)	19 (5%)	2	16
All	All	13911/14094 (99%)	12913 (93%)	763 (6%)	235 (2%)	9	34

All (235) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	d	31	THR
4	d	50	SER
6	f	14	SER
5	E	16	SER
13	6	27	ASP
13	6	138	SER
15	W	190	ILE
16	V	171	ARG
16	V	217	HIS
17	T	97	SER
19	Y	3	THR
20	Z	24	THR
20	Z	85	VAL
20	Z	728	LYS
20	Z	870	ALA
21	N	17	GLN
21	N	175	ASP
21	N	832	HIS
21	N	863	SER
22	S	47	THR
22	S	84	ASP
24	Q	68	MET
24	Q	384	LYS
24	Q	387	TYR
25	R	73	ASN
25	R	280	ILE
28	H	141	GLU
29	I	86	GLU
29	I	290	LYS
29	I	317	ASP
30	K	219	LYS
30	K	284	ALA
31	L	101	ILE

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Mol	Chain	Res	Type
31	L	290	ARG
31	L	343	LEU
32	M	172	VAL
32	M	322	LYS
32	M	339	ARG
32	M	343	LEU
33	J	212	ARG
4	d	205	THR
9	i	175	LEU
10	j	7	ILE
10	j	40	PHE
11	k	73	TYR
13	m	27	ASP
6	F	14	SER
15	W	179	ARG
18	X	21	SER
18	X	29	VAL
18	X	106	SER
20	Z	82	MET
20	Z	255	LEU
21	N	612	SER
21	N	742	TRP
21	N	790	GLU
22	S	108	ALA
23	P	273	TYR
24	Q	149	LYS
25	R	182	ASN
28	H	112	SER
28	H	343	PHE
28	H	348	ASN
29	I	115	ASP
29	I	126	PRO
29	I	173	MET
29	I	229	LYS
30	K	104	ASP
30	K	160	VAL
31	L	177	GLU
31	L	292	SER
31	L	322	LYS
32	M	344	ASP
33	J	4	ALA
33	J	69	GLY

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Mol	Chain	Res	Type
33	J	72	VAL
33	J	119	SER
33	J	261	SER
33	J	285	SER
2	b	41	ASN
5	e	53	ARG
6	f	58	SER
6	f	203	ASP
8	h	49	LYS
9	i	212	ASP
9	i	223	ASN
10	j	56	LEU
11	k	4	ILE
5	E	126	GLY
5	E	128	SER
5	E	169	ALA
9	2	60	CYS
10	3	157	ASN
11	4	150	PRO
14	7	60	LEU
14	7	173	PRO
15	W	149	GLN
15	W	166	GLU
19	Y	49	ILE
19	Y	55	THR
20	Z	611	THR
20	Z	825	ALA
20	Z	887	GLY
20	Z	926	ASN
20	Z	940	GLY
21	N	87	ASP
21	N	123	PHE
21	N	393	SER
22	S	97	THR
22	S	172	ASN
23	P	109	SER
23	P	328	ALA
27	O	71	ASP
27	O	204	SER
28	H	94	GLU
28	H	181	TYR
30	K	167	PRO

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Mol	Chain	Res	Type
30	K	206	PRO
30	K	334	LEU
32	M	296	SER
33	J	82	LYS
33	J	180	ALA
33	J	281	GLY
4	d	40	ASN
5	e	16	SER
5	e	126	GLY
8	h	101	ASN
8	h	154	ASN
10	j	8	ASN
11	k	176	PHE
13	m	208	ASP
14	n	249	ASN
9	2	174	ASP
11	4	11	ASP
12	5	93	SER
14	7	80	ASP
19	Y	32	ASP
20	Z	142	ASP
20	Z	205	LEU
20	Z	233	LEU
20	Z	578	GLY
20	Z	947	GLY
21	N	842	ASN
21	N	861	TYR
22	S	448	LEU
22	S	450	ASN
23	P	3	ARG
23	P	68	SER
24	Q	46	VAL
24	Q	67	THR
24	Q	110	SER
24	Q	170	ASP
24	Q	230	LYS
26	U	42	ASN
28	H	124	ASN
28	H	139	ASP
29	I	134	SER
30	K	308	GLN
30	K	327	ALA

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Mol	Chain	Res	Type
32	M	223	PRO
33	J	228	ARG
33	J	252	SER
2	b	17	LYS
4	d	217	PRO
6	f	205	SER
8	h	138	SER
10	j	157	ASN
11	k	11	ASP
14	n	35	GLN
13	6	48	GLU
14	7	43	SER
15	W	180	LEU
16	V	175	SER
16	V	262	THR
18	X	55	LYS
19	Y	31	GLU
20	Z	25	PRO
20	Z	65	GLU
20	Z	463	HIS
20	Z	557	GLU
20	Z	789	GLN
21	N	397	SER
23	P	89	LEU
24	Q	48	ASP
24	Q	289	GLU
24	Q	309	ARG
25	R	72	VAL
25	R	125	GLU
27	O	70	TYR
27	O	120	LYS
28	H	152	ILE
28	H	203	LYS
28	H	282	LYS
32	M	105	ASN
32	M	151	ASP
32	M	179	THR
32	M	230	LEU
33	J	141	LYS
33	J	213	VAL
33	J	221	LYS
33	J	251	ASP

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Mol	Chain	Res	Type
33	J	280	ASP
33	J	287	ASN
33	J	341	ILE
1	a	60	PRO
1	a	75	ILE
5	E	13	SER
5	E	53	ARG
13	6	40	ASP
16	V	185	ILE
17	T	171	ILE
18	X	39	GLU
20	Z	802	ASP
22	S	44	THR
22	S	113	SER
27	O	56	PRO
32	M	215	PRO
6	f	11	VAL
13	m	12	PRO
11	4	9	VAL
15	W	117	PRO
16	V	72	PRO
21	N	744	PRO
16	V	46	PRO
23	P	130	ILE
32	M	91	ILE
7	g	131	PRO
8	h	32	GLY
20	Z	886	VAL
28	H	314	VAL
30	K	415	VAL
4	d	102	ASP
10	j	102	PRO
8	1	123	PRO
30	K	274	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/206 (100%)	204 (99%)	2 (1%)	68	76
1	a	206/206 (100%)	201 (98%)	5 (2%)	43	62
2	B	208/208 (100%)	207 (100%)	1 (0%)	81	82
2	b	208/208 (100%)	204 (98%)	4 (2%)	50	66
3	C	203/203 (100%)	202 (100%)	1 (0%)	81	82
3	c	203/203 (100%)	197 (97%)	6 (3%)	36	56
4	D	210/224 (94%)	209 (100%)	1 (0%)	81	82
4	d	224/224 (100%)	216 (96%)	8 (4%)	31	52
5	E	200/200 (100%)	196 (98%)	4 (2%)	48	65
5	e	200/200 (100%)	190 (95%)	10 (5%)	22	42
6	F	190/190 (100%)	189 (100%)	1 (0%)	81	82
6	f	190/190 (100%)	182 (96%)	8 (4%)	26	47
7	G	200/200 (100%)	196 (98%)	4 (2%)	48	65
7	g	200/200 (100%)	189 (94%)	11 (6%)	19	40
8	1	162/162 (100%)	157 (97%)	5 (3%)	35	55
8	h	162/162 (100%)	155 (96%)	7 (4%)	26	47
9	2	185/185 (100%)	181 (98%)	4 (2%)	45	63
9	i	185/185 (100%)	179 (97%)	6 (3%)	34	55
10	3	172/172 (100%)	168 (98%)	4 (2%)	44	63
10	j	172/172 (100%)	167 (97%)	5 (3%)	37	57
11	4	173/173 (100%)	169 (98%)	4 (2%)	44	63
11	k	173/173 (100%)	170 (98%)	3 (2%)	53	67
12	5	169/169 (100%)	165 (98%)	4 (2%)	43	62
12	l	169/169 (100%)	165 (98%)	4 (2%)	43	62
13	6	185/185 (100%)	182 (98%)	3 (2%)	55	69
13	m	185/185 (100%)	178 (96%)	7 (4%)	29	50
14	7	195/198 (98%)	187 (96%)	8 (4%)	27	48
14	n	198/198 (100%)	192 (97%)	6 (3%)	36	56
15	W	171/171 (100%)	163 (95%)	8 (5%)	23	44
16	V	253/253 (100%)	251 (99%)	2 (1%)	73	78
17	T	249/249 (100%)	241 (97%)	8 (3%)	34	55
18	X	116/116 (100%)	111 (96%)	5 (4%)	26	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	Y	81/81 (100%)	79 (98%)	2 (2%)	42	61
20	Z	773/828 (93%)	754 (98%)	19 (2%)	42	61
21	N	776/776 (100%)	760 (98%)	16 (2%)	47	64
22	S	447/447 (100%)	436 (98%)	11 (2%)	42	61
23	P	412/412 (100%)	407 (99%)	5 (1%)	63	74
24	Q	391/391 (100%)	378 (97%)	13 (3%)	33	54
25	R	356/356 (100%)	348 (98%)	8 (2%)	45	63
26	U	277/277 (100%)	268 (97%)	9 (3%)	34	55
27	O	363/363 (100%)	349 (96%)	14 (4%)	28	49
28	H	352/352 (100%)	345 (98%)	7 (2%)	48	65
29	I	342/342 (100%)	331 (97%)	11 (3%)	34	55
30	K	346/346 (100%)	333 (96%)	13 (4%)	29	50
31	L	332/332 (100%)	321 (97%)	11 (3%)	33	54
32	M	364/364 (100%)	357 (98%)	7 (2%)	50	66
33	J	352/352 (100%)	337 (96%)	15 (4%)	26	47
All	All	12086/12158 (99%)	11766 (97%)	320 (3%)	41	60

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	45	VAL
1	a	78	THR
1	a	86	PRO
1	a	95	LEU
1	a	175	GLN
2	b	84	VAL
2	b	97	TYR
2	b	119	GLN
2	b	217	GLU
3	c	11	THR
3	c	54	SER
3	c	108	VAL
3	c	111	LEU
3	c	141	ASP
3	c	163	ILE
4	d	11	PHE
4	d	42	VAL

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Mol	Chain	Res	Type
4	d	119	ARG
4	d	126	VAL
4	d	158	SER
4	d	187	THR
4	d	240	LYS
4	d	243	GLN
5	e	21	LEU
5	e	36	THR
5	e	47	VAL
5	e	71	ASP
5	e	110	GLU
5	e	121	LEU
5	e	142	LEU
5	e	188	HIS
5	e	214	GLU
5	e	225	GLN
6	f	7	ASP
6	f	12	THR
6	f	23	GLU
6	f	67	ASP
6	f	72	LEU
6	f	92	CYS
6	f	189	LEU
6	f	226	ASP
7	g	9	ASP
7	g	46	VAL
7	g	50	VAL
7	g	69	VAL
7	g	109	ILE
7	g	129	VAL
7	g	175	GLU
7	g	185	GLU
7	g	202	LEU
7	g	212	PHE
7	g	220	SER
8	h	16	THR
8	h	18	LYS
8	h	40	THR
8	h	90	VAL
8	h	185	VAL
8	h	188	THR
8	h	199	PRO

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Mol	Chain	Res	Type
9	i	97	LEU
9	i	109	LEU
9	i	148	THR
9	i	206	VAL
9	i	212	ASP
9	i	246	ILE
10	j	11	ILE
10	j	61	THR
10	j	156	PRO
10	j	172	LEU
10	j	183	TRP
11	k	93	ARG
11	k	141	PHE
11	k	180	ILE
12	l	79	LEU
12	l	174	THR
12	l	186	THR
12	l	215	LEU
13	m	94	ILE
13	m	109	ARG
13	m	115	VAL
13	m	167	GLN
13	m	180	LEU
13	m	201	GLU
13	m	217	LYS
14	n	36	GLN
14	n	55	ILE
14	n	137	ARG
14	n	165	LEU
14	n	189	ARG
14	n	258	ILE
1	A	139	VAL
1	A	175	GLN
2	B	119	GLN
3	C	152	ASN
4	D	11	PHE
5	E	22	PHE
5	E	68	VAL
5	E	121	LEU
5	E	136	ARG
6	F	21	GLN
7	G	121	GLN

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Mol	Chain	Res	Type
7	G	185	GLU
7	G	212	PHE
7	G	218	TRP
8	1	66	ASP
8	1	116	LYS
8	1	135	ILE
8	1	144	TYR
8	1	199	PRO
9	2	88	ILE
9	2	147	SER
9	2	233	LYS
9	2	236	ARG
10	3	51	LEU
10	3	147	PHE
10	3	166	THR
10	3	172	LEU
11	4	29	LYS
11	4	40	PRO
11	4	72	ASP
11	4	186	LYS
12	5	151	VAL
12	5	186	THR
12	5	193	ASP
12	5	195	THR
13	6	20	ILE
13	6	39	THR
13	6	61	SER
14	7	34	THR
14	7	39	VAL
14	7	53	VAL
14	7	96	ILE
14	7	115	ASP
14	7	131	THR
14	7	214	MET
14	7	230	LEU
15	W	103	ASN
15	W	139	VAL
15	W	155	ASP
15	W	171	LEU
15	W	174	VAL
15	W	187	SER
15	W	191	ILE

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Mol	Chain	Res	Type
15	W	194	GLU
16	V	58	VAL
16	V	189	ILE
17	T	46	ILE
17	T	78	PHE
17	T	96	LEU
17	T	150	ARG
17	T	200	LEU
17	T	224	ARG
17	T	238	GLN
17	T	257	THR
18	X	11	ARG
18	X	14	VAL
18	X	33	ILE
18	X	36	LYS
18	X	78	ILE
19	Y	3	THR
19	Y	66	ASP
20	Z	27	LYS
20	Z	57	LYS
20	Z	156	HIS
20	Z	171	LYS
20	Z	221	VAL
20	Z	222	ASP
20	Z	255	LEU
20	Z	386	VAL
20	Z	563	VAL
20	Z	566	LEU
20	Z	613	ASP
20	Z	624	LEU
20	Z	728	LYS
20	Z	729	GLU
20	Z	734	ASP
20	Z	748	LEU
20	Z	842	GLN
20	Z	927	VAL
20	Z	951	GLN
21	N	71	ASN
21	N	79	VAL
21	N	98	VAL
21	N	104	LYS
21	N	343	THR

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Mol	Chain	Res	Type
21	N	373	VAL
21	N	434	SER
21	N	496	GLU
21	N	534	ASP
21	N	665	ILE
21	N	823	PRO
21	N	829	LYS
21	N	840	GLU
21	N	871	MET
21	N	873	ARG
21	N	900	ASN
22	S	57	LEU
22	S	72	GLU
22	S	89	LYS
22	S	93	LEU
22	S	101	LYS
22	S	145	PHE
22	S	169	CYS
22	S	219	LYS
22	S	339	GLN
22	S	353	LYS
22	S	455	GLU
23	P	6	PRO
23	P	75	LEU
23	P	224	LEU
23	P	370	ASP
23	P	396	PRO
24	Q	64	LEU
24	Q	66	VAL
24	Q	79	PRO
24	Q	91	SER
24	Q	94	VAL
24	Q	214	THR
24	Q	233	LYS
24	Q	323	LYS
24	Q	359	ILE
24	Q	384	LYS
24	Q	385	ILE
24	Q	389	VAL
24	Q	406	ASP
25	R	146	ASP
25	R	162	ILE

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Mol	Chain	Res	Type
25	R	168	ILE
25	R	243	LEU
25	R	336	LYS
25	R	337	VAL
25	R	375	LYS
25	R	413	LYS
26	U	13	LEU
26	U	28	LYS
26	U	125	VAL
26	U	130	VAL
26	U	161	ILE
26	U	212	ASP
26	U	223	HIS
26	U	224	THR
26	U	268	LYS
27	O	47	LYS
27	O	78	VAL
27	O	87	LYS
27	O	173	SER
27	O	198	THR
27	O	207	LEU
27	O	258	LEU
27	O	270	ILE
27	O	320	PRO
27	O	329	MET
27	O	348	VAL
27	O	350	ILE
27	O	355	PRO
27	O	393	VAL
28	H	44	PRO
28	H	59	ILE
28	H	217	GLN
28	H	219	GLU
28	H	267	THR
28	H	360	THR
28	H	375	VAL
29	I	66	LYS
29	I	71	LEU
29	I	112	ILE
29	I	120	VAL
29	I	133	LEU
29	I	171	MET

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Mol	Chain	Res	Type
29	I	181	TYR
29	I	187	LEU
29	I	192	GLN
29	I	344	ILE
29	I	352	ASN
30	K	51	LEU
30	K	67	TYR
30	K	89	ILE
30	K	121	ARG
30	K	135	MET
30	K	161	MET
30	K	183	GLU
30	K	206	PRO
30	K	236	ARG
30	K	310	THR
30	K	379	SER
30	K	387	MET
30	K	401	VAL
31	L	63	LYS
31	L	135	VAL
31	L	137	ARG
31	L	199	LEU
31	L	261	ARG
31	L	284	ASP
31	L	312	MET
31	L	321	THR
31	L	333	LEU
31	L	415	LEU
31	L	432	ILE
32	M	18	LEU
32	M	62	ILE
32	M	94	LYS
32	M	146	VAL
32	M	172	VAL
32	M	256	ILE
32	M	426	LYS
33	J	2	THR
33	J	22	TYR
33	J	32	LEU
33	J	53	ASP
33	J	83	LYS
33	J	145	SER

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Mol	Chain	Res	Type
33	J	228	ARG
33	J	289	LYS
33	J	299	ILE
33	J	304	LEU
33	J	309	ARG
33	J	310	ILE
33	J	338	THR
33	J	358	VAL
33	J	388	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (336) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	41	ASN
1	a	56	GLN
1	a	92	ASN
1	a	209	HIS
1	a	251	GLN
2	b	94	HIS
2	b	119	GLN
2	b	139	HIS
2	b	149	GLN
3	c	31	HIS
3	c	94	HIS
3	c	96	GLN
3	c	152	ASN
4	d	19	GLN
4	d	70	HIS
4	d	96	HIS
4	d	117	GLN
4	d	118	GLN
4	d	122	GLN
4	d	149	GLN
4	d	230	ASN
5	e	73	HIS
5	e	188	HIS
6	f	4	ASN
6	f	43	HIS
6	f	69	HIS
6	f	117	GLN
7	g	12	ASN
7	g	68	GLN

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Mol	Chain	Res	Type
7	g	204	HIS
7	g	207	ASN
8	h	37	ASN
8	h	47	HIS
8	h	62	GLN
8	h	101	ASN
9	i	38	ASN
9	i	39	ASN
9	i	173	GLN
9	i	189	GLN
9	i	201	ASN
9	i	223	ASN
9	i	248	ASN
9	i	253	GLN
10	j	38	ASN
10	j	48	HIS
10	j	72	ASN
10	j	113	ASN
10	j	145	GLN
10	j	204	GLN
11	k	65	GLN
11	k	86	GLN
11	k	101	ASN
11	k	118	GLN
11	k	146	HIS
11	k	147	HIS
12	l	128	GLN
12	l	141	HIS
12	l	254	HIS
12	l	266	HIS
12	l	283	ASN
13	m	11	ASN
13	m	78	ASN
13	m	87	HIS
13	m	100	ASN
13	m	103	HIS
13	m	161	GLN
13	m	167	GLN
13	m	173	ASN
14	n	70	ASN
14	n	111	ASN
14	n	236	ASN

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Mol	Chain	Res	Type
1	A	15	HIS
1	A	175	GLN
1	A	181	ASN
1	A	184	ASN
1	A	185	HIS
1	A	209	HIS
1	A	221	ASN
2	B	20	GLN
2	B	149	GLN
2	B	190	HIS
2	B	205	ASN
2	B	218	ASN
2	B	244	ASN
3	C	21	GLN
3	C	31	HIS
3	C	221	ASN
3	C	227	GLN
3	C	233	GLN
4	D	16	HIS
4	D	19	GLN
4	D	231	GLN
4	D	235	GLN
5	E	99	HIS
5	E	154	GLN
5	E	206	GLN
5	E	216	ASN
5	E	225	GLN
6	F	117	GLN
6	F	121	GLN
6	F	210	ASN
7	G	12	ASN
7	G	68	GLN
7	G	87	HIS
7	G	121	GLN
7	G	123	HIS
7	G	183	HIS
7	G	195	GLN
7	G	204	HIS
7	G	248	ASN
8	1	37	ASN
8	1	101	ASN
8	1	154	ASN

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Mol	Chain	Res	Type
9	2	91	ASN
9	2	248	ASN
10	3	8	ASN
10	3	48	HIS
10	3	64	ASN
10	3	113	ASN
11	4	10	GLN
11	4	63	ASN
11	4	78	GLN
11	4	99	GLN
11	4	101	ASN
11	4	118	GLN
11	4	133	HIS
11	4	146	HIS
12	5	141	HIS
12	5	164	GLN
12	5	241	HIS
12	5	251	ASN
12	5	263	HIS
13	6	11	ASN
13	6	16	ASN
13	6	63	ASN
13	6	78	ASN
13	6	84	HIS
13	6	87	HIS
13	6	160	ASN
13	6	163	ASN
13	6	203	HIS
14	7	35	GLN
14	7	36	GLN
14	7	51	ASN
14	7	107	ASN
14	7	155	ASN
14	7	182	HIS
15	W	12	ASN
15	W	42	ASN
15	W	77	HIS
15	W	86	HIS
15	W	106	GLN
15	W	136	ASN
15	W	170	HIS
16	V	40	HIS

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Mol	Chain	Res	Type
16	V	111	HIS
16	V	167	ASN
16	V	181	ASN
16	V	195	HIS
16	V	217	HIS
16	V	291	ASN
17	T	38	ASN
17	T	53	ASN
17	T	74	ASN
17	T	117	ASN
17	T	123	HIS
17	T	158	GLN
17	T	204	ASN
17	T	212	ASN
17	T	236	ASN
17	T	238	GLN
17	T	258	ASN
18	X	30	GLN
18	X	38	ASN
18	X	94	ASN
18	X	112	ASN
18	X	130	ASN
18	X	131	ASN
19	Y	9	GLN
19	Y	58	ASN
19	Y	75	ASN
20	Z	23	GLN
20	Z	214	HIS
20	Z	307	HIS
20	Z	380	ASN
20	Z	429	ASN
20	Z	434	GLN
20	Z	502	ASN
20	Z	532	HIS
20	Z	539	ASN
20	Z	577	GLN
20	Z	622	HIS
20	Z	628	ASN
20	Z	760	HIS
20	Z	763	HIS
20	Z	766	HIS
20	Z	769	ASN

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Mol	Chain	Res	Type
20	Z	789	GLN
20	Z	897	HIS
20	Z	926	ASN
20	Z	931	GLN
20	Z	938	GLN
20	Z	958	ASN
21	N	17	GLN
21	N	256	GLN
21	N	305	ASN
21	N	340	HIS
21	N	352	ASN
21	N	361	ASN
21	N	430	ASN
21	N	444	HIS
21	N	472	ASN
21	N	509	GLN
21	N	510	HIS
21	N	580	ASN
21	N	613	HIS
21	N	616	HIS
21	N	690	HIS
21	N	703	GLN
21	N	707	ASN
21	N	719	ASN
21	N	738	GLN
21	N	870	ASN
21	N	900	ASN
22	S	20	HIS
22	S	139	HIS
22	S	191	HIS
22	S	206	GLN
22	S	225	HIS
22	S	334	HIS
22	S	339	GLN
22	S	378	GLN
22	S	386	ASN
22	S	417	GLN
23	P	86	HIS
23	P	164	GLN
23	P	178	GLN
23	P	263	HIS
23	P	277	GLN

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Mol	Chain	Res	Type
23	P	278	ASN
23	P	282	HIS
23	P	296	GLN
23	P	348	HIS
23	P	366	ASN
23	P	394	ASN
23	P	407	ASN
23	P	413	ASN
23	P	425	HIS
23	P	431	HIS
23	P	440	HIS
24	Q	21	ASN
24	Q	87	GLN
24	Q	159	ASN
24	Q	248	ASN
24	Q	273	ASN
24	Q	372	GLN
25	R	89	ASN
25	R	96	GLN
25	R	118	GLN
25	R	314	ASN
25	R	325	HIS
25	R	366	ASN
25	R	397	ASN
25	R	401	HIS
26	U	21	HIS
26	U	30	ASN
26	U	62	ASN
26	U	70	HIS
26	U	75	ASN
26	U	84	ASN
26	U	94	HIS
26	U	107	ASN
26	U	115	GLN
26	U	127	GLN
26	U	156	HIS
26	U	192	ASN
26	U	222	ASN
26	U	234	ASN
26	U	256	ASN
26	U	280	ASN
26	U	298	ASN

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Mol	Chain	Res	Type
27	O	28	GLN
27	O	40	GLN
27	O	105	GLN
27	O	183	ASN
27	O	256	ASN
27	O	282	GLN
27	O	289	GLN
27	O	345	ASN
28	H	80	HIS
28	H	95	HIS
28	H	109	ASN
28	H	120	ASN
28	H	124	ASN
28	H	128	ASN
28	H	130	ASN
28	H	281	GLN
28	H	413	ASN
29	I	68	HIS
29	I	150	HIS
29	I	151	HIS
29	I	161	GLN
29	I	204	HIS
29	I	352	ASN
29	I	365	HIS
29	I	426	ASN
30	K	36	ASN
30	K	90	GLN
30	K	244	HIS
30	K	388	GLN
31	L	58	ASN
31	L	67	HIS
31	L	73	GLN
31	L	79	GLN
31	L	99	GLN
31	L	189	GLN
32	M	28	GLN
32	M	31	GLN
32	M	55	ASN
32	M	72	ASN
32	M	74	GLN
32	M	96	ASN
32	M	105	ASN

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Mol	Chain	Res	Type
32	M	189	GLN
32	M	310	ASN
32	M	359	GLN
32	M	375	ASN
32	M	390	GLN
32	M	405	ASN
32	M	412	HIS
33	J	15	HIS
33	J	47	GLN
33	J	89	GLN
33	J	123	HIS
33	J	240	HIS
33	J	331	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
36	ATP	K	501	35	32,33,33	4.47	5 (15%)	48,52,52	1.75	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	ADP	H	501	35	28,29,29	1.52	4 (14%)	43,45,45	1.66	7 (16%)
36	ATP	J	501	35	32,33,33	3.77	6 (18%)	48,52,52	1.37	6 (12%)
36	ATP	I	501	35	32,33,33	4.48	6 (18%)	48,52,52	1.72	11 (22%)
34	ADP	M	501	35	28,29,29	2.34	8 (28%)	43,45,45	1.53	6 (13%)
36	ATP	L	501	35	32,33,33	4.45	6 (18%)	48,52,52	1.70	9 (18%)

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
36	ATP	K	501	35	-	4/22/38/38	0/3/3/3
34	ADP	H	501	35	-	4/16/32/32	0/3/3/3
36	ATP	J	501	35	-	5/22/38/38	0/3/3/3
36	ATP	I	501	35	-	5/22/38/38	0/3/3/3
34	ADP	M	501	35	-	4/16/32/32	0/3/3/3
36	ATP	L	501	35	-	6/22/38/38	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	I	501	ATP	PB-O3B	19.33	1.80	1.59
36	L	501	ATP	PB-O3B	19.22	1.80	1.59
36	K	501	ATP	PB-O3B	19.17	1.80	1.59
36	J	501	ATP	PB-O3A	14.78	1.75	1.59
36	J	501	ATP	PB-O3B	13.00	1.73	1.59
36	K	501	ATP	PB-O3A	12.79	1.73	1.59
36	I	501	ATP	PB-O3A	12.68	1.73	1.59
36	L	501	ATP	PB-O3A	12.67	1.73	1.59
36	L	501	ATP	PA-O3A	8.57	1.68	1.59
36	K	501	ATP	PA-O3A	8.57	1.68	1.59
36	I	501	ATP	PA-O3A	8.51	1.68	1.59
34	M	501	ADP	PA-O3A	8.01	1.68	1.59
36	J	501	ATP	PA-O3A	6.03	1.66	1.59
34	H	501	ADP	PA-O3A	5.04	1.64	1.59
34	M	501	ADP	O4'-C4'	4.88	1.55	1.45
34	M	501	ADP	C4-N9	4.41	1.46	1.37
34	M	501	ADP	C4-N3	-3.35	1.28	1.34
34	H	501	ADP	C2'-C3'	-3.21	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	L	501	ATP	C2-N3	2.84	1.39	1.33
36	K	501	ATP	C2-N3	2.83	1.39	1.33
36	I	501	ATP	C2-N3	2.82	1.38	1.33
36	J	501	ATP	C2-N1	-2.65	1.29	1.33
36	K	501	ATP	C5-C4	-2.65	1.34	1.39
36	L	501	ATP	C5-C4	-2.62	1.34	1.39
36	I	501	ATP	C5-C4	-2.60	1.34	1.39
34	H	501	ADP	C5-N7	-2.57	1.34	1.39
34	M	501	ADP	C6-N6	2.50	1.40	1.34
34	H	501	ADP	C6-N1	2.27	1.42	1.35
36	J	501	ATP	C2-N3	2.23	1.37	1.33
36	J	501	ATP	C4-N9	2.20	1.42	1.37
34	M	501	ADP	PB-O2B	-2.08	1.47	1.54
34	M	501	ADP	C5-C4	-2.08	1.35	1.39
34	M	501	ADP	C2-N3	2.07	1.37	1.33
36	I	501	ATP	C2-N1	-2.04	1.30	1.33
36	L	501	ATP	C2-N1	-2.03	1.30	1.33

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	M	501	ADP	C4-N9-C8	-5.80	99.65	105.74
34	H	501	ADP	N3-C2-N1	5.17	136.41	128.58
36	K	501	ATP	O4'-C1'-N9	4.70	117.11	108.09
36	I	501	ATP	O4'-C1'-N9	4.69	117.09	108.09
36	L	501	ATP	O4'-C1'-N9	4.66	117.04	108.09
34	H	501	ADP	N6-C6-N1	4.22	127.77	118.38
36	J	501	ATP	N3-C2-N1	4.09	134.78	128.58
34	H	501	ADP	C2-N1-C6	-4.01	112.15	118.73
34	M	501	ADP	N6-C6-N1	3.89	127.03	118.38
36	L	501	ATP	N6-C6-N1	3.81	126.85	118.38
36	I	501	ATP	N6-C6-N1	3.78	126.81	118.38
36	K	501	ATP	N6-C6-N1	3.77	126.78	118.38
34	H	501	ADP	C5-C6-N6	-3.71	114.09	123.29
36	J	501	ATP	N6-C6-N1	3.67	126.55	118.38
36	I	501	ATP	N9-C8-N7	-3.54	108.92	113.94
36	K	501	ATP	N9-C8-N7	-3.50	108.97	113.94
36	L	501	ATP	N9-C8-N7	-3.47	109.01	113.94
36	I	501	ATP	C4-N9-C8	3.44	109.35	105.74
36	L	501	ATP	C4-N9-C8	3.41	109.32	105.74
36	K	501	ATP	C4-N9-C8	3.38	109.29	105.74
36	K	501	ATP	C6-C5-C4	3.24	121.60	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	I	501	ATP	C6-C5-C4	3.23	121.58	117.18
36	L	501	ATP	C6-C5-C4	3.21	121.56	117.18
34	H	501	ADP	O4'-C1'-N9	3.06	113.96	108.09
36	J	501	ATP	C5-C4-N9	-2.64	102.94	105.81
36	L	501	ATP	C5-C6-N6	-2.62	116.80	123.29
36	K	501	ATP	O3B-PB-O1B	-2.60	102.87	110.70
36	L	501	ATP	O3B-PB-O1B	-2.60	102.88	110.70
36	K	501	ATP	C5-C6-N6	-2.59	116.86	123.29
36	I	501	ATP	C5-C6-N6	-2.59	116.87	123.29
36	K	501	ATP	O3A-PA-O1A	-2.49	103.20	110.70
36	J	501	ATP	C5-C6-N6	-2.48	117.14	123.29
36	I	501	ATP	O3A-PA-O1A	-2.47	103.28	110.70
34	M	501	ADP	C5-C4-N9	2.47	108.50	105.81
36	J	501	ATP	C2-N3-C4	-2.29	106.25	111.83
36	I	501	ATP	N3-C4-N9	2.26	131.02	127.17
36	I	501	ATP	O3G-PG-O2G	2.26	116.27	107.80
36	K	501	ATP	C2-N1-C6	-2.25	115.03	118.73
36	K	501	ATP	O3G-PG-O2G	2.24	116.22	107.80
36	L	501	ATP	N3-C4-N9	2.23	130.97	127.17
34	M	501	ADP	O3B-PB-O2B	2.23	116.16	107.80
36	L	501	ATP	C2-N1-C6	-2.23	115.07	118.73
34	H	501	ADP	O2B-PB-O3A	2.22	112.07	104.64
36	K	501	ATP	N3-C4-N9	2.21	130.93	127.17
36	I	501	ATP	C2-N1-C6	-2.21	115.10	118.73
34	M	501	ADP	C5-C6-N6	-2.14	117.98	123.29
34	M	501	ADP	C5'-C4'-C3'	2.11	122.82	115.21
36	I	501	ATP	C5-N7-C8	2.06	106.68	103.45
34	H	501	ADP	O4'-C4'-C5'	2.03	115.85	109.33
36	J	501	ATP	O3G-PG-O2G	2.01	115.35	107.80
36	K	501	ATP	C5-N7-C8	2.01	106.61	103.45

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	H	501	ADP	C5'-O5'-PA-O2A
34	H	501	ADP	C5'-O5'-PA-O3A
34	M	501	ADP	C5'-O5'-PA-O1A
34	M	501	ADP	C5'-O5'-PA-O3A
36	I	501	ATP	PB-O3B-PG-O2G
36	K	501	ATP	PB-O3B-PG-O2G
36	L	501	ATP	PB-O3B-PG-O2G

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

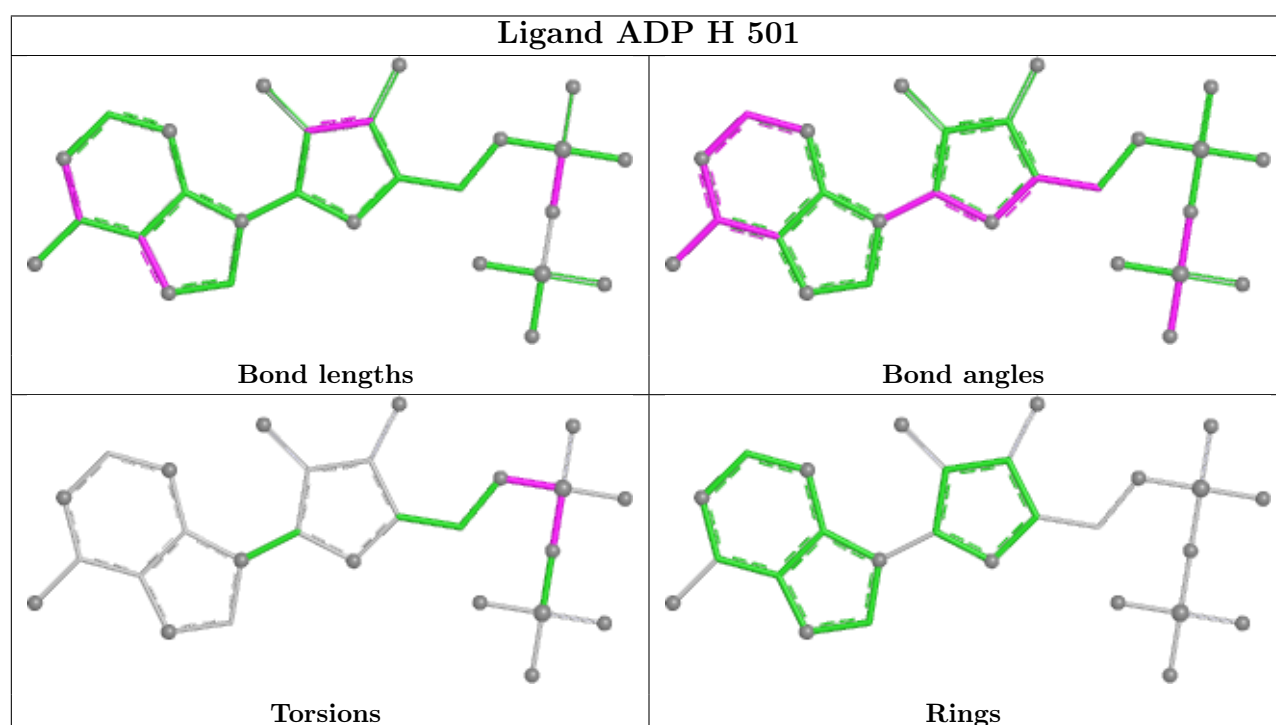
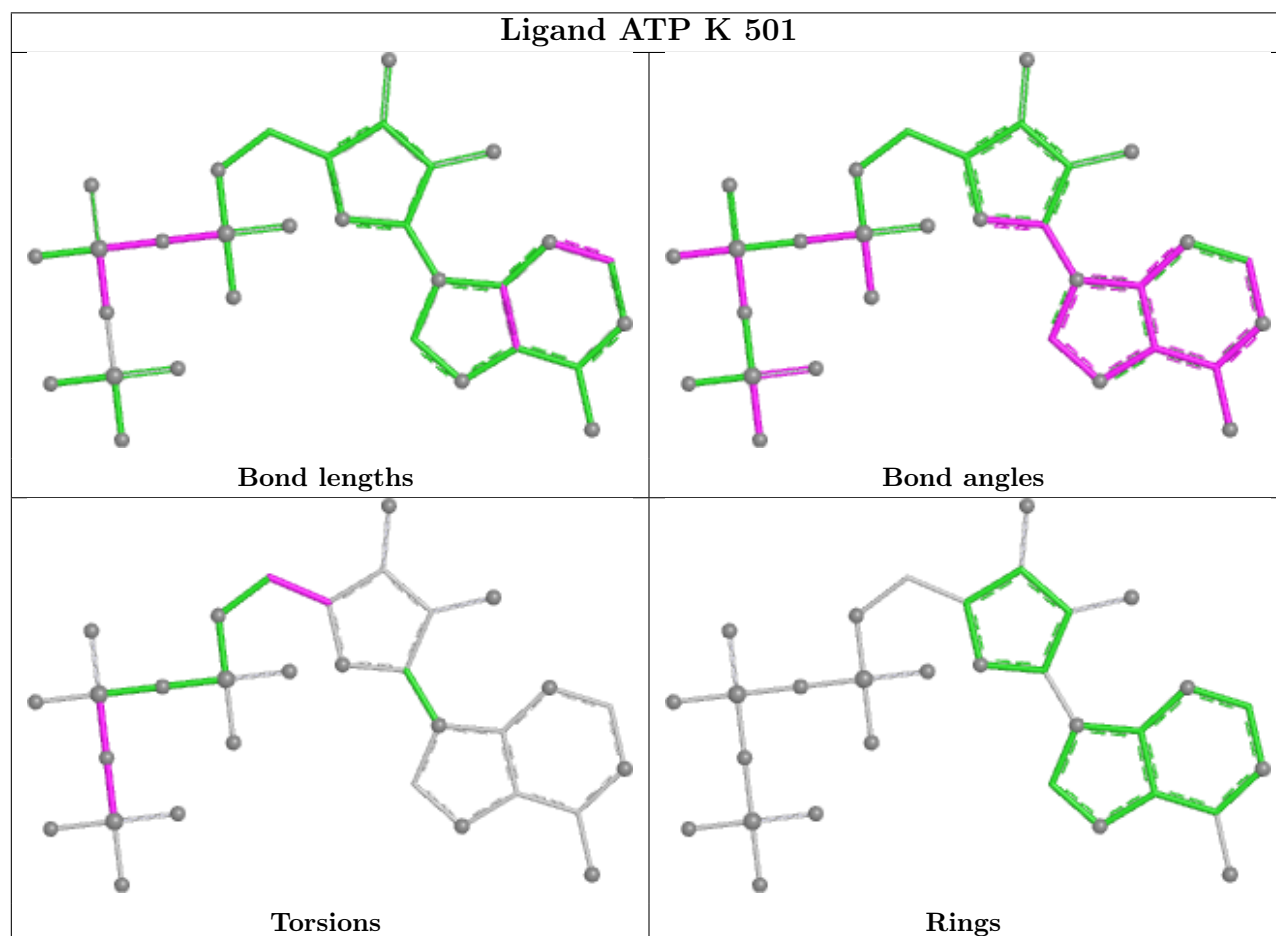
There are no ring outliers.

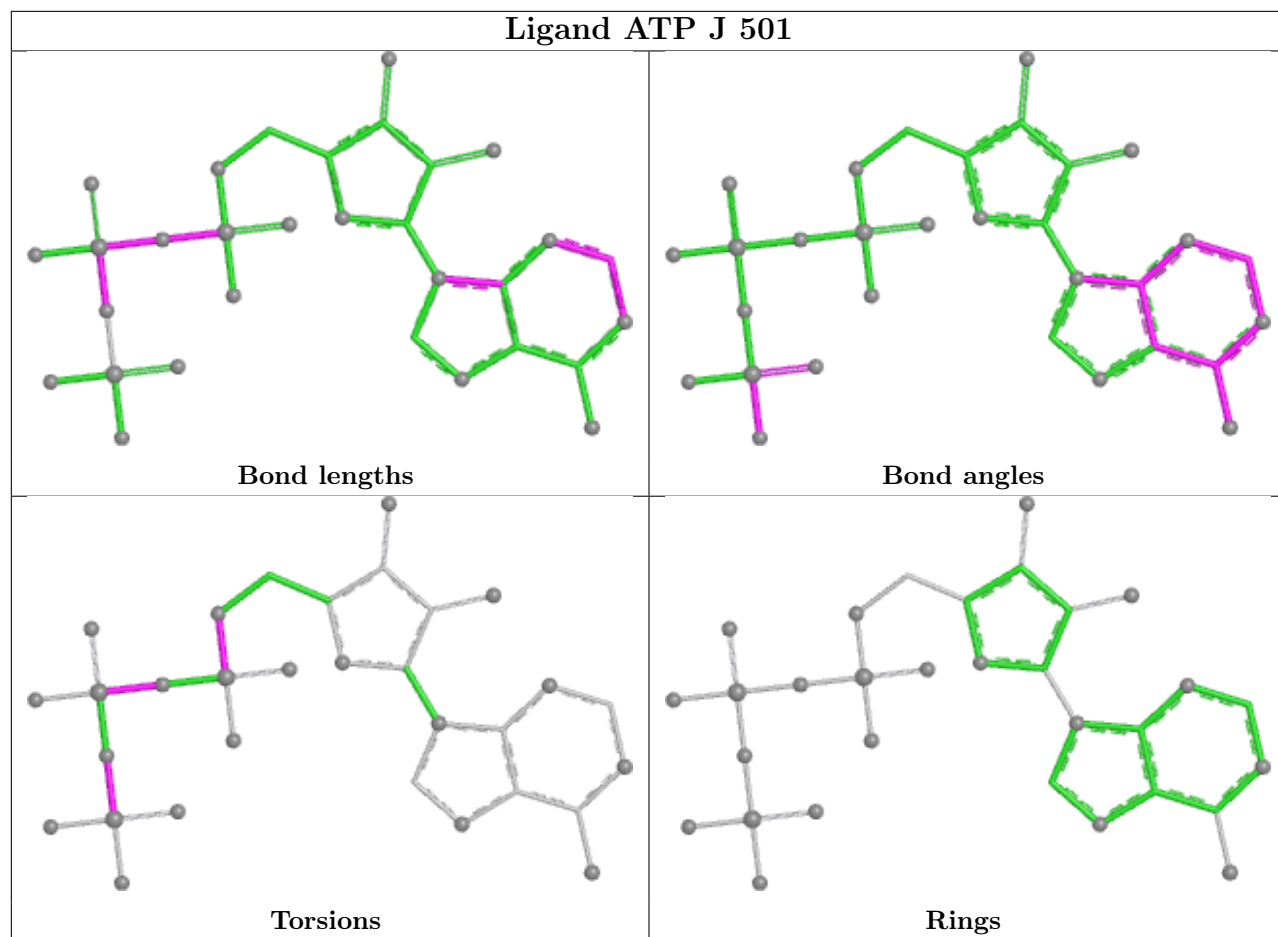
5 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	K	501	ATP	10	0
34	H	501	ADP	14	0
36	J	501	ATP	4	0
36	I	501	ATP	10	0
36	L	501	ATP	13	0

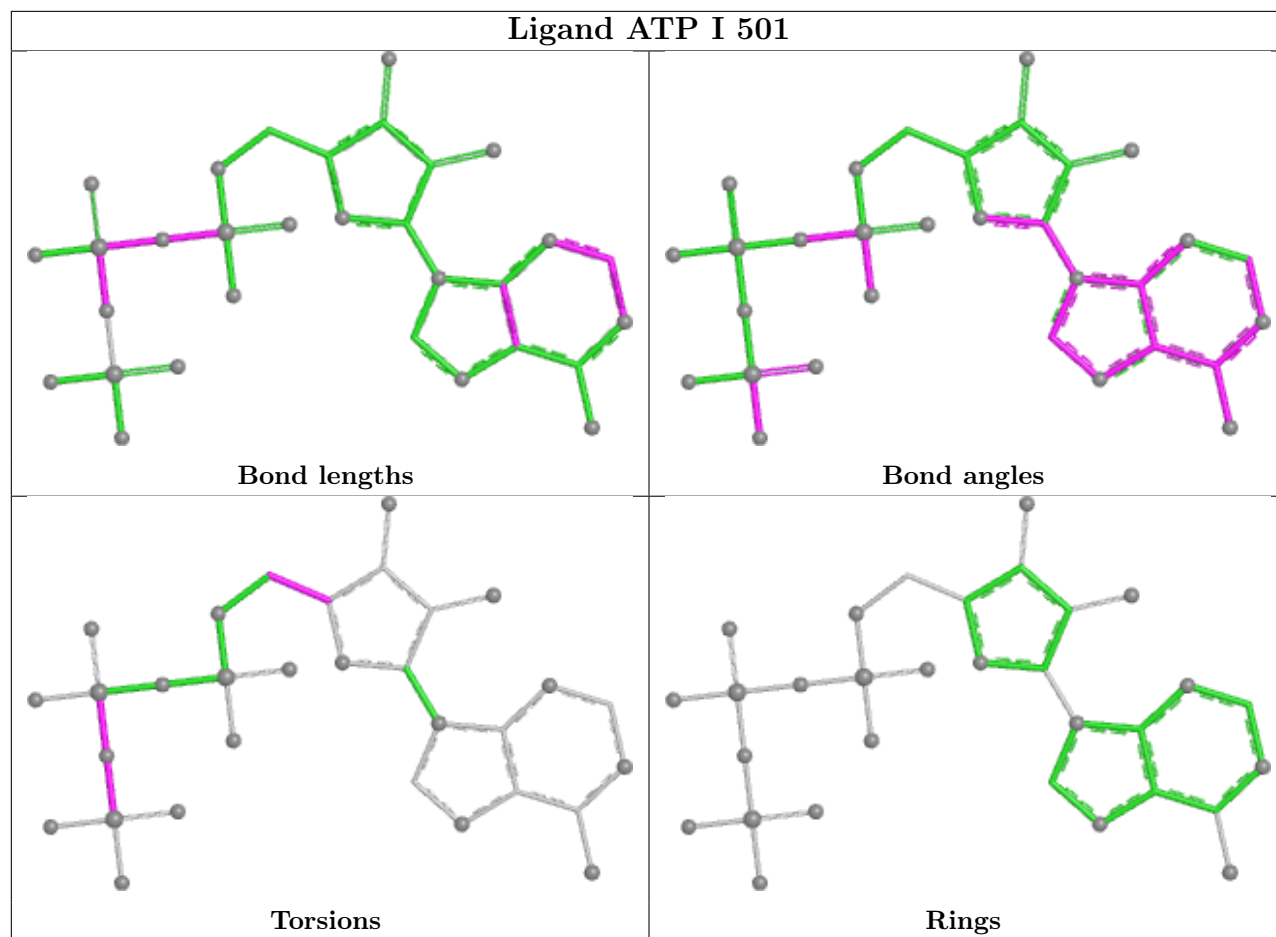
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

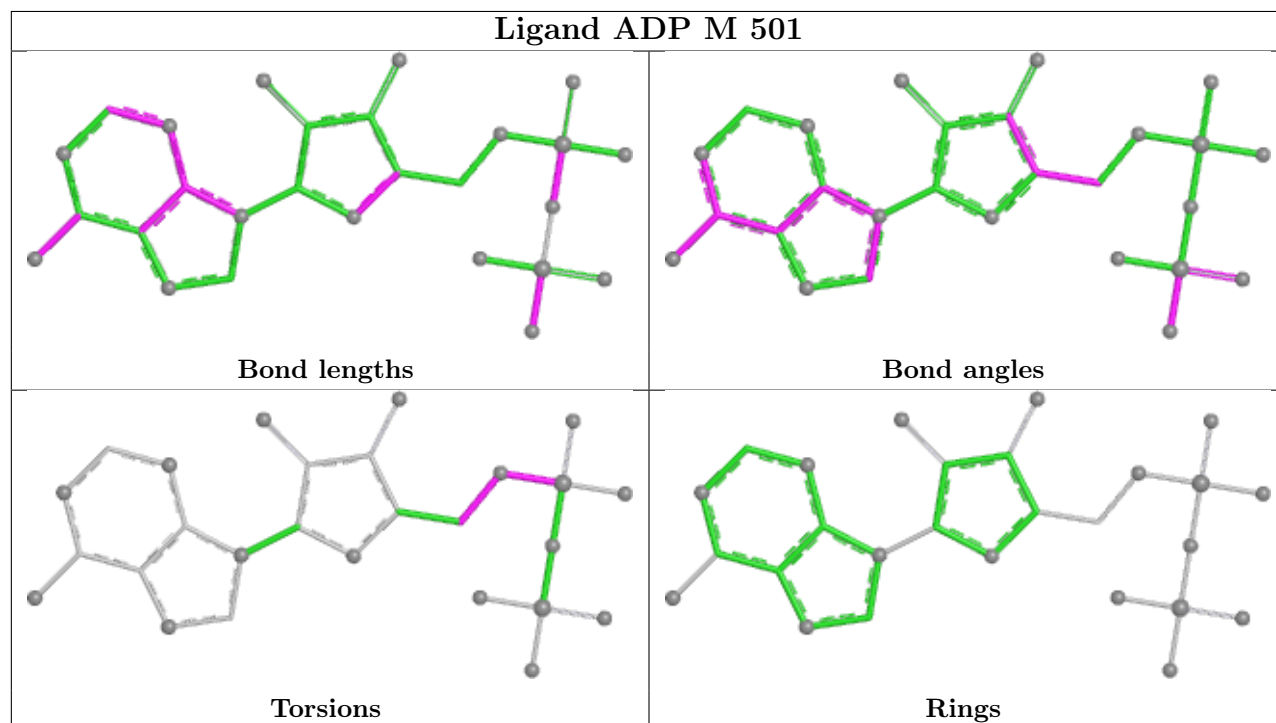


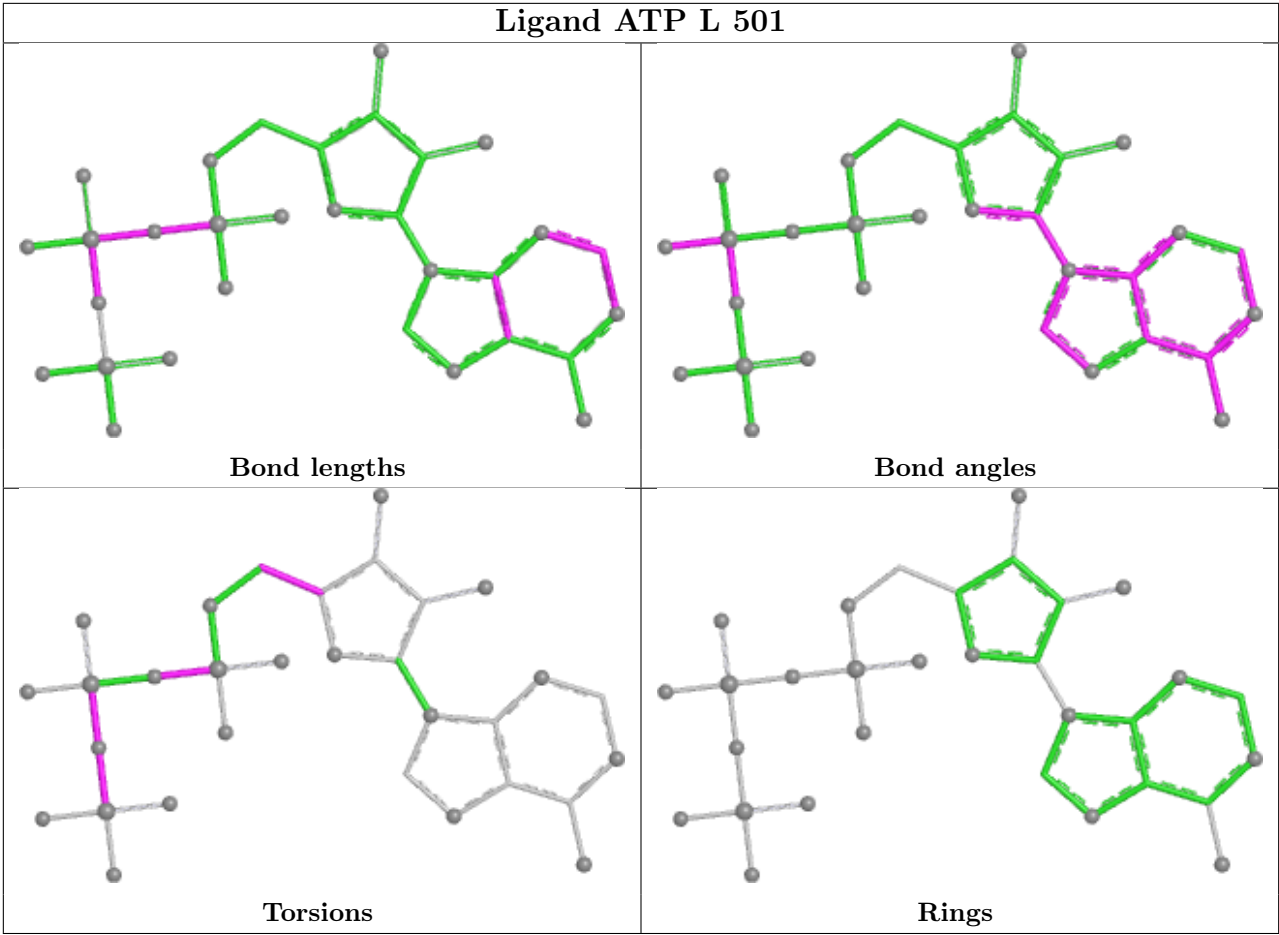


Ligand ATP I 501



Ligand ADP M 501





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
29	I	2
32	M	2
33	J	2
31	L	1
30	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	180:PHE	C	181:ASP	N	2.67

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	183:ASP	C	184:ILE	N	2.58
1	I	186:GLY	C	187:LEU	N	2.56
1	M	338:LEU	C	339:ARG	N	1.69
1	J	212:ARG	C	213:VAL	N	1.68
1	M	342:ARG	C	343:LEU	N	1.18
1	K	220:THR	C	221:MET	N	0.91
1	J	211:ILE	C	212:ARG	N	0.52

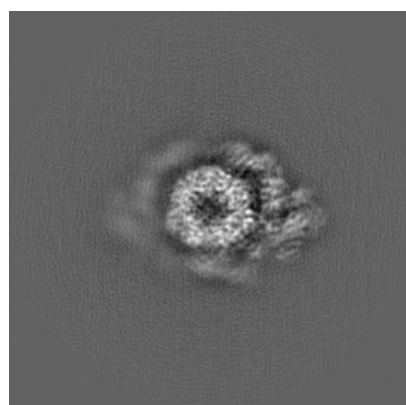
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4321. These allow visual inspection of the internal detail of the map and identification of artifacts.

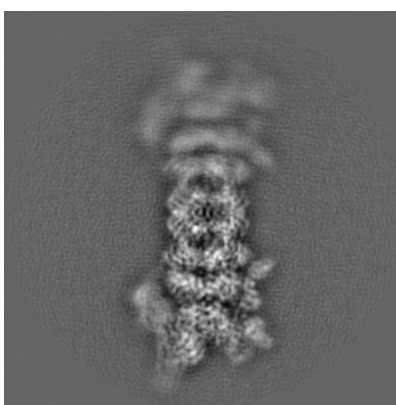
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

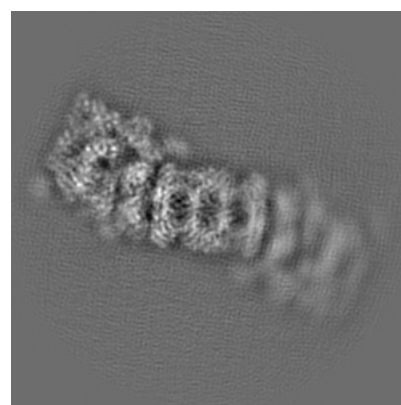
6.1.1 Primary map



X



Y

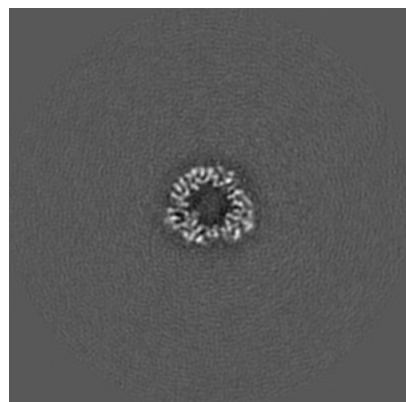


Z

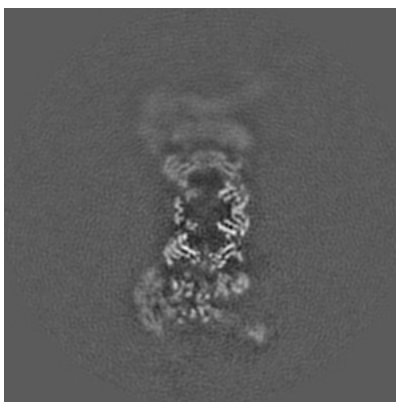
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

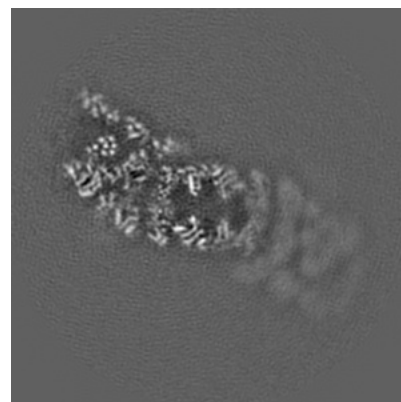
6.2.1 Primary map



X Index: 192



Y Index: 192

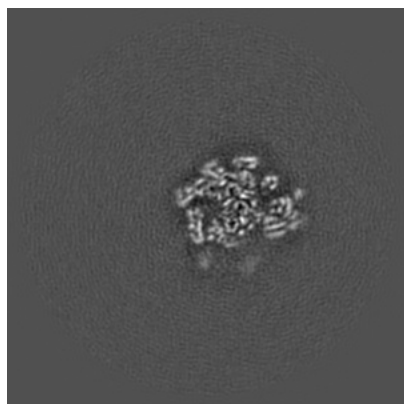


Z Index: 192

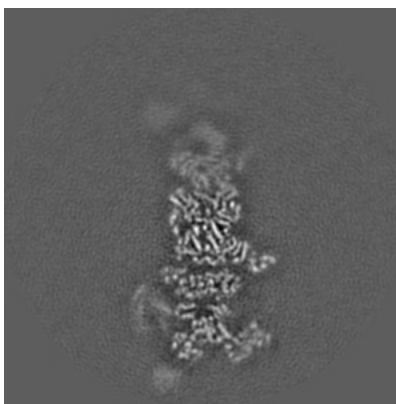
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

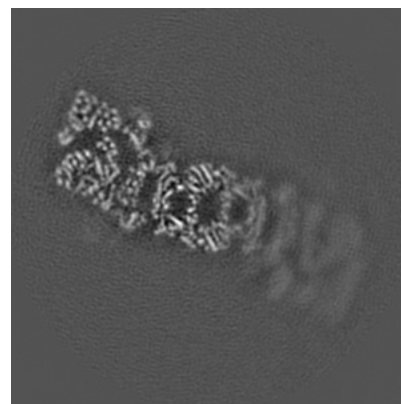
6.3.1 Primary map



X Index: 122



Y Index: 213

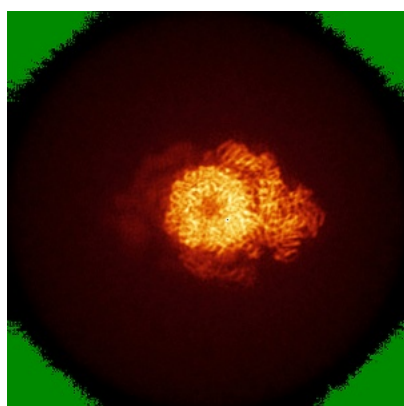


Z Index: 182

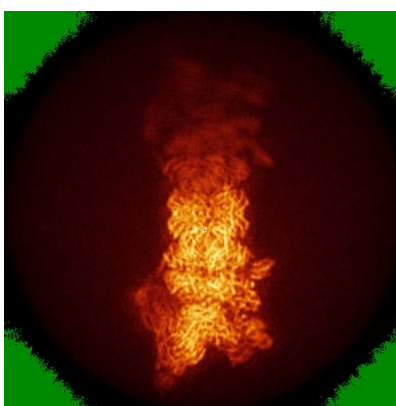
The images above show the largest variance slices of the map in three orthogonal directions.

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

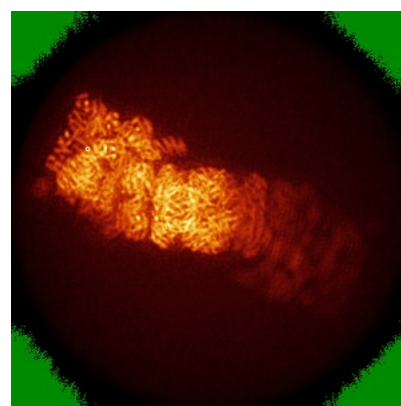
6.4.1 Primary map



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

This section was not generated.

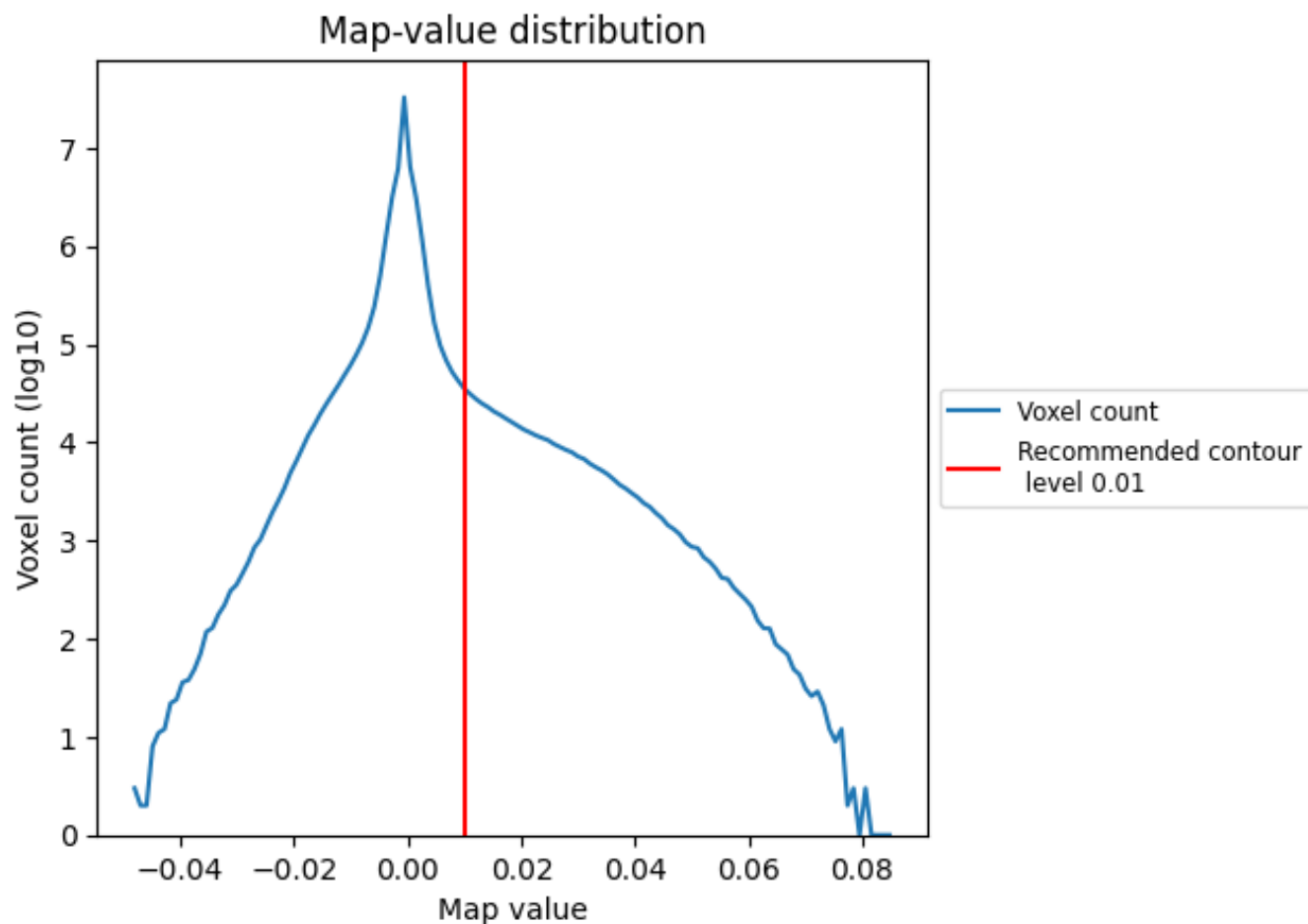
6.6 Mask visualisation

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

7 Map analysis [i](#)

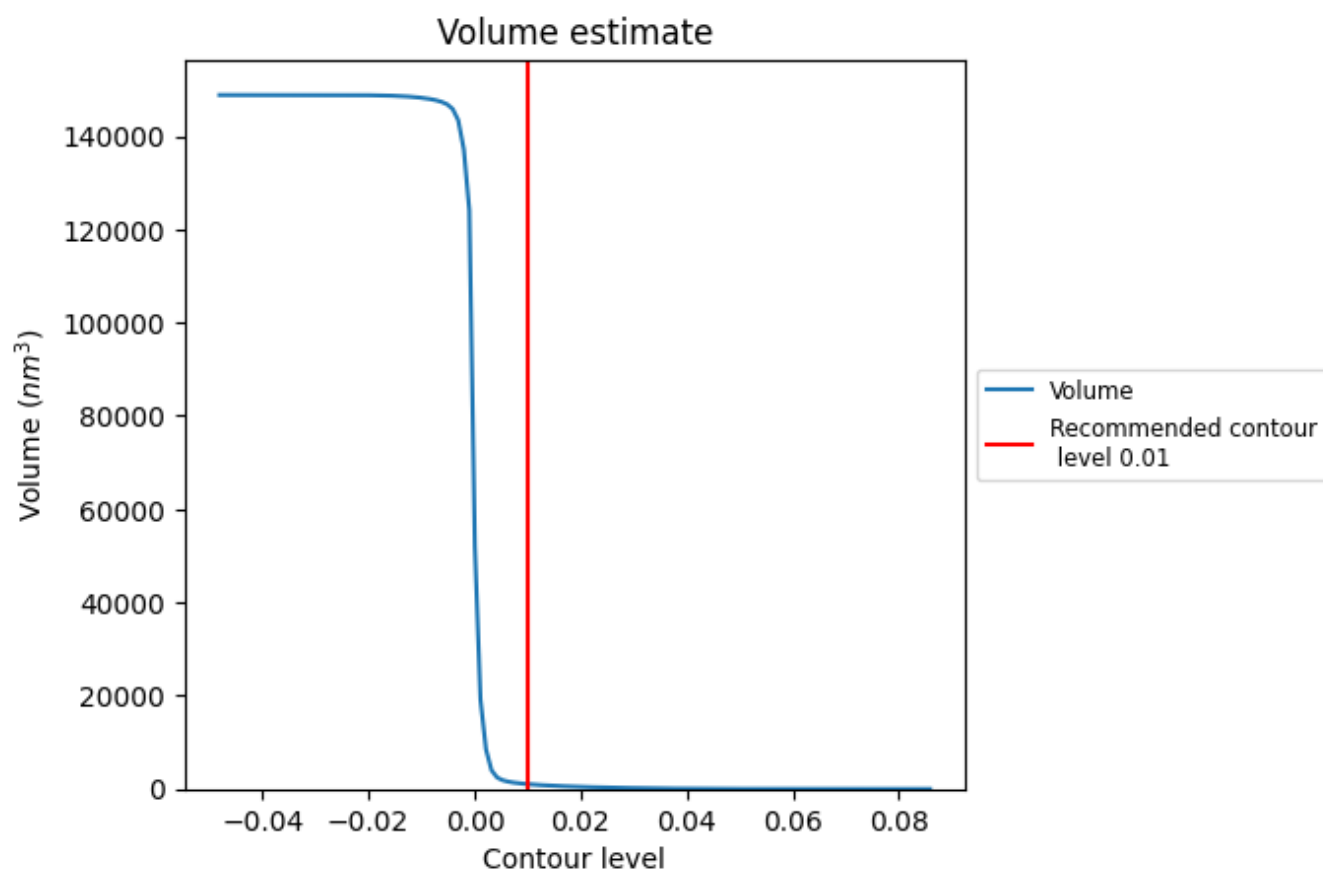
This section contains the results of statistical analysis of the map.

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.

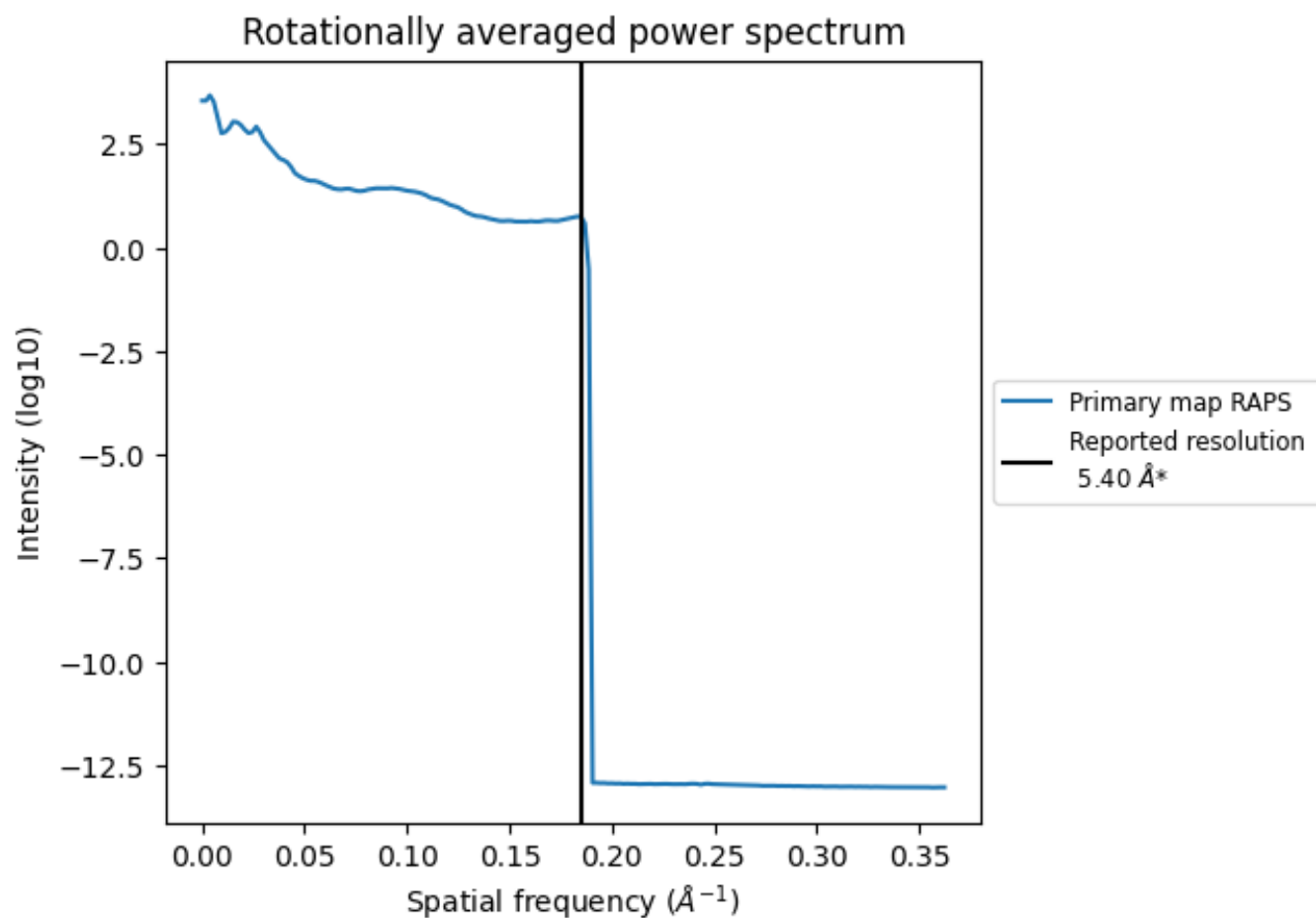
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1039 nm^3 ; this corresponds to an approximate mass of 938 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 0.185 Å⁻¹

8 Fourier-Shell correlation

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

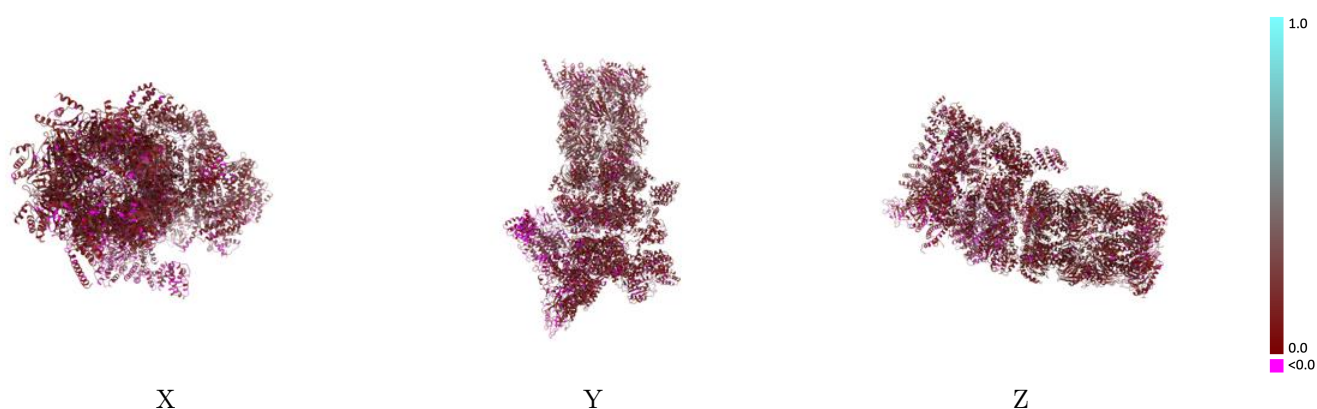
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4321 and PDB model 6FVV. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)

This section was not generated.

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

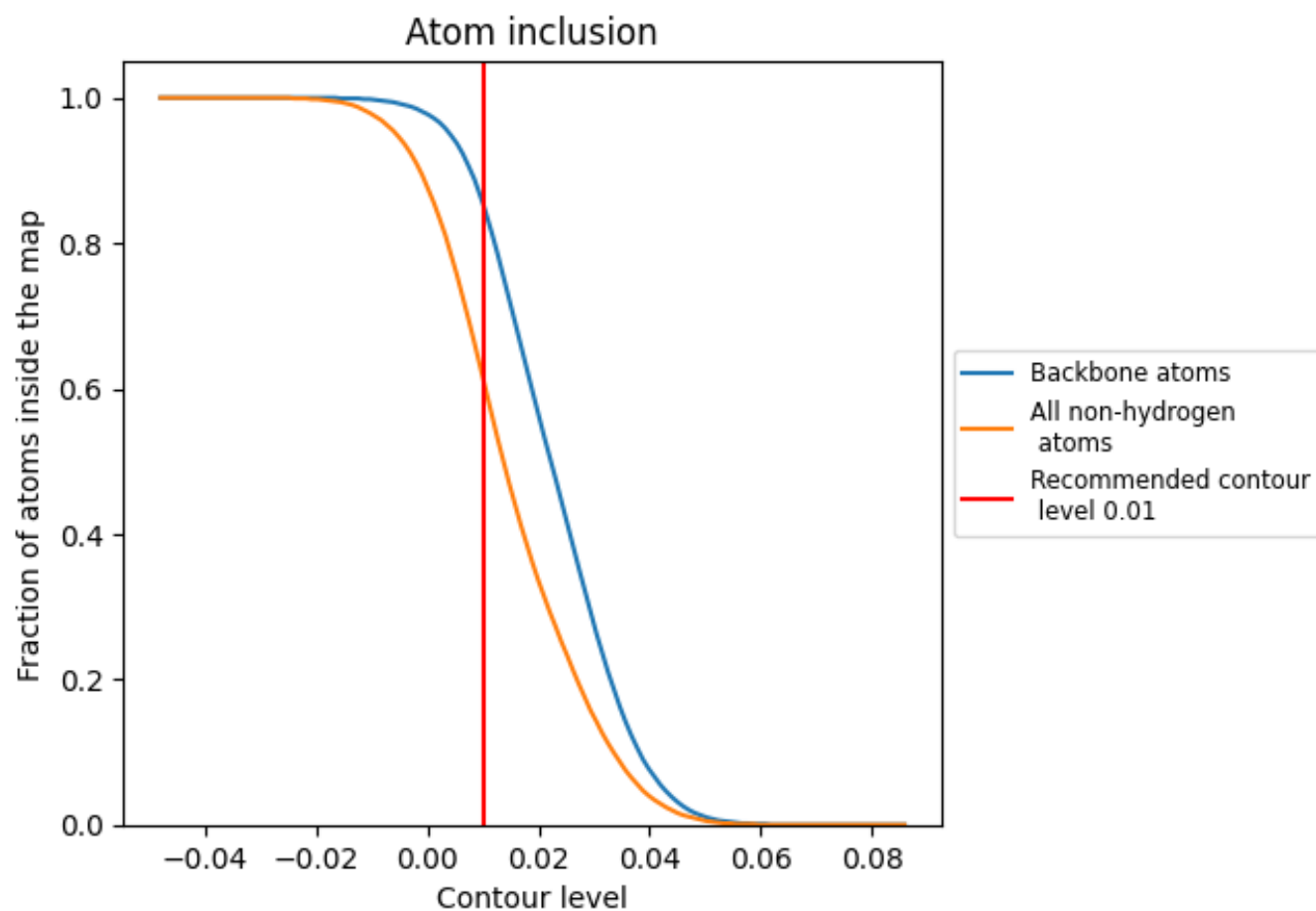


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 61% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6140	 0.1490
1	 0.7310	 0.1860
2	 0.7210	 0.1970
3	 0.6850	 0.1880
4	 0.7140	 0.1830
5	 0.7400	 0.1850
6	 0.7100	 0.1840
7	 0.7230	 0.1830
A	 0.7000	 0.1800
B	 0.6810	 0.1950
C	 0.6880	 0.1850
D	 0.7000	 0.1870
E	 0.6740	 0.1750
F	 0.7100	 0.1830
G	 0.7100	 0.1820
H	 0.5850	 0.1240
I	 0.5760	 0.1380
J	 0.5790	 0.1250
K	 0.5990	 0.1410
L	 0.6450	 0.1490
M	 0.5990	 0.1300
N	 0.6510	 0.1540
O	 0.6890	 0.1520
P	 0.7390	 0.1520
Q	 0.6930	 0.1450
R	 0.6900	 0.1450
S	 0.6220	 0.1380
T	 0.6380	 0.1340
U	 0.6130	 0.1490
V	 0.6500	 0.1610
W	 0.6020	 0.1360
X	 0.2610	 0.0510
Y	 0.4140	 0.0670
Z	 0.3350	 0.0590
a	 0.5000	 0.1460



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Chain	Atom inclusion	Q-score
b	 0.4420	 0.1550
c	 0.4700	 0.1370
d	 0.4520	 0.1300
e	 0.4500	 0.1420
f	 0.5230	 0.1570
g	 0.5170	 0.1430
h	 0.6950	 0.1650
i	 0.6780	 0.1790
j	 0.6600	 0.1750
k	 0.6760	 0.1760
l	 0.6870	 0.1680
m	 0.6530	 0.1690
n	 0.6640	 0.1710