



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 09:30 PM UTC

PDB ID : 5MPC / pdb_00005mpc
EMDB ID : EMD-3537
Title : 26S proteasome in presence of BeFx (s4)
Authors : Wehmer, M.; Rudack, T.; Beck, F.; Aufderheide, A.; Pfeifer, G.; Plitzko, J.M.;
Foerster, F.; Schulten, K.; Baumeister, W.; Sakata, E.
Deposited on : 2016-12-16
Resolution : 7.70 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:

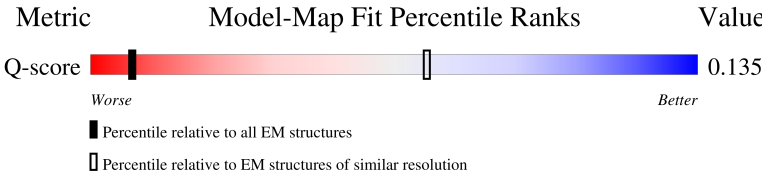
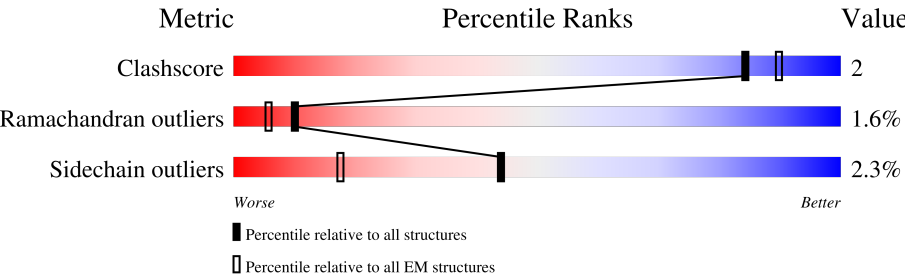
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 7.70 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	384 (7.20 - 8.20)

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	252	15% 44% 47% • •
1	a	252	21% 45% 45% 5% • •
2	B	250	20% 45% 50% 6%
2	b	250	30% 46% 51% •

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Mol	Chain	Length	Quality of chain
3	C	258	
3	c	258	
4	D	254	
4	d	254	
5	E	260	
5	e	260	
6	F	234	
6	f	234	
7	G	288	
7	g	288	
8	l	215	
8	h	215	
9	2	261	
9	i	261	
10	3	205	
10	j	205	
11	4	198	
11	k	198	
12	5	287	
12	l	287	
13	6	241	
13	m	241	
14	7	266	
14	n	266	
15	H	467	

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Mol	Chain	Length	Quality of chain
16	I	437	
17	K	428	
18	L	437	
19	M	434	
20	J	405	
21	W	268	
22	V	306	
23	T	274	
24	X	156	
25	Y	89	
26	Z	993	
27	N	945	
28	S	523	
29	P	445	
30	Q	434	
31	R	429	
32	U	338	
33	O	393	
34	8	499	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 112042 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
			1907	1214	320	365	8		
1	A	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		
2	B	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		

- 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
			1904	1201	321	379	3		
3	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		
4	D	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		
5	E	242	Total	C	N	O	S	0	0
			1861	1162	314	378	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	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	243	Total	C	N	O	S	0	0
			1892	1203	329	356	4		
7	G	243	Total	C	N	O	S	0	0
			1892	1203	329	356	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
			1719	1082	298	332	7		
9	2	226	Total	C	N	O	S	0	0
			1719	1082	298	332	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
			1561	992	264	299	6		
11	4	195	Total	C	N	O	S	0	0
			1561	992	264	299	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
			1815	1148	311	349	7		
14	7	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		

- Molecule 15 is a protein called 26S protease regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	380	Total	C	N	O	S	0	0
			2967	1869	531	551	16		

- Molecule 16 is a protein called 26S protease regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	385	Total	C	N	O	S	0	0
			3022	1899	508	598	17		

- Molecule 17 is a protein called 26S protease regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	389	Total	C	N	O	S	0	0
			3078	1933	540	595	10		

- Molecule 18 is a protein called 26S protease subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	388	Total	C	N	O	S	0	0
			3082	1942	548	580	12		

- Molecule 19 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	381	Total	C	N	O	S	0	0
			2986	1870	524	580	12		

- Molecule 20 is a protein called 26S protease regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	393	Total	C	N	O	S	0	0
			3089	1944	552	576	17		

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN10.

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

- Molecule 22 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

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

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN12.

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

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN13.

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

- Molecule 25 is a protein called 26S proteasome complex subunit SEM1.

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

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

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

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN2.

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

- Molecule 28 is a protein called 26S proteasome regulatory subunit RPN3.

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

- Molecule 29 is a protein called 26S proteasome regulatory subunit RPN5.

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

- Molecule 30 is a protein called 26S proteasome regulatory subunit RPN6.

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

- Molecule 31 is a protein called 26S proteasome regulatory subunit RPN7.

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

- Molecule 32 is a protein called 26S proteasome regulatory subunit RPN8.

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

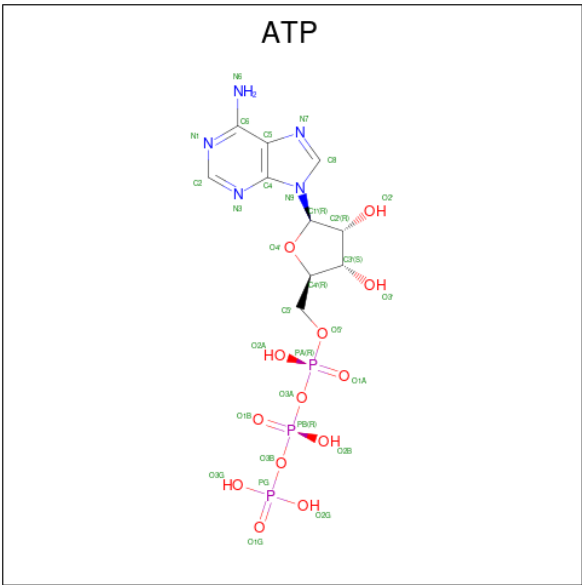
- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN9.

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

- Molecule 34 is a protein called Ubiquitin carboxyl-terminal hydrolase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	395	Total	C	N	O	S	0	0
			3219	2029	554	623	13		

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

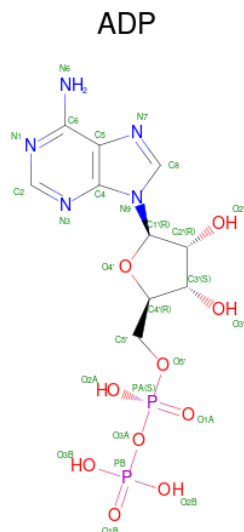


Mol	Chain	Residues	Atoms					AltConf
35	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	M	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

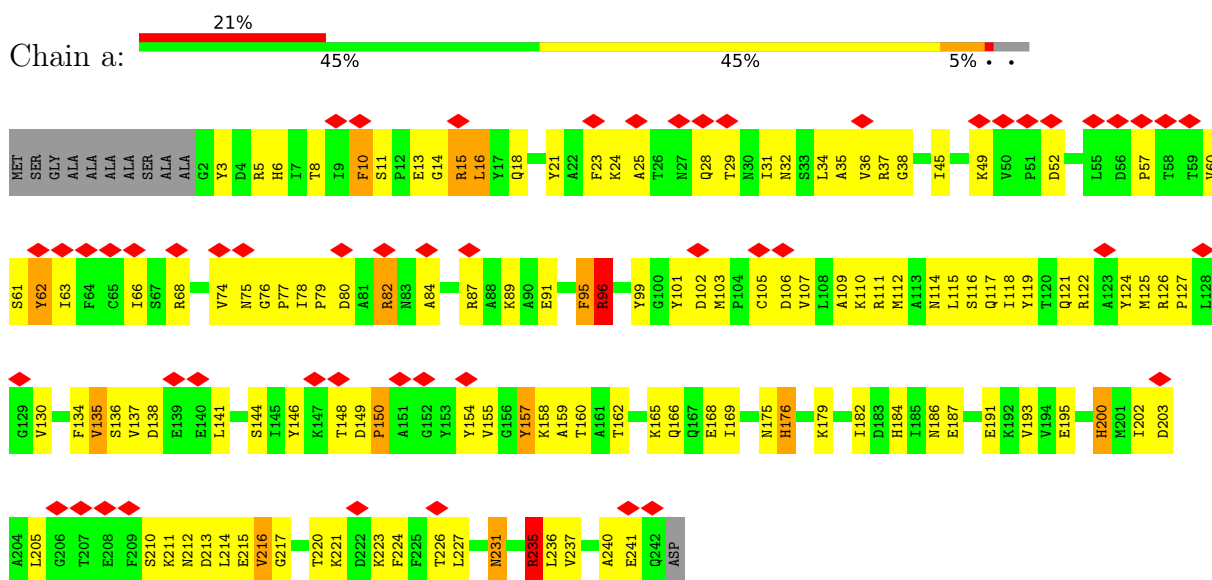


Mol	Chain	Residues	Atoms					AltConf
37	K	1	Total 27	C 10	N 5	O 10	P 2	0
37	L	1	Total 27	C 10	N 5	O 10	P 2	0

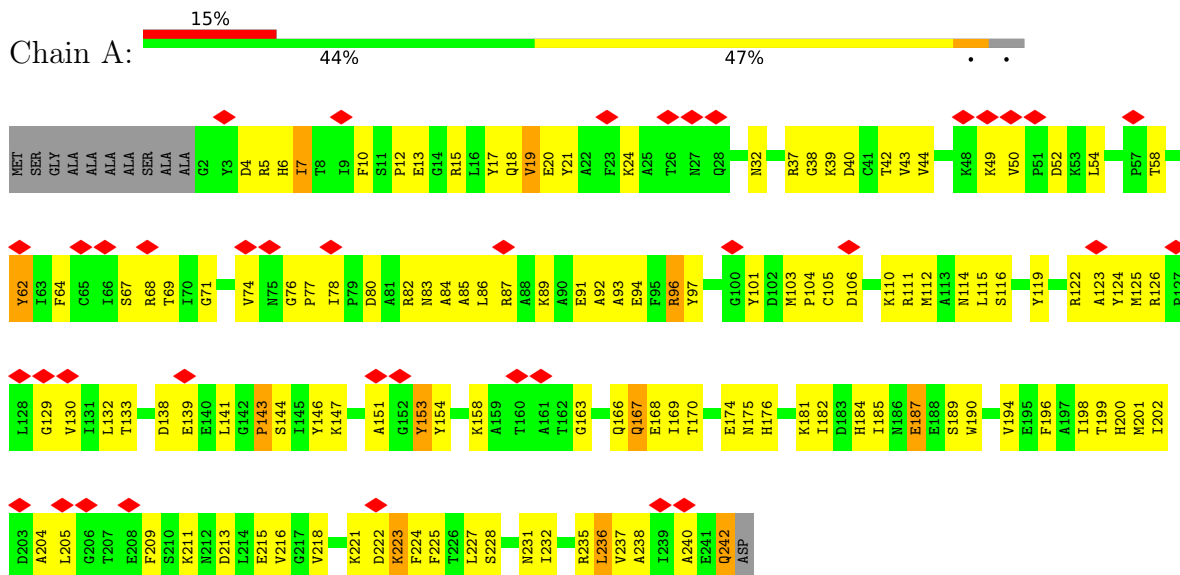
3 Residue-property plots

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

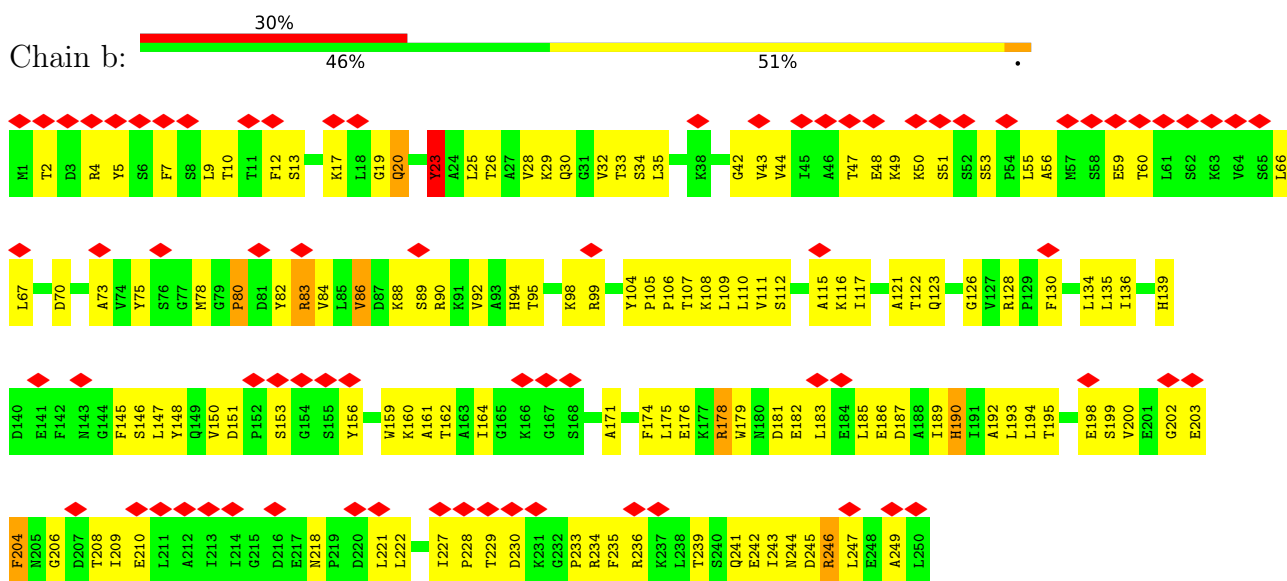
- Molecule 1: Proteasome subunit alpha type-1



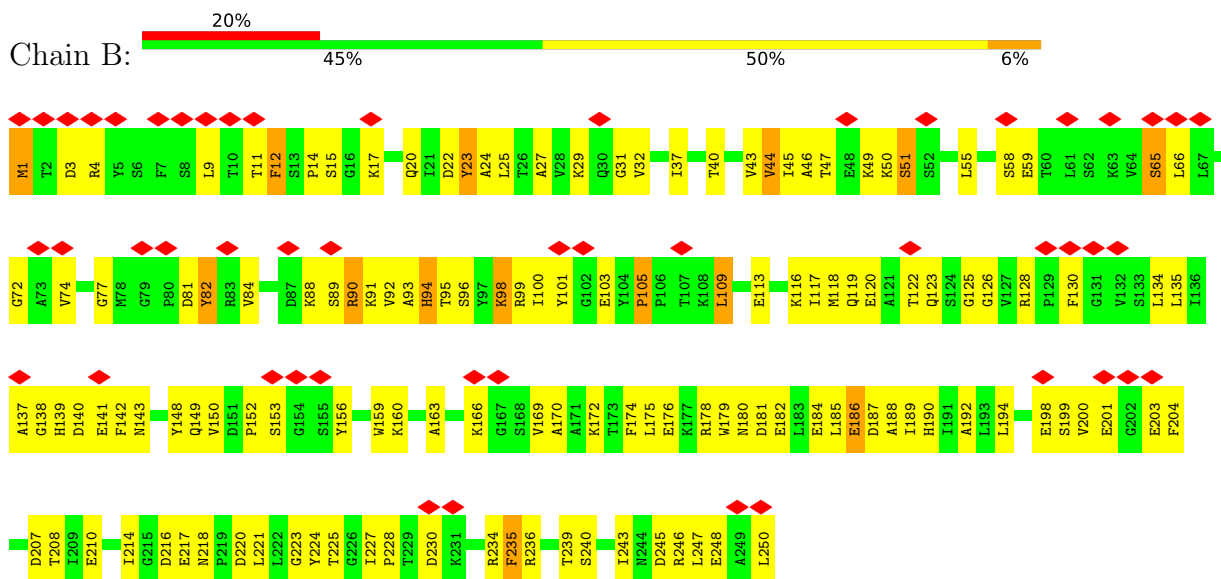
- Molecule 1: Proteasome subunit alpha type-1



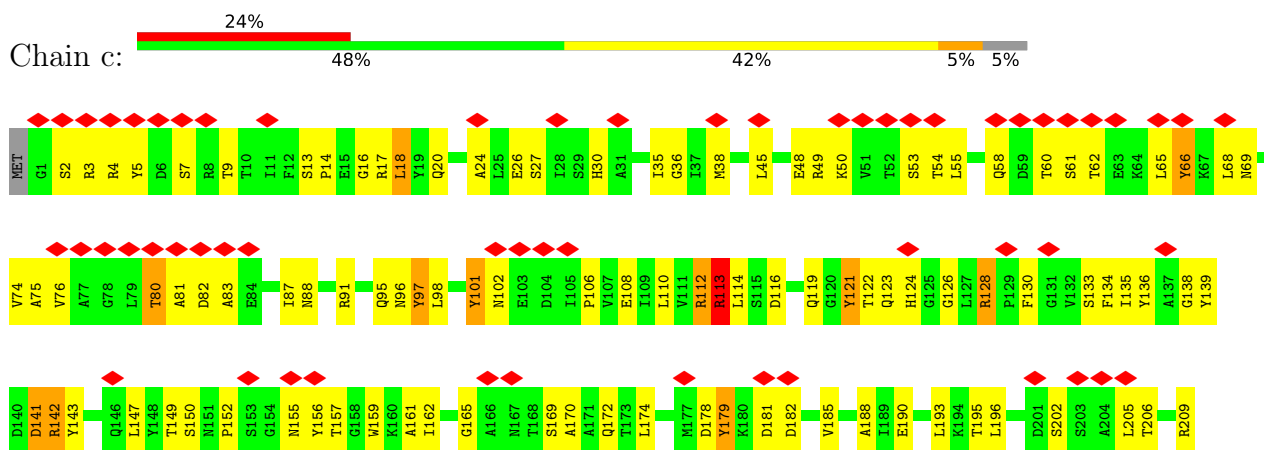
- Molecule 2: Proteasome subunit alpha type-2

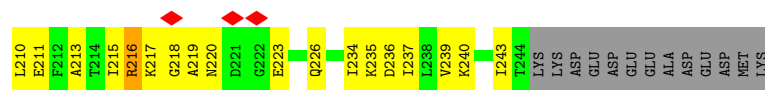


• Molecule 2: Proteasome subunit alpha type-2

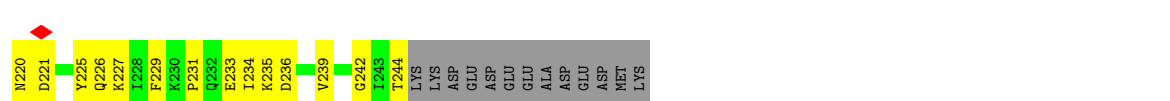
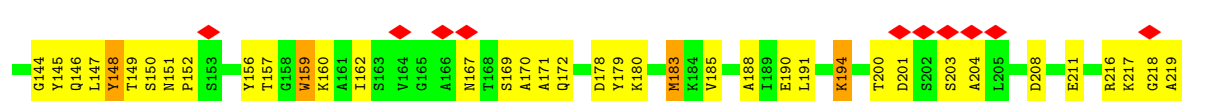
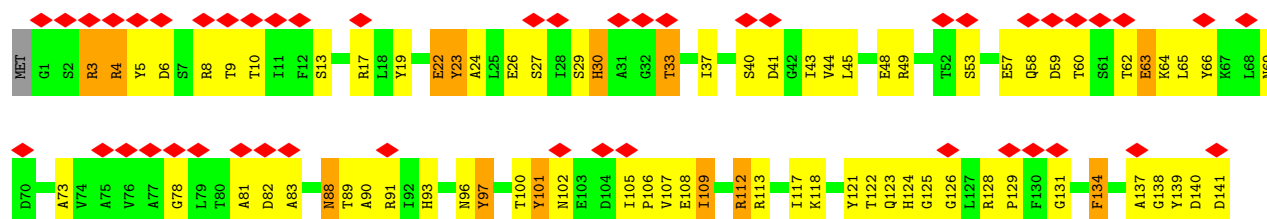
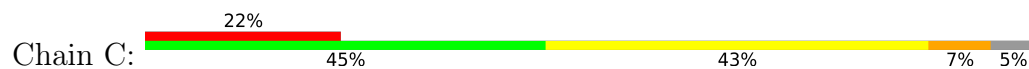


• Molecule 3: Proteasome subunit alpha type-3





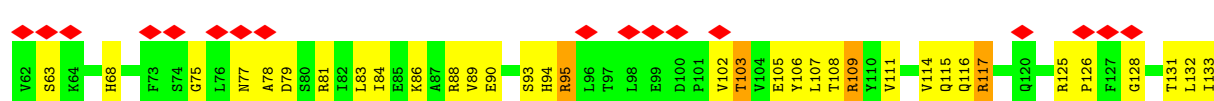
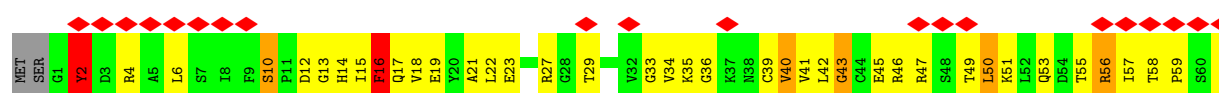
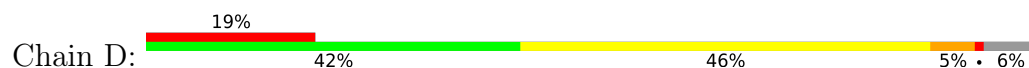
• Molecule 3: Proteasome subunit alpha type-3

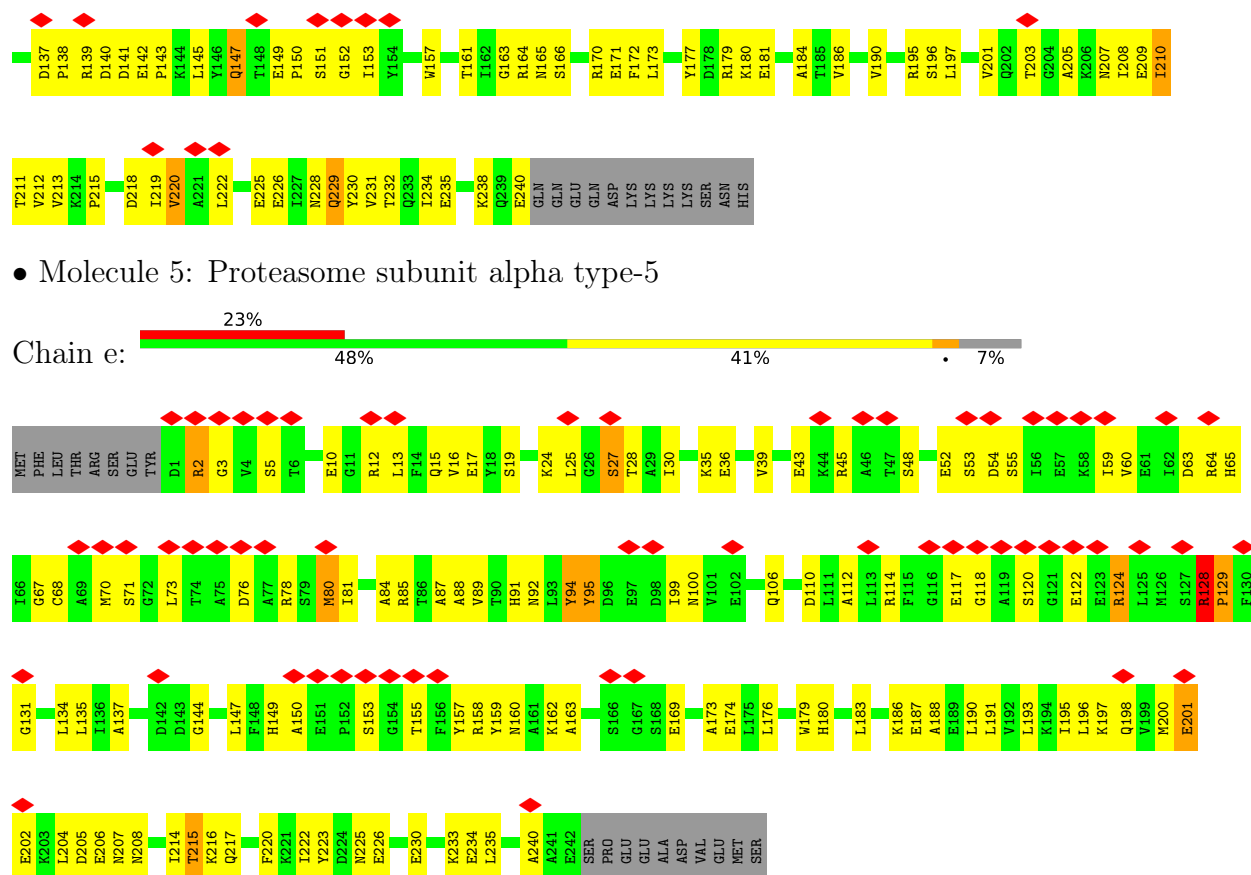


• Molecule 4: Proteasome subunit alpha type-4



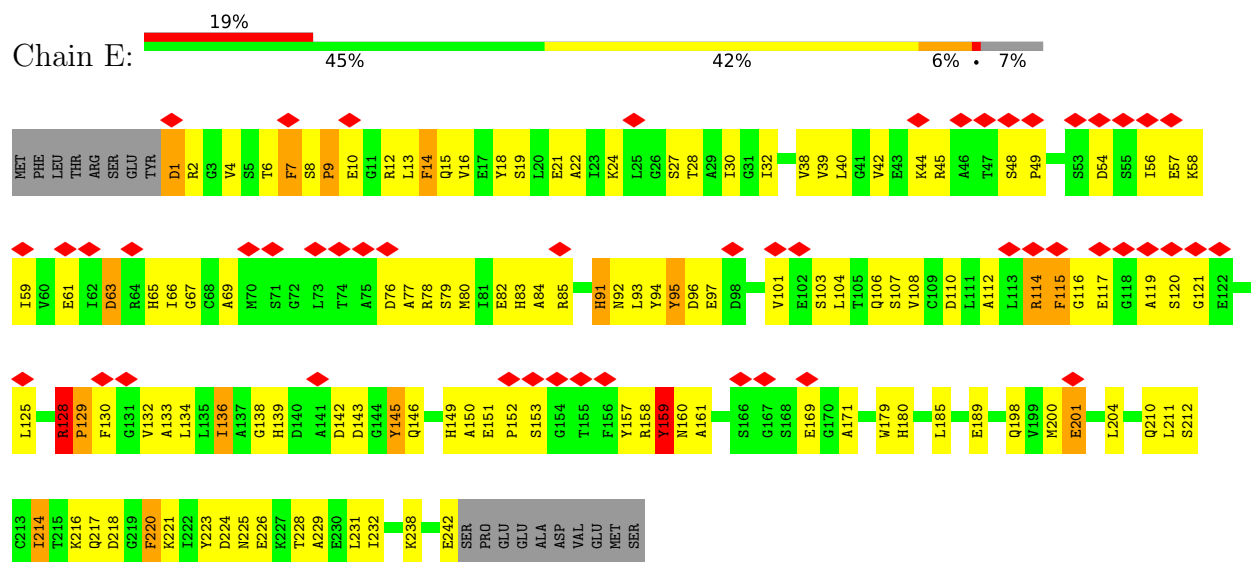
• Molecule 4: Proteasome subunit alpha type-4



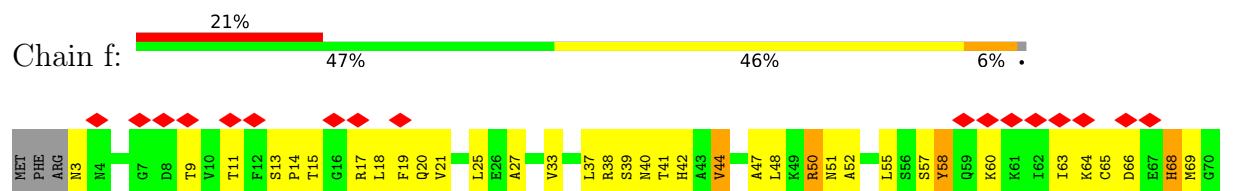


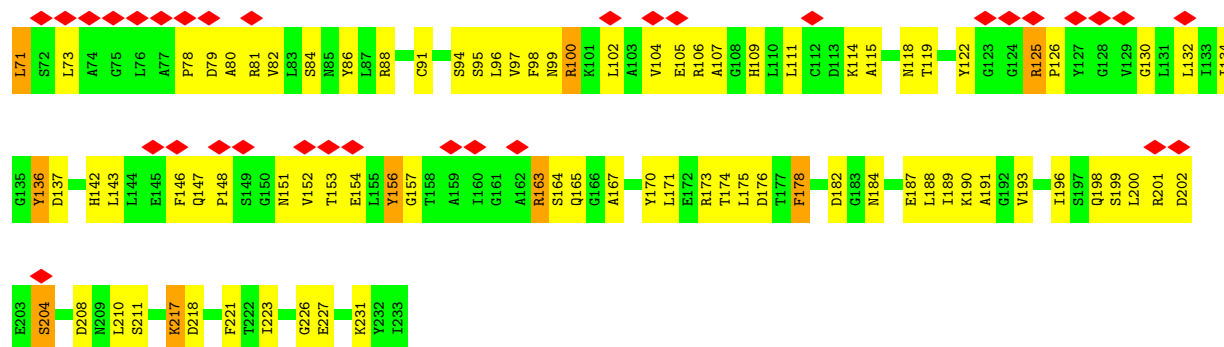
• Molecule 5: Proteasome subunit alpha type-5

• Molecule 5: Proteasome subunit alpha type-5

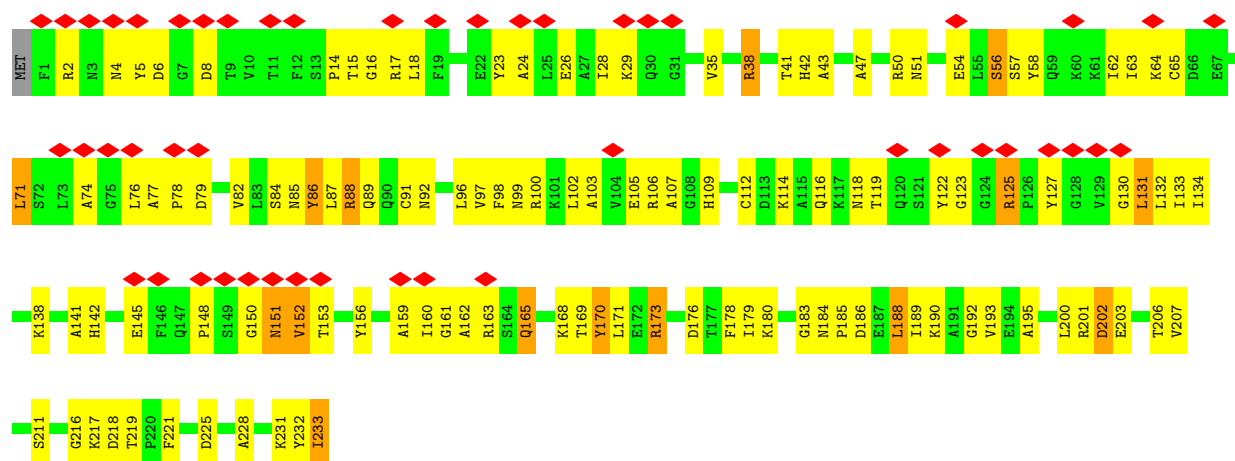


• Molecule 6: Proteasome subunit alpha type-6

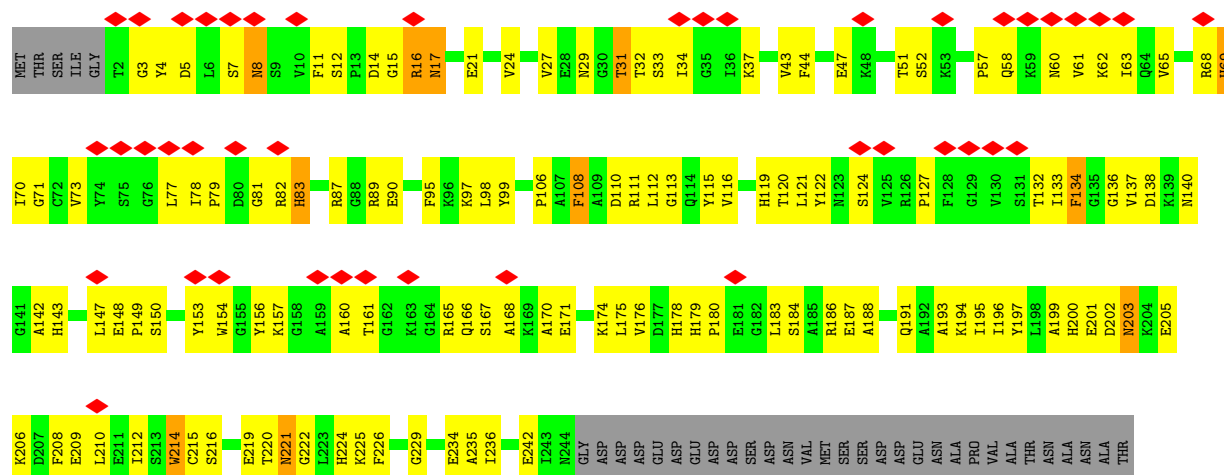




• Molecule 6: Proteasome subunit alpha type-6



• Molecule 7: Probable proteasome subunit alpha type-7



THR
ASP
GLN
GLU
GLY
ASP
ILE
HIS
LEU
GLU

Chain G:

Sequence logo for Chain G showing amino acid conservation across 222 positions. The y-axis represents information content in bits (0.00 to 1.00). The x-axis shows positions 1 to 222. A bar chart at the top indicates the percentage of residues in each conservation bin: 12% (red), 43% (green), 36% (yellow), 5% (orange), and 16% (grey). Red diamonds mark positions 14, 15, 16, 18, 20, 22, 24, 26, 28, 30, 32, 34, 36, 38, 40, 42, 44, 46, 48, 50, 52, 54, 56, 58, 60, 62, 64, 66, 68, 70, 72, 74, 76, 78, 80, 82, 84, 86, 88, 90, 92, 94, 96, 98, 100, 102, 104, 106, 108, 110, 112, 114, 116, 118, 120, 122, 124, 126, 128, 130, 132, 134, 136, 138, 140, 142, 144, 146, 148, 150, 152, 154, 156, 158, 160, 162, 164, 166, 168, 170, 172, 174, 176, 178, 180, 182, 184, 186, 188, 190, 192, 194, 196, 198, 200, 202, 204, 206, 208, 210, 212, 214, 216, 218, 220, 222.

Chain h:

13% 42% 42% 7% 9%

MET ASN GLY ILE GLN VAL ASP ILE ASP ASN ARG ARG LEU LYS LYS GLY GLY VAL SER LEU GLY T1 S2 I3 M4 F8 K9 V12 I13 L14 D17 S18 R19 T20 T21 A24 T25 I26 A27 N28 R29 V30 T31 D32 K33 L34 T35 R36 V37 H38 D39 K40 T41 W42 C43 C44 R45 S46 G47 S48 A49 A50 D51 T52 Q53 A54 I55 A56 V59 G60 Y61 H62 L63 E64 L65 Y66 T67 Y70 A78 A79 S80 V81 F82 Y87 K90 D91 N92 L93 T94 A95 G96 I97 L98 Y102 D103 D104 K107 G108 E109 V110 Y111 T112 Y113 P114 L115 G116 G117 S118 V119 H120 K121 A125 I126 G130 S131 T132 F133 I134 Y135 C138 R143 E144 N145 M146 S147 K148 E149 D153 F154 I155 K156 H157 S158 L159 S160 Q161 A162 I163 K164 G167 S168 S169 G170 G171 V172 I173 R174 M175 V176 V177 L178 T179 A180 G181 G182 V183 E184 R185 L186 I187 F188 Y189 P190 D191 E192 L196

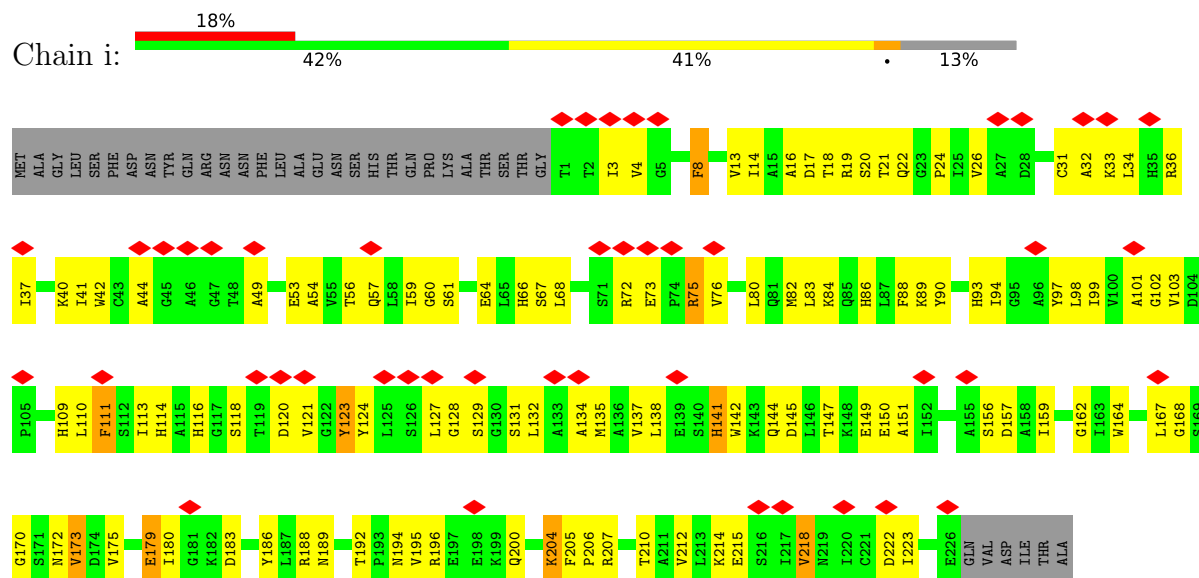
Chain 1:

12% 40% 47% 9%

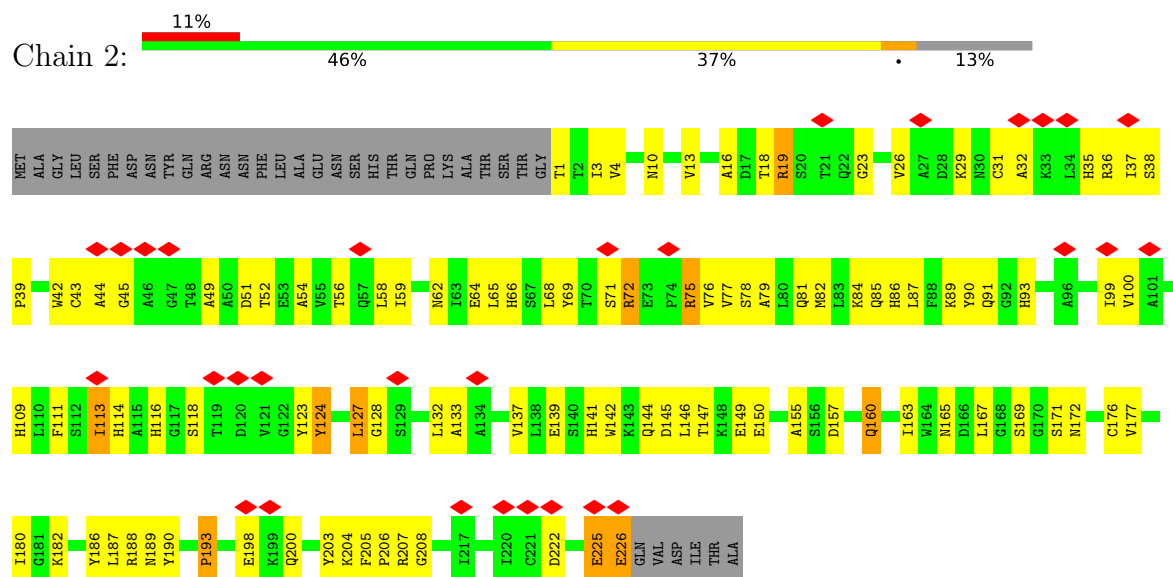
Met, Asn, Gly, Ile, Val, Asp, Ile, Arg, Leu, Lys, Gly, Val, Ser, Leu, Gly, T1, S2, T3, M4, A5, Y6, T7, F8, I13, L14, G15, A16, L17, S18, R19, T20, T21, Y25, I26, A27, Y28, R29, V30, T31, D32, K33, L34, T35, R36, V37, H38, D39, K40, T41, A42, R45, S46, A49, A50, D51, T52, Q53, D57, I58, V59, G60, F61, H62, L63, T67, S68, G69, Y70, G71, S74, T75, F76, T77, A78, A79, S80, R81, V82, R83, E84, L85, C86, Y87, E88, R89, K90, D91, N92, L93, T94, A95, V96, G97, T98, A99, A100, D104, K105, L106, K107, T112, I113, P114, L115, Y116, G117, H120, K121, L122, Y123, A124, A125, I126, S131, T132, F133, Y137, C138, F142, R143, E144, N145, E149, E150, T151, V152, D153, F154, I155, K156, L157, S158, L159, S160, Q161, W165, D166, G167, V172, L173, R174, M175, V176, V177, L178, T179, A180, A181, G182, V183, E184, R185, L186, Y189, E192, Y193, E194, Q195

◆
L196

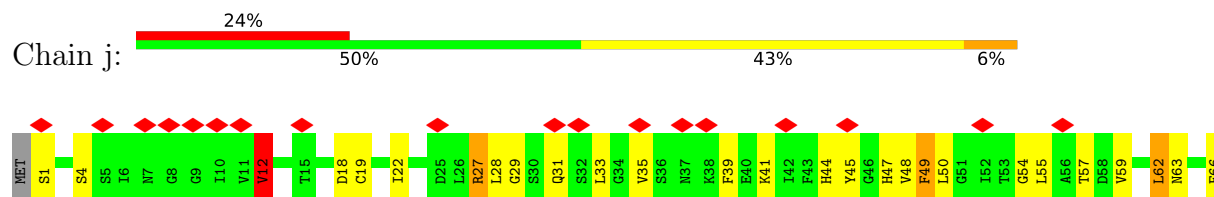
• Molecule 9: Proteasome subunit beta type-2

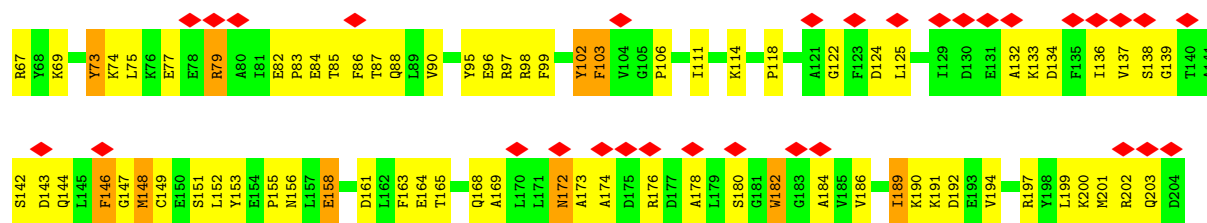


• Molecule 9: Proteasome subunit beta type-2

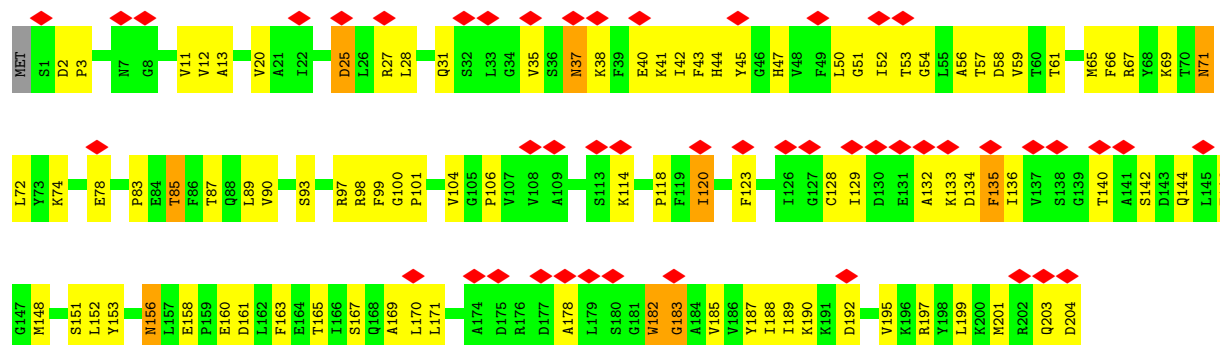


• Molecule 10: Proteasome subunit beta type-3

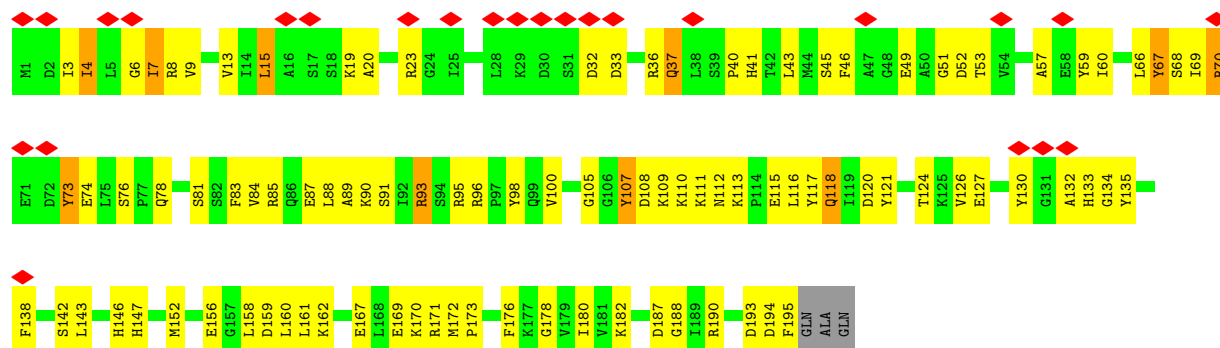




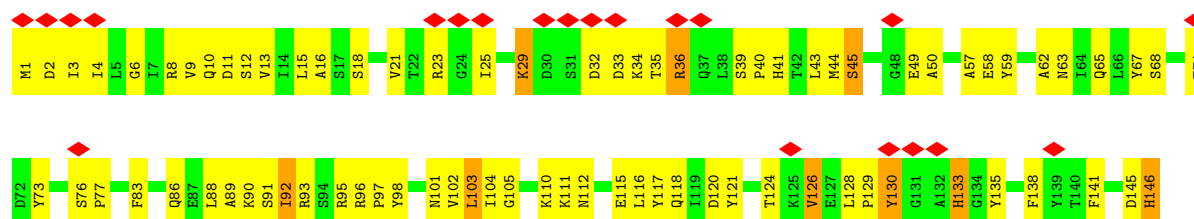
• Molecule 10: Proteasome subunit beta type-3



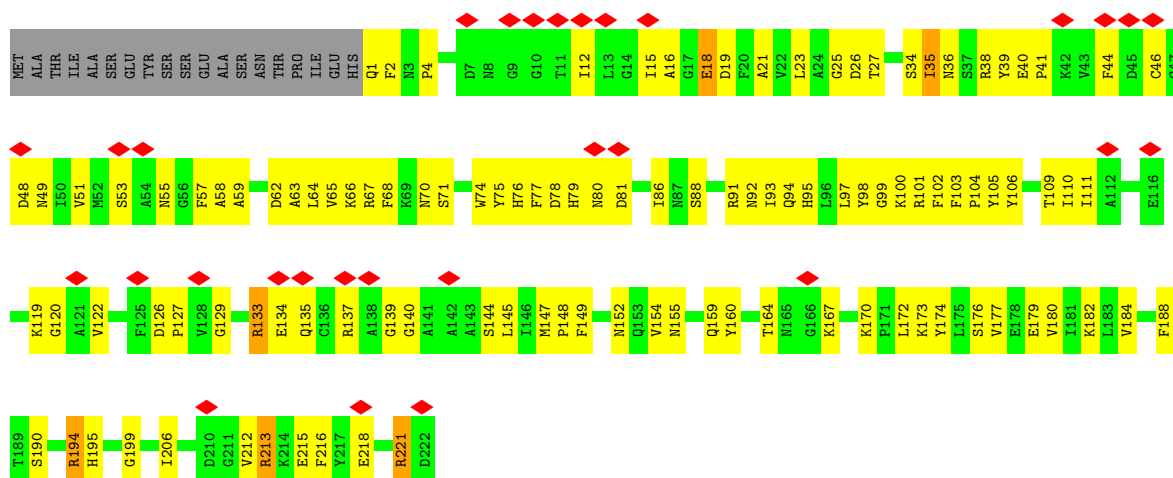
• Molecule 11: Proteasome subunit beta type-4



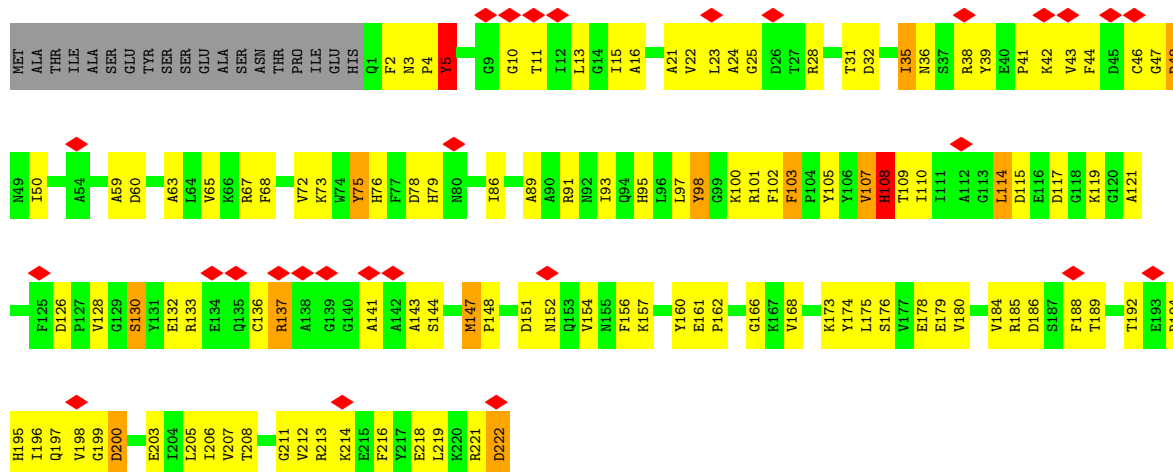
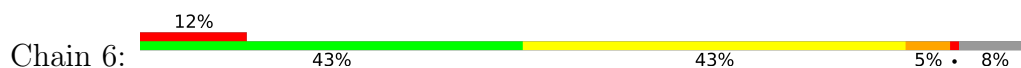
• Molecule 11: Proteasome subunit beta type-4



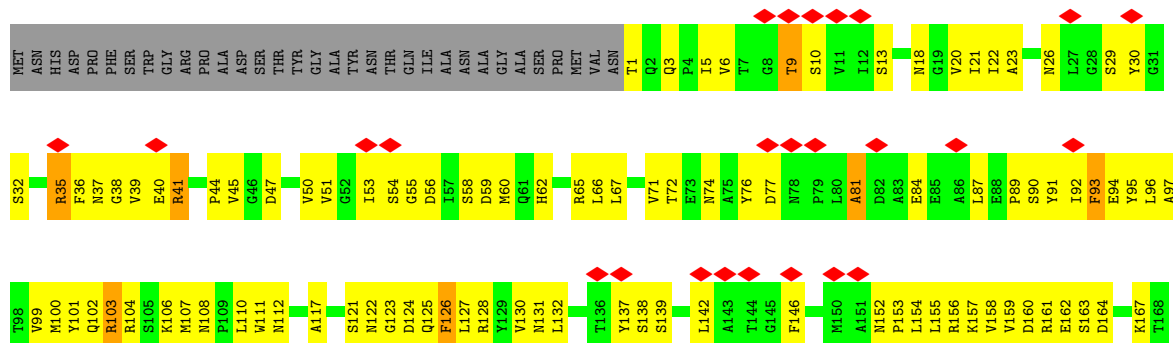


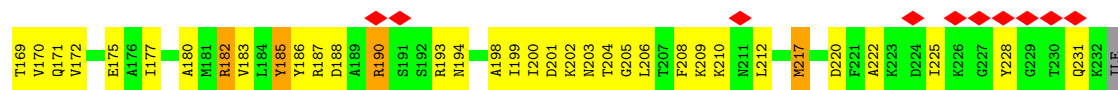


• Molecule 13: Proteasome subunit beta type-6

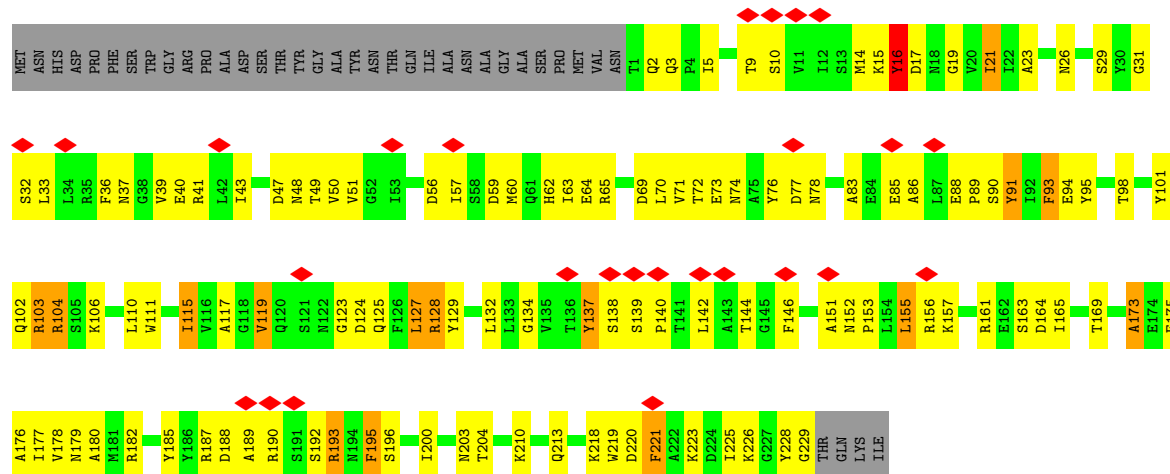


• Molecule 14: Proteasome subunit beta type-7

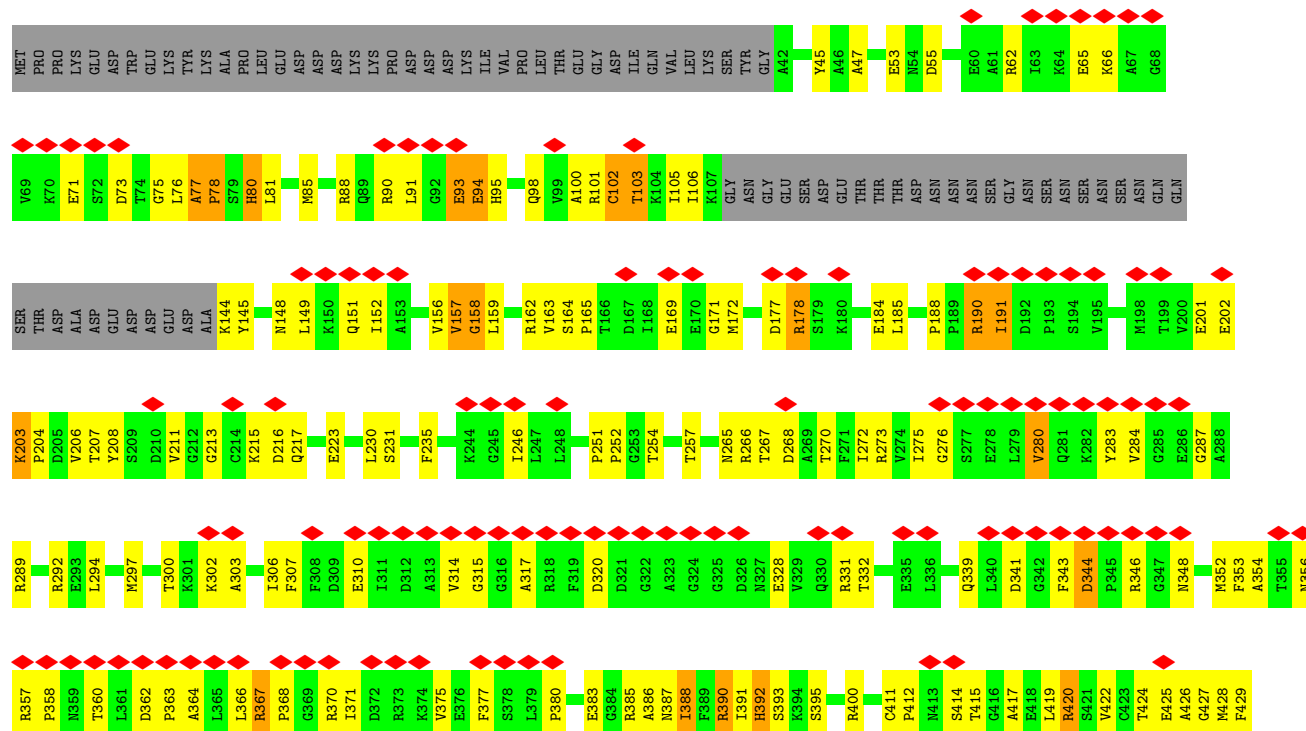


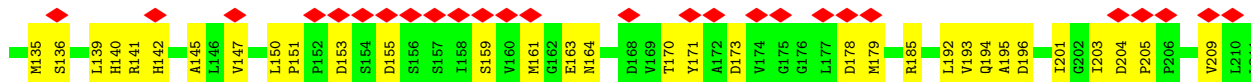


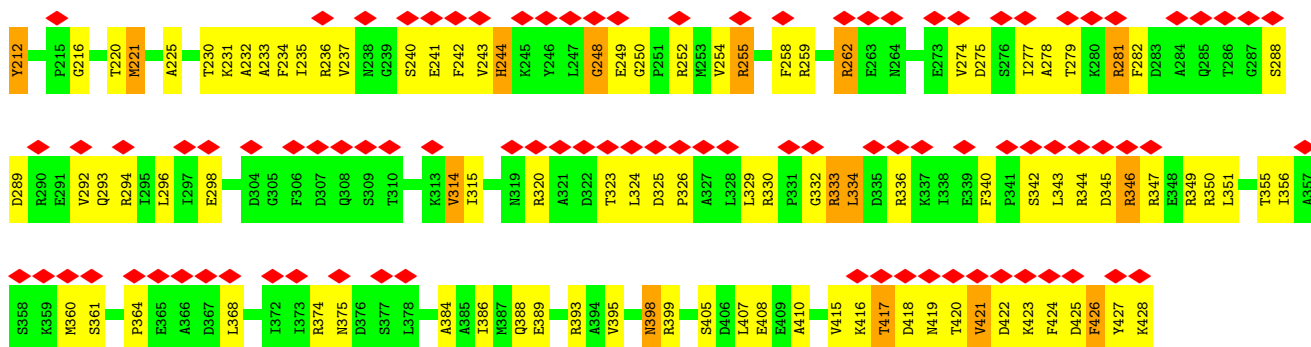
• Molecule 14: Proteasome subunit beta type-7



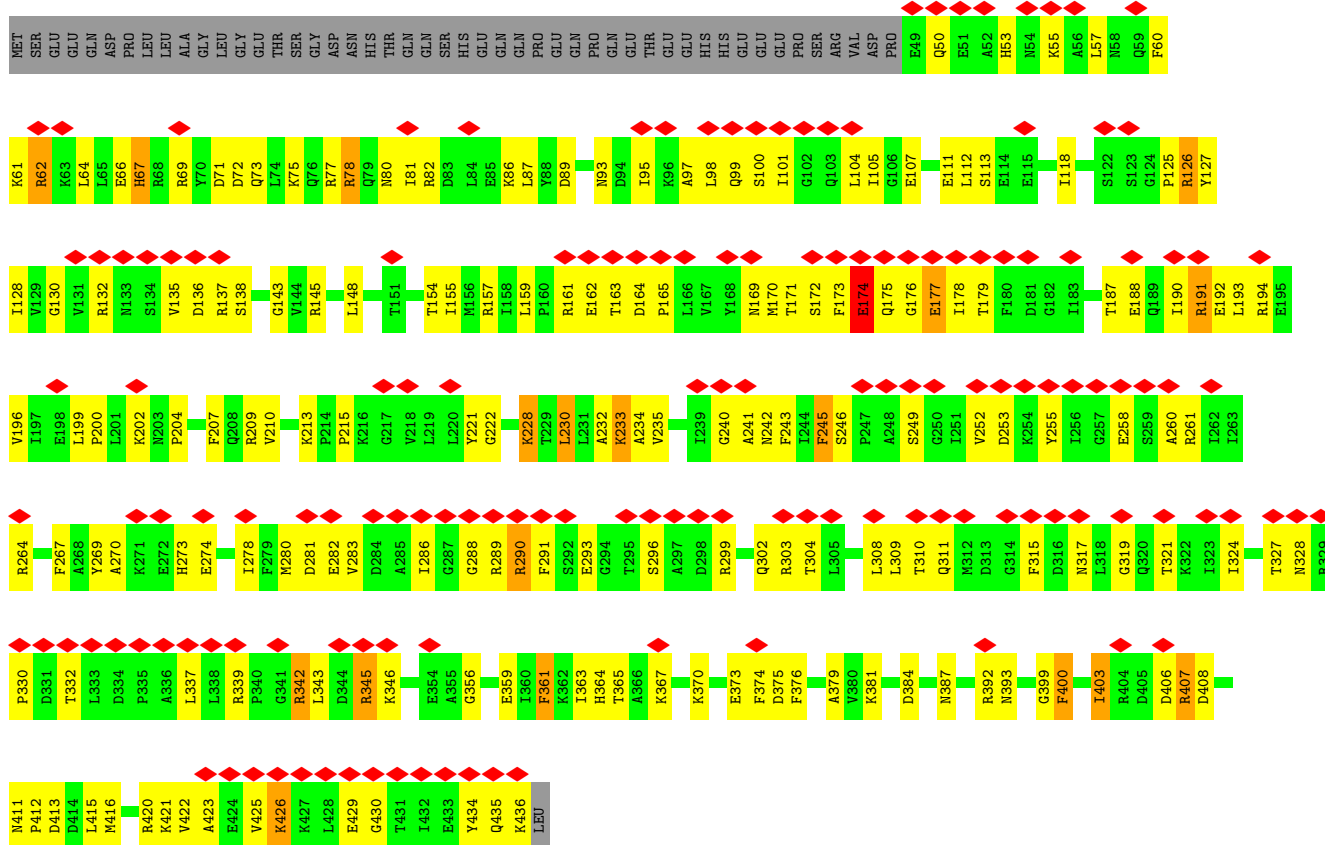
• Molecule 15: 26S protease regulatory subunit 7 homolog



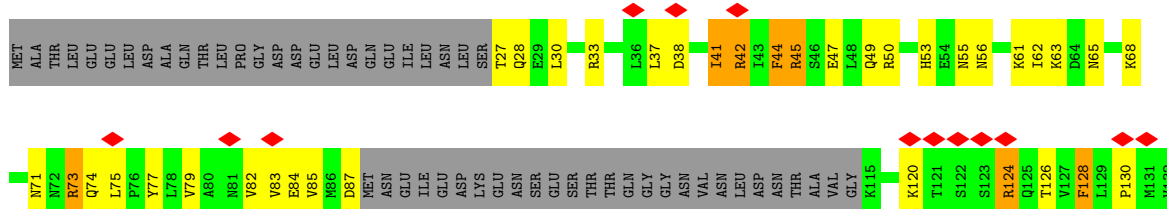


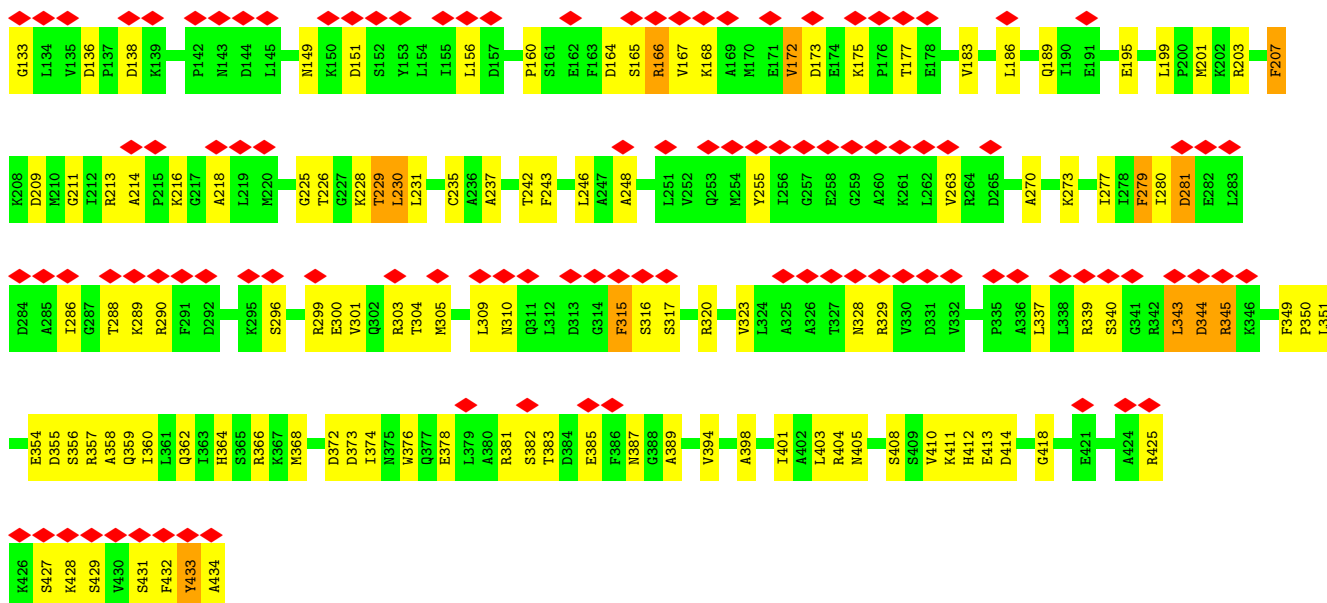


• Molecule 18: 26S protease subunit RPT4

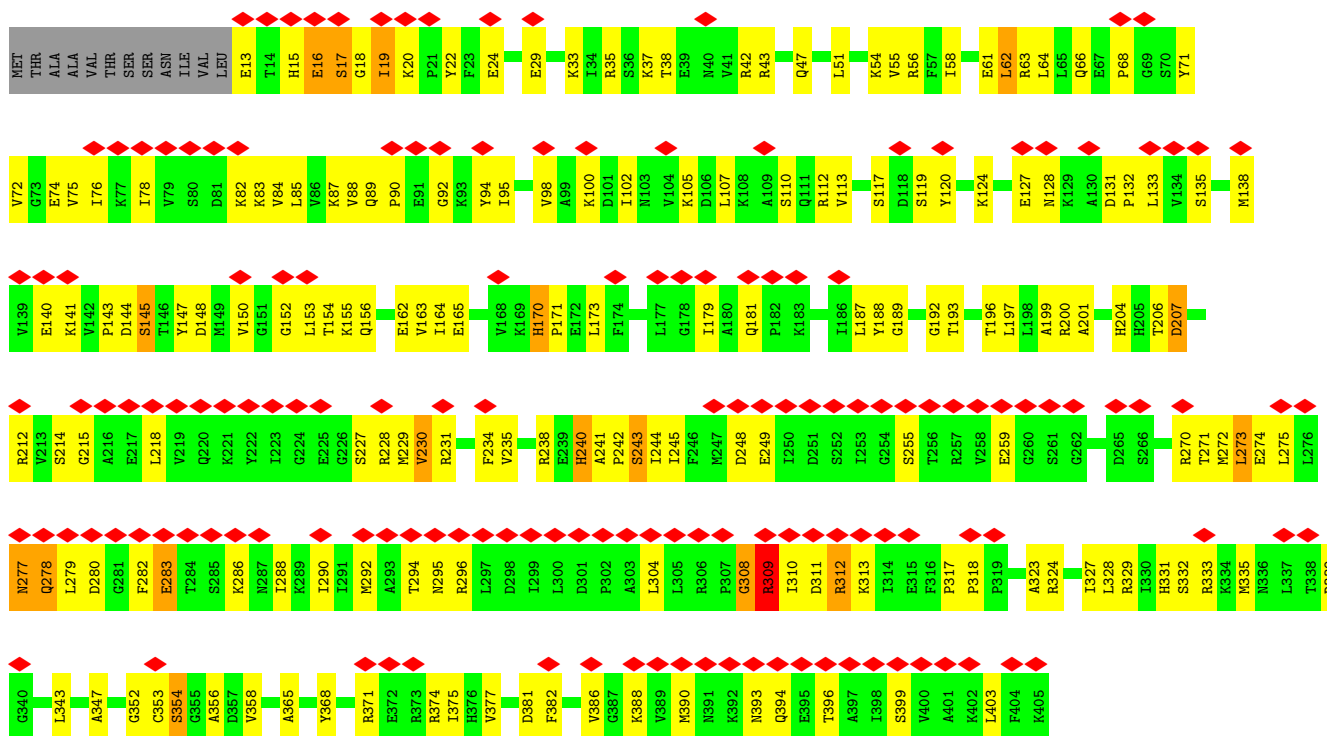
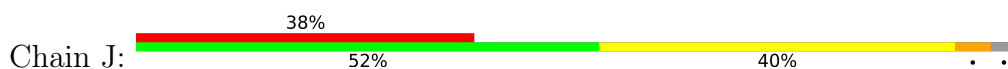


• Molecule 19: 26S protease regulatory subunit 6A





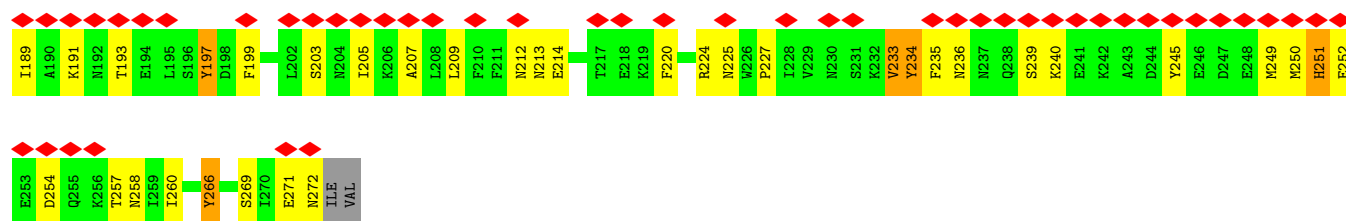
- Molecule 20: 26S protease regulatory subunit 8 homolog



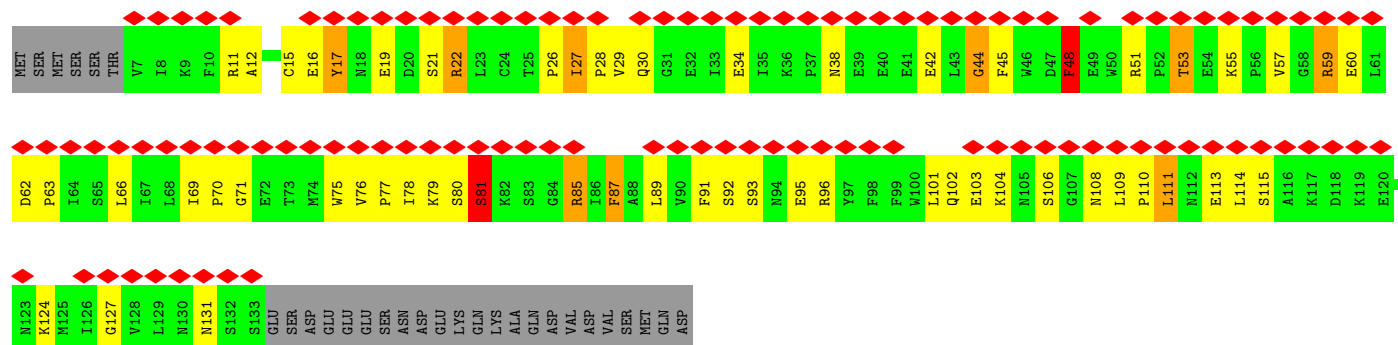
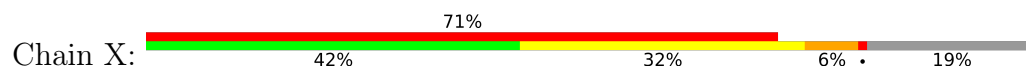
- Molecule 21: 26S proteasome regulatory subunit RPN10



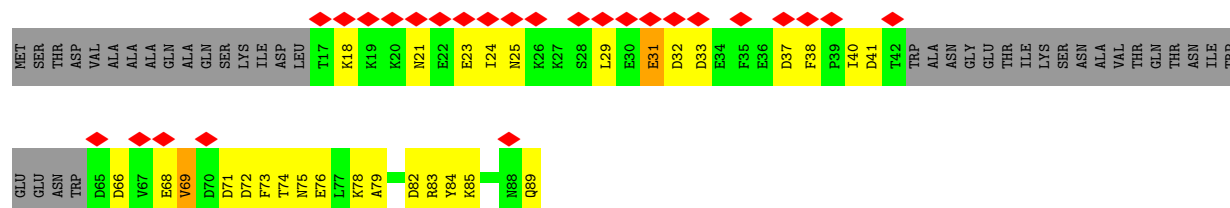
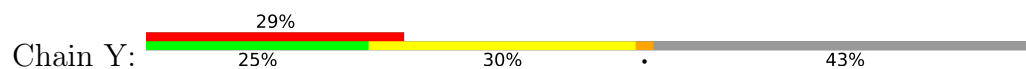




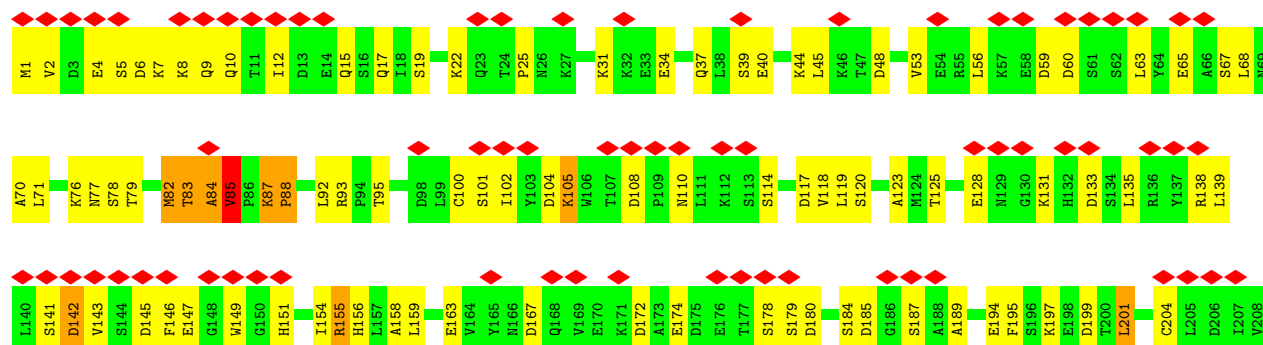
• Molecule 24: 26S proteasome regulatory subunit RPN13

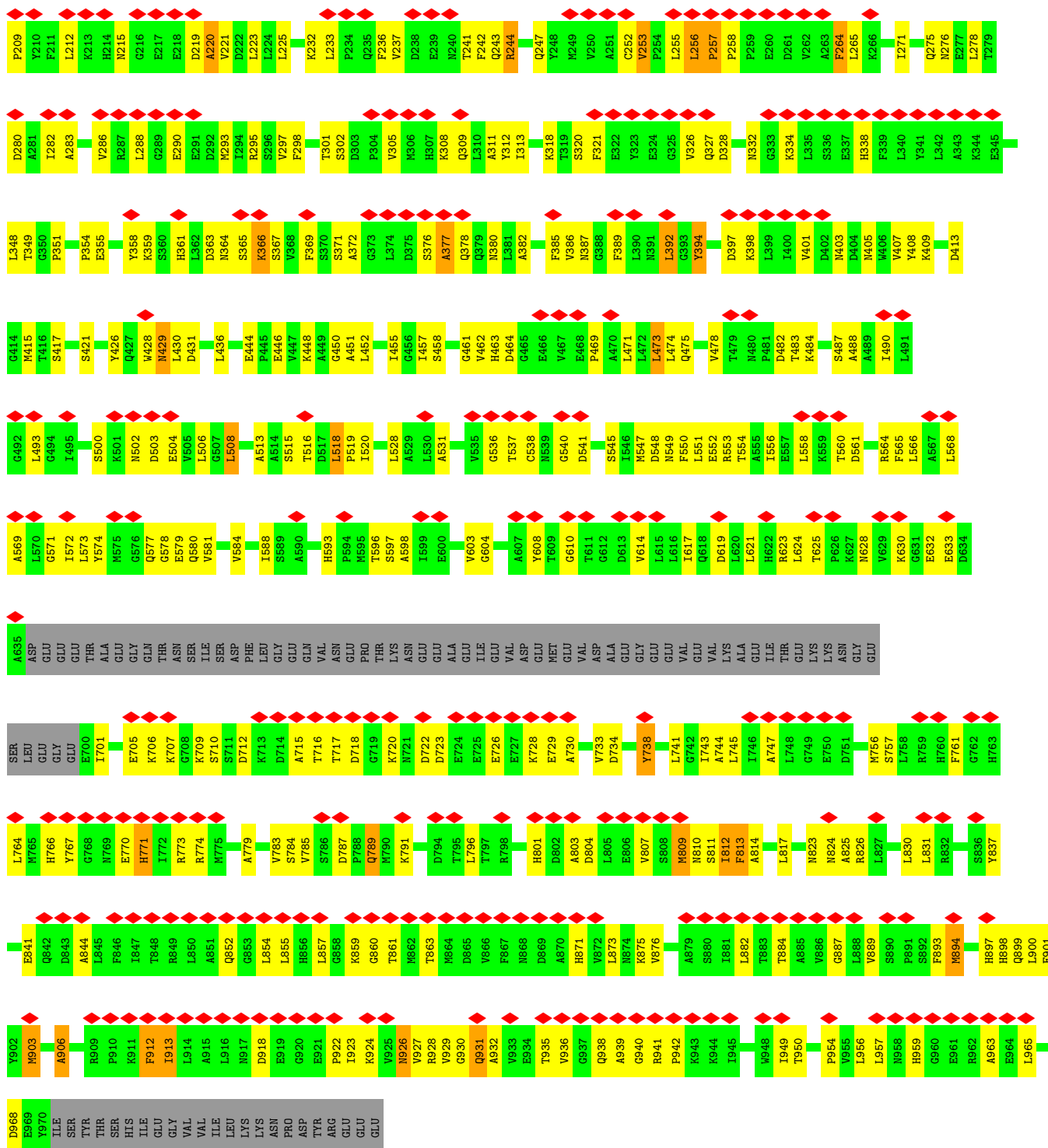


• Molecule 25: 26S proteasome complex subunit SEM1

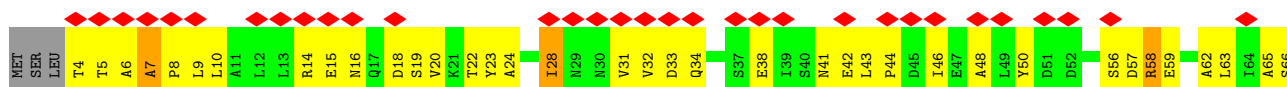


• Molecule 26: 26S proteasome regulatory subunit RPN1

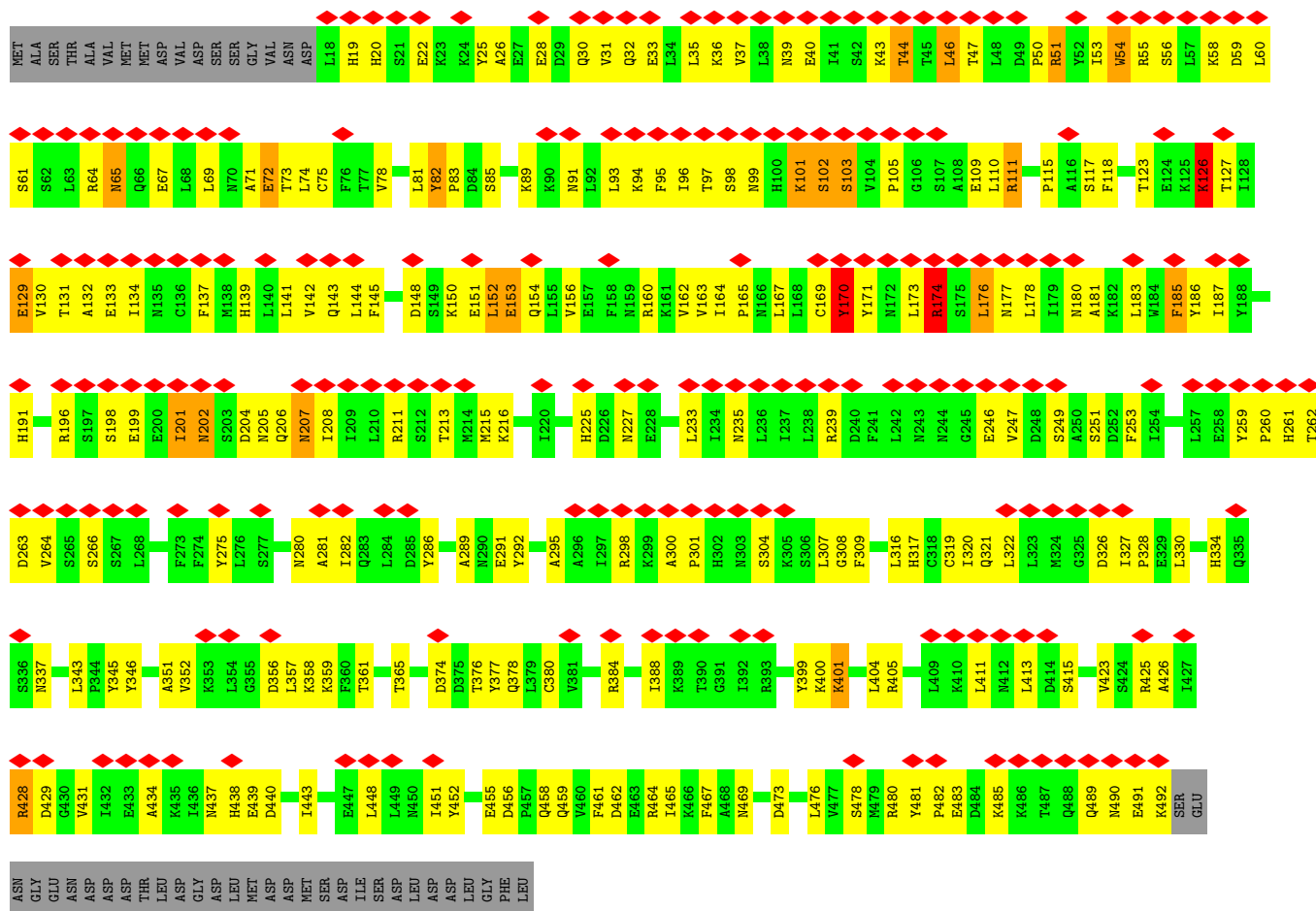




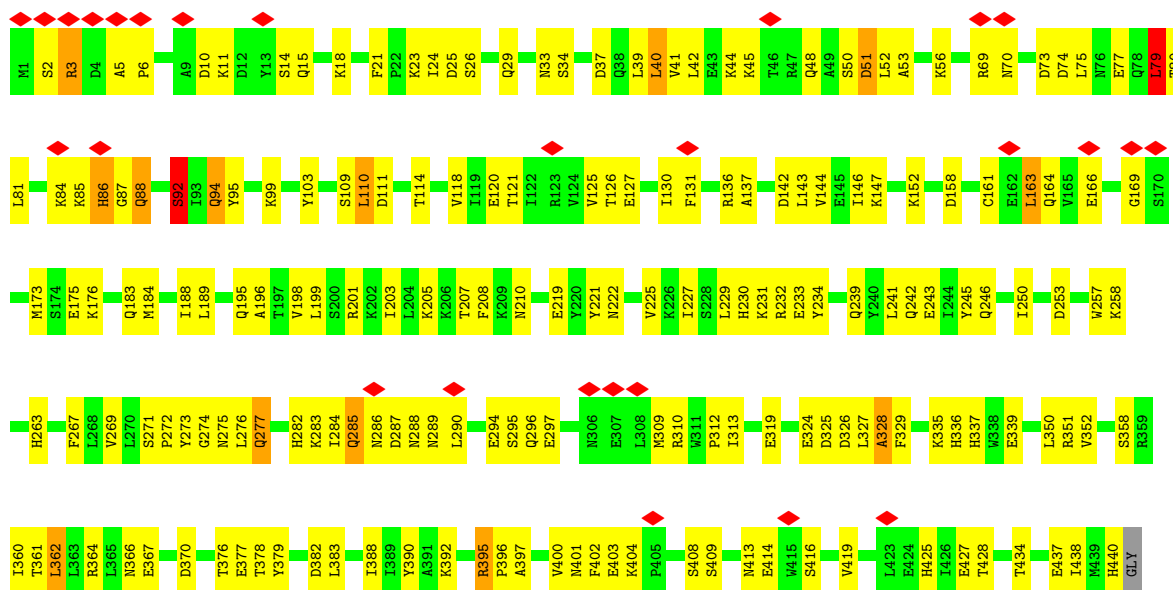
• Molecule 27: 26S proteasome regulatory subunit RPN2





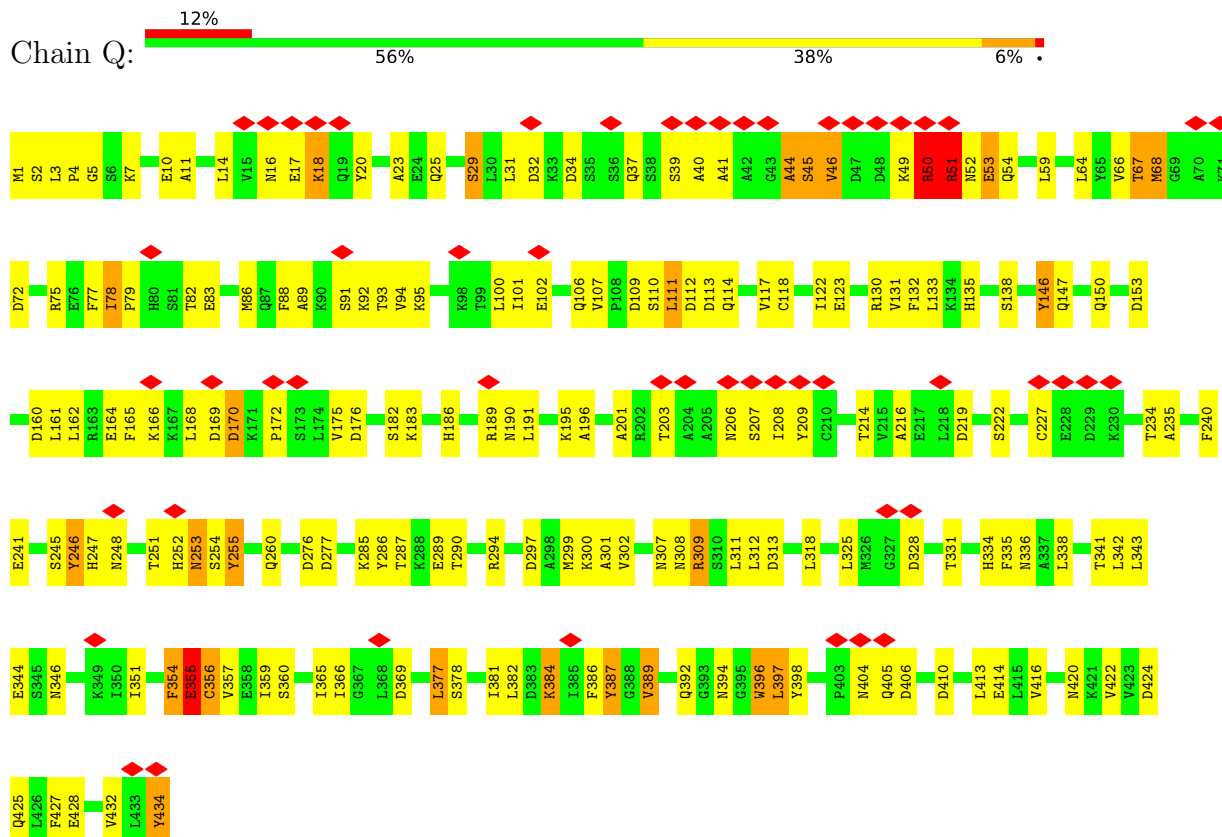


• Molecule 29: 26S proteasome regulatory subunit RPN5

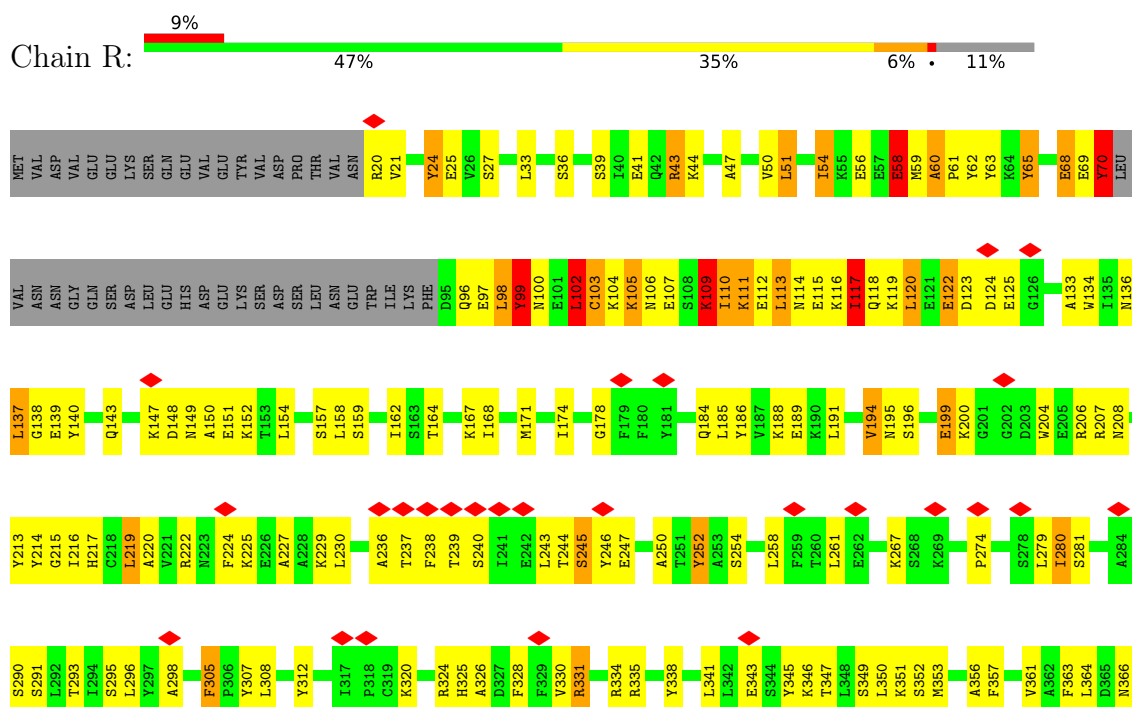


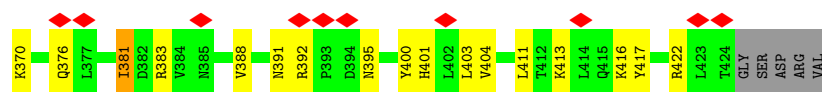
LEU
GLN
ALA
LYS

• Molecule 30: 26S proteasome regulatory subunit RPN6

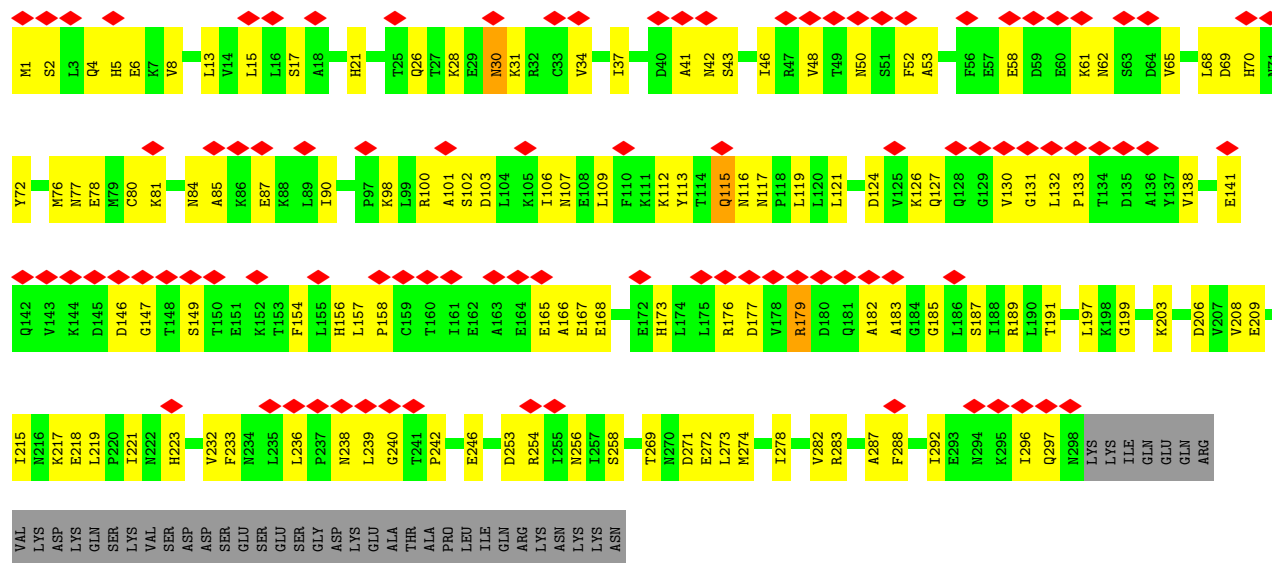


• Molecule 31: 26S proteasome regulatory subunit RPN7

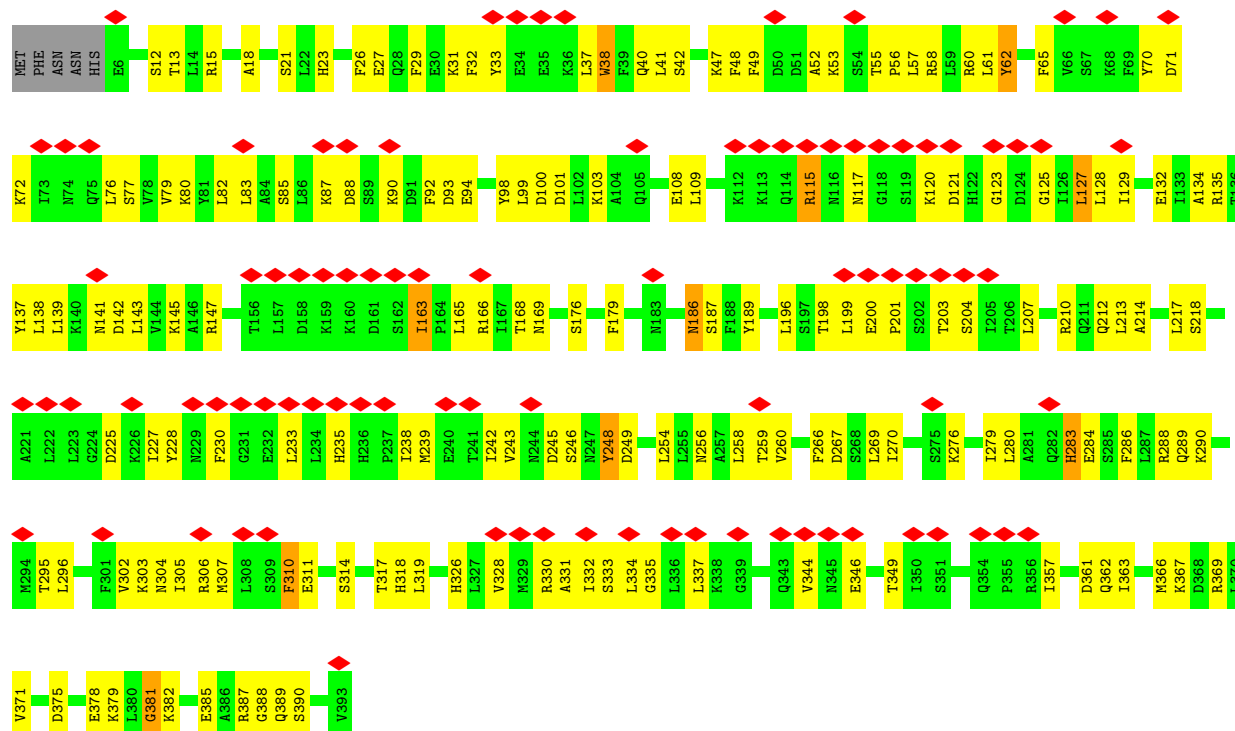




• Molecule 32: 26S proteasome regulatory subunit RPN8



• Molecule 33: 26S proteasome regulatory subunit RPN9



Chain 8:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27600	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.117	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	561.60004, 561.60004, 561.60004	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3500001, 1.3500001, 1.3500001	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	2.26	70/1945 (3.6%)	2.45	134/2634 (5.1%)
1	a	2.34	88/1945 (4.5%)	2.42	109/2634 (4.1%)
2	B	2.28	87/1952 (4.5%)	2.31	95/2642 (3.6%)
2	b	2.27	77/1952 (3.9%)	2.34	108/2642 (4.1%)
3	C	2.25	68/1934 (3.5%)	2.33	108/2618 (4.1%)
3	c	2.24	62/1934 (3.2%)	2.33	114/2618 (4.4%)
4	D	2.36	96/1910 (5.0%)	2.38	120/2586 (4.6%)
4	d	2.33	71/1910 (3.7%)	2.38	104/2586 (4.0%)
5	E	2.33	85/1886 (4.5%)	2.30	98/2541 (3.9%)
5	e	2.29	76/1886 (4.0%)	2.30	92/2541 (3.6%)
6	F	2.32	83/1823 (4.6%)	2.37	110/2463 (4.5%)
6	f	2.31	72/1800 (4.0%)	2.32	97/2433 (4.0%)
7	G	2.25	74/1932 (3.8%)	2.37	112/2609 (4.3%)
7	g	2.31	87/1932 (4.5%)	2.47	125/2609 (4.8%)
8	1	2.28	60/1541 (3.9%)	2.27	81/2087 (3.9%)
8	h	2.30	63/1541 (4.1%)	2.39	100/2087 (4.8%)
9	2	2.27	66/1750 (3.8%)	2.33	84/2373 (3.5%)
9	i	2.28	65/1750 (3.7%)	2.36	100/2373 (4.2%)
10	3	2.28	59/1611 (3.7%)	2.23	67/2174 (3.1%)
10	j	2.31	72/1611 (4.5%)	2.34	82/2174 (3.8%)
11	4	2.33	75/1589 (4.7%)	2.29	72/2142 (3.4%)
11	k	2.27	61/1589 (3.8%)	2.34	80/2142 (3.7%)
12	5	2.33	76/1681 (4.5%)	2.44	114/2274 (5.0%)
12	l	2.30	64/1681 (3.8%)	2.40	108/2274 (4.7%)
13	6	2.30	79/1795 (4.4%)	2.23	76/2420 (3.1%)
13	m	2.27	73/1795 (4.1%)	2.33	98/2420 (4.0%)
14	7	2.24	65/1821 (3.6%)	2.36	103/2470 (4.2%)
14	n	2.37	87/1846 (4.7%)	2.37	101/2503 (4.0%)
15	H	2.14	77/3014 (2.6%)	2.27	147/4058 (3.6%)
16	I	2.12	67/3061 (2.2%)	2.30	154/4121 (3.7%)
17	K	2.14	98/3121 (3.1%)	2.28	149/4213 (3.5%)
18	L	2.13	87/3128 (2.8%)	2.32	190/4204 (4.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	M	2.08	75/3023 (2.5%)	2.27	144/4070 (3.5%)
20	J	2.08	80/3130 (2.6%)	2.29	152/4203 (3.6%)
21	W	2.02	40/1557 (2.6%)	2.24	86/2111 (4.1%)
22	V	1.99	57/2309 (2.5%)	2.15	103/3115 (3.3%)
23	T	1.92	33/2235 (1.5%)	2.31	127/3017 (4.2%)
24	X	2.11	32/1058 (3.0%)	2.13	45/1432 (3.1%)
25	Y	2.07	11/438 (2.5%)	2.36	32/583 (5.5%)
26	Z	2.02	163/7122 (2.3%)	2.21	370/9645 (3.8%)
27	N	2.04	183/6994 (2.6%)	2.25	351/9455 (3.7%)
28	S	2.16	93/3966 (2.3%)	2.35	253/5355 (4.7%)
29	P	1.95	63/3663 (1.7%)	2.28	196/4940 (4.0%)
30	Q	2.00	95/3556 (2.7%)	2.32	192/4787 (4.0%)
31	R	2.09	82/3110 (2.6%)	2.43	198/4193 (4.7%)
32	U	2.05	60/2407 (2.5%)	2.13	94/3258 (2.9%)
33	O	2.01	77/3247 (2.4%)	2.29	175/4380 (4.0%)
34	8	2.22	112/3278 (3.4%)	2.36	192/4402 (4.4%)
All	All	2.17	3646/113759 (3.2%)	2.31	6142/153611 (4.0%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	3	0	1
10	j	0	6
11	4	0	5
11	k	0	7
12	5	0	4
12	l	0	12
13	6	0	8
13	m	0	9
14	7	0	10
14	n	0	11
15	H	0	6
16	I	0	7
17	K	0	13
18	L	0	12
19	M	0	13
20	J	0	6
21	W	0	4
22	V	0	4
23	T	0	9
24	X	0	4
26	Z	0	3
27	N	0	10
28	S	0	10
29	P	0	10
30	Q	0	6
31	R	0	16
32	U	0	2
33	O	0	7
34	8	0	11
All	All	0	347

All (3646) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S	126	LYS	CA-CB	-51.12	0.67	1.53
27	N	861	TYR	CA-CB	15.65	1.88	1.53
29	P	86	HIS	CA-CB	15.34	1.79	1.53
31	R	102	LEU	CA-C	-12.37	1.36	1.52
13	6	222	ASP	C-OXT	-11.57	1.00	1.23
10	3	204	ASP	C-O	-11.57	1.00	1.23
17	K	428	LYS	C-OXT	-11.57	1.00	1.23
7	G	244	ASN	C-O	-11.57	1.00	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	89	GLN	C-OXT	-11.57	1.00	1.23
8	1	196	LEU	C-OXT	-11.56	1.00	1.23
2	B	250	LEU	C-O	-11.56	1.00	1.23
12	5	212	GLY	C-OXT	-11.56	1.00	1.23
14	7	229	GLY	C-O	-11.56	1.00	1.23
25	Y	89	GLN	C-O	-11.56	1.00	1.23
30	Q	434	TYR	C-OXT	-11.56	1.00	1.23
18	L	436	LYS	C-O	-11.55	1.00	1.23
4	D	240	GLU	C-O	-11.55	1.00	1.23
16	I	437	LEU	C-OXT	-11.55	1.00	1.23
19	M	434	ALA	C-OXT	-11.55	1.00	1.23
6	F	233	ILE	C-OXT	-11.55	1.00	1.23
10	3	204	ASP	C-OXT	-11.55	1.00	1.23
11	4	195	PHE	C-O	-11.55	1.00	1.23
12	5	212	GLY	C-O	-11.55	1.00	1.23
16	I	437	LEU	C-O	-11.54	1.00	1.23
17	K	428	LYS	C-O	-11.54	1.00	1.23
19	M	434	ALA	C-O	-11.54	1.00	1.23
30	Q	434	TYR	C-O	-11.54	1.00	1.23
2	B	250	LEU	C-OXT	-11.54	1.00	1.23
28	S	492	LYS	C-O	-11.54	1.00	1.23
1	A	242	GLN	C-O	-11.54	1.00	1.23
8	1	196	LEU	C-O	-11.53	1.00	1.23
3	C	244	THR	C-O	-11.53	1.00	1.23
13	6	222	ASP	C-O	-11.53	1.00	1.23
9	2	226	GLU	C-O	-11.53	1.00	1.23
5	E	242	GLU	C-O	-11.53	1.00	1.23
27	N	925	ASP	C-O	-11.53	1.00	1.23
29	P	440	HIS	C-O	-11.53	1.00	1.23
6	F	233	ILE	C-O	-11.53	1.00	1.23
6	f	148	PRO	N-CA	-11.18	1.32	1.47
6	F	153	THR	CA-C	-11.16	1.39	1.52
1	A	185	ILE	CA-C	11.05	1.64	1.52
9	i	102	GLY	CA-C	-10.99	1.39	1.51
2	B	227	ILE	CA-C	-10.93	1.43	1.52
7	g	73	VAL	N-CA	-10.89	1.33	1.46
27	N	604	ARG	CD-NE	10.82	1.61	1.46
12	5	69	ARG	NE-CZ	10.57	1.44	1.33
33	O	279	ILE	N-CA	-10.46	1.33	1.46
11	4	138	PHE	CA-C	-10.37	1.39	1.52
12	l	166	HIS	CA-C	-10.33	1.40	1.52
16	I	135	PHE	CA-C	-10.30	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	70	ILE	C-N	10.11	1.43	1.33
31	R	47	ALA	CA-C	-10.07	1.40	1.52
2	b	110	LEU	N-CA	-10.05	1.33	1.46
31	R	110	ILE	C-N	-10.01	1.20	1.33
26	Z	722	ASP	CA-C	-10.01	1.39	1.52
4	d	53	GLN	CA-C	-9.93	1.40	1.52
11	4	105	GLY	CA-C	-9.93	1.45	1.52
14	7	43	ILE	N-CA	-9.91	1.37	1.46
2	B	204	PHE	CA-C	-9.91	1.41	1.53
4	d	139	ARG	CA-C	-9.88	1.39	1.53
1	A	43	VAL	CA-CB	-9.71	1.42	1.54
8	h	134	ILE	CA-CB	-9.67	1.44	1.54
6	f	134	ILE	CA-C	-9.64	1.40	1.52
18	L	273	HIS	ND1-CE1	9.54	1.42	1.32
4	D	137	ASP	C-N	9.53	1.44	1.33
8	h	184	GLU	CA-C	-9.49	1.41	1.52
19	M	74	GLN	CA-C	-9.49	1.40	1.52
1	a	6	HIS	CG-CD2	9.47	1.46	1.35
19	M	366	ARG	CD-NE	9.46	1.59	1.46
31	R	105	LYS	CA-CB	9.46	1.69	1.53
4	d	86	LYS	N-CA	-9.43	1.34	1.46
15	H	366	LEU	CA-CB	9.42	1.68	1.53
4	d	165	ASN	CA-C	-9.40	1.41	1.53
9	2	172	ASN	CA-C	-9.39	1.41	1.52
20	J	377	VAL	CA-C	-9.32	1.44	1.52
8	1	182	GLY	CA-C	-9.30	1.41	1.52
11	k	15	LEU	CA-C	-9.26	1.41	1.52
4	D	164	ARG	CD-NE	9.26	1.59	1.46
14	7	51	VAL	C-N	9.26	1.39	1.33
30	Q	122	ILE	CA-C	9.18	1.64	1.52
26	Z	194	GLU	CA-C	-9.18	1.40	1.52
4	D	150	PRO	CA-C	-9.17	1.43	1.52
34	8	449	GLN	CA-C	-9.15	1.41	1.52
11	4	190	ARG	NE-CZ	9.14	1.43	1.33
14	7	41	ARG	NE-CZ	9.13	1.43	1.33
6	f	125	ARG	NE-CZ	9.09	1.43	1.33
1	a	237	VAL	CA-CB	9.02	1.65	1.54
6	f	152	VAL	CA-CB	-8.99	1.43	1.54
5	e	157	TYR	CA-C	-8.99	1.41	1.52
17	K	78	GLU	CA-C	-8.98	1.41	1.52
10	j	197	ARG	CA-C	-8.97	1.42	1.52
17	K	69	LYS	CA-C	-8.96	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	222	GLY	C-N	8.95	1.45	1.33
34	8	242	LYS	CA-C	-8.95	1.42	1.52
6	f	107	ALA	CA-C	-8.94	1.41	1.52
16	I	346	ARG	CD-NE	8.94	1.58	1.46
8	1	174	ARG	NE-CZ	8.89	1.42	1.33
26	Z	469	PRO	C-N	8.89	1.45	1.34
13	6	35	ILE	N-CA	-8.89	1.35	1.46
6	F	47	ALA	CA-C	-8.88	1.41	1.52
4	d	19	GLU	N-CA	-8.86	1.35	1.46
30	Q	51	ARG	CD-NE	8.85	1.58	1.46
27	N	430	ASN	C-N	8.84	1.45	1.33
1	a	202	ILE	CA-C	-8.82	1.42	1.52
7	g	137	VAL	C-N	8.82	1.40	1.33
1	a	63	ILE	CA-C	-8.81	1.42	1.52
6	f	163	ARG	CA-C	-8.80	1.42	1.53
20	J	286	LYS	CA-C	-8.79	1.44	1.53
22	V	126	GLN	N-CA	-8.78	1.35	1.46
10	j	29	GLY	CA-C	-8.77	1.44	1.52
1	a	87	ARG	NE-CZ	8.77	1.42	1.33
34	8	462	TYR	CA-C	-8.77	1.42	1.52
9	i	192	THR	CA-C	8.77	1.60	1.52
3	C	93	HIS	CE1-NE2	8.76	1.41	1.32
15	H	178	ARG	NE-CZ	8.76	1.42	1.33
29	P	42	LEU	CA-C	-8.72	1.41	1.52
24	X	85	ARG	NE-CZ	8.67	1.42	1.33
14	7	156	ARG	NE-CZ	8.66	1.42	1.33
11	4	90	LYS	CA-C	-8.64	1.42	1.52
6	f	106	ARG	NE-CZ	8.64	1.42	1.33
30	Q	396	TRP	CA-C	-8.64	1.42	1.52
8	h	174	ARG	NE-CZ	8.55	1.42	1.33
12	5	86	LEU	C-N	8.55	1.44	1.33
33	O	109	LEU	CA-C	-8.53	1.41	1.52
27	N	15	GLU	CA-CB	8.52	1.67	1.53
9	2	100	VAL	CA-C	-8.51	1.41	1.52
8	1	75	THR	N-CA	-8.50	1.36	1.46
6	f	78	PRO	CA-C	-8.49	1.39	1.52
8	1	29	ARG	NE-CZ	8.49	1.42	1.33
4	d	238	LYS	N-CA	-8.49	1.35	1.46
29	P	147	LYS	N-CA	-8.48	1.34	1.46
9	i	173	VAL	CA-C	-8.47	1.42	1.52
1	A	198	ILE	CA-C	-8.47	1.42	1.52
4	D	149	GLU	C-N	8.47	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	235	PHE	CA-C	-8.47	1.41	1.52
11	4	128	LEU	CA-C	-8.46	1.44	1.52
1	A	235	ARG	NE-CZ	8.45	1.42	1.33
27	N	482	ALA	CA-C	-8.44	1.42	1.52
27	N	547	LEU	N-CA	-8.43	1.35	1.46
24	X	11	ARG	CD-NE	8.43	1.58	1.46
23	T	11	LEU	C-N	8.42	1.45	1.33
14	7	110	LEU	CA-CB	8.40	1.64	1.53
7	g	200	HIS	ND1-CE1	8.40	1.41	1.32
10	3	67	ARG	CD-NE	8.39	1.57	1.46
2	b	17	LYS	N-CA	-8.37	1.36	1.46
5	E	30	ILE	CA-C	-8.37	1.42	1.52
27	N	296	CYS	CA-C	-8.36	1.42	1.52
28	S	25	TYR	N-CA	-8.35	1.36	1.46
5	E	121	GLY	C-N	8.35	1.44	1.33
11	k	76	SER	CA-C	-8.35	1.44	1.53
12	5	2	THR	CA-C	-8.34	1.42	1.52
29	P	37	ASP	N-CA	-8.33	1.36	1.46
30	Q	31	LEU	N-CA	-8.33	1.36	1.46
26	Z	596	THR	CA-C	-8.32	1.41	1.52
11	4	159	ASP	N-CA	-8.32	1.36	1.46
2	B	236	ARG	NE-CZ	8.31	1.42	1.33
6	F	82	VAL	CA-C	-8.31	1.42	1.52
25	Y	73	PHE	CA-C	-8.30	1.42	1.52
33	O	83	LEU	CA-C	-8.29	1.42	1.52
7	g	147	LEU	CA-CB	8.29	1.65	1.53
27	N	345	ASP	N-CA	-8.29	1.35	1.46
19	M	82	VAL	CA-C	-8.27	1.42	1.52
34	8	121	ASN	CA-CB	8.27	1.66	1.53
12	l	115	VAL	CA-C	-8.25	1.43	1.52
2	b	179	TRP	C-N	8.24	1.44	1.33
23	T	81	TYR	CA-C	-8.24	1.42	1.52
18	L	163	THR	CA-C	-8.24	1.42	1.52
27	N	899	ASN	CA-C	-8.23	1.42	1.52
4	d	191	LYS	N-CA	-8.22	1.36	1.46
16	I	100	ARG	CA-CB	8.21	1.63	1.52
30	Q	241	GLU	CA-C	-8.21	1.41	1.52
13	6	198	VAL	C-N	8.21	1.41	1.32
8	h	54	ALA	C-N	8.20	1.44	1.33
4	D	173	LEU	N-CA	-8.19	1.36	1.46
31	R	109	LYS	N-CA	-8.19	1.36	1.46
11	4	149	ARG	NE-CZ	8.17	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	93	ARG	NE-CZ	8.17	1.42	1.33
7	g	69	HIS	ND1-CE1	8.16	1.40	1.32
26	Z	801	HIS	N-CA	-8.15	1.35	1.46
1	a	175	ASN	N-CA	-8.15	1.36	1.46
2	B	243	ILE	CA-C	-8.15	1.42	1.52
14	n	199	ILE	CA-C	-8.15	1.43	1.52
12	l	198	TRP	NE1-CE2	-8.14	1.28	1.37
14	n	222	ALA	CA-C	-8.14	1.42	1.52
16	I	95	GLN	N-CA	-8.14	1.36	1.46
33	O	337	LEU	CA-C	-8.13	1.42	1.52
9	i	75	ARG	CD-NE	8.12	1.57	1.46
27	N	353	LEU	CA-C	8.12	1.63	1.52
32	U	21	HIS	ND1-CE1	8.12	1.40	1.32
27	N	753	PHE	CA-C	-8.12	1.42	1.52
11	k	156	GLU	CA-C	-8.11	1.42	1.52
14	7	165	ILE	CA-C	8.11	1.60	1.52
11	4	98	TYR	CA-C	-8.10	1.43	1.52
27	N	510	HIS	CA-C	-8.09	1.43	1.52
10	j	83	PRO	N-CA	-8.09	1.36	1.47
6	f	100	ARG	CD-NE	8.08	1.57	1.46
13	m	79	HIS	ND1-CE1	8.08	1.40	1.32
1	A	111	ARG	NE-CZ	8.08	1.42	1.33
6	F	109	HIS	CB-CG	-8.08	1.38	1.50
17	K	294	ARG	NE-CZ	8.08	1.42	1.33
30	Q	245	SER	CA-C	-8.08	1.42	1.52
30	Q	123	GLU	CA-C	8.07	1.63	1.52
26	Z	959	HIS	ND1-CE1	8.06	1.40	1.32
16	I	350	PHE	CA-C	-8.05	1.42	1.52
22	V	52	LEU	CA-C	-8.05	1.43	1.52
10	j	22	ILE	N-CA	-8.04	1.36	1.46
18	L	165	PRO	N-CA	-8.03	1.36	1.47
27	N	352	ASN	CA-CB	8.04	1.65	1.52
34	8	395	GLU	CA-C	-8.03	1.42	1.52
5	E	67	GLY	N-CA	-8.02	1.36	1.45
9	i	72	ARG	NE-CZ	8.02	1.41	1.33
5	e	149	HIS	CA-C	-8.00	1.42	1.52
11	k	118	GLN	CA-C	-8.00	1.42	1.52
4	D	140	ASP	N-CA	-8.00	1.36	1.46
10	3	178	ALA	N-CA	-8.00	1.36	1.46
28	S	225	HIS	ND1-CE1	8.00	1.40	1.32
34	8	111	PHE	CA-C	-7.99	1.43	1.52
5	e	30	ILE	CA-CB	-7.99	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	289	ARG	N-CA	-7.98	1.35	1.46
12	5	191	HIS	CA-C	-7.98	1.43	1.52
34	8	389	THR	CA-C	7.97	1.62	1.53
10	j	27	ARG	NE-CZ	7.97	1.41	1.33
9	2	35	HIS	CA-C	-7.97	1.43	1.52
27	N	605	ILE	CA-C	-7.97	1.42	1.52
4	d	169	VAL	C-N	7.97	1.44	1.33
10	j	114	LYS	CA-C	-7.97	1.41	1.52
21	W	5	ALA	CA-C	-7.95	1.43	1.52
4	D	170	ARG	NE-CZ	7.95	1.41	1.33
31	R	69	GLU	CA-C	-7.95	1.41	1.52
33	O	326	HIS	N-CA	-7.95	1.36	1.46
3	C	144	GLY	CA-C	-7.95	1.42	1.52
16	I	127	ASP	N-CA	-7.95	1.36	1.45
2	B	224	TYR	CA-C	-7.94	1.43	1.53
5	e	59	ILE	CA-CB	7.94	1.63	1.54
1	A	7	ILE	CA-C	-7.93	1.43	1.52
1	A	218	VAL	CA-CB	-7.93	1.44	1.54
15	H	346	ARG	NE-CZ	7.93	1.41	1.33
5	E	229	ALA	CA-C	-7.92	1.42	1.52
16	I	246	ARG	NE-CZ	7.92	1.41	1.33
8	1	115	LEU	C-N	7.91	1.44	1.33
26	Z	767	TYR	CA-C	-7.91	1.42	1.52
27	N	6	ALA	CA-C	-7.90	1.42	1.52
9	2	31	CYS	CA-C	-7.89	1.42	1.52
26	Z	537	THR	CA-C	-7.89	1.43	1.52
17	K	259	ARG	CD-NE	7.88	1.57	1.46
2	B	99	ARG	NE-CZ	7.88	1.41	1.33
19	M	280	ILE	CA-C	-7.88	1.43	1.52
31	R	116	LYS	N-CA	-7.87	1.37	1.46
17	K	139	LEU	N-CA	-7.87	1.36	1.46
1	A	200	HIS	ND1-CE1	7.87	1.40	1.32
10	j	27	ARG	CD-NE	7.86	1.57	1.46
2	b	185	LEU	CA-C	-7.86	1.42	1.52
22	V	57	PHE	CA-C	-7.86	1.43	1.52
10	3	99	PHE	CA-CB	7.86	1.63	1.53
10	3	195	VAL	N-CA	-7.85	1.36	1.46
14	n	193	ARG	N-CA	-7.85	1.36	1.46
4	D	133	ILE	CA-C	-7.85	1.42	1.52
27	N	78	ALA	N-CA	-7.84	1.37	1.46
4	D	149	GLU	N-CA	-7.84	1.40	1.46
30	Q	355	GLU	CA-C	-7.83	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	66	TYR	CA-C	-7.83	1.42	1.52
20	J	98	VAL	C-N	7.83	1.43	1.33
7	g	87	ARG	CD-NE	7.81	1.57	1.46
11	4	58	GLU	N-CA	-7.81	1.36	1.46
11	k	52	ASP	N-CA	-7.81	1.36	1.46
27	N	179	THR	C-N	7.81	1.44	1.33
30	Q	123	GLU	C-N	7.81	1.44	1.33
10	3	67	ARG	NE-CZ	7.81	1.41	1.33
28	S	426	ALA	C-N	7.81	1.42	1.33
13	m	139	GLY	CA-C	7.80	1.58	1.52
4	D	131	THR	CA-C	-7.80	1.43	1.52
15	H	251	PRO	CA-C	7.80	1.59	1.52
4	D	47	ARG	CZ-NH2	7.79	1.43	1.33
6	F	183	GLY	C-N	7.78	1.39	1.33
8	1	36	ARG	CD-NE	7.78	1.57	1.46
31	R	364	LEU	CA-C	-7.78	1.43	1.52
16	I	246	ARG	CD-NE	7.78	1.57	1.46
21	W	174	VAL	CA-C	-7.77	1.42	1.52
21	W	178	PRO	N-CD	-7.77	1.36	1.47
8	h	161	GLN	CA-C	-7.76	1.43	1.52
14	n	44	PRO	CA-C	-7.76	1.42	1.52
18	L	89	ASP	CA-C	-7.76	1.42	1.52
21	W	75	GLY	CA-C	-7.76	1.43	1.52
27	N	201	LYS	N-CA	-7.76	1.37	1.46
31	R	104	LYS	CA-C	-7.75	1.43	1.52
34	8	190	LYS	N-CA	-7.75	1.36	1.46
14	n	187	ARG	CD-NE	7.74	1.57	1.46
3	c	133	SER	CA-C	-7.74	1.43	1.52
6	f	165	GLN	N-CA	7.74	1.55	1.46
3	C	216	ARG	CD-NE	7.74	1.57	1.46
29	P	403	GLU	CA-C	-7.74	1.43	1.52
15	H	95	HIS	ND1-CE1	7.73	1.40	1.32
6	F	130	GLY	CA-C	7.72	1.58	1.52
6	F	132	LEU	CA-C	-7.72	1.43	1.52
18	L	145	ARG	NE-CZ	7.71	1.41	1.33
4	D	225	GLU	CA-C	-7.71	1.42	1.52
8	1	121	LYS	CA-C	-7.71	1.42	1.52
2	b	236	ARG	CZ-NH1	7.70	1.43	1.32
10	3	44	HIS	CA-C	-7.70	1.43	1.52
5	e	13	LEU	N-CA	7.70	1.55	1.46
27	N	327	LEU	CA-C	-7.69	1.43	1.52
27	N	786	ARG	CA-CB	7.69	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	114	HIS	CA-C	7.69	1.63	1.52
28	S	473	ASP	N-CA	-7.68	1.36	1.46
26	Z	726	GLU	CA-C	-7.68	1.42	1.52
12	5	103	GLY	C-N	7.68	1.43	1.33
14	n	122	ASN	CA-CB	7.67	1.66	1.53
7	g	113	GLY	CA-C	-7.67	1.43	1.52
23	T	209	LEU	CA-C	-7.66	1.42	1.52
4	D	88	ARG	CD-NE	7.66	1.56	1.46
34	8	331	ARG	NE-CZ	7.66	1.41	1.33
11	4	149	ARG	CZ-NH1	7.65	1.43	1.32
20	J	356	ALA	CA-C	-7.65	1.43	1.52
23	T	19	ASP	CA-C	-7.65	1.43	1.53
6	F	65	CYS	N-CA	-7.65	1.36	1.46
21	W	26	PHE	N-CA	-7.65	1.37	1.46
11	k	147	HIS	CE1-NE2	7.64	1.40	1.32
8	1	25	TYR	C-N	7.64	1.42	1.33
17	K	150	LEU	CA-C	-7.64	1.42	1.52
11	k	162	LYS	N-CA	-7.63	1.37	1.46
16	I	76	VAL	CA-C	-7.63	1.43	1.52
9	2	207	ARG	CZ-NH2	7.62	1.43	1.33
26	Z	923	ILE	CA-C	7.62	1.62	1.52
5	E	85	ARG	CZ-NH2	7.62	1.43	1.33
26	Z	547	MET	N-CA	-7.62	1.37	1.46
16	I	154	MET	N-CA	-7.60	1.36	1.46
11	4	6	GLY	N-CA	-7.60	1.37	1.45
14	n	47	ASP	N-CA	-7.60	1.35	1.46
7	G	139	LYS	CA-C	-7.60	1.43	1.52
26	Z	146	PHE	CA-C	-7.59	1.43	1.52
20	J	371	ARG	NE-CZ	7.59	1.41	1.33
26	Z	709	LYS	N-CA	-7.58	1.37	1.46
24	X	63	PRO	N-CA	-7.58	1.38	1.47
27	N	747	HIS	ND1-CE1	7.58	1.40	1.32
10	j	158	GLU	CA-CB	7.57	1.64	1.53
9	2	177	VAL	CA-CB	-7.57	1.45	1.54
12	5	68	LEU	CA-C	-7.57	1.43	1.52
3	c	88	ASN	CA-C	-7.57	1.43	1.52
2	B	152	PRO	C-N	7.57	1.44	1.33
8	1	100	ALA	CA-C	-7.56	1.43	1.52
4	d	154	TYR	CA-C	-7.56	1.43	1.52
1	A	86	LEU	CA-CB	7.55	1.65	1.53
18	L	434	TYR	CA-C	-7.54	1.43	1.52
10	j	151	SER	N-CA	7.54	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	72	CYS	C-N	7.54	1.42	1.33
4	D	49	THR	CA-C	7.54	1.63	1.52
1	a	96	ARG	NE-CZ	7.54	1.41	1.33
9	2	206	PRO	N-CA	-7.54	1.38	1.47
26	Z	101	SER	N-CA	-7.54	1.37	1.46
9	2	200	GLN	CA-CB	7.53	1.65	1.53
12	5	179	HIS	ND1-CE1	7.53	1.40	1.32
10	j	98	ARG	NE-CZ	7.52	1.41	1.33
9	2	66	HIS	CA-C	-7.52	1.43	1.52
15	H	280	VAL	CA-CB	7.52	1.64	1.54
29	P	440	HIS	ND1-CE1	7.52	1.40	1.32
32	U	141	GLU	CA-C	-7.52	1.43	1.52
6	F	221	PHE	CA-C	-7.52	1.43	1.52
14	7	51	VAL	CA-C	-7.51	1.43	1.52
6	f	81	ARG	CD-NE	7.51	1.56	1.46
12	5	165	ALA	N-CA	-7.51	1.37	1.46
27	N	892	PRO	C-N	7.50	1.43	1.33
27	N	549	TYR	CA-C	-7.50	1.43	1.52
34	8	180	LEU	C-N	7.50	1.39	1.33
34	8	299	VAL	CA-C	-7.50	1.43	1.52
2	B	101	TYR	C-N	7.50	1.40	1.33
6	f	63	ILE	CA-C	-7.49	1.43	1.52
19	M	355	ASP	N-CA	-7.49	1.37	1.46
34	8	151	ALA	N-CA	-7.49	1.36	1.46
34	8	129	ARG	CD-NE	7.49	1.56	1.46
13	6	28	ARG	NE-CZ	7.48	1.41	1.33
27	N	103	SER	CA-C	-7.48	1.43	1.52
13	6	157	LYS	N-CA	-7.48	1.36	1.46
10	j	133	LYS	N-CA	-7.47	1.36	1.46
14	n	93	PHE	CA-C	-7.47	1.43	1.52
8	h	185	ARG	N-CA	-7.47	1.37	1.45
18	L	69	ARG	CZ-NH2	7.47	1.43	1.33
26	Z	547	MET	CA-C	-7.47	1.43	1.52
26	Z	625	THR	C-O	-7.46	1.17	1.24
10	3	71	ASN	CA-C	-7.46	1.43	1.52
4	d	195	ARG	CZ-NH1	7.46	1.43	1.32
27	N	230	VAL	N-CA	-7.46	1.37	1.46
5	E	107	SER	CA-CB	7.45	1.65	1.53
23	T	124	SER	C-N	7.45	1.43	1.33
33	O	389	GLN	CA-C	-7.44	1.43	1.52
15	H	392	HIS	ND1-CE1	7.44	1.40	1.32
17	K	364	PRO	CA-C	-7.44	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S	141	LEU	CA-C	-7.44	1.43	1.52
32	U	15	LEU	N-CA	-7.44	1.37	1.46
13	m	133	ARG	NE-CZ	7.43	1.41	1.33
27	N	89	PHE	C-N	7.43	1.44	1.34
9	i	90	TYR	CA-C	-7.43	1.42	1.52
5	E	149	HIS	CA-CB	7.43	1.64	1.53
26	Z	712	ASP	CA-CB	7.42	1.64	1.53
3	C	22	GLU	N-CA	-7.41	1.37	1.46
30	Q	294	ARG	NE-CZ	7.41	1.41	1.33
5	E	228	THR	CA-CB	7.41	1.64	1.53
3	c	142	ARG	NE-CZ	7.40	1.41	1.33
14	7	103	ARG	CD-NE	7.40	1.56	1.46
32	U	41	ALA	CA-CB	7.40	1.63	1.53
12	5	7	ARG	NE-CZ	7.40	1.41	1.33
27	N	742	TRP	C-N	7.40	1.41	1.33
4	D	16	PHE	CA-C	-7.39	1.42	1.52
16	I	151	HIS	C-N	7.39	1.43	1.33
2	b	83	ARG	NE-CZ	7.39	1.41	1.33
32	U	288	PHE	CA-C	-7.39	1.43	1.52
6	f	218	ASP	CA-C	7.38	1.62	1.52
8	h	36	ARG	N-CA	-7.38	1.37	1.46
20	J	47	GLN	CA-C	-7.38	1.43	1.52
7	G	179	HIS	ND1-CE1	7.38	1.40	1.32
26	Z	705	GLU	C-N	7.38	1.43	1.33
14	7	15	LYS	N-CA	-7.38	1.36	1.45
5	E	40	LEU	N-CA	-7.37	1.36	1.46
16	I	54	ARG	CZ-NH1	7.37	1.43	1.32
20	J	283	GLU	N-CA	-7.37	1.37	1.46
14	7	189	ALA	N-CA	-7.36	1.36	1.46
3	C	137	ALA	N-CA	-7.36	1.37	1.46
7	g	21	GLU	CA-CB	7.36	1.65	1.53
11	4	11	ASP	CA-C	-7.36	1.43	1.52
26	Z	584	VAL	CA-C	7.35	1.60	1.52
29	P	241	LEU	N-CA	-7.35	1.36	1.46
3	C	159	TRP	N-CA	-7.35	1.36	1.45
4	d	56	ARG	NE-CZ	7.35	1.41	1.33
5	E	78	ARG	N-CA	-7.34	1.37	1.46
13	6	107	VAL	CA-C	-7.34	1.43	1.52
14	n	205	GLY	CA-C	-7.34	1.43	1.52
5	e	65	HIS	ND1-CE1	7.33	1.39	1.32
31	R	296	LEU	CA-CB	7.33	1.64	1.53
32	U	217	LYS	C-N	7.33	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	186	VAL	CA-C	-7.33	1.43	1.52
17	K	350	ARG	N-CA	-7.33	1.37	1.46
12	l	41	LEU	N-CA	-7.32	1.37	1.46
14	n	90	SER	CA-CB	7.32	1.65	1.53
26	Z	899	GLN	CA-C	-7.32	1.44	1.53
27	N	594	VAL	C-N	7.32	1.44	1.33
2	B	91	LYS	C-N	7.32	1.42	1.33
12	l	159	ARG	NE-CZ	7.32	1.41	1.33
14	7	111	TRP	NE1-CE2	7.32	1.45	1.37
34	8	335	PHE	CA-C	-7.31	1.43	1.52
1	a	119	TYR	N-CA	-7.31	1.37	1.46
28	S	439	GLU	CA-CB	7.31	1.65	1.53
3	C	227	LYS	N-CA	-7.30	1.37	1.46
22	V	24	LYS	CA-C	-7.30	1.43	1.52
2	b	145	PHE	C-N	7.30	1.42	1.33
8	1	20	THR	C-N	7.30	1.44	1.33
18	L	132	ARG	NE-CZ	7.30	1.41	1.33
12	5	199	LYS	CA-C	-7.29	1.43	1.52
29	P	203	ILE	C-N	7.29	1.43	1.33
13	m	180	VAL	CA-C	7.29	1.62	1.52
13	6	13	LEU	N-CA	-7.28	1.37	1.46
4	D	79	ASP	CA-C	-7.27	1.43	1.52
2	B	4	ARG	NE-CZ	7.27	1.41	1.33
10	3	57	THR	CA-CB	-7.27	1.41	1.53
13	6	185	ARG	NE-CZ	7.27	1.41	1.33
27	N	526	TYR	C-N	7.27	1.44	1.33
8	h	53	GLN	N-CA	-7.26	1.37	1.46
30	Q	130	ARG	N-CA	-7.26	1.36	1.45
34	8	357	ARG	NE-CZ	7.26	1.41	1.33
17	K	74	HIS	CE1-NE2	-7.26	1.25	1.32
19	M	49	GLN	C-N	7.26	1.43	1.33
26	Z	163	GLU	N-CA	-7.26	1.37	1.46
2	B	246	ARG	CD-NE	7.25	1.56	1.46
3	C	160	LYS	N-CA	-7.25	1.37	1.46
28	S	151	GLU	CA-C	-7.25	1.44	1.53
34	8	156	ILE	CA-CB	-7.25	1.45	1.54
5	e	87	ALA	CA-C	-7.25	1.43	1.52
3	c	62	THR	CA-C	-7.25	1.44	1.52
14	7	88	GLU	CA-CB	7.25	1.62	1.54
2	B	88	LYS	C-N	7.25	1.43	1.33
5	e	214	ILE	CA-C	-7.25	1.43	1.52
34	8	161	VAL	N-CA	-7.24	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	69	ARG	CA-C	-7.24	1.43	1.52
1	A	69	THR	CA-C	-7.24	1.43	1.52
10	3	167	SER	N-CA	-7.24	1.37	1.46
27	N	914	VAL	N-CA	-7.24	1.38	1.46
18	L	78	ARG	NE-CZ	7.23	1.41	1.33
34	8	316	ARG	NE-CZ	7.23	1.41	1.33
8	1	62	HIS	ND1-CE1	7.23	1.39	1.32
15	H	302	LYS	CA-C	-7.23	1.43	1.52
10	3	20	VAL	N-CA	-7.22	1.38	1.46
2	b	190	HIS	ND1-CE1	7.21	1.39	1.32
14	n	58	SER	N-CA	-7.21	1.37	1.46
1	A	182	ILE	N-CA	-7.21	1.37	1.46
13	m	133	ARG	CD-NE	7.21	1.56	1.46
14	7	128	ARG	CZ-NH2	7.21	1.42	1.33
13	m	221	ARG	NE-CZ	7.21	1.41	1.33
4	D	212	VAL	CA-C	-7.20	1.44	1.52
33	O	128	LEU	CA-C	-7.20	1.43	1.52
29	P	263	HIS	C-N	7.20	1.43	1.34
3	C	216	ARG	N-CA	-7.20	1.37	1.46
31	R	350	LEU	CA-C	-7.19	1.43	1.52
18	L	392	ARG	NE-CZ	7.19	1.41	1.33
16	I	107	GLY	N-CA	-7.19	1.38	1.45
4	d	197	LEU	CA-C	-7.18	1.43	1.52
3	c	190	GLU	N-CA	-7.18	1.37	1.46
9	i	207	ARG	NE-CZ	7.18	1.41	1.33
5	e	180	HIS	CG-CD2	7.18	1.43	1.35
12	5	180	VAL	CA-CB	-7.18	1.45	1.53
7	g	111	ARG	CZ-NH2	7.17	1.42	1.33
4	d	83	LEU	CA-C	-7.17	1.43	1.52
9	i	196	ARG	CD-NE	7.17	1.56	1.46
26	Z	10	GLN	N-CA	-7.17	1.37	1.46
2	b	44	VAL	CA-CB	-7.17	1.45	1.54
30	Q	325	LEU	C-N	7.17	1.43	1.33
4	d	188	GLU	CA-CB	7.16	1.64	1.53
9	2	56	THR	CA-C	7.16	1.62	1.52
17	K	161	MET	CA-C	-7.16	1.43	1.52
31	R	206	ARG	CZ-NH1	7.16	1.42	1.32
9	2	167	LEU	CA-CB	7.15	1.65	1.53
34	8	453	ARG	CA-C	-7.15	1.43	1.52
2	B	208	THR	C-N	7.15	1.42	1.33
2	b	239	THR	C-N	-7.14	1.24	1.33
12	l	120	THR	N-CA	-7.14	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	22	ASP	CA-CB	7.14	1.65	1.53
14	n	198	ALA	CA-C	-7.14	1.44	1.52
23	T	224	ARG	CD-NE	7.14	1.56	1.46
18	L	345	ARG	NE-CZ	7.14	1.40	1.33
9	i	93	HIS	ND1-CE1	7.13	1.39	1.32
5	E	6	THR	CA-C	-7.13	1.44	1.52
2	b	234	ARG	CD-NE	7.13	1.56	1.46
2	B	89	SER	CA-C	-7.13	1.43	1.52
26	Z	604	GLY	CA-C	-7.13	1.43	1.51
13	m	88	SER	CA-C	-7.13	1.43	1.52
14	n	29	SER	C-N	7.13	1.44	1.33
18	L	159	LEU	CA-C	-7.13	1.44	1.52
32	U	254	ARG	NE-CZ	7.13	1.40	1.33
13	6	59	ALA	C-N	7.12	1.43	1.33
1	a	82	ARG	CZ-NH2	7.12	1.42	1.33
7	g	111	ARG	CA-C	-7.12	1.43	1.52
9	2	71	SER	C-N	7.12	1.42	1.33
27	N	570	ARG	CZ-NH2	7.12	1.42	1.33
29	P	121	THR	N-CA	-7.12	1.37	1.46
13	m	149	PHE	CA-C	-7.12	1.43	1.52
12	5	210	VAL	CA-C	-7.12	1.44	1.52
18	L	172	SER	CA-C	-7.11	1.43	1.52
9	i	121	VAL	CA-C	-7.11	1.43	1.52
7	G	54	LEU	C-N	7.11	1.42	1.33
31	R	103	CYS	N-CA	-7.11	1.37	1.46
4	d	22	LEU	CA-CB	7.11	1.64	1.53
6	F	14	PRO	C-O	-7.11	1.15	1.24
24	X	59	ARG	NE-CZ	7.11	1.40	1.33
26	Z	180	ASP	CA-C	-7.10	1.47	1.52
11	4	93	ARG	NE-CZ	7.10	1.40	1.33
4	d	4	ARG	NE-CZ	7.10	1.40	1.33
11	4	95	ARG	NE-CZ	7.09	1.40	1.33
31	R	122	GLU	CA-CB	7.09	1.64	1.53
7	G	186	ARG	NE-CZ	7.09	1.40	1.33
1	a	175	ASN	C-N	7.09	1.42	1.33
9	2	222	ASP	CA-C	-7.09	1.43	1.52
28	S	53	ILE	C-N	7.08	1.42	1.33
7	G	89	ARG	CD-NE	7.08	1.56	1.46
10	j	90	VAL	C-N	7.08	1.42	1.33
15	H	427	GLY	CA-C	-7.08	1.43	1.51
12	5	19	ARG	CD-NE	7.08	1.56	1.46
16	I	84	PRO	N-CA	-7.07	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	58	GLU	N-CA	-7.07	1.37	1.46
31	R	115	GLU	CA-CB	7.07	1.65	1.53
3	C	69	ASN	CA-C	-7.07	1.44	1.52
26	Z	68	LEU	CA-C	-7.06	1.44	1.52
8	h	37	VAL	CA-CB	-7.06	1.46	1.54
6	F	159	ALA	C-N	7.06	1.43	1.33
8	h	19	ARG	NE-CZ	7.06	1.40	1.33
1	a	155	VAL	CA-CB	-7.06	1.48	1.55
11	k	190	ARG	CD-NE	7.06	1.56	1.46
6	F	134	ILE	CA-C	-7.05	1.43	1.52
10	j	86	PHE	N-CA	-7.05	1.37	1.46
30	Q	413	LEU	N-CA	7.05	1.55	1.46
1	a	130	VAL	CA-C	-7.04	1.45	1.52
23	T	92	ASN	N-CA	-7.04	1.37	1.46
7	g	27	VAL	CA-C	-7.04	1.43	1.52
7	g	165	ARG	CZ-NH1	7.04	1.42	1.32
34	8	352	GLU	N-CA	-7.04	1.37	1.46
14	n	23	ALA	N-CA	-7.03	1.37	1.45
26	Z	154	ILE	N-CA	-7.03	1.38	1.46
26	Z	789	GLN	N-CA	-7.03	1.37	1.46
20	J	143	PRO	C-N	7.03	1.42	1.33
26	Z	204	CYS	CA-C	-7.03	1.43	1.52
4	d	157	TRP	NE1-CE2	7.02	1.45	1.37
12	l	66	HIS	ND1-CE1	7.02	1.39	1.32
12	5	26	VAL	CA-C	-7.02	1.45	1.53
23	T	159	LYS	N-CA	-7.02	1.37	1.46
31	R	353	MET	CA-C	-7.02	1.43	1.52
14	n	182	ARG	CZ-NH2	7.01	1.42	1.33
33	O	76	LEU	N-CA	-7.00	1.37	1.46
14	n	142	LEU	CA-C	-7.00	1.43	1.52
7	g	183	LEU	CA-C	-7.00	1.43	1.52
4	D	4	ARG	N-CA	-6.99	1.37	1.46
10	3	41	LYS	C-N	6.99	1.42	1.33
15	H	62	ARG	CD-NE	6.98	1.56	1.46
4	d	62	VAL	N-CA	-6.98	1.37	1.46
9	2	187	LEU	N-CA	-6.97	1.37	1.46
17	K	242	PHE	C-N	6.97	1.42	1.33
3	c	211	GLU	CA-C	-6.97	1.44	1.52
18	L	303	ARG	NE-CZ	6.97	1.40	1.33
22	V	102	GLN	CA-C	-6.97	1.44	1.52
2	B	90	ARG	CZ-NH2	6.97	1.42	1.33
12	5	159	ARG	CD-NE	6.97	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	M	166	ARG	NE-CZ	6.97	1.40	1.33
4	D	164	ARG	NE-CZ	6.97	1.40	1.33
1	a	157	TYR	CA-C	-6.96	1.44	1.52
2	b	56	ALA	CA-C	-6.96	1.44	1.52
16	I	433	GLU	C-N	6.96	1.39	1.33
2	b	135	LEU	CA-C	-6.96	1.44	1.52
28	S	160	ARG	NE-CZ	6.96	1.40	1.33
8	h	177	VAL	CA-C	-6.96	1.44	1.52
6	f	81	ARG	CA-C	-6.95	1.43	1.52
6	f	201	ARG	NE-CZ	6.95	1.40	1.33
19	M	345	ARG	CA-C	-6.95	1.43	1.52
7	G	73	VAL	N-CA	-6.95	1.38	1.46
26	Z	462	VAL	C-O	6.95	1.30	1.24
8	h	186	LEU	C-N	6.94	1.42	1.33
10	3	66	PHE	N-CA	-6.94	1.37	1.46
14	7	94	GLU	CA-C	-6.94	1.43	1.52
9	i	20	SER	CA-C	-6.93	1.44	1.52
27	N	659	ALA	C-N	6.93	1.43	1.33
1	a	182	ILE	CA-CB	-6.93	1.44	1.54
10	j	33	LEU	CA-CB	6.93	1.61	1.53
3	c	216	ARG	NE-CZ	6.93	1.40	1.33
3	C	48	GLU	CA-C	-6.93	1.44	1.52
20	J	163	VAL	N-CA	-6.92	1.38	1.46
4	d	27	ARG	NE-CZ	6.92	1.40	1.33
4	D	4	ARG	CD-NE	6.92	1.55	1.46
28	S	401	LYS	C-N	6.92	1.42	1.33
22	V	105	VAL	N-CA	-6.92	1.37	1.46
19	M	42	ARG	CD-NE	6.91	1.55	1.46
15	H	207	THR	C-N	6.91	1.43	1.34
9	2	188	ARG	NE-CZ	6.91	1.40	1.33
30	Q	146	TYR	CA-C	-6.91	1.43	1.52
8	1	172	VAL	N-CA	-6.90	1.37	1.46
13	6	100	LYS	CA-C	-6.90	1.44	1.52
13	6	144	SER	C-N	6.90	1.43	1.33
7	g	78	ILE	CA-CB	-6.90	1.50	1.54
29	P	11	LYS	C-N	6.90	1.43	1.33
32	U	283	ARG	NE-CZ	6.90	1.40	1.33
34	8	189	ARG	C-N	6.90	1.43	1.33
27	N	555	ILE	C-N	6.90	1.42	1.33
19	M	33	ARG	CD-NE	6.90	1.55	1.46
11	4	182	LYS	CA-C	-6.89	1.44	1.52
18	L	342	ARG	CD-NE	6.89	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	331	ARG	NE-CZ	6.89	1.40	1.33
2	B	59	GLU	CA-C	-6.89	1.43	1.52
31	R	346	LYS	N-CA	-6.88	1.37	1.46
17	K	426	PHE	N-CA	-6.88	1.40	1.46
4	D	190	VAL	CA-C	-6.88	1.44	1.52
11	k	134	GLY	CA-C	-6.87	1.45	1.52
16	I	424	MET	C-N	6.87	1.42	1.33
26	Z	938	GLN	CA-C	-6.86	1.44	1.53
2	B	55	LEU	C-N	6.86	1.43	1.33
5	E	93	LEU	CA-C	-6.86	1.43	1.52
5	e	235	LEU	N-CA	-6.86	1.38	1.46
12	5	66	HIS	ND1-CE1	6.86	1.39	1.32
32	U	126	LYS	N-CA	-6.85	1.37	1.46
34	8	339	LEU	CA-C	-6.85	1.44	1.52
13	6	213	ARG	CA-C	-6.85	1.44	1.52
7	g	236	ILE	CB-CG1	6.84	1.67	1.53
2	b	203	GLU	CA-C	-6.84	1.43	1.52
3	c	17	ARG	NE-CZ	6.84	1.40	1.33
5	E	132	VAL	C-N	6.84	1.42	1.33
4	d	148	THR	CA-C	-6.83	1.44	1.52
14	7	104	ARG	CA-C	-6.83	1.44	1.52
17	K	356	ILE	CA-C	-6.83	1.44	1.52
1	A	216	VAL	C-N	6.83	1.40	1.33
11	4	96	ARG	C-O	-6.83	1.19	1.25
16	I	327	ALA	CA-C	-6.83	1.44	1.52
6	F	15	THR	N-CA	-6.83	1.37	1.46
3	c	30	HIS	CG-ND1	-6.83	1.30	1.38
26	Z	484	LYS	C-N	6.83	1.42	1.33
13	6	101	ARG	CD-NE	6.83	1.55	1.46
26	Z	561	ASP	C-N	6.83	1.42	1.33
32	U	106	ILE	N-CA	-6.83	1.38	1.46
5	E	12	ARG	NE-CZ	6.82	1.40	1.33
10	3	160	GLU	CA-C	6.82	1.62	1.52
22	V	119	SER	CA-CB	6.82	1.63	1.53
30	Q	366	ILE	N-CA	-6.82	1.38	1.46
1	a	13	GLU	N-CA	-6.82	1.38	1.46
19	M	237	ALA	CA-C	-6.82	1.44	1.52
8	h	132	THR	CA-C	-6.82	1.44	1.52
2	b	123	GLN	CA-C	-6.81	1.44	1.52
9	i	214	LYS	CA-CB	6.81	1.65	1.53
4	D	46	ARG	CD-NE	6.81	1.55	1.46
10	3	201	MET	CA-C	-6.81	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	37	ASN	C-N	6.81	1.42	1.33
2	B	23	TYR	C-N	6.81	1.43	1.33
6	F	64	LYS	CA-C	-6.81	1.44	1.52
30	Q	34	ASP	CA-C	-6.81	1.44	1.52
17	K	346	ARG	NE-CZ	6.80	1.40	1.33
18	L	261	ARG	NE-CZ	6.80	1.40	1.33
12	l	170	TYR	C-N	6.80	1.43	1.33
12	l	204	GLU	CA-CB	6.80	1.64	1.53
11	k	68	SER	CA-C	-6.80	1.44	1.52
32	U	121	LEU	CA-CB	6.80	1.62	1.53
4	D	117	ARG	CZ-NH1	6.79	1.42	1.32
20	J	259	GLU	N-CA	-6.79	1.37	1.46
18	L	100	SER	C-N	6.79	1.42	1.33
27	N	405	LEU	CA-CB	6.78	1.64	1.53
2	B	234	ARG	CD-NE	6.78	1.55	1.46
14	7	119	VAL	C-N	6.78	1.42	1.33
2	B	172	LYS	CA-C	-6.78	1.44	1.52
12	l	69	ARG	NE-CZ	6.77	1.40	1.33
15	H	62	ARG	CZ-NH2	6.77	1.42	1.33
24	X	66	LEU	CA-C	-6.77	1.44	1.52
34	8	129	ARG	CZ-NH1	6.77	1.42	1.32
14	n	13	SER	C-N	6.77	1.41	1.33
12	5	162	LEU	CA-C	-6.77	1.44	1.52
32	U	274	MET	N-CA	-6.77	1.38	1.46
15	H	363	PRO	N-CA	-6.76	1.38	1.47
26	Z	936	VAL	N-CA	-6.76	1.38	1.46
3	C	121	TYR	C-N	6.76	1.42	1.33
26	Z	7	LYS	C-N	6.76	1.43	1.33
26	Z	942	PRO	CA-C	-6.76	1.44	1.52
7	G	28	GLU	C-N	6.76	1.43	1.33
14	7	190	ARG	CZ-NH2	6.76	1.42	1.33
7	G	216	SER	CA-C	-6.76	1.44	1.52
15	H	387	ASN	C-N	6.76	1.42	1.33
10	j	28	LEU	CA-C	-6.75	1.44	1.52
13	m	137	ARG	CD-NE	6.75	1.55	1.46
3	C	49	ARG	NE-CZ	6.75	1.40	1.33
9	i	113	ILE	CA-C	6.75	1.60	1.52
1	A	170	THR	CA-C	-6.75	1.44	1.52
26	Z	225	LEU	N-CA	-6.75	1.38	1.46
34	8	334	VAL	CA-C	-6.75	1.44	1.52
1	a	118	ILE	CA-C	-6.75	1.44	1.52
27	N	652	VAL	CA-C	-6.75	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	166	HIS	CA-CB	6.74	1.64	1.53
1	A	215	GLU	CA-C	-6.74	1.44	1.52
6	f	57	SER	CA-C	-6.74	1.44	1.53
10	3	203	GLN	CA-C	-6.74	1.44	1.52
27	N	394	ARG	NE-CZ	6.74	1.40	1.33
3	C	172	GLN	N-CA	-6.74	1.38	1.46
19	M	362	GLN	C-N	6.74	1.42	1.33
4	d	122	GLY	CA-C	-6.73	1.45	1.52
8	h	59	VAL	CA-C	-6.73	1.44	1.52
9	i	19	ARG	NE-CZ	6.73	1.40	1.33
31	R	21	VAL	CA-CB	6.73	1.57	1.54
9	i	36	ARG	NE-CZ	6.73	1.40	1.33
34	8	476	LYS	N-CA	-6.72	1.38	1.46
13	m	95	HIS	N-CA	-6.72	1.37	1.46
14	n	194	ASN	CA-C	-6.72	1.44	1.52
26	Z	436	LEU	CA-CB	6.72	1.64	1.53
32	U	242	PRO	C-N	6.72	1.43	1.34
3	c	30	HIS	ND1-CE1	6.72	1.39	1.32
13	m	195	HIS	ND1-CE1	6.71	1.39	1.32
4	D	109	ARG	NE-CZ	6.71	1.40	1.33
20	J	283	GLU	CA-C	-6.71	1.44	1.52
13	6	103	PHE	CA-C	-6.71	1.46	1.52
14	7	210	LYS	N-CA	-6.71	1.37	1.45
29	P	351	ARG	NE-CZ	6.70	1.40	1.33
7	G	64	GLN	N-CA	-6.70	1.37	1.46
3	c	226	GLN	CA-CB	6.69	1.62	1.53
17	K	235	ILE	N-CA	-6.69	1.36	1.46
17	K	173	ASP	C-N	6.69	1.41	1.33
22	V	79	SER	CA-C	-6.69	1.44	1.52
1	a	134	PHE	N-CA	-6.69	1.37	1.46
14	7	62	HIS	CA-CB	6.69	1.63	1.53
5	E	146	GLN	CA-C	-6.69	1.44	1.52
18	L	363	ILE	CA-C	-6.69	1.44	1.52
3	C	112	ARG	N-CA	-6.68	1.38	1.46
1	a	110	LYS	N-CA	-6.68	1.38	1.46
1	A	126	ARG	CD-NE	6.68	1.55	1.46
12	l	166	HIS	N-CA	-6.68	1.38	1.46
1	A	87	ARG	NE-CZ	6.68	1.40	1.33
13	m	119	LYS	C-N	6.68	1.39	1.33
28	S	365	THR	C-N	6.68	1.43	1.33
33	O	103	LYS	N-CA	-6.68	1.38	1.46
13	6	38	ARG	CD-NE	6.67	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	X	96	ARG	N-CA	6.67	1.54	1.46
31	R	207	ARG	N-CA	-6.67	1.38	1.46
11	4	96	ARG	NE-CZ	6.67	1.40	1.33
27	N	867	LYS	CA-CB	6.67	1.63	1.53
6	f	173	ARG	CZ-NH2	6.67	1.42	1.33
28	S	405	ARG	CZ-NH2	6.67	1.42	1.33
3	c	66	TYR	CA-C	-6.67	1.44	1.52
19	M	73	ARG	CZ-NH2	6.67	1.42	1.33
13	m	100	LYS	CA-CB	6.67	1.62	1.53
3	C	148	TYR	C-O	6.66	1.32	1.23
27	N	296	CYS	N-CA	-6.66	1.38	1.46
5	e	174	GLU	CA-C	-6.66	1.44	1.52
5	e	204	LEU	CA-C	-6.66	1.44	1.52
7	g	179	HIS	CA-C	6.66	1.61	1.52
3	C	89	THR	C-O	-6.66	1.16	1.24
28	S	462	ASP	C-N	6.66	1.42	1.33
29	P	402	PHE	N-CA	-6.66	1.38	1.46
12	l	110	PRO	CA-CB	6.66	1.62	1.53
13	m	12	ILE	C-N	6.66	1.42	1.33
4	D	46	ARG	NE-CZ	6.66	1.40	1.33
31	R	237	THR	CA-C	-6.65	1.43	1.52
5	e	52	GLU	CA-C	-6.65	1.44	1.53
16	I	291	ARG	NE-CZ	6.64	1.40	1.33
5	e	100	ASN	CA-C	-6.64	1.44	1.52
16	I	54	ARG	CD-NE	6.64	1.55	1.46
12	5	69	ARG	C-N	6.64	1.43	1.33
26	Z	554	THR	N-CA	-6.64	1.38	1.46
15	H	211	VAL	C-N	6.64	1.43	1.33
18	L	364	HIS	CA-C	-6.64	1.44	1.52
2	B	45	ILE	CA-C	6.63	1.60	1.52
9	2	86	HIS	CE1-NE2	-6.63	1.25	1.32
6	f	42	HIS	CA-C	-6.63	1.44	1.52
32	U	90	ILE	N-CA	-6.63	1.40	1.46
8	h	175	MET	CA-C	-6.63	1.44	1.52
14	n	193	ARG	NE-CZ	6.63	1.40	1.33
5	E	119	ALA	N-CA	-6.63	1.37	1.45
9	2	59	ILE	CA-C	-6.63	1.44	1.52
14	n	206	LEU	N-CA	-6.62	1.38	1.46
7	g	167	SER	CA-C	-6.62	1.44	1.52
2	B	143	ASN	CA-C	-6.62	1.44	1.52
7	g	58	GLN	CA-C	-6.62	1.45	1.53
15	H	88	ARG	NE-CZ	6.62	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	432	ARG	CZ-NH1	6.62	1.42	1.32
26	Z	531	ALA	CA-C	-6.62	1.44	1.52
26	Z	756	MET	N-CA	-6.62	1.37	1.46
14	n	26	ASN	N-CA	-6.62	1.38	1.46
6	F	163	ARG	NE-CZ	6.62	1.40	1.33
28	S	110	LEU	C-N	6.62	1.42	1.33
7	G	111	ARG	CD-NE	6.61	1.55	1.46
6	f	105	GLU	CA-C	-6.61	1.44	1.52
27	N	801	THR	CA-CB	-6.61	1.42	1.53
3	c	240	LYS	N-CA	-6.61	1.38	1.46
11	k	53	THR	CA-CB	-6.61	1.43	1.53
30	Q	150	GLN	CA-C	-6.61	1.44	1.53
5	e	99	ILE	CA-C	-6.61	1.46	1.53
1	A	110	LYS	CA-C	-6.61	1.44	1.52
18	L	53	HIS	ND1-CE1	6.61	1.39	1.32
29	P	201	ARG	N-CA	-6.60	1.37	1.46
18	L	196	VAL	N-CA	-6.60	1.38	1.46
22	V	42	ARG	CZ-NH2	6.60	1.42	1.33
27	N	570	ARG	NE-CZ	6.60	1.40	1.33
13	6	185	ARG	CZ-NH2	6.60	1.42	1.33
5	e	64	ARG	NE-CZ	6.59	1.40	1.33
33	O	239	MET	CA-C	-6.59	1.44	1.52
26	Z	723	ASP	N-CA	-6.59	1.38	1.46
27	N	635	GLN	C-N	6.59	1.42	1.33
5	e	112	ALA	C-N	6.59	1.41	1.33
3	C	105	ILE	N-CA	-6.59	1.38	1.47
16	I	222	TYR	CA-C	-6.59	1.44	1.52
18	L	230	LEU	C-N	6.59	1.42	1.33
29	P	425	HIS	CA-C	-6.59	1.44	1.52
4	D	47	ARG	NE-CZ	6.58	1.40	1.33
32	U	127	GLN	CA-C	-6.58	1.45	1.53
13	m	99	GLY	C-N	6.57	1.43	1.33
22	V	159	ILE	C-N	6.57	1.42	1.33
2	b	108	LYS	CA-C	-6.57	1.44	1.52
7	G	128	PHE	CA-C	6.57	1.61	1.52
13	6	25	GLY	CA-C	-6.57	1.44	1.51
20	J	270	ARG	NE-CZ	6.56	1.40	1.33
12	l	25	TRP	N-CA	-6.56	1.38	1.46
1	A	5	ARG	NE-CZ	6.55	1.40	1.33
15	H	455	LYS	CA-C	-6.55	1.44	1.52
19	M	345	ARG	NE-CZ	6.55	1.40	1.33
17	K	349	ARG	CD-NE	6.55	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	155	ALA	N-CA	-6.55	1.38	1.46
1	a	111	ARG	NE-CZ	6.55	1.40	1.33
27	N	496	GLU	CA-CB	6.55	1.63	1.53
30	Q	131	VAL	C-N	6.55	1.42	1.33
3	c	17	ARG	N-CA	-6.55	1.38	1.46
15	H	289	ARG	CD-NE	6.55	1.55	1.46
26	Z	119	LEU	N-CA	-6.54	1.38	1.46
4	D	89	VAL	N-CA	-6.54	1.38	1.46
4	D	111	VAL	N-CA	-6.54	1.39	1.46
8	1	178	LEU	CA-C	-6.54	1.44	1.52
18	L	213	LYS	CA-C	6.54	1.59	1.53
13	m	144	SER	N-CA	6.53	1.54	1.46
16	I	300	ARG	CZ-NH2	6.53	1.42	1.33
10	j	50	LEU	N-CA	-6.53	1.38	1.46
12	5	141	ASP	CA-C	-6.53	1.44	1.52
20	J	329	ARG	CD-NE	6.53	1.55	1.46
27	N	426	ILE	C-N	6.53	1.42	1.33
11	4	104	ILE	C-N	6.53	1.37	1.33
7	g	195	ILE	CA-CB	6.53	1.62	1.54
11	4	118	GLN	C-O	-6.53	1.16	1.24
12	5	34	VAL	CA-CB	-6.52	1.46	1.54
19	M	364	HIS	ND1-CE1	6.52	1.39	1.32
29	P	297	GLU	N-CA	-6.52	1.38	1.46
5	E	211	LEU	C-N	6.52	1.41	1.33
13	m	195	HIS	CA-CB	6.52	1.65	1.53
7	G	200	HIS	N-CA	6.52	1.54	1.46
12	l	52	CYS	C-N	6.52	1.41	1.33
4	D	195	ARG	CZ-NH2	6.51	1.42	1.33
24	X	111	LEU	N-CA	-6.51	1.38	1.46
11	4	102	VAL	CA-C	-6.51	1.44	1.52
15	H	163	VAL	CA-CB	-6.51	1.45	1.54
9	i	110	LEU	N-CA	-6.51	1.38	1.46
10	3	3	PRO	CA-CB	6.51	1.62	1.53
32	U	133	PRO	CA-C	6.51	1.59	1.52
33	O	18	ALA	CA-C	-6.51	1.44	1.52
20	J	245	ILE	CA-C	-6.50	1.44	1.52
33	O	319	LEU	C-N	6.50	1.41	1.33
26	Z	457	ILE	N-CA	-6.50	1.38	1.46
18	L	240	GLY	C-N	6.50	1.42	1.33
1	A	147	LYS	CA-C	-6.50	1.44	1.52
13	m	67	ARG	NE-CZ	6.50	1.40	1.33
5	E	189	GLU	CA-C	-6.50	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	392	HIS	N-CA	-6.50	1.38	1.46
27	N	789	GLU	C-N	6.50	1.42	1.33
9	2	23	GLY	C-N	6.50	1.40	1.33
7	g	44	PHE	CA-C	-6.49	1.44	1.52
1	a	106	ASP	CA-CB	6.49	1.63	1.53
13	m	176	SER	CA-C	-6.49	1.44	1.52
22	V	51	GLY	CA-C	-6.49	1.43	1.51
5	e	137	ALA	C-N	6.49	1.39	1.33
5	E	28	THR	N-CA	-6.49	1.38	1.46
1	a	235	ARG	CZ-NH1	6.48	1.41	1.32
10	3	66	PHE	CA-C	-6.48	1.43	1.52
31	R	392	ARG	CZ-NH2	6.48	1.41	1.33
12	l	19	ARG	NE-CZ	6.48	1.40	1.33
1	A	85	ALA	N-CA	-6.48	1.38	1.46
13	m	101	ARG	NE-CZ	6.48	1.40	1.33
2	B	46	ALA	N-CA	-6.48	1.38	1.46
6	F	228	ALA	CA-C	-6.48	1.43	1.52
17	K	249	GLU	N-CA	-6.48	1.38	1.46
26	Z	450	GLY	N-CA	-6.48	1.37	1.45
28	S	469	ASN	C-N	6.48	1.42	1.33
9	i	72	ARG	CZ-NH1	6.48	1.41	1.32
6	F	17	ARG	N-CA	-6.48	1.38	1.46
4	d	109	ARG	CZ-NH2	6.47	1.41	1.33
31	R	331	ARG	NE-CZ	6.47	1.40	1.33
8	h	192	GLU	C-N	6.47	1.43	1.33
6	F	193	VAL	C-O	6.47	1.31	1.24
18	L	407	ARG	CD-NE	6.47	1.55	1.46
17	K	170	THR	CA-C	-6.47	1.44	1.52
19	M	53	HIS	ND1-CE1	6.47	1.39	1.32
24	X	15	CYS	CA-C	-6.47	1.44	1.52
2	B	192	ALA	N-CA	6.47	1.54	1.46
5	e	64	ARG	CD-NE	6.46	1.55	1.46
3	C	227	LYS	CA-C	-6.46	1.45	1.52
5	E	139	HIS	N-CA	-6.46	1.37	1.46
34	8	234	ARG	CZ-NH2	6.46	1.41	1.33
34	8	319	TRP	N-CA	-6.46	1.38	1.46
10	j	203	GLN	N-CA	-6.45	1.37	1.46
11	4	18	SER	N-CA	-6.45	1.38	1.46
12	5	99	THR	CA-C	-6.45	1.44	1.52
3	c	82	ASP	CA-CB	6.45	1.63	1.53
12	l	125	ASP	C-N	6.45	1.41	1.33
2	B	200	VAL	N-CA	-6.45	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	P	275	ASN	CA-CB	6.45	1.63	1.53
32	U	26	GLN	CA-C	-6.44	1.44	1.53
27	N	332	VAL	C-N	6.44	1.42	1.33
18	L	126	ARG	CD-NE	6.44	1.55	1.46
29	P	137	ALA	CA-C	-6.44	1.44	1.52
33	O	235	HIS	ND1-CE1	6.44	1.39	1.32
34	8	287	ARG	CZ-NH2	6.44	1.41	1.33
2	B	160	LYS	CA-C	-6.43	1.44	1.52
14	7	71	VAL	C-N	6.43	1.42	1.33
7	g	82	ARG	CD-NE	6.43	1.55	1.46
26	Z	172	ASP	C-N	6.43	1.40	1.33
21	W	108	GLN	N-CA	-6.43	1.38	1.46
33	O	145	LYS	CA-C	-6.43	1.44	1.52
3	C	128	ARG	NE-CZ	6.42	1.40	1.33
19	M	343	LEU	CA-C	-6.42	1.45	1.52
26	Z	392	LEU	CA-C	-6.42	1.44	1.52
30	Q	25	GLN	C-N	6.42	1.42	1.33
34	8	109	VAL	CA-C	-6.42	1.47	1.52
14	n	77	ASP	CA-C	-6.42	1.44	1.53
28	S	64	ARG	CD-NE	6.42	1.55	1.46
1	a	193	VAL	CA-C	-6.42	1.45	1.52
2	B	116	LYS	C-O	-6.42	1.16	1.24
14	7	182	ARG	NE-CZ	6.42	1.40	1.33
10	j	114	LYS	CA-CB	6.41	1.64	1.53
2	B	169	VAL	N-CA	-6.41	1.38	1.46
4	D	165	ASN	CA-C	-6.41	1.44	1.53
32	U	296	ILE	C-N	6.41	1.42	1.33
20	J	332	SER	CA-CB	6.41	1.63	1.53
9	i	31	CYS	N-CA	-6.41	1.38	1.46
16	I	64	ARG	NE-CZ	6.41	1.40	1.33
33	O	238	ILE	N-CA	-6.41	1.39	1.46
21	W	122	ARG	NE-CZ	6.41	1.40	1.33
5	e	114	ARG	CZ-NH1	6.41	1.41	1.32
20	J	196	THR	CA-C	-6.41	1.44	1.52
27	N	134	THR	CA-C	6.41	1.61	1.52
4	d	115	GLN	C-N	6.40	1.42	1.33
13	6	137	ARG	CA-C	-6.40	1.45	1.52
22	V	295	VAL	C-N	6.40	1.42	1.33
27	N	489	MET	N-CA	-6.40	1.38	1.46
33	O	128	LEU	C-N	6.40	1.41	1.33
4	d	136	PHE	CA-C	-6.40	1.45	1.52
4	D	235	GLU	CA-C	-6.40	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	225	LYS	CA-C	-6.40	1.44	1.52
14	n	117	ALA	C-N	6.40	1.40	1.33
5	E	63	ASP	CA-C	-6.40	1.44	1.52
13	6	137	ARG	N-CA	-6.40	1.38	1.46
14	n	84	GLU	C-N	6.39	1.42	1.33
10	3	104	VAL	C-N	6.39	1.43	1.33
33	O	362	GLN	N-CA	-6.39	1.38	1.46
12	l	19	ARG	CZ-NH2	6.39	1.41	1.33
13	m	1	GLN	C-N	6.39	1.42	1.33
14	7	31	GLY	C-N	6.39	1.42	1.33
30	Q	277	ASP	CA-C	-6.39	1.44	1.52
4	D	81	ARG	NE-CZ	6.39	1.40	1.33
26	Z	385	PHE	CA-C	-6.39	1.44	1.52
32	U	189	ARG	CA-C	-6.39	1.43	1.52
8	1	19	ARG	NE-CZ	6.38	1.40	1.33
13	6	203	GLU	CA-CB	6.38	1.62	1.53
13	m	18	GLU	CA-C	-6.38	1.45	1.52
34	8	178	SER	CA-C	-6.38	1.44	1.52
5	E	27	SER	CA-C	-6.38	1.44	1.52
9	2	145	ASP	C-N	6.38	1.41	1.33
28	S	127	THR	C-N	6.38	1.42	1.33
2	b	99	ARG	NE-CZ	6.38	1.40	1.33
6	F	88	ARG	CZ-NH2	6.38	1.41	1.33
13	6	79	HIS	CA-CB	6.38	1.62	1.53
1	A	231	ASN	CA-C	-6.37	1.44	1.52
22	V	237	ASN	CA-C	-6.37	1.44	1.52
10	3	54	GLY	C-O	6.37	1.28	1.24
31	R	204	TRP	CG-CD2	6.37	1.55	1.43
14	7	29	SER	CA-C	-6.37	1.44	1.52
20	J	113	VAL	C-N	6.37	1.42	1.33
33	O	387	ARG	CD-NE	6.37	1.55	1.46
4	d	56	ARG	CZ-NH2	6.37	1.41	1.33
7	g	186	ARG	CA-C	-6.37	1.44	1.52
7	G	130	VAL	N-CA	-6.37	1.39	1.46
2	b	178	ARG	N-CA	-6.37	1.37	1.46
5	e	2	ARG	NE-CZ	6.37	1.40	1.33
26	Z	566	LEU	CA-CB	6.37	1.63	1.53
9	i	75	ARG	NE-CZ	6.37	1.40	1.33
5	E	112	ALA	C-N	6.37	1.42	1.33
30	Q	14	LEU	N-CA	6.37	1.54	1.46
31	R	109	LYS	C-N	6.37	1.42	1.33
17	K	130	LEU	C-N	6.36	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	277	LYS	CA-C	-6.36	1.44	1.52
28	S	239	ARG	CA-C	-6.36	1.44	1.52
27	N	500	ASP	CA-CB	6.36	1.63	1.53
11	4	18	SER	CA-C	-6.36	1.44	1.52
28	S	481	TYR	N-CA	-6.36	1.40	1.46
7	G	114	GLN	CA-C	-6.36	1.44	1.52
16	I	203	THR	CA-C	-6.36	1.44	1.52
2	b	60	THR	CA-C	6.36	1.60	1.52
3	C	13	SER	CA-C	-6.36	1.46	1.53
30	Q	64	LEU	CA-C	-6.36	1.44	1.52
32	U	158	PRO	CA-C	-6.36	1.45	1.52
26	Z	123	ALA	N-CA	-6.35	1.38	1.46
19	M	382	SER	C-N	6.35	1.42	1.33
26	Z	156	HIS	ND1-CE1	6.35	1.39	1.32
3	c	91	ARG	NE-CZ	6.35	1.40	1.33
26	Z	178	SER	CA-C	-6.35	1.44	1.52
5	E	45	ARG	CA-CB	6.35	1.62	1.53
26	Z	117	ASP	C-N	6.35	1.41	1.33
26	Z	295	ARG	C-N	6.35	1.42	1.33
17	K	205	PRO	CA-C	-6.34	1.48	1.51
5	e	73	LEU	N-CA	-6.34	1.38	1.46
7	G	124	SER	CA-CB	6.34	1.63	1.53
12	5	73	ARG	CD-NE	6.34	1.55	1.46
12	5	78	ALA	C-N	6.34	1.42	1.33
24	X	57	VAL	N-CA	-6.34	1.38	1.46
26	Z	65	GLU	N-CA	-6.34	1.38	1.46
13	m	38	ARG	CZ-NH2	6.34	1.41	1.33
4	D	157	TRP	CA-C	6.34	1.60	1.52
24	X	55	LYS	C-N	6.34	1.41	1.34
33	O	166	ARG	N-CA	-6.34	1.38	1.46
7	g	132	THR	CA-C	-6.33	1.45	1.52
7	g	68	ARG	NE-CZ	6.33	1.40	1.33
6	F	211	SER	CA-C	-6.33	1.44	1.52
29	P	370	ASP	CA-CB	6.33	1.63	1.53
33	O	200	GLU	C-N	6.33	1.40	1.34
26	Z	552	GLU	N-CA	-6.33	1.38	1.46
27	N	693	GLY	CA-C	-6.33	1.44	1.52
25	Y	33	ASP	N-CA	-6.33	1.38	1.47
27	N	891	VAL	CA-CB	-6.33	1.46	1.54
6	f	176	ASP	N-CA	-6.32	1.37	1.46
14	7	190	ARG	CD-NE	6.32	1.55	1.46
34	8	456	LEU	N-CA	-6.32	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	235	LEU	C-O	-6.32	1.16	1.24
7	g	196	ILE	CA-CB	-6.32	1.46	1.54
9	2	45	GLY	CA-C	-6.32	1.47	1.52
28	S	461	PHE	CA-C	-6.32	1.44	1.52
29	P	232	ARG	CD-NE	6.32	1.55	1.46
13	m	71	SER	C-N	6.31	1.41	1.33
15	H	442	ASP	CA-C	-6.31	1.44	1.52
12	5	121	ARG	NE-CZ	6.31	1.40	1.33
15	H	71	GLU	N-CA	-6.31	1.38	1.46
27	N	140	MET	C-N	6.31	1.41	1.33
17	K	252	ARG	CA-C	-6.31	1.44	1.52
2	B	46	ALA	CA-C	-6.31	1.44	1.52
28	S	298	ARG	NE-CZ	6.31	1.40	1.33
27	N	518	ALA	CA-C	-6.31	1.44	1.52
7	G	78	ILE	C-N	6.30	1.42	1.34
26	Z	215	ASN	C-N	6.30	1.40	1.33
26	Z	928	ARG	CZ-NH1	6.30	1.41	1.32
3	C	159	TRP	NE1-CE2	-6.30	1.30	1.37
11	4	12	SER	N-CA	-6.30	1.38	1.46
4	D	152	GLY	C-N	6.30	1.42	1.33
7	G	98	LEU	CA-C	-6.30	1.44	1.52
14	n	111	TRP	N-CA	-6.30	1.38	1.46
5	E	85	ARG	CA-C	-6.30	1.44	1.52
33	O	228	TYR	N-CA	-6.30	1.40	1.46
14	n	30	TYR	CA-C	-6.29	1.45	1.53
18	L	172	SER	N-CA	6.29	1.53	1.46
1	a	109	ALA	C-N	6.29	1.42	1.33
20	J	74	GLU	C-N	6.29	1.39	1.33
13	6	137	ARG	CZ-NH1	6.29	1.41	1.32
21	W	47	ASN	CA-C	-6.29	1.44	1.52
23	T	103	SER	C-N	6.29	1.41	1.33
26	Z	930	GLY	C-N	6.29	1.42	1.33
28	S	485	LYS	CA-CB	6.29	1.63	1.53
5	E	2	ARG	NE-CZ	6.28	1.40	1.33
2	B	113	GLU	C-N	6.28	1.41	1.33
17	K	336	ARG	NE-CZ	6.28	1.40	1.33
3	c	112	ARG	CD-NE	6.28	1.55	1.46
26	Z	628	ASN	C-N	6.28	1.41	1.33
3	c	49	ARG	NE-CZ	6.28	1.40	1.33
6	f	201	ARG	CD-NE	6.28	1.55	1.46
10	j	29	GLY	N-CA	-6.28	1.38	1.44
26	Z	243	GLN	N-CA	-6.28	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	664	LEU	C-N	6.28	1.41	1.33
32	U	272	GLU	CA-C	-6.28	1.44	1.52
15	H	388	ILE	C-O	-6.27	1.16	1.24
1	a	57	PRO	CA-CB	-6.27	1.43	1.54
3	c	50	LYS	C-N	6.27	1.41	1.33
4	d	116	GLN	N-CA	-6.27	1.39	1.46
10	j	50	LEU	CA-CB	6.27	1.63	1.53
7	G	119	HIS	ND1-CE1	6.27	1.38	1.32
10	3	100	GLY	CA-C	6.27	1.60	1.51
27	N	271	GLU	N-CA	-6.27	1.39	1.46
5	e	204	LEU	N-CA	-6.27	1.38	1.46
6	f	88	ARG	NE-CZ	6.27	1.40	1.33
27	N	459	ASN	CA-C	-6.27	1.45	1.52
4	D	83	LEU	CA-CB	6.27	1.63	1.53
3	C	73	ALA	CA-C	6.26	1.60	1.52
7	g	111	ARG	NE-CZ	6.26	1.40	1.33
6	F	178	PHE	C-N	6.26	1.41	1.33
29	P	409	SER	CA-C	-6.26	1.44	1.52
1	a	137	VAL	C-N	6.26	1.41	1.33
10	3	25	ASP	CA-C	-6.25	1.44	1.53
13	6	221	ARG	CZ-NH2	6.25	1.41	1.33
15	H	353	PHE	CA-C	-6.25	1.45	1.52
12	5	61	SER	CA-CB	6.25	1.63	1.53
27	N	86	LYS	C-N	6.25	1.42	1.33
27	N	104	LYS	C-N	6.25	1.42	1.33
34	8	187	THR	N-CA	-6.25	1.38	1.46
4	d	95	ARG	CA-C	-6.25	1.44	1.52
6	F	88	ARG	NE-CZ	6.25	1.40	1.33
30	Q	252	HIS	CA-CB	6.25	1.63	1.53
31	R	326	ALA	CA-C	-6.25	1.44	1.52
34	8	391	ARG	NE-CZ	6.25	1.40	1.33
31	R	291	SER	N-CA	-6.25	1.38	1.46
6	f	154	GLU	C-N	6.25	1.41	1.33
27	N	784	TYR	CA-CB	6.24	1.63	1.53
34	8	377	ARG	NE-CZ	6.24	1.40	1.33
15	H	203	LYS	CA-CB	6.24	1.63	1.53
11	4	65	GLN	CA-C	-6.24	1.44	1.52
18	L	130	GLY	N-CA	-6.24	1.39	1.44
7	g	63	ILE	CA-C	-6.24	1.45	1.52
2	b	55	LEU	CA-C	-6.24	1.44	1.52
4	D	218	ASP	N-CA	-6.24	1.38	1.46
1	A	82	ARG	CZ-NH1	6.23	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	97	VAL	CA-C	-6.23	1.44	1.52
5	E	120	SER	CA-C	-6.23	1.44	1.52
12	l	9	GLN	N-CA	6.23	1.54	1.46
17	K	121	ARG	CD-NE	6.23	1.54	1.46
26	Z	568	LEU	CA-C	-6.23	1.44	1.52
1	A	111	ARG	C-N	6.23	1.42	1.34
34	8	385	GLU	CA-C	-6.23	1.44	1.52
14	n	41	ARG	CD-NE	6.23	1.54	1.46
3	C	201	ASP	CA-C	-6.23	1.45	1.52
13	6	133	ARG	CZ-NH1	6.23	1.41	1.32
9	i	212	VAL	CA-CB	-6.23	1.46	1.54
29	P	126	THR	C-N	6.23	1.41	1.33
5	E	159	TYR	N-CA	-6.22	1.38	1.45
8	h	54	ALA	N-CA	-6.22	1.38	1.46
15	H	101	ARG	CZ-NH2	6.22	1.41	1.33
20	J	141	LYS	C-N	6.22	1.40	1.33
26	Z	359	LYS	CA-C	-6.22	1.44	1.52
28	S	246	GLU	CA-C	-6.22	1.45	1.53
12	5	114	TYR	CA-C	-6.22	1.45	1.52
17	K	73	ARG	CZ-NH2	6.22	1.41	1.33
14	n	5	ILE	N-CA	-6.22	1.38	1.46
16	I	102	ASN	C-O	-6.22	1.16	1.24
24	X	96	ARG	CZ-NH2	6.22	1.41	1.33
30	Q	397	LEU	CA-C	-6.22	1.45	1.52
7	G	69	HIS	CA-C	-6.22	1.44	1.52
15	H	435	ARG	NE-CZ	6.22	1.39	1.33
11	4	169	GLU	C-O	6.22	1.31	1.24
20	J	249	GLU	N-CA	-6.21	1.39	1.46
8	1	117	GLY	CA-C	-6.21	1.43	1.51
14	7	180	ALA	CA-C	-6.21	1.44	1.52
2	B	81	ASP	C-N	6.21	1.41	1.33
6	F	219	THR	C-N	6.21	1.41	1.33
3	c	128	ARG	CZ-NH1	6.21	1.41	1.32
1	A	201	MET	CA-C	-6.21	1.45	1.52
2	B	137	ALA	C-N	6.21	1.40	1.33
17	K	237	VAL	N-CA	-6.21	1.39	1.46
9	i	21	THR	N-CA	-6.21	1.38	1.45
9	i	157	ASP	C-O	-6.21	1.17	1.24
9	2	82	MET	N-CA	-6.21	1.38	1.46
31	R	54	ILE	CA-C	-6.21	1.44	1.52
14	n	159	VAL	CA-CB	-6.21	1.46	1.53
11	4	23	ARG	NE-CZ	6.21	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	ARG	NE-CZ	6.20	1.39	1.33
33	O	286	PHE	CA-C	-6.20	1.45	1.52
28	S	388	ILE	C-N	6.20	1.42	1.33
15	H	213	GLY	C-N	6.20	1.42	1.33
34	8	155	GLU	CA-C	-6.20	1.44	1.52
5	e	45	ARG	C-N	6.19	1.42	1.33
18	L	82	ARG	CA-C	-6.19	1.44	1.52
26	Z	167	ASP	CA-C	-6.19	1.44	1.52
6	f	136	TYR	N-CA	-6.19	1.38	1.46
14	n	53	ILE	CA-C	-6.19	1.45	1.52
8	1	167	GLY	CA-C	-6.19	1.43	1.51
20	J	63	ARG	CZ-NH1	6.19	1.41	1.32
33	O	306	ARG	CZ-NH2	6.19	1.41	1.33
28	S	467	PHE	C-N	6.19	1.42	1.33
1	a	235	ARG	NE-CZ	6.19	1.39	1.33
5	e	89	VAL	N-CA	-6.19	1.37	1.46
8	h	174	ARG	CD-NE	6.19	1.54	1.46
12	l	167	ARG	NE-CZ	6.19	1.39	1.33
13	m	53	SER	CA-C	-6.19	1.45	1.52
5	e	85	ARG	CZ-NH1	6.19	1.41	1.32
10	3	72	LEU	CA-C	-6.19	1.44	1.52
7	g	16	ARG	CA-C	-6.18	1.45	1.52
9	i	56	THR	C-N	6.18	1.42	1.33
14	n	163	SER	CA-C	-6.18	1.44	1.52
19	M	126	THR	CA-C	-6.18	1.45	1.52
34	8	319	TRP	CA-CB	6.18	1.60	1.53
13	6	168	VAL	N-CA	-6.18	1.37	1.46
34	8	390	PRO	C-O	-6.18	1.16	1.24
6	F	118	ASN	N-CA	-6.18	1.38	1.46
10	3	58	ASP	C-N	6.18	1.41	1.33
2	b	190	HIS	CG-ND1	6.18	1.45	1.38
23	T	9	LYS	C-N	6.18	1.42	1.33
12	l	159	ARG	CD-NE	6.17	1.54	1.46
14	n	96	LEU	CA-C	-6.17	1.44	1.52
4	D	229	GLN	C-O	-6.17	1.16	1.24
14	7	128	ARG	NE-CZ	6.17	1.39	1.33
1	a	176	HIS	C-N	6.17	1.42	1.34
27	N	595	LEU	N-CA	-6.17	1.38	1.46
6	F	168	LYS	CA-C	-6.17	1.44	1.52
22	V	111	HIS	CD2-NE2	6.17	1.44	1.37
32	U	168	GLU	N-CA	-6.17	1.38	1.46
9	2	155	ALA	C-N	6.17	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	207	ARG	CZ-NH2	6.17	1.41	1.33
9	i	218	VAL	CA-CB	-6.17	1.45	1.54
3	C	30	HIS	N-CA	-6.17	1.39	1.46
30	Q	216	ALA	CA-C	-6.17	1.45	1.52
16	I	346	ARG	NE-CZ	6.17	1.39	1.33
19	M	320	ARG	NE-CZ	6.17	1.39	1.33
31	R	41	GLU	N-CA	-6.17	1.39	1.46
8	h	79	ALA	CA-C	-6.16	1.44	1.52
11	4	163	LEU	C-N	6.16	1.42	1.33
11	4	194	ASP	CA-CB	6.16	1.63	1.53
18	L	77	ARG	NE-CZ	6.16	1.39	1.33
30	Q	300	LYS	N-CA	6.16	1.54	1.46
16	I	98	GLU	N-CA	-6.16	1.39	1.46
27	N	550	GLY	C-N	6.16	1.42	1.33
2	b	9	LEU	CA-CB	6.16	1.64	1.53
18	L	210	VAL	C-N	6.16	1.41	1.33
19	M	120	LYS	CA-C	-6.16	1.45	1.52
1	A	112	MET	SD-CE	6.16	1.95	1.79
7	G	140	ASN	CA-CB	-6.16	1.45	1.53
14	7	156	ARG	CZ-NH2	6.16	1.41	1.33
3	C	239	VAL	CA-CB	-6.15	1.45	1.54
7	G	123	ASN	N-CA	-6.15	1.39	1.46
21	W	152	GLU	CA-CB	6.15	1.60	1.53
34	8	463	LYS	CA-C	-6.15	1.45	1.52
9	2	43	CYS	CA-C	-6.15	1.45	1.52
11	4	112	ASN	CA-CB	6.15	1.63	1.53
28	S	103	SER	C-N	6.15	1.38	1.32
5	e	54	ASP	N-CA	-6.15	1.39	1.46
8	h	14	LEU	CA-C	6.15	1.60	1.52
26	Z	779	ALA	CA-C	-6.15	1.44	1.52
18	L	255	TYR	N-CA	-6.15	1.38	1.45
2	b	2	THR	CA-C	-6.14	1.45	1.53
12	l	19	ARG	CD-NE	6.14	1.54	1.46
28	S	246	GLU	C-N	6.14	1.41	1.33
2	b	78	MET	CA-C	-6.14	1.44	1.52
10	j	184	ALA	C-N	6.14	1.41	1.33
11	4	193	ASP	CA-CB	6.14	1.62	1.53
17	K	281	ARG	CZ-NH1	6.14	1.41	1.32
24	X	76	VAL	CA-C	-6.14	1.47	1.52
26	Z	40	GLU	N-CA	-6.14	1.38	1.46
34	8	219	HIS	CE1-NE2	-6.14	1.26	1.32
5	E	151	GLU	CA-CB	6.14	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S	35	LEU	C-N	6.14	1.41	1.33
10	3	97	ARG	CZ-NH2	6.14	1.41	1.33
13	6	5	TYR	CA-C	-6.14	1.45	1.52
15	H	73	ASP	CA-C	-6.14	1.45	1.52
34	8	217	LEU	CA-C	-6.14	1.44	1.52
19	M	357	ARG	NE-CZ	6.14	1.39	1.33
1	a	124	TYR	N-CA	-6.14	1.38	1.46
2	B	135	LEU	N-CA	-6.14	1.38	1.46
11	k	182	LYS	CA-C	-6.13	1.45	1.52
20	J	35	ARG	C-N	6.13	1.42	1.33
18	L	425	VAL	C-N	6.13	1.42	1.33
23	T	48	ASN	CA-C	-6.13	1.45	1.52
31	R	220	ALA	CA-C	-6.13	1.44	1.52
34	8	321	ARG	CA-C	-6.13	1.44	1.52
1	A	170	THR	CB-OG1	-6.13	1.33	1.43
4	D	238	LYS	N-CA	-6.13	1.38	1.46
13	6	4	PRO	C-N	6.13	1.41	1.33
34	8	234	ARG	CZ-NH1	6.13	1.41	1.32
6	F	50	ARG	NE-CZ	6.13	1.39	1.33
20	J	51	LEU	N-CA	-6.12	1.38	1.46
3	c	35	ILE	C-N	6.12	1.38	1.33
7	g	193	ALA	N-CA	-6.12	1.38	1.46
28	S	54	TRP	C-N	6.12	1.41	1.33
1	A	84	ALA	N-CA	-6.12	1.39	1.46
30	Q	114	GLN	N-CA	6.12	1.53	1.46
13	6	147	MET	C-O	-6.12	1.18	1.24
29	P	70	ASN	CA-C	-6.12	1.45	1.52
14	7	182	ARG	CZ-NH1	6.12	1.41	1.32
13	m	4	PRO	N-CD	-6.12	1.39	1.47
11	4	116	LEU	CA-C	-6.12	1.45	1.52
4	D	94	HIS	N-CA	-6.12	1.39	1.46
4	D	179	ARG	CA-C	-6.12	1.44	1.52
11	k	108	ASP	N-CA	-6.11	1.38	1.46
26	Z	244	ARG	NE-CZ	6.11	1.39	1.33
24	X	69	ILE	CA-C	6.11	1.58	1.52
28	S	352	VAL	N-CA	-6.11	1.39	1.46
32	U	77	ASN	N-CA	-6.11	1.39	1.46
8	1	137	TYR	N-CA	-6.11	1.39	1.46
1	a	8	THR	N-CA	-6.11	1.38	1.46
13	m	25	GLY	C-N	6.11	1.41	1.33
14	7	63	ILE	C-N	6.11	1.42	1.33
27	N	7	ALA	CA-C	6.11	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	184	VAL	CA-CB	-6.10	1.46	1.54
22	V	104	VAL	C-N	6.10	1.40	1.33
3	c	60	THR	N-CA	-6.10	1.38	1.46
10	3	61	THR	CA-C	-6.10	1.45	1.52
33	O	85	SER	C-N	6.10	1.42	1.33
2	b	228	PRO	C-N	6.10	1.42	1.33
10	j	12	VAL	N-CA	-6.10	1.39	1.46
2	B	224	TYR	CA-CB	6.10	1.59	1.53
17	K	326	PRO	C-N	6.10	1.42	1.33
18	L	228	LYS	CA-C	-6.10	1.44	1.52
27	N	77	SER	CA-C	6.10	1.60	1.52
10	3	51	GLY	C-N	6.10	1.41	1.33
5	E	214	ILE	C-O	-6.09	1.17	1.24
19	M	53	HIS	CB-CG	6.09	1.58	1.50
1	a	240	ALA	CA-C	-6.09	1.45	1.52
12	l	101	ILE	CA-CB	6.09	1.60	1.53
4	D	51	LYS	C-N	6.09	1.41	1.33
13	6	10	GLY	CA-C	-6.09	1.46	1.52
27	N	904	VAL	N-CA	-6.09	1.39	1.46
2	b	34	SER	C-N	6.09	1.41	1.33
10	3	69	LYS	C-N	6.09	1.42	1.34
16	I	289	THR	C-N	6.09	1.41	1.33
4	d	77	ASN	CA-CB	6.09	1.63	1.53
1	a	60	VAL	N-CA	-6.09	1.38	1.46
5	e	150	ALA	C-O	-6.09	1.16	1.24
22	V	42	ARG	CD-NE	6.09	1.54	1.46
7	G	208	PHE	N-CA	-6.08	1.38	1.45
20	J	244	ILE	CA-C	-6.08	1.44	1.52
27	N	907	ASP	CA-C	-6.08	1.45	1.52
2	b	28	VAL	CA-C	-6.08	1.45	1.52
7	g	62	LYS	CA-C	-6.08	1.45	1.52
8	h	143	ARG	CZ-NH1	6.08	1.41	1.32
28	S	357	LEU	N-CA	-6.08	1.38	1.46
8	h	143	ARG	CZ-NH2	6.08	1.41	1.33
33	O	333	SER	CA-C	-6.08	1.44	1.52
24	X	124	LYS	N-CA	-6.08	1.39	1.46
9	2	124	TYR	N-CA	-6.08	1.38	1.46
10	3	187	TYR	CZ-OH	6.08	1.50	1.38
28	S	428	ARG	NE-CZ	6.08	1.39	1.33
16	I	262	ARG	NE-CZ	6.08	1.39	1.33
1	a	214	LEU	CB-CG	6.07	1.65	1.53
14	7	37	ASN	CA-CB	6.07	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	80	ALA	N-CA	-6.07	1.39	1.46
6	F	176	ASP	N-CA	-6.07	1.38	1.46
12	5	35	ILE	N-CA	-6.07	1.38	1.46
23	T	176	SER	CA-CB	6.07	1.63	1.53
14	7	104	ARG	NE-CZ	6.07	1.39	1.33
20	J	230	VAL	CA-C	-6.07	1.45	1.52
4	D	153	ILE	CA-C	-6.07	1.46	1.52
6	F	160	ILE	N-CA	-6.07	1.39	1.46
8	h	87	TYR	N-CA	-6.06	1.39	1.46
10	j	73	TYR	CA-C	-6.06	1.45	1.52
18	L	278	ILE	CA-C	-6.06	1.45	1.52
6	f	52	ALA	CA-C	-6.06	1.44	1.52
11	k	41	HIS	CA-C	-6.06	1.45	1.53
10	j	67	ARG	NE-CZ	6.06	1.39	1.33
6	F	218	ASP	N-CA	-6.06	1.38	1.46
13	6	219	LEU	CA-C	-6.06	1.45	1.52
26	Z	93	ARG	CA-CB	6.06	1.61	1.53
26	Z	338	HIS	CD2-NE2	6.06	1.44	1.37
34	8	181	PRO	CA-C	-6.06	1.46	1.52
2	B	126	GLY	CA-C	-6.06	1.43	1.51
13	m	199	GLY	N-CA	6.05	1.50	1.45
33	O	382	LYS	CA-C	-6.05	1.45	1.52
20	J	240	HIS	CA-C	-6.05	1.44	1.52
30	Q	165	PHE	N-CA	-6.05	1.38	1.46
11	4	90	LYS	C-N	6.05	1.41	1.33
14	n	131	ASN	CA-C	-6.05	1.45	1.52
6	F	77	ALA	C-N	6.04	1.41	1.34
11	k	49	GLU	CA-CB	6.04	1.63	1.53
3	C	108	GLU	CA-CB	6.04	1.62	1.53
15	H	204	PRO	CA-C	-6.04	1.45	1.52
27	N	215	MET	CA-CB	6.04	1.62	1.53
21	W	95	GLN	N-CA	-6.04	1.39	1.46
27	N	619	CYS	C-N	6.04	1.41	1.33
31	R	247	GLU	CA-C	-6.04	1.45	1.52
28	S	170	TYR	C-N	6.04	1.42	1.33
31	R	139	GLU	N-CA	-6.04	1.39	1.46
1	a	87	ARG	CZ-NH1	6.04	1.41	1.32
16	I	78	ASN	CA-CB	6.04	1.62	1.53
28	S	60	LEU	CA-CB	6.04	1.62	1.53
13	m	34	SER	CA-C	-6.04	1.45	1.52
17	K	333	ARG	CD-NE	6.04	1.54	1.46
21	W	100	HIS	ND1-CE1	6.04	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	102	LEU	CA-CB	6.04	1.63	1.53
12	5	167	ARG	CZ-NH1	6.03	1.41	1.32
11	4	8	ARG	NE-CZ	6.03	1.39	1.33
27	N	72	LEU	CA-CB	6.03	1.62	1.53
29	P	362	LEU	CA-C	-6.03	1.44	1.52
10	3	203	GLN	N-CA	-6.03	1.38	1.46
16	I	226	GLY	CA-C	6.03	1.59	1.51
14	n	54	SER	CA-C	-6.03	1.45	1.52
5	E	91	HIS	CG-CD2	6.03	1.42	1.35
34	8	280	LEU	C-N	6.03	1.41	1.33
6	f	143	LEU	CA-CB	6.03	1.63	1.53
3	C	26	GLU	CA-C	-6.03	1.45	1.52
7	g	70	ILE	N-CA	-6.02	1.38	1.46
7	g	219	GLU	C-N	6.02	1.42	1.33
15	H	273	ARG	N-CA	-6.02	1.38	1.46
30	Q	309	ARG	NE-CZ	6.02	1.39	1.33
31	R	236	ALA	CA-C	-6.02	1.45	1.52
5	E	54	ASP	N-CA	-6.02	1.39	1.46
12	5	144	TYR	CA-CB	6.02	1.61	1.53
1	a	68	ARG	CD-NE	6.02	1.54	1.46
1	A	122	ARG	NE-CZ	6.02	1.39	1.33
1	A	170	THR	N-CA	6.02	1.53	1.46
11	4	45	SER	CA-CB	6.02	1.63	1.53
1	a	126	ARG	CA-CB	6.02	1.62	1.53
3	C	17	ARG	CA-C	-6.02	1.45	1.53
19	M	71	ASN	C-N	6.02	1.42	1.33
26	Z	578	GLY	CA-C	-6.02	1.43	1.51
28	S	65	ASN	C-N	6.02	1.41	1.33
26	Z	968	ASP	CA-C	-6.02	1.45	1.52
13	6	137	ARG	NE-CZ	6.01	1.39	1.33
19	M	203	ARG	NE-CZ	6.01	1.39	1.33
28	S	129	GLU	CA-C	-6.01	1.45	1.52
1	a	95	PHE	CA-C	-6.01	1.45	1.52
2	b	159	TRP	CZ2-CH2	6.01	1.48	1.37
6	f	69	MET	C-N	6.01	1.40	1.33
4	D	147	GLN	N-CA	-6.01	1.38	1.45
6	F	17	ARG	CA-CB	6.01	1.62	1.53
25	Y	40	ILE	CA-C	-6.01	1.45	1.52
13	m	179	GLU	CA-C	-6.01	1.45	1.52
9	2	35	HIS	ND1-CE1	6.01	1.38	1.32
21	W	178	PRO	N-CA	-6.01	1.40	1.47
23	T	110	LEU	N-CA	-6.01	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	M	189	GLN	C-N	6.01	1.41	1.33
26	Z	558	LEU	C-O	-6.01	1.17	1.24
34	8	228	LYS	C-N	6.01	1.42	1.33
32	U	256	ASN	C-N	6.00	1.41	1.33
14	n	154	LEU	C-N	6.00	1.42	1.34
26	Z	899	GLN	C-N	6.00	1.42	1.33
29	P	99	LYS	N-CA	-6.00	1.38	1.46
30	Q	102	GLU	C-N	6.00	1.41	1.33
8	h	168	SER	N-CA	6.00	1.53	1.46
1	A	227	LEU	CA-C	-6.00	1.45	1.53
13	6	75	TYR	CA-CB	6.00	1.62	1.53
14	7	163	SER	N-CA	-6.00	1.38	1.46
17	K	350	ARG	CZ-NH2	6.00	1.41	1.33
7	g	234	GLU	C-N	6.00	1.41	1.33
31	R	343	GLU	CA-C	-6.00	1.44	1.52
8	1	185	ARG	NE-CZ	6.00	1.39	1.33
5	E	19	SER	CA-C	-6.00	1.45	1.52
20	J	76	ILE	C-N	6.00	1.41	1.33
33	O	276	LYS	CA-C	-6.00	1.45	1.52
34	8	114	MET	N-CA	-6.00	1.41	1.47
3	c	223	GLU	CA-C	-5.99	1.44	1.52
12	l	52	CYS	N-CA	-5.99	1.39	1.46
4	D	14	HIS	CA-C	-5.99	1.45	1.52
9	2	36	ARG	CA-C	-5.99	1.45	1.52
30	Q	404	ASN	CA-C	-5.99	1.45	1.52
4	d	121	SER	N-CA	-5.99	1.38	1.46
3	C	203	SER	C-N	5.99	1.42	1.33
16	I	303	GLN	CA-CB	5.99	1.62	1.53
4	D	36	GLY	C-N	5.99	1.42	1.33
8	1	34	LEU	CA-C	-5.99	1.45	1.52
9	2	180	ILE	N-CA	-5.99	1.38	1.46
17	K	255	ARG	CZ-NH2	5.99	1.41	1.33
9	2	127	LEU	C-N	5.99	1.41	1.32
2	b	99	ARG	CD-NE	5.99	1.54	1.46
12	5	55	TRP	NE1-CE2	5.99	1.44	1.37
13	m	4	PRO	C-O	-5.98	1.16	1.24
5	E	180	HIS	ND1-CE1	5.98	1.38	1.32
17	K	88	ARG	NE-CZ	5.98	1.39	1.33
27	N	581	ASP	CA-C	-5.98	1.44	1.52
31	R	254	SER	C-N	5.98	1.41	1.33
4	D	61	LYS	CA-C	-5.98	1.45	1.52
7	G	82	ARG	CZ-NH1	5.98	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	89	PRO	CA-C	-5.98	1.42	1.52
4	d	234	ILE	C-N	5.98	1.42	1.34
11	k	170	LYS	N-CA	-5.98	1.39	1.46
33	O	121	ASP	CA-C	-5.98	1.45	1.52
34	8	368	ASN	C-N	5.98	1.41	1.33
13	m	134	GLU	N-CA	-5.98	1.38	1.45
10	j	49	PHE	C-O	-5.97	1.16	1.23
10	j	106	PRO	N-CD	-5.97	1.39	1.47
26	Z	17	GLN	C-O	-5.97	1.17	1.24
30	Q	427	PHE	CA-C	-5.97	1.45	1.52
34	8	198	ARG	CZ-NH1	5.97	1.41	1.32
2	b	235	PHE	C-N	5.97	1.41	1.33
8	1	183	VAL	CA-CB	-5.97	1.46	1.54
9	2	150	GLU	CA-C	-5.97	1.44	1.52
28	S	139	HIS	CG-CD2	5.97	1.42	1.35
13	m	154	VAL	CA-C	-5.97	1.45	1.52
4	D	145	LEU	N-CA	-5.97	1.38	1.46
9	2	145	ASP	CA-C	-5.97	1.46	1.53
10	j	182	TRP	C-N	5.96	1.42	1.33
11	4	171	ARG	CZ-NH1	5.96	1.41	1.32
18	L	61	LYS	CA-CB	5.96	1.62	1.53
12	l	141	ASP	N-CA	-5.96	1.39	1.46
13	6	79	HIS	N-CA	-5.96	1.39	1.46
11	k	9	VAL	N-CA	-5.96	1.39	1.46
13	m	164	THR	N-CA	-5.96	1.39	1.46
9	2	90	TYR	N-CA	-5.96	1.38	1.46
16	I	242	ALA	CA-CB	5.96	1.62	1.53
26	Z	500	SER	CA-C	-5.96	1.45	1.52
28	S	40	GLU	CA-CB	5.96	1.62	1.53
34	8	221	MET	CA-CB	5.96	1.62	1.53
3	c	113	ARG	C-N	5.96	1.42	1.34
8	h	92	ASN	N-CA	-5.96	1.39	1.46
20	J	228	ARG	NE-CZ	5.96	1.39	1.33
26	Z	901	PHE	CA-C	-5.96	1.45	1.52
13	m	122	VAL	N-CA	-5.95	1.39	1.46
27	N	170	LEU	CA-C	-5.95	1.45	1.52
33	O	12	SER	C-N	5.95	1.41	1.33
5	E	134	LEU	CA-C	-5.95	1.45	1.52
7	G	74	TYR	C-N	5.95	1.41	1.33
21	W	31	ASP	CA-CB	5.95	1.62	1.53
23	T	163	LEU	N-CA	-5.95	1.38	1.46
1	a	146	TYR	CA-C	-5.95	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	HIS	N-CA	-5.95	1.38	1.46
18	L	148	LEU	CA-C	-5.95	1.45	1.52
24	X	75	TRP	CZ2-CH2	5.95	1.48	1.37
26	Z	783	VAL	N-CA	-5.95	1.39	1.46
1	a	96	ARG	CD-NE	5.95	1.54	1.46
7	g	24	VAL	N-CA	-5.95	1.39	1.46
4	d	74	SER	C-N	5.95	1.42	1.33
3	C	9	THR	C-O	5.95	1.31	1.24
4	d	179	ARG	CZ-NH1	5.95	1.41	1.32
4	d	212	VAL	N-CA	-5.95	1.39	1.46
7	G	183	LEU	N-CA	5.95	1.53	1.45
12	5	206	SER	C-N	5.94	1.42	1.33
5	e	60	VAL	C-O	-5.94	1.18	1.24
30	Q	343	LEU	CA-C	-5.94	1.45	1.52
22	V	37	MET	C-N	5.94	1.41	1.33
2	b	116	LYS	C-N	5.94	1.41	1.33
5	E	85	ARG	CZ-NH1	5.94	1.41	1.32
26	Z	528	LEU	C-N	5.94	1.42	1.33
5	e	193	LEU	CA-C	-5.94	1.45	1.52
15	H	289	ARG	NE-CZ	5.94	1.39	1.33
17	K	99	PHE	CA-CB	5.94	1.62	1.53
7	g	73	VAL	C-N	5.93	1.41	1.33
1	A	167	GLN	N-CA	-5.93	1.39	1.46
8	1	174	ARG	CA-CB	5.93	1.62	1.53
23	T	43	ASP	C-N	5.93	1.41	1.33
27	N	33	ASP	CA-CB	5.93	1.62	1.53
27	N	324	LYS	C-N	5.93	1.41	1.33
33	O	37	LEU	N-CA	-5.93	1.38	1.46
2	b	112	SER	N-CA	-5.93	1.39	1.46
16	I	360	LYS	CA-CB	5.93	1.62	1.53
19	M	235	CYS	C-N	5.93	1.41	1.33
6	F	169	THR	CA-C	-5.93	1.45	1.52
13	6	133	ARG	CD-NE	5.93	1.54	1.46
14	7	127	LEU	N-CA	-5.93	1.39	1.46
32	U	78	GLU	C-N	5.93	1.42	1.33
32	U	253	ASP	CA-CB	5.93	1.62	1.53
8	h	27	ALA	N-CA	-5.93	1.38	1.46
15	H	427	GLY	N-CA	5.93	1.53	1.45
27	N	487	LEU	CA-C	-5.93	1.45	1.52
27	N	821	LYS	N-CA	-5.93	1.39	1.46
27	N	351	ALA	C-N	5.93	1.40	1.33
6	F	91	CYS	C-N	5.92	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	62	HIS	CA-C	-5.92	1.45	1.52
26	Z	118	VAL	CA-C	-5.92	1.45	1.52
34	8	433	ILE	N-CA	-5.92	1.39	1.46
7	G	127	PRO	N-CA	-5.92	1.40	1.47
20	J	304	LEU	C-N	5.92	1.41	1.33
27	N	877	GLN	CA-C	-5.92	1.45	1.52
18	L	381	LYS	CA-C	-5.92	1.45	1.52
10	j	189	ILE	CA-CB	-5.92	1.46	1.53
4	D	106	TYR	CA-C	-5.92	1.45	1.52
15	H	178	ARG	CD-NE	5.92	1.54	1.46
19	M	124	ARG	NE-CZ	5.92	1.39	1.33
7	g	78	ILE	N-CA	-5.92	1.39	1.46
12	l	7	ARG	NE-CZ	5.92	1.39	1.33
5	E	117	GLU	C-N	5.92	1.38	1.33
16	I	80	GLU	CA-CB	5.92	1.63	1.53
21	W	179	ARG	CD-NE	5.92	1.54	1.46
20	J	75	VAL	CA-C	-5.91	1.46	1.53
10	3	151	SER	C-N	5.91	1.42	1.33
2	b	192	ALA	CA-C	-5.91	1.45	1.52
7	g	176	VAL	CA-C	5.91	1.60	1.52
10	3	185	VAL	N-CA	-5.91	1.39	1.46
17	K	185	ARG	NE-CZ	5.91	1.39	1.33
30	Q	392	GLN	N-CA	5.91	1.53	1.46
34	8	165	LYS	N-CA	-5.91	1.39	1.46
4	d	47	ARG	NE-CZ	5.91	1.39	1.33
18	L	50	GLN	CA-C	-5.91	1.45	1.52
11	4	193	ASP	C-N	5.91	1.41	1.33
10	j	106	PRO	N-CA	-5.91	1.40	1.46
29	P	33	ASN	C-N	5.91	1.41	1.33
9	i	67	SER	C-N	5.90	1.42	1.33
14	n	51	VAL	CA-C	-5.90	1.45	1.52
17	K	79	LEU	CA-CB	5.90	1.62	1.53
28	S	358	LYS	N-CA	-5.90	1.39	1.46
6	F	2	ARG	NE-CZ	5.90	1.39	1.33
18	L	200	PRO	N-CD	-5.90	1.39	1.47
29	P	144	VAL	N-CA	5.90	1.53	1.46
6	f	100	ARG	NE-CZ	5.90	1.39	1.33
14	n	137	TYR	CZ-OH	5.90	1.50	1.38
8	l	6	VAL	N-CA	-5.90	1.39	1.46
18	L	191	ARG	NE-CZ	5.90	1.39	1.33
11	k	96	ARG	NE-CZ	5.90	1.39	1.33
11	4	89	ALA	CA-C	-5.90	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	63	ASP	N-CA	-5.90	1.38	1.45
9	2	204	LYS	CA-C	-5.89	1.45	1.52
22	V	86	VAL	C-O	-5.89	1.17	1.24
25	Y	23	GLU	N-CA	-5.89	1.39	1.46
29	P	75	LEU	CA-C	-5.89	1.45	1.52
32	U	154	PHE	C-O	-5.89	1.17	1.24
3	c	161	ALA	C-N	5.89	1.40	1.33
7	G	87	ARG	CD-NE	5.89	1.54	1.46
15	H	435	ARG	CD-NE	5.89	1.54	1.46
27	N	215	MET	C-N	5.89	1.41	1.33
28	S	404	LEU	N-CA	5.89	1.53	1.46
34	8	392	GLU	C-N	5.89	1.41	1.33
30	Q	334	HIS	CG-ND1	5.89	1.44	1.38
5	e	225	ASN	N-CA	-5.89	1.38	1.46
8	h	185	ARG	NE-CZ	5.89	1.39	1.33
11	4	43	LEU	C-N	5.89	1.41	1.33
28	S	423	VAL	C-N	5.89	1.41	1.33
6	f	115	ALA	CA-C	-5.88	1.45	1.52
5	E	97	GLU	CA-C	-5.88	1.45	1.52
14	7	123	GLY	CA-C	-5.88	1.43	1.51
26	Z	108	ASP	N-CA	-5.88	1.37	1.46
28	S	89	LYS	CA-C	-5.88	1.45	1.52
4	d	117	ARG	NE-CZ	5.88	1.39	1.33
12	l	146	TRP	CA-C	-5.88	1.44	1.52
1	A	182	ILE	C-N	5.88	1.41	1.33
26	Z	541	ASP	N-CA	-5.88	1.37	1.46
26	Z	787	ASP	CA-C	-5.88	1.45	1.53
27	N	795	GLU	C-N	5.88	1.41	1.33
4	d	87	ALA	N-CA	-5.88	1.39	1.46
9	i	131	SER	N-CA	5.88	1.53	1.46
10	j	90	VAL	C-O	-5.88	1.17	1.24
11	k	187	ASP	C-N	5.88	1.38	1.33
4	D	55	THR	C-N	5.88	1.41	1.33
17	K	356	ILE	C-N	5.88	1.42	1.34
6	F	180	LYS	CA-C	-5.88	1.45	1.52
31	R	416	LYS	CA-C	-5.88	1.45	1.52
32	U	42	ASN	CA-C	-5.88	1.46	1.53
10	j	138	SER	CA-C	-5.87	1.45	1.52
8	1	78	ALA	N-CA	-5.87	1.39	1.46
13	6	130	SER	CA-C	-5.87	1.45	1.52
12	5	136	ALA	N-CA	-5.87	1.39	1.46
1	A	93	ALA	N-CA	-5.87	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	W	127	ARG	NE-CZ	5.87	1.39	1.33
5	e	223	TYR	CA-CB	5.87	1.63	1.53
7	G	81	GLY	CA-C	-5.87	1.43	1.51
32	U	297	GLN	C-N	5.87	1.41	1.33
14	n	104	ARG	CZ-NH1	5.87	1.41	1.32
1	A	181	LYS	C-N	5.87	1.41	1.33
22	V	257	GLU	CA-C	-5.87	1.45	1.52
27	N	604	ARG	NE-CZ	5.87	1.39	1.33
34	8	320	LYS	CA-CB	5.87	1.60	1.53
2	b	23	TYR	N-CA	5.86	1.53	1.46
10	j	85	THR	N-CA	-5.86	1.39	1.46
12	l	38	ASN	CA-CB	5.86	1.62	1.53
11	4	133	HIS	CA-C	-5.86	1.45	1.52
13	6	21	ALA	CA-C	-5.86	1.45	1.52
32	U	138	VAL	N-CA	-5.86	1.39	1.46
1	a	96	ARG	CZ-NH1	5.86	1.41	1.32
3	c	182	ASP	CA-CB	5.86	1.61	1.53
10	3	78	GLU	C-N	5.86	1.40	1.33
10	3	118	PRO	N-CA	-5.86	1.40	1.47
25	Y	79	ALA	CA-C	-5.86	1.45	1.52
5	E	42	VAL	C-N	5.86	1.41	1.33
6	f	19	PHE	N-CA	-5.86	1.38	1.46
10	3	101	PRO	CA-C	-5.86	1.44	1.52
15	H	377	PHE	CA-C	-5.86	1.45	1.52
26	Z	34	GLU	CA-C	-5.86	1.45	1.52
26	Z	715	ALA	CA-C	-5.86	1.44	1.52
27	N	34	GLN	CA-C	-5.86	1.45	1.52
1	a	184	HIS	ND1-CE1	5.86	1.38	1.32
10	3	153	TYR	N-CA	-5.86	1.38	1.46
21	W	101	ARG	CZ-NH2	5.85	1.41	1.33
26	Z	295	ARG	NE-CZ	5.85	1.39	1.33
29	P	229	LEU	CA-CB	5.85	1.62	1.53
1	a	159	ALA	N-CA	-5.85	1.38	1.45
1	A	225	PHE	C-N	5.85	1.41	1.33
6	F	192	GLY	N-CA	-5.85	1.38	1.45
21	W	35	PHE	CA-C	5.85	1.60	1.52
23	T	224	ARG	NE-CZ	5.85	1.39	1.33
26	Z	950	THR	N-CA	-5.85	1.38	1.46
27	N	650	ASP	N-CA	-5.85	1.39	1.46
18	L	89	ASP	CA-CB	5.85	1.62	1.53
8	h	26	ILE	N-CA	-5.85	1.39	1.46
11	k	84	VAL	N-CA	-5.85	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	16	GLY	C-N	5.85	1.41	1.33
18	L	171	THR	CA-CB	-5.85	1.44	1.53
19	M	167	VAL	CA-C	5.85	1.60	1.52
3	c	217	LYS	CA-C	5.85	1.60	1.52
19	M	339	ARG	NE-CZ	5.85	1.39	1.33
19	M	381	ARG	CD-NE	5.85	1.54	1.46
26	Z	884	THR	CA-C	-5.85	1.45	1.52
33	O	318	HIS	C-N	5.85	1.40	1.33
21	W	61	VAL	N-CA	-5.85	1.39	1.46
31	R	143	GLN	CA-C	-5.85	1.44	1.52
5	E	228	THR	N-CA	-5.84	1.39	1.46
10	j	18	ASP	CA-CB	5.84	1.62	1.53
4	d	39	CYS	N-CA	-5.84	1.38	1.46
17	K	423	LYS	CA-C	-5.84	1.45	1.52
1	a	175	ASN	CA-C	-5.84	1.45	1.52
32	U	278	ILE	C-N	5.84	1.41	1.33
3	c	17	ARG	CA-CB	5.84	1.64	1.53
16	I	421	GLU	CA-C	-5.84	1.45	1.52
26	Z	811	SER	CA-C	-5.84	1.45	1.52
34	8	371	GLU	C-N	5.84	1.41	1.33
2	B	236	ARG	CZ-NH1	5.83	1.41	1.32
4	D	111	VAL	CA-C	-5.83	1.45	1.52
2	B	128	ARG	CZ-NH1	5.83	1.41	1.32
20	J	68	PRO	N-CA	-5.83	1.41	1.46
22	V	50	MET	CA-C	-5.83	1.45	1.52
23	T	189	ILE	CA-C	-5.83	1.45	1.52
28	S	411	LEU	CA-C	-5.83	1.45	1.52
31	R	361	VAL	N-CA	-5.83	1.39	1.46
33	O	94	GLU	N-CA	-5.83	1.39	1.46
9	i	207	ARG	CA-C	-5.83	1.45	1.52
11	k	60	ILE	CA-C	5.83	1.60	1.52
5	E	179	TRP	CA-CB	5.83	1.63	1.53
6	F	88	ARG	N-CA	-5.83	1.39	1.46
18	L	261	ARG	CD-NE	5.83	1.54	1.46
28	S	480	ARG	CZ-NH2	5.83	1.41	1.33
20	J	238	ARG	CD-NE	5.83	1.54	1.46
23	T	251	HIS	ND1-CE1	5.83	1.38	1.32
32	U	70	HIS	CG-CD2	5.83	1.42	1.35
2	b	86	VAL	C-O	-5.83	1.17	1.24
8	h	62	HIS	CA-C	-5.83	1.45	1.52
11	k	4	ILE	CA-C	-5.83	1.45	1.52
15	H	449	LYS	C-N	5.83	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S	36	LYS	N-CA	-5.83	1.39	1.46
29	P	400	VAL	N-CA	-5.83	1.39	1.46
31	R	122	GLU	C-N	5.83	1.41	1.33
17	K	281	ARG	CD-NE	5.82	1.54	1.46
18	L	69	ARG	CD-NE	5.82	1.54	1.46
31	R	167	LYS	N-CA	-5.82	1.39	1.46
33	O	33	TYR	CA-C	5.82	1.60	1.52
3	c	152	PRO	C-N	5.82	1.42	1.33
10	3	40	GLU	CA-C	-5.82	1.45	1.52
11	k	132	ALA	CA-C	-5.82	1.45	1.52
13	m	129	GLY	C-N	5.82	1.41	1.33
19	M	77	TYR	CA-C	-5.82	1.45	1.52
26	Z	928	ARG	CD-NE	5.82	1.54	1.46
2	b	115	ALA	N-CA	-5.82	1.39	1.46
14	7	89	PRO	N-CA	-5.82	1.39	1.47
17	K	368	LEU	CA-CB	5.82	1.62	1.53
1	A	228	SER	C-N	5.82	1.41	1.33
17	K	298	GLU	N-CA	5.82	1.53	1.46
6	f	51	ASN	CA-C	-5.82	1.45	1.52
3	C	41	ASP	C-N	5.82	1.39	1.32
5	E	80	MET	N-CA	-5.82	1.39	1.46
17	K	236	ARG	NE-CZ	5.82	1.39	1.33
2	b	121	ALA	N-CA	-5.81	1.38	1.46
6	f	44	VAL	N-CA	-5.81	1.39	1.46
10	j	194	VAL	N-CA	-5.81	1.38	1.46
8	l	52	THR	C-O	-5.81	1.17	1.24
7	G	224	HIS	ND1-CE1	5.81	1.38	1.32
27	N	753	PHE	C-O	-5.81	1.17	1.23
8	h	102	TYR	N-CA	-5.81	1.39	1.46
4	D	22	LEU	CA-CB	5.81	1.62	1.53
4	D	83	LEU	CA-C	-5.81	1.45	1.52
27	N	155	GLY	C-N	5.81	1.41	1.33
30	Q	428	GLU	N-CA	-5.81	1.39	1.46
2	b	88	LYS	CA-C	-5.81	1.45	1.52
3	C	100	THR	CA-C	-5.81	1.45	1.52
8	l	45	ARG	CZ-NH1	5.81	1.40	1.32
27	N	718	GLU	CA-C	-5.81	1.45	1.52
2	b	139	HIS	CA-C	-5.80	1.45	1.52
9	i	194	ASN	CA-CB	5.80	1.63	1.53
13	m	15	ILE	CA-C	-5.80	1.45	1.52
3	c	95	GLN	C-N	5.80	1.41	1.33
19	M	337	LEU	C-N	5.80	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	1	GLN	N-CA	5.80	1.57	1.46
2	B	44	VAL	C-N	5.80	1.41	1.33
27	N	769	PRO	C-N	5.80	1.42	1.33
30	Q	276	ASP	CA-CB	5.80	1.62	1.53
2	B	187	ASP	N-CA	-5.80	1.39	1.46
6	F	163	ARG	CZ-NH1	5.80	1.40	1.32
17	K	85	GLU	CA-C	-5.80	1.45	1.52
31	R	204	TRP	CA-CB	5.80	1.62	1.53
4	D	39	CYS	CA-C	-5.79	1.45	1.52
7	G	67	ASP	C-O	-5.79	1.19	1.24
8	h	44	CYS	C-O	-5.79	1.17	1.24
4	D	125	ARG	NE-CZ	5.79	1.39	1.33
24	X	80	SER	C-N	5.79	1.41	1.33
27	N	62	ALA	C-N	5.79	1.41	1.33
13	6	36	ASN	CA-C	-5.79	1.45	1.52
34	8	303	ILE	CA-C	-5.79	1.45	1.52
20	J	61	GLU	N-CA	-5.79	1.39	1.46
26	Z	774	ARG	N-CA	-5.79	1.38	1.46
10	j	122	GLY	N-CA	-5.79	1.39	1.44
13	6	93	ILE	C-N	5.79	1.41	1.33
23	T	193	THR	CA-C	-5.78	1.44	1.52
2	B	82	TYR	N-CA	-5.78	1.39	1.46
17	K	74	HIS	N-CA	-5.78	1.39	1.46
32	U	168	GLU	CA-CB	5.78	1.62	1.53
2	b	239	THR	CA-C	-5.78	1.45	1.52
3	c	38	MET	CA-CB	5.78	1.62	1.53
2	B	130	PHE	CA-C	-5.78	1.45	1.52
14	7	164	ASP	CA-CB	5.78	1.63	1.53
7	g	4	TYR	N-CA	-5.78	1.39	1.46
18	L	283	VAL	N-CA	-5.78	1.39	1.46
24	X	21	SER	CA-C	-5.78	1.45	1.52
34	8	452	ILE	CB-CG1	5.78	1.65	1.53
3	c	123	GLN	CA-C	-5.77	1.45	1.52
11	k	36	ARG	CD-NE	5.77	1.54	1.46
7	G	104	PRO	CA-C	-5.77	1.45	1.52
1	a	15	ARG	NE-CZ	5.77	1.39	1.33
1	a	191	GLU	N-CA	-5.77	1.39	1.46
10	j	178	ALA	N-CA	-5.77	1.39	1.46
17	K	345	ASP	CA-CB	5.77	1.62	1.53
14	n	32	SER	CA-C	5.77	1.60	1.52
2	B	188	ALA	N-CA	-5.77	1.39	1.46
4	D	34	VAL	N-CA	-5.77	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	385	ARG	CZ-NH1	5.77	1.40	1.32
27	N	500	ASP	C-N	5.77	1.41	1.33
31	R	392	ARG	CD-NE	5.77	1.54	1.46
2	b	204	PHE	N-CA	-5.77	1.40	1.46
34	8	198	ARG	NE-CZ	5.77	1.39	1.33
12	l	49	ALA	C-O	-5.76	1.17	1.24
4	D	95	ARG	C-O	-5.76	1.17	1.24
12	5	75	SER	N-CA	5.76	1.53	1.45
26	Z	817	LEU	CA-C	-5.76	1.45	1.52
4	d	200	VAL	N-CA	-5.76	1.41	1.46
5	E	69	ALA	CA-C	-5.76	1.45	1.52
6	f	175	LEU	C-O	-5.76	1.17	1.24
7	g	199	ALA	C-N	5.76	1.42	1.33
13	m	77	PHE	CA-C	-5.76	1.45	1.52
13	6	42	LYS	N-CA	-5.76	1.39	1.46
17	K	278	ALA	C-O	5.76	1.31	1.24
33	O	288	ARG	NE-CZ	5.76	1.39	1.33
34	8	459	ASN	N-CA	-5.76	1.39	1.46
5	e	169	GLU	N-CA	-5.76	1.39	1.46
11	4	21	VAL	CA-C	-5.76	1.45	1.52
27	N	729	SER	N-CA	-5.76	1.39	1.46
32	U	166	ALA	N-CA	-5.76	1.39	1.46
6	f	21	VAL	CA-CB	-5.75	1.47	1.54
13	m	120	GLY	CA-C	-5.75	1.46	1.52
26	Z	720	LYS	CA-C	-5.75	1.45	1.52
12	5	40	PHE	N-CA	-5.75	1.38	1.46
3	c	170	ALA	C-O	-5.75	1.17	1.24
11	k	133	HIS	CD2-NE2	5.75	1.44	1.37
21	W	118	ILE	CA-CB	-5.75	1.48	1.54
27	N	819	LYS	N-CA	-5.75	1.39	1.46
9	2	118	SER	N-CA	5.75	1.53	1.46
15	H	420	ARG	CD-NE	5.75	1.54	1.46
23	T	203	SER	C-N	5.75	1.41	1.34
10	j	149	CYS	CA-C	-5.74	1.45	1.52
9	2	44	ALA	CA-C	-5.74	1.45	1.52
12	5	129	VAL	C-N	5.74	1.39	1.32
34	8	168	PHE	N-CA	-5.74	1.39	1.46
4	D	170	ARG	CA-CB	5.74	1.62	1.53
11	4	110	LYS	CA-C	-5.74	1.44	1.52
13	6	144	SER	N-CA	-5.74	1.39	1.46
34	8	120	LEU	N-CA	-5.74	1.39	1.46
2	b	2	THR	C-N	5.74	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	56	SER	C-N	5.74	1.41	1.33
22	V	106	GLY	CA-C	-5.74	1.45	1.52
34	8	136	MET	CA-C	-5.74	1.45	1.52
7	g	200	HIS	CB-CG	5.74	1.58	1.50
7	G	94	SER	CA-C	-5.74	1.45	1.52
17	K	347	ARG	NE-CZ	5.74	1.39	1.33
32	U	149	SER	C-N	5.74	1.41	1.33
32	U	179	ARG	CD-NE	5.74	1.54	1.46
11	4	32	ASP	CA-C	-5.74	1.45	1.52
15	H	90	ARG	CA-C	-5.74	1.45	1.52
12	l	174	SER	C-N	5.73	1.40	1.33
18	L	154	THR	C-O	5.73	1.30	1.23
26	Z	451	ALA	N-CA	-5.73	1.39	1.46
10	j	133	LYS	C-N	5.73	1.41	1.33
12	l	93	ALA	N-CA	-5.73	1.38	1.46
14	n	125	GLN	CA-C	-5.73	1.45	1.52
27	N	762	ARG	NE-CZ	5.73	1.39	1.33
7	g	127	PRO	CA-CB	5.73	1.61	1.53
13	m	109	THR	N-CA	-5.73	1.39	1.46
13	m	221	ARG	N-CA	-5.73	1.38	1.45
4	D	139	ARG	NE-CZ	5.73	1.39	1.33
9	2	4	VAL	CA-C	-5.73	1.46	1.52
6	F	54	GLU	CA-C	-5.73	1.45	1.52
26	Z	588	ILE	N-CA	-5.73	1.39	1.46
27	N	503	THR	C-N	5.73	1.41	1.33
30	Q	138	SER	C-N	5.73	1.40	1.33
33	O	141	ASN	C-N	5.73	1.39	1.33
3	C	29	SER	N-CA	-5.72	1.38	1.46
1	a	82	ARG	N-CA	-5.72	1.39	1.46
10	j	199	LEU	N-CA	-5.72	1.38	1.45
27	N	396	SER	C-N	5.72	1.40	1.33
11	k	130	TYR	C-N	-5.72	1.25	1.33
23	T	271	GLU	C-N	5.72	1.41	1.33
27	N	740	TRP	NE1-CE2	-5.72	1.31	1.37
28	S	415	SER	CA-C	-5.72	1.45	1.52
31	R	110	ILE	N-CA	5.72	1.53	1.46
4	d	59	PRO	C-N	5.72	1.41	1.33
4	d	156	SER	C-N	5.72	1.41	1.33
27	N	187	ASN	N-CA	-5.72	1.39	1.46
27	N	352	ASN	CG-ND2	5.72	1.45	1.33
32	U	100	ARG	CD-NE	5.72	1.54	1.46
21	W	139	VAL	CA-C	-5.72	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	8	442	ASN	C-N	5.72	1.41	1.33
4	d	107	LEU	N-CA	-5.72	1.39	1.46
8	h	163	ILE	CA-CB	-5.72	1.47	1.54
14	7	182	ARG	CZ-NH2	5.72	1.40	1.33
7	g	12	SER	C-N	5.71	1.40	1.34
19	M	343	LEU	N-CA	-5.71	1.39	1.46
30	Q	377	LEU	CA-C	-5.71	1.45	1.52
10	j	97	ARG	CZ-NH2	5.71	1.40	1.33
1	A	224	PHE	CA-C	-5.71	1.45	1.52
10	j	161	ASP	N-CA	-5.71	1.38	1.46
7	G	104	PRO	N-CA	-5.71	1.40	1.47
9	2	49	ALA	CA-C	-5.71	1.45	1.52
12	5	121	ARG	CD-NE	5.71	1.54	1.46
14	n	104	ARG	CA-C	-5.71	1.45	1.52
4	D	219	ILE	CA-C	-5.71	1.45	1.52
10	3	104	VAL	CA-CB	-5.71	1.45	1.55
2	B	118	MET	C-O	5.71	1.30	1.24
9	2	78	SER	CA-C	-5.71	1.45	1.52
14	7	78	ASN	C-N	5.71	1.40	1.34
28	S	164	ILE	CA-C	5.71	1.58	1.52
11	k	85	ARG	CZ-NH1	5.71	1.40	1.32
17	K	135	MET	N-CA	-5.71	1.39	1.46
14	7	182	ARG	CD-NE	5.71	1.54	1.46
20	J	78	ILE	CA-C	5.70	1.59	1.52
26	Z	110	ASN	CA-C	-5.70	1.45	1.52
27	N	138	GLU	CA-CB	5.70	1.62	1.53
27	N	508	THR	CA-C	-5.70	1.45	1.52
2	B	235	PHE	N-CA	-5.70	1.39	1.46
3	C	65	LEU	CA-C	-5.70	1.45	1.52
30	Q	387	TYR	N-CA	5.70	1.53	1.46
1	a	122	ARG	CZ-NH1	5.70	1.40	1.32
11	k	70	ARG	NE-CZ	5.70	1.39	1.33
20	J	66	GLN	CA-C	-5.70	1.45	1.52
26	Z	863	THR	C-N	5.70	1.42	1.33
6	F	38	ARG	CZ-NH1	5.70	1.40	1.32
11	4	194	ASP	CA-C	-5.70	1.45	1.52
6	F	118	ASN	CA-CB	5.70	1.63	1.53
8	1	25	TYR	CA-CB	5.70	1.62	1.53
34	8	166	ARG	CZ-NH2	5.70	1.40	1.33
9	i	41	ILE	C-N	5.69	1.41	1.33
12	5	108	GLU	N-CA	-5.69	1.38	1.46
13	6	73	LYS	C-N	5.69	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	M	55	ASN	N-CA	-5.69	1.39	1.46
20	J	35	ARG	CD-NE	5.69	1.54	1.46
21	W	78	ASP	C-N	5.69	1.40	1.33
6	f	102	LEU	CB-CG	5.69	1.64	1.53
10	j	33	LEU	CA-C	-5.69	1.45	1.52
1	A	10	PHE	CA-C	-5.69	1.45	1.52
22	V	302	SER	CA-CB	5.69	1.62	1.53
32	U	209	GLU	N-CA	-5.69	1.39	1.46
34	8	306	LEU	CA-CB	5.69	1.62	1.52
11	k	74	GLU	N-CA	-5.69	1.38	1.46
14	n	183	VAL	C-O	-5.69	1.17	1.24
6	F	5	TYR	CA-C	-5.69	1.45	1.53
6	f	58	TYR	N-CA	-5.69	1.38	1.45
8	h	182	GLY	CA-C	-5.69	1.46	1.52
18	L	299	ARG	C-N	5.69	1.41	1.33
12	5	168	ASP	CA-C	-5.69	1.45	1.52
18	L	304	THR	C-N	5.69	1.41	1.33
1	A	168	GLU	CA-CB	5.68	1.62	1.53
5	E	116	GLY	CA-C	-5.68	1.45	1.52
15	H	292	ARG	CA-CB	5.68	1.62	1.53
26	Z	147	GLU	C-O	-5.68	1.17	1.24
28	S	199	GLU	C-N	5.68	1.40	1.33
5	e	198	GLN	CA-C	-5.68	1.45	1.52
2	B	11	THR	C-N	5.68	1.41	1.33
20	J	92	GLY	CA-C	-5.68	1.44	1.51
5	e	91	HIS	CA-CB	5.68	1.62	1.53
33	O	385	GLU	N-CA	5.68	1.53	1.46
13	m	91	ARG	NE-CZ	5.68	1.39	1.33
14	n	20	VAL	N-CA	-5.68	1.40	1.46
2	B	47	THR	N-CA	5.68	1.53	1.46
5	E	84	ALA	N-CA	-5.68	1.39	1.46
12	5	73	ARG	NE-CZ	5.68	1.39	1.33
28	S	174	ARG	NE-CZ	5.68	1.39	1.33
13	m	40	GLU	C-N	5.68	1.40	1.33
2	b	99	ARG	C-N	5.68	1.41	1.33
1	A	15	ARG	NE-CZ	5.68	1.39	1.33
5	E	232	ILE	CA-C	-5.68	1.45	1.52
29	P	289	ASN	CA-C	-5.68	1.45	1.52
1	a	117	GLN	C-N	5.67	1.41	1.33
9	i	66	HIS	CB-CG	-5.67	1.42	1.50
11	k	162	LYS	CA-CB	-5.67	1.44	1.53
9	2	165	ASN	CA-C	5.67	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	150	PRO	N-CA	-5.67	1.40	1.47
11	4	121	TYR	C-O	-5.67	1.17	1.24
16	I	311	ASN	N-CA	-5.67	1.39	1.46
24	X	17	TYR	N-CA	-5.67	1.39	1.46
1	a	76	GLY	N-CA	5.67	1.52	1.44
28	S	156	VAL	C-O	-5.67	1.17	1.24
8	h	185	ARG	CZ-NH1	5.67	1.40	1.32
13	m	94	GLN	N-CA	-5.67	1.39	1.46
3	C	62	THR	C-N	5.67	1.41	1.33
14	7	72	THR	C-N	5.67	1.41	1.33
26	Z	876	VAL	N-CA	-5.67	1.39	1.46
27	N	455	MET	CA-CB	5.67	1.62	1.53
17	K	296	LEU	C-N	5.67	1.41	1.33
3	c	169	SER	N-CA	-5.66	1.39	1.46
2	B	140	ASP	CA-CB	5.66	1.64	1.53
4	D	132	LEU	CB-CG	5.66	1.64	1.53
17	K	407	LEU	CA-CB	5.66	1.62	1.53
3	c	155	ASN	C-N	5.66	1.41	1.33
8	h	56	ALA	C-N	5.66	1.41	1.33
6	F	190	LYS	CA-C	-5.66	1.45	1.52
12	5	191	HIS	ND1-CE1	5.66	1.38	1.32
26	Z	276	ASN	N-CA	5.66	1.53	1.46
26	Z	785	VAL	N-CA	5.66	1.53	1.46
1	A	54	LEU	CA-CB	5.66	1.62	1.53
12	5	47	GLY	CA-C	-5.66	1.46	1.52
26	Z	830	LEU	N-CA	-5.66	1.39	1.46
13	6	179	GLU	N-CA	-5.66	1.39	1.46
26	Z	745	LEU	CA-C	-5.66	1.45	1.52
3	c	55	LEU	C-N	5.66	1.41	1.33
8	h	29	ARG	NE-CZ	5.66	1.39	1.33
14	n	217	MET	CA-C	-5.66	1.45	1.52
19	M	246	LEU	N-CA	-5.66	1.38	1.45
28	S	180	ASN	CA-C	-5.66	1.44	1.52
13	m	190	SER	CA-CB	5.66	1.62	1.53
4	D	39	CYS	N-CA	-5.66	1.38	1.45
7	G	143	HIS	CG-CD2	5.66	1.42	1.35
11	4	35	THR	CA-CB	-5.66	1.43	1.53
20	J	339	ARG	NE-CZ	5.66	1.39	1.33
31	R	334	ARG	NE-CZ	5.66	1.39	1.33
33	O	196	LEU	CA-C	-5.66	1.45	1.52
16	I	384	LYS	CA-C	-5.65	1.45	1.52
29	P	136	ARG	CA-C	-5.65	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	183	GLY	C-N	5.65	1.40	1.33
26	Z	12	ILE	CA-C	-5.65	1.46	1.52
26	Z	401	VAL	CA-C	5.65	1.59	1.52
10	j	164	GLU	N-CA	-5.65	1.39	1.46
30	Q	389	VAL	CA-C	-5.65	1.45	1.52
32	U	185	GLY	C-N	5.65	1.41	1.33
34	8	302	LYS	CA-C	-5.65	1.46	1.52
14	7	111	TRP	N-CA	-5.65	1.39	1.46
2	b	210	GLU	CA-C	5.65	1.59	1.52
17	K	417	THR	C-N	5.65	1.41	1.33
18	L	430	GLY	C-N	5.65	1.41	1.33
20	J	38	THR	C-O	-5.65	1.17	1.24
20	J	75	VAL	C-N	5.65	1.41	1.33
27	N	782	PHE	N-CA	-5.65	1.38	1.46
2	B	3	ASP	CA-C	-5.65	1.45	1.53
17	K	141	ARG	CD-NE	5.65	1.54	1.46
30	Q	183	LYS	CA-C	-5.65	1.45	1.52
31	R	222	ARG	NE-CZ	5.65	1.39	1.33
21	W	11	ASP	C-N	5.64	1.41	1.33
27	N	607	GLN	CA-C	-5.64	1.45	1.52
4	d	170	ARG	C-N	5.64	1.41	1.33
11	4	62	ALA	N-CA	-5.64	1.39	1.46
27	N	129	ILE	CA-C	-5.64	1.48	1.53
3	c	116	ASP	C-O	-5.64	1.17	1.24
19	M	199	LEU	CA-C	-5.64	1.45	1.52
27	N	924	LYS	C-N	5.64	1.41	1.33
20	J	110	SER	CA-C	-5.64	1.44	1.52
24	X	11	ARG	NE-CZ	5.64	1.39	1.33
30	Q	392	GLN	C-N	5.64	1.40	1.33
33	O	87	LYS	N-CA	-5.64	1.39	1.46
3	c	196	LEU	N-CA	-5.64	1.39	1.46
1	A	123	ALA	N-CA	-5.64	1.39	1.46
7	G	232	LEU	CA-CB	5.64	1.62	1.53
33	O	260	VAL	CA-CB	-5.64	1.47	1.54
3	c	219	ALA	C-N	5.63	1.41	1.33
5	e	39	VAL	CA-C	5.63	1.59	1.52
5	e	186	LYS	CA-C	-5.63	1.45	1.52
17	K	255	ARG	CD-NE	5.63	1.54	1.46
28	S	437	ASN	CA-C	-5.63	1.46	1.53
32	U	189	ARG	NE-CZ	5.63	1.39	1.33
5	e	150	ALA	CA-C	-5.63	1.45	1.52
1	a	28	GLN	CA-C	-5.63	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	95	ARG	CZ-NH2	5.63	1.40	1.33
10	j	146	PHE	CA-C	-5.63	1.45	1.52
8	1	143	ARG	NE-CZ	5.63	1.39	1.33
12	5	204	GLU	CA-CB	5.63	1.62	1.53
19	M	427	SER	CA-C	5.63	1.59	1.52
26	Z	812	ILE	C-N	5.63	1.41	1.33
27	N	629	CYS	N-CA	-5.63	1.39	1.46
3	c	80	THR	C-N	5.63	1.41	1.33
6	F	153	THR	C-O	5.63	1.30	1.23
7	G	87	ARG	NE-CZ	5.63	1.39	1.33
18	L	308	LEU	C-N	5.63	1.41	1.33
31	R	267	LYS	CA-C	-5.63	1.45	1.52
8	1	89	ASN	N-CA	-5.62	1.39	1.46
18	L	422	VAL	CA-C	5.62	1.59	1.52
5	e	230	GLU	CA-C	-5.62	1.45	1.52
13	m	93	ILE	C-N	5.62	1.41	1.33
6	F	165	GLN	CA-C	-5.62	1.45	1.52
9	2	72	ARG	CA-CB	5.62	1.63	1.53
13	6	222	ASP	CA-CB	5.62	1.64	1.53
22	V	107	TRP	CA-C	-5.62	1.45	1.52
33	O	390	SER	CA-C	-5.62	1.45	1.52
6	f	167	ALA	C-N	5.62	1.41	1.33
2	B	77	GLY	N-CA	5.62	1.53	1.45
15	H	445	LYS	C-N	5.62	1.41	1.33
16	I	377	LEU	N-CA	-5.62	1.39	1.46
18	L	97	ALA	C-N	5.62	1.41	1.33
32	U	221	ILE	N-CA	-5.62	1.39	1.46
10	j	118	PRO	N-CA	-5.62	1.40	1.47
12	5	67	GLU	C-N	5.62	1.41	1.33
17	K	192	LEU	CA-CB	5.62	1.62	1.53
26	Z	87	LYS	CA-C	-5.62	1.46	1.52
4	d	27	ARG	N-CA	-5.62	1.39	1.46
6	F	102	LEU	CA-C	-5.62	1.45	1.52
27	N	70	TYR	CA-CB	5.62	1.62	1.53
4	d	50	LEU	N-CA	-5.61	1.38	1.45
9	2	19	ARG	NE-CZ	5.61	1.39	1.33
17	K	79	LEU	C-N	5.61	1.41	1.33
32	U	278	ILE	N-CA	-5.61	1.39	1.46
3	c	143	TYR	C-N	-5.61	1.26	1.33
4	d	92	GLN	CA-CB	5.61	1.62	1.53
10	3	152	LEU	CA-CB	5.61	1.62	1.53
18	L	339	ARG	CZ-NH2	5.61	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	207	ARG	CD-NE	5.61	1.54	1.46
11	4	155	GLU	CA-CB	5.61	1.62	1.53
1	A	153	TYR	CZ-OH	5.61	1.49	1.38
32	U	102	SER	CA-C	-5.61	1.44	1.52
34	8	192	TYR	C-N	5.61	1.40	1.34
6	f	198	GLN	CA-CB	5.60	1.62	1.53
6	F	170	TYR	CA-C	-5.60	1.45	1.52
11	4	59	TYR	CZ-OH	5.60	1.49	1.38
19	M	63	LYS	N-CA	-5.60	1.39	1.46
26	Z	515	SER	C-N	5.60	1.42	1.33
4	D	170	ARG	CZ-NH2	5.60	1.40	1.33
28	S	74	LEU	C-N	5.60	1.41	1.33
1	A	125	MET	CA-C	5.60	1.60	1.52
26	Z	873	LEU	N-CA	5.60	1.53	1.46
28	S	78	VAL	CA-CB	-5.60	1.47	1.54
34	8	133	LEU	C-O	-5.60	1.17	1.24
7	g	242	GLU	C-N	5.60	1.40	1.33
8	h	185	ARG	CA-CB	5.60	1.62	1.53
13	m	16	ALA	CA-C	-5.60	1.46	1.52
14	7	219	TRP	N-CA	-5.60	1.41	1.46
20	J	33	LYS	C-N	5.60	1.41	1.33
2	B	1	MET	C-N	5.60	1.40	1.33
16	I	404	LEU	N-CA	-5.60	1.39	1.46
21	W	116	SER	CA-C	-5.60	1.46	1.52
33	O	311	GLU	C-N	5.60	1.41	1.34
4	D	105	GLU	C-N	5.59	1.41	1.33
32	U	17	SER	N-CA	-5.59	1.39	1.46
33	O	203	THR	N-CA	-5.59	1.39	1.46
1	a	37	ARG	NE-CZ	5.59	1.39	1.33
5	e	91	HIS	ND1-CE1	5.59	1.38	1.32
10	j	55	LEU	N-CA	-5.59	1.39	1.46
15	H	357	ARG	CA-C	5.59	1.58	1.52
22	V	101	ASP	C-N	5.59	1.40	1.33
13	m	63	ALA	N-CA	-5.59	1.39	1.46
5	E	200	MET	C-N	5.59	1.41	1.33
8	1	174	ARG	CZ-NH2	5.59	1.40	1.33
1	a	103	MET	CA-CB	5.59	1.61	1.53
8	1	99	VAL	CA-C	-5.59	1.45	1.52
12	5	83	LEU	CA-C	-5.59	1.45	1.52
14	7	23	ALA	C-N	5.59	1.40	1.33
22	V	42	ARG	CA-C	-5.59	1.45	1.52
1	a	125	MET	N-CA	-5.59	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	84	SER	CA-CB	5.59	1.62	1.53
7	g	206	LYS	N-CA	-5.59	1.39	1.45
6	f	193	VAL	C-N	5.58	1.41	1.34
33	O	12	SER	CA-CB	5.58	1.62	1.53
4	d	179	ARG	CZ-NH2	5.58	1.40	1.33
14	n	71	VAL	CA-C	-5.58	1.45	1.52
1	A	174	GLU	N-CA	-5.58	1.39	1.46
27	N	756	THR	C-N	5.58	1.40	1.33
31	R	320	LYS	CA-C	-5.58	1.45	1.52
10	j	44	HIS	CE1-NE2	-5.58	1.26	1.32
9	2	132	LEU	N-CA	-5.58	1.39	1.46
15	H	390	ARG	CZ-NH2	5.58	1.40	1.33
20	J	18	GLY	N-CA	-5.58	1.38	1.45
1	a	182	ILE	N-CA	-5.58	1.39	1.46
3	c	91	ARG	N-CA	-5.58	1.39	1.46
3	C	145	TYR	CA-C	-5.58	1.45	1.52
6	f	198	GLN	CA-C	-5.58	1.45	1.52
8	1	88	GLU	CA-C	-5.58	1.45	1.52
13	6	89	ALA	CA-C	-5.58	1.45	1.52
26	Z	59	ASP	CA-CB	5.58	1.60	1.53
33	O	139	LEU	CA-C	-5.58	1.45	1.52
34	8	392	GLU	CA-CB	5.58	1.62	1.53
17	K	375	ASN	N-CA	5.58	1.53	1.46
21	W	130	LYS	CA-C	-5.58	1.45	1.52
14	n	65	ARG	CA-C	-5.58	1.45	1.52
1	a	168	GLU	C-N	5.57	1.41	1.33
7	g	127	PRO	C-N	5.57	1.41	1.33
11	k	100	VAL	CA-C	-5.57	1.45	1.52
13	6	28	ARG	CZ-NH2	5.57	1.40	1.33
15	H	434	ARG	N-CA	-5.57	1.39	1.46
7	G	115	TYR	CA-C	-5.57	1.45	1.52
4	D	33	GLY	N-CA	-5.57	1.40	1.45
16	I	365	HIS	CA-CB	5.57	1.62	1.53
32	U	53	ALA	C-N	5.57	1.40	1.33
13	m	66	LYS	C-O	-5.57	1.17	1.24
20	J	229	MET	CA-C	-5.57	1.47	1.53
14	n	44	PRO	C-O	-5.57	1.17	1.23
4	D	231	VAL	CA-C	5.57	1.59	1.52
7	G	114	GLN	CA-CB	5.57	1.62	1.53
2	B	178	ARG	C-N	5.57	1.40	1.33
19	M	433	TYR	CA-C	-5.57	1.46	1.52
26	Z	929	VAL	N-CA	5.57	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	P	52	LEU	CA-C	-5.57	1.45	1.52
4	d	102	VAL	N-CA	-5.56	1.39	1.46
5	e	65	HIS	CD2-NE2	5.56	1.44	1.37
9	2	149	GLU	N-CA	-5.56	1.39	1.46
14	7	26	ASN	CA-C	-5.56	1.45	1.53
26	Z	810	ASN	CA-C	-5.56	1.45	1.52
9	i	53	GLU	CA-C	-5.56	1.45	1.52
5	E	133	ALA	CA-C	-5.56	1.46	1.52
27	N	24	ALA	CA-C	-5.56	1.45	1.52
30	Q	160	ASP	N-CA	5.56	1.53	1.46
5	E	217	GLN	CA-CB	5.56	1.62	1.53
13	6	180	VAL	C-N	5.56	1.40	1.33
1	a	223	LYS	CA-C	-5.56	1.45	1.52
9	2	18	THR	CA-C	-5.56	1.45	1.52
31	R	245	SER	CA-C	-5.56	1.45	1.52
1	a	35	ALA	CA-C	5.56	1.59	1.52
3	C	138	GLY	CA-C	-5.56	1.45	1.51
24	X	92	SER	CA-C	-5.56	1.46	1.53
33	O	92	PHE	N-CA	-5.56	1.38	1.46
10	j	47	HIS	C-N	5.56	1.40	1.33
10	j	111	ILE	N-CA	-5.56	1.39	1.46
11	4	174	MET	C-N	5.56	1.41	1.33
10	3	135	PHE	CA-CB	5.55	1.62	1.53
11	4	33	ASP	CA-C	-5.55	1.45	1.52
17	K	102	PRO	C-N	5.55	1.39	1.33
17	K	161	MET	N-CA	-5.55	1.38	1.45
18	L	66	GLU	CA-C	-5.55	1.45	1.52
27	N	686	ILE	CA-C	-5.55	1.45	1.52
17	K	325	ASP	CA-CB	5.55	1.61	1.53
13	6	117	ASP	CA-C	-5.55	1.45	1.52
28	S	452	TYR	CA-C	-5.55	1.45	1.52
30	Q	168	LEU	C-N	5.55	1.41	1.33
2	b	242	GLU	C-N	5.55	1.41	1.33
4	d	19	GLU	CA-C	-5.55	1.45	1.52
7	g	3	GLY	N-CA	-5.55	1.36	1.45
7	g	210	LEU	N-CA	-5.55	1.38	1.46
6	F	79	ASP	N-CA	-5.55	1.39	1.46
27	N	279	ALA	CA-C	-5.55	1.45	1.52
32	U	239	LEU	CA-CB	5.55	1.63	1.53
1	a	186	ASN	N-CA	-5.55	1.38	1.46
5	e	188	ALA	CA-C	-5.55	1.45	1.52
27	N	183	VAL	N-CA	5.55	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	25	TRP	NE1-CE2	5.55	1.43	1.37
13	m	27	THR	CA-C	-5.55	1.44	1.52
3	c	36	GLY	CA-C	-5.54	1.48	1.52
8	1	194	GLU	N-CA	-5.54	1.39	1.46
26	Z	293	MET	N-CA	-5.54	1.39	1.46
11	4	133	HIS	CB-CG	-5.54	1.42	1.50
30	Q	91	SER	N-CA	-5.54	1.39	1.46
9	2	85	GLN	CA-C	-5.54	1.45	1.52
19	M	425	ARG	CZ-NH1	5.54	1.40	1.32
22	V	300	VAL	C-N	5.54	1.41	1.33
2	b	115	ALA	C-N	5.54	1.41	1.33
5	e	25	LEU	N-CA	-5.54	1.39	1.46
11	k	167	GLU	CA-CB	-5.54	1.44	1.53
2	B	189	ILE	N-CA	5.54	1.53	1.46
2	B	207	ASP	CA-C	-5.54	1.45	1.52
4	D	18	VAL	N-CA	-5.54	1.40	1.46
6	F	168	LYS	C-N	5.54	1.41	1.33
13	6	121	ALA	CA-C	-5.54	1.45	1.52
19	M	84	GLU	N-CA	-5.54	1.39	1.46
28	S	286	TYR	CA-C	-5.54	1.45	1.52
28	S	352	VAL	CA-CB	5.54	1.61	1.54
30	Q	290	THR	CA-C	-5.54	1.45	1.52
32	U	76	MET	CA-C	-5.54	1.45	1.52
1	A	15	ARG	C-O	-5.54	1.17	1.24
2	B	109	LEU	CA-CB	5.54	1.62	1.53
15	H	346	ARG	CZ-NH1	5.54	1.40	1.32
30	Q	17	GLU	C-N	5.54	1.41	1.33
33	O	166	ARG	NE-CZ	5.54	1.39	1.33
11	k	124	THR	C-O	-5.53	1.17	1.23
2	B	170	ALA	N-CA	-5.53	1.39	1.46
13	6	176	SER	CA-C	-5.53	1.45	1.53
18	L	392	ARG	CZ-NH1	5.53	1.40	1.32
20	J	273	LEU	C-N	5.53	1.41	1.34
5	e	43	GLU	CA-C	-5.53	1.45	1.52
29	P	329	PHE	N-CA	-5.53	1.39	1.46
30	Q	357	VAL	N-CA	-5.53	1.39	1.46
12	l	29	GLN	CA-C	-5.53	1.45	1.52
8	1	126	ILE	C-N	5.53	1.40	1.33
14	7	106	LYS	CA-CB	5.53	1.61	1.53
26	Z	114	SER	CA-CB	5.53	1.62	1.53
34	8	196	ALA	C-N	5.53	1.40	1.33
6	F	41	THR	CA-CB	-5.53	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	7	ARG	C-N	5.53	1.39	1.33
26	Z	741	LEU	N-CA	5.53	1.53	1.46
27	N	389	TYR	C-N	5.53	1.41	1.33
3	c	139	TYR	CZ-OH	5.53	1.49	1.38
27	N	786	ARG	CA-C	-5.53	1.45	1.53
29	P	408	SER	CA-C	-5.53	1.45	1.52
32	U	37	ILE	C-O	-5.53	1.18	1.24
10	j	202	ARG	CD-NE	5.53	1.53	1.46
11	k	81	SER	N-CA	-5.53	1.39	1.46
12	5	161	ILE	N-CA	-5.53	1.39	1.46
2	b	194	LEU	CA-C	-5.52	1.45	1.52
4	d	160	GLN	CA-C	-5.52	1.45	1.52
16	I	265	ARG	CZ-NH2	5.52	1.40	1.33
17	K	282	PHE	N-CA	-5.52	1.39	1.45
4	D	195	ARG	NE-CZ	5.52	1.39	1.33
4	d	198	LEU	CA-CB	5.52	1.62	1.53
6	F	29	LYS	CA-C	-5.52	1.45	1.52
12	5	135	PHE	CA-C	-5.52	1.45	1.52
14	n	103	ARG	CZ-NH2	5.52	1.40	1.33
3	C	218	GLY	CA-C	-5.52	1.44	1.51
4	D	172	PHE	C-O	-5.52	1.17	1.24
8	1	149	GLU	C-N	5.52	1.41	1.33
34	8	203	GLY	C-N	5.52	1.40	1.33
10	j	139	GLY	C-O	5.52	1.30	1.23
23	T	245	TYR	C-N	5.52	1.41	1.33
27	N	563	GLY	C-N	5.52	1.41	1.33
6	F	62	ILE	CA-C	-5.51	1.46	1.52
16	I	354	ASP	CA-CB	5.51	1.61	1.53
11	k	76	SER	N-CA	-5.51	1.38	1.45
30	Q	182	SER	CA-C	-5.51	1.45	1.52
30	Q	206	ASN	CA-C	-5.51	1.45	1.52
11	k	88	LEU	C-N	5.51	1.41	1.33
11	k	95	ARG	NE-CZ	5.51	1.39	1.33
7	G	126	ARG	CZ-NH2	5.51	1.40	1.33
6	f	82	VAL	N-CA	-5.51	1.40	1.46
14	n	21	ILE	C-N	5.51	1.41	1.33
11	4	76	SER	CA-C	5.51	1.59	1.53
26	Z	145	ASP	CA-CB	5.51	1.60	1.53
5	e	233	LYS	C-N	5.51	1.41	1.33
9	2	51	ASP	C-N	5.51	1.40	1.33
9	i	207	ARG	C-N	5.50	1.40	1.33
11	k	37	GLN	CA-C	5.50	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	19	GLY	CA-C	-5.50	1.44	1.51
9	i	180	ILE	C-N	5.50	1.40	1.33
14	n	190	ARG	CZ-NH2	5.50	1.40	1.33
16	I	85	PHE	CA-C	5.50	1.57	1.52
8	l	31	THR	C-O	5.50	1.30	1.23
28	S	380	CYS	N-CA	-5.50	1.39	1.46
33	O	55	THR	CA-C	5.50	1.59	1.53
26	Z	906	ALA	CA-CB	-5.50	1.44	1.53
14	n	203	ASN	CA-C	-5.50	1.45	1.52
15	H	66	LYS	N-CA	-5.50	1.39	1.46
15	H	103	THR	C-O	5.50	1.30	1.23
20	J	270	ARG	C-N	5.50	1.41	1.33
26	Z	220	ALA	CA-C	-5.50	1.45	1.52
31	R	335	ARG	N-CA	-5.50	1.39	1.46
8	h	47	GLY	C-N	5.50	1.41	1.33
3	C	233	GLU	CA-C	-5.50	1.45	1.52
19	M	195	GLU	CA-CB	5.50	1.61	1.53
19	M	329	ARG	CA-CB	5.50	1.61	1.53
7	g	188	ALA	N-CA	-5.50	1.39	1.46
28	S	126	LYS	CB-CG	5.50	1.69	1.52
3	c	124	HIS	CA-C	-5.49	1.46	1.52
1	A	115	LEU	CA-C	5.49	1.59	1.52
7	G	211	GLU	CA-C	-5.49	1.45	1.52
27	N	212	ASP	CA-C	-5.49	1.45	1.52
28	S	55	ARG	CA-C	-5.49	1.45	1.52
2	b	50	LYS	CA-CB	5.49	1.62	1.53
8	h	178	LEU	CA-C	-5.49	1.45	1.52
19	M	376	TRP	N-CA	-5.49	1.39	1.46
26	Z	53	VAL	C-N	5.49	1.41	1.33
8	l	16	ALA	N-CA	-5.49	1.39	1.46
16	I	110	GLU	C-N	5.49	1.40	1.33
23	T	251	HIS	CA-CB	5.49	1.62	1.53
26	Z	844	ALA	CA-C	-5.49	1.46	1.53
30	Q	294	ARG	CD-NE	5.49	1.53	1.46
10	j	19	CYS	CA-C	-5.49	1.45	1.52
13	m	63	ALA	C-N	5.49	1.40	1.33
6	F	50	ARG	CZ-NH1	5.49	1.40	1.32
1	A	190	TRP	CZ2-CH2	5.49	1.47	1.37
5	E	201	GLU	CA-C	-5.49	1.45	1.52
20	J	212	ARG	NE-CZ	5.49	1.39	1.33
27	N	19	SER	CA-C	-5.49	1.45	1.52
6	F	173	ARG	NE-CZ	5.49	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	44	MET	CA-C	-5.49	1.46	1.52
13	6	194	ARG	CD-NE	5.48	1.53	1.46
6	f	200	LEU	N-CA	-5.48	1.39	1.45
7	g	142	ALA	C-N	5.48	1.40	1.33
10	j	180	SER	CA-C	-5.48	1.46	1.52
11	k	126	VAL	C-O	5.48	1.29	1.24
2	B	149	GLN	CD-NE2	5.48	1.44	1.33
22	V	80	VAL	N-CA	-5.48	1.40	1.46
27	N	78	ALA	CA-C	-5.48	1.45	1.52
4	d	158	SER	N-CA	-5.48	1.39	1.46
12	5	19	ARG	CZ-NH1	5.48	1.40	1.32
17	K	84	GLU	N-CA	-5.48	1.39	1.46
17	K	101	GLU	CA-CB	5.48	1.60	1.54
3	C	129	PRO	CA-C	-5.48	1.45	1.52
28	S	326	ASP	C-N	5.48	1.38	1.33
12	l	137	TYR	CA-C	5.48	1.59	1.52
6	f	106	ARG	CZ-NH1	5.48	1.40	1.32
10	3	187	TYR	N-CA	-5.47	1.39	1.46
31	R	324	ARG	NE-CZ	5.47	1.39	1.33
34	8	447	HIS	CG-ND1	5.47	1.44	1.38
3	C	167	ASN	CG-ND2	5.47	1.44	1.33
7	G	62	LYS	CA-C	-5.47	1.45	1.52
19	M	270	ALA	N-CA	-5.47	1.39	1.46
31	R	403	LEU	CA-C	-5.47	1.45	1.52
8	h	188	PHE	N-CA	-5.47	1.39	1.46
1	A	144	SER	CA-C	-5.47	1.45	1.52
9	2	176	CYS	C-N	5.47	1.40	1.33
20	J	312	ARG	CD-NE	5.47	1.53	1.46
31	R	208	ASN	CA-C	-5.47	1.45	1.52
32	U	282	VAL	CA-CB	-5.47	1.47	1.54
8	h	93	LEU	CA-C	-5.47	1.46	1.52
13	6	203	GLU	C-O	-5.47	1.17	1.24
26	Z	338	HIS	ND1-CE1	5.47	1.38	1.32
30	Q	122	ILE	N-CA	-5.47	1.40	1.46
17	K	116	MET	CA-CB	5.47	1.61	1.53
2	b	134	LEU	CA-C	-5.47	1.46	1.52
14	n	161	ARG	CD-NE	5.47	1.53	1.46
31	R	39	SER	CA-C	-5.47	1.46	1.52
31	R	134	TRP	CA-CB	5.47	1.62	1.53
14	n	108	ASN	C-N	5.46	1.39	1.33
3	C	131	GLY	C-N	5.46	1.40	1.33
7	G	50	ILE	CA-C	-5.46	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	143	HIS	ND1-CE1	5.46	1.38	1.32
28	S	191	HIS	ND1-CE1	5.46	1.38	1.32
5	e	106	GLN	C-O	-5.46	1.17	1.24
8	1	157	HIS	CG-ND1	-5.46	1.32	1.38
17	K	74	HIS	ND1-CE1	5.46	1.38	1.32
20	J	62	LEU	N-CA	-5.46	1.39	1.46
6	F	125	ARG	CA-C	-5.46	1.46	1.52
28	S	458	GLN	C-N	5.46	1.41	1.33
31	R	239	THR	CA-C	-5.46	1.46	1.52
9	i	162	GLY	C-N	5.46	1.40	1.33
11	4	77	PRO	N-CA	-5.46	1.40	1.47
12	5	161	ILE	CA-C	-5.46	1.44	1.52
14	7	157	LYS	C-N	-5.46	1.26	1.33
34	8	379	PHE	CA-C	-5.46	1.46	1.52
12	5	159	ARG	CZ-NH1	5.46	1.40	1.32
15	H	184	GLU	CA-CB	5.46	1.62	1.53
26	Z	135	LEU	CA-C	-5.46	1.45	1.52
30	Q	276	ASP	CA-C	-5.46	1.45	1.52
30	Q	169	ASP	CA-CB	5.46	1.60	1.53
1	a	211	LYS	C-N	5.45	1.41	1.33
5	e	202	GLU	N-CA	-5.45	1.39	1.46
12	l	102	CYS	N-CA	-5.45	1.39	1.46
4	D	114	VAL	CA-CB	5.45	1.61	1.54
34	8	141	ASN	CA-C	5.45	1.57	1.52
1	a	184	HIS	CA-C	-5.45	1.45	1.52
8	h	19	ARG	CD-NE	5.45	1.53	1.46
3	C	30	HIS	CA-C	-5.45	1.46	1.52
5	E	108	VAL	CA-C	-5.45	1.45	1.52
5	e	180	HIS	ND1-CE1	5.45	1.38	1.32
17	K	50	LYS	CA-CB	5.45	1.61	1.53
18	L	155	ILE	CA-C	-5.45	1.46	1.52
18	L	302	GLN	C-N	5.45	1.41	1.33
27	N	427	ILE	N-CA	-5.45	1.40	1.46
1	a	107	VAL	CA-C	-5.45	1.45	1.52
5	e	160	ASN	CA-CB	5.45	1.61	1.54
7	g	216	SER	CA-C	-5.45	1.45	1.52
2	B	125	GLY	CA-C	-5.45	1.47	1.52
6	F	78	PRO	CA-C	5.45	1.59	1.52
18	L	264	ARG	NE-CZ	5.45	1.39	1.33
18	L	293	GLU	C-N	5.45	1.40	1.33
2	b	187	ASP	CA-C	-5.44	1.45	1.52
12	l	196	LEU	CA-C	-5.44	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	125	ARG	NE-CZ	5.44	1.39	1.33
10	j	87	THR	CA-C	5.44	1.60	1.52
1	A	37	ARG	CZ-NH2	5.44	1.40	1.33
5	E	223	TYR	N-CA	-5.44	1.39	1.46
6	F	86	TYR	CA-C	-5.44	1.45	1.52
11	4	115	GLU	C-N	5.44	1.40	1.33
27	N	234	ASP	CA-CB	5.44	1.61	1.53
28	S	262	THR	N-CA	-5.44	1.39	1.46
16	I	154	MET	CA-C	-5.44	1.45	1.52
25	Y	69	VAL	N-CA	-5.44	1.39	1.46
28	S	131	THR	C-N	5.44	1.41	1.33
3	C	147	LEU	C-N	5.44	1.40	1.33
13	6	211	GLY	C-N	5.44	1.40	1.33
34	8	252	VAL	CA-CB	-5.44	1.47	1.54
4	d	62	VAL	CA-C	-5.44	1.46	1.52
5	E	220	PHE	C-N	5.44	1.40	1.33
9	2	169	SER	C-N	5.44	1.39	1.33
18	L	172	SER	C-N	5.44	1.41	1.33
26	Z	624	LEU	C-O	-5.44	1.17	1.24
32	U	70	HIS	CE1-NE2	5.44	1.38	1.32
9	i	34	LEU	C-N	5.44	1.40	1.33
14	n	171	GLN	C-N	5.44	1.40	1.33
6	F	145	GLU	N-CA	-5.43	1.39	1.46
7	G	199	ALA	N-CA	-5.43	1.39	1.46
23	T	174	PHE	CA-CB	5.43	1.62	1.53
9	i	111	PHE	C-N	5.43	1.41	1.33
9	i	212	VAL	C-N	5.43	1.40	1.33
16	I	277	SER	C-N	5.43	1.40	1.33
17	K	393	ARG	CD-NE	5.43	1.53	1.46
27	N	281	GLY	C-N	5.43	1.41	1.33
28	S	72	GLU	N-CA	-5.43	1.39	1.46
34	8	213	LEU	N-CA	-5.43	1.39	1.46
13	m	36	ASN	CA-CB	5.43	1.62	1.53
15	H	455	LYS	C-O	-5.43	1.17	1.24
31	R	157	SER	CA-C	-5.43	1.45	1.52
2	b	174	PHE	CA-CB	5.43	1.61	1.53
8	h	34	LEU	CA-C	-5.43	1.46	1.52
28	S	491	GLU	C-N	5.43	1.41	1.33
12	5	25	TRP	CA-C	-5.43	1.45	1.52
13	6	16	ALA	CA-CB	5.43	1.60	1.53
15	H	95	HIS	CG-CD2	5.43	1.41	1.35
15	H	190	ARG	CZ-NH2	5.43	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	X	81	SER	N-CA	-5.43	1.39	1.46
26	Z	894	MET	CA-C	-5.43	1.45	1.52
29	P	131	PHE	N-CA	-5.43	1.40	1.46
28	S	207	ASN	CA-CB	5.43	1.61	1.53
19	M	289	LYS	C-N	5.42	1.40	1.33
20	J	200	ARG	CZ-NH1	5.42	1.40	1.32
27	N	738	GLN	N-CA	-5.42	1.39	1.46
21	W	21	PHE	CA-CB	5.42	1.61	1.53
29	P	29	GLN	C-N	5.42	1.41	1.33
1	a	158	LYS	CA-C	-5.42	1.45	1.52
2	b	89	SER	CA-CB	5.42	1.61	1.53
13	m	194	ARG	CZ-NH1	5.42	1.40	1.32
7	G	65	VAL	CA-C	-5.42	1.45	1.52
3	c	75	ALA	CA-CB	5.42	1.60	1.53
5	e	197	LYS	CA-C	-5.42	1.46	1.52
5	E	185	LEU	C-O	-5.42	1.17	1.24
32	U	48	VAL	N-CA	-5.42	1.40	1.46
6	F	176	ASP	CA-C	-5.42	1.45	1.52
8	1	59	VAL	CA-C	-5.42	1.45	1.52
10	3	85	THR	CA-C	-5.42	1.45	1.52
20	J	42	ARG	CZ-NH2	5.42	1.40	1.33
5	e	200	MET	CA-C	-5.42	1.46	1.52
13	6	67	ARG	CZ-NH1	5.42	1.40	1.32
21	W	84	LYS	N-CA	-5.42	1.39	1.46
4	d	37	LYS	N-CA	-5.42	1.39	1.46
9	i	132	LEU	CA-C	-5.42	1.46	1.52
3	C	227	LYS	CA-CB	5.42	1.61	1.53
4	D	51	LYS	CA-C	5.42	1.59	1.52
15	H	426	ALA	CA-C	-5.42	1.45	1.52
8	h	26	ILE	CA-C	-5.41	1.46	1.52
27	N	760	GLY	CA-C	-5.41	1.45	1.52
8	1	8	PHE	N-CA	-5.41	1.38	1.46
1	a	220	THR	CA-C	-5.41	1.46	1.52
8	1	185	ARG	CD-NE	5.41	1.53	1.46
9	2	141	HIS	ND1-CE1	5.41	1.38	1.32
12	5	157	GLY	C-N	5.41	1.41	1.33
20	J	374	ARG	CD-NE	5.41	1.53	1.46
22	V	90	LYS	C-O	-5.41	1.17	1.24
32	U	206	ASP	CA-CB	5.41	1.61	1.53
3	c	159	TRP	CA-CB	5.41	1.62	1.53
5	e	65	HIS	CE1-NE2	5.41	1.38	1.32
7	g	215	CYS	CA-CB	5.41	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	172	VAL	CA-C	-5.41	1.44	1.52
6	F	225	ASP	CA-C	-5.41	1.46	1.52
20	J	313	LYS	C-N	5.41	1.40	1.33
27	N	570	ARG	C-O	-5.41	1.17	1.24
2	B	185	LEU	N-CA	-5.41	1.39	1.46
5	E	143	ASP	C-N	5.41	1.41	1.33
18	L	303	ARG	CD-NE	5.41	1.53	1.46
21	W	158	ILE	C-N	5.41	1.41	1.33
27	N	639	ASP	C-N	5.41	1.40	1.33
11	k	167	GLU	CA-C	-5.41	1.45	1.52
3	C	30	HIS	C-N	5.41	1.40	1.33
18	L	299	ARG	CA-C	-5.41	1.45	1.52
23	T	191	LYS	CA-C	5.41	1.59	1.52
27	N	97	PHE	C-N	5.41	1.41	1.33
29	P	351	ARG	N-CA	-5.41	1.39	1.46
33	O	49	PHE	CA-CB	5.41	1.62	1.53
20	J	56	ARG	NE-CZ	5.40	1.39	1.33
14	n	186	TYR	N-CA	-5.40	1.39	1.46
9	2	193	PRO	N-CD	-5.40	1.40	1.47
12	5	127	PHE	CA-C	-5.40	1.46	1.52
22	V	128	SER	CA-C	5.40	1.59	1.52
32	U	107	ASN	CA-C	-5.40	1.45	1.52
1	a	226	THR	CA-CB	-5.40	1.45	1.53
2	B	203	GLU	CA-CB	5.40	1.63	1.53
3	C	208	ASP	N-CA	-5.40	1.38	1.46
10	3	140	THR	CA-C	-5.40	1.46	1.52
11	4	96	ARG	CA-C	5.40	1.58	1.52
18	L	125	PRO	CA-C	5.40	1.59	1.52
22	V	20	ARG	NE-CZ	5.40	1.39	1.33
24	X	101	LEU	N-CA	-5.40	1.39	1.46
34	8	204	PHE	C-O	-5.40	1.18	1.24
8	h	145	ASN	CA-C	-5.40	1.47	1.53
10	j	77	GLU	N-CA	-5.40	1.38	1.46
7	G	59	LYS	C-O	5.40	1.30	1.24
13	6	43	VAL	C-N	5.40	1.41	1.33
7	g	98	LEU	C-N	5.40	1.41	1.33
4	D	209	GLU	C-N	5.40	1.40	1.33
26	Z	770	GLU	C-N	5.40	1.40	1.33
27	N	150	LEU	N-CA	-5.40	1.38	1.46
30	Q	189	ARG	CD-NE	5.40	1.53	1.46
33	O	267	ASP	C-N	5.40	1.40	1.33
34	8	311	THR	C-N	5.40	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	8	315	VAL	N-CA	-5.40	1.39	1.46
6	f	157	GLY	C-O	-5.40	1.16	1.23
14	n	13	SER	CA-C	-5.40	1.45	1.52
3	C	73	ALA	C-N	5.40	1.40	1.33
10	3	123	PHE	N-CA	-5.40	1.39	1.45
27	N	100	THR	CA-C	-5.40	1.46	1.52
27	N	795	GLU	CA-CB	5.40	1.61	1.53
30	Q	32	ASP	N-CA	-5.40	1.39	1.46
4	d	81	ARG	NE-CZ	5.39	1.39	1.33
4	d	216	ASP	N-CA	-5.39	1.39	1.46
8	h	66	TYR	N-CA	-5.39	1.40	1.46
14	n	66	LEU	CB-CG	5.39	1.64	1.53
27	N	412	TYR	CA-CB	5.39	1.61	1.53
33	O	79	VAL	C-N	5.39	1.41	1.33
13	m	79	HIS	CE1-NE2	-5.39	1.27	1.32
8	1	42	TRP	CE2-CZ2	-5.39	1.28	1.39
22	V	234	GLU	CA-C	-5.39	1.46	1.52
9	2	149	GLU	CA-C	-5.39	1.46	1.52
7	G	232	LEU	C-N	5.39	1.41	1.33
14	7	115	ILE	C-N	5.39	1.40	1.33
15	H	383	GLU	N-CA	-5.39	1.39	1.46
18	L	164	ASP	C-N	5.39	1.40	1.33
29	P	88	GLN	CA-C	-5.39	1.46	1.53
22	V	132	LEU	CA-CB	5.39	1.61	1.53
19	M	349	PHE	CA-C	-5.38	1.47	1.53
28	S	365	THR	N-CA	-5.38	1.39	1.46
32	U	85	ALA	N-CA	-5.38	1.39	1.46
33	O	99	LEU	CA-C	-5.38	1.46	1.52
3	c	113	ARG	CZ-NH1	5.38	1.40	1.32
9	i	16	ALA	N-CA	-5.38	1.39	1.45
21	W	101	ARG	CZ-NH1	5.38	1.40	1.32
26	Z	900	LEU	N-CA	-5.38	1.39	1.46
27	N	633	GLY	CA-C	-5.38	1.44	1.51
34	8	235	ILE	CA-CB	5.38	1.60	1.54
3	c	138	GLY	CA-C	5.38	1.56	1.51
33	O	61	LEU	CA-CB	5.38	1.62	1.53
34	8	166	ARG	CD-NE	5.38	1.53	1.46
34	8	426	PRO	C-O	-5.38	1.17	1.24
1	A	126	ARG	CZ-NH1	5.38	1.40	1.32
15	H	215	LYS	CA-CB	5.38	1.62	1.53
6	f	14	PRO	N-CA	-5.38	1.40	1.47
4	D	126	PRO	N-CD	-5.38	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	144	SER	CA-CB	5.38	1.62	1.53
16	I	307	LEU	N-CA	-5.38	1.40	1.46
27	N	740	TRP	CD2-CE3	-5.38	1.31	1.40
6	f	37	LEU	C-N	5.37	1.40	1.33
7	g	16	ARG	NE-CZ	5.37	1.39	1.33
4	D	141	ASP	N-CA	5.37	1.51	1.46
15	H	80	HIS	C-N	5.37	1.41	1.33
17	K	405	SER	N-CA	-5.37	1.39	1.46
5	e	149	HIS	CG-CD2	5.37	1.41	1.35
14	7	226	LYS	C-N	5.37	1.40	1.33
5	e	89	VAL	C-N	5.37	1.41	1.33
12	l	66	HIS	N-CA	-5.37	1.39	1.46
2	B	58	SER	CA-C	-5.37	1.45	1.52
6	f	65	CYS	CA-CB	5.37	1.62	1.53
12	l	157	GLY	CA-C	-5.37	1.45	1.52
22	V	130	GLU	N-CA	-5.37	1.39	1.46
34	8	470	SER	CA-C	-5.37	1.46	1.52
1	A	71	GLY	C-N	5.37	1.40	1.33
3	c	17	ARG	CA-C	-5.37	1.46	1.52
12	l	183	ASP	CA-CB	5.37	1.62	1.53
7	G	66	VAL	N-CA	-5.37	1.39	1.46
10	3	45	TYR	CZ-OH	5.37	1.49	1.38
27	N	20	VAL	CA-C	-5.37	1.45	1.52
34	8	128	TYR	N-CA	-5.37	1.39	1.46
5	E	56	ILE	C-N	5.36	1.40	1.33
22	V	156	PHE	CA-C	-5.36	1.46	1.52
26	Z	913	ILE	N-CA	-5.36	1.39	1.46
11	4	95	ARG	CA-CB	5.36	1.61	1.53
3	C	183	MET	CA-CB	5.36	1.62	1.53
5	E	210	GLN	N-CA	-5.36	1.39	1.46
5	E	226	GLU	C-N	5.36	1.41	1.33
8	1	33	LYS	N-CA	5.36	1.52	1.46
15	H	231	SER	CA-C	-5.36	1.46	1.52
1	a	217	GLY	CA-C	-5.36	1.47	1.52
12	l	52	CYS	CA-CB	5.36	1.61	1.53
4	D	49	THR	N-CA	-5.36	1.39	1.46
26	Z	841	GLU	N-CA	-5.36	1.39	1.46
4	d	23	GLU	CA-C	-5.36	1.45	1.52
6	f	164	SER	C-N	5.36	1.41	1.33
6	F	188	LEU	N-CA	5.36	1.52	1.46
17	K	140	HIS	ND1-CE1	5.36	1.38	1.32
20	J	393	ASN	CA-C	-5.36	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	204	HIS	C-N	5.36	1.40	1.33
5	E	114	ARG	CZ-NH2	5.35	1.40	1.33
17	K	374	ARG	CD-NE	5.35	1.53	1.46
14	n	81	ALA	C-N	5.35	1.40	1.33
9	2	42	TRP	CA-C	-5.35	1.46	1.52
12	5	106	ARG	CZ-NH1	5.35	1.40	1.32
27	N	190	LEU	CA-CB	5.35	1.61	1.53
32	U	166	ALA	CA-C	5.35	1.59	1.52
4	d	45	GLU	N-CA	-5.35	1.39	1.46
5	e	162	LYS	N-CA	-5.35	1.39	1.45
6	f	48	LEU	CA-C	-5.35	1.46	1.52
10	j	84	GLU	CA-CB	5.35	1.61	1.53
9	2	29	LYS	C-N	5.35	1.41	1.33
22	V	269	ARG	CD-NE	5.35	1.53	1.46
5	E	106	GLN	N-CA	-5.35	1.40	1.46
18	L	435	GLN	C-N	5.35	1.40	1.33
30	Q	107	VAL	C-N	5.35	1.40	1.33
31	R	352	SER	C-O	-5.35	1.18	1.24
5	e	81	ILE	CA-C	-5.35	1.46	1.52
11	k	33	ASP	CA-C	-5.35	1.46	1.52
13	6	101	ARG	CZ-NH2	5.35	1.40	1.33
12	l	125	ASP	CA-CB	5.35	1.62	1.53
7	g	174	LYS	CA-CB	5.34	1.61	1.53
11	k	143	LEU	CA-C	-5.34	1.46	1.52
14	n	99	VAL	CA-CB	-5.34	1.47	1.54
12	5	17	ASP	N-CA	-5.34	1.39	1.46
25	Y	18	LYS	N-CA	-5.34	1.39	1.46
30	Q	336	ASN	C-N	5.34	1.41	1.33
33	O	204	SER	C-N	5.34	1.39	1.33
2	b	49	LYS	CA-C	-5.34	1.45	1.52
3	C	57	GLU	CA-C	-5.34	1.46	1.52
10	3	132	ALA	CA-C	-5.34	1.45	1.52
20	J	171	PRO	C-N	5.34	1.41	1.33
8	1	94	THR	CA-C	-5.34	1.46	1.52
17	K	136	SER	CA-CB	5.34	1.62	1.53
27	N	14	ARG	CZ-NH2	5.34	1.40	1.33
27	N	162	ARG	NE-CZ	5.34	1.39	1.33
27	N	180	SER	CA-C	-5.34	1.45	1.52
27	N	303	LEU	CA-C	5.34	1.59	1.52
31	R	112	GLU	N-CA	-5.34	1.40	1.46
6	f	27	ALA	C-N	5.34	1.40	1.33
12	l	199	LYS	CA-C	-5.34	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	188	ILE	C-N	5.34	1.40	1.33
20	J	43	ARG	NE-CZ	5.34	1.39	1.33
6	f	227	GLU	N-CA	-5.34	1.39	1.46
5	E	45	ARG	CZ-NH1	5.34	1.40	1.32
6	F	74	ALA	CA-CB	5.34	1.62	1.53
17	K	196	ASP	CA-C	-5.34	1.45	1.52
19	M	165	SER	CA-CB	5.34	1.62	1.53
30	Q	106	GLN	CA-C	-5.34	1.46	1.52
8	h	94	THR	C-N	5.33	1.40	1.33
17	K	204	ASP	CA-C	-5.33	1.47	1.53
1	a	62	TYR	CZ-OH	5.33	1.49	1.38
5	e	68	CYS	N-CA	-5.33	1.39	1.45
10	j	50	LEU	C-N	5.33	1.38	1.33
3	C	112	ARG	C-N	5.33	1.40	1.33
3	C	236	ASP	C-N	5.33	1.40	1.33
6	F	96	LEU	CA-C	-5.33	1.46	1.52
7	G	204	LYS	CA-C	-5.33	1.45	1.52
27	N	703	GLN	C-N	5.33	1.41	1.33
27	N	773	MET	CA-C	-5.33	1.46	1.52
14	n	209	LYS	CA-C	5.33	1.59	1.52
4	D	208	ILE	CA-C	-5.33	1.46	1.52
19	M	357	ARG	CD-NE	5.33	1.53	1.46
30	Q	360	SER	N-CA	-5.33	1.40	1.46
1	a	150	PRO	CA-C	-5.33	1.43	1.52
17	K	145	ALA	CA-C	-5.33	1.46	1.52
31	R	366	ASN	CA-C	5.33	1.59	1.52
7	g	31	THR	N-CA	-5.33	1.38	1.45
13	m	15	ILE	C-N	5.33	1.41	1.33
5	E	8	SER	CA-C	-5.33	1.47	1.53
26	Z	882	LEU	C-N	5.33	1.41	1.34
27	N	48	ALA	CA-C	-5.33	1.45	1.52
30	Q	196	ALA	C-N	5.33	1.41	1.33
33	O	125	GLY	N-CA	-5.33	1.39	1.45
1	a	80	ASP	C-N	5.33	1.40	1.33
20	J	17	SER	C-N	5.33	1.40	1.33
30	Q	51	ARG	CZ-NH2	5.33	1.40	1.33
11	k	66	LEU	CA-CB	5.32	1.61	1.53
1	A	111	ARG	N-CA	-5.32	1.40	1.46
5	E	115	PHE	N-CA	5.32	1.52	1.45
6	F	65	CYS	C-N	5.32	1.40	1.33
1	a	61	SER	N-CA	-5.32	1.39	1.46
7	g	215	CYS	CA-C	-5.32	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	111	ILE	CB-CG1	5.32	1.64	1.53
3	C	109	ILE	C-O	-5.32	1.18	1.24
18	L	80	ASN	N-CA	-5.32	1.39	1.46
23	T	36	LYS	N-CA	-5.32	1.39	1.46
31	R	356	ALA	N-CA	-5.32	1.40	1.46
27	N	434	SER	CA-C	-5.32	1.48	1.52
3	c	209	ARG	CZ-NH2	5.32	1.40	1.33
3	C	229	PHE	CA-C	-5.32	1.46	1.52
7	G	207	ASP	C-N	5.32	1.40	1.33
10	3	185	VAL	CA-C	5.32	1.59	1.52
12	5	182	GLU	N-CA	5.32	1.52	1.46
13	6	65	VAL	CA-C	-5.32	1.46	1.52
18	L	210	VAL	CA-C	-5.32	1.46	1.52
33	O	201	PRO	N-CD	-5.32	1.40	1.47
34	8	273	ARG	CZ-NH2	5.32	1.40	1.33
2	b	192	ALA	N-CA	-5.32	1.40	1.46
14	n	156	ARG	NE-CZ	5.32	1.38	1.33
7	G	33	SER	C-O	5.32	1.30	1.23
8	1	36	ARG	NE-CZ	5.32	1.38	1.33
21	W	101	ARG	NE-CZ	5.32	1.38	1.33
27	N	196	THR	N-CA	-5.32	1.39	1.46
29	P	73	ASP	N-CA	-5.32	1.40	1.46
1	a	38	GLY	C-N	5.31	1.41	1.33
8	h	104	ASP	C-N	5.31	1.41	1.33
8	h	176	VAL	CA-C	-5.31	1.46	1.52
13	6	95	HIS	ND1-CE1	5.31	1.37	1.32
16	I	68	HIS	CA-CB	5.31	1.61	1.53
14	n	117	ALA	C-O	-5.31	1.17	1.24
2	B	66	LEU	CA-CB	5.31	1.61	1.53
3	C	33	THR	C-N	5.31	1.41	1.33
3	C	211	GLU	C-N	5.31	1.40	1.33
33	O	218	SER	C-N	5.31	1.40	1.33
34	8	264	HIS	CA-C	-5.31	1.45	1.52
7	g	196	ILE	CA-C	-5.31	1.46	1.52
8	1	34	LEU	CA-CB	5.31	1.59	1.53
2	b	156	TYR	CZ-OH	5.31	1.49	1.38
5	e	19	SER	CA-C	5.31	1.59	1.52
11	k	66	LEU	C-N	-5.31	1.26	1.33
12	l	77	ALA	C-O	-5.31	1.18	1.24
7	G	52	SER	C-O	-5.31	1.17	1.23
8	1	154	PHE	CA-C	-5.31	1.45	1.52
34	8	376	ARG	CZ-NH1	5.31	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	176	GLU	CA-C	-5.31	1.46	1.52
9	2	225	GLU	C-O	5.31	1.30	1.24
30	Q	405	GLN	C-N	5.31	1.41	1.33
5	E	39	VAL	C-N	5.31	1.41	1.33
30	Q	285	LYS	CA-CB	5.31	1.62	1.53
5	e	81	ILE	N-CA	-5.30	1.40	1.46
10	j	176	ARG	CZ-NH2	5.30	1.40	1.33
11	4	3	ILE	N-CA	-5.30	1.40	1.46
12	5	91	LYS	CA-CB	5.30	1.62	1.53
5	e	222	ILE	N-CA	-5.30	1.40	1.46
10	3	27	ARG	CZ-NH1	5.30	1.40	1.32
19	M	286	ILE	N-CA	-5.30	1.39	1.46
2	b	209	ILE	C-O	5.30	1.29	1.24
3	C	200	THR	CA-C	-5.30	1.46	1.52
7	G	71	GLY	N-CA	-5.30	1.38	1.45
26	Z	859	LYS	CA-C	-5.30	1.45	1.52
34	8	305	ARG	NE-CZ	5.30	1.38	1.33
1	a	66	ILE	CA-CB	-5.30	1.47	1.54
1	a	127	PRO	C-N	5.30	1.40	1.33
3	c	124	HIS	CB-CG	5.30	1.57	1.50
7	G	196	ILE	C-N	5.30	1.41	1.33
8	1	152	VAL	CA-C	-5.30	1.46	1.52
20	J	102	ILE	N-CA	-5.30	1.40	1.46
2	b	176	GLU	C-N	5.30	1.41	1.34
16	I	76	VAL	CA-CB	-5.30	1.48	1.54
6	f	88	ARG	CD-NE	5.30	1.53	1.46
2	B	74	VAL	CA-C	-5.30	1.46	1.52
2	B	128	ARG	CZ-NH2	5.30	1.40	1.33
22	V	68	VAL	C-N	5.30	1.40	1.33
24	X	60	GLU	C-N	5.30	1.41	1.33
33	O	346	GLU	C-N	5.30	1.41	1.33
34	8	190	LYS	CA-C	-5.30	1.46	1.52
6	f	202	ASP	CA-CB	5.29	1.61	1.53
9	i	4	VAL	N-CA	-5.29	1.40	1.46
9	i	13	VAL	CA-C	-5.29	1.46	1.52
8	1	104	ASP	N-CA	-5.29	1.39	1.46
24	X	104	LYS	N-CA	-5.29	1.39	1.46
27	N	623	PHE	N-CA	-5.29	1.40	1.46
33	O	330	ARG	NE-CZ	5.29	1.38	1.33
3	C	141	ASP	N-CA	-5.29	1.39	1.46
4	D	46	ARG	N-CA	-5.29	1.40	1.46
22	V	116	CYS	CA-CB	5.29	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	646	LYS	C-N	5.29	1.41	1.33
5	e	100	ASN	CA-CB	5.29	1.62	1.53
9	i	84	LYS	N-CA	-5.29	1.40	1.46
11	4	128	LEU	C-O	5.29	1.28	1.24
34	8	108	PRO	N-CA	-5.29	1.41	1.46
1	a	57	PRO	CA-C	-5.29	1.46	1.52
14	7	124	ASP	CA-C	-5.29	1.46	1.52
14	7	125	GLN	C-N	5.29	1.40	1.33
4	d	32	VAL	CA-C	-5.28	1.46	1.52
13	m	49	ASN	N-CA	-5.28	1.38	1.46
5	E	101	VAL	C-N	5.28	1.40	1.33
14	7	196	SER	CA-CB	5.28	1.64	1.53
18	L	246	SER	N-CA	-5.28	1.40	1.46
2	b	51	SER	CA-C	-5.28	1.45	1.52
13	m	51	VAL	CA-C	-5.28	1.46	1.52
6	F	87	LEU	CA-C	-5.28	1.46	1.52
17	K	66	ASP	C-O	-5.28	1.18	1.24
14	7	117	ALA	C-N	5.28	1.39	1.33
33	O	196	LEU	C-O	5.28	1.30	1.24
5	e	35	LYS	N-CA	-5.28	1.39	1.46
9	i	109	HIS	ND1-CE1	5.28	1.37	1.32
7	G	176	VAL	N-CA	-5.28	1.40	1.46
1	a	84	ALA	N-CA	-5.28	1.40	1.46
6	f	217	LYS	CA-C	-5.28	1.46	1.52
11	k	143	LEU	N-CA	5.28	1.52	1.46
6	F	38	ARG	CZ-NH2	5.28	1.40	1.33
7	G	16	ARG	NE-CZ	5.28	1.38	1.33
11	4	179	VAL	C-N	5.28	1.41	1.33
13	6	63	ALA	CA-C	-5.28	1.46	1.52
29	P	164	GLN	C-N	5.28	1.40	1.33
1	a	68	ARG	CZ-NH2	5.28	1.40	1.33
7	g	165	ARG	C-N	5.28	1.40	1.33
11	k	116	LEU	CA-C	-5.28	1.46	1.52
14	n	6	VAL	CA-CB	-5.28	1.48	1.54
2	B	150	VAL	CA-C	-5.28	1.46	1.52
7	G	148	GLU	C-N	5.28	1.39	1.33
16	I	227	THR	CA-C	-5.28	1.45	1.52
31	R	383	ARG	CD-NE	5.28	1.53	1.46
2	B	128	ARG	NE-CZ	5.27	1.38	1.33
15	H	273	ARG	CA-CB	5.27	1.60	1.53
17	K	122	ILE	N-CA	-5.27	1.40	1.46
2	b	139	HIS	CG-CD2	-5.27	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	15	ALA	N-CA	-5.27	1.39	1.46
24	X	77	PRO	CA-C	-5.27	1.44	1.52
12	l	152	ASP	CA-C	-5.27	1.45	1.52
20	J	63	ARG	C-N	5.27	1.40	1.33
21	W	179	ARG	CA-C	-5.27	1.45	1.52
13	6	24	ALA	C-N	5.27	1.39	1.33
20	J	309	ARG	NE-CZ	5.27	1.38	1.33
21	W	110	ILE	C-N	5.27	1.40	1.33
25	Y	83	ARG	CA-C	-5.27	1.46	1.52
32	U	87	GLU	N-CA	-5.27	1.39	1.46
7	g	153	TYR	N-CA	-5.27	1.39	1.45
13	6	148	PRO	N-CA	-5.27	1.40	1.47
17	K	92	VAL	CA-CB	5.27	1.60	1.54
21	W	157	PHE	N-CA	-5.27	1.39	1.46
30	Q	420	ASN	N-CA	-5.27	1.40	1.46
10	j	174	ALA	CA-C	-5.27	1.46	1.52
7	G	17	ASN	N-CA	-5.27	1.39	1.46
28	S	85	SER	CA-C	5.27	1.59	1.52
27	N	685	VAL	CA-C	5.26	1.59	1.52
7	G	52	SER	N-CA	-5.26	1.40	1.46
10	3	128	CYS	CA-C	-5.26	1.46	1.52
12	5	97	MET	CA-C	-5.26	1.46	1.52
26	Z	156	HIS	N-CA	-5.26	1.40	1.46
28	S	37	VAL	C-N	5.26	1.40	1.33
28	S	482	PRO	C-N	5.26	1.41	1.34
11	k	190	ARG	NE-CZ	5.26	1.38	1.33
20	J	388	LYS	CA-CB	5.26	1.61	1.53
7	G	172	LEU	CA-C	-5.26	1.45	1.52
22	V	121	VAL	C-O	-5.26	1.17	1.24
26	Z	538	CYS	C-N	5.26	1.40	1.33
34	8	327	SER	N-CA	-5.26	1.39	1.46
2	b	161	ALA	N-CA	-5.26	1.39	1.46
8	1	61	TYR	CA-C	-5.26	1.46	1.52
33	O	331	ALA	C-N	5.26	1.40	1.33
1	A	83	ASN	CA-C	-5.26	1.46	1.52
1	A	103	MET	CA-C	-5.26	1.47	1.53
20	J	371	ARG	CZ-NH1	5.26	1.40	1.32
2	b	7	PHE	CA-C	-5.25	1.45	1.52
6	f	68	HIS	CB-CG	5.25	1.57	1.50
4	d	136	PHE	C-N	5.25	1.41	1.33
13	6	23	LEU	C-O	-5.25	1.18	1.24
4	d	221	ALA	CA-C	-5.25	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	12	ARG	N-CA	-5.25	1.39	1.45
26	Z	621	LEU	C-O	-5.25	1.17	1.24
27	N	137	PHE	N-CA	-5.25	1.40	1.46
6	f	154	GLU	CA-C	-5.25	1.46	1.52
9	i	175	VAL	C-N	5.25	1.40	1.33
24	X	93	SER	CA-C	-5.25	1.45	1.52
30	Q	82	THR	N-CA	-5.25	1.39	1.46
11	k	96	ARG	CD-NE	5.25	1.53	1.46
2	b	67	LEU	C-N	5.25	1.44	1.33
27	N	637	ALA	N-CA	-5.25	1.40	1.46
6	f	190	LYS	N-CA	-5.25	1.40	1.46
30	Q	72	ASP	N-CA	-5.25	1.39	1.46
1	a	89	LYS	N-CA	5.24	1.52	1.46
2	B	152	PRO	CA-CB	-5.24	1.45	1.53
9	2	10	ASN	CA-C	-5.24	1.46	1.53
12	5	119	GLY	C-N	5.24	1.40	1.33
28	S	438	HIS	ND1-CE1	5.24	1.37	1.32
6	f	111	LEU	N-CA	-5.24	1.39	1.46
8	h	81	VAL	CA-CB	-5.24	1.47	1.54
17	K	368	LEU	C-N	5.24	1.41	1.33
22	V	49	VAL	N-CA	-5.24	1.40	1.46
27	N	566	SER	N-CA	-5.24	1.40	1.46
27	N	769	PRO	CA-C	-5.24	1.45	1.52
7	g	168	ALA	N-CA	-5.24	1.40	1.46
12	l	201	LYS	C-N	5.24	1.40	1.33
11	4	76	SER	CA-CB	5.24	1.61	1.53
14	7	195	PHE	N-CA	-5.24	1.39	1.45
23	T	49	ASP	C-N	5.24	1.40	1.33
26	Z	903	MET	N-CA	-5.24	1.39	1.46
3	c	20	GLN	N-CA	-5.24	1.40	1.46
4	d	134	ALA	C-N	5.24	1.39	1.33
11	k	67	TYR	C-N	5.24	1.40	1.33
11	4	145	ASP	C-O	5.24	1.30	1.24
12	5	153	ALA	C-O	-5.24	1.18	1.24
19	M	428	LYS	CA-C	-5.24	1.45	1.52
27	N	686	ILE	C-N	5.24	1.40	1.33
30	Q	106	GLN	C-N	5.24	1.39	1.33
32	U	4	GLN	C-N	5.24	1.41	1.33
8	h	107	LYS	CA-C	-5.23	1.45	1.52
26	Z	358	TYR	N-CA	-5.23	1.39	1.46
26	Z	378	GLN	C-N	5.23	1.41	1.33
28	S	320	ILE	N-CA	-5.23	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	27	SER	C-N	5.23	1.40	1.33
13	m	194	ARG	CZ-NH2	5.23	1.40	1.33
8	1	152	VAL	C-N	5.23	1.40	1.33
10	3	93	SER	C-N	5.23	1.40	1.33
27	N	66	SER	C-N	5.23	1.40	1.33
1	a	18	GLN	CA-C	5.23	1.59	1.52
11	k	96	ARG	CA-C	5.23	1.57	1.52
4	D	56	ARG	NE-CZ	5.23	1.38	1.33
15	H	289	ARG	N-CA	5.23	1.52	1.46
17	K	44	ASN	N-CA	-5.23	1.40	1.46
26	Z	138	ARG	CZ-NH1	5.23	1.40	1.32
26	Z	429	ASN	C-N	5.23	1.41	1.33
27	N	57	ASP	CA-CB	5.23	1.60	1.53
28	S	211	ARG	CA-CB	5.23	1.61	1.53
29	P	358	SER	CA-CB	5.23	1.61	1.53
34	8	472	VAL	N-CA	-5.23	1.38	1.45
7	g	68	ARG	CZ-NH2	5.23	1.40	1.33
9	i	83	LEU	N-CA	-5.23	1.40	1.46
11	k	169	GLU	CA-CB	5.23	1.62	1.53
6	f	19	PHE	C-O	-5.23	1.17	1.24
18	L	107	GLU	C-N	5.23	1.40	1.33
26	Z	712	ASP	C-N	5.23	1.41	1.33
2	B	96	SER	C-N	5.23	1.41	1.33
11	4	71	GLU	CA-CB	5.23	1.62	1.53
27	N	76	GLU	C-O	-5.23	1.17	1.24
7	g	119	HIS	CB-CG	5.22	1.57	1.50
8	h	4	MET	C-N	5.22	1.41	1.33
14	n	139	SER	C-O	-5.22	1.18	1.24
20	J	333	ARG	CZ-NH1	5.22	1.40	1.32
27	N	539	MET	N-CA	-5.22	1.40	1.46
30	Q	34	ASP	CA-CB	5.22	1.61	1.53
11	4	190	ARG	CZ-NH1	5.22	1.40	1.32
12	5	41	LEU	N-CA	-5.22	1.39	1.45
12	5	50	ALA	N-CA	-5.22	1.40	1.46
19	M	37	LEU	CA-C	5.22	1.59	1.52
20	J	331	HIS	CG-ND1	5.22	1.44	1.38
29	P	328	ALA	CA-C	-5.22	1.45	1.52
1	A	68	ARG	NE-CZ	5.22	1.38	1.33
6	f	68	HIS	CA-CB	-5.22	1.46	1.53
12	l	129	VAL	CA-C	-5.22	1.46	1.52
21	W	142	ILE	N-CA	-5.22	1.40	1.46
33	O	254	LEU	CA-C	-5.22	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	122	THR	CA-CB	-5.22	1.46	1.54
8	h	56	ALA	CA-C	5.22	1.59	1.52
8	h	173	ILE	CA-C	-5.22	1.46	1.52
7	G	84	LEU	CA-C	5.22	1.59	1.52
22	V	195	HIS	CG-ND1	5.22	1.44	1.38
4	d	127	PHE	CA-CB	5.22	1.61	1.53
7	g	24	VAL	C-N	5.22	1.41	1.34
11	k	147	HIS	CG-ND1	5.22	1.44	1.38
14	n	204	THR	N-CA	-5.22	1.39	1.46
4	D	19	GLU	CA-C	-5.22	1.45	1.52
27	N	145	LEU	N-CA	-5.22	1.39	1.46
33	O	296	LEU	N-CA	-5.22	1.40	1.46
10	j	153	TYR	C-N	5.21	1.41	1.33
16	I	407	ARG	NE-CZ	5.21	1.38	1.33
17	K	67	TYR	CA-C	-5.21	1.46	1.52
27	N	132	LYS	N-CA	-5.21	1.40	1.46
31	R	44	LYS	CA-C	-5.21	1.45	1.52
5	e	173	ALA	C-N	5.21	1.40	1.33
14	7	161	ARG	NE-CZ	5.21	1.38	1.33
26	Z	855	LEU	N-CA	-5.21	1.39	1.46
30	Q	425	GLN	CA-C	-5.21	1.46	1.52
6	F	63	ILE	C-N	5.21	1.40	1.33
7	G	27	VAL	CA-CB	-5.21	1.48	1.54
7	G	165	ARG	CZ-NH1	5.21	1.40	1.32
26	Z	504	GLU	N-CA	-5.21	1.40	1.46
28	S	19	HIS	C-N	5.21	1.40	1.33
29	P	309	MET	N-CA	-5.21	1.40	1.46
30	Q	39	SER	C-N	5.21	1.41	1.33
7	g	167	SER	C-N	5.21	1.40	1.33
26	Z	221	VAL	C-N	5.21	1.41	1.33
5	e	5	SER	CA-C	-5.21	1.46	1.52
5	e	202	GLU	CA-C	5.21	1.60	1.52
6	f	153	THR	N-CA	-5.21	1.39	1.46
12	5	73	ARG	C-N	5.21	1.40	1.33
17	K	91	SER	C-O	-5.21	1.16	1.23
22	V	100	ARG	CZ-NH2	5.21	1.40	1.33
34	8	354	VAL	C-N	5.21	1.41	1.33
23	T	23	CYS	CA-CB	5.21	1.61	1.53
34	8	397	GLN	N-CA	5.21	1.52	1.46
14	n	208	PHE	CA-CB	5.21	1.60	1.53
15	H	163	VAL	C-N	5.21	1.40	1.33
17	K	399	ARG	CZ-NH1	5.21	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	J	279	LEU	N-CA	-5.21	1.39	1.46
31	R	118	GLN	N-CA	-5.21	1.40	1.46
1	a	200	HIS	CD2-NE2	5.20	1.43	1.37
4	d	93	SER	CA-C	-5.20	1.46	1.52
4	d	125	ARG	CZ-NH2	5.20	1.40	1.33
9	i	103	VAL	CA-C	-5.20	1.46	1.52
14	n	108	ASN	N-CA	-5.20	1.41	1.46
2	B	194	LEU	CA-CB	5.20	1.61	1.53
7	G	190	LYS	CA-CB	5.20	1.61	1.53
20	J	188	TYR	CA-C	-5.20	1.46	1.52
23	T	172	SER	CA-C	-5.20	1.45	1.52
24	X	79	LYS	C-N	5.20	1.41	1.33
33	O	72	LYS	CA-C	-5.20	1.46	1.52
4	d	5	ALA	CA-C	5.20	1.59	1.52
12	l	55	TRP	N-CA	-5.20	1.39	1.46
14	n	41	ARG	CA-C	-5.20	1.44	1.52
8	1	71	GLY	C-N	5.20	1.41	1.33
10	3	13	ALA	N-CA	5.20	1.52	1.45
19	M	354	GLU	CA-C	-5.20	1.46	1.52
22	V	190	HIS	ND1-CE1	5.20	1.37	1.32
2	B	182	GLU	N-CA	-5.20	1.39	1.46
28	S	111	ARG	CD-NE	5.20	1.53	1.46
28	S	455	GLU	N-CA	-5.20	1.39	1.46
5	E	44	LYS	N-CA	-5.20	1.39	1.46
30	Q	5	GLY	CA-C	-5.20	1.46	1.52
12	l	112	ILE	C-N	5.20	1.40	1.33
1	A	129	GLY	N-CA	-5.20	1.37	1.45
15	H	422	VAL	CA-CB	-5.20	1.47	1.54
18	L	98	LEU	C-N	5.20	1.41	1.33
18	L	202	LYS	CA-CB	5.20	1.61	1.53
8	h	9	LYS	CA-CB	5.19	1.61	1.53
16	I	408	ARG	CZ-NH2	5.19	1.40	1.33
7	g	89	ARG	CZ-NH1	5.19	1.40	1.32
16	I	306	MET	CA-C	-5.19	1.46	1.52
20	J	324	ARG	NE-CZ	5.19	1.38	1.33
29	P	94	GLN	CA-C	-5.19	1.45	1.52
12	5	106	ARG	CD-NE	5.19	1.53	1.46
17	K	320	ARG	NE-CZ	5.19	1.38	1.33
31	R	171	MET	CA-CB	5.19	1.61	1.53
15	H	102	CYS	N-CA	-5.19	1.39	1.46
27	N	780	ASP	CA-CB	5.19	1.61	1.53
2	B	153	SER	CA-C	-5.19	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	39	PRO	C-N	5.19	1.41	1.33
11	4	41	HIS	N-CA	-5.19	1.40	1.46
20	J	120	TYR	N-CA	-5.19	1.39	1.46
26	Z	282	ILE	C-N	5.19	1.40	1.33
27	N	725	LEU	C-N	5.19	1.41	1.33
30	Q	312	LEU	N-CA	-5.19	1.40	1.46
1	a	241	GLU	CA-C	5.19	1.60	1.52
15	H	370	ARG	C-N	5.19	1.41	1.33
20	J	235	VAL	N-CA	5.19	1.52	1.46
19	M	329	ARG	CD-NE	5.18	1.53	1.46
26	Z	764	LEU	CA-C	-5.18	1.46	1.52
27	N	172	SER	CA-CB	5.18	1.62	1.53
27	N	548	ARG	CA-CB	5.18	1.61	1.53
31	R	392	ARG	NE-CZ	5.18	1.38	1.33
2	b	42	GLY	C-N	5.18	1.39	1.33
3	c	150	SER	CA-C	-5.18	1.46	1.52
4	d	181	GLU	CA-CB	5.18	1.60	1.52
5	E	83	HIS	ND1-CE1	5.18	1.37	1.32
21	W	194	GLU	C-N	5.18	1.40	1.33
31	R	400	TYR	CA-C	-5.18	1.46	1.52
2	b	28	VAL	N-CA	-5.18	1.40	1.46
5	e	24	LYS	CA-CB	5.18	1.61	1.53
12	l	186	ILE	CA-C	-5.18	1.46	1.52
29	P	69	ARG	CZ-NH1	5.18	1.40	1.32
17	K	100	LEU	C-N	5.18	1.39	1.32
33	O	349	THR	CA-C	-5.18	1.46	1.52
4	d	88	ARG	CA-CB	-5.18	1.45	1.53
1	A	175	ASN	CB-CG	5.18	1.65	1.52
10	j	103	PHE	C-N	5.18	1.40	1.33
11	k	95	ARG	CZ-NH2	5.18	1.40	1.33
3	C	59	ASP	CA-CB	5.18	1.61	1.53
11	4	148	TYR	CZ-OH	5.18	1.49	1.38
16	I	304	ARG	NE-CZ	5.18	1.38	1.33
19	M	381	ARG	C-N	5.18	1.41	1.33
12	l	190	ASN	CA-C	-5.17	1.46	1.52
4	D	219	ILE	C-O	-5.17	1.18	1.24
8	1	17	ASP	CA-C	-5.17	1.45	1.52
10	3	114	LYS	N-CA	-5.17	1.38	1.45
22	V	44	GLY	CA-C	-5.17	1.43	1.51
26	Z	734	ASP	N-CA	-5.17	1.40	1.46
6	f	102	LEU	C-N	5.17	1.41	1.33
13	6	136	CYS	CA-C	-5.17	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	163	ALA	CA-CB	-5.17	1.45	1.53
6	F	133	ILE	C-N	5.17	1.41	1.33
16	I	363	GLY	C-N	5.17	1.40	1.33
19	M	290	ARG	NE-CZ	5.17	1.38	1.33
1	a	187	GLU	C-N	5.17	1.41	1.34
4	d	123	GLY	CA-C	-5.17	1.44	1.51
17	K	288	SER	N-CA	-5.17	1.39	1.46
22	V	171	ARG	CZ-NH2	5.17	1.40	1.33
29	P	158	ASP	CA-C	-5.17	1.46	1.52
2	B	81	ASP	C-O	-5.17	1.18	1.24
6	F	203	GLU	CA-C	5.17	1.59	1.52
9	2	29	LYS	CA-C	5.17	1.59	1.52
34	8	485	GLU	C-N	-5.17	1.26	1.33
15	H	346	ARG	CD-NE	5.17	1.53	1.46
23	T	187	ASP	CA-C	-5.17	1.46	1.52
26	Z	508	LEU	N-CA	-5.17	1.40	1.46
31	R	250	ALA	N-CA	-5.17	1.40	1.46
8	h	12	VAL	C-O	-5.16	1.18	1.24
8	h	37	VAL	CA-C	-5.16	1.45	1.52
13	6	39	TYR	N-CA	5.16	1.52	1.46
28	S	201	ILE	N-CA	-5.16	1.39	1.46
5	E	139	HIS	C-N	5.16	1.40	1.33
14	n	190	ARG	CA-CB	5.16	1.62	1.53
3	C	60	THR	C-N	5.16	1.40	1.33
10	3	90	VAL	C-N	5.16	1.40	1.33
12	5	76	VAL	CA-C	5.16	1.59	1.52
18	L	199	LEU	CA-CB	5.16	1.60	1.53
19	M	263	VAL	N-CA	-5.16	1.40	1.46
26	Z	813	PHE	N-CA	-5.16	1.40	1.46
2	b	66	LEU	CA-C	-5.16	1.46	1.52
9	i	151	ALA	C-N	5.16	1.40	1.33
9	i	223	ILE	CA-C	-5.16	1.46	1.52
10	j	143	ASP	CA-C	-5.16	1.46	1.52
2	B	90	ARG	CD-NE	5.16	1.53	1.46
14	7	65	ARG	NE-CZ	5.16	1.38	1.33
17	K	43	VAL	CA-C	-5.16	1.46	1.52
19	M	73	ARG	NE-CZ	5.16	1.38	1.33
13	m	212	VAL	C-O	-5.16	1.18	1.24
18	L	222	GLY	C-N	-5.16	1.27	1.33
4	D	84	ILE	N-CA	-5.16	1.40	1.46
22	V	194	ARG	NE-CZ	5.16	1.38	1.33
26	Z	490	ILE	N-CA	5.15	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	381	GLU	N-CA	-5.15	1.40	1.46
28	S	451	ILE	C-O	-5.15	1.18	1.24
13	6	41	PRO	N-CA	-5.15	1.40	1.47
9	i	188	ARG	CZ-NH2	5.15	1.40	1.33
11	k	52	ASP	CA-CB	5.15	1.61	1.53
4	D	81	ARG	CD-NE	5.15	1.53	1.46
12	5	64	ARG	CZ-NH1	5.15	1.40	1.32
14	7	62	HIS	C-O	-5.15	1.18	1.24
17	K	66	ASP	N-CA	-5.15	1.40	1.46
17	K	240	SER	CA-CB	5.15	1.61	1.53
7	G	205	GLU	CA-C	5.15	1.59	1.52
33	O	147	ARG	CD-NE	5.15	1.53	1.46
34	8	299	VAL	N-CA	-5.15	1.39	1.46
1	a	5	ARG	NE-CZ	5.14	1.38	1.33
8	h	27	ALA	CA-C	-5.14	1.46	1.52
20	J	200	ARG	NE-CZ	5.14	1.38	1.33
10	j	132	ALA	N-CA	-5.14	1.39	1.46
14	n	53	ILE	N-CA	-5.14	1.40	1.46
14	n	138	SER	CA-CB	5.14	1.65	1.53
6	F	206	THR	CA-CB	-5.14	1.44	1.53
8	1	25	TYR	CA-C	-5.14	1.46	1.52
31	R	189	GLU	CA-CB	5.14	1.61	1.53
31	R	227	ALA	C-N	5.14	1.40	1.33
6	f	173	ARG	C-N	5.14	1.40	1.33
7	g	52	SER	CA-C	-5.14	1.46	1.52
24	X	16	GLU	N-CA	5.14	1.52	1.46
27	N	124	TYR	C-N	5.14	1.40	1.33
7	g	95	PHE	CA-C	5.14	1.59	1.52
10	j	161	ASP	C-N	5.14	1.40	1.33
18	L	107	GLU	N-CA	-5.14	1.39	1.46
2	b	145	PHE	CA-CB	5.14	1.61	1.53
9	2	1	THR	C-N	5.14	1.40	1.33
27	N	566	SER	C-O	-5.14	1.18	1.24
29	P	282	HIS	N-CA	-5.14	1.39	1.46
8	h	34	LEU	C-N	5.14	1.40	1.33
13	m	190	SER	CA-C	-5.14	1.46	1.52
24	X	51	ARG	CA-C	5.14	1.58	1.52
27	N	154	LEU	CA-C	5.14	1.59	1.52
32	U	124	ASP	N-CA	-5.14	1.39	1.46
34	8	181	PRO	CA-CB	5.14	1.59	1.53
3	c	202	SER	CA-CB	5.13	1.60	1.53
9	i	61	SER	CA-CB	5.13	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	122	THR	N-CA	-5.13	1.39	1.45
7	G	178	HIS	ND1-CE1	5.13	1.37	1.32
23	T	260	ILE	N-CA	-5.13	1.40	1.46
27	N	586	ALA	N-CA	-5.13	1.40	1.46
2	b	175	LEU	CA-C	-5.13	1.46	1.52
12	l	184	GLY	C-N	5.13	1.40	1.33
20	J	22	TYR	CA-CB	5.13	1.61	1.53
26	Z	545	SER	C-O	5.13	1.30	1.24
34	8	150	GLY	C-N	5.13	1.40	1.33
20	J	396	THR	CA-C	-5.13	1.46	1.52
28	S	490	ASN	C-N	5.13	1.40	1.33
30	Q	331	THR	CA-C	-5.13	1.46	1.52
33	O	52	ALA	N-CA	-5.13	1.39	1.46
4	D	109	ARG	CA-CB	5.13	1.61	1.53
17	K	262	ARG	NE-CZ	5.13	1.38	1.33
29	P	230	HIS	C-N	5.13	1.40	1.33
32	U	119	LEU	N-CA	-5.13	1.39	1.46
34	8	189	ARG	CD-NE	5.13	1.53	1.46
34	8	213	LEU	C-O	-5.13	1.18	1.24
4	D	181	GLU	C-N	5.13	1.39	1.33
15	H	266	ARG	CZ-NH1	5.13	1.40	1.32
17	K	63	LEU	N-CA	5.13	1.52	1.46
22	V	291	ASN	C-N	5.13	1.40	1.33
28	S	31	VAL	CA-C	-5.13	1.46	1.52
33	O	21	SER	CA-C	-5.13	1.45	1.52
1	a	231	ASN	N-CA	-5.13	1.40	1.46
7	g	79	PRO	N-CA	-5.13	1.40	1.47
13	m	58	ALA	C-N	5.13	1.40	1.33
14	n	60	MET	CA-CB	5.13	1.61	1.53
5	E	153	SER	C-N	5.13	1.40	1.33
7	G	65	VAL	CA-CB	5.13	1.61	1.54
18	L	62	ARG	CA-C	-5.13	1.46	1.52
22	V	264	GLU	N-CA	-5.13	1.40	1.46
27	N	364	LYS	N-CA	-5.13	1.40	1.46
31	R	125	GLU	N-CA	-5.13	1.40	1.46
13	6	91	ARG	NE-CZ	5.12	1.38	1.33
34	8	397	GLN	CA-C	-5.12	1.45	1.52
6	f	152	VAL	N-CA	-5.12	1.40	1.46
7	g	140	ASN	N-CA	-5.12	1.39	1.46
9	i	72	ARG	CA-CB	5.12	1.62	1.53
3	C	124	HIS	ND1-CE1	5.12	1.37	1.32
12	5	122	LEU	C-O	-5.12	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	W	65	PHE	CA-CB	5.12	1.61	1.53
22	V	31	SER	C-N	5.12	1.40	1.33
23	T	85	LEU	N-CA	-5.12	1.40	1.46
26	Z	949	ILE	N-CA	-5.12	1.40	1.46
27	N	720	ALA	N-CA	-5.12	1.39	1.46
3	c	172	GLN	CA-CB	5.12	1.61	1.53
4	D	93	SER	CA-C	-5.12	1.46	1.52
6	F	103	ALA	CA-C	-5.12	1.46	1.52
7	G	26	ALA	CA-CB	5.12	1.62	1.53
20	J	329	ARG	NE-CZ	5.12	1.38	1.33
10	3	190	LYS	C-N	5.12	1.40	1.34
3	c	7	SER	C-N	5.12	1.40	1.33
11	k	146	HIS	CA-CB	5.12	1.61	1.53
14	n	126	PHE	CA-C	-5.12	1.46	1.52
12	5	142	SER	CA-C	-5.12	1.45	1.52
19	M	211	GLY	C-N	5.12	1.39	1.33
27	N	433	THR	CA-C	-5.12	1.46	1.52
30	Q	234	THR	CA-C	5.12	1.59	1.52
3	c	126	GLY	C-O	-5.12	1.20	1.24
6	F	179	ILE	N-CA	5.12	1.53	1.46
2	b	146	SER	C-O	-5.12	1.17	1.23
6	f	38	ARG	NE-CZ	5.12	1.38	1.33
13	m	104	PRO	C-N	5.12	1.40	1.33
5	E	221	LYS	CA-CB	5.12	1.61	1.53
13	6	156	PHE	CA-C	-5.12	1.45	1.53
26	Z	515	SER	CA-C	-5.12	1.46	1.52
29	P	419	VAL	N-CA	-5.12	1.40	1.46
2	B	120	GLU	N-CA	-5.11	1.39	1.46
15	H	294	LEU	CA-CB	5.11	1.61	1.53
18	L	136	ASP	C-N	5.11	1.41	1.33
20	J	201	ALA	C-N	5.11	1.40	1.33
28	S	476	LEU	C-O	5.11	1.30	1.24
31	R	400	TYR	C-N	5.11	1.40	1.33
34	8	378	LYS	CA-C	-5.11	1.45	1.52
30	Q	93	THR	C-N	5.11	1.40	1.33
4	D	210	ILE	C-N	5.11	1.40	1.33
9	2	190	TYR	CA-C	-5.11	1.46	1.52
28	S	216	LYS	N-CA	-5.11	1.40	1.46
29	P	161	CYS	C-N	5.11	1.40	1.33
30	Q	366	ILE	C-N	5.11	1.40	1.33
12	5	63	CYS	CA-CB	5.11	1.61	1.53
14	7	70	LEU	CB-CG	5.11	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	138	ASP	CA-C	-5.11	1.46	1.52
7	g	208	PHE	C-N	-5.11	1.26	1.33
12	l	85	ASN	CA-CB	5.11	1.61	1.53
14	7	40	GLU	C-N	5.11	1.41	1.33
17	K	49	PHE	CA-C	-5.11	1.46	1.52
18	L	78	ARG	N-CA	-5.11	1.40	1.46
18	L	126	ARG	CZ-NH1	5.11	1.40	1.32
6	f	41	THR	CA-C	-5.11	1.46	1.52
10	j	1	SER	CA-CB	5.11	1.63	1.53
2	B	140	ASP	CA-C	-5.11	1.46	1.52
4	D	4	ARG	CZ-NH1	5.11	1.39	1.32
15	H	164	SER	CA-CB	5.11	1.60	1.53
27	N	585	ARG	CA-C	-5.11	1.46	1.52
7	G	135	GLY	N-CA	-5.10	1.39	1.45
12	5	59	LEU	N-CA	5.10	1.52	1.46
6	f	142	HIS	ND1-CE1	5.10	1.37	1.32
12	l	180	VAL	CA-CB	5.10	1.60	1.54
9	2	157	ASP	CA-C	5.10	1.59	1.52
11	4	15	LEU	CA-C	-5.10	1.46	1.52
12	5	198	TRP	CA-C	-5.10	1.46	1.52
13	6	185	ARG	CA-C	-5.10	1.46	1.52
15	H	252	PRO	CA-C	-5.10	1.46	1.52
22	V	267	LYS	N-CA	-5.10	1.39	1.46
12	l	66	HIS	CA-C	-5.10	1.46	1.52
12	l	112	ILE	C-O	5.10	1.29	1.24
1	a	154	TYR	CA-C	-5.10	1.46	1.52
7	g	43	VAL	CA-C	-5.10	1.46	1.52
11	k	3	ILE	CA-C	-5.10	1.45	1.53
11	4	43	LEU	C-O	-5.10	1.17	1.23
26	Z	931	GLN	N-CA	-5.10	1.39	1.46
27	N	499	HIS	ND1-CE1	5.10	1.37	1.32
33	O	88	ASP	N-CA	-5.10	1.39	1.46
34	8	326	LYS	N-CA	-5.10	1.39	1.46
10	j	143	ASP	N-CA	-5.10	1.40	1.46
10	j	190	LYS	CA-CB	5.10	1.61	1.53
14	n	188	ASP	C-O	-5.10	1.18	1.23
9	2	91	GLN	N-CA	-5.10	1.39	1.46
19	M	213	ARG	NE-CZ	5.10	1.38	1.33
19	M	413	GLU	C-N	5.10	1.40	1.33
27	N	467	LYS	N-CA	-5.10	1.40	1.46
30	Q	18	LYS	CA-CB	5.10	1.62	1.53
31	R	195	ASN	N-CA	5.10	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	8	346	THR	C-O	-5.10	1.17	1.24
14	n	190	ARG	CD-NE	5.10	1.53	1.46
1	A	154	TYR	CA-C	-5.10	1.46	1.52
27	N	406	TYR	C-N	5.10	1.40	1.33
7	g	138	ASP	C-N	5.09	1.40	1.33
3	C	44	VAL	CA-CB	-5.09	1.48	1.54
25	Y	41	ASP	CA-C	-5.09	1.46	1.52
4	d	180	LYS	C-O	-5.09	1.17	1.24
4	D	4	ARG	CA-C	-5.09	1.45	1.52
26	Z	540	GLY	N-CA	-5.09	1.38	1.45
4	D	197	LEU	C-N	5.09	1.40	1.34
8	1	15	GLY	CA-C	-5.09	1.47	1.51
30	Q	432	VAL	N-CA	-5.09	1.39	1.46
3	c	136	TYR	N-CA	-5.09	1.39	1.46
7	g	148	GLU	CA-C	-5.09	1.47	1.53
13	6	91	ARG	CA-C	-5.09	1.46	1.52
15	H	357	ARG	CD-NE	5.09	1.53	1.46
17	K	45	SER	C-N	5.09	1.41	1.34
2	B	72	GLY	N-CA	5.09	1.49	1.44
27	N	283	ASP	C-N	5.09	1.39	1.34
28	S	431	VAL	N-CA	-5.09	1.39	1.46
7	g	209	GLU	C-N	5.09	1.40	1.33
8	1	125	ALA	C-N	5.09	1.40	1.33
17	K	259	ARG	N-CA	-5.09	1.40	1.46
17	K	262	ARG	CZ-NH1	5.09	1.39	1.32
22	V	78	VAL	N-CA	-5.09	1.39	1.46
10	j	102	TYR	CA-C	5.08	1.59	1.52
26	Z	926	ASN	CA-C	-5.08	1.46	1.52
2	b	185	LEU	N-CA	-5.08	1.40	1.46
8	h	96	GLY	C-N	5.08	1.40	1.33
9	i	194	ASN	N-CA	-5.08	1.39	1.46
4	D	42	LEU	CA-CB	5.08	1.61	1.53
16	I	346	ARG	CZ-NH2	5.08	1.40	1.33
26	Z	482	ASP	N-CA	-5.08	1.39	1.46
29	P	294	GLU	N-CA	-5.08	1.39	1.46
1	a	136	SER	C-N	5.08	1.41	1.33
3	c	170	ALA	C-N	5.08	1.40	1.33
7	g	87	ARG	C-O	-5.08	1.18	1.24
7	g	87	ARG	NE-CZ	5.08	1.38	1.33
6	F	100	ARG	CZ-NH2	5.08	1.40	1.33
13	6	192	THR	CA-C	-5.08	1.46	1.52
19	M	85	VAL	C-N	5.08	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	45	VAL	CA-C	5.08	1.58	1.52
24	X	77	PRO	N-CA	-5.08	1.41	1.47
27	N	890	PHE	C-N	5.08	1.39	1.33
29	P	246	GLN	C-N	5.08	1.40	1.33
2	b	25	LEU	CA-C	-5.08	1.46	1.52
13	m	12	ILE	N-CA	-5.08	1.40	1.46
4	D	45	GLU	N-CA	-5.08	1.39	1.46
5	E	220	PHE	CA-C	-5.08	1.46	1.52
18	L	132	ARG	CZ-NH1	5.08	1.39	1.32
26	Z	320	SER	CA-C	-5.08	1.46	1.52
3	c	81	ALA	N-CA	-5.08	1.40	1.46
9	i	120	ASP	C-N	5.08	1.41	1.33
13	m	213	ARG	NE-CZ	5.08	1.38	1.33
14	n	65	ARG	CA-CB	5.08	1.61	1.53
10	3	65	MET	N-CA	-5.08	1.40	1.46
13	6	178	GLU	C-N	5.08	1.40	1.33
16	I	152	LYS	N-CA	-5.08	1.40	1.46
27	N	548	ARG	CZ-NH2	5.08	1.40	1.33
31	R	335	ARG	NE-CZ	5.08	1.38	1.33
33	O	176	SER	C-N	5.08	1.40	1.33
13	m	25	GLY	CA-C	-5.08	1.44	1.51
1	A	213	ASP	CA-CB	5.08	1.61	1.53
4	D	14	HIS	N-CA	-5.08	1.40	1.46
18	L	245	PHE	CA-C	-5.08	1.46	1.52
30	Q	301	ALA	C-N	5.08	1.40	1.33
12	l	108	GLU	CA-C	-5.08	1.45	1.52
4	D	125	ARG	CD-NE	5.08	1.53	1.46
14	7	73	GLU	CA-CB	5.08	1.61	1.53
16	I	322	VAL	CA-C	-5.08	1.46	1.52
30	Q	424	ASP	C-N	5.08	1.40	1.33
3	c	213	ALA	C-N	5.07	1.40	1.33
7	g	7	SER	CA-CB	5.07	1.64	1.54
11	4	36	ARG	CA-C	-5.07	1.46	1.52
11	4	43	LEU	CA-C	-5.07	1.46	1.52
13	6	186	ASP	N-CA	-5.07	1.40	1.46
16	I	160	LEU	C-N	5.07	1.39	1.33
21	W	179	ARG	CZ-NH2	5.07	1.40	1.33
23	T	225	ASN	CA-CB	5.07	1.60	1.53
30	Q	289	GLU	CA-C	-5.07	1.46	1.52
31	R	289	ILE	C-N	5.07	1.40	1.33
32	U	176	ARG	C-N	5.07	1.40	1.33
34	8	321	ARG	NE-CZ	5.07	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	368	PRO	N-CA	-5.07	1.41	1.47
17	K	241	GLU	N-CA	-5.07	1.40	1.46
18	L	75	LYS	CA-C	-5.07	1.46	1.52
30	Q	50	ARG	NE-CZ	5.07	1.38	1.33
2	B	138	GLY	C-O	-5.07	1.18	1.23
13	6	212	VAL	N-CA	-5.07	1.40	1.46
20	J	54	LYS	N-CA	-5.07	1.40	1.46
29	P	276	LEU	CA-C	-5.07	1.46	1.52
7	g	201	GLU	C-N	5.07	1.40	1.33
14	n	193	ARG	CZ-NH2	5.07	1.40	1.33
15	H	169	GLU	C-N	5.07	1.40	1.33
9	i	68	LEU	N-CA	-5.07	1.40	1.46
4	D	180	LYS	CA-C	-5.07	1.46	1.52
6	F	38	ARG	CD-NE	5.07	1.53	1.46
7	G	202	ASP	C-N	5.07	1.40	1.33
30	Q	186	HIS	ND1-CE1	5.07	1.37	1.32
30	Q	190	ASN	CA-C	-5.07	1.46	1.52
2	B	160	LYS	N-CA	-5.07	1.40	1.46
2	B	234	ARG	C-N	-5.07	1.26	1.33
14	7	78	ASN	CA-CB	5.07	1.61	1.53
17	K	408	GLU	CA-CB	5.07	1.61	1.53
20	J	215	GLY	C-N	5.07	1.40	1.33
29	P	118	VAL	CA-C	-5.07	1.46	1.52
13	m	95	HIS	CB-CG	5.06	1.57	1.50
5	E	96	ASP	CA-CB	5.06	1.60	1.53
22	V	304	ALA	N-CA	-5.06	1.40	1.46
12	l	15	ALA	C-O	-5.06	1.18	1.24
13	m	155	ASN	CA-CB	5.06	1.61	1.53
4	D	163	GLY	C-N	5.06	1.40	1.33
13	6	38	ARG	CA-C	-5.06	1.46	1.52
22	V	297	THR	N-CA	-5.06	1.40	1.46
27	N	546	LEU	N-CA	-5.06	1.40	1.46
8	1	86	CYS	CA-C	-5.06	1.46	1.52
12	5	59	LEU	CB-CG	5.06	1.63	1.53
2	B	91	LYS	C-O	-5.06	1.18	1.24
5	E	133	ALA	C-N	5.06	1.40	1.33
13	6	46	CYS	C-N	5.06	1.40	1.33
15	H	306	ILE	CA-C	-5.06	1.46	1.52
13	m	167	LYS	C-N	5.06	1.40	1.33
8	1	53	GLN	CA-C	-5.06	1.46	1.52
21	W	74	ALA	CA-C	-5.06	1.46	1.52
26	Z	448	LYS	N-CA	-5.06	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	95	ARG	NE-CZ	5.06	1.38	1.33
10	j	200	LYS	CA-C	-5.06	1.46	1.52
5	E	78	ARG	CD-NE	5.06	1.53	1.46
11	4	130	TYR	N-CA	-5.06	1.39	1.46
24	X	45	PHE	N-CA	5.06	1.52	1.46
34	8	208	GLN	CA-C	-5.06	1.46	1.52
7	g	229	GLY	N-CA	-5.05	1.38	1.45
1	A	146	TYR	C-N	5.05	1.40	1.33
9	2	142	TRP	NE1-CE2	5.05	1.43	1.37
26	Z	409	LYS	C-N	5.05	1.40	1.33
27	N	698	GLY	CA-C	-5.05	1.46	1.52
14	n	51	VAL	C-O	-5.05	1.18	1.24
16	I	145	CYS	C-O	-5.05	1.17	1.23
28	S	126	LYS	CA-C	-5.05	1.46	1.52
33	O	198	THR	N-CA	-5.05	1.39	1.46
5	e	94	TYR	CA-C	-5.05	1.46	1.52
9	i	121	VAL	CA-CB	-5.05	1.47	1.54
13	m	126	ASP	CG-OD2	5.05	1.34	1.25
28	S	85	SER	C-N	-5.05	1.27	1.33
30	Q	100	LEU	N-CA	-5.05	1.40	1.46
33	O	189	TYR	CA-C	-5.05	1.46	1.52
14	n	22	ILE	N-CA	-5.05	1.40	1.46
14	n	128	ARG	CZ-NH1	5.05	1.39	1.32
5	E	38	VAL	CA-C	-5.05	1.46	1.52
10	3	53	THR	CA-C	-5.05	1.46	1.53
16	I	64	ARG	CZ-NH1	5.05	1.39	1.32
17	K	131	LEU	N-CA	-5.05	1.40	1.46
27	N	497	ALA	C-N	5.05	1.40	1.33
28	S	253	PHE	CA-C	-5.05	1.46	1.52
30	Q	428	GLU	C-N	5.05	1.40	1.33
33	O	249	ASP	CA-C	-5.05	1.48	1.53
7	g	47	GLU	N-CA	-5.05	1.40	1.46
7	g	191	GLN	C-N	5.05	1.40	1.33
9	i	129	SER	C-N	5.05	1.40	1.33
2	B	148	TYR	CA-C	-5.05	1.46	1.52
16	I	263	LEU	C-N	5.05	1.40	1.33
7	g	32	THR	CA-C	-5.04	1.46	1.52
7	g	154	TRP	NE1-CE2	-5.04	1.31	1.37
7	g	166	GLN	N-CA	-5.04	1.40	1.46
12	l	133	GLN	CA-C	-5.04	1.45	1.52
5	E	58	LYS	C-N	5.04	1.39	1.33
16	I	422	ARG	CZ-NH2	5.04	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Q	201	ALA	C-O	-5.04	1.18	1.24
33	O	242	ILE	N-CA	-5.04	1.40	1.46
6	f	40	ASN	N-CA	-5.04	1.40	1.46
5	E	83	HIS	CA-CB	5.04	1.61	1.53
19	M	45	ARG	CA-C	-5.04	1.46	1.52
20	J	107	LEU	N-CA	-5.04	1.39	1.45
22	V	66	VAL	N-CA	-5.04	1.40	1.46
26	Z	151	HIS	ND1-CE1	5.04	1.37	1.32
31	R	148	ASP	CA-CB	5.04	1.61	1.53
33	O	187	SER	CA-CB	5.04	1.61	1.53
1	a	75	ASN	CA-C	-5.04	1.46	1.52
5	e	118	GLY	CA-C	-5.04	1.44	1.51
1	A	44	VAL	CA-C	-5.04	1.46	1.52
1	A	92	ALA	CA-C	-5.04	1.46	1.52
9	2	82	MET	CA-C	-5.04	1.46	1.52
11	4	34	LYS	CA-C	-5.04	1.47	1.53
15	H	307	PHE	CA-CB	5.04	1.60	1.53
15	H	375	VAL	N-CA	-5.04	1.40	1.46
30	Q	107	VAL	C-O	-5.04	1.18	1.24
34	8	184	LEU	CA-C	-5.04	1.46	1.52
12	l	100	MET	N-CA	-5.04	1.40	1.46
12	l	136	ALA	N-CA	5.04	1.52	1.46
14	7	193	ARG	N-CA	-5.04	1.40	1.46
5	e	150	ALA	C-N	5.04	1.40	1.33
14	n	231	GLN	CA-C	5.04	1.59	1.52
1	A	37	ARG	NE-CZ	5.04	1.38	1.33
2	B	12	PHE	CA-C	5.04	1.59	1.52
5	E	79	SER	N-CA	-5.04	1.40	1.46
9	2	86	HIS	ND1-CE1	5.04	1.37	1.32
21	W	16	SER	CA-C	-5.04	1.45	1.52
26	Z	889	VAL	N-CA	-5.04	1.39	1.46
29	P	258	LYS	N-CA	5.04	1.53	1.46
30	Q	135	HIS	N-CA	-5.04	1.39	1.46
2	b	150	VAL	C-O	-5.04	1.18	1.24
17	K	84	GLU	C-N	5.04	1.40	1.33
27	N	575	ALA	C-O	-5.04	1.18	1.24
34	8	148	ASN	CA-C	-5.04	1.46	1.52
34	8	453	ARG	NE-CZ	5.04	1.38	1.33
14	n	104	ARG	NE-CZ	5.04	1.38	1.33
26	Z	854	LEU	CB-CG	5.04	1.63	1.53
33	O	332	ILE	N-CA	-5.04	1.40	1.46
14	n	177	ILE	CA-CB	-5.03	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	10	GLU	N-CA	-5.03	1.40	1.46
5	E	40	LEU	C-N	5.03	1.39	1.33
27	N	114	SER	C-N	5.03	1.40	1.33
29	P	56	LYS	CA-CB	5.03	1.61	1.53
6	f	163	ARG	CD-NE	5.03	1.53	1.46
3	C	82	ASP	CA-C	-5.03	1.46	1.52
27	N	777	ALA	CA-C	-5.03	1.46	1.52
1	A	24	LYS	CA-CB	5.03	1.61	1.53
1	A	138	ASP	CA-C	-5.03	1.46	1.53
2	B	174	PHE	C-N	5.03	1.40	1.33
6	F	76	LEU	N-CA	-5.03	1.40	1.46
12	5	123	LYS	CA-CB	5.03	1.61	1.53
18	L	311	GLN	CA-C	-5.03	1.46	1.52
7	g	14	ASP	CA-CB	5.03	1.61	1.53
14	7	138	SER	CA-C	-5.03	1.46	1.52
24	X	124	LYS	C-N	5.03	1.40	1.33
26	Z	283	ALA	CA-C	-5.03	1.46	1.52
34	8	487	ASP	CA-C	5.03	1.58	1.52
5	e	64	ARG	N-CA	-5.03	1.39	1.46
11	k	171	ARG	CZ-NH2	5.03	1.40	1.33
18	L	194	ARG	CA-C	-5.03	1.45	1.52
26	Z	392	LEU	C-N	5.03	1.41	1.33
27	N	554	THR	C-O	-5.03	1.18	1.24
29	P	103	TYR	C-O	-5.03	1.17	1.24
9	i	164	TRP	C-O	-5.02	1.18	1.24
14	n	100	MET	CA-CB	5.02	1.61	1.53
13	6	196	ILE	CA-C	-5.02	1.45	1.52
19	M	41	ILE	C-O	-5.02	1.18	1.24
20	J	173	LEU	N-CA	5.02	1.52	1.46
29	P	103	TYR	C-N	5.02	1.40	1.33
29	P	242	GLN	CA-C	-5.02	1.46	1.52
30	Q	252	HIS	N-CA	-5.02	1.40	1.46
2	b	29	LYS	CA-C	-5.02	1.46	1.52
2	b	160	LYS	C-N	5.02	1.40	1.33
3	C	88	ASN	CA-CB	-5.02	1.45	1.53
9	2	137	VAL	CA-C	-5.02	1.46	1.52
31	R	291	SER	CA-C	-5.02	1.46	1.52
22	V	51	GLY	N-CA	-5.02	1.39	1.45
34	8	337	PHE	C-N	5.02	1.40	1.33
6	f	9	THR	C-O	-5.02	1.18	1.24
12	l	63	CYS	C-N	5.02	1.40	1.33
5	E	204	LEU	C-N	5.02	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	M	124	ARG	CD-NE	5.02	1.53	1.46
30	Q	1	MET	C-N	5.02	1.40	1.33
1	a	186	ASN	CA-C	-5.02	1.45	1.52
9	i	44	ALA	C-N	-5.02	1.27	1.33
3	C	91	ARG	CZ-NH2	5.02	1.40	1.33
6	F	156	TYR	CA-CB	-5.02	1.45	1.53
19	M	166	ARG	CZ-NH2	5.02	1.40	1.33
26	Z	519	PRO	C-N	5.02	1.39	1.33
26	Z	809	MET	N-CA	5.02	1.52	1.46
33	O	369	ARG	CZ-NH2	5.02	1.40	1.33
8	h	39	ASP	N-CA	-5.02	1.40	1.46
9	i	118	SER	CA-C	-5.02	1.46	1.52
5	E	139	HIS	ND1-CE1	5.02	1.37	1.32
7	G	159	ALA	C-O	-5.02	1.18	1.23
29	P	169	GLY	C-N	5.02	1.40	1.33
1	a	240	ALA	N-CA	-5.01	1.40	1.46
2	b	117	ILE	CA-CB	-5.01	1.48	1.54
12	l	75	SER	CA-C	-5.01	1.46	1.53
13	m	76	HIS	ND1-CE1	5.01	1.37	1.32
13	6	41	PRO	C-O	5.01	1.29	1.23
19	M	385	GLU	CA-CB	5.01	1.61	1.53
21	W	119	SER	CA-CB	5.01	1.61	1.53
27	N	818	LYS	C-N	5.01	1.40	1.33
28	S	289	ALA	CA-CB	5.01	1.61	1.53
10	j	173	ALA	N-CA	-5.01	1.40	1.46
14	n	29	SER	N-CA	-5.01	1.40	1.46
4	D	213	VAL	C-N	5.01	1.39	1.32
7	G	239	ALA	C-N	5.01	1.40	1.33
19	M	164	ASP	CA-CB	5.01	1.60	1.53
19	M	374	ILE	CA-C	-5.01	1.46	1.52
27	N	109	TYR	C-N	5.01	1.40	1.33
31	R	158	LEU	CA-CB	5.01	1.61	1.53
31	R	392	ARG	CZ-NH1	5.01	1.39	1.32
2	b	130	PHE	CA-C	-5.01	1.46	1.52
2	b	222	LEU	CA-CB	5.01	1.61	1.53
6	F	100	ARG	CA-C	-5.01	1.46	1.52
6	F	171	LEU	C-N	5.01	1.40	1.33
11	4	29	LYS	CA-C	-5.01	1.46	1.52
16	I	106	ILE	CA-C	-5.01	1.47	1.52
16	I	191	ILE	CA-C	-5.01	1.45	1.52
18	L	104	LEU	CA-C	-5.01	1.46	1.52
20	J	55	VAL	CA-C	5.01	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	W	2	VAL	CA-CB	-5.01	1.49	1.54
28	S	59	ASP	CA-C	-5.01	1.46	1.52
34	8	437	THR	CA-C	-5.01	1.46	1.52
9	i	59	ILE	C-O	-5.01	1.18	1.24
29	P	285	GLN	C-N	5.01	1.40	1.33
5	E	145	TYR	CA-C	5.01	1.59	1.52
8	l	156	LYS	N-CA	-5.01	1.40	1.46
19	M	255	TYR	CA-CB	5.01	1.61	1.53
19	M	383	THR	N-CA	-5.01	1.39	1.46
9	i	188	ARG	NE-CZ	5.00	1.38	1.33
13	m	149	PHE	CA-CB	5.00	1.61	1.53
9	i	36	ARG	CZ-NH2	5.00	1.40	1.33
9	i	82	MET	N-CA	-5.00	1.40	1.46
11	k	180	ILE	CA-C	-5.00	1.46	1.52
5	E	136	ILE	CA-C	-5.00	1.46	1.52
19	M	299	ARG	CD-NE	5.00	1.53	1.46
31	R	281	SER	CA-CB	5.00	1.60	1.53
5	e	191	LEU	N-CA	-5.00	1.40	1.46
8	h	62	HIS	CD2-NE2	5.00	1.43	1.37
11	k	146	HIS	CA-C	-5.00	1.46	1.52
11	k	160	LEU	C-O	-5.00	1.17	1.24
12	l	24	ASN	C-O	5.00	1.30	1.24
1	A	74	VAL	N-CA	-5.00	1.40	1.46
27	N	452	LEU	C-N	5.00	1.40	1.34
28	S	280	ASN	N-CA	-5.00	1.40	1.46
33	O	310	PHE	CA-C	-5.00	1.46	1.52

All (6142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	86	HIS	CB-CA-C	-25.80	59.08	110.42
29	P	86	HIS	N-CA-CB	23.36	149.97	110.49
27	N	861	TYR	N-CA-CB	-18.62	78.83	111.42
30	Q	123	GLU	N-CA-C	16.80	129.59	111.28
30	Q	123	GLU	CA-C-N	16.60	143.12	120.38
30	Q	123	GLU	C-N-CA	16.60	143.12	120.38
22	V	188	LEU	N-CA-CB	12.85	129.35	109.82
1	a	216	VAL	CA-C-N	12.82	131.69	122.33
1	a	216	VAL	C-N-CA	12.82	131.69	122.33
26	Z	253	VAL	O-C-N	-12.70	111.06	120.07
30	Q	67	THR	CA-C-N	12.19	143.64	121.70
30	Q	67	THR	C-N-CA	12.19	143.64	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	4	25	ILE	N-CA-C	-11.94	101.52	113.10
9	2	200	GLN	OE1-CD-NE2	11.68	134.28	122.60
31	R	102	LEU	CA-C-N	11.63	136.32	120.38
31	R	102	LEU	C-N-CA	11.63	136.32	120.38
26	Z	859	LYS	CA-C-N	11.54	133.02	120.44
26	Z	859	LYS	C-N-CA	11.54	133.02	120.44
31	R	110	ILE	O-C-N	-11.54	108.14	122.57
12	5	37	ILE	N-CA-C	-11.47	99.75	110.53
31	R	70	TYR	CA-CB-CG	11.47	134.54	113.90
28	S	126	LYS	N-CA-CB	11.46	129.86	110.49
31	R	102	LEU	N-CA-CB	11.44	129.83	110.49
26	Z	142	ASP	CA-CB-CG	-11.42	101.18	112.60
7	g	187	GLU	O-C-N	11.33	134.13	122.12
31	R	110	ILE	N-CA-CB	11.30	129.88	111.23
12	5	181	THR	CA-C-N	11.25	135.79	120.38
12	5	181	THR	C-N-CA	11.25	135.79	120.38
29	P	277	GLN	CA-C-N	11.21	136.37	120.79
29	P	277	GLN	C-N-CA	11.21	136.37	120.79
30	Q	123	GLU	CA-C-O	-11.15	108.73	120.55
13	m	44	PHE	CA-CB-CG	-10.87	102.93	113.80
29	P	18	LYS	N-CA-C	-10.87	100.15	113.41
7	g	65	VAL	N-CA-CB	10.87	122.57	110.72
31	R	100	ASN	CA-CB-CG	-10.87	101.73	112.60
34	8	290	LEU	N-CA-C	-10.80	99.84	113.23
26	Z	252	CYS	CA-C-N	10.79	127.03	120.24
26	Z	252	CYS	C-N-CA	10.79	127.03	120.24
31	R	109	LYS	CA-C-O	-10.78	109.50	120.82
3	C	151	ASN	CA-CB-CG	-10.74	101.86	112.60
27	N	99	GLU	N-CA-C	-10.69	98.98	113.30
27	N	576	VAL	CB-CA-C	-10.68	97.94	112.24
3	C	134	PHE	CA-CB-CG	-10.66	103.14	113.80
30	Q	308	ASN	CA-CB-CG	-10.65	101.95	112.60
31	R	391	ASN	CA-CB-CG	-10.64	101.96	112.60
8	1	133	PHE	CA-CB-CG	-10.59	103.21	113.80
30	Q	355	GLU	N-CA-CB	10.54	128.30	110.49
28	S	439	GLU	N-CA-C	-10.52	99.98	112.92
24	X	53	THR	N-CA-C	-10.50	102.65	114.62
28	S	170	TYR	CA-CB-CG	10.49	132.79	113.90
12	l	139	VAL	CB-CA-C	-10.45	97.80	112.22
30	Q	41	ALA	N-CA-C	-10.45	102.71	114.62
12	l	207	PHE	CA-CB-CG	-10.40	103.40	113.80
27	N	237	LEU	CA-C-N	10.39	133.94	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	237	LEU	C-N-CA	10.39	133.94	120.44
24	X	87	PHE	CA-CB-CG	-10.37	103.43	113.80
6	f	98	PHE	CA-CB-CG	-10.28	103.52	113.80
8	h	30	VAL	N-CA-C	-10.28	100.99	111.88
31	R	376	GLN	N-CA-C	-10.27	102.91	114.62
23	T	50	ILE	N-CA-C	-10.26	100.89	110.53
10	3	156	ASN	CA-CB-CG	-10.24	102.36	112.60
11	k	4	ILE	N-CA-CB	10.23	125.73	111.82
1	A	77	PRO	CA-C-N	10.22	126.68	120.24
1	A	77	PRO	C-N-CA	10.22	126.68	120.24
18	L	281	ASP	CA-CB-CG	-10.20	102.40	112.60
28	S	127	THR	N-CA-C	-10.19	101.35	113.88
14	7	111	TRP	CB-CG-CD2	-10.16	112.57	126.80
4	D	207	ASN	CA-CB-CG	-10.15	102.45	112.60
7	g	150	SER	N-CA-C	-10.15	100.22	111.28
1	A	196	PHE	CA-CB-CG	-10.14	103.66	113.80
34	8	267	GLY	N-CA-C	-10.13	99.91	112.68
33	O	56	PRO	CA-C-N	10.13	134.25	120.38
33	O	56	PRO	C-N-CA	10.13	134.25	120.38
1	A	89	LYS	N-CA-C	-10.08	100.25	111.14
27	N	56	SER	N-CA-C	-10.07	100.48	113.17
30	Q	252	HIS	CA-CB-CG	10.04	123.84	113.80
24	X	79	LYS	N-CA-C	-9.99	102.16	114.75
6	F	201	ARG	N-CA-C	-9.97	101.30	112.57
10	3	31	GLN	CA-C-N	9.97	133.64	120.28
10	3	31	GLN	C-N-CA	9.97	133.64	120.28
13	m	62	ASP	CA-CB-CG	-9.95	102.66	112.60
28	S	126	LYS	CA-CB-CG	-9.93	94.25	114.10
8	1	113	ILE	N-CA-C	-9.92	98.33	108.15
8	1	122	LEU	O-C-N	-9.89	114.85	121.88
31	R	70	TYR	CA-C-O	-9.87	104.02	120.80
26	Z	405	ASN	CA-CB-CG	-9.86	102.75	112.60
13	m	164	THR	N-CA-C	-9.85	99.12	112.03
13	m	140	GLY	O-C-N	9.85	131.05	122.88
27	N	91	ILE	CA-C-N	9.85	134.46	120.28
27	N	91	ILE	C-N-CA	9.85	134.46	120.28
34	8	219	HIS	ND1-CE1-NE2	9.84	118.24	108.40
5	E	1	ASP	CA-CB-CG	-9.79	102.81	112.60
20	J	311	ASP	CA-CB-CG	9.78	122.38	112.60
32	U	101	ALA	N-CA-C	-9.77	101.36	113.38
14	7	111	TRP	CB-CG-CD1	9.77	141.55	126.90
3	c	195	THR	CA-C-N	9.73	133.31	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	195	THR	C-N-CA	9.73	133.31	120.28
27	N	77	SER	N-CA-C	-9.72	100.76	111.36
31	R	98	LEU	CA-C-N	9.67	133.59	120.44
31	R	98	LEU	C-N-CA	9.67	133.59	120.44
15	H	357	ARG	CA-C-N	9.65	129.31	119.56
15	H	357	ARG	C-N-CA	9.65	129.31	119.56
20	J	234	PHE	CA-C-N	9.64	132.70	120.56
20	J	234	PHE	C-N-CA	9.64	132.70	120.56
6	F	107	ALA	CA-C-N	9.63	130.67	119.98
6	F	107	ALA	C-N-CA	9.63	130.67	119.98
2	B	214	ILE	N-CA-C	-9.62	94.65	108.11
6	f	80	ALA	N-CA-C	9.60	121.74	111.28
2	B	105	PRO	CA-C-O	-9.53	113.20	120.73
13	m	102	PHE	CA-CB-CG	-9.53	104.27	113.80
28	S	249	SER	CA-C-N	9.52	133.04	120.28
28	S	249	SER	C-N-CA	9.52	133.04	120.28
33	O	90	LYS	N-CA-C	-9.52	100.04	112.41
15	H	283	TYR	N-CA-C	-9.50	99.58	112.03
5	e	117	GLU	N-CA-C	-9.46	101.74	113.28
1	A	176	HIS	CE1-NE2-CD2	-9.46	99.54	109.00
26	Z	253	VAL	CB-CA-C	-9.43	104.35	114.35
20	J	248	ASP	CA-CB-CG	-9.40	103.20	112.60
33	O	366	MET	CA-C-N	9.40	132.87	120.28
33	O	366	MET	C-N-CA	9.40	132.87	120.28
11	4	156	GLU	CA-C-N	9.39	130.41	119.98
11	4	156	GLU	C-N-CA	9.39	130.41	119.98
13	m	58	ALA	CA-C-O	-9.38	110.61	120.55
30	Q	123	GLU	N-CA-CB	-9.37	96.35	110.12
20	J	127	GLU	N-CA-C	-9.34	101.05	111.14
11	k	69	ILE	N-CA-CB	9.34	121.47	110.55
14	n	185	TYR	CA-C-N	9.27	133.45	120.29
14	n	185	TYR	C-N-CA	9.27	133.45	120.29
1	A	176	HIS	O-C-N	9.27	131.94	122.12
23	T	214	GLU	CA-C-N	9.25	132.67	120.28
23	T	214	GLU	C-N-CA	9.25	132.67	120.28
18	L	93	ASN	CA-CB-CG	9.23	121.83	112.60
5	E	14	PHE	CA-CB-CG	-9.21	104.59	113.80
34	8	466	ASP	CA-CB-CG	-9.21	103.39	112.60
5	E	4	VAL	N-CA-C	-9.20	104.97	113.71
1	A	222	ASP	CA-CB-CG	-9.20	103.40	112.60
19	M	349	PHE	CA-CB-CG	-9.20	104.60	113.80
4	d	106	TYR	O-C-N	9.20	131.54	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	625	THR	CA-C-N	9.17	128.78	119.24
26	Z	625	THR	C-N-CA	9.17	128.78	119.24
11	k	52	ASP	CA-CB-CG	-9.16	103.44	112.60
16	I	116	ASP	CA-CB-CG	-9.14	103.46	112.60
14	7	220	ASP	N-CA-C	-9.12	100.74	112.23
16	I	135	PHE	CA-CB-CG	-9.11	104.69	113.80
7	g	77	LEU	CA-C-N	9.08	127.59	120.33
7	g	77	LEU	C-N-CA	9.08	127.59	120.33
21	W	142	ILE	N-CA-C	-9.07	93.99	107.51
9	i	189	ASN	CA-CB-CG	9.03	121.63	112.60
15	H	443	PHE	CA-CB-CG	-9.03	104.77	113.80
26	Z	461	GLY	N-CA-C	-9.03	104.12	115.31
8	h	191	ASP	CA-CB-CG	-9.02	103.58	112.60
12	5	38	ASN	CA-C-N	9.00	131.09	119.84
12	5	38	ASN	C-N-CA	9.00	131.09	119.84
18	L	81	ILE	N-CA-C	-8.95	101.83	110.42
12	l	33	LYS	N-CA-C	-8.94	102.10	113.72
23	T	124	SER	CA-C-N	8.94	132.26	120.28
23	T	124	SER	C-N-CA	8.94	132.26	120.28
27	N	23	TYR	CA-C-N	8.94	132.98	120.29
27	N	23	TYR	C-N-CA	8.94	132.98	120.29
4	D	205	ALA	CA-C-O	-8.94	110.99	120.55
11	4	141	PHE	CA-CB-CG	-8.92	104.88	113.80
7	g	170	ALA	N-CA-CB	8.91	123.21	109.94
7	G	238	PHE	N-CA-C	-8.90	101.55	111.07
2	b	136	ILE	N-CA-CB	8.88	123.18	111.64
34	8	157	HIS	CG-CD2-NE2	8.88	116.08	107.20
21	W	190	ILE	N-CA-C	-8.85	105.30	113.71
26	Z	201	LEU	N-CA-C	-8.85	100.80	111.69
1	a	31	ILE	CB-CA-C	-8.84	99.50	110.99
28	S	72	GLU	CA-C-N	8.84	131.93	120.44
28	S	72	GLU	C-N-CA	8.84	131.93	120.44
11	k	135	TYR	CA-CB-CG	-8.83	98.00	113.90
12	5	147	ASP	CA-CB-CG	-8.83	103.77	112.60
5	E	48	SER	CA-C-O	-8.82	112.22	120.34
31	R	200	LYS	N-CA-C	-8.82	101.74	111.36
20	J	382	PHE	CA-CB-CG	-8.81	104.99	113.80
15	H	98	GLN	OE1-CD-NE2	8.80	131.41	122.60
13	m	76	HIS	CE1-NE2-CD2	-8.80	100.20	109.00
13	m	91	ARG	CA-C-O	8.79	129.86	120.55
3	C	62	THR	N-CA-C	-8.78	96.16	108.54
3	C	26	GLU	CA-C-N	8.78	132.04	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	26	GLU	C-N-CA	8.78	132.04	120.28
9	i	205	PHE	CA-CB-CG	-8.77	105.03	113.80
34	8	376	ARG	O-C-N	8.76	131.41	122.12
26	Z	199	ASP	CA-C-O	-8.74	111.28	120.55
30	Q	111	LEU	CA-C-N	8.73	132.92	120.79
30	Q	111	LEU	C-N-CA	8.73	132.92	120.79
33	O	286	PHE	N-CA-CB	8.73	122.67	110.01
7	G	70	ILE	CA-C-O	8.72	129.46	120.39
3	C	229	PHE	CA-CB-CG	-8.71	105.09	113.80
27	N	350	LYS	CA-C-O	-8.70	111.33	120.55
34	8	393	GLN	CA-C-N	8.70	131.94	120.28
34	8	393	GLN	C-N-CA	8.70	131.94	120.28
19	M	38	ASP	CA-CB-CG	-8.69	103.91	112.60
1	a	57	PRO	N-CA-C	-8.69	102.46	114.80
5	E	61	GLU	N-CA-C	-8.68	95.98	109.25
3	C	102	ASN	CA-CB-CG	-8.66	103.94	112.60
28	S	431	VAL	N-CA-C	-8.66	103.39	111.45
31	R	158	LEU	N-CA-CB	8.66	122.98	110.16
31	R	154	LEU	CA-C-N	8.66	129.52	120.00
31	R	154	LEU	C-N-CA	8.66	129.52	120.00
22	V	71	MET	CA-C-N	8.65	130.65	119.84
22	V	71	MET	C-N-CA	8.65	130.65	119.84
9	2	65	LEU	CA-C-O	-8.64	111.65	120.90
19	M	226	THR	N-CA-C	-8.64	102.28	113.17
33	O	286	PHE	CA-CB-CG	-8.63	105.17	113.80
10	j	143	ASP	CA-CB-CG	8.62	121.22	112.60
31	R	109	LYS	CB-CA-C	8.62	124.41	110.88
10	3	106	PRO	CA-C-O	-8.61	111.17	121.67
15	H	191	ILE	N-CA-C	-8.58	103.38	113.42
16	I	65	ILE	N-CA-C	-8.58	104.08	113.43
9	2	81	GLN	OE1-CD-NE2	8.57	131.17	122.60
26	Z	369	PHE	N-CA-C	-8.57	102.14	112.59
27	N	898	GLY	N-CA-C	-8.56	102.05	115.67
12	5	203	GLU	N-CA-C	8.56	120.69	111.36
15	H	257	THR	CA-C-N	8.55	131.56	120.44
15	H	257	THR	C-N-CA	8.55	131.56	120.44
6	f	189	ILE	O-C-N	8.54	130.63	121.83
19	M	372	ASP	CA-CB-CG	-8.53	104.07	112.60
23	T	75	PHE	CA-CB-CG	-8.53	105.27	113.80
28	S	163	VAL	N-CA-C	8.53	119.32	110.62
17	K	163	GLU	N-CA-C	-8.53	104.90	114.62
26	Z	826	ARG	CA-C-N	8.53	132.40	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	826	ARG	C-N-CA	8.53	132.40	120.29
2	b	10	THR	N-CA-C	-8.52	101.91	111.71
10	j	97	ARG	N-CA-CB	8.52	124.67	110.53
1	A	199	THR	CA-C-O	-8.52	111.88	120.82
7	G	83	HIS	CE1-NE2-CD2	-8.52	100.48	109.00
6	F	225	ASP	CA-CB-CG	-8.51	104.09	112.60
9	2	56	THR	O-C-N	8.50	131.13	122.12
17	K	63	LEU	N-CA-CB	8.50	122.73	110.16
28	S	26	ALA	CA-C-N	8.48	131.47	120.44
28	S	26	ALA	C-N-CA	8.48	131.47	120.44
14	7	5	ILE	O-C-N	-8.48	111.97	122.57
12	5	57	THR	N-CA-C	-8.48	101.26	111.69
32	U	80	CYS	O-C-N	8.48	134.16	122.46
34	8	176	PHE	CA-CB-CG	-8.48	105.32	113.80
25	Y	23	GLU	CA-C-N	8.47	132.45	120.42
25	Y	23	GLU	C-N-CA	8.47	132.45	120.42
27	N	598	ASP	N-CA-C	-8.47	94.45	108.34
32	U	130	VAL	N-CA-C	-8.47	102.57	110.53
27	N	71	ASN	CA-C-N	8.47	131.63	120.28
27	N	71	ASN	C-N-CA	8.47	131.63	120.28
15	H	106	ILE	N-CA-C	-8.46	95.40	107.75
30	Q	122	ILE	CA-C-O	-8.44	112.27	121.05
6	f	125	ARG	CA-C-N	8.44	128.38	120.03
6	f	125	ARG	C-N-CA	8.44	128.38	120.03
26	Z	45	LEU	CA-C-N	8.44	131.41	120.44
26	Z	45	LEU	C-N-CA	8.44	131.41	120.44
8	h	114	PRO	O-C-N	8.40	133.40	122.89
27	N	743	PHE	CA-C-N	8.40	129.45	120.12
27	N	743	PHE	C-N-CA	8.40	129.45	120.12
12	5	135	PHE	CA-CB-CG	-8.40	105.40	113.80
23	T	125	GLU	CA-C-O	8.40	129.46	120.55
14	n	110	LEU	N-CA-C	-8.39	95.66	108.67
17	K	66	ASP	CA-C-N	8.39	131.52	120.28
17	K	66	ASP	C-N-CA	8.39	131.52	120.28
26	Z	766	HIS	N-CA-C	8.37	120.18	111.14
7	G	161	THR	CA-CB-OG1	8.35	122.13	109.60
28	S	127	THR	N-CA-CB	8.35	121.69	110.59
16	I	384	LYS	N-CA-CB	8.35	122.24	109.97
31	R	70	TYR	CB-CG-CD1	8.35	133.32	120.80
32	U	242	PRO	N-CA-C	-8.35	103.77	114.03
1	a	224	PHE	CA-CB-CG	-8.34	105.46	113.80
8	h	62	HIS	CE1-NE2-CD2	-8.34	100.66	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	179	GLU	CA-C-N	8.34	132.26	120.42
13	m	179	GLU	C-N-CA	8.34	132.26	120.42
33	O	207	LEU	CA-C-N	8.34	132.13	120.29
33	O	207	LEU	C-N-CA	8.34	132.13	120.29
7	g	121	LEU	N-CA-C	-8.33	103.56	114.31
16	I	370	ASN	N-CA-C	-8.33	95.32	109.24
9	2	13	VAL	CA-C-O	8.33	129.92	120.76
4	D	105	GLU	N-CA-CB	-8.32	97.84	110.16
18	L	324	ILE	N-CA-C	-8.32	96.46	108.11
14	n	81	ALA	CA-C-N	8.32	131.77	120.54
14	n	81	ALA	C-N-CA	8.32	131.77	120.54
7	G	101	THR	O-C-N	-8.32	113.58	122.06
31	R	27	SER	N-CA-C	8.32	120.34	111.28
34	8	141	ASN	CA-CB-CG	-8.32	104.28	112.60
10	j	163	PHE	CA-CB-CG	-8.31	105.49	113.80
1	A	138	ASP	CA-CB-CG	-8.31	104.29	112.60
28	S	154	GLN	CA-C-N	8.31	131.42	120.28
28	S	154	GLN	C-N-CA	8.31	131.42	120.28
13	6	216	PHE	CA-CB-CG	-8.31	105.49	113.80
7	g	220	THR	CA-C-O	8.30	128.19	119.05
25	Y	37	ASP	N-CA-C	-8.30	102.31	111.36
27	N	861	TYR	CA-CB-CG	8.30	128.84	113.90
11	4	103	LEU	N-CA-C	-8.29	95.38	108.90
1	a	77	PRO	CA-C-N	8.28	125.46	120.24
1	a	77	PRO	C-N-CA	8.28	125.46	120.24
2	B	184	GLU	CA-C-N	8.28	132.05	120.29
2	B	184	GLU	C-N-CA	8.28	132.05	120.29
20	J	87	LYS	N-CA-C	-8.27	94.06	108.20
30	Q	20	TYR	CA-C-N	8.26	131.70	120.38
30	Q	20	TYR	C-N-CA	8.26	131.70	120.38
32	U	236	LEU	O-C-N	-8.26	115.03	121.47
14	n	5	ILE	O-C-N	8.26	128.13	121.85
14	n	35	ARG	NE-CZ-NH2	-8.26	111.77	119.20
3	c	142	ARG	NE-CZ-NH2	-8.25	111.77	119.20
11	k	109	LYS	N-CA-C	-8.24	103.22	113.28
29	P	127	GLU	O-C-N	8.24	130.56	122.07
3	c	138	GLY	O-C-N	8.24	131.22	123.56
33	O	186	ASN	CA-CB-CG	-8.24	104.36	112.60
26	Z	155	ARG	N-CA-C	8.23	120.25	111.28
7	g	202	ASP	N-CA-C	-8.22	102.80	112.92
14	n	203	ASN	CA-CB-CG	-8.22	104.38	112.60
34	8	121	ASN	OD1-CG-ND2	8.22	130.82	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	128	GLY	N-CA-C	-8.22	101.26	112.52
27	N	861	TYR	CB-CA-C	8.21	130.73	110.46
7	g	122	TYR	CA-C-O	8.20	129.34	120.32
18	L	190	ILE	O-C-N	8.21	129.95	121.91
8	1	84	GLU	N-CA-C	-8.20	102.42	111.36
19	M	387	ASN	CA-C-N	8.20	129.26	119.99
19	M	387	ASN	C-N-CA	8.20	129.26	119.99
3	c	181	ASP	CA-CB-CG	-8.20	104.40	112.60
14	7	9	THR	CA-C-N	8.20	133.52	121.31
14	7	9	THR	C-N-CA	8.20	133.52	121.31
31	R	291	SER	CA-C-N	8.20	131.26	120.28
31	R	291	SER	C-N-CA	8.20	131.26	120.28
28	S	440	ASP	CA-CB-CG	-8.18	104.42	112.60
1	a	66	ILE	N-CA-C	-8.17	102.89	110.82
23	T	88	TYR	N-CA-C	-8.17	102.33	111.07
10	j	77	GLU	N-CA-C	-8.16	103.11	113.23
20	J	51	LEU	N-CA-C	-8.16	102.47	111.36
14	n	97	ALA	CA-C-N	8.16	131.04	120.44
14	n	97	ALA	C-N-CA	8.16	131.04	120.44
14	7	134	GLY	CA-C-N	8.16	133.22	121.80
14	7	134	GLY	C-N-CA	8.16	133.22	121.80
8	h	37	VAL	N-CA-C	-8.15	105.54	113.53
20	J	85	LEU	N-CA-C	-8.15	95.93	109.46
10	3	161	ASP	CA-C-N	8.15	131.20	120.28
10	3	161	ASP	C-N-CA	8.15	131.20	120.28
18	L	273	HIS	CE1-NE2-CD2	-8.14	100.86	109.00
2	B	100	ILE	N-CA-C	-8.14	103.88	111.45
34	8	476	LYS	N-CA-C	-8.14	102.41	111.28
8	h	98	ILE	N-CA-C	-8.13	95.39	107.51
14	7	213	GLN	N-CA-CB	8.13	126.17	111.37
16	I	365	HIS	CG-CD2-NE2	8.13	115.33	107.20
23	T	161	TRP	CA-C-N	8.13	131.01	120.44
23	T	161	TRP	C-N-CA	8.13	131.01	120.44
34	8	341	VAL	CA-C-N	8.13	131.52	120.38
34	8	341	VAL	C-N-CA	8.13	131.52	120.38
30	Q	53	GLU	N-CA-C	8.12	120.86	111.11
27	N	696	LYS	N-CA-CB	8.12	122.05	110.12
3	c	147	LEU	CB-CA-C	8.12	124.39	109.70
19	M	398	ALA	CA-C-N	8.12	130.53	120.22
19	M	398	ALA	C-N-CA	8.12	130.53	120.22
20	J	283	GLU	N-CA-CB	8.11	121.83	110.07
19	M	149	ASN	CA-C-N	8.11	130.99	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	149	ASN	C-N-CA	8.11	130.99	120.44
18	L	193	LEU	N-CA-C	8.11	120.12	111.28
3	C	204	ALA	N-CA-C	-8.11	102.96	113.17
18	L	412	PRO	N-CA-CB	8.11	111.00	103.46
14	n	39	VAL	N-CA-CB	8.10	119.81	110.82
5	E	103	SER	CA-C-N	8.10	131.13	120.28
5	E	103	SER	C-N-CA	8.10	131.13	120.28
9	2	145	ASP	CA-CB-CG	-8.10	104.50	112.60
31	R	150	ALA	CA-C-O	-8.10	112.32	120.82
2	b	171	ALA	N-CA-C	8.09	119.73	111.07
26	Z	403	ASN	CA-CB-CG	-8.09	104.51	112.60
7	G	47	GLU	CB-CG-CD	-8.09	98.85	112.60
7	g	110	ASP	N-CA-C	-8.08	102.41	111.14
5	E	169	GLU	N-CA-CB	8.08	122.11	110.16
12	5	92	GLY	N-CA-C	-8.07	102.83	115.67
25	Y	66	ASP	N-CA-C	-8.07	103.22	113.72
2	b	245	ASP	CA-CB-CG	-8.07	104.53	112.60
8	h	49	ALA	CA-C-N	8.07	131.43	120.54
8	h	49	ALA	C-N-CA	8.07	131.43	120.54
6	F	98	PHE	CA-CB-CG	-8.07	105.73	113.80
32	U	70	HIS	CE1-NE2-CD2	-8.07	100.93	109.00
16	I	345	ASP	CA-CB-CG	-8.06	104.54	112.60
15	H	425	GLU	CA-C-O	-8.06	111.88	120.42
28	S	170	TYR	CA-C-N	-8.06	111.70	122.42
28	S	170	TYR	C-N-CA	-8.06	111.70	122.42
14	7	164	ASP	CA-CB-CG	-8.05	104.55	112.60
22	V	125	THR	CA-C-N	8.05	131.07	120.28
22	V	125	THR	C-N-CA	8.05	131.07	120.28
3	C	217	LYS	N-CA-C	-8.05	103.25	113.23
22	V	208	LYS	N-CA-C	-8.05	101.58	111.40
31	R	115	GLU	CA-C-N	8.05	131.27	120.65
31	R	115	GLU	C-N-CA	8.05	131.27	120.65
9	i	109	HIS	CB-CG-CD2	-8.05	120.74	131.20
11	4	83	PHE	CA-CB-CG	-8.04	105.76	113.80
26	Z	581	VAL	N-CA-C	-8.04	101.19	113.16
14	n	139	SER	O-C-N	8.03	127.58	121.88
34	8	361	ARG	N-CA-CB	8.03	121.92	110.12
21	W	58	ASN	CA-C-N	8.02	129.87	119.84
21	W	58	ASN	C-N-CA	8.02	129.87	119.84
26	Z	209	PRO	N-CA-CB	8.02	110.82	103.20
13	m	137	ARG	NE-CZ-NH2	8.01	126.41	119.20
7	g	14	ASP	N-CA-C	-8.01	102.96	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	46	LEU	CA-C-N	8.01	136.84	121.54
28	S	46	LEU	C-N-CA	8.01	136.84	121.54
1	a	52	ASP	N-CA-C	-8.00	100.93	111.24
33	O	290	LYS	O-C-N	8.00	130.60	122.12
30	Q	31	LEU	CA-C-N	8.00	131.33	120.54
30	Q	31	LEU	C-N-CA	8.00	131.33	120.54
27	N	659	ALA	CA-C-N	7.99	130.99	120.28
27	N	659	ALA	C-N-CA	7.99	130.99	120.28
28	S	55	ARG	CA-C-O	-7.99	112.43	120.82
9	i	179	GLU	CA-C-N	7.99	131.26	120.63
9	i	179	GLU	C-N-CA	7.99	131.26	120.63
26	Z	258	PRO	CA-C-O	-7.99	108.98	120.56
4	d	79	ASP	CA-C-N	7.98	132.04	120.38
4	d	79	ASP	C-N-CA	7.98	132.04	120.38
27	N	63	LEU	CA-C-N	7.98	131.40	120.46
27	N	63	LEU	C-N-CA	7.98	131.40	120.46
8	1	14	LEU	CA-C-N	7.98	127.75	121.61
8	1	14	LEU	C-N-CA	7.98	127.75	121.61
8	h	138	CYS	N-CA-CB	7.97	121.96	110.16
11	4	135	TYR	CA-C-N	7.97	130.96	120.28
11	4	135	TYR	C-N-CA	7.97	130.96	120.28
26	Z	478	VAL	N-CA-C	-7.97	102.67	110.72
4	D	41	VAL	CB-CA-C	-7.97	100.00	110.84
29	P	205	LYS	CA-C-N	7.97	130.96	120.28
29	P	205	LYS	C-N-CA	7.97	130.96	120.28
1	a	11	SER	CA-C-N	7.96	127.68	119.56
1	a	11	SER	C-N-CA	7.96	127.68	119.56
7	g	186	ARG	CA-C-N	7.96	130.95	120.28
7	g	186	ARG	C-N-CA	7.96	130.95	120.28
14	7	185	TYR	CA-C-O	-7.96	111.98	120.42
2	b	42	GLY	CA-C-N	7.95	135.05	122.33
2	b	42	GLY	C-N-CA	7.95	135.05	122.33
17	K	340	PHE	CA-CB-CG	-7.95	105.85	113.80
29	P	196	ALA	CA-C-O	-7.94	112.13	120.55
5	e	110	ASP	CA-C-N	7.94	131.56	120.29
5	e	110	ASP	C-N-CA	7.94	131.56	120.29
31	R	20	ARG	CA-C-N	7.94	126.68	120.33
31	R	20	ARG	C-N-CA	7.94	126.68	120.33
8	1	82	PHE	CA-C-O	-7.93	112.49	120.82
30	Q	414	GLU	CA-C-N	7.93	130.91	120.28
30	Q	414	GLU	C-N-CA	7.93	130.91	120.28
10	j	161	ASP	CA-C-N	7.92	130.90	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	161	ASP	C-N-CA	7.92	130.90	120.28
4	d	126	PRO	N-CA-CB	7.92	110.36	103.31
23	T	160	ALA	CA-C-N	7.92	130.89	120.28
23	T	160	ALA	C-N-CA	7.92	130.89	120.28
9	2	160	GLN	N-CA-CB	7.91	121.93	110.06
27	N	450	ILE	CA-C-N	7.91	128.70	120.00
27	N	450	ILE	C-N-CA	7.91	128.70	120.00
30	Q	287	THR	N-CA-C	7.90	119.97	111.36
3	c	74	VAL	CA-C-N	7.90	134.11	123.05
3	c	74	VAL	C-N-CA	7.90	134.11	123.05
28	S	67	GLU	CA-C-N	7.90	133.86	122.40
28	S	67	GLU	C-N-CA	7.90	133.86	122.40
31	R	70	TYR	CB-CG-CD2	-7.90	108.95	120.80
2	B	218	ASN	OD1-CG-ND2	7.89	130.49	122.60
21	W	9	VAL	CA-C-O	-7.88	111.43	120.65
26	Z	837	TYR	CA-C-N	7.88	130.84	120.28
26	Z	837	TYR	C-N-CA	7.88	130.84	120.28
34	8	159	GLN	OE1-CD-NE2	-7.88	114.72	122.60
7	g	108	PHE	CA-C-N	7.87	130.82	120.28
7	g	108	PHE	C-N-CA	7.87	130.82	120.28
33	O	134	ALA	CA-C-N	7.86	131.46	120.29
33	O	134	ALA	C-N-CA	7.86	131.46	120.29
2	b	199	SER	O-C-N	7.86	130.16	122.07
12	5	144	TYR	CA-C-O	7.85	129.22	120.43
23	T	84	GLN	CA-C-N	7.84	131.12	120.54
23	T	84	GLN	C-N-CA	7.84	131.12	120.54
28	S	110	LEU	N-CA-C	-7.83	101.51	113.89
31	R	70	TYR	CB-CA-C	7.83	124.97	110.10
12	l	25	TRP	CG-CD2-CE3	-7.82	126.08	133.90
11	k	100	VAL	O-C-N	7.82	131.51	123.07
11	k	96	ARG	NE-CZ-NH1	7.81	129.31	121.50
5	E	149	HIS	CA-C-O	7.81	128.60	120.40
16	I	138	LYS	CA-C-N	7.81	130.60	120.44
16	I	138	LYS	C-N-CA	7.81	130.60	120.44
31	R	124	ASP	CA-CB-CG	-7.81	104.79	112.60
11	k	133	HIS	CA-CB-CG	-7.81	105.99	113.80
22	V	264	GLU	CA-C-N	7.81	130.75	120.28
22	V	264	GLU	C-N-CA	7.81	130.75	120.28
32	U	223	HIS	CA-CB-CG	7.81	121.61	113.80
30	Q	311	LEU	CA-C-N	7.81	130.74	120.28
30	Q	311	LEU	C-N-CA	7.81	130.74	120.28
2	b	59	GLU	CA-C-N	7.80	130.58	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	59	GLU	C-N-CA	7.80	130.58	120.44
12	5	87	VAL	N-CA-C	7.80	118.60	110.72
1	A	50	VAL	N-CA-CB	7.80	119.39	111.36
20	J	187	LEU	N-CA-C	-7.80	96.52	109.07
27	N	280	GLN	CA-C-N	7.79	134.81	120.87
27	N	280	GLN	C-N-CA	7.79	134.81	120.87
14	7	59	ASP	CA-CB-CG	-7.79	104.81	112.60
19	M	358	ALA	N-CA-C	-7.79	102.87	111.36
10	j	168	GLN	N-CA-CB	7.78	121.30	110.01
19	M	53	HIS	CA-CB-CG	7.78	121.58	113.80
20	J	280	ASP	CA-CB-CG	-7.78	104.82	112.60
14	7	139	SER	CA-C-N	7.78	127.84	119.28
14	7	139	SER	C-N-CA	7.78	127.84	119.28
7	G	83	HIS	ND1-CE1-NE2	7.77	116.17	108.40
27	N	18	ASP	CA-C-N	7.77	130.69	120.28
27	N	18	ASP	C-N-CA	7.77	130.69	120.28
12	l	191	HIS	CE1-NE2-CD2	-7.77	101.23	109.00
33	O	53	LYS	CA-C-N	7.77	131.03	120.38
33	O	53	LYS	C-N-CA	7.77	131.03	120.38
18	L	258	GLU	CA-C-N	7.77	130.69	120.28
18	L	258	GLU	C-N-CA	7.77	130.69	120.28
27	N	689	LYS	N-CA-C	-7.77	102.86	112.88
7	g	17	ASN	CA-CB-CG	7.76	120.36	112.60
31	R	21	VAL	O-C-N	-7.76	115.45	120.42
1	A	196	PHE	N-CA-C	-7.76	102.82	111.28
8	h	108	GLY	O-C-N	-7.75	114.85	122.84
23	T	22	ALA	CA-C-N	7.75	130.67	120.28
23	T	22	ALA	C-N-CA	7.75	130.67	120.28
18	L	137	ARG	CA-C-N	7.75	131.29	120.29
18	L	137	ARG	C-N-CA	7.75	131.29	120.29
26	Z	78	SER	N-CA-C	-7.75	102.77	111.14
7	G	122	TYR	CA-C-N	7.74	130.97	120.44
7	G	122	TYR	C-N-CA	7.74	130.97	120.44
17	K	343	LEU	N-CA-C	-7.74	102.92	111.36
34	8	376	ARG	CA-C-O	-7.73	112.36	120.55
1	A	123	ALA	N-CA-C	-7.73	101.97	111.40
27	N	869	ASP	CA-CB-CG	-7.72	104.88	112.60
29	P	45	LYS	CA-C-N	7.72	130.63	120.28
29	P	45	LYS	C-N-CA	7.72	130.63	120.28
8	h	41	ILE	N-CA-C	-7.72	94.27	107.24
9	i	76	VAL	CA-C-N	7.72	132.96	120.30
9	i	76	VAL	C-N-CA	7.72	132.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	865	PRO	CA-C-O	-7.72	112.44	121.86
34	8	475	GLU	CA-C-O	-7.72	112.37	120.55
1	a	49	LYS	N-CA-CB	7.72	121.49	109.83
11	4	10	GLN	N-CA-C	7.72	120.37	111.11
12	l	158	LYS	N-CA-CB	7.72	121.26	110.07
1	a	134	PHE	CA-CB-CG	-7.71	106.09	113.80
23	T	141	LEU	CA-C-N	7.71	131.39	120.28
23	T	141	LEU	C-N-CA	7.71	131.39	120.28
34	8	398	VAL	CA-C-N	7.71	130.62	120.28
34	8	398	VAL	C-N-CA	7.71	130.62	120.28
28	S	32	GLN	CA-C-N	7.71	130.95	120.54
28	S	32	GLN	C-N-CA	7.71	130.95	120.54
17	K	250	GLY	CA-C-N	7.71	127.76	119.28
17	K	250	GLY	C-N-CA	7.71	127.76	119.28
19	M	317	SER	N-CA-C	-7.71	104.01	113.41
4	d	212	VAL	CB-CA-C	-7.70	100.66	111.21
4	D	94	HIS	CE1-NE2-CD2	-7.70	101.30	109.00
28	S	415	SER	CA-C-N	7.70	130.60	120.28
28	S	415	SER	C-N-CA	7.70	130.60	120.28
4	d	49	THR	N-CA-C	-7.70	103.89	113.28
22	V	153	ILE	N-CA-C	-7.70	96.93	108.17
26	Z	397	ASP	N-CA-C	-7.70	101.94	112.03
16	I	295	ASN	N-CA-C	-7.69	101.01	111.55
8	l	37	VAL	N-CA-C	-7.69	104.42	113.42
19	M	360	ILE	N-CA-C	-7.69	102.95	110.72
7	g	11	PHE	N-CA-CB	7.68	121.44	109.69
28	S	400	LYS	N-CA-C	-7.68	100.98	112.04
12	l	188	HIS	CA-CB-CG	-7.68	106.12	113.80
1	A	205	LEU	N-CA-C	-7.68	102.55	112.23
6	F	92	ASN	CA-CB-CG	7.68	120.28	112.60
21	W	178	PRO	CA-C-O	-7.68	112.95	121.32
26	Z	77	ASN	CA-C-N	7.67	130.88	120.44
26	Z	77	ASN	C-N-CA	7.67	130.88	120.44
27	N	602	VAL	N-CA-CB	7.67	115.33	110.50
7	g	226	PHE	CA-CB-CG	-7.66	106.14	113.80
2	B	199	SER	N-CA-CB	7.66	121.11	110.01
6	F	42	HIS	CA-CB-CG	7.65	121.45	113.80
7	G	49	LEU	CA-C-N	7.65	132.88	122.01
7	G	49	LEU	C-N-CA	7.65	132.88	122.01
8	h	164	LYS	N-CA-C	7.65	120.51	111.71
12	l	69	ARG	NE-CZ-NH1	7.64	129.15	121.50
26	Z	941	ARG	CA-C-O	-7.64	109.69	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9	LEU	N-CA-C	-7.64	103.06	113.30
27	N	382	GLY	CA-C-N	7.64	131.14	120.29
27	N	382	GLY	C-N-CA	7.64	131.14	120.29
30	Q	77	PHE	CB-CA-C	-7.64	97.86	110.85
14	n	108	ASN	CA-C-N	7.64	127.79	120.31
14	n	108	ASN	C-N-CA	7.64	127.79	120.31
18	L	80	ASN	CA-CB-CG	-7.64	104.96	112.60
26	Z	311	ALA	N-CA-C	7.63	119.24	111.07
27	N	554	THR	N-CA-C	-7.63	103.04	111.36
30	Q	247	HIS	CA-CB-CG	7.63	121.43	113.80
32	U	70	HIS	ND1-CE1-NE2	7.63	116.03	108.40
31	R	204	TRP	CE2-CD2-CE3	7.63	126.43	118.80
1	a	79	PRO	CA-C-N	7.63	131.26	120.28
1	a	79	PRO	C-N-CA	7.63	131.26	120.28
10	j	192	ASP	CA-CB-CG	-7.63	104.97	112.60
14	n	121	SER	CA-C-N	7.62	131.26	120.28
14	n	121	SER	C-N-CA	7.62	131.26	120.28
12	5	51	ASP	CA-C-O	7.62	128.63	120.55
6	F	169	THR	CA-C-N	7.62	130.49	120.28
6	F	169	THR	C-N-CA	7.62	130.49	120.28
10	j	50	LEU	CA-C-N	7.61	129.75	122.36
10	j	50	LEU	C-N-CA	7.61	129.75	122.36
23	T	92	ASN	N-CA-CB	7.61	123.36	110.49
31	R	120	LEU	CA-C-O	-7.61	112.83	120.82
29	P	111	ASP	CA-C-N	7.61	130.33	120.44
29	P	111	ASP	C-N-CA	7.61	130.33	120.44
10	j	148	MET	CB-CA-C	-7.60	98.89	110.90
29	P	5	ALA	CA-C-N	7.59	128.28	119.47
29	P	5	ALA	C-N-CA	7.59	128.28	119.47
9	i	49	ALA	CA-C-N	7.59	130.45	120.28
9	i	49	ALA	C-N-CA	7.59	130.45	120.28
14	n	112	ASN	CA-CB-CG	-7.59	105.01	112.60
26	Z	85	VAL	CA-C-N	-7.58	110.36	119.84
26	Z	85	VAL	C-N-CA	-7.58	110.36	119.84
13	6	200	ASP	N-CA-CB	7.58	123.31	110.49
7	g	60	ASN	N-CA-C	-7.58	104.00	112.57
29	P	50	SER	N-CA-C	-7.58	103.49	112.89
1	a	215	GLU	N-CA-C	-7.58	95.28	108.69
2	B	25	LEU	N-CA-C	7.58	120.42	111.71
4	D	14	HIS	CA-C-N	7.58	132.12	121.66
4	D	14	HIS	C-N-CA	7.58	132.12	121.66
31	R	195	ASN	N-CA-C	-7.57	103.30	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	30	HIS	CE1-NE2-CD2	-7.57	101.43	109.00
2	B	123	GLN	N-CA-C	-7.57	101.47	111.24
1	a	176	HIS	CE1-NE2-CD2	-7.57	101.43	109.00
16	I	220	ILE	N-CA-CB	7.57	122.57	111.52
15	H	246	ILE	N-CA-C	-7.57	97.25	108.45
7	g	71	GLY	O-C-N	-7.56	115.62	123.48
27	N	454	ALA	N-CA-C	-7.56	104.10	112.72
3	c	9	THR	N-CA-C	-7.56	103.78	113.16
7	g	81	GLY	CA-C-O	-7.56	112.65	120.66
23	T	82	PHE	CA-C-N	7.56	130.75	120.54
23	T	82	PHE	C-N-CA	7.56	130.75	120.54
16	I	316	PHE	CA-CB-CG	-7.56	106.24	113.80
20	J	354	SER	N-CA-C	-7.55	97.23	108.79
29	P	50	SER	CA-C-N	7.55	130.40	120.28
29	P	50	SER	C-N-CA	7.55	130.40	120.28
29	P	326	ASP	CA-C-N	7.55	135.96	121.54
29	P	326	ASP	C-N-CA	7.55	135.96	121.54
5	e	5	SER	N-CA-C	-7.55	102.41	111.69
3	C	118	LYS	CA-C-N	7.55	130.25	120.44
3	C	118	LYS	C-N-CA	7.55	130.25	120.44
15	H	164	SER	CA-C-N	7.54	127.42	119.05
15	H	164	SER	C-N-CA	7.54	127.42	119.05
26	Z	139	LEU	N-CA-C	-7.54	104.05	113.55
10	j	4	SER	N-CA-C	-7.54	103.54	112.89
20	J	156	GLN	OE1-CD-NE2	-7.54	115.06	122.60
27	N	28	ILE	CB-CA-C	-7.54	101.97	112.14
31	R	159	SER	CB-CA-C	-7.53	99.05	110.88
14	7	146	PHE	CA-C-N	7.53	129.56	120.14
14	7	146	PHE	C-N-CA	7.53	129.56	120.14
7	G	54	LEU	N-CA-C	-7.53	102.75	112.23
6	f	118	ASN	CA-CB-CG	-7.53	105.07	112.60
30	Q	114	GLN	CA-C-N	7.52	131.10	120.42
30	Q	114	GLN	C-N-CA	7.52	131.10	120.42
1	A	103	MET	CA-C-O	-7.52	112.13	120.25
4	D	6	LEU	N-CA-C	-7.52	103.18	113.18
23	T	254	ASP	CA-CB-CG	7.52	120.12	112.60
26	Z	720	LYS	N-CA-C	-7.52	103.17	111.36
18	L	175	GLN	CA-C-N	7.52	127.24	120.10
18	L	175	GLN	C-N-CA	7.52	127.24	120.10
10	j	41	LYS	CA-C-N	-7.51	113.46	122.93
10	j	41	LYS	C-N-CA	-7.51	113.46	122.93
15	H	442	ASP	CA-CB-CG	-7.51	105.09	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	536	GLY	N-CA-C	-7.51	104.96	115.32
33	O	361	ASP	N-CA-C	7.51	119.10	111.07
28	S	73	THR	CA-CB-CG2	7.51	123.26	110.50
12	5	76	VAL	N-CA-C	-7.50	103.14	110.72
33	O	12	SER	O-C-N	-7.50	114.17	122.12
26	Z	377	ALA	N-CA-C	7.50	119.71	108.31
30	Q	3	LEU	CA-C-N	7.50	127.04	119.24
30	Q	3	LEU	C-N-CA	7.50	127.04	119.24
28	S	115	PRO	N-CA-C	-7.50	104.15	114.80
4	D	12	ASP	CA-CB-CG	-7.49	105.11	112.60
24	X	27	ILE	CA-C-O	-7.49	113.73	119.20
3	c	243	ILE	N-CA-C	-7.49	104.19	112.80
4	d	54	ASP	N-CA-CB	7.49	122.31	110.55
7	G	86	ASN	CA-C-N	7.49	130.32	120.28
7	G	86	ASN	C-N-CA	7.49	130.32	120.28
12	5	48	GLY	CA-C-N	7.49	130.18	120.44
12	5	48	GLY	C-N-CA	7.49	130.18	120.44
17	K	355	THR	CA-C-N	7.49	131.05	120.42
17	K	355	THR	C-N-CA	7.49	131.05	120.42
27	N	242	PHE	CA-CB-CG	-7.48	106.32	113.80
13	6	36	ASN	CA-CB-CG	-7.48	105.12	112.60
26	Z	455	ILE	N-CA-C	-7.48	103.17	110.72
9	i	116	HIS	N-CA-C	-7.47	104.19	113.38
2	B	32	VAL	N-CA-C	7.47	121.30	110.09
2	B	51	SER	N-CA-C	-7.47	102.81	112.23
15	H	371	ILE	CA-C-N	7.47	130.60	120.44
15	H	371	ILE	C-N-CA	7.47	130.60	120.44
1	a	115	LEU	CA-C-O	-7.46	112.51	120.42
10	j	74	LYS	CA-C-O	-7.46	112.64	120.55
26	Z	313	ILE	CA-C-N	7.46	130.14	120.44
26	Z	313	ILE	C-N-CA	7.46	130.14	120.44
26	Z	359	LYS	N-CA-C	-7.46	103.23	111.36
4	D	84	ILE	CA-C-O	-7.45	112.78	121.05
5	E	121	GLY	O-C-N	-7.45	113.01	122.70
26	Z	302	SER	CA-C-N	7.45	130.41	120.58
26	Z	302	SER	C-N-CA	7.45	130.41	120.58
26	Z	729	GLU	CA-C-N	7.45	133.32	120.58
26	Z	729	GLU	C-N-CA	7.45	133.32	120.58
12	5	51	ASP	CA-CB-CG	-7.45	105.15	112.60
26	Z	614	VAL	N-CA-C	-7.45	104.59	111.67
6	F	203	GLU	N-CA-C	-7.44	102.32	111.40
9	i	76	VAL	N-CA-C	-7.44	101.47	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	435	GLN	OE1-CD-NE2	7.44	130.04	122.60
29	P	25	ASP	CA-C-N	7.44	130.85	120.29
29	P	25	ASP	C-N-CA	7.44	130.85	120.29
1	A	4	ASP	CA-CB-CG	-7.44	105.16	112.60
31	R	111	LYS	N-CA-C	7.44	119.39	111.28
25	Y	78	LYS	N-CA-C	7.43	119.03	111.07
3	C	9	THR	N-CA-C	-7.43	103.26	111.36
8	1	179	THR	N-CA-C	-7.43	98.39	108.86
29	P	312	PRO	N-CA-C	-7.43	104.25	114.80
29	P	401	ASN	CA-CB-CG	-7.43	105.17	112.60
17	K	205	PRO	CA-C-O	-7.42	115.56	120.90
9	2	64	GLU	CA-C-N	7.41	130.55	120.54
9	2	64	GLU	C-N-CA	7.41	130.55	120.54
23	T	12	SER	O-C-N	7.41	129.98	122.12
31	R	157	SER	CA-C-N	7.41	130.81	120.29
31	R	157	SER	C-N-CA	7.41	130.81	120.29
20	J	95	ILE	N-CA-C	-7.40	97.78	108.36
27	N	298	TYR	N-CA-C	-7.40	103.29	111.36
13	m	40	GLU	CA-C-N	7.40	127.36	120.03
13	m	40	GLU	C-N-CA	7.40	127.36	120.03
31	R	109	LYS	CG-CD-CE	7.40	128.32	111.30
14	7	102	GLN	N-CA-CB	7.39	121.10	110.16
15	H	332	THR	CA-C-N	7.39	130.18	120.28
15	H	332	THR	C-N-CA	7.39	130.18	120.28
28	S	164	ILE	CA-C-N	7.38	127.40	119.28
28	S	164	ILE	C-N-CA	7.38	127.40	119.28
30	Q	381	ILE	N-CA-C	-7.38	103.26	110.72
28	S	110	LEU	CA-C-N	7.38	130.03	120.44
28	S	110	LEU	C-N-CA	7.38	130.03	120.44
12	l	40	PHE	CB-CA-C	-7.38	97.17	109.27
6	F	116	GLN	O-C-N	-7.38	113.20	122.27
14	7	33	LEU	CA-C-O	7.37	129.13	120.58
6	F	26	GLU	N-CA-C	-7.37	103.27	111.82
30	Q	246	TYR	N-CA-C	7.37	119.31	111.28
3	C	96	ASN	CA-CB-CG	7.37	119.97	112.60
31	R	104	LYS	CA-C-O	-7.37	113.27	121.00
10	3	71	ASN	N-CA-CB	7.36	120.94	110.12
14	n	175	GLU	CA-C-O	-7.36	113.09	120.82
2	b	244	ASN	CA-C-N	7.36	131.50	120.31
2	b	244	ASN	C-N-CA	7.36	131.50	120.31
7	g	71	GLY	N-CA-C	-7.36	98.08	111.25
14	n	126	PHE	CA-CB-CG	-7.36	106.44	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	112	ASN	CA-CB-CG	-7.35	105.25	112.60
26	Z	741	LEU	N-CA-C	-7.35	103.27	111.28
16	I	416	PHE	CA-CB-CG	7.35	121.15	113.80
11	k	173	PRO	N-CA-C	-7.35	104.68	113.86
12	5	207	PHE	CA-CB-CG	-7.35	106.45	113.80
9	i	56	THR	N-CA-CB	7.35	120.92	110.12
14	7	228	TYR	CA-CB-CG	-7.35	100.68	113.90
19	M	351	LEU	CA-C-O	-7.34	112.39	120.69
33	O	142	ASP	N-CA-C	-7.34	98.69	109.11
4	D	41	VAL	N-CA-CB	7.34	119.80	110.99
20	J	347	ALA	CA-C-O	-7.34	113.14	120.70
26	Z	518	LEU	CB-CA-C	-7.34	102.84	110.33
22	V	210	THR	CA-C-N	7.34	130.11	120.28
22	V	210	THR	C-N-CA	7.34	130.11	120.28
4	d	14	HIS	CB-CG-CD2	-7.33	121.67	131.20
7	g	133	ILE	N-CA-C	-7.33	97.87	108.36
22	V	196	TYR	CA-CB-CG	-7.33	100.70	113.90
5	e	220	PHE	N-CA-CB	7.33	120.76	109.85
14	7	14	MET	O-C-N	-7.32	115.58	123.42
5	e	195	ILE	N-CA-C	-7.32	103.33	110.72
9	i	57	GLN	O-C-N	-7.32	113.81	122.15
14	n	44	PRO	N-CA-CB	7.32	109.82	103.31
12	5	134	THR	N-CA-C	-7.32	103.39	111.36
7	g	108	PHE	CA-CB-CG	-7.31	106.49	113.80
9	i	205	PHE	CA-C-N	7.31	127.75	119.92
9	i	205	PHE	C-N-CA	7.31	127.75	119.92
30	Q	153	ASP	CA-CB-CG	-7.31	105.29	112.60
34	8	318	PHE	O-C-N	-7.31	115.60	123.42
2	B	55	LEU	N-CA-C	-7.31	104.36	113.28
4	d	176	ASN	O-C-N	-7.31	114.66	122.19
12	l	71	LYS	N-CA-C	-7.31	101.29	111.52
10	j	169	ALA	CB-CA-C	-7.31	98.66	110.79
2	B	236	ARG	N-CA-C	-7.31	95.75	108.69
17	K	275	ASP	CA-CB-CG	-7.31	105.29	112.60
23	T	108	LEU	O-C-N	7.31	130.48	122.15
12	5	201	LYS	CA-C-N	7.31	130.38	120.44
12	5	201	LYS	C-N-CA	7.31	130.38	120.44
26	Z	108	ASP	CA-C-N	7.30	127.65	119.32
26	Z	108	ASP	C-N-CA	7.30	127.65	119.32
4	d	176	ASN	N-CA-C	-7.30	103.81	114.39
30	Q	77	PHE	CA-CB-CG	7.30	121.10	113.80
3	c	121	TYR	CB-CA-C	-7.30	96.66	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	n	94	GLU	N-CA-C	-7.30	103.36	111.82
31	R	100	ASN	CA-C-N	7.29	131.76	120.82
31	R	100	ASN	C-N-CA	7.29	131.76	120.82
3	c	185	VAL	CA-CB-CG2	7.29	122.80	110.40
9	2	186	TYR	N-CA-C	-7.29	97.36	108.96
15	H	148	ASN	CA-CB-CG	7.29	119.89	112.60
17	K	235	ILE	CA-C-O	7.29	127.46	120.31
26	Z	871	HIS	CA-CB-CG	-7.29	106.51	113.80
26	Z	860	GLY	N-CA-C	-7.29	104.31	112.33
7	G	44	PHE	CA-CB-CG	-7.28	106.52	113.80
11	4	110	LYS	N-CA-C	7.28	121.40	112.23
27	N	336	ASN	CA-C-N	7.28	128.06	119.98
27	N	336	ASN	C-N-CA	7.28	128.06	119.98
16	I	329	ASN	CA-C-N	7.28	135.44	121.54
16	I	329	ASN	C-N-CA	7.28	135.44	121.54
30	Q	25	GLN	CA-C-N	7.28	129.73	120.56
30	Q	25	GLN	C-N-CA	7.28	129.73	120.56
18	L	199	LEU	CA-C-O	-7.27	111.28	118.34
33	O	42	SER	CA-C-O	-7.27	113.21	120.70
17	K	171	TYR	N-CA-C	-7.27	103.39	111.82
10	3	37	ASN	CA-CB-CG	-7.27	105.33	112.60
26	Z	621	LEU	N-CA-C	-7.27	103.44	111.36
31	R	102	LEU	CB-CA-C	-7.27	95.96	110.42
3	c	113	ARG	CD-NE-CZ	7.26	134.56	124.40
13	m	160	TYR	CA-CB-CG	-7.26	100.84	113.90
8	1	74	SER	N-CA-C	-7.26	99.47	110.14
15	H	272	ILE	N-CA-C	-7.26	96.97	107.78
21	W	96	LEU	CA-C-N	7.26	130.00	120.28
21	W	96	LEU	C-N-CA	7.26	130.00	120.28
7	g	140	ASN	CA-CB-CG	-7.25	105.35	112.60
3	C	53	SER	CA-C-O	-7.25	113.03	121.16
30	Q	252	HIS	ND1-CE1-NE2	7.25	115.65	108.40
2	B	220	ASP	CB-CA-C	-7.25	98.76	110.79
4	D	86	LYS	N-CA-C	-7.25	103.38	111.28
28	S	44	THR	O-C-N	-7.25	112.95	122.59
26	Z	791	LYS	N-CA-C	-7.24	104.42	113.18
5	E	115	PHE	N-CA-C	-7.24	98.07	109.07
2	b	147	LEU	O-C-N	-7.24	114.58	123.33
13	m	190	SER	N-CA-C	-7.24	103.39	111.28
4	D	150	PRO	N-CA-C	-7.24	106.31	114.92
29	P	404	LYS	N-CA-C	-7.24	100.98	110.39
7	G	108	PHE	CA-C-O	-7.23	112.75	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	21	TYR	O-C-N	7.23	130.40	122.15
25	Y	85	LYS	CA-C-N	7.23	130.29	120.38
25	Y	85	LYS	C-N-CA	7.23	130.29	120.38
12	l	59	LEU	N-CA-C	-7.23	103.40	111.71
22	V	195	HIS	N-CA-CB	7.23	120.46	109.91
12	l	58	TRP	CB-CG-CD2	-7.23	116.68	126.80
7	G	13	PRO	N-CA-C	-7.22	104.52	114.27
18	L	286	ILE	CA-C-N	7.22	126.85	119.92
18	L	286	ILE	C-N-CA	7.22	126.85	119.92
19	M	359	GLN	CA-C-O	-7.22	112.77	120.42
34	8	437	THR	CA-C-O	7.22	130.30	121.56
31	R	207	ARG	NE-CZ-NH1	7.22	128.72	121.50
5	e	173	ALA	CA-C-N	7.22	129.95	120.28
5	e	173	ALA	C-N-CA	7.22	129.95	120.28
2	b	243	ILE	N-CA-C	-7.22	103.26	110.62
2	B	243	ILE	O-C-N	7.22	129.26	121.83
2	b	80	PRO	O-C-N	7.21	132.37	122.64
1	A	37	ARG	NE-CZ-NH1	7.21	128.71	121.50
32	U	157	LEU	CB-CA-C	-7.21	100.47	110.13
3	c	124	HIS	CE1-NE2-CD2	-7.21	101.79	109.00
31	R	293	THR	CA-C-N	7.20	129.63	120.56
31	R	293	THR	C-N-CA	7.20	129.63	120.56
33	O	129	ILE	N-CA-CB	7.20	118.97	110.55
34	8	462	TYR	N-CA-CB	7.20	122.17	110.43
28	S	327	ILE	N-CA-C	-7.20	99.52	107.73
21	W	76	LEU	CA-C-O	-7.20	111.69	119.97
33	O	23	HIS	CE1-NE2-CD2	-7.20	101.80	109.00
2	b	186	GLU	CA-C-N	7.20	129.92	120.28
2	b	186	GLU	C-N-CA	7.20	129.92	120.28
6	f	126	PRO	N-CA-CB	7.19	110.93	103.38
31	R	239	THR	N-CA-C	-7.19	97.18	108.90
17	K	361	SER	CA-C-O	7.19	129.10	121.19
26	Z	747	ALA	CA-C-N	7.19	129.79	120.44
26	Z	747	ALA	C-N-CA	7.19	129.79	120.44
31	R	69	GLU	N-CA-CB	7.19	122.12	110.40
27	N	239	LEU	CA-C-O	7.19	128.17	120.55
23	T	64	VAL	CA-C-N	7.18	129.34	120.22
23	T	64	VAL	C-N-CA	7.18	129.34	120.22
26	Z	223	LEU	CA-C-N	7.18	129.91	120.28
26	Z	223	LEU	C-N-CA	7.18	129.91	120.28
29	P	275	ASN	CA-C-N	7.18	129.78	120.44
29	P	275	ASN	C-N-CA	7.18	129.78	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	363	PHE	CA-CB-CG	-7.18	106.62	113.80
1	a	76	GLY	CA-C-N	7.18	128.82	119.84
1	a	76	GLY	C-N-CA	7.18	128.82	119.84
23	T	10	SER	N-CA-CB	7.18	120.79	110.16
9	i	120	ASP	CA-CB-CG	-7.18	105.42	112.60
12	5	203	GLU	O-C-N	-7.18	113.97	122.15
2	b	153	SER	N-CA-C	-7.17	103.54	111.36
31	R	185	LEU	CA-C-N	7.17	129.77	120.44
31	R	185	LEU	C-N-CA	7.17	129.77	120.44
1	A	78	ILE	CB-CA-C	-7.17	106.75	114.35
14	n	77	ASP	CA-CB-CG	7.17	119.77	112.60
31	R	110	ILE	CA-C-O	7.17	129.74	120.78
1	a	195	GLU	N-CA-CB	7.17	120.66	110.12
16	I	370	ASN	CA-CB-CG	-7.17	105.44	112.60
10	j	155	PRO	CA-C-N	7.16	135.22	121.54
10	j	155	PRO	C-N-CA	7.16	135.22	121.54
26	Z	67	SER	CB-CA-C	-7.16	99.58	110.90
26	Z	488	ALA	N-CA-C	-7.16	103.41	111.14
34	8	464	PHE	CA-CB-CG	-7.16	106.64	113.80
12	l	190	ASN	CA-CB-CG	-7.16	105.44	112.60
9	2	87	LEU	CA-C-O	7.16	128.13	120.55
28	S	233	LEU	CA-C-N	7.15	130.26	120.46
28	S	233	LEU	C-N-CA	7.15	130.26	120.46
30	Q	23	ALA	CA-C-N	7.15	129.87	120.28
30	Q	23	ALA	C-N-CA	7.15	129.87	120.28
5	e	48	SER	CB-CA-C	-7.15	100.19	109.92
11	k	91	SER	N-CA-C	7.15	119.08	111.28
1	A	6	HIS	CG-CD2-NE2	7.15	114.35	107.20
26	Z	545	SER	CA-C-N	7.15	130.25	120.46
26	Z	545	SER	C-N-CA	7.15	130.25	120.46
30	Q	252	HIS	CE1-NE2-CD2	-7.15	101.85	109.00
20	J	327	ILE	CA-C-N	7.14	130.43	120.29
20	J	327	ILE	C-N-CA	7.14	130.43	120.29
34	8	291	THR	CA-C-O	7.14	127.92	119.56
21	W	156	GLU	O-C-N	7.14	129.69	122.12
14	n	96	LEU	CA-C-N	7.13	130.42	120.29
14	n	96	LEU	C-N-CA	7.13	130.42	120.29
13	6	108	HIS	CA-CB-CG	-7.13	106.67	113.80
7	G	112	LEU	N-CA-C	-7.13	103.51	111.71
17	K	244	HIS	CE1-NE2-CD2	-7.13	101.87	109.00
29	P	352	VAL	O-C-N	7.13	128.79	121.87
1	A	24	LYS	N-CA-CB	7.13	120.72	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	229	THR	N-CA-CB	7.13	120.71	110.16
12	5	164	ALA	CA-C-N	7.13	129.83	120.28
12	5	164	ALA	C-N-CA	7.13	129.83	120.28
17	K	41	SER	CA-C-N	7.13	129.71	120.44
17	K	41	SER	C-N-CA	7.13	129.71	120.44
19	M	299	ARG	NE-CZ-NH2	-7.13	112.79	119.20
4	d	98	LEU	N-CA-C	-7.12	104.59	113.28
13	6	143	ALA	CA-C-N	7.12	131.14	120.31
13	6	143	ALA	C-N-CA	7.12	131.14	120.31
22	V	156	PHE	N-CA-CB	7.12	124.09	111.69
27	N	209	LYS	N-CA-C	7.12	119.04	111.28
30	Q	346	ASN	CA-C-N	7.12	129.83	120.28
30	Q	346	ASN	C-N-CA	7.12	129.83	120.28
26	Z	187	SER	N-CA-C	-7.12	102.70	112.03
17	K	204	ASP	CA-C-N	7.12	124.86	119.66
17	K	204	ASP	C-N-CA	7.12	124.86	119.66
10	3	47	HIS	CG-CD2-NE2	7.12	114.32	107.20
28	S	443	ILE	O-C-N	7.12	130.94	123.26
30	Q	101	ILE	N-CA-C	7.12	118.73	110.62
1	a	87	ARG	N-CA-C	-7.11	103.61	111.36
22	V	180	LEU	N-CA-C	-7.11	97.31	108.90
26	Z	37	GLN	N-CA-C	-7.11	104.61	113.28
20	J	189	GLY	O-C-N	-7.11	114.66	121.77
27	N	782	PHE	N-CA-C	-7.11	101.14	111.30
5	E	180	HIS	N-CA-CB	7.10	122.78	111.56
26	Z	968	ASP	N-CA-C	-7.10	96.94	108.52
20	J	148	ASP	CA-C-N	7.10	129.80	120.28
20	J	148	ASP	C-N-CA	7.10	129.80	120.28
6	f	227	GLU	CA-C-N	7.09	129.78	120.28
6	f	227	GLU	C-N-CA	7.09	129.78	120.28
5	E	91	HIS	ND1-CE1-NE2	7.09	115.49	108.40
23	T	240	LYS	CA-C-N	7.09	129.65	120.44
23	T	240	LYS	C-N-CA	7.09	129.65	120.44
26	Z	871	HIS	CE1-NE2-CD2	-7.09	101.91	109.00
29	P	103	TYR	N-CA-C	7.09	119.86	111.71
29	P	208	PHE	CA-CB-CG	-7.09	106.71	113.80
17	K	98	GLN	CB-CA-C	7.08	121.05	110.14
5	E	117	GLU	CA-C-N	7.08	126.72	119.92
5	E	117	GLU	C-N-CA	7.08	126.72	119.92
10	3	28	LEU	N-CA-C	-7.08	97.36	108.90
12	5	103	GLY	CA-C-O	-7.08	113.65	121.37
18	L	273	HIS	CG-CD2-NE2	7.08	114.28	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	117	GLU	N-CA-C	-7.08	104.51	113.43
34	8	157	HIS	CE1-NE2-CD2	-7.08	101.92	109.00
34	8	140	TYR	N-CA-CB	7.08	120.92	109.95
4	d	14	HIS	ND1-CE1-NE2	7.08	115.48	108.40
9	i	93	HIS	CG-CD2-NE2	7.08	114.28	107.20
1	A	130	VAL	CA-C-N	7.08	131.85	122.93
1	A	130	VAL	C-N-CA	7.08	131.85	122.93
31	R	109	LYS	N-CA-C	-7.08	103.50	111.07
19	M	408	SER	CA-C-N	7.07	130.91	120.87
19	M	408	SER	C-N-CA	7.07	130.91	120.87
2	b	202	GLY	CA-C-N	7.07	130.85	120.95
2	b	202	GLY	C-N-CA	7.07	130.85	120.95
20	J	241	ALA	CA-C-O	-7.07	112.81	120.17
26	Z	918	ASP	N-CA-C	-7.07	105.84	114.75
2	B	22	ASP	CA-CB-CG	7.07	119.67	112.60
4	D	50	LEU	N-CA-CB	7.07	120.68	109.51
4	d	94	HIS	CA-CB-CG	7.06	120.86	113.80
14	7	139	SER	O-C-N	-7.06	116.91	121.85
22	V	64	ASN	OD1-CG-ND2	7.06	129.66	122.60
26	Z	65	GLU	CA-C-N	7.06	130.31	120.29
26	Z	65	GLU	C-N-CA	7.06	130.31	120.29
2	b	20	GLN	CB-CA-C	-7.05	96.39	110.42
4	D	181	GLU	CA-C-O	-7.05	114.09	119.59
4	d	94	HIS	ND1-CE1-NE2	7.05	115.45	108.40
8	h	94	THR	CA-C-O	7.05	128.07	120.32
1	A	169	ILE	O-C-N	7.05	128.71	121.87
16	I	365	HIS	CE1-NE2-CD2	-7.05	101.95	109.00
7	g	77	LEU	N-CA-CB	7.04	121.21	109.94
2	B	15	SER	N-CA-C	-7.04	103.68	111.36
12	l	179	HIS	CE1-NE2-CD2	-7.04	101.96	109.00
9	2	26	VAL	CA-C-N	7.04	130.02	120.44
9	2	26	VAL	C-N-CA	7.04	130.02	120.44
9	2	87	LEU	CA-C-N	7.04	129.72	120.28
9	2	87	LEU	C-N-CA	7.04	129.72	120.28
30	Q	394	ASN	N-CA-C	-7.04	104.18	114.39
32	U	61	LYS	N-CA-C	-7.04	103.03	111.69
18	L	113	SER	N-CA-CB	7.04	122.30	111.46
1	A	76	GLY	CA-C-N	7.04	127.08	119.90
1	A	76	GLY	C-N-CA	7.04	127.08	119.90
6	f	226	GLY	O-C-N	7.04	129.11	123.41
24	X	44	GLY	CA-C-N	-7.03	113.70	122.84
24	X	44	GLY	C-N-CA	-7.03	113.70	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	60	VAL	N-CA-CB	7.03	120.53	111.67
29	P	376	THR	CA-C-N	7.03	129.70	120.28
29	P	376	THR	C-N-CA	7.03	129.70	120.28
28	S	91	ASN	CA-CB-CG	-7.03	105.57	112.60
16	I	98	GLU	CB-CG-CD	-7.03	100.65	112.60
17	K	194	GLN	CA-C-N	7.03	130.27	120.29
17	K	194	GLN	C-N-CA	7.03	130.27	120.29
1	A	32	ASN	CA-CB-CG	-7.03	105.57	112.60
7	G	148	GLU	N-CA-C	-7.03	99.85	110.39
10	3	87	THR	CB-CA-C	7.03	122.45	110.79
7	g	187	GLU	CA-C-O	-7.02	113.11	120.55
12	l	78	ALA	N-CA-C	-7.02	103.70	111.36
10	j	83	PRO	N-CA-CB	7.02	111.05	103.33
15	H	276	GLY	CA-C-N	7.02	130.39	120.28
15	H	276	GLY	C-N-CA	7.02	130.39	120.28
9	i	93	HIS	CE1-NE2-CD2	-7.02	101.98	109.00
13	m	48	ASP	CA-C-N	7.02	132.10	122.34
13	m	48	ASP	C-N-CA	7.02	132.10	122.34
3	C	128	ARG	CA-C-N	7.02	126.99	119.76
3	C	128	ARG	C-N-CA	7.02	126.99	119.76
10	3	171	LEU	CA-C-O	-7.02	113.45	120.82
16	I	419	ALA	N-CA-C	-7.01	103.64	111.28
4	D	142	GLU	CA-C-O	-7.01	114.13	119.32
34	8	409	LEU	CA-C-O	7.01	127.98	120.55
4	d	106	TYR	CA-C-O	-7.01	113.46	120.82
23	T	105	LEU	CA-C-N	7.01	130.06	120.46
23	T	105	LEU	C-N-CA	7.01	130.06	120.46
24	X	63	PRO	CA-C-O	-7.01	112.90	121.31
14	n	62	HIS	N-CA-C	-7.00	103.58	111.07
9	2	68	LEU	CA-C-N	7.00	129.67	120.28
9	2	68	LEU	C-N-CA	7.00	129.67	120.28
12	5	157	GLY	CA-C-N	7.00	130.24	120.29
12	5	157	GLY	C-N-CA	7.00	130.24	120.29
27	N	147	ALA	CA-C-N	7.00	132.06	122.19
27	N	147	ALA	C-N-CA	7.00	132.06	122.19
28	S	152	LEU	CA-C-N	7.00	134.91	121.54
28	S	152	LEU	C-N-CA	7.00	134.91	121.54
31	R	150	ALA	CA-C-N	7.00	129.54	120.44
31	R	150	ALA	C-N-CA	7.00	129.54	120.44
6	F	18	LEU	CA-C-N	7.00	130.95	120.31
6	F	18	LEU	C-N-CA	7.00	130.95	120.31
20	J	365	ALA	CB-CA-C	-7.00	99.17	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	62	VAL	N-CA-CB	7.00	118.92	110.31
23	T	38	ASN	OD1-CG-ND2	7.00	129.60	122.60
27	N	782	PHE	CA-CB-CG	-7.00	106.80	113.80
33	O	304	ASN	N-CA-C	-7.00	104.55	113.23
34	8	304	SER	O-C-N	7.00	130.39	122.27
19	M	315	PHE	CA-CB-CG	7.00	120.80	113.80
1	a	75	ASN	N-CA-C	-6.99	96.94	108.76
16	I	401	LEU	CA-C-N	6.99	130.22	120.29
16	I	401	LEU	C-N-CA	6.99	130.22	120.29
27	N	804	LEU	N-CA-C	6.99	118.90	111.28
16	I	86	GLU	CA-C-N	6.99	129.98	120.54
16	I	86	GLU	C-N-CA	6.99	129.98	120.54
2	B	122	THR	N-CA-C	-6.99	105.29	114.31
4	D	27	ARG	CA-C-O	-6.99	113.01	120.42
8	h	50	ALA	N-CA-C	6.99	119.50	111.11
31	R	109	LYS	CA-CB-CG	6.99	128.07	114.10
27	N	780	ASP	O-C-N	6.99	129.52	122.12
3	C	125	GLY	CA-C-N	6.98	128.93	120.13
3	C	125	GLY	C-N-CA	6.98	128.93	120.13
5	E	129	PRO	N-CA-C	6.98	126.85	112.47
30	Q	260	GLN	CA-C-N	6.98	130.33	120.42
30	Q	260	GLN	C-N-CA	6.98	130.33	120.42
10	j	35	VAL	N-CA-CB	6.98	123.47	111.82
13	m	36	ASN	N-CA-C	-6.98	102.89	111.40
29	P	92	SER	CA-C-N	6.98	130.02	120.46
29	P	92	SER	C-N-CA	6.98	130.02	120.46
1	A	80	ASP	CA-CB-CG	-6.97	105.63	112.60
27	N	387	ALA	CA-C-O	-6.97	110.60	120.16
5	e	65	HIS	CA-CB-CG	6.97	120.77	113.80
29	P	152	LYS	N-CA-C	-6.97	104.77	112.72
2	b	159	TRP	CB-CG-CD2	-6.97	117.04	126.80
22	V	103	MET	CA-C-N	6.97	130.95	120.77
22	V	103	MET	C-N-CA	6.97	130.95	120.77
8	h	102	TYR	N-CA-C	-6.97	96.91	108.34
2	b	49	LYS	CA-C-O	-6.97	112.98	120.92
1	A	104	PRO	O-C-N	6.96	130.95	123.23
1	A	209	PHE	CA-C-O	6.96	128.22	120.70
28	S	58	LYS	CA-C-N	6.96	129.60	120.28
28	S	58	LYS	C-N-CA	6.96	129.60	120.28
2	B	152	PRO	N-CA-C	-6.95	105.48	114.03
3	C	58	GLN	O-C-N	6.95	130.08	122.15
11	k	187	ASP	CA-CB-CG	-6.95	105.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	150	SER	O-C-N	6.95	129.49	122.12
26	Z	803	ALA	CA-C-O	6.95	128.62	120.70
4	d	164	ARG	NE-CZ-NH2	6.95	125.45	119.20
29	P	440	HIS	CA-C-O	-6.95	108.99	120.80
33	O	57	LEU	CA-C-O	6.95	128.13	120.63
9	2	226	GLU	CA-C-O	-6.95	108.99	120.80
11	k	23	ARG	O-C-N	6.95	131.18	122.84
11	4	195	PHE	CA-C-O	-6.95	108.99	120.80
27	N	877	GLN	CA-C-N	6.95	130.28	120.28
27	N	877	GLN	C-N-CA	6.95	130.28	120.28
16	I	86	GLU	N-CA-CB	6.94	119.73	110.29
17	K	361	SER	O-C-N	-6.94	114.33	122.87
32	U	240	GLY	N-CA-C	-6.94	105.74	115.32
10	j	165	THR	CB-CA-C	-6.94	99.98	110.88
23	T	17	ASN	O-C-N	6.94	130.06	122.15
27	N	925	ASP	CA-C-O	-6.94	109.00	120.80
4	D	240	GLU	CA-C-O	-6.94	109.01	120.80
28	S	492	LYS	CA-C-O	-6.94	109.01	120.80
28	S	74	LEU	CA-C-N	6.94	129.90	120.54
28	S	74	LEU	C-N-CA	6.94	129.90	120.54
7	G	244	ASN	CA-C-O	-6.93	109.01	120.80
27	N	280	GLN	O-C-N	6.93	130.80	122.27
6	F	62	ILE	CA-C-O	6.93	127.83	120.48
18	L	436	LYS	CA-C-O	-6.93	109.02	120.80
1	A	211	LYS	CA-C-N	6.93	130.26	120.28
1	A	211	LYS	C-N-CA	6.93	130.26	120.28
1	A	242	GLN	CA-C-O	-6.93	109.02	120.80
13	6	128	VAL	N-CA-CB	6.93	122.50	110.65
9	i	172	ASN	O-C-N	-6.93	115.13	122.96
5	E	242	GLU	CA-C-O	-6.93	109.02	120.80
34	8	459	ASN	CA-C-N	6.93	133.92	122.07
34	8	459	ASN	C-N-CA	6.93	133.92	122.07
27	N	214	LEU	CA-C-N	6.93	129.56	120.28
27	N	214	LEU	C-N-CA	6.93	129.56	120.28
31	R	118	GLN	N-CA-C	6.93	118.83	111.28
2	b	112	SER	CA-C-O	-6.92	113.21	120.55
13	m	102	PHE	N-CA-C	-6.92	104.58	113.16
5	E	231	LEU	CA-C-O	-6.92	112.01	119.97
8	h	43	CYS	O-C-N	6.92	131.30	123.27
3	C	244	THR	CA-C-O	-6.92	109.03	120.80
11	4	135	TYR	O-C-N	6.92	131.70	122.43
4	d	189	CYS	N-CA-C	-6.92	103.82	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	4	103	LEU	CA-C-O	6.92	127.83	120.36
23	T	42	PRO	CA-C-N	6.92	131.95	122.34
23	T	42	PRO	C-N-CA	6.92	131.95	122.34
26	Z	502	ASN	N-CA-CB	6.92	124.39	111.52
4	D	90	GLU	CA-C-N	6.91	129.43	120.44
4	D	90	GLU	C-N-CA	6.91	129.43	120.44
3	c	68	LEU	N-CA-C	-6.91	102.09	112.04
27	N	569	LYS	N-CA-C	-6.91	103.75	111.28
30	Q	201	ALA	N-CA-C	-6.91	103.68	111.07
34	8	255	ASN	CA-CB-CG	6.91	119.50	112.60
7	G	58	GLN	OE1-CD-NE2	6.90	129.50	122.60
15	H	348	ASN	OD1-CG-ND2	6.90	129.50	122.60
21	W	81	ILE	CA-C-O	6.90	126.25	119.97
27	N	230	VAL	CA-C-O	-6.90	113.53	120.85
3	c	209	ARG	NE-CZ-NH1	6.90	128.40	121.50
15	H	437	VAL	N-CA-C	-6.90	98.19	108.12
30	Q	359	ILE	CA-C-N	6.90	129.82	120.44
30	Q	359	ILE	C-N-CA	6.90	129.82	120.44
5	E	152	PRO	N-CA-C	-6.89	105.01	114.80
23	T	252	GLU	N-CA-C	-6.89	105.49	114.04
30	Q	37	GLN	CA-C-N	6.89	129.40	120.44
30	Q	37	GLN	C-N-CA	6.89	129.40	120.44
31	R	124	ASP	N-CA-C	-6.89	105.00	113.41
17	K	80	LYS	N-CA-CB	6.89	120.36	110.16
31	R	366	ASN	OD1-CG-ND2	6.89	129.49	122.60
14	n	160	ASP	N-CA-C	-6.89	102.36	111.24
9	i	116	HIS	CG-CD2-NE2	6.88	114.08	107.20
2	B	181	ASP	O-C-N	6.88	129.42	122.12
26	Z	398	LYS	CA-C-O	-6.88	113.53	120.90
27	N	352	ASN	CA-CB-CG	-6.88	105.72	112.60
8	h	138	CYS	CA-C-N	6.88	129.39	120.44
8	h	138	CYS	C-N-CA	6.88	129.39	120.44
7	G	99	TYR	N-CA-C	-6.88	104.92	113.38
11	k	100	VAL	CA-C-O	-6.88	112.94	120.43
9	2	147	THR	CA-C-N	6.88	129.38	120.44
9	2	147	THR	C-N-CA	6.88	129.38	120.44
15	H	90	ARG	CA-C-N	6.88	130.06	120.29
15	H	90	ARG	C-N-CA	6.88	130.06	120.29
27	N	655	ALA	CA-C-N	6.88	129.49	120.28
27	N	655	ALA	C-N-CA	6.88	129.49	120.28
31	R	43	ARG	CA-C-N	6.88	132.37	120.68
31	R	43	ARG	C-N-CA	6.88	132.37	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	8	204	PHE	CA-C-O	6.88	127.53	120.24
21	W	165	GLN	N-CA-C	-6.88	98.56	108.60
1	A	237	VAL	N-CA-CB	6.87	119.89	110.54
2	B	186	GLU	CA-C-N	6.87	129.49	120.28
2	B	186	GLU	C-N-CA	6.87	129.49	120.28
17	K	124	SER	CA-C-N	6.87	132.63	122.74
17	K	124	SER	C-N-CA	6.87	132.63	122.74
10	j	63	ASN	N-CA-C	-6.87	103.87	111.36
14	7	17	ASP	CA-CB-CG	6.87	119.47	112.60
14	7	161	ARG	NE-CZ-NH2	-6.87	113.02	119.20
32	U	130	VAL	CA-C-O	-6.87	113.43	121.05
4	d	116	GLN	CB-CA-C	-6.86	100.10	110.88
5	E	32	ILE	CA-C-O	6.86	127.04	120.25
34	8	264	HIS	CE1-NE2-CD2	-6.86	102.14	109.00
4	D	95	ARG	N-CA-CB	6.86	120.32	110.16
7	G	15	GLY	O-C-N	-6.86	114.44	122.60
26	Z	621	LEU	CA-C-O	-6.86	113.15	120.42
26	Z	770	GLU	N-CA-CB	6.86	120.19	109.83
27	N	758	VAL	N-CA-CB	6.86	118.19	110.72
34	8	177	LYS	N-CA-C	-6.86	105.07	113.50
1	a	32	ASN	CA-CB-CG	-6.86	105.75	112.60
29	P	79	LEU	N-CA-C	6.86	125.40	110.80
14	n	152	ASN	CA-C-O	-6.85	112.02	118.33
17	K	410	ALA	CA-C-N	6.85	129.46	120.28
17	K	410	ALA	C-N-CA	6.85	129.46	120.28
26	Z	598	ALA	N-CA-C	-6.85	103.89	111.36
31	R	99	TYR	N-CA-CB	6.85	120.01	110.07
2	B	14	PRO	CA-C-N	6.85	130.02	120.29
2	B	14	PRO	C-N-CA	6.85	130.02	120.29
20	J	272	MET	CA-C-N	6.85	130.02	120.29
20	J	272	MET	C-N-CA	6.85	130.02	120.29
13	m	111	ILE	O-C-N	6.85	130.10	122.98
18	L	315	PHE	CA-CB-CG	-6.85	106.95	113.80
27	N	58	ARG	N-CA-CB	-6.85	100.06	110.12
28	S	225	HIS	CA-CB-CG	-6.85	106.95	113.80
7	g	191	GLN	OE1-CD-NE2	-6.84	115.76	122.60
6	F	92	ASN	N-CA-C	6.84	118.74	111.28
26	Z	189	ALA	CA-C-N	6.84	129.34	120.44
26	Z	189	ALA	C-N-CA	6.84	129.34	120.44
20	J	286	LYS	N-CA-CB	6.84	118.01	110.35
26	Z	936	VAL	CB-CA-C	-6.84	102.69	110.96
32	U	117	ASN	CA-C-N	6.84	127.21	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	U	117	ASN	C-N-CA	6.84	127.21	119.83
5	E	145	TYR	O-C-N	-6.83	114.46	122.87
12	5	133	GLN	N-CA-C	-6.83	103.83	111.28
18	L	159	LEU	O-C-N	-6.83	115.24	121.66
21	W	102	GLN	N-CA-C	-6.83	103.83	111.28
4	D	171	GLU	CA-C-O	-6.83	113.31	120.55
30	Q	176	ASP	CA-CB-CG	-6.83	105.77	112.60
34	8	117	THR	N-CA-C	-6.83	102.40	113.19
1	a	109	ALA	CA-C-N	6.83	129.99	120.29
1	a	109	ALA	C-N-CA	6.83	129.99	120.29
6	F	152	VAL	N-CA-CB	6.83	120.83	111.41
1	A	196	PHE	CA-C-O	-6.83	113.31	120.55
27	N	16	ASN	CA-C-O	-6.83	114.21	121.99
27	N	573	HIS	CA-C-O	-6.83	113.19	120.42
15	H	450	VAL	N-CA-C	6.82	117.58	110.62
8	h	156	LYS	CA-C-N	6.82	129.31	120.44
8	h	156	LYS	C-N-CA	6.82	129.31	120.44
12	5	58	TRP	O-C-N	6.82	129.10	122.07
27	N	237	LEU	N-CA-CB	6.82	120.15	110.12
22	V	219	GLU	N-CA-C	-6.82	104.99	113.38
15	H	216	ASP	CA-C-N	6.82	129.42	120.28
15	H	216	ASP	C-N-CA	6.82	129.42	120.28
3	c	82	ASP	CA-CB-CG	-6.82	105.78	112.60
5	e	149	HIS	CE1-NE2-CD2	-6.82	102.18	109.00
30	Q	4	PRO	CA-C-N	6.82	127.51	119.94
30	Q	4	PRO	C-N-CA	6.82	127.51	119.94
31	R	214	TYR	CA-C-N	6.82	127.51	119.94
31	R	214	TYR	C-N-CA	6.82	127.51	119.94
26	Z	244	ARG	NE-CZ-NH1	-6.81	114.69	121.50
7	G	145	TYR	N-CA-C	-6.81	98.97	109.52
2	b	32	VAL	O-C-N	6.81	129.85	122.57
6	F	38	ARG	CA-C-O	6.81	128.73	121.45
2	B	65	SER	O-C-N	-6.80	115.20	123.30
27	N	499	HIS	CE1-NE2-CD2	-6.80	102.19	109.00
31	R	150	ALA	N-CA-C	-6.80	103.79	111.07
5	E	24	LYS	O-C-N	-6.80	115.06	122.07
19	M	412	HIS	CE1-NE2-CD2	-6.80	102.20	109.00
27	N	716	GLN	CA-C-N	6.80	129.69	120.44
27	N	716	GLN	C-N-CA	6.80	129.69	120.44
5	e	124	ARG	CA-C-N	6.80	132.33	121.18
5	e	124	ARG	C-N-CA	6.80	132.33	121.18
27	N	508	THR	CA-C-N	6.80	133.03	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	508	THR	C-N-CA	6.80	133.03	122.49
34	8	258	ASP	CA-CB-CG	-6.80	105.80	112.60
12	5	107	LYS	N-CA-C	-6.79	103.33	111.69
24	X	59	ARG	CA-C-N	6.79	129.68	120.44
24	X	59	ARG	C-N-CA	6.79	129.68	120.44
12	l	32	LYS	O-C-N	6.79	130.97	123.22
30	Q	209	TYR	N-CA-C	-6.79	104.61	113.17
13	m	64	LEU	CA-C-N	6.79	129.12	120.56
13	m	64	LEU	C-N-CA	6.79	129.12	120.56
8	1	85	LEU	N-CA-C	-6.79	103.96	111.36
28	S	93	LEU	CA-C-N	6.79	129.38	120.28
28	S	93	LEU	C-N-CA	6.79	129.38	120.28
10	j	29	GLY	O-C-N	6.79	129.60	123.42
5	E	85	ARG	NE-CZ-NH1	6.79	128.29	121.50
16	I	343	ARG	N-CA-C	-6.79	104.55	114.39
18	L	164	ASP	CA-C-N	6.79	126.75	119.28
18	L	164	ASP	C-N-CA	6.79	126.75	119.28
26	Z	6	ASP	N-CA-C	-6.79	104.62	113.17
2	b	7	PHE	N-CA-C	-6.79	103.68	112.23
12	5	194	GLY	O-C-N	6.79	128.85	122.13
31	R	147	LYS	N-CA-CB	6.79	120.80	110.28
19	M	173	ASP	CA-C-N	6.79	129.37	120.28
19	M	173	ASP	C-N-CA	6.79	129.37	120.28
20	J	82	LYS	N-CA-C	-6.79	104.30	112.58
33	O	284	GLU	CA-C-N	6.79	129.26	120.44
33	O	284	GLU	C-N-CA	6.79	129.26	120.44
26	Z	897	HIS	CA-CB-CG	6.78	120.58	113.80
7	G	86	ASN	CA-C-O	-6.78	113.23	120.42
12	l	160	SER	CA-C-N	6.78	130.05	120.42
12	l	160	SER	C-N-CA	6.78	130.05	120.42
1	A	40	ASP	CA-C-O	6.78	126.20	119.08
17	K	142	HIS	CA-CB-CG	-6.78	107.02	113.80
17	K	315	ILE	CA-C-O	-6.78	113.00	120.72
19	M	61	LYS	CB-CA-C	-6.78	98.09	110.63
20	J	145	SER	CA-C-N	6.78	130.98	120.75
20	J	145	SER	C-N-CA	6.78	130.98	120.75
28	S	438	HIS	CA-CB-CG	-6.78	107.03	113.80
24	X	95	GLU	N-CA-C	-6.77	102.33	113.50
5	E	220	PHE	CA-CB-CG	-6.77	107.03	113.80
22	V	191	GLY	CA-C-N	6.77	130.03	120.28
22	V	191	GLY	C-N-CA	6.77	130.03	120.28
4	d	109	ARG	O-C-N	6.77	129.29	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	113	ILE	O-C-N	-6.77	115.54	123.05
14	7	23	ALA	O-C-N	6.77	131.06	123.48
21	W	62	LEU	N-CA-C	-6.77	105.15	113.41
34	8	248	ASN	N-CA-C	-6.77	103.83	111.07
3	C	81	ALA	CA-C-N	6.77	129.90	120.29
3	C	81	ALA	C-N-CA	6.77	129.90	120.29
29	P	324	GLU	N-CA-C	-6.76	105.03	113.28
19	M	218	ALA	CA-C-N	6.76	132.33	123.00
19	M	218	ALA	C-N-CA	6.76	132.33	123.00
33	O	280	LEU	CA-C-N	6.76	129.89	120.29
33	O	280	LEU	C-N-CA	6.76	129.89	120.29
5	e	64	ARG	NE-CZ-NH2	6.76	125.28	119.20
10	j	54	GLY	CA-C-N	6.76	130.35	120.82
10	j	54	GLY	C-N-CA	6.76	130.35	120.82
23	T	193	THR	N-CA-C	-6.76	104.78	113.16
34	8	247	ASP	CA-CB-CG	-6.76	105.84	112.60
6	f	95	SER	N-CA-C	6.76	118.64	111.28
7	g	212	ILE	CA-C-O	6.76	129.12	121.28
18	L	260	ALA	CA-C-O	-6.76	113.39	120.55
33	O	286	PHE	CB-CA-C	-6.76	100.27	110.88
32	U	232	VAL	CA-C-O	-6.75	114.01	121.17
12	5	7	ARG	N-CA-CB	6.75	121.42	110.41
12	5	57	THR	CA-C-N	6.75	129.22	120.44
12	5	57	THR	C-N-CA	6.75	129.22	120.44
22	V	212	MET	N-CA-CB	6.75	120.16	110.16
7	G	200	HIS	CG-CD2-NE2	6.75	113.95	107.20
19	M	138	ASP	CA-CB-CG	-6.75	105.85	112.60
13	m	79	HIS	CG-CD2-NE2	6.75	113.95	107.20
27	N	179	THR	N-CA-C	6.75	118.63	111.28
34	8	304	SER	CA-C-O	-6.75	111.48	118.90
3	c	76	VAL	O-C-N	-6.75	115.90	123.18
31	R	325	HIS	CE1-NE2-CD2	-6.74	102.26	109.00
27	N	740	TRP	CA-C-N	6.74	129.61	120.44
27	N	740	TRP	C-N-CA	6.74	129.61	120.44
10	j	84	GLU	CA-C-N	6.74	129.86	120.29
10	j	84	GLU	C-N-CA	6.74	129.86	120.29
13	6	78	ASP	N-CA-C	6.74	121.34	113.18
27	N	269	LEU	CA-C-N	6.74	129.31	120.28
27	N	269	LEU	C-N-CA	6.74	129.31	120.28
12	l	91	LYS	N-CA-C	-6.74	101.00	110.50
30	Q	182	SER	N-CA-CB	6.74	120.02	110.12
12	l	66	HIS	CA-CB-CG	6.73	120.53	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	55	ASN	O-C-N	6.73	129.26	122.12
26	Z	77	ASN	OD1-CG-ND2	-6.73	115.87	122.60
29	P	80	THR	N-CA-C	6.73	122.47	111.37
13	m	81	ASP	CA-CB-CG	-6.73	105.87	112.60
24	X	30	GLN	N-CA-C	-6.73	96.47	110.80
22	V	119	SER	CA-C-N	6.73	129.29	120.28
22	V	119	SER	C-N-CA	6.73	129.29	120.28
8	1	45	ARG	CB-CA-C	-6.72	98.09	109.72
10	3	99	PHE	CA-CB-CG	-6.72	107.08	113.80
24	X	62	ASP	N-CA-CB	6.72	119.64	109.75
20	J	165	GLU	CA-C-O	-6.72	113.78	120.70
29	P	56	LYS	N-CA-C	6.72	118.61	111.28
29	P	195	GLN	OE1-CD-NE2	6.72	129.32	122.60
11	4	163	LEU	O-C-N	-6.72	115.00	122.12
11	4	181	VAL	N-CA-C	-6.72	98.70	108.11
13	6	36	ASN	CB-CG-ND2	-6.72	106.32	116.40
1	A	184	HIS	CE1-NE2-CD2	-6.72	102.28	109.00
19	M	389	ALA	CA-C-N	6.72	129.61	120.54
19	M	389	ALA	C-N-CA	6.72	129.61	120.54
20	J	55	VAL	N-CA-C	-6.72	103.94	110.72
34	8	277	LEU	N-CA-C	6.72	118.26	111.07
2	b	30	GLN	OE1-CD-NE2	-6.71	115.89	122.60
21	W	181	LEU	CA-C-N	6.71	129.28	120.28
21	W	181	LEU	C-N-CA	6.71	129.28	120.28
2	B	17	LYS	N-CA-C	-6.71	97.58	108.52
22	V	98	THR	N-CA-C	-6.71	105.09	113.28
27	N	798	LYS	N-CA-C	6.71	118.25	111.07
34	8	416	PHE	CB-CA-C	-6.71	98.92	109.52
26	Z	179	SER	CA-C-N	6.71	130.35	121.90
26	Z	179	SER	C-N-CA	6.71	130.35	121.90
8	1	98	ILE	N-CA-C	-6.70	98.78	108.17
14	n	157	LYS	N-CA-C	-6.70	104.05	111.82
10	3	98	ARG	CA-C-N	6.70	131.34	122.30
10	3	98	ARG	C-N-CA	6.70	131.34	122.30
32	U	271	ASP	CA-CB-CG	6.70	119.30	112.60
6	f	91	CYS	CA-C-N	6.70	129.25	120.28
6	f	91	CYS	C-N-CA	6.70	129.25	120.28
12	l	166	HIS	CA-CB-CG	6.70	120.50	113.80
5	E	180	HIS	CE1-NE2-CD2	-6.70	102.30	109.00
27	N	42	GLU	CA-C-N	6.70	128.46	120.09
27	N	42	GLU	C-N-CA	6.70	128.46	120.09
3	C	169	SER	N-CA-C	6.69	118.58	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	100	LYS	N-CA-C	-6.69	97.50	108.41
33	O	60	ARG	NE-CZ-NH2	6.69	125.22	119.20
11	4	145	ASP	CA-CB-CG	-6.69	105.91	112.60
30	Q	10	GLU	CA-C-N	6.69	129.14	120.44
30	Q	10	GLU	C-N-CA	6.69	129.14	120.44
33	O	375	ASP	CA-C-O	-6.69	112.54	120.10
7	g	166	GLN	N-CA-CB	6.69	119.95	110.12
9	2	10	ASN	N-CA-C	-6.69	102.44	111.87
26	Z	131	LYS	N-CA-C	-6.69	105.03	113.72
12	l	51	ASP	CA-CB-CG	-6.68	105.92	112.60
1	A	78	ILE	N-CA-C	6.68	122.30	112.61
19	M	277	ILE	N-CA-C	-6.68	97.82	107.78
29	P	388	ILE	N-CA-C	-6.68	104.25	110.53
13	m	182	LYS	N-CA-CB	6.68	119.94	110.12
13	6	44	PHE	CA-CB-CG	-6.68	107.12	113.80
13	6	188	PHE	N-CA-CB	6.68	120.04	110.16
21	W	24	THR	CA-C-N	6.68	130.46	120.31
21	W	24	THR	C-N-CA	6.68	130.46	120.31
5	e	208	ASN	CA-CB-CG	6.68	119.28	112.60
8	l	177	VAL	N-CA-CB	6.67	119.02	111.21
28	S	261	HIS	N-CA-C	-6.67	102.24	112.99
5	e	73	LEU	CA-C-O	6.67	127.60	120.46
8	h	134	ILE	CA-CB-CG1	6.67	121.74	110.40
2	B	149	GLN	CB-CG-CD	-6.67	101.26	112.60
4	D	34	VAL	O-C-N	-6.67	115.86	123.07
4	D	229	GLN	N-CA-C	-6.67	104.09	111.36
23	T	170	ASN	CA-C-N	6.67	129.44	120.50
23	T	170	ASN	C-N-CA	6.67	129.44	120.50
26	Z	195	PHE	CA-CB-CG	-6.67	107.13	113.80
26	Z	257	PRO	N-CA-C	6.67	118.84	110.70
28	S	309	PHE	CA-C-N	6.67	129.54	120.54
28	S	309	PHE	C-N-CA	6.67	129.54	120.54
4	d	224	SER	N-CA-CB	6.66	119.92	110.12
10	j	66	PHE	N-CA-C	-6.66	104.63	112.89
10	j	142	SER	CA-C-N	6.66	129.75	120.29
10	j	142	SER	C-N-CA	6.66	129.75	120.29
3	C	167	ASN	CA-CB-CG	6.66	119.26	112.60
19	M	405	ASN	N-CA-CB	6.66	119.92	110.12
7	G	187	GLU	N-CA-CB	6.66	120.61	110.28
28	S	429	ASP	N-CA-C	-6.66	105.12	113.18
5	E	59	ILE	N-CA-C	-6.66	98.85	108.17
28	S	434	ALA	CA-C-O	6.66	128.42	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	175	GLU	CA-C-N	6.66	129.75	120.29
29	P	175	GLU	C-N-CA	6.66	129.75	120.29
31	R	363	PHE	N-CA-CB	6.66	120.02	110.16
9	i	123	TYR	N-CA-C	-6.66	104.11	111.36
14	7	185	TYR	O-C-N	6.65	129.74	122.15
27	N	626	GLY	N-CA-C	-6.65	104.78	112.50
13	6	162	PRO	N-CA-CB	6.65	109.26	103.27
15	H	45	TYR	CA-C-O	6.65	126.22	118.90
5	e	226	GLU	O-C-N	6.65	129.73	122.15
7	G	110	ASP	O-C-N	6.65	129.27	122.09
9	2	62	ASN	CA-CB-CG	6.65	119.25	112.60
33	O	135	ARG	CA-C-N	6.65	129.19	120.28
33	O	135	ARG	C-N-CA	6.65	129.19	120.28
4	d	68	HIS	ND1-CE1-NE2	6.65	115.05	108.40
16	I	283	GLU	CA-C-N	6.65	129.90	120.53
16	I	283	GLU	C-N-CA	6.65	129.90	120.53
30	Q	118	CYS	N-CA-C	6.64	119.08	111.11
8	h	133	PHE	CA-CB-CG	-6.64	107.16	113.80
2	B	103	GLU	N-CA-CB	6.64	121.69	111.46
31	R	105	LYS	CB-CA-C	6.64	123.63	110.42
4	d	47	ARG	N-CA-C	-6.63	97.92	108.73
14	n	170	VAL	N-CA-CB	6.63	119.56	110.54
8	h	159	LEU	N-CA-CB	6.63	120.56	110.28
14	7	70	LEU	CA-C-N	6.63	129.05	120.56
14	7	70	LEU	C-N-CA	6.63	129.05	120.56
18	L	286	ILE	N-CA-C	-6.63	105.06	113.22
26	Z	9	GLN	CB-CG-CD	-6.63	101.33	112.60
21	W	83	GLY	O-C-N	-6.63	114.08	122.70
5	E	128	ARG	CA-C-O	-6.63	111.08	120.16
6	F	165	GLN	CA-C-O	-6.63	113.52	120.55
15	H	391	ILE	CA-C-N	6.63	129.70	120.29
15	H	391	ILE	C-N-CA	6.63	129.70	120.29
16	I	209	GLU	CA-C-N	6.63	129.16	120.28
16	I	209	GLU	C-N-CA	6.63	129.16	120.28
17	K	44	ASN	CA-C-N	6.63	129.70	120.29
17	K	44	ASN	C-N-CA	6.63	129.70	120.29
20	J	199	ALA	CB-CA-C	-6.63	99.58	110.85
21	W	65	PHE	CA-CB-CG	-6.62	107.18	113.80
13	6	93	ILE	CA-C-O	6.62	127.87	120.85
32	U	273	LEU	CB-CA-C	-6.62	100.48	110.88
11	k	81	SER	N-CA-C	6.62	118.58	111.36
22	V	183	ALA	N-CA-C	6.62	119.35	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	42	TRP	CB-CG-CD1	6.62	136.83	126.90
3	C	221	ASP	CA-CB-CG	-6.62	105.98	112.60
31	R	119	LYS	CA-C-N	6.62	129.04	120.44
31	R	119	LYS	C-N-CA	6.62	129.04	120.44
6	F	85	ASN	CA-CB-CG	-6.62	105.98	112.60
26	Z	852	GLN	CA-C-O	6.62	127.34	119.60
11	k	194	ASP	CA-CB-CG	-6.61	105.99	112.60
1	A	151	ALA	O-C-N	6.61	129.69	122.15
2	B	29	LYS	N-CA-CB	6.61	119.94	110.16
19	M	350	PRO	N-CA-CB	6.61	110.19	103.25
19	M	55	ASN	CA-C-O	-6.61	113.55	120.55
14	n	55	GLY	CA-C-N	6.61	130.80	121.02
14	n	55	GLY	C-N-CA	6.61	130.80	121.02
8	h	183	VAL	CA-CB-CG1	6.60	121.62	110.40
13	m	137	ARG	NE-CZ-NH1	-6.60	114.90	121.50
8	l	50	ALA	CA-C-O	6.60	127.75	120.82
17	K	254	VAL	O-C-N	6.60	128.63	121.83
18	L	161	ARG	O-C-N	-6.60	114.75	122.87
27	N	616	HIS	CA-C-N	6.60	129.50	120.46
27	N	616	HIS	C-N-CA	6.60	129.50	120.46
1	a	16	LEU	CA-C-N	6.59	131.89	120.68
1	a	16	LEU	C-N-CA	6.59	131.89	120.68
34	8	291	THR	O-C-N	-6.59	114.43	122.34
7	g	83	HIS	N-CA-C	-6.59	104.17	111.36
16	I	107	GLY	CA-C-O	6.59	127.47	121.47
11	4	23	ARG	NE-CZ-NH1	-6.59	114.91	121.50
27	N	264	SER	N-CA-C	6.59	119.74	111.24
32	U	8	VAL	N-CA-CB	6.59	120.78	111.82
5	E	225	ASN	N-CA-C	-6.59	104.18	111.82
28	S	337	ASN	CA-CB-CG	6.59	119.19	112.60
12	5	209	ASN	CA-C-N	6.59	129.39	120.63
12	5	209	ASN	C-N-CA	6.59	129.39	120.63
5	e	135	LEU	N-CA-C	-6.58	97.79	108.52
10	3	65	MET	O-C-N	6.58	129.10	122.12
19	M	376	TRP	CA-C-N	6.58	129.00	120.44
19	M	376	TRP	C-N-CA	6.58	129.00	120.44
22	V	288	LEU	O-C-N	6.58	128.85	122.07
26	Z	475	GLN	CA-C-N	6.58	129.10	120.28
26	Z	475	GLN	C-N-CA	6.58	129.10	120.28
28	S	39	ASN	CA-C-N	6.58	129.10	120.28
28	S	39	ASN	C-N-CA	6.58	129.10	120.28
3	C	41	ASP	CA-C-O	6.58	126.36	119.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	124	TYR	O-C-N	-6.58	115.75	123.25
18	L	228	LYS	CA-C-N	6.58	129.09	120.28
18	L	228	LYS	C-N-CA	6.58	129.09	120.28
5	e	201	GLU	N-CA-C	-6.57	104.19	111.36
6	F	23	TYR	CB-CG-CD2	-6.57	110.94	120.80
13	6	161	GLU	CA-C-N	6.57	126.93	119.83
13	6	161	GLU	C-N-CA	6.57	126.93	119.83
13	6	200	ASP	CA-CB-CG	-6.57	106.03	112.60
11	4	1	MET	CA-C-N	6.57	134.09	121.54
11	4	1	MET	C-N-CA	6.57	134.09	121.54
30	Q	378	SER	CA-C-O	6.57	127.51	120.55
23	T	236	ASN	CA-CB-CG	6.57	119.17	112.60
26	Z	733	VAL	N-CA-C	-6.57	104.09	110.72
5	e	190	LEU	CA-C-O	-6.57	113.46	120.42
9	2	31	CYS	N-CA-C	-6.57	96.82	110.80
16	I	301	GLU	N-CA-C	6.57	118.23	111.14
27	N	308	ASN	N-CA-C	-6.56	97.58	108.34
16	I	288	GLY	CA-C-N	6.56	129.07	120.28
16	I	288	GLY	C-N-CA	6.56	129.07	120.28
26	Z	142	ASP	N-CA-C	6.56	124.78	110.80
28	S	64	ARG	CA-C-O	-6.56	113.85	121.07
33	O	256	ASN	CA-CB-CG	6.56	119.16	112.60
14	n	210	LYS	CA-C-O	6.56	129.50	121.56
9	2	189	ASN	CA-C-N	6.56	128.97	120.44
9	2	189	ASN	C-N-CA	6.56	128.97	120.44
18	L	95	ILE	N-CA-C	-6.56	104.10	110.72
16	I	117	HIS	N-CA-C	-6.55	99.34	109.24
19	M	209	ASP	O-C-N	6.55	129.17	122.09
26	Z	365	SER	N-CA-C	-6.55	104.76	112.89
3	c	58	GLN	CB-CG-CD	-6.55	101.46	112.60
27	N	512	ASN	CA-C-N	6.55	129.72	120.42
27	N	512	ASN	C-N-CA	6.55	129.72	120.42
4	d	94	HIS	CA-C-N	6.55	129.59	120.29
4	d	94	HIS	C-N-CA	6.55	129.59	120.29
8	h	64	GLU	CB-CA-C	-6.55	99.71	110.85
3	C	122	THR	N-CA-C	-6.55	104.93	113.12
28	S	91	ASN	CA-C-N	6.55	128.95	120.44
28	S	91	ASN	C-N-CA	6.55	128.95	120.44
12	l	34	VAL	N-CA-CB	6.55	119.36	111.31
7	G	220	THR	N-CA-CB	6.54	121.47	111.06
18	L	242	ASN	CA-CB-CG	6.54	119.14	112.60
18	L	411	ASN	N-CA-C	-6.54	101.83	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	20	HIS	ND1-CE1-NE2	6.54	114.94	108.40
28	S	94	LYS	CA-C-O	-6.54	113.61	120.55
1	a	223	LYS	CA-C-O	6.54	128.39	121.33
4	d	86	LYS	CA-C-N	6.54	129.58	120.29
4	d	86	LYS	C-N-CA	6.54	129.58	120.29
10	3	142	SER	N-CA-CB	6.54	119.73	110.12
28	S	50	PRO	CA-C-N	6.54	129.05	120.28
28	S	50	PRO	C-N-CA	6.54	129.05	120.28
6	F	6	ASP	CA-CB-CG	6.54	119.14	112.60
25	Y	68	GLU	N-CA-CB	6.54	122.58	111.66
27	N	795	GLU	CA-C-N	6.54	128.80	120.56
27	N	795	GLU	C-N-CA	6.54	128.80	120.56
4	D	234	ILE	N-CA-C	-6.54	104.12	110.72
34	8	232	ASP	CA-C-N	6.54	130.24	120.17
34	8	232	ASP	C-N-CA	6.54	130.24	120.17
20	J	193	THR	CA-CB-OG1	-6.54	99.80	109.60
26	Z	503	ASP	N-CA-C	-6.54	104.16	111.28
31	R	104	LYS	N-CA-CB	6.54	119.45	109.91
33	O	270	ILE	N-CA-C	6.54	117.29	110.62
4	d	223	SER	CA-C-N	6.53	129.03	120.28
4	d	223	SER	C-N-CA	6.53	129.03	120.28
10	j	57	THR	CA-C-O	-6.53	113.62	120.55
4	D	103	THR	N-CA-CB	6.53	120.52	109.87
2	B	166	LYS	CA-C-O	6.53	127.47	120.55
17	K	194	GLN	O-C-N	-6.53	114.50	123.12
27	N	465	ALA	N-CA-CB	6.53	119.48	110.01
4	D	170	ARG	CA-C-O	-6.53	113.50	120.42
27	N	580	ASN	O-C-N	-6.53	114.84	122.87
8	h	13	ILE	CB-CA-C	-6.53	101.50	110.77
8	h	62	HIS	ND1-CE1-NE2	6.53	114.93	108.40
29	P	361	THR	CA-C-N	6.53	129.68	120.28
29	P	361	THR	C-N-CA	6.53	129.68	120.28
28	S	164	ILE	O-C-N	-6.53	113.66	121.10
13	m	70	ASN	CA-C-N	6.52	129.02	120.28
13	m	70	ASN	C-N-CA	6.52	129.02	120.28
6	F	42	HIS	CB-CG-CD2	-6.52	122.72	131.20
23	T	234	TYR	N-CA-C	-6.52	96.91	110.80
23	T	258	ASN	CA-C-N	6.52	129.68	120.42
23	T	258	ASN	C-N-CA	6.52	129.68	120.42
9	2	146	LEU	N-CA-CB	6.52	119.55	109.97
15	H	98	GLN	N-CA-C	-6.52	100.63	110.28
33	O	92	PHE	N-CA-CB	6.52	120.11	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	61	SER	N-CA-CB	6.52	119.67	109.83
4	D	186	VAL	CA-C-N	6.52	128.91	120.44
4	D	186	VAL	C-N-CA	6.52	128.91	120.44
17	K	99	PHE	CA-CB-CG	-6.52	107.28	113.80
20	J	15	HIS	CA-CB-CG	-6.52	107.28	113.80
21	W	188	SER	N-CA-CB	6.52	118.84	110.04
9	i	141	HIS	CB-CG-CD2	-6.52	122.73	131.20
33	O	306	ARG	N-CA-C	-6.52	103.94	112.41
10	j	201	MET	O-C-N	-6.51	115.82	123.25
26	Z	871	HIS	ND1-CE1-NE2	6.51	114.92	108.40
5	E	13	LEU	CA-C-N	6.51	129.01	120.28
5	E	13	LEU	C-N-CA	6.51	129.01	120.28
3	c	217	LYS	N-CA-C	-6.51	104.65	112.59
27	N	469	VAL	N-CA-C	-6.51	104.14	110.72
29	P	207	THR	CA-C-N	6.51	129.66	120.28
29	P	207	THR	C-N-CA	6.51	129.66	120.28
8	h	189	TYR	CA-C-N	6.51	126.44	119.28
8	h	189	TYR	C-N-CA	6.51	126.44	119.28
15	H	363	PRO	CA-C-N	6.50	128.90	120.44
15	H	363	PRO	C-N-CA	6.50	128.90	120.44
15	H	55	ASP	CA-C-N	6.50	129.00	120.28
15	H	55	ASP	C-N-CA	6.50	129.00	120.28
14	n	142	LEU	O-C-N	6.50	131.02	123.41
2	B	239	THR	N-CA-CB	6.50	121.48	110.49
14	7	173	ALA	N-CA-C	-6.50	104.19	111.28
19	M	364	HIS	CA-C-N	6.50	131.73	120.68
19	M	364	HIS	C-N-CA	6.50	131.73	120.68
32	U	282	VAL	CA-C-N	6.50	129.64	120.28
32	U	282	VAL	C-N-CA	6.50	129.64	120.28
27	N	314	LEU	CB-CA-C	-6.50	100.68	110.88
15	H	157	VAL	CA-C-O	-6.49	112.66	120.78
9	i	99	ILE	N-CA-CB	6.49	118.80	111.21
16	I	352	ASN	CA-CB-CG	-6.49	106.11	112.60
9	i	109	HIS	ND1-CE1-NE2	6.49	114.89	108.40
9	2	54	ALA	N-CA-CB	6.49	119.76	110.16
17	K	164	ASN	N-CA-CB	6.49	119.48	110.07
6	f	164	SER	N-CA-C	-6.49	105.23	113.01
11	k	159	ASP	N-CA-C	-6.49	104.29	111.36
13	m	188	PHE	CA-CB-CG	-6.49	107.31	113.80
27	N	123	PHE	CA-C-N	6.48	131.55	120.72
27	N	123	PHE	C-N-CA	6.48	131.55	120.72
5	e	2	ARG	NE-CZ-NH1	6.48	127.98	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	287	ASP	N-CA-C	-6.48	97.71	108.34
26	Z	133	ASP	CA-CB-CG	-6.48	106.12	112.60
12	l	147	ASP	N-CA-C	-6.48	104.62	113.30
29	P	24	ILE	O-C-N	6.48	128.50	121.83
6	f	78	PRO	CA-C-N	6.48	129.60	120.28
6	f	78	PRO	C-N-CA	6.48	129.60	120.28
1	A	69	THR	N-CA-CB	6.48	121.43	110.49
22	V	89	ALA	N-CA-C	-6.47	104.30	111.36
4	d	68	HIS	CA-CB-CG	6.47	120.27	113.80
4	d	164	ARG	NE-CZ-NH1	-6.47	115.03	121.50
17	K	279	THR	CA-C-N	6.47	128.95	120.28
17	K	279	THR	C-N-CA	6.47	128.95	120.28
9	i	60	GLY	CA-C-O	-6.47	114.08	120.75
12	l	53	GLN	CG-CD-NE2	-6.47	106.69	116.40
14	n	202	LYS	N-CA-CB	6.47	119.39	110.01
9	i	40	LYS	N-CA-C	-6.47	103.67	113.89
7	G	93	ALA	O-C-N	6.47	128.73	122.07
9	2	116	HIS	CB-CG-CD2	-6.47	122.79	131.20
25	Y	31	GLU	CA-C-N	6.47	133.89	121.54
25	Y	31	GLU	C-N-CA	6.47	133.89	121.54
28	S	307	LEU	N-CA-CB	6.47	119.63	110.12
29	P	87	GLY	N-CA-C	-6.47	106.66	113.58
4	d	4	ARG	NE-CZ-NH2	6.46	125.02	119.20
12	5	61	SER	O-C-N	-6.46	115.11	122.09
16	I	183	ASP	N-CA-C	-6.46	104.31	111.36
3	c	50	LYS	CA-C-N	6.46	129.33	120.35
3	c	50	LYS	C-N-CA	6.46	129.33	120.35
4	d	108	THR	CA-C-O	-6.46	113.65	120.63
12	5	134	THR	N-CA-CB	6.46	119.72	110.16
14	7	21	ILE	O-C-N	-6.46	116.20	123.18
14	7	203	ASN	CA-CB-CG	-6.46	106.14	112.60
32	U	46	ILE	N-CA-C	-6.46	99.28	108.58
12	5	191	HIS	CA-CB-CG	-6.46	107.34	113.80
27	N	443	LEU	N-CA-C	-6.46	104.44	112.90
10	j	86	PHE	CA-CB-CG	-6.46	107.34	113.80
12	l	196	LEU	CA-C-O	6.46	127.40	120.55
22	V	76	THR	N-CA-C	-6.46	105.15	113.16
26	Z	452	LEU	N-CA-C	6.46	118.32	111.28
12	l	160	SER	CA-C-O	6.46	127.26	120.42
13	m	94	GLN	OE1-CD-NE2	6.46	129.06	122.60
20	J	162	GLU	CA-C-O	6.46	127.39	120.55
26	Z	257	PRO	CA-C-N	6.46	127.03	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	257	PRO	C-N-CA	6.46	127.03	120.38
31	R	401	HIS	CA-C-N	6.46	128.93	120.28
31	R	401	HIS	C-N-CA	6.46	128.93	120.28
13	m	15	ILE	CA-C-O	6.45	127.47	120.43
22	V	285	ASP	CA-C-O	-6.45	113.58	120.42
1	a	165	LYS	N-CA-C	-6.45	103.75	112.26
7	g	15	GLY	CA-C-O	6.45	126.17	119.27
7	g	112	LEU	CB-CA-C	-6.45	100.08	110.79
12	5	87	VAL	N-CA-CB	6.45	120.26	110.58
17	K	47	ILE	N-CA-C	-6.45	104.23	110.42
18	L	406	ASP	N-CA-CB	6.45	121.39	110.49
29	P	434	THR	N-CA-C	-6.45	104.33	111.36
16	I	302	ILE	CA-C-N	6.45	129.25	120.54
16	I	302	ILE	C-N-CA	6.45	129.25	120.54
26	Z	569	ALA	CA-C-N	6.45	128.82	120.44
26	Z	569	ALA	C-N-CA	6.45	128.82	120.44
31	R	286	LEU	CA-C-O	6.45	127.26	120.42
1	A	13	GLU	N-CA-CB	6.45	120.27	110.28
20	J	381	ASP	CA-C-O	-6.45	113.59	120.42
2	b	13	SER	CA-C-N	6.44	126.13	119.56
2	b	13	SER	C-N-CA	6.44	126.13	119.56
1	a	223	LYS	O-C-N	-6.44	115.91	123.25
2	b	2	THR	CA-C-O	6.44	128.97	120.98
13	m	212	VAL	CB-CA-C	-6.44	102.16	110.98
6	F	161	GLY	CA-C-N	6.44	133.84	121.54
6	F	161	GLY	C-N-CA	6.44	133.84	121.54
27	N	546	LEU	CA-C-O	6.44	127.58	120.82
27	N	329	HIS	CE1-NE2-CD2	-6.44	102.56	109.00
29	P	146	ILE	N-CA-C	-6.44	104.24	110.42
3	C	78	GLY	CA-C-N	6.44	133.83	121.54
3	C	78	GLY	C-N-CA	6.44	133.83	121.54
27	N	468	GLU	CA-C-N	6.43	129.56	120.42
27	N	468	GLU	C-N-CA	6.43	129.56	120.42
7	G	117	GLN	OE1-CD-NE2	-6.43	116.17	122.60
28	S	95	PHE	N-CA-CB	-6.43	100.69	110.01
8	1	120	HIS	CE1-NE2-CD2	-6.43	102.57	109.00
11	4	73	TYR	CA-C-N	-6.43	112.40	121.72
11	4	73	TYR	C-N-CA	-6.43	112.40	121.72
26	Z	366	LYS	CA-C-N	6.43	130.53	121.02
26	Z	366	LYS	C-N-CA	6.43	130.53	121.02
31	R	69	GLU	CB-CA-C	-6.43	96.56	109.99
33	O	344	VAL	N-CA-C	-6.43	106.06	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	120	THR	N-CA-C	-6.43	105.31	113.02
14	n	38	GLY	O-C-N	6.43	130.29	122.32
7	G	123	ASN	N-CA-CB	6.43	119.39	110.07
14	7	219	TRP	CA-C-O	6.43	125.53	118.65
5	E	78	ARG	CA-C-N	6.42	129.41	120.29
5	E	78	ARG	C-N-CA	6.42	129.41	120.29
21	W	163	ASN	O-C-N	-6.42	115.86	121.71
10	j	75	LEU	CA-C-O	-6.42	113.61	120.42
10	3	170	LEU	CA-C-N	6.42	128.79	120.44
10	3	170	LEU	C-N-CA	6.42	128.79	120.44
14	7	33	LEU	O-C-N	-6.42	114.87	122.96
22	V	76	THR	CA-C-N	6.42	133.99	121.41
22	V	76	THR	C-N-CA	6.42	133.99	121.41
6	F	211	SER	CA-C-N	-6.42	114.02	122.94
6	F	211	SER	C-N-CA	-6.42	114.02	122.94
16	I	417	LYS	N-CA-C	-6.42	104.14	112.23
8	1	142	PHE	CB-CG-CD2	-6.42	109.79	120.70
18	L	60	PHE	CB-CG-CD1	6.42	131.61	120.70
3	C	37	ILE	N-CA-C	-6.42	99.13	108.11
7	g	136	GLY	CA-C-O	6.41	125.33	120.91
12	l	191	HIS	ND1-CE1-NE2	6.41	114.81	108.40
13	6	198	VAL	O-C-N	-6.41	115.91	123.03
34	8	391	ARG	NE-CZ-NH1	6.41	127.91	121.50
21	W	79	THR	CA-C-N	6.41	131.01	120.94
21	W	79	THR	C-N-CA	6.41	131.01	120.94
27	N	473	ASP	N-CA-C	-6.41	103.33	111.92
18	L	315	PHE	CA-C-N	6.41	130.43	120.75
18	L	315	PHE	C-N-CA	6.41	130.43	120.75
6	F	207	VAL	N-CA-C	-6.41	104.08	110.62
11	k	32	ASP	O-C-N	6.41	131.11	122.59
14	n	87	LEU	N-CA-CB	6.41	119.45	110.04
20	J	124	LYS	O-C-N	-6.41	115.42	123.17
26	Z	550	PHE	CA-C-N	6.41	128.77	120.44
26	Z	550	PHE	C-N-CA	6.41	128.77	120.44
18	L	128	ILE	N-CA-C	-6.40	98.51	107.80
5	e	53	SER	N-CA-C	6.40	118.26	111.28
13	m	177	VAL	CA-C-N	6.40	129.15	120.38
13	m	177	VAL	C-N-CA	6.40	129.15	120.38
17	K	203	ILE	CA-C-N	6.40	129.79	120.51
17	K	203	ILE	C-N-CA	6.40	129.79	120.51
34	8	324	ASN	N-CA-CB	6.40	121.64	111.91
3	C	44	VAL	O-C-N	-6.40	116.35	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	378	GLU	N-CA-C	6.40	118.34	111.36
28	S	51	ARG	CB-CA-C	-6.40	100.17	110.79
28	S	225	HIS	CE1-NE2-CD2	-6.40	102.60	109.00
2	b	249	ALA	N-CA-C	-6.40	102.61	110.61
5	E	49	PRO	N-CA-C	-6.40	105.71	114.80
15	H	317	ALA	CA-C-N	6.40	129.80	120.71
15	H	317	ALA	C-N-CA	6.40	129.80	120.71
27	N	280	GLN	CA-C-O	-6.40	112.61	119.97
6	f	182	ASP	CA-CB-CG	-6.40	106.20	112.60
9	i	24	PRO	N-CA-C	-6.40	106.36	114.35
15	H	246	ILE	CA-C-N	6.40	132.00	123.05
15	H	246	ILE	C-N-CA	6.40	132.00	123.05
15	H	450	VAL	N-CA-CB	6.40	119.24	110.54
27	N	315	ASN	N-CA-C	6.40	118.33	111.36
3	c	122	THR	CA-C-N	6.39	129.37	120.29
3	c	122	THR	C-N-CA	6.39	129.37	120.29
22	V	19	GLY	CA-C-N	6.39	133.75	121.54
22	V	19	GLY	C-N-CA	6.39	133.75	121.54
25	Y	84	TYR	N-CA-CB	6.39	119.47	109.94
32	U	282	VAL	N-CA-C	6.39	117.14	110.62
4	d	116	GLN	O-C-N	6.39	128.65	122.07
1	A	167	GLN	N-CA-C	6.39	118.25	111.28
27	N	329	HIS	ND1-CE1-NE2	6.39	114.79	108.40
6	f	55	LEU	CA-C-O	-6.39	113.78	120.55
26	Z	382	ALA	CA-C-N	6.39	128.84	120.28
26	Z	382	ALA	C-N-CA	6.39	128.84	120.28
32	U	113	TYR	CB-CA-C	-6.39	100.81	110.90
27	N	466	LEU	CA-C-N	6.39	128.84	120.28
27	N	466	LEU	C-N-CA	6.39	128.84	120.28
7	g	179	HIS	CE1-NE2-CD2	-6.39	102.61	109.00
2	B	198	GLU	N-CA-C	-6.38	104.40	111.36
16	I	356	SER	N-CA-C	6.38	119.22	111.82
31	R	109	LYS	CA-C-N	6.38	133.46	121.97
31	R	109	LYS	C-N-CA	6.38	133.46	121.97
8	h	186	LEU	N-CA-C	-6.38	99.41	109.50
9	2	56	THR	N-CA-CB	6.38	119.50	110.12
6	f	173	ARG	NE-CZ-NH1	6.38	127.88	121.50
5	E	79	SER	CB-CA-C	-6.38	100.00	110.85
20	J	15	HIS	CE1-NE2-CD2	-6.38	102.62	109.00
28	S	478	SER	CA-C-N	6.38	128.83	120.28
28	S	478	SER	C-N-CA	6.38	128.83	120.28
7	g	134	PHE	CA-CB-CG	-6.38	107.42	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	433	GLU	N-CA-C	-6.38	100.53	110.42
11	4	163	LEU	CA-C-O	6.38	127.52	120.63
20	J	89	GLN	CA-C-O	-6.38	111.43	120.16
8	h	24	ALA	N-CA-C	-6.37	105.50	113.28
9	2	75	ARG	O-C-N	-6.37	115.52	122.79
31	R	230	LEU	N-CA-C	-6.37	104.41	111.36
22	V	111	HIS	ND1-CE1-NE2	6.37	114.77	108.40
26	Z	446	GLU	O-C-N	-6.37	115.21	122.09
29	P	370	ASP	CA-CB-CG	-6.37	106.23	112.60
7	G	179	HIS	CE1-NE2-CD2	-6.37	102.63	109.00
23	T	249	MET	N-CA-CB	6.37	121.27	111.46
34	8	204	PHE	N-CA-CB	6.37	120.77	110.77
9	i	86	HIS	O-C-N	6.37	128.97	122.09
10	j	136	ILE	N-CA-C	-6.37	98.95	108.12
17	K	384	ALA	CA-C-N	6.37	128.81	120.28
17	K	384	ALA	C-N-CA	6.37	128.81	120.28
20	J	135	SER	CA-C-N	6.37	128.81	120.28
20	J	135	SER	C-N-CA	6.37	128.81	120.28
4	d	15	ILE	O-C-N	6.36	129.56	122.75
5	e	207	ASN	CA-CB-CG	-6.36	106.24	112.60
12	l	8	PHE	CA-CB-CG	-6.36	107.44	113.80
22	V	238	LEU	CA-C-N	6.36	129.05	120.65
22	V	238	LEU	C-N-CA	6.36	129.05	120.65
24	X	106	SER	N-CA-C	-6.36	104.77	113.30
31	R	174	ILE	CA-C-N	6.36	128.81	120.28
31	R	174	ILE	C-N-CA	6.36	128.81	120.28
6	f	37	LEU	N-CA-CB	6.36	121.42	111.56
11	k	147	HIS	CE1-NE2-CD2	-6.36	102.64	109.00
15	H	45	TYR	N-CA-C	-6.36	105.28	114.12
18	L	337	LEU	N-CA-C	-6.36	105.48	113.18
6	F	57	SER	N-CA-CB	6.36	119.42	109.69
15	H	411	CYS	CA-C-N	6.36	127.79	119.84
15	H	411	CYS	C-N-CA	6.36	127.79	119.84
19	M	368	MET	N-CA-CB	6.36	119.09	110.38
26	Z	506	LEU	N-CA-CB	6.36	119.47	110.12
26	Z	738	TYR	N-CA-C	-6.36	104.27	111.14
26	Z	771	HIS	CA-C-O	6.36	127.50	120.82
31	R	136	ASN	CA-C-N	6.36	128.80	120.28
31	R	136	ASN	C-N-CA	6.36	128.80	120.28
34	8	127	LEU	CA-C-N	6.36	128.80	120.28
34	8	127	LEU	C-N-CA	6.36	128.80	120.28
15	H	432	ARG	NE-CZ-NH2	6.36	124.92	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	144	VAL	CB-CA-C	6.36	120.72	112.14
6	f	60	LYS	CA-C-O	6.36	128.12	120.81
9	i	147	THR	N-CA-CB	6.36	120.63	110.46
6	F	151	ASN	N-CA-C	6.36	119.59	110.24
33	O	371	VAL	CA-C-N	6.36	129.12	120.54
33	O	371	VAL	C-N-CA	6.36	129.12	120.54
10	j	59	VAL	N-CA-CB	6.36	117.56	110.51
12	l	63	CYS	CA-C-O	-6.36	114.15	120.82
19	M	65	ASN	CA-C-N	6.36	129.32	120.29
19	M	65	ASN	C-N-CA	6.36	129.32	120.29
23	T	74	ASN	CA-C-N	6.36	129.12	120.54
23	T	74	ASN	C-N-CA	6.36	129.12	120.54
26	Z	31	LYS	N-CA-CB	6.36	119.29	110.07
33	O	378	GLU	O-C-N	6.36	128.62	122.07
4	D	95	ARG	NE-CZ-NH1	-6.35	115.15	121.50
1	A	123	ALA	CA-C-N	6.35	128.79	120.28
1	A	123	ALA	C-N-CA	6.35	128.79	120.28
19	M	364	HIS	CB-CG-CD2	-6.35	122.94	131.20
26	Z	487	SER	CA-C-O	6.35	127.15	120.42
3	c	83	ALA	N-CA-CB	6.35	119.45	110.12
12	5	53	GLN	O-C-N	6.35	128.61	122.07
17	K	405	SER	CA-C-O	-6.35	113.69	120.42
27	N	110	VAL	N-CA-CB	-6.35	101.91	110.54
5	e	78	ARG	NE-CZ-NH2	-6.35	113.49	119.20
5	e	153	SER	N-CA-C	-6.35	104.58	112.90
6	f	156	TYR	CB-CA-C	-6.35	99.49	110.09
8	h	80	SER	N-CA-C	6.35	118.20	111.28
14	n	162	GLU	N-CA-CB	6.35	119.45	110.12
27	N	235	ALA	CA-C-N	6.35	126.98	120.00
27	N	235	ALA	C-N-CA	6.35	126.98	120.00
6	f	147	GLN	CB-CG-CD	-6.35	101.81	112.60
21	W	135	ASN	N-CA-C	-6.35	105.17	113.17
9	2	203	TYR	N-CA-C	-6.34	102.83	110.44
2	B	221	LEU	N-CA-CB	6.34	119.82	110.56
7	G	221	ASN	CA-CB-CG	-6.34	106.26	112.60
15	H	47	ALA	N-CA-C	-6.34	105.51	113.18
19	M	79	VAL	O-C-N	6.34	129.61	123.14
27	N	217	MET	O-C-N	-6.34	115.49	121.20
3	C	43	ILE	N-CA-C	-6.34	99.09	108.85
4	D	165	ASN	CA-CB-CG	-6.34	106.26	112.60
20	J	64	LEU	CA-C-N	6.34	129.41	120.28
20	J	64	LEU	C-N-CA	6.34	129.41	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	130	LEU	CA-C-N	6.34	128.77	120.28
17	K	130	LEU	C-N-CA	6.34	128.77	120.28
19	M	214	ALA	CA-C-N	6.34	126.71	119.93
19	M	214	ALA	C-N-CA	6.34	126.71	119.93
4	d	81	ARG	N-CA-CB	6.34	119.20	110.01
31	R	112	GLU	N-CA-CB	6.34	120.49	109.72
32	U	58	GLU	N-CA-CB	6.34	121.32	110.68
1	a	14	GLY	N-CA-C	-6.33	106.39	114.37
14	7	88	GLU	CB-CG-CD	-6.33	101.83	112.60
27	N	576	VAL	N-CA-CB	6.33	121.14	110.56
7	G	192	ALA	O-C-N	6.33	128.83	122.12
16	I	279	VAL	N-CA-CB	6.33	119.65	111.67
27	N	459	ASN	CA-CB-CG	-6.33	106.27	112.60
26	Z	142	ASP	CA-C-N	6.33	129.41	120.42
26	Z	142	ASP	C-N-CA	6.33	129.41	120.42
9	i	89	LYS	N-CA-C	6.33	118.18	111.28
1	A	166	GLN	OE1-CD-NE2	-6.33	116.27	122.60
7	G	202	ASP	N-CA-C	-6.33	104.12	113.61
14	7	37	ASN	OD1-CG-ND2	-6.33	116.27	122.60
22	V	144	ILE	CB-CA-C	-6.33	101.85	112.16
27	N	873	ARG	NE-CZ-NH1	6.33	127.83	121.50
31	R	189	GLU	CA-C-N	6.33	128.76	120.28
31	R	189	GLU	C-N-CA	6.33	128.76	120.28
6	f	86	TYR	N-CA-C	-6.33	104.47	111.36
12	l	179	HIS	CG-CD2-NE2	6.33	113.53	107.20
18	L	209	ARG	NE-CZ-NH1	-6.33	115.17	121.50
23	T	102	LYS	N-CA-C	6.33	118.70	111.11
29	P	437	GLU	N-CA-C	-6.33	103.91	111.69
32	U	269	THR	CA-C-N	6.32	129.39	120.28
32	U	269	THR	C-N-CA	6.32	129.39	120.28
8	h	9	LYS	N-CA-CB	6.32	119.52	110.16
32	U	98	LYS	CA-C-N	6.32	130.87	120.94
32	U	98	LYS	C-N-CA	6.32	130.87	120.94
1	a	200	HIS	CE1-NE2-CD2	-6.32	102.68	109.00
11	4	32	ASP	N-CA-CB	6.32	119.26	109.97
27	N	71	ASN	N-CA-C	6.32	119.15	111.82
7	G	85	VAL	N-CA-C	-6.32	104.12	111.00
16	I	75	PHE	CA-C-N	6.32	128.52	120.56
16	I	75	PHE	C-N-CA	6.32	128.52	120.56
34	8	161	VAL	N-CA-C	-6.32	104.34	110.72
2	B	220	ASP	CA-CB-CG	-6.31	106.29	112.60
3	C	10	THR	CA-C-O	-6.31	113.73	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	23	TYR	O-C-N	-6.31	114.51	122.27
6	F	178	PHE	N-CA-C	-6.31	104.28	112.23
27	N	647	ASP	O-C-N	-6.31	115.15	121.27
28	S	131	THR	CA-C-O	-6.31	112.34	119.79
6	f	111	LEU	CB-CA-C	-6.31	98.96	110.63
20	J	277	ASN	N-CA-C	-6.31	105.24	114.39
27	N	254	SER	CA-C-N	6.31	128.73	120.28
27	N	254	SER	C-N-CA	6.31	128.73	120.28
33	O	12	SER	CA-C-O	6.31	127.24	120.55
3	C	124	HIS	CE1-NE2-CD2	-6.31	102.69	109.00
18	L	235	VAL	CA-C-O	-6.30	114.39	120.95
21	W	150	ASN	OD1-CG-ND2	-6.30	116.30	122.60
21	W	156	GLU	CA-C-O	-6.30	113.87	120.55
12	l	203	GLU	N-CA-C	6.30	117.95	111.14
7	G	244	ASN	CB-CA-C	-6.30	98.12	110.10
4	d	40	VAL	N-CA-CB	6.30	120.11	111.41
6	f	136	TYR	CA-C-O	6.30	127.04	120.30
1	A	93	ALA	CB-CA-C	-6.30	100.33	110.79
13	6	43	VAL	N-CA-C	-6.30	100.57	108.89
22	V	147	VAL	N-CA-C	-6.30	106.99	113.10
27	N	359	ALA	N-CA-C	6.30	118.92	110.35
7	G	123	ASN	N-CA-C	-6.30	104.34	111.14
18	L	267	PHE	CA-CB-CG	-6.30	107.50	113.80
9	i	31	CYS	N-CA-C	-6.30	97.38	110.80
1	a	176	HIS	ND1-CE1-NE2	6.30	114.70	108.40
11	4	154	THR	N-CA-C	-6.30	104.50	111.36
13	6	189	THR	N-CA-CB	6.30	119.38	110.12
18	L	319	GLY	CA-C-N	6.30	128.72	120.28
18	L	319	GLY	C-N-CA	6.30	128.72	120.28
13	m	95	HIS	N-CA-C	6.29	119.12	111.82
18	L	296	SER	CA-C-N	6.29	129.34	120.28
18	L	296	SER	C-N-CA	6.29	129.34	120.28
31	R	138	GLY	CA-C-N	6.29	129.22	120.29
31	R	138	GLY	C-N-CA	6.29	129.22	120.29
13	m	48	ASP	CA-CB-CG	-6.29	106.31	112.60
32	U	173	HIS	CE1-NE2-CD2	-6.29	102.71	109.00
26	Z	580	GLN	N-CA-C	-6.29	105.61	113.28
27	N	41	ASN	N-CA-C	-6.29	104.43	111.28
29	P	84	LYS	CA-C-O	-6.29	113.88	120.55
31	R	184	GLN	CA-C-N	6.29	129.22	120.29
31	R	184	GLN	C-N-CA	6.29	129.22	120.29
2	b	159	TRP	CA-C-N	6.29	128.99	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	159	TRP	C-N-CA	6.29	128.99	120.44
1	a	236	LEU	CA-C-N	6.29	129.07	120.46
1	a	236	LEU	C-N-CA	6.29	129.07	120.46
19	M	156	LEU	N-CA-C	-6.29	102.99	112.04
29	P	196	ALA	O-C-N	6.29	128.78	122.12
9	2	139	GLU	CB-CG-CD	-6.28	101.92	112.60
17	K	235	ILE	O-C-N	-6.28	116.94	123.03
23	T	95	LYS	CA-C-N	6.28	133.54	121.54
23	T	95	LYS	C-N-CA	6.28	133.54	121.54
27	N	198	THR	N-CA-C	-6.28	106.20	114.31
33	O	233	LEU	N-CA-C	6.28	118.13	111.28
3	c	135	ILE	N-CA-C	-6.28	98.58	107.75
6	F	99	ASN	OD1-CG-ND2	6.28	128.88	122.60
30	Q	11	ALA	CA-C-O	-6.28	114.22	120.82
5	E	139	HIS	ND1-CE1-NE2	6.28	114.68	108.40
20	J	295	ASN	CA-CB-CG	-6.28	106.32	112.60
22	V	183	ALA	CA-C-O	-6.28	114.89	121.55
28	S	154	GLN	N-CA-C	6.28	117.79	111.07
28	S	343	LEU	CA-C-N	6.28	126.19	119.28
28	S	343	LEU	C-N-CA	6.28	126.19	119.28
15	H	217	GLN	CA-C-N	6.28	129.06	120.46
15	H	217	GLN	C-N-CA	6.28	129.06	120.46
22	V	90	LYS	CA-C-N	6.28	129.20	120.29
22	V	90	LYS	C-N-CA	6.28	129.20	120.29
33	O	27	GLU	CA-C-N	6.28	128.69	120.28
33	O	27	GLU	C-N-CA	6.28	128.69	120.28
19	M	62	ILE	N-CA-C	-6.28	104.22	110.62
14	7	179	ASN	N-CA-C	-6.27	104.36	111.14
1	a	102	ASP	CA-CB-CG	6.27	118.87	112.60
9	i	168	GLY	N-CA-C	-6.27	105.88	115.66
20	J	38	THR	N-CA-C	-6.27	104.52	111.36
31	R	171	MET	CA-C-O	6.27	127.20	120.55
31	R	219	LEU	CA-C-N	6.27	129.19	120.29
31	R	219	LEU	C-N-CA	6.27	129.19	120.29
3	c	16	GLY	N-CA-C	-6.27	106.47	114.37
2	B	198	GLU	CB-CG-CD	-6.27	101.94	112.60
3	C	123	GLN	N-CA-C	-6.27	104.53	111.36
4	D	17	GLN	CB-CA-C	-6.27	99.03	110.63
24	X	71	GLY	N-CA-C	-6.27	106.04	115.32
7	g	12	SER	O-C-N	-6.27	116.02	121.35
5	E	8	SER	O-C-N	6.27	128.45	121.43
34	8	204	PHE	CA-CB-CG	-6.27	107.53	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	239	ARG	CA-C-N	6.27	128.68	120.28
28	S	239	ARG	C-N-CA	6.27	128.68	120.28
6	f	191	ALA	CA-C-O	-6.26	113.86	120.63
7	g	37	LYS	CA-C-N	6.26	132.19	121.29
7	g	37	LYS	C-N-CA	6.26	132.19	121.29
17	K	205	PRO	CA-C-N	6.26	126.29	119.90
17	K	205	PRO	C-N-CA	6.26	126.29	119.90
26	Z	817	LEU	CA-C-O	-6.26	113.85	120.55
28	S	281	ALA	N-CA-C	6.26	118.11	111.28
31	R	305	PHE	CA-C-O	-6.26	111.58	120.16
8	h	171	GLY	CA-C-N	6.26	129.13	120.49
8	h	171	GLY	C-N-CA	6.26	129.13	120.49
26	Z	297	VAL	N-CA-CB	6.26	117.88	110.55
26	Z	630	LYS	N-CA-C	6.26	118.11	111.28
1	a	217	GLY	CA-C-O	6.26	126.52	120.57
19	M	344	ASP	CA-C-N	6.26	133.50	121.54
19	M	344	ASP	C-N-CA	6.26	133.50	121.54
30	Q	255	TYR	CA-C-N	6.26	129.18	120.29
30	Q	255	TYR	C-N-CA	6.26	129.18	120.29
1	a	15	ARG	NE-CZ-NH2	-6.26	113.57	119.20
3	c	119	GLN	N-CA-C	6.26	118.10	111.28
10	3	74	LYS	N-CA-C	-6.26	104.54	111.36
29	P	15	GLN	O-C-N	6.26	128.51	122.07
8	h	82	PHE	CA-CB-CG	-6.25	107.55	113.80
31	R	151	GLU	CB-CA-C	-6.25	101.06	110.88
33	O	100	ASP	CA-C-N	6.25	129.17	120.29
33	O	100	ASP	C-N-CA	6.25	129.17	120.29
6	f	223	ILE	N-CA-C	-6.25	98.73	107.80
9	2	157	ASP	N-CA-C	-6.25	104.54	111.36
17	K	140	HIS	N-CA-CB	6.25	119.23	110.04
28	S	28	GLU	CA-C-N	6.25	128.98	120.54
28	S	28	GLU	C-N-CA	6.25	128.98	120.54
28	S	319	CYS	CA-C-N	6.25	129.03	120.46
28	S	319	CYS	C-N-CA	6.25	129.03	120.46
8	h	65	LEU	CA-C-N	6.25	128.57	120.44
8	h	65	LEU	C-N-CA	6.25	128.57	120.44
4	D	212	VAL	CB-CA-C	-6.25	101.52	110.83
16	I	400	GLY	CA-C-N	6.25	128.66	120.28
16	I	400	GLY	C-N-CA	6.25	128.66	120.28
27	N	118	THR	N-CA-C	-6.25	104.52	111.71
2	B	24	ALA	N-CA-C	-6.25	104.55	111.36
3	C	108	GLU	CB-CG-CD	-6.25	101.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	571	GLY	CA-C-N	6.25	129.29	120.42
26	Z	571	GLY	C-N-CA	6.25	129.29	120.42
26	Z	475	GLN	N-CA-C	6.25	118.09	111.28
27	N	14	ARG	N-CA-CB	6.25	119.92	110.30
27	N	560	ALA	CB-CA-C	-6.25	99.35	109.72
28	S	384	ARG	CA-C-N	6.25	128.65	120.28
28	S	384	ARG	C-N-CA	6.25	128.65	120.28
7	g	7	SER	CA-C-N	6.24	132.33	120.97
7	g	7	SER	C-N-CA	6.24	132.33	120.97
3	C	23	TYR	CA-C-N	6.24	128.65	120.28
3	C	23	TYR	C-N-CA	6.24	128.65	120.28
11	4	23	ARG	NE-CZ-NH2	6.24	124.82	119.20
33	O	115	ARG	NE-CZ-NH2	-6.24	113.58	119.20
8	1	149	GLU	N-CA-CB	6.24	119.40	110.16
17	K	66	ASP	CA-CB-CG	6.24	118.84	112.60
27	N	815	LYS	O-C-N	6.24	128.74	122.12
1	A	154	TYR	N-CA-CB	6.24	122.42	111.13
4	D	109	ARG	CA-C-N	6.24	128.55	120.44
4	D	109	ARG	C-N-CA	6.24	128.55	120.44
6	F	202	ASP	N-CA-CB	6.24	121.03	110.49
18	L	204	PRO	CA-C-N	6.24	128.64	120.28
18	L	204	PRO	C-N-CA	6.24	128.64	120.28
4	d	204	GLY	N-CA-C	-6.24	98.40	113.18
13	m	160	TYR	N-CA-CB	6.24	119.28	110.36
26	Z	804	ASP	CA-C-N	6.24	131.25	122.46
26	Z	804	ASP	C-N-CA	6.24	131.25	122.46
33	O	248	TYR	CB-CA-C	-6.24	100.65	110.94
6	F	148	PRO	CA-C-N	6.23	128.63	120.28
6	F	148	PRO	C-N-CA	6.23	128.63	120.28
7	G	224	HIS	CB-CG-ND1	-6.23	113.35	122.70
20	J	283	GLU	CA-C-N	6.23	128.92	120.44
20	J	283	GLU	C-N-CA	6.23	128.92	120.44
3	c	45	LEU	CB-CA-C	-6.23	100.70	110.74
3	c	178	ASP	CA-CB-CG	-6.23	106.37	112.60
16	I	220	ILE	CB-CA-C	-6.23	101.23	110.33
16	I	418	GLN	CA-C-N	6.23	128.63	120.28
16	I	418	GLN	C-N-CA	6.23	128.63	120.28
21	W	84	LYS	CA-C-N	6.23	129.56	120.71
21	W	84	LYS	C-N-CA	6.23	129.56	120.71
18	L	72	ASP	CA-C-N	6.23	128.63	120.28
18	L	72	ASP	C-N-CA	6.23	128.63	120.28
20	J	328	LEU	CA-C-N	6.23	128.63	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	328	LEU	C-N-CA	6.23	128.63	120.28
26	Z	593	HIS	CB-CG-ND1	6.23	132.04	122.70
33	O	187	SER	CA-C-N	6.23	128.95	120.54
33	O	187	SER	C-N-CA	6.23	128.95	120.54
6	f	3	ASN	CA-CB-CG	-6.23	106.37	112.60
8	l	51	ASP	CB-CA-C	-6.23	100.26	110.85
9	i	31	CYS	N-CA-CB	6.23	121.01	110.49
29	P	290	LEU	N-CA-CB	6.23	119.81	110.22
16	I	355	LEU	CA-C-O	-6.23	113.95	120.55
6	F	207	VAL	CA-C-N	6.22	128.62	120.28
6	F	207	VAL	C-N-CA	6.22	128.62	120.28
33	O	98	TYR	CA-C-N	6.22	128.53	120.44
33	O	98	TYR	C-N-CA	6.22	128.53	120.44
18	L	143	GLY	N-CA-C	-6.22	106.50	115.27
14	n	212	LEU	N-CA-CB	6.22	119.12	110.17
16	I	122	SER	CA-C-N	6.22	125.91	119.56
16	I	122	SER	C-N-CA	6.22	125.91	119.56
25	Y	71	ASP	CA-CB-CG	-6.22	106.38	112.60
30	Q	384	LYS	N-CA-CB	6.22	121.00	110.49
32	U	147	GLY	N-CA-C	-6.22	106.33	115.72
7	g	187	GLU	CA-C-N	6.22	128.61	120.28
7	g	187	GLU	C-N-CA	6.22	128.61	120.28
2	B	31	GLY	O-C-N	6.22	128.99	122.59
5	E	91	HIS	CE1-NE2-CD2	-6.22	102.78	109.00
15	H	202	GLU	N-CA-CB	6.22	120.30	110.23
22	V	123	VAL	CA-C-N	6.22	129.12	120.29
22	V	123	VAL	C-N-CA	6.22	129.12	120.29
23	T	21	ALA	CA-C-O	6.22	127.01	120.42
27	N	31	VAL	CB-CA-C	-6.22	104.19	112.46
3	c	18	LEU	CA-C-N	6.21	128.61	120.28
3	c	18	LEU	C-N-CA	6.21	128.61	120.28
3	c	162	ILE	CA-CB-CG1	6.21	120.96	110.40
21	W	179	ARG	NE-CZ-NH2	6.21	124.79	119.20
26	Z	730	ALA	N-CA-C	-6.21	104.05	111.69
34	8	201	GLN	N-CA-CB	6.21	119.18	110.04
32	U	238	ASN	N-CA-C	-6.21	99.88	109.14
13	m	55	ASN	CA-CB-CG	-6.21	106.39	112.60
18	L	280	MET	N-CA-CB	6.21	119.61	110.35
28	S	32	GLN	N-CA-C	6.21	117.72	111.07
33	O	62	TYR	CB-CG-CD2	-6.21	111.48	120.80
4	D	232	THR	N-CA-CB	6.21	119.35	110.16
28	S	208	ILE	CA-C-N	6.21	128.97	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	208	ILE	C-N-CA	6.21	128.97	120.46
13	m	147	MET	CA-C-O	-6.21	112.32	118.34
27	N	570	ARG	CB-CA-C	-6.21	101.13	110.88
11	k	176	PHE	CA-CB-CG	-6.21	107.59	113.80
29	P	250	ILE	N-CA-C	6.21	116.95	110.62
8	h	21	THR	CA-C-O	6.21	127.40	120.70
12	5	143	ASN	OD1-CG-ND2	6.21	128.81	122.60
12	l	50	ALA	CA-C-O	-6.20	113.84	120.42
3	C	53	SER	N-CA-C	-6.20	101.10	110.28
27	N	251	GLU	CA-C-N	6.20	126.87	119.98
27	N	251	GLU	C-N-CA	6.20	126.87	119.98
13	6	119	LYS	CA-C-O	-6.20	114.80	121.56
6	f	211	SER	O-C-N	6.20	130.92	123.36
15	H	101	ARG	CD-NE-CZ	6.20	133.08	124.40
23	T	51	TYR	CB-CG-CD2	-6.20	111.50	120.80
10	j	95	TYR	CA-C-N	6.20	128.50	120.44
10	j	95	TYR	C-N-CA	6.20	128.50	120.44
11	k	41	HIS	CG-CD2-NE2	6.20	113.40	107.20
3	C	194	LYS	CG-CD-CE	6.20	125.56	111.30
16	I	408	ARG	CA-C-N	6.20	128.91	120.54
16	I	408	ARG	C-N-CA	6.20	128.91	120.54
30	Q	50	ARG	CA-C-N	6.20	133.38	121.54
30	Q	50	ARG	C-N-CA	6.20	133.38	121.54
5	e	36	GLU	CA-C-O	6.20	126.60	119.35
27	N	339	MET	N-CA-C	6.20	118.55	111.11
7	g	179	HIS	CA-C-N	6.20	126.73	120.04
7	g	179	HIS	C-N-CA	6.20	126.73	120.04
9	2	200	GLN	O-C-N	6.20	128.69	122.12
10	3	160	GLU	CA-C-N	6.20	128.87	120.44
10	3	160	GLU	C-N-CA	6.20	128.87	120.44
30	Q	133	LEU	CA-C-N	6.20	128.50	120.44
30	Q	133	LEU	C-N-CA	6.20	128.50	120.44
33	O	283	HIS	ND1-CE1-NE2	6.20	114.60	108.40
3	c	235	LYS	CA-C-N	6.19	128.58	120.28
3	c	235	LYS	C-N-CA	6.19	128.58	120.28
32	U	30	ASN	CA-CB-CG	-6.19	106.41	112.60
1	a	23	PHE	CA-C-N	6.19	128.58	120.28
1	a	23	PHE	C-N-CA	6.19	128.58	120.28
14	n	124	ASP	CA-CB-CG	6.19	118.79	112.60
2	B	90	ARG	CA-C-N	6.19	128.86	120.44
2	B	90	ARG	C-N-CA	6.19	128.86	120.44
9	2	65	LEU	O-C-N	6.19	128.53	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	100	ASN	OD1-CG-ND2	6.19	128.79	122.60
9	i	135	MET	N-CA-C	-6.19	104.59	111.71
17	K	243	VAL	CA-C-N	6.19	133.36	121.54
17	K	243	VAL	C-N-CA	6.19	133.36	121.54
27	N	553	PHE	CA-CB-CG	-6.19	107.61	113.80
28	S	19	HIS	CA-C-N	6.19	128.49	120.44
28	S	19	HIS	C-N-CA	6.19	128.49	120.44
34	8	418	PRO	CB-CA-C	-6.19	102.09	111.44
4	D	173	LEU	N-CA-CB	6.19	119.22	110.12
5	e	64	ARG	NE-CZ-NH1	-6.19	115.31	121.50
1	A	19	VAL	N-CA-C	6.19	116.97	110.72
3	C	126	GLY	CA-C-N	6.19	131.21	121.56
3	C	126	GLY	C-N-CA	6.19	131.21	121.56
7	g	157	LYS	N-CA-C	-6.18	104.80	112.90
24	X	108	ASN	CB-CA-C	-6.18	101.17	110.88
26	Z	814	ALA	CA-C-N	6.18	129.07	120.29
26	Z	814	ALA	C-N-CA	6.18	129.07	120.29
34	8	443	SER	N-CA-C	-6.18	104.22	112.94
3	c	4	ARG	NE-CZ-NH2	-6.18	113.64	119.20
10	j	49	PHE	N-CA-C	-6.18	99.62	109.76
3	C	30	HIS	CA-C-O	6.18	127.07	120.70
6	F	28	ILE	CA-C-O	6.18	127.40	120.85
16	I	252	LEU	N-CA-C	-6.18	104.91	112.88
2	b	122	THR	N-CA-C	-6.18	106.71	114.56
10	j	172	ASN	CA-CB-CG	-6.18	106.42	112.60
19	M	56	ASN	CA-C-N	6.18	128.92	120.46
19	M	56	ASN	C-N-CA	6.18	128.92	120.46
28	S	177	ASN	CA-C-N	6.18	129.18	120.28
28	S	177	ASN	C-N-CA	6.18	129.18	120.28
28	S	317	HIS	CE1-NE2-CD2	-6.18	102.82	109.00
11	k	46	PHE	CA-CB-CG	-6.18	107.62	113.80
2	B	210	GLU	N-CA-C	-6.18	98.45	108.52
27	N	687	THR	N-CA-C	-6.18	104.55	111.28
34	8	214	PHE	CA-CB-CG	-6.18	107.62	113.80
23	T	53	ASN	OD1-CG-ND2	6.17	128.78	122.60
1	a	221	LYS	N-CA-CB	6.17	119.14	109.69
7	G	73	VAL	O-C-N	-6.17	116.21	123.00
27	N	157	ALA	CA-C-O	-6.17	113.88	120.42
23	T	118	ASN	CA-C-N	6.17	128.83	120.44
23	T	118	ASN	C-N-CA	6.17	128.83	120.44
24	X	48	PHE	N-CA-CB	6.17	120.71	110.47
12	5	85	ASN	CB-CA-C	-6.17	101.19	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	233	ALA	N-CA-C	6.17	118.26	110.24
18	L	359	GLU	N-CA-C	-6.17	104.56	111.28
20	J	148	ASP	N-CA-CB	6.17	119.19	110.12
26	Z	371	SER	N-CA-C	-6.17	99.93	109.24
27	N	485	MET	N-CA-C	6.17	117.67	111.07
27	N	589	ILE	CA-C-N	6.17	129.16	120.28
27	N	589	ILE	C-N-CA	6.17	129.16	120.28
32	U	103	ASP	N-CA-C	-6.17	105.72	113.18
12	l	54	PHE	CA-CB-CG	-6.17	107.63	113.80
12	l	82	ILE	N-CA-CB	6.17	117.77	110.55
26	Z	328	ASP	O-C-N	6.17	128.42	122.07
27	N	585	ARG	CA-C-N	6.17	128.54	120.28
27	N	585	ARG	C-N-CA	6.17	128.54	120.28
28	S	162	VAL	N-CA-C	6.17	116.34	110.42
33	O	77	SER	CA-C-O	-6.17	114.02	120.55
33	O	367	LYS	CB-CA-C	-6.16	100.56	110.79
16	I	414	GLU	N-CA-C	6.16	118.08	111.36
18	L	64	LEU	N-CA-C	-6.16	104.64	111.36
18	L	379	ALA	CA-C-N	6.16	130.21	120.47
18	L	379	ALA	C-N-CA	6.16	130.21	120.47
10	j	57	THR	N-CA-CB	6.16	119.17	110.12
4	D	88	ARG	NE-CZ-NH2	-6.16	113.66	119.20
16	I	387	LEU	CA-C-N	6.16	129.88	120.82
16	I	387	LEU	C-N-CA	6.16	129.88	120.82
31	R	395	ASN	CA-C-N	6.16	129.15	120.28
31	R	395	ASN	C-N-CA	6.16	129.15	120.28
13	m	76	HIS	CG-CD2-NE2	6.16	113.36	107.20
17	K	98	GLN	OE1-CD-NE2	-6.16	116.44	122.60
19	M	401	ILE	O-C-N	6.16	127.84	121.87
29	P	23	LYS	CA-C-N	6.16	129.17	120.42
29	P	23	LYS	C-N-CA	6.16	129.17	120.42
27	N	154	LEU	N-CA-C	6.16	117.66	111.07
30	Q	117	VAL	CA-C-O	-6.16	114.64	121.17
3	c	196	LEU	N-CA-C	-6.15	104.57	111.28
9	i	17	ASP	O-C-N	6.15	129.86	122.85
9	2	145	ASP	N-CA-CB	6.15	121.46	111.74
3	c	149	THR	N-CA-C	-6.15	99.70	109.23
9	i	56	THR	N-CA-C	-6.15	104.58	111.28
22	V	158	LEU	N-CA-C	6.15	118.96	110.35
25	Y	82	ASP	CA-C-O	-6.15	114.32	120.90
29	P	110	LEU	N-CA-C	-6.15	97.70	110.80
7	g	111	ARG	CA-C-O	6.15	127.03	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	GLN	CB-CA-C	-6.15	100.58	110.79
23	T	10	SER	N-CA-C	-6.15	104.66	111.36
34	8	401	ASN	O-C-N	6.15	128.64	122.12
6	f	96	LEU	N-CA-CB	6.15	119.26	110.16
1	A	194	VAL	N-CA-C	-6.15	104.51	110.72
1	a	138	ASP	N-CA-CB	6.14	119.02	110.17
10	j	45	TYR	N-CA-C	-6.14	97.27	108.02
16	I	205	PRO	N-CA-C	-6.14	105.97	114.27
33	O	363	ILE	CA-C-N	6.14	128.51	120.28
33	O	363	ILE	C-N-CA	6.14	128.51	120.28
15	H	80	HIS	CA-CB-CG	-6.14	107.66	113.80
26	Z	48	ASP	CA-CB-CG	-6.14	106.46	112.60
28	S	143	GLN	CB-CG-CD	-6.14	102.16	112.60
32	U	287	ALA	N-CA-C	6.14	118.06	111.36
34	8	406	ASP	CA-C-N	6.14	128.43	120.44
34	8	406	ASP	C-N-CA	6.14	128.43	120.44
4	D	89	VAL	N-CA-C	-6.14	104.76	110.53
12	l	139	VAL	CA-C-N	6.14	128.75	120.65
12	l	139	VAL	C-N-CA	6.14	128.75	120.65
24	X	92	SER	CA-C-N	6.14	134.56	124.31
24	X	92	SER	C-N-CA	6.14	134.56	124.31
27	N	89	PHE	N-CA-C	-6.14	105.95	113.50
31	R	224	PHE	CA-C-N	6.14	128.79	120.44
31	R	224	PHE	C-N-CA	6.14	128.79	120.44
34	8	425	ASN	CA-C-O	-6.14	113.62	120.25
27	N	622	ALA	CB-CA-C	-6.14	100.42	110.85
28	S	227	ASN	N-CA-C	6.14	118.05	111.36
4	d	165	ASN	CA-CB-CG	-6.14	106.46	112.60
27	N	560	ALA	N-CA-CB	6.14	119.10	109.83
32	U	131	GLY	CA-C-N	6.14	132.86	121.69
32	U	131	GLY	C-N-CA	6.14	132.86	121.69
23	T	272	ASN	OD1-CG-ND2	6.13	128.74	122.60
22	V	172	GLN	N-CA-C	-6.13	104.71	111.82
29	P	231	LYS	N-CA-C	-6.13	105.38	112.92
31	R	117	ILE	N-CA-CB	6.13	118.88	110.54
2	b	67	LEU	N-CA-C	-6.13	103.21	112.04
7	G	138	ASP	N-CA-C	-6.13	99.38	109.80
14	7	128	ARG	NE-CZ-NH1	6.13	127.63	121.50
18	L	174	GLU	N-CA-CB	6.13	120.85	110.49
23	T	115	SER	N-CA-C	-6.13	105.06	112.54
3	c	218	GLY	O-C-N	6.13	130.43	122.71
12	5	53	GLN	CA-C-N	6.13	128.81	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	53	GLN	C-N-CA	6.13	128.81	120.54
2	b	23	TYR	N-CA-CB	6.13	119.23	110.16
8	h	42	TRP	CG-CD2-CE3	-6.13	127.77	133.90
13	6	148	PRO	N-CA-CB	6.13	110.01	103.39
16	I	279	VAL	CB-CA-C	-6.13	102.67	111.19
1	A	58	THR	CA-C-O	6.12	127.04	120.55
2	B	139	HIS	N-CA-CB	6.12	121.10	110.81
3	C	13	SER	O-C-N	-6.12	114.57	121.43
13	6	15	ILE	CA-C-N	6.12	130.80	122.84
13	6	15	ILE	C-N-CA	6.12	130.80	122.84
17	K	195	ALA	CA-C-N	6.12	128.49	120.28
17	K	195	ALA	C-N-CA	6.12	128.49	120.28
21	W	86	HIS	ND1-CE1-NE2	6.12	114.52	108.40
28	S	98	SER	N-CA-CB	6.12	119.18	109.51
34	8	181	PRO	N-CA-C	-6.12	106.84	114.68
2	B	239	THR	CA-C-N	6.12	128.76	120.38
2	B	239	THR	C-N-CA	6.12	128.76	120.38
4	D	111	VAL	N-CA-C	6.12	116.30	110.42
19	M	165	SER	N-CA-C	-6.12	104.72	111.82
32	U	158	PRO	CA-N-CD	6.12	120.57	112.00
28	S	82	TYR	CA-C-O	6.12	125.37	119.62
33	O	335	GLY	N-CA-C	-6.12	106.48	115.72
34	8	202	GLY	CA-C-O	-6.12	109.92	120.57
13	6	110	ILE	CA-C-O	6.12	127.10	120.43
18	L	425	VAL	O-C-N	6.12	128.72	121.80
28	S	275	TYR	CB-CG-CD2	6.12	129.98	120.80
29	P	147	LYS	CA-C-N	6.12	128.98	120.29
29	P	147	LYS	C-N-CA	6.12	128.98	120.29
7	G	21	GLU	CA-C-N	6.12	128.47	120.28
7	G	21	GLU	C-N-CA	6.12	128.47	120.28
1	A	176	HIS	CG-CD2-NE2	6.11	113.31	107.20
31	R	134	TRP	O-C-N	-6.11	114.75	122.27
3	c	218	GLY	N-CA-C	-6.11	107.08	114.66
4	d	169	VAL	CA-CB-CG1	6.11	120.79	110.40
6	f	13	SER	O-C-N	-6.11	115.12	121.60
4	D	166	SER	N-CA-C	-6.11	105.65	113.23
26	Z	355	GLU	CB-CG-CD	-6.11	102.21	112.60
6	F	122	TYR	N-CA-CB	6.11	119.11	109.71
34	8	197	GLU	N-CA-CB	6.11	119.09	110.36
2	b	88	LYS	CA-C-N	6.11	128.96	120.29
2	b	88	LYS	C-N-CA	6.11	128.96	120.29
17	K	241	GLU	CA-C-O	6.11	126.89	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	25	TYR	CA-C-N	6.10	128.38	120.44
28	S	25	TYR	C-N-CA	6.10	128.38	120.44
7	g	90	GLU	CB-CG-CD	-6.10	102.22	112.60
13	m	26	ASP	N-CA-CB	6.10	119.56	110.29
7	G	168	ALA	N-CA-C	6.10	117.93	111.28
28	S	425	ARG	N-CA-CB	6.10	119.09	110.12
29	P	121	THR	N-CA-C	6.10	118.01	111.36
26	Z	861	THR	O-C-N	-6.10	114.47	122.59
1	a	213	ASP	O-C-N	6.10	129.40	122.20
15	H	80	HIS	N-CA-C	-6.10	106.16	113.97
26	Z	17	GLN	CA-C-O	6.10	127.22	120.82
26	Z	707	LYS	CA-C-N	6.10	126.88	119.99
26	Z	707	LYS	C-N-CA	6.10	126.88	119.99
32	U	132	LEU	N-CA-C	-6.10	101.05	109.71
1	A	42	THR	CA-C-O	6.10	126.82	120.30
3	C	101	TYR	CA-C-O	6.10	125.61	118.90
26	Z	271	ILE	O-C-N	6.10	128.11	121.83
27	N	622	ALA	N-CA-CB	6.10	119.18	110.16
30	Q	49	LYS	CA-C-N	6.10	128.95	120.29
30	Q	49	LYS	C-N-CA	6.10	128.95	120.29
31	R	36	SER	CB-CA-C	-6.10	99.86	110.17
34	8	202	GLY	O-C-N	6.10	130.63	122.70
8	1	42	TRP	N-CA-C	-6.10	100.22	109.85
7	g	143	HIS	CA-CB-CG	6.09	119.89	113.80
26	Z	2	VAL	N-CA-C	-6.09	106.80	112.83
3	C	124	HIS	CG-CD2-NE2	6.09	113.29	107.20
9	i	170	GLY	CA-C-O	6.09	127.11	121.38
13	m	35	ILE	N-CA-CB	6.09	118.33	111.21
13	m	76	HIS	ND1-CE1-NE2	6.09	114.49	108.40
7	G	123	ASN	CA-C-N	6.09	128.44	120.28
7	G	123	ASN	C-N-CA	6.09	128.44	120.28
1	a	213	ASP	CA-CB-CG	-6.09	106.51	112.60
26	Z	197	LYS	CA-C-O	-6.09	114.43	120.82
30	Q	398	TYR	N-CA-C	-6.09	99.79	109.59
34	8	247	ASP	CA-C-N	6.09	128.35	120.44
34	8	247	ASP	C-N-CA	6.09	128.35	120.44
14	n	55	GLY	O-C-N	6.08	128.13	122.90
10	3	42	ILE	CA-C-N	6.08	132.14	122.59
10	3	42	ILE	C-N-CA	6.08	132.14	122.59
11	4	117	TYR	N-CA-CB	6.08	120.12	110.57
19	M	394	VAL	CA-C-N	6.08	128.35	120.44
19	M	394	VAL	C-N-CA	6.08	128.35	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	147	GLU	CA-C-N	6.08	126.86	119.99
26	Z	147	GLU	C-N-CA	6.08	126.86	119.99
8	h	42	TRP	CD2-CE2-CZ2	-6.08	116.32	122.40
26	Z	351	PRO	N-CA-C	-6.08	107.68	114.92
26	Z	928	ARG	N-CA-CB	6.08	120.08	110.23
33	O	269	LEU	CB-CA-C	-6.08	101.29	110.90
17	K	277	ILE	N-CA-C	-6.08	105.14	111.58
13	m	68	PHE	CA-CB-CG	-6.08	107.72	113.80
15	H	450	VAL	CB-CA-C	-6.08	103.94	112.14
26	Z	610	GLY	O-C-N	-6.08	114.80	122.70
29	P	199	LEU	O-C-N	6.08	128.56	122.12
1	a	36	VAL	N-CA-CB	6.08	121.02	112.52
7	g	170	ALA	CA-C-N	6.08	128.42	120.28
7	g	170	ALA	C-N-CA	6.08	128.42	120.28
12	5	66	HIS	CA-CB-CG	6.08	119.88	113.80
21	W	69	PHE	CA-C-N	6.08	126.68	120.00
21	W	69	PHE	C-N-CA	6.08	126.68	120.00
21	W	178	PRO	O-C-N	6.08	130.26	122.85
28	S	206	GLN	CA-C-N	6.08	128.92	120.29
28	S	206	GLN	C-N-CA	6.08	128.92	120.29
4	d	226	GLU	CB-CG-CD	-6.07	102.27	112.60
11	k	8	ARG	CA-C-N	6.07	132.90	121.97
11	k	8	ARG	C-N-CA	6.07	132.90	121.97
7	G	180	PRO	CA-C-N	6.07	128.33	120.44
7	G	180	PRO	C-N-CA	6.07	128.33	120.44
10	3	114	LYS	CA-C-O	-6.07	112.37	119.05
22	V	250	GLN	CA-C-O	6.07	126.95	119.97
27	N	331	ALA	CA-C-N	6.07	128.78	120.46
27	N	331	ALA	C-N-CA	6.07	128.78	120.46
28	S	60	LEU	CA-C-N	6.07	128.42	120.28
28	S	60	LEU	C-N-CA	6.07	128.42	120.28
29	P	364	ARG	CA-C-N	6.07	128.91	120.29
29	P	364	ARG	C-N-CA	6.07	128.91	120.29
8	1	189	TYR	CB-CG-CD1	6.07	129.91	120.80
18	L	416	MET	CA-C-N	6.07	128.41	120.28
18	L	416	MET	C-N-CA	6.07	128.41	120.28
20	J	133	LEU	CA-C-N	6.07	128.21	120.56
20	J	133	LEU	C-N-CA	6.07	128.21	120.56
10	3	69	LYS	CA-C-N	6.07	129.53	120.31
10	3	69	LYS	C-N-CA	6.07	129.53	120.31
21	W	102	GLN	CB-CG-CD	-6.07	102.28	112.60
27	N	378	ASN	CA-C-N	6.07	129.02	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	378	ASN	C-N-CA	6.07	129.02	120.28
1	a	200	HIS	ND1-CE1-NE2	6.07	114.47	108.40
4	d	112	ALA	CA-C-N	6.07	127.93	120.22
4	d	112	ALA	C-N-CA	6.07	127.93	120.22
5	e	149	HIS	ND1-CE1-NE2	6.07	114.47	108.40
14	n	180	ALA	CB-CA-C	-6.07	100.53	110.85
8	l	157	HIS	CE1-NE2-CD2	-6.07	102.93	109.00
13	6	213	ARG	CA-C-O	6.07	128.02	121.16
17	K	48	TYR	CA-CB-CG	-6.07	102.98	113.90
26	Z	536	GLY	CA-C-O	-6.07	112.27	119.06
34	8	249	ASP	CA-CB-CG	-6.07	106.53	112.60
6	F	98	PHE	CA-C-N	6.07	133.12	121.54
6	F	98	PHE	C-N-CA	6.07	133.12	121.54
12	5	94	GLY	N-CA-C	-6.07	105.74	115.08
15	H	165	PRO	CA-C-N	6.06	130.84	120.72
15	H	165	PRO	C-N-CA	6.06	130.84	120.72
20	J	20	LYS	CA-C-O	-6.06	112.75	118.33
25	Y	25	ASN	OD1-CG-ND2	-6.06	116.54	122.60
28	S	176	LEU	CA-C-N	6.06	128.40	120.28
28	S	176	LEU	C-N-CA	6.06	128.40	120.28
34	8	437	THR	CA-C-N	6.06	132.08	122.62
34	8	437	THR	C-N-CA	6.06	132.08	122.62
1	a	82	ARG	CA-C-N	6.06	128.32	120.44
1	a	82	ARG	C-N-CA	6.06	128.32	120.44
8	h	92	ASN	CA-CB-CG	-6.06	106.54	112.60
6	F	150	GLY	CA-C-N	6.06	129.72	121.05
6	F	150	GLY	C-N-CA	6.06	129.72	121.05
16	I	82	LEU	N-CA-CB	6.06	118.80	110.01
24	X	79	LYS	N-CA-CB	6.06	120.00	111.15
7	g	14	ASP	CA-CB-CG	-6.06	106.54	112.60
1	A	176	HIS	ND1-CE1-NE2	6.06	114.46	108.40
6	F	119	THR	N-CA-C	-6.06	105.55	113.12
26	Z	197	LYS	CA-C-N	6.06	128.72	120.54
26	Z	197	LYS	C-N-CA	6.06	128.72	120.54
3	c	18	LEU	N-CA-C	6.05	119.14	110.24
11	k	161	LEU	N-CA-C	6.05	117.88	111.28
3	C	226	GLN	OE1-CD-NE2	6.05	128.65	122.60
1	a	25	ALA	CA-C-N	6.05	128.99	120.28
1	a	25	ALA	C-N-CA	6.05	128.99	120.28
19	M	87	ASP	N-CA-CB	6.05	120.78	110.50
7	g	194	LYS	O-C-N	-6.05	115.71	122.12
13	m	71	SER	CB-CA-C	-6.05	100.75	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	287	GLY	CA-C-N	6.05	128.38	120.28
15	H	287	GLY	C-N-CA	6.05	128.38	120.28
29	P	53	ALA	O-C-N	6.05	128.30	122.07
30	Q	355	GLU	CA-C-N	-6.05	112.25	121.26
30	Q	355	GLU	C-N-CA	-6.05	112.25	121.26
17	K	427	TYR	CB-CA-C	-6.04	100.50	110.72
31	R	114	ASN	N-CA-CB	6.04	120.71	110.49
3	c	26	GLU	CB-CG-CD	-6.04	102.33	112.60
4	d	119	THR	N-CA-CB	6.04	119.00	110.12
5	e	158	ARG	CA-C-N	6.04	132.00	122.21
5	e	158	ARG	C-N-CA	6.04	132.00	122.21
11	k	171	ARG	N-CA-C	-6.04	105.67	113.16
4	D	170	ARG	CD-NE-CZ	6.04	132.86	124.40
16	I	212	GLY	CA-C-N	6.04	129.57	120.75
16	I	212	GLY	C-N-CA	6.04	129.57	120.75
18	L	364	HIS	CE1-NE2-CD2	-6.04	102.96	109.00
30	Q	92	LYS	CA-C-N	6.04	128.38	120.28
30	Q	92	LYS	C-N-CA	6.04	128.38	120.28
8	h	96	GLY	CA-C-N	6.04	131.05	123.14
8	h	96	GLY	C-N-CA	6.04	131.05	123.14
14	n	201	ASP	CA-CB-CG	-6.04	106.56	112.60
29	P	337	HIS	CA-C-N	6.04	128.87	120.29
29	P	337	HIS	C-N-CA	6.04	128.87	120.29
15	H	434	ARG	CA-C-N	6.04	132.25	122.29
15	H	434	ARG	C-N-CA	6.04	132.25	122.29
14	n	186	TYR	CA-C-O	-6.04	114.02	120.42
3	C	242	GLY	CA-C-O	-6.04	112.12	119.06
15	H	55	ASP	CB-CA-C	-6.04	101.40	110.88
17	K	244	HIS	CG-CD2-NE2	6.04	113.24	107.20
28	S	202	ASN	N-CA-C	-6.04	104.62	112.23
28	S	328	PRO	CA-C-O	-6.04	114.35	122.08
11	k	193	ASP	CA-CB-CG	-6.04	106.56	112.60
2	b	107	THR	CA-C-N	6.04	128.86	120.29
2	b	107	THR	C-N-CA	6.04	128.86	120.29
12	l	29	GLN	N-CA-C	-6.03	105.10	112.88
1	A	236	LEU	CA-C-N	6.03	128.73	120.46
1	A	236	LEU	C-N-CA	6.03	128.73	120.46
6	F	125	ARG	CA-C-O	-6.03	113.76	119.55
9	2	77	VAL	O-C-N	-6.03	114.98	121.80
27	N	466	LEU	CA-C-O	6.03	126.79	119.31
33	O	304	ASN	CA-C-O	6.03	126.33	119.27
34	8	320	LYS	N-CA-CB	6.03	119.50	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	281	ALA	N-CA-CB	6.03	118.99	110.12
33	O	379	LYS	O-C-N	6.03	128.51	122.12
9	i	22	GLN	N-CA-C	-6.03	97.29	108.02
27	N	609	LEU	N-CA-C	-6.03	105.57	113.17
34	8	373	GLU	O-C-N	-6.03	114.35	122.43
3	C	140	ASP	CA-CB-CG	-6.03	106.57	112.60
26	Z	608	TYR	N-CA-C	-6.03	105.92	113.28
34	8	380	ASP	CA-CB-CG	-6.03	106.57	112.60
6	f	173	ARG	NH1-CZ-NH2	-6.03	111.46	119.30
9	i	206	PRO	CA-C-O	-6.03	114.42	121.95
4	D	77	ASN	CA-C-N	6.03	128.28	120.44
4	D	77	ASN	C-N-CA	6.03	128.28	120.44
6	F	141	ALA	CA-C-O	6.03	127.91	121.16
7	G	136	GLY	N-CA-C	-6.03	102.32	111.42
19	M	300	GLU	CA-C-N	6.03	128.72	120.46
19	M	300	GLU	C-N-CA	6.03	128.72	120.46
27	N	375	HIS	CA-C-N	6.03	129.27	120.71
27	N	375	HIS	C-N-CA	6.03	129.27	120.71
7	G	87	ARG	CA-C-N	6.03	126.67	119.98
7	G	87	ARG	C-N-CA	6.03	126.67	119.98
19	M	304	THR	N-CA-C	-6.03	105.89	113.18
3	C	93	HIS	CA-CB-CG	-6.02	107.78	113.80
6	F	123	GLY	O-C-N	-6.02	117.18	122.90
20	J	318	PRO	O-C-N	6.02	124.08	121.31
33	O	203	THR	N-CA-C	-6.02	105.24	112.59
13	m	135	GLN	N-CA-C	-6.02	104.64	111.14
30	Q	95	LYS	N-CA-CB	6.02	119.07	110.16
1	a	169	ILE	O-C-N	-6.02	116.03	121.87
7	g	214	TRP	CG-CD2-CE3	-6.02	127.88	133.90
14	n	122	ASN	O-C-N	6.02	129.26	122.22
1	A	224	PHE	N-CA-C	-6.02	99.59	109.40
8	1	142	PHE	O-C-N	6.02	130.41	122.95
12	5	199	LYS	CA-C-N	6.02	128.70	120.46
12	5	199	LYS	C-N-CA	6.02	128.70	120.46
26	Z	5	SER	CA-C-O	-6.02	112.78	119.34
6	f	20	GLN	CB-CG-CD	-6.01	102.38	112.60
6	f	199	SER	O-C-N	-6.01	115.88	122.07
14	n	92	ILE	CA-C-O	6.01	127.23	120.85
10	3	83	PRO	CB-CA-C	-6.01	103.53	112.55
18	L	118	ILE	N-CA-C	-6.01	99.76	108.36
21	W	94	ALA	CA-C-N	6.01	128.83	120.29
21	W	94	ALA	C-N-CA	6.01	128.83	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	68	VAL	CA-C-O	-6.01	114.47	120.85
26	Z	807	VAL	O-C-N	-6.01	115.00	121.80
24	X	17	TYR	CA-C-N	6.01	132.35	121.89
24	X	17	TYR	C-N-CA	6.01	132.35	121.89
10	3	135	PHE	CA-CB-CG	6.01	119.81	113.80
10	3	163	PHE	CA-C-O	-6.01	114.18	120.55
15	H	425	GLU	CA-C-N	6.01	128.33	120.28
15	H	425	GLU	C-N-CA	6.01	128.33	120.28
16	I	213	ILE	N-CA-C	-6.01	101.81	109.80
30	Q	132	PHE	CA-CB-CG	-6.01	107.79	113.80
31	R	96	GLN	N-CA-CB	6.01	120.37	110.39
6	f	11	THR	N-CA-CB	6.01	120.90	110.81
6	f	122	TYR	CA-C-O	-6.01	114.58	121.19
25	Y	66	ASP	CA-C-N	6.01	128.95	120.42
25	Y	66	ASP	C-N-CA	6.01	128.95	120.42
30	Q	307	ASN	CA-CB-CG	-6.01	106.59	112.60
6	F	225	ASP	CA-C-O	-6.01	115.01	121.38
7	G	105	ILE	CA-C-O	-6.01	113.74	118.85
23	T	170	ASN	N-CA-C	-6.01	103.10	110.61
26	Z	363	ASP	CA-CB-CG	6.01	118.61	112.60
33	O	310	PHE	CA-CB-CG	-6.01	107.79	113.80
33	O	388	GLY	CA-C-N	6.01	128.82	120.29
33	O	388	GLY	C-N-CA	6.01	128.82	120.29
21	W	119	SER	N-CA-C	-6.00	104.07	113.02
18	L	177	GLU	CA-C-O	-6.00	114.08	120.92
12	l	208	ASN	OD1-CG-ND2	6.00	128.60	122.60
12	l	49	ALA	N-CA-C	6.00	117.82	111.28
27	N	120	ASP	O-C-N	-6.00	116.39	123.41
18	L	376	PHE	CA-C-N	6.00	128.32	120.28
18	L	376	PHE	C-N-CA	6.00	128.32	120.28
31	R	258	LEU	CA-C-N	6.00	128.24	120.44
31	R	258	LEU	C-N-CA	6.00	128.24	120.44
33	O	198	THR	CA-C-N	6.00	133.00	121.54
33	O	198	THR	C-N-CA	6.00	133.00	121.54
12	l	76	VAL	N-CA-C	-6.00	104.66	110.72
8	1	81	VAL	CB-CA-C	-6.00	103.94	112.22
28	S	43	LYS	CA-C-N	6.00	132.99	121.54
28	S	43	LYS	C-N-CA	6.00	132.99	121.54
29	P	189	LEU	CA-C-N	6.00	128.92	120.28
29	P	189	LEU	C-N-CA	6.00	128.92	120.28
6	F	216	GLY	CA-C-O	6.00	127.62	121.21
20	J	399	SER	CA-C-N	6.00	129.94	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	399	SER	C-N-CA	6.00	129.94	120.47
31	R	417	TYR	CA-C-O	-6.00	114.07	120.42
1	A	238	ALA	CA-C-O	5.99	126.77	120.42
16	I	97	GLU	CA-C-N	5.99	129.12	120.79
16	I	97	GLU	C-N-CA	5.99	129.12	120.79
16	I	151	HIS	CE1-NE2-CD2	-5.99	103.01	109.00
31	R	195	ASN	O-C-N	-5.99	114.40	122.43
33	O	381	GLY	N-CA-C	-5.99	104.87	113.86
20	J	377	VAL	CA-C-O	5.99	126.41	121.68
33	O	71	ASP	CA-C-N	5.99	128.23	120.44
33	O	71	ASP	C-N-CA	5.99	128.23	120.44
33	O	259	THR	CA-CB-OG1	5.99	118.59	109.60
4	d	138	PRO	CA-C-N	5.99	131.37	122.74
4	d	138	PRO	C-N-CA	5.99	131.37	122.74
2	B	43	VAL	N-CA-C	-5.99	99.42	108.17
4	D	27	ARG	O-C-N	5.99	128.98	122.15
24	X	70	PRO	CA-C-O	-5.99	114.12	121.31
18	L	176	GLY	N-CA-C	-5.99	105.05	111.93
23	T	207	ALA	CA-C-N	5.99	128.30	120.28
23	T	207	ALA	C-N-CA	5.99	128.30	120.28
14	7	72	THR	CA-C-O	-5.99	114.20	120.55
15	H	455	LYS	N-CA-CB	5.99	118.66	109.98
31	R	147	LYS	CA-C-O	-5.99	113.09	119.97
16	I	361	ILE	CA-C-N	5.98	128.30	120.28
16	I	361	ILE	C-N-CA	5.98	128.30	120.28
29	P	295	SER	CA-C-N	5.98	128.79	120.29
29	P	295	SER	C-N-CA	5.98	128.79	120.29
19	M	349	PHE	N-CA-CB	5.98	118.57	110.14
23	T	56	MET	N-CA-C	-5.98	104.67	111.07
27	N	338	PHE	CA-CB-CG	5.98	119.78	113.80
30	Q	222	SER	CA-C-N	5.98	126.58	119.94
30	Q	222	SER	C-N-CA	5.98	126.58	119.94
33	O	302	VAL	CA-C-N	5.98	129.36	120.87
33	O	302	VAL	C-N-CA	5.98	129.36	120.87
33	O	318	HIS	ND1-CE1-NE2	5.98	114.38	108.40
3	c	215	ILE	N-CA-C	-5.98	98.52	107.37
7	g	235	ALA	CA-C-N	5.98	128.09	120.56
7	g	235	ALA	C-N-CA	5.98	128.09	120.56
18	L	365	THR	CA-C-N	5.98	128.29	120.28
18	L	365	THR	C-N-CA	5.98	128.29	120.28
23	T	53	ASN	CA-C-N	5.98	129.40	120.31
23	T	53	ASN	C-N-CA	5.98	129.40	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	124	ASP	CA-C-N	5.98	128.57	120.44
10	j	124	ASP	C-N-CA	5.98	128.57	120.44
13	m	159	GLN	O-C-N	5.98	130.22	122.87
18	L	270	ALA	CA-C-N	5.98	128.29	120.28
18	L	270	ALA	C-N-CA	5.98	128.29	120.28
26	Z	4	GLU	N-CA-C	-5.98	105.81	112.57
33	O	245	ASP	CA-CB-CG	-5.98	106.62	112.60
2	b	104	TYR	CA-C-N	-5.98	114.22	120.38
2	b	104	TYR	C-N-CA	-5.98	114.22	120.38
7	g	220	THR	O-C-N	-5.98	115.00	122.35
8	1	38	HIS	ND1-CE1-NE2	5.98	114.38	108.40
8	1	144	GLU	N-CA-CB	5.97	120.38	110.52
7	g	224	HIS	CB-CG-CD2	-5.97	123.44	131.20
16	I	239	GLN	CA-C-N	5.97	128.88	120.28
16	I	239	GLN	C-N-CA	5.97	128.88	120.28
17	K	63	LEU	CA-C-N	5.97	128.28	120.28
17	K	63	LEU	C-N-CA	5.97	128.28	120.28
17	K	43	VAL	CA-C-N	5.97	128.28	120.28
17	K	43	VAL	C-N-CA	5.97	128.28	120.28
18	L	269	TYR	CA-C-O	5.97	126.75	120.42
33	O	283	HIS	CE1-NE2-CD2	-5.97	103.03	109.00
7	g	31	THR	CA-C-N	5.97	129.32	120.90
7	g	31	THR	C-N-CA	5.97	129.32	120.90
9	2	144	GLN	CB-CA-C	-5.97	100.59	109.90
19	M	351	LEU	CA-C-N	5.97	125.93	119.78
19	M	351	LEU	C-N-CA	5.97	125.93	119.78
28	S	204	ASP	CA-CB-CG	-5.97	106.63	112.60
6	F	109	HIS	CB-CG-CD2	-5.97	123.44	131.20
6	F	186	ASP	CA-C-N	5.97	129.38	120.31
6	F	186	ASP	C-N-CA	5.97	129.38	120.31
2	b	7	PHE	N-CA-CB	5.97	119.49	110.30
17	K	292	VAL	CA-C-N	5.97	128.20	120.44
17	K	292	VAL	C-N-CA	5.97	128.20	120.44
31	R	104	LYS	CB-CA-C	-5.97	101.77	110.96
4	D	68	HIS	CG-CD2-NE2	5.96	113.17	107.20
15	H	320	ASP	N-CA-CB	5.96	119.09	110.20
20	J	282	PHE	CB-CA-C	-5.96	97.84	110.31
26	Z	513	ALA	N-CA-C	-5.96	105.97	113.72
32	U	80	CYS	CA-C-O	-5.96	111.91	119.31
34	8	120	LEU	N-CA-C	-5.96	104.86	111.36
4	d	221	ALA	O-C-N	-5.96	116.21	123.19
23	T	151	TRP	CE2-CD2-CE3	5.96	124.76	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	33	ASP	CA-C-N	5.96	128.19	120.44
27	N	33	ASP	C-N-CA	5.96	128.19	120.44
14	n	112	ASN	CA-C-N	5.96	131.39	122.99
14	n	112	ASN	C-N-CA	5.96	131.39	122.99
6	F	127	TYR	N-CA-CB	5.96	118.81	109.69
27	N	203	ARG	CA-C-O	5.96	127.07	120.63
27	N	340	HIS	O-C-N	5.96	129.59	122.26
27	N	534	ASP	N-CA-C	-5.96	104.69	111.07
9	i	218	VAL	N-CA-CB	5.96	120.86	112.52
2	B	123	GLN	N-CA-CB	5.96	118.83	110.07
12	5	70	GLU	N-CA-C	-5.96	105.97	113.72
28	S	102	SER	N-CA-C	-5.96	98.11	110.80
11	k	117	TYR	CA-CB-CG	-5.96	103.18	113.90
1	A	84	ALA	CA-C-N	5.96	128.26	120.28
1	A	84	ALA	C-N-CA	5.96	128.26	120.28
16	I	99	ILE	CA-C-O	5.96	127.66	121.05
19	M	27	THR	CA-C-N	5.96	128.75	120.29
19	M	27	THR	C-N-CA	5.96	128.75	120.29
6	f	105	GLU	N-CA-C	-5.95	104.87	111.36
15	H	386	ALA	N-CA-C	-5.95	104.87	111.36
27	N	873	ARG	NE-CZ-NH2	-5.95	113.84	119.20
30	Q	369	ASP	CA-CB-CG	5.95	118.55	112.60
31	R	274	PRO	CA-C-N	5.95	128.26	120.28
31	R	274	PRO	C-N-CA	5.95	128.26	120.28
27	N	335	ALA	CA-C-N	5.95	128.26	120.28
27	N	335	ALA	C-N-CA	5.95	128.26	120.28
34	8	372	ARG	CB-CA-C	-5.95	100.56	110.68
12	l	158	LYS	CB-CA-C	-5.95	101.50	110.90
33	O	41	LEU	N-CA-C	-5.95	104.87	111.36
4	d	193	THR	CA-C-N	5.95	128.61	120.46
4	d	193	THR	C-N-CA	5.95	128.61	120.46
14	7	57	ILE	N-CA-C	-5.95	104.71	110.72
33	O	101	ASP	CA-CB-CG	-5.95	106.65	112.60
33	O	246	SER	N-CA-CB	5.95	118.87	110.12
12	l	89	GLN	N-CA-CB	5.95	119.38	110.22
19	M	412	HIS	CA-CB-CG	-5.95	107.85	113.80
27	N	721	ASP	CA-CB-CG	-5.95	106.65	112.60
9	2	32	ALA	N-CA-CB	5.95	118.71	109.97
20	J	283	GLU	CA-C-O	-5.95	114.58	120.70
29	P	257	TRP	N-CA-CB	5.95	119.50	110.28
1	a	60	VAL	N-CA-C	-5.94	98.58	107.37
6	f	119	THR	N-CA-C	-5.94	106.16	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	227	ILE	N-CA-C	-5.94	98.32	107.71
5	E	115	PHE	CA-CB-CG	-5.94	107.86	113.80
6	f	174	THR	N-CA-C	-5.94	105.89	113.02
7	g	179	HIS	ND1-CE1-NE2	5.94	114.34	108.40
20	J	290	ILE	N-CA-CB	5.94	118.73	111.60
26	Z	518	LEU	CA-C-N	5.94	125.62	119.56
26	Z	518	LEU	C-N-CA	5.94	125.62	119.56
7	g	87	ARG	CA-C-N	5.94	127.56	120.14
7	g	87	ARG	C-N-CA	5.94	127.56	120.14
13	6	67	ARG	O-C-N	-5.94	115.38	122.15
1	A	20	GLU	N-CA-C	-5.94	104.81	111.28
18	L	159	LEU	CA-C-N	5.94	127.26	119.84
18	L	159	LEU	C-N-CA	5.94	127.26	119.84
28	S	20	HIS	CE1-NE2-CD2	-5.94	103.06	109.00
32	U	246	GLU	N-CA-C	5.94	117.75	111.28
33	O	357	ILE	CA-C-N	5.94	129.85	121.66
33	O	357	ILE	C-N-CA	5.94	129.85	121.66
34	8	222	SER	N-CA-CB	5.94	118.85	110.12
34	8	337	PHE	CB-CG-CD1	-5.94	110.61	120.70
12	l	42	LEU	N-CA-CB	5.94	121.16	110.83
1	A	153	TYR	O-C-N	-5.94	115.51	122.81
29	P	395	ARG	CA-C-O	-5.94	113.17	118.63
30	Q	7	LYS	CA-C-N	5.94	128.16	120.44
30	Q	7	LYS	C-N-CA	5.94	128.16	120.44
10	j	67	ARG	N-CA-C	-5.93	104.73	111.14
2	B	190	HIS	CA-C-N	5.93	128.59	120.46
2	B	190	HIS	C-N-CA	5.93	128.59	120.46
34	8	309	PHE	CA-CB-CG	-5.93	107.87	113.80
8	1	40	LYS	N-CA-C	-5.93	103.29	110.88
16	I	167	MET	CA-C-N	5.93	128.03	120.56
16	I	167	MET	C-N-CA	5.93	128.03	120.56
18	L	408	ASP	N-CA-C	-5.93	104.70	112.41
19	M	166	ARG	CA-C-N	5.93	128.84	120.42
19	M	166	ARG	C-N-CA	5.93	128.84	120.42
26	Z	824	ASN	CA-C-O	5.93	125.55	119.97
15	H	356	ASN	OD1-CG-ND2	-5.93	116.67	122.60
22	V	209	GLU	CA-C-N	5.93	128.23	120.28
22	V	209	GLU	C-N-CA	5.93	128.23	120.28
25	Y	29	LEU	CA-C-N	5.93	129.32	120.31
25	Y	29	LEU	C-N-CA	5.93	129.32	120.31
31	R	325	HIS	ND1-CE1-NE2	5.93	114.33	108.40
8	1	62	HIS	CE1-NE2-CD2	-5.93	103.07	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	456	ASP	CA-C-O	-5.93	112.04	120.16
9	i	57	GLN	CA-C-O	5.93	126.70	120.42
3	c	190	GLU	CA-C-N	5.93	128.22	120.28
3	c	190	GLU	C-N-CA	5.93	128.22	120.28
9	i	37	ILE	N-CA-C	-5.93	105.94	111.45
12	5	20	ALA	N-CA-CB	5.93	120.37	110.59
19	M	412	HIS	ND1-CE1-NE2	5.93	114.33	108.40
21	W	127	ARG	CB-CA-C	-5.93	100.78	110.85
20	J	90	PRO	N-CA-CB	5.92	109.20	103.51
23	T	121	LYS	CA-C-N	5.92	128.14	120.44
23	T	121	LYS	C-N-CA	5.92	128.14	120.44
27	N	399	PHE	CA-CB-CG	-5.92	107.88	113.80
6	f	231	LYS	O-C-N	-5.92	115.84	122.12
21	W	178	PRO	N-CA-CB	5.92	108.52	103.19
7	g	203	ASN	N-CA-C	-5.92	104.27	112.03
8	h	81	VAL	O-C-N	5.92	127.93	121.83
15	H	303	ALA	N-CA-CB	5.92	120.50	110.49
4	d	116	GLN	CA-C-O	-5.92	114.61	120.82
14	7	48	ASN	O-C-N	5.92	128.39	122.12
18	L	379	ALA	O-C-N	-5.92	115.85	122.12
34	8	400	LEU	N-CA-CB	5.92	118.59	110.01
7	G	149	PRO	N-CA-C	-5.92	106.95	114.35
20	J	206	THR	CA-CB-OG1	5.92	118.47	109.60
30	Q	336	ASN	CA-CB-CG	-5.92	106.68	112.60
7	g	61	VAL	N-CA-CB	5.92	120.07	110.13
4	D	171	GLU	N-CA-C	-5.92	104.83	111.28
9	2	37	ILE	N-CA-C	-5.91	105.08	110.82
11	4	158	LEU	CB-CA-C	-5.91	100.80	110.85
13	m	57	PHE	N-CA-CB	5.91	118.81	109.71
12	l	55	TRP	CB-CG-CD2	-5.91	118.53	126.80
2	B	201	GLU	CB-CA-C	-5.91	99.71	109.99
6	F	206	THR	N-CA-CB	5.91	118.73	110.04
10	3	189	ILE	N-CA-C	-5.91	99.12	107.75
17	K	334	LEU	CA-C-N	5.91	129.29	120.31
17	K	334	LEU	C-N-CA	5.91	129.29	120.31
20	J	63	ARG	CA-C-O	-5.91	113.17	119.97
28	S	131	THR	N-CA-CB	5.91	119.40	110.30
4	d	220	VAL	O-C-N	-5.91	116.49	123.05
9	i	88	PHE	CA-CB-CG	-5.91	107.89	113.80
2	B	240	SER	CA-C-N	5.91	128.20	120.28
2	B	240	SER	C-N-CA	5.91	128.20	120.28
4	D	13	GLY	N-CA-C	-5.91	107.50	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	351	LEU	CA-C-O	-5.91	114.29	120.55
28	S	123	THR	O-C-N	5.91	128.38	122.12
30	Q	46	VAL	CA-C-N	5.91	132.82	121.54
30	Q	46	VAL	C-N-CA	5.91	132.82	121.54
20	J	75	VAL	N-CA-C	-5.91	100.20	108.12
24	X	71	GLY	O-C-N	-5.91	115.35	122.38
11	k	98	TYR	CB-CA-C	-5.91	102.84	111.23
12	5	51	ASP	CA-C-N	5.91	128.12	120.44
12	5	51	ASP	C-N-CA	5.91	128.12	120.44
3	c	82	ASP	CA-C-N	5.90	128.19	120.28
3	c	82	ASP	C-N-CA	5.90	128.19	120.28
5	E	92	ASN	N-CA-CB	5.90	119.43	110.28
28	S	462	ASP	O-C-N	5.90	128.38	122.12
30	Q	235	ALA	CA-C-N	5.90	128.19	120.28
30	Q	235	ALA	C-N-CA	5.90	128.19	120.28
2	b	117	ILE	N-CA-C	-5.90	104.60	110.62
1	A	126	ARG	CA-C-N	5.90	125.66	119.76
1	A	126	ARG	C-N-CA	5.90	125.66	119.76
27	N	499	HIS	N-CA-C	-5.90	104.93	111.36
30	Q	254	SER	N-CA-C	-5.90	106.08	113.28
8	h	112	THR	N-CA-CB	5.90	120.59	110.68
8	l	177	VAL	N-CA-C	-5.90	99.38	107.99
13	6	97	LEU	CB-CA-C	-5.90	100.82	110.85
8	l	45	ARG	N-CA-C	5.90	118.57	109.07
15	H	428	MET	N-CA-C	5.90	117.79	111.36
26	Z	959	HIS	N-CA-C	-5.90	103.81	111.71
5	e	174	GLU	N-CA-CB	5.89	118.78	110.12
18	L	67	HIS	CE1-NE2-CD2	-5.89	103.11	109.00
14	n	76	TYR	N-CA-CB	5.89	118.66	110.17
14	n	225	ILE	CB-CA-C	5.89	119.23	111.33
2	B	94	HIS	CA-C-O	5.89	126.67	120.42
4	D	33	GLY	CA-C-O	-5.89	116.34	120.94
12	5	90	TYR	N-CA-C	5.89	120.47	113.16
29	P	438	ILE	N-CA-C	-5.89	104.58	111.00
1	a	116	SER	CB-CA-C	-5.89	101.01	110.79
5	e	122	GLU	CA-C-O	5.89	127.59	120.99
4	D	10	SER	N-CA-CB	5.89	120.85	110.37
5	E	85	ARG	NE-CZ-NH2	-5.89	113.90	119.20
12	5	166	HIS	CB-CG-ND1	5.89	131.54	122.70
16	I	102	ASN	CA-CB-CG	-5.89	106.71	112.60
27	N	146	LYS	CA-C-O	-5.89	114.18	120.42
11	k	9	VAL	CA-C-N	5.89	128.17	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	9	VAL	C-N-CA	5.89	128.17	120.28
10	3	182	TRP	CB-CG-CD2	-5.89	118.56	126.80
15	H	275	ILE	N-CA-CB	5.89	119.64	112.10
33	O	93	ASP	N-CA-CB	5.89	118.87	110.16
4	D	42	LEU	CA-C-O	5.88	126.48	120.24
6	F	190	LYS	N-CA-C	5.88	118.17	111.11
23	T	26	LEU	N-CA-C	-5.88	106.26	113.50
6	f	187	GLU	N-CA-C	-5.88	105.00	111.82
6	f	151	ASN	N-CA-CB	5.88	120.00	110.77
11	k	19	LYS	CG-CD-CE	5.88	124.83	111.30
1	A	196	PHE	CB-CA-C	-5.88	101.03	110.79
5	E	180	HIS	O-C-N	-5.88	116.34	123.10
33	O	328	VAL	CA-CB-CG2	-5.88	100.40	110.40
3	c	179	TYR	N-CA-CB	5.88	118.61	109.85
14	7	220	ASP	CA-CB-CG	-5.88	106.72	112.60
19	M	207	PHE	CA-CB-CG	-5.88	107.92	113.80
1	a	78	ILE	O-C-N	-5.88	115.90	120.07
10	3	152	LEU	N-CA-CB	5.88	118.86	110.16
16	I	271	ALA	CA-C-N	5.88	126.47	120.00
16	I	271	ALA	C-N-CA	5.88	126.47	120.00
8	h	102	TYR	N-CA-CB	5.88	119.99	110.77
27	N	85	ALA	CA-C-N	5.88	130.51	122.34
27	N	85	ALA	C-N-CA	5.88	130.51	122.34
1	A	133	THR	CA-C-O	5.87	126.57	120.40
12	5	79	ALA	N-CA-C	5.87	117.76	111.36
23	T	183	SER	CA-C-N	5.87	128.15	120.28
23	T	183	SER	C-N-CA	5.87	128.15	120.28
34	8	108	PRO	N-CD-CG	5.87	112.01	103.20
14	n	155	LEU	N-CA-CB	-5.87	101.18	110.28
6	F	92	ASN	OD1-CG-ND2	5.87	128.47	122.60
9	2	111	PHE	CB-CA-C	-5.87	97.75	109.79
15	H	159	LEU	N-CA-CB	5.87	118.63	110.17
34	8	391	ARG	CD-NE-CZ	-5.87	116.18	124.40
2	b	195	THR	N-CA-CB	-5.87	101.49	110.12
12	l	164	ALA	N-CA-C	-5.87	104.79	111.07
15	H	429	PHE	CB-CA-C	-5.87	99.40	110.67
16	I	354	ASP	CA-CB-CG	5.87	118.47	112.60
28	S	186	TYR	CB-CG-CD2	-5.87	112.00	120.80
34	8	174	LYS	N-CA-CB	5.87	119.38	110.28
34	8	276	LEU	CA-C-O	-5.87	114.33	120.55
1	a	212	ASN	CA-CB-CG	5.87	118.47	112.60
21	W	86	HIS	CE1-NE2-CD2	-5.87	103.13	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	50	LYS	CA-C-O	5.87	126.98	120.82
26	Z	633	GLU	N-CA-C	-5.87	105.02	111.82
32	U	292	ILE	CA-C-N	5.87	129.22	120.31
32	U	292	ILE	C-N-CA	5.87	129.22	120.31
9	i	114	HIS	CE1-NE2-CD2	-5.86	103.14	109.00
13	m	97	LEU	CA-C-O	-5.86	114.33	120.55
14	n	220	ASP	N-CA-CB	5.86	118.74	110.12
3	C	113	ARG	CA-C-O	-5.86	114.66	120.82
18	L	253	ASP	CA-CB-CG	5.86	118.46	112.60
19	M	71	ASN	OD1-CG-ND2	5.86	128.46	122.60
21	W	21	PHE	CA-CB-CG	-5.86	107.94	113.80
21	W	182	TYR	CA-C-N	5.86	128.62	120.29
21	W	182	TYR	C-N-CA	5.86	128.62	120.29
28	S	101	LYS	CA-C-N	5.86	132.74	121.54
28	S	101	LYS	C-N-CA	5.86	132.74	121.54
32	U	34	VAL	N-CA-C	-5.86	99.68	108.12
26	Z	332	ASN	CA-CB-CG	-5.86	106.74	112.60
12	l	19	ARG	CA-C-N	5.86	131.09	123.00
12	l	19	ARG	C-N-CA	5.86	131.09	123.00
17	K	98	GLN	CG-CD-OE1	5.86	132.52	120.80
17	K	417	THR	CB-CA-C	5.86	120.05	111.73
31	R	244	THR	CA-C-N	5.86	132.73	121.54
31	R	244	THR	C-N-CA	5.86	132.73	121.54
7	g	95	PHE	CA-CB-CG	-5.86	107.94	113.80
2	B	101	TYR	N-CA-C	-5.86	105.45	113.30
20	J	64	LEU	CB-CA-C	-5.86	101.64	110.90
13	6	203	GLU	O-C-N	5.86	130.18	123.27
17	K	347	ARG	CA-C-N	5.86	128.13	120.28
17	K	347	ARG	C-N-CA	5.86	128.13	120.28
20	J	201	ALA	N-CA-CB	5.86	118.83	110.16
27	N	301	THR	N-CA-CB	5.86	118.83	110.16
34	8	192	TYR	CA-C-N	5.86	125.96	119.87
34	8	192	TYR	C-N-CA	5.86	125.96	119.87
7	g	178	HIS	CE1-NE2-CD2	-5.86	103.14	109.00
26	Z	386	VAL	CA-C-N	5.86	128.40	120.38
26	Z	386	VAL	C-N-CA	5.86	128.40	120.38
29	P	176	LYS	CB-CA-C	-5.86	100.90	110.85
5	E	180	HIS	CB-CA-C	-5.85	97.80	111.09
30	Q	338	LEU	CA-C-N	5.85	128.44	120.54
30	Q	338	LEU	C-N-CA	5.85	128.44	120.54
3	c	113	ARG	O-C-N	5.85	128.10	122.07
1	A	94	GLU	CA-C-N	5.85	128.12	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	GLU	C-N-CA	5.85	128.12	120.28
5	E	76	ASP	N-CA-CB	5.85	119.23	110.22
21	W	8	LEU	CA-C-N	5.85	129.69	122.37
21	W	8	LEU	C-N-CA	5.85	129.69	122.37
26	Z	807	VAL	N-CA-C	-5.85	103.77	111.09
8	1	132	THR	CA-C-N	5.85	129.20	120.31
8	1	132	THR	C-N-CA	5.85	129.20	120.31
15	H	53	GLU	N-CA-C	5.85	117.66	111.28
14	n	40	GLU	CA-C-N	5.85	131.03	122.08
14	n	40	GLU	C-N-CA	5.85	131.03	122.08
26	Z	56	LEU	N-CA-C	-5.85	105.99	114.12
30	Q	78	ILE	CA-C-N	5.85	125.95	119.87
30	Q	78	ILE	C-N-CA	5.85	125.95	119.87
30	Q	365	ILE	N-CA-C	5.85	116.03	110.53
32	U	215	ILE	CA-C-O	-5.85	114.12	119.91
8	h	55	ILE	N-CA-C	-5.85	104.81	110.42
19	M	288	THR	N-CA-C	5.85	119.31	111.24
27	N	429	GLU	CA-C-O	5.85	126.72	120.70
12	l	7	ARG	CB-CA-C	-5.85	99.89	109.53
12	l	55	TRP	N-CA-CB	5.85	119.93	110.40
21	W	5	ALA	N-CA-C	-5.85	99.37	108.90
28	S	206	GLN	OE1-CD-NE2	-5.84	116.76	122.60
31	R	261	LEU	CA-C-N	5.84	130.75	120.87
31	R	261	LEU	C-N-CA	5.84	130.75	120.87
34	8	488	SER	CA-C-N	5.84	129.01	120.71
34	8	488	SER	C-N-CA	5.84	129.01	120.71
11	k	7	ILE	CA-C-N	5.84	131.23	123.05
11	k	7	ILE	C-N-CA	5.84	131.23	123.05
7	G	178	HIS	CE1-NE2-CD2	-5.84	103.16	109.00
16	I	172	LYS	N-CA-CB	5.84	119.18	109.60
30	Q	166	LYS	N-CA-C	-5.84	105.04	111.82
1	a	61	SER	N-CA-CB	5.84	118.56	109.97
6	f	97	VAL	CA-C-O	5.84	126.96	120.71
14	n	169	THR	CA-C-N	5.84	128.46	120.46
14	n	169	THR	C-N-CA	5.84	128.46	120.46
26	Z	717	THR	N-CA-CB	5.84	118.91	110.20
27	N	63	LEU	N-CA-CB	5.84	118.54	110.07
16	I	165	ASP	CA-CB-CG	-5.84	106.76	112.60
26	Z	201	LEU	N-CA-CB	5.84	118.90	110.20
26	Z	603	VAL	N-CA-C	-5.84	104.38	112.50
34	8	304	SER	N-CA-C	-5.84	106.00	114.12
9	i	200	GLN	CA-C-O	5.84	126.61	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	218	GLU	CA-C-O	5.84	128.18	121.47
11	k	138	PHE	N-CA-C	-5.84	106.16	113.28
4	D	151	SER	CB-CA-C	5.84	120.52	110.01
18	L	423	ALA	CA-C-O	-5.84	114.36	120.55
25	Y	74	THR	O-C-N	5.84	128.31	122.12
13	m	105	TYR	N-CA-C	-5.83	99.01	108.52
11	4	92	ILE	N-CA-C	-5.83	104.39	112.50
22	V	149	GLY	CA-C-N	5.83	128.68	120.28
22	V	149	GLY	C-N-CA	5.83	128.68	120.28
8	h	31	THR	CA-C-N	5.83	130.72	122.09
8	h	31	THR	C-N-CA	5.83	130.72	122.09
1	A	58	THR	CA-C-N	5.83	128.57	120.29
1	A	58	THR	C-N-CA	5.83	128.57	120.29
12	5	117	SER	CB-CA-C	-5.83	101.11	110.79
28	S	260	PRO	N-CA-C	-5.83	102.70	111.57
34	8	458	GLU	CA-C-O	5.83	126.56	119.38
6	f	88	ARG	CA-C-N	5.83	128.09	120.28
6	f	88	ARG	C-N-CA	5.83	128.09	120.28
29	P	40	LEU	CA-C-O	-5.83	114.37	120.55
6	f	39	SER	N-CA-C	-5.83	101.57	110.14
6	F	109	HIS	ND1-CE1-NE2	5.83	114.23	108.40
17	K	82	ALA	N-CA-CB	5.83	118.79	110.16
26	Z	710	SER	N-CA-CB	5.83	118.79	110.16
10	j	144	GLN	CA-C-O	5.83	126.94	120.82
12	l	26	VAL	N-CA-CB	5.83	118.15	111.39
9	2	198	GLU	N-CA-CB	5.83	118.61	109.69
18	L	330	PRO	CB-CA-C	-5.83	101.94	111.56
23	T	65	GLY	CA-C-N	5.83	128.57	120.29
23	T	65	GLY	C-N-CA	5.83	128.57	120.29
28	S	431	VAL	CA-C-O	5.83	127.94	120.83
6	f	33	VAL	N-CA-CB	5.83	117.47	110.95
1	A	166	GLN	N-CA-CB	5.83	119.19	110.22
7	G	153	TYR	CA-C-O	-5.83	114.30	121.06
11	k	73	TYR	N-CA-C	-5.82	98.11	108.13
30	Q	186	HIS	N-CA-CB	5.82	118.78	110.16
34	8	182	ILE	N-CA-C	-5.82	105.06	110.53
1	a	99	TYR	O-C-N	5.82	128.19	122.19
3	c	110	LEU	CA-C-N	5.82	128.69	120.42
3	c	110	LEU	C-N-CA	5.82	128.69	120.42
14	n	35	ARG	NH1-CZ-NH2	5.82	126.86	119.30
11	k	78	GLN	CA-C-N	5.82	128.55	120.29
11	k	78	GLN	C-N-CA	5.82	128.55	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	T	214	GLU	CB-CG-CD	-5.82	102.71	112.60
26	Z	709	LYS	CB-CA-C	-5.82	101.71	110.90
5	e	128	ARG	NE-CZ-NH2	-5.82	113.97	119.20
17	K	205	PRO	N-CA-CB	5.82	106.45	103.19
22	V	199	LEU	CA-C-N	5.82	129.10	120.90
22	V	199	LEU	C-N-CA	5.82	129.10	120.90
33	O	58	ARG	N-CA-C	5.82	118.40	111.71
4	D	78	ALA	N-CA-CB	5.81	118.44	110.01
9	2	193	PRO	N-CA-CB	5.81	109.36	103.25
11	4	76	SER	CA-C-N	5.81	125.49	119.56
11	4	76	SER	C-N-CA	5.81	125.49	119.56
20	J	181	GLN	CA-C-N	5.81	126.14	119.92
20	J	181	GLN	C-N-CA	5.81	126.14	119.92
27	N	350	LYS	O-C-N	5.81	128.28	122.12
27	N	716	GLN	OE1-CD-NE2	-5.81	116.79	122.60
27	N	770	LYS	CA-C-N	5.81	131.75	122.10
27	N	770	LYS	C-N-CA	5.81	131.75	122.10
28	S	99	ASN	CA-CB-CG	-5.81	106.79	112.60
32	U	50	ASN	CA-C-N	5.81	131.80	121.75
32	U	50	ASN	C-N-CA	5.81	131.80	121.75
3	c	87	ILE	CB-CA-C	-5.81	104.53	111.97
14	n	161	ARG	CA-C-N	5.81	128.07	120.28
14	n	161	ARG	C-N-CA	5.81	128.07	120.28
29	P	416	SER	CB-CA-C	-5.81	101.14	110.79
12	l	3	THR	CA-C-O	-5.81	114.31	121.11
16	I	352	ASN	N-CA-C	-5.81	102.33	109.65
20	J	127	GLU	CA-C-N	5.81	132.63	121.54
20	J	127	GLU	C-N-CA	5.81	132.63	121.54
27	N	310	ASP	CA-CB-CG	-5.81	106.79	112.60
4	d	73	PHE	CA-C-O	5.81	127.60	121.33
5	e	92	ASN	CA-CB-CG	-5.81	106.79	112.60
14	n	59	ASP	O-C-N	5.81	130.11	122.33
3	C	152	PRO	N-CA-C	-5.81	106.60	113.86
16	I	350	PHE	CA-CB-CG	-5.81	107.99	113.80
17	K	374	ARG	N-CA-C	-5.81	105.03	111.36
8	1	87	TYR	N-CA-C	5.81	117.69	111.36
25	Y	68	GLU	CA-C-N	5.81	132.42	121.97
25	Y	68	GLU	C-N-CA	5.81	132.42	121.97
10	j	201	MET	N-CA-C	-5.80	100.25	109.07
7	G	17	ASN	CA-CB-CG	-5.80	106.80	112.60
16	I	145	CYS	O-C-N	-5.80	116.56	123.06
26	Z	593	HIS	CA-C-N	5.80	125.67	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	593	HIS	C-N-CA	5.80	125.67	119.28
34	8	170	ASN	N-CA-C	5.80	117.69	111.36
7	g	115	TYR	N-CA-C	5.80	117.61	111.28
5	E	39	VAL	CB-CA-C	-5.80	102.04	110.63
8	h	163	ILE	CA-C-O	-5.80	114.70	120.85
12	l	53	GLN	N-CA-CB	5.80	118.64	109.82
11	4	83	PHE	N-CA-CB	5.80	118.64	109.82
18	L	170	MET	CA-C-N	5.80	128.53	120.29
18	L	170	MET	C-N-CA	5.80	128.53	120.29
27	N	565	ASN	CA-C-N	5.80	128.05	120.28
27	N	565	ASN	C-N-CA	5.80	128.05	120.28
28	S	183	LEU	CA-C-N	5.80	128.63	120.28
28	S	183	LEU	C-N-CA	5.80	128.63	120.28
28	S	374	ASP	CA-CB-CG	-5.80	106.80	112.60
29	P	125	VAL	CA-C-N	5.80	132.62	121.54
29	P	125	VAL	C-N-CA	5.80	132.62	121.54
34	8	130	VAL	CA-C-N	5.80	127.98	120.44
34	8	130	VAL	C-N-CA	5.80	127.98	120.44
3	C	234	ILE	O-C-N	-5.80	116.23	121.91
9	2	13	VAL	N-CA-C	-5.80	99.87	108.45
28	S	145	PHE	CA-C-N	5.80	127.98	120.44
28	S	145	PHE	C-N-CA	5.80	127.98	120.44
12	l	183	ASP	CA-CB-CG	-5.80	106.80	112.60
4	D	40	VAL	N-CA-C	-5.80	99.99	108.11
12	5	61	SER	N-CA-CB	5.80	118.48	110.07
27	N	923	MET	N-CA-CB	5.80	118.64	110.12
2	b	84	VAL	CB-CA-C	-5.80	104.22	112.22
9	i	33	LYS	CA-C-O	5.80	126.64	119.97
11	k	83	PHE	O-C-N	5.80	128.04	122.07
16	I	114	ASP	CA-CB-CG	-5.80	106.80	112.60
23	T	155	GLY	N-CA-C	-5.80	106.99	115.63
31	R	341	LEU	CA-C-O	-5.80	114.28	120.42
22	V	222	GLN	CB-CG-CD	-5.79	102.75	112.60
2	B	117	ILE	O-C-N	5.79	127.49	121.87
12	5	196	LEU	CD1-CG-CD2	-5.79	98.05	110.80
18	L	157	ARG	CA-C-N	5.79	128.40	120.35
18	L	157	ARG	C-N-CA	5.79	128.40	120.35
23	T	45	SER	N-CA-C	-5.79	106.38	113.50
26	Z	236	PHE	CA-C-N	5.79	132.40	121.97
26	Z	236	PHE	C-N-CA	5.79	132.40	121.97
27	N	129	ILE	CB-CA-C	-5.79	106.08	112.68
2	b	221	LEU	N-CA-CB	5.79	119.06	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	LEU	CA-C-N	5.79	128.51	120.29
1	A	86	LEU	C-N-CA	5.79	128.51	120.29
14	7	32	SER	O-C-N	5.79	128.26	122.12
24	X	12	ALA	CA-C-N	-5.79	117.32	122.47
24	X	12	ALA	C-N-CA	-5.79	117.32	122.47
8	h	60	GLN	OE1-CD-NE2	-5.79	116.81	122.60
3	C	148	TYR	N-CA-CB	5.79	121.76	111.69
20	J	331	HIS	CG-CD2-NE2	5.79	112.99	107.20
26	Z	92	LEU	CA-C-N	5.79	129.54	120.97
26	Z	92	LEU	C-N-CA	5.79	129.54	120.97
27	N	690	HIS	CA-C-O	5.79	125.75	119.15
32	U	258	SER	CA-C-N	5.79	128.51	120.29
32	U	258	SER	C-N-CA	5.79	128.51	120.29
34	8	219	HIS	CG-ND1-CE1	-5.79	99.46	109.30
32	U	2	SER	N-CA-C	-5.79	102.34	110.50
2	b	109	LEU	CA-C-O	-5.79	114.74	120.70
9	i	134	ALA	O-C-N	5.79	129.75	122.23
13	m	93	ILE	CA-C-O	5.79	126.97	120.95
6	F	28	ILE	O-C-N	-5.79	115.87	121.83
20	J	75	VAL	N-CA-CB	5.79	117.65	111.46
34	8	182	ILE	CA-C-O	-5.79	114.63	121.05
34	8	306	LEU	N-CA-CB	5.79	117.85	110.04
3	c	196	LEU	N-CA-CB	5.78	118.62	110.12
19	M	168	LYS	CA-C-N	5.78	128.50	120.29
19	M	168	LYS	C-N-CA	5.78	128.50	120.29
4	D	228	ASN	CA-C-N	5.78	128.50	120.29
4	D	228	ASN	C-N-CA	5.78	128.50	120.29
3	c	134	PHE	CA-CB-CG	-5.78	108.02	113.80
13	m	41	PRO	CA-N-CD	-5.78	103.91	112.00
18	L	367	LYS	N-CA-CB	5.78	118.39	110.01
31	R	164	THR	N-CA-C	-5.78	104.98	111.28
13	6	126	ASP	CA-C-N	5.78	125.31	119.19
13	6	126	ASP	C-N-CA	5.78	125.31	119.19
30	Q	39	SER	CA-C-N	5.78	132.58	121.54
30	Q	39	SER	C-N-CA	5.78	132.58	121.54
12	l	87	VAL	N-CA-CB	5.78	120.53	110.65
1	A	106	ASP	CA-CB-CG	-5.78	106.82	112.60
6	F	76	LEU	CA-C-O	5.78	127.45	120.81
16	I	251	GLU	N-CA-C	-5.78	106.19	113.18
28	S	65	ASN	CA-C-N	5.78	128.34	120.54
28	S	65	ASN	C-N-CA	5.78	128.34	120.54
29	P	319	GLU	N-CA-CB	5.78	118.91	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	112	ILE	CB-CA-C	-5.78	101.90	110.33
12	l	115	VAL	CA-CB-CG1	5.78	120.22	110.40
6	F	43	ALA	CA-C-O	5.78	127.38	120.28
6	F	190	LYS	CA-C-N	5.78	128.02	120.28
6	F	190	LYS	C-N-CA	5.78	128.02	120.28
18	L	392	ARG	N-CA-C	-5.78	104.98	111.28
20	J	280	ASP	N-CA-CB	5.78	120.25	110.49
26	Z	560	THR	CA-C-O	5.78	126.54	120.42
27	N	617	VAL	CA-C-N	5.78	128.60	120.28
27	N	617	VAL	C-N-CA	5.78	128.60	120.28
20	J	204	HIS	CE1-NE2-CD2	-5.77	103.23	109.00
11	k	51	GLY	CA-C-N	5.77	128.49	120.29
11	k	51	GLY	C-N-CA	5.77	128.49	120.29
6	F	195	ALA	CA-C-O	-5.77	114.30	120.42
10	3	59	VAL	N-CA-CB	5.77	117.30	110.55
9	i	150	GLU	CB-CG-CD	-5.77	102.79	112.60
10	3	132	ALA	N-CA-CB	5.77	118.52	109.69
12	5	161	ILE	CA-C-O	-5.77	114.24	120.47
16	I	78	ASN	CA-C-O	-5.77	114.44	120.55
22	V	131	GLN	CA-C-N	5.77	128.26	120.65
22	V	131	GLN	C-N-CA	5.77	128.26	120.65
26	Z	349	THR	O-C-N	5.77	128.73	122.15
27	N	365	PHE	CA-C-O	-5.77	114.30	120.42
27	N	798	LYS	CA-C-N	5.77	128.36	120.46
27	N	798	LYS	C-N-CA	5.77	128.36	120.46
34	8	257	SER	CA-C-O	-5.77	115.06	121.23
12	l	204	GLU	N-CA-CB	5.77	119.44	110.44
30	Q	203	THR	N-CA-C	-5.77	105.07	111.36
13	6	184	VAL	N-CA-C	-5.77	104.90	110.72
24	X	34	GLU	N-CA-C	-5.77	98.69	108.26
5	e	155	THR	N-CA-CB	5.76	118.51	109.69
15	H	449	LYS	N-CA-CB	5.76	118.33	109.91
34	8	281	ASN	CB-CG-ND2	-5.76	107.75	116.40
6	f	130	GLY	N-CA-C	-5.76	100.45	110.71
7	g	82	ARG	CA-C-N	5.76	128.47	120.29
7	g	82	ARG	C-N-CA	5.76	128.47	120.29
16	I	309	LEU	CA-C-N	5.76	127.93	120.44
16	I	309	LEU	C-N-CA	5.76	127.93	120.44
2	b	111	VAL	CA-CB-CG1	5.76	120.19	110.40
3	c	106	PRO	CA-C-O	-5.76	114.88	121.56
7	g	57	PRO	O-C-N	5.76	130.01	123.10
10	j	35	VAL	CB-CA-C	-5.76	105.77	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	n	172	VAL	CA-C-O	5.76	126.96	120.85
19	M	37	LEU	N-CA-C	-5.76	105.75	112.89
34	8	132	ASP	CA-CB-CG	-5.76	106.84	112.60
7	g	175	LEU	N-CA-C	-5.76	105.14	111.82
12	l	166	HIS	CE1-NE2-CD2	-5.76	103.24	109.00
13	6	208	THR	CA-C-O	5.76	128.26	121.58
21	W	76	LEU	CA-C-N	5.76	128.57	120.28
21	W	76	LEU	C-N-CA	5.76	128.57	120.28
25	Y	75	ASN	CA-C-N	5.76	128.31	120.54
25	Y	75	ASN	C-N-CA	5.76	128.31	120.54
27	N	125	THR	CA-C-N	5.76	129.98	120.94
27	N	125	THR	C-N-CA	5.76	129.98	120.94
28	S	448	LEU	N-CA-C	-5.76	106.88	114.31
33	O	254	LEU	CA-C-N	5.76	127.93	120.44
33	O	254	LEU	C-N-CA	5.76	127.93	120.44
16	I	372	SER	N-CA-C	-5.76	105.17	114.09
28	S	225	HIS	ND1-CE1-NE2	5.76	114.16	108.40
5	e	131	GLY	CA-C-N	5.76	131.29	122.25
5	e	131	GLY	C-N-CA	5.76	131.29	122.25
8	h	80	SER	CB-CA-C	-5.76	101.23	110.79
13	m	199	GLY	CA-C-N	5.76	132.54	121.54
13	m	199	GLY	C-N-CA	5.76	132.54	121.54
4	D	114	VAL	N-CA-C	-5.76	104.73	111.00
21	W	107	HIS	ND1-CE1-NE2	5.76	114.16	108.40
26	Z	326	VAL	CA-C-N	5.76	127.99	120.28
26	Z	326	VAL	C-N-CA	5.76	127.99	120.28
29	P	39	LEU	CB-CA-C	-5.76	100.17	110.70
5	e	195	ILE	CB-CA-C	5.75	120.16	112.22
26	Z	242	PHE	N-CA-C	-5.75	105.01	111.28
27	N	421	ASP	CA-CB-CG	-5.75	106.84	112.60
5	e	55	SER	CA-C-O	-5.75	114.45	120.55
5	E	14	PHE	CA-C-N	5.75	127.99	120.28
5	E	14	PHE	C-N-CA	5.75	127.99	120.28
27	N	584	ARG	CA-C-N	5.75	127.99	120.28
27	N	584	ARG	C-N-CA	5.75	127.99	120.28
29	P	34	SER	CA-C-N	5.75	128.26	120.44
29	P	34	SER	C-N-CA	5.75	128.26	120.44
4	D	68	HIS	CB-CG-ND1	5.75	131.33	122.70
7	G	111	ARG	N-CA-CB	5.75	118.35	110.01
20	J	24	GLU	N-CA-CB	5.75	118.67	110.16
20	J	274	GLU	CB-CA-C	-5.75	99.62	110.67
33	O	283	HIS	CG-CD2-NE2	5.75	112.95	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Q	16	ASN	N-CA-C	-5.75	106.12	113.02
15	H	284	VAL	N-CA-CB	5.75	120.72	111.23
17	K	289	ASP	CA-C-N	5.75	127.98	120.28
17	K	289	ASP	C-N-CA	5.75	127.98	120.28
26	Z	71	LEU	N-CA-C	-5.75	105.15	111.82
29	P	276	LEU	N-CA-C	-5.75	104.92	111.07
33	O	33	TYR	CA-C-N	5.75	128.45	120.29
33	O	33	TYR	C-N-CA	5.75	128.45	120.29
14	n	56	ASP	CA-C-N	5.75	129.72	120.30
14	n	56	ASP	C-N-CA	5.75	129.72	120.30
16	I	72	GLU	CA-C-N	5.75	128.30	120.54
16	I	72	GLU	C-N-CA	5.75	128.30	120.54
26	Z	540	GLY	N-CA-C	-5.75	107.53	114.66
30	Q	67	THR	O-C-N	-5.75	114.95	122.59
30	Q	95	LYS	CA-C-N	5.75	127.80	120.56
30	Q	95	LYS	C-N-CA	5.75	127.80	120.56
31	R	229	LYS	N-CA-C	5.75	117.35	111.14
7	g	180	PRO	N-CA-C	-5.75	106.52	114.27
8	h	179	THR	CA-C-N	5.75	128.55	120.28
8	h	179	THR	C-N-CA	5.75	128.55	120.28
15	H	328	GLU	CA-C-N	5.75	129.72	120.30
15	H	328	GLU	C-N-CA	5.75	129.72	120.30
27	N	616	HIS	CE1-NE2-CD2	-5.75	103.25	109.00
2	b	179	TRP	CB-CG-CD2	-5.74	118.76	126.80
4	D	215	PRO	CB-CA-C	-5.74	103.71	111.12
20	J	196	THR	O-C-N	5.74	128.21	122.12
27	N	801	THR	O-C-N	-5.74	115.60	122.15
1	A	198	ILE	CA-C-N	5.74	127.90	120.44
1	A	198	ILE	C-N-CA	5.74	127.90	120.44
16	I	349	LEU	N-CA-C	-5.74	99.16	108.52
13	6	198	VAL	CA-C-N	5.74	129.49	121.22
13	6	198	VAL	C-N-CA	5.74	129.49	121.22
18	L	413	ASP	CA-CB-CG	-5.74	106.86	112.60
3	C	150	SER	O-C-N	-5.74	116.60	123.31
4	D	57	ILE	CA-C-O	-5.74	112.25	119.48
13	m	213	ARG	CA-C-N	-5.74	114.33	122.94
13	m	213	ARG	C-N-CA	-5.74	114.33	122.94
19	M	228	LYS	CA-C-N	5.74	132.50	121.54
19	M	228	LYS	C-N-CA	5.74	132.50	121.54
19	M	281	ASP	CA-CB-CG	-5.74	106.86	112.60
3	c	54	THR	CA-C-N	5.74	127.97	120.28
3	c	54	THR	C-N-CA	5.74	127.97	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	n	30	TYR	N-CA-C	-5.74	96.44	107.57
12	5	40	PHE	N-CA-C	-5.74	106.41	113.41
16	I	348	ILE	CA-CB-CG1	5.73	120.15	110.40
2	B	248	GLU	N-CA-C	-5.73	106.29	113.28
4	D	79	ASP	N-CA-CB	5.73	118.64	110.16
6	F	102	LEU	N-CA-CB	5.73	118.39	109.85
22	V	60	ASP	N-CA-C	-5.73	103.89	112.54
24	X	26	PRO	N-CA-CB	5.73	108.67	103.34
28	S	281	ALA	CB-CA-C	-5.73	101.27	110.79
31	R	295	SER	CA-C-N	5.73	127.89	120.44
31	R	295	SER	C-N-CA	5.73	127.89	120.44
31	R	328	PHE	CA-CB-CG	5.73	119.53	113.80
2	b	189	ILE	CB-CA-C	-5.73	104.41	112.14
3	c	24	ALA	N-CA-C	5.73	117.53	111.28
9	i	223	ILE	CA-C-O	5.73	127.49	121.59
13	m	148	PRO	N-CA-C	-5.73	106.06	113.57
2	B	228	PRO	CA-C-N	5.73	127.96	120.28
2	B	228	PRO	C-N-CA	5.73	127.96	120.28
15	H	235	PHE	CA-CB-CG	-5.73	108.07	113.80
19	M	225	GLY	N-CA-C	-5.73	107.35	115.43
29	P	267	PHE	CA-CB-CG	-5.73	108.07	113.80
33	O	92	PHE	CA-CB-CG	-5.73	108.07	113.80
34	8	176	PHE	O-C-N	-5.73	116.69	123.22
8	h	120	HIS	CA-CB-CG	5.73	119.53	113.80
5	e	179	TRP	CB-CG-CD1	5.73	135.49	126.90
2	B	141	GLU	CA-C-N	5.73	127.96	120.28
2	B	141	GLU	C-N-CA	5.73	127.96	120.28
9	2	141	HIS	N-CA-C	-5.73	107.28	114.56
18	L	78	ARG	CA-C-N	5.73	127.95	120.28
18	L	78	ARG	C-N-CA	5.73	127.95	120.28
27	N	583	VAL	N-CA-C	-5.73	105.15	110.53
32	U	182	ALA	N-CA-C	-5.73	106.16	114.12
12	l	197	PHE	CB-CA-C	-5.73	101.65	110.81
18	L	213	LYS	N-CA-C	-5.73	102.37	109.64
8	1	82	PHE	N-CA-C	-5.72	104.95	111.07
8	1	145	ASN	CA-CB-CG	-5.72	106.88	112.60
19	M	47	GLU	CA-C-N	5.72	127.95	120.28
19	M	47	GLU	C-N-CA	5.72	127.95	120.28
11	4	128	LEU	CA-C-N	5.72	125.40	119.05
11	4	128	LEU	C-N-CA	5.72	125.40	119.05
16	I	67	ASP	CA-C-O	-5.72	114.78	120.90
23	T	106	ILE	CA-C-O	-5.72	115.00	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	903	MET	CA-C-N	5.72	128.22	120.44
26	Z	903	MET	C-N-CA	5.72	128.22	120.44
27	N	699	ALA	CA-C-O	5.72	126.83	120.82
28	S	359	LYS	O-C-N	5.72	128.19	122.12
7	G	224	HIS	CB-CG-CD2	5.72	138.64	131.20
28	S	75	CYS	N-CA-CB	5.72	118.46	109.94
23	T	28	PRO	CA-C-N	5.72	125.40	119.05
23	T	28	PRO	C-N-CA	5.72	125.40	119.05
27	N	785	PRO	CA-C-N	5.72	131.13	120.95
27	N	785	PRO	C-N-CA	5.72	131.13	120.95
16	I	151	HIS	ND1-CE1-NE2	5.72	114.12	108.40
12	l	169	ALA	O-C-N	5.72	128.18	122.12
5	E	83	HIS	CG-CD2-NE2	5.72	112.92	107.20
18	L	290	ARG	N-CA-C	5.72	117.51	111.28
20	J	227	SER	N-CA-CB	5.72	118.62	110.16
26	Z	757	SER	N-CA-C	-5.72	105.19	111.82
28	S	376	THR	N-CA-C	-5.72	106.26	113.18
1	a	186	ASN	CA-CB-CG	5.71	118.31	112.60
13	6	189	THR	CA-CB-CG2	5.71	120.22	110.50
15	H	358	PRO	N-CA-C	-5.71	106.72	113.86
20	J	100	LYS	CA-C-N	5.71	128.41	120.29
20	J	100	LYS	C-N-CA	5.71	128.41	120.29
28	S	111	ARG	CA-C-N	5.71	132.21	123.47
28	S	111	ARG	C-N-CA	5.71	132.21	123.47
30	Q	66	VAL	CA-C-O	5.71	127.01	120.90
13	m	2	PHE	N-CA-CB	5.71	118.97	109.60
3	C	58	GLN	OE1-CD-NE2	5.71	128.31	122.60
8	1	74	SER	CA-C-N	5.71	127.94	120.28
8	1	74	SER	C-N-CA	5.71	127.94	120.28
19	M	207	PHE	N-CA-CB	5.71	118.52	110.12
28	S	181	ALA	N-CA-C	-5.71	105.57	112.54
5	e	39	VAL	N-CA-C	-5.71	100.11	108.11
11	k	93	ARG	NE-CZ-NH2	5.71	124.34	119.20
14	n	18	ASN	CB-CA-C	-5.71	101.07	110.72
28	S	264	VAL	CA-C-N	5.71	128.82	120.71
28	S	264	VAL	C-N-CA	5.71	128.82	120.71
28	S	440	ASP	N-CA-C	-5.71	98.64	110.80
15	H	354	ALA	N-CA-CB	5.71	119.67	110.65
16	I	192	GLN	N-CA-C	-5.71	103.73	111.55
18	L	346	LYS	N-CA-C	-5.71	95.77	107.70
27	N	496	GLU	O-C-N	-5.71	116.07	122.12
30	Q	3	LEU	CA-C-O	-5.71	113.38	118.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	73	ARG	CB-CG-CD	5.71	124.43	111.30
8	1	33	LYS	N-CA-C	-5.71	105.71	114.16
26	Z	809	MET	N-CA-C	-5.71	105.06	111.28
27	N	620	GLY	O-C-N	5.71	129.13	122.68
14	7	62	HIS	CB-CG-CD2	-5.71	123.78	131.20
18	L	393	ASN	CA-CB-CG	-5.71	106.89	112.60
26	Z	493	LEU	CA-C-N	5.71	126.42	120.03
26	Z	493	LEU	C-N-CA	5.71	126.42	120.03
3	c	124	HIS	CG-CD2-NE2	5.70	112.90	107.20
14	n	193	ARG	NE-CZ-NH2	-5.70	114.07	119.20
3	C	107	VAL	CA-C-N	5.70	127.92	120.28
3	C	107	VAL	C-N-CA	5.70	127.92	120.28
9	2	200	GLN	CA-C-O	-5.70	114.47	120.63
13	6	115	ASP	N-CA-C	-5.70	102.48	110.35
34	8	407	GLN	N-CA-C	-5.70	104.97	111.07
1	a	205	LEU	N-CA-CB	5.70	119.41	110.46
18	L	241	ALA	N-CA-CB	5.70	118.44	109.83
26	Z	898	HIS	N-CA-C	-5.70	105.66	113.30
33	O	127	LEU	CB-CA-C	-5.70	101.16	110.85
5	e	100	ASN	CA-CB-CG	-5.70	106.90	112.60
5	e	225	ASN	CA-CB-CG	5.70	118.30	112.60
10	j	199	LEU	N-CA-CB	5.70	119.70	110.41
26	Z	431	ASP	N-CA-CB	5.70	118.63	109.28
26	Z	547	MET	N-CA-CB	5.70	118.34	110.07
27	N	781	ALA	O-C-N	5.70	128.16	122.12
29	P	77	GLU	O-C-N	5.70	128.16	122.12
32	U	43	SER	CA-C-N	5.70	127.85	120.44
32	U	43	SER	C-N-CA	5.70	127.85	120.44
9	i	42	TRP	CB-CG-CD2	-5.70	118.82	126.80
9	i	142	TRP	CB-CG-CD1	5.70	135.45	126.90
14	n	94	GLU	CB-CG-CD	-5.70	102.91	112.60
7	G	180	PRO	N-CA-C	-5.70	106.74	113.86
17	K	53	LYS	CB-CA-C	-5.70	101.33	110.79
17	K	255	ARG	CB-CA-C	-5.70	101.16	110.85
26	Z	184	SER	CA-C-O	5.70	126.38	119.31
28	S	330	LEU	CA-C-N	5.70	128.19	120.38
28	S	330	LEU	C-N-CA	5.70	128.19	120.38
4	D	43	GLY	N-CA-C	-5.70	101.99	110.71
13	6	60	ASP	CA-CB-CG	-5.70	106.90	112.60
26	Z	364	ASN	N-CA-C	5.70	117.17	111.07
27	N	555	ILE	N-CA-C	-5.70	104.81	110.62
30	Q	45	SER	N-CA-CB	5.70	120.12	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	147	SER	N-CA-CB	5.70	118.34	109.97
10	3	148	MET	O-C-N	5.70	128.24	122.09
17	K	71	GLU	CA-C-O	-5.70	114.38	120.42
30	Q	88	PHE	O-C-N	5.70	128.64	122.15
1	a	210	SER	CA-C-O	5.69	128.10	121.49
15	H	85	MET	CA-C-N	5.69	127.26	120.14
15	H	85	MET	C-N-CA	5.69	127.26	120.14
26	Z	278	LEU	CA-C-O	5.69	126.31	119.59
27	N	881	TYR	CA-CB-CG	-5.69	103.65	113.90
4	d	105	GLU	N-CA-C	5.69	117.48	111.28
7	g	176	VAL	CA-C-N	5.69	127.91	120.28
7	g	176	VAL	C-N-CA	5.69	127.91	120.28
6	F	207	VAL	CA-C-O	5.69	126.87	120.95
21	W	86	HIS	CG-CD2-NE2	5.69	112.89	107.20
6	f	152	VAL	CA-CB-CG2	5.69	120.07	110.40
7	g	79	PRO	N-CA-CB	5.69	109.55	103.52
13	6	93	ILE	O-C-N	-5.69	115.97	121.83
26	Z	717	THR	N-CA-C	-5.69	104.69	111.69
27	N	226	ASN	CA-C-N	5.69	127.91	120.28
27	N	226	ASN	C-N-CA	5.69	127.91	120.28
7	g	122	TYR	O-C-N	-5.69	116.56	123.27
10	3	144	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	A	204	ALA	N-CA-C	-5.69	105.00	111.14
33	O	169	ASN	CA-C-N	5.69	128.37	120.29
33	O	169	ASN	C-N-CA	5.69	128.37	120.29
12	l	166	HIS	ND1-CE1-NE2	5.68	114.08	108.40
33	O	62	TYR	CB-CG-CD1	5.68	129.33	120.80
1	A	190	TRP	CA-C-O	5.68	126.50	119.97
10	3	158	GLU	CA-C-O	-5.68	114.26	120.17
7	G	241	LYS	O-C-N	-5.68	115.67	122.15
8	1	93	LEU	CA-C-O	5.68	126.84	120.70
20	J	242	PRO	N-CD-CG	5.68	110.62	103.80
21	W	131	THR	CA-C-N	5.68	127.89	120.28
21	W	131	THR	C-N-CA	5.68	127.89	120.28
3	c	27	SER	CA-C-N	5.68	128.24	120.46
3	c	27	SER	C-N-CA	5.68	128.24	120.46
7	g	142	ALA	N-CA-C	-5.68	101.23	110.20
11	k	195	PHE	CA-CB-CG	5.68	119.48	113.80
7	G	112	LEU	CA-C-N	5.68	126.25	120.00
7	G	112	LEU	C-N-CA	5.68	126.25	120.00
16	I	402	LEU	CA-C-N	5.68	128.36	120.29
16	I	402	LEU	C-N-CA	5.68	128.36	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	190	HIS	ND1-CE1-NE2	5.68	114.08	108.40
3	c	202	SER	O-C-N	-5.68	116.60	123.13
14	7	16	TYR	CA-C-N	5.68	128.46	120.28
14	7	16	TYR	C-N-CA	5.68	128.46	120.28
31	R	114	ASN	CA-C-N	5.68	128.46	120.28
31	R	114	ASN	C-N-CA	5.68	128.46	120.28
4	d	2	TYR	N-CA-C	-5.68	105.01	111.14
6	f	38	ARG	CA-C-N	5.68	133.21	123.05
6	f	38	ARG	C-N-CA	5.68	133.21	123.05
8	h	149	GLU	CA-C-N	5.68	127.89	120.28
8	h	149	GLU	C-N-CA	5.68	127.89	120.28
8	h	179	THR	N-CA-C	-5.68	100.91	108.34
11	k	152	MET	N-CA-CB	5.68	118.48	109.51
8	l	62	HIS	CG-CD2-NE2	5.68	112.88	107.20
8	l	174	ARG	NE-CZ-NH2	-5.68	114.09	119.20
28	S	321	GLN	CB-CG-CD	-5.68	102.95	112.60
1	a	24	LYS	N-CA-CB	5.67	118.46	110.12
18	L	99	GLN	CB-CG-CD	-5.67	102.95	112.60
23	T	107	SER	N-CA-C	-5.67	105.01	111.14
28	S	19	HIS	ND1-CE1-NE2	5.67	114.08	108.40
28	S	261	HIS	CA-C-O	5.67	125.04	119.08
14	n	72	THR	N-CA-CB	5.67	118.46	110.12
29	P	163	LEU	N-CA-C	5.67	117.14	111.07
9	i	26	VAL	N-CA-CB	5.67	117.53	111.46
13	6	115	ASP	CA-CB-CG	5.67	118.27	112.60
18	L	273	HIS	ND1-CE1-NE2	5.67	114.07	108.40
19	M	411	LYS	N-CA-C	-5.67	101.35	110.14
26	Z	572	ILE	N-CA-C	-5.67	104.99	110.72
26	Z	932	ALA	CA-C-N	-5.67	114.06	122.23
26	Z	932	ALA	C-N-CA	-5.67	114.06	122.23
9	i	90	TYR	CA-C-N	5.67	130.18	122.19
9	i	90	TYR	C-N-CA	5.67	130.18	122.19
10	j	82	GLU	CA-C-N	5.67	125.34	119.05
10	j	82	GLU	C-N-CA	5.67	125.34	119.05
4	D	163	GLY	CA-C-N	5.67	128.89	120.90
4	D	163	GLY	C-N-CA	5.67	128.89	120.90
29	P	288	ASN	CA-CB-CG	-5.67	106.93	112.60
29	P	377	GLU	CA-C-N	5.67	127.88	120.28
29	P	377	GLU	C-N-CA	5.67	127.88	120.28
31	R	148	ASP	N-CA-C	5.67	117.54	111.36
3	c	68	LEU	N-CA-CB	5.67	118.97	110.19
6	F	219	THR	N-CA-CB	5.67	118.97	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	133	LYS	N-CA-C	-5.67	106.35	113.72
14	n	107	MET	N-CA-CB	5.67	120.06	110.49
19	M	124	ARG	N-CA-CB	5.67	120.06	110.49
4	D	115	GLN	CA-C-O	5.66	126.42	120.42
13	6	11	THR	N-CA-C	-5.66	99.43	109.06
17	K	275	ASP	N-CA-CB	5.66	119.02	110.30
27	N	815	LYS	CA-C-O	-5.66	114.55	120.55
34	8	438	HIS	CA-CB-CG	5.66	119.46	113.80
1	A	39	LYS	CA-C-O	-5.66	114.42	120.42
4	D	195	ARG	NE-CZ-NH1	5.66	127.16	121.50
7	G	239	ALA	CA-C-N	5.66	127.87	120.28
7	G	239	ALA	C-N-CA	5.66	127.87	120.28
18	L	356	GLY	CA-C-N	5.66	128.33	120.29
18	L	356	GLY	C-N-CA	5.66	128.33	120.29
3	c	141	ASP	CA-C-O	-5.66	114.42	120.42
28	S	99	ASN	O-C-N	-5.66	115.65	123.12
11	k	113	LYS	CA-C-N	-5.66	113.95	119.78
11	k	113	LYS	C-N-CA	-5.66	113.95	119.78
28	S	170	TYR	N-CA-C	5.66	118.86	110.48
23	T	227	PRO	CA-C-O	-5.66	115.11	122.12
26	Z	255	LEU	CA-C-O	5.66	126.53	120.70
27	N	434	SER	CA-C-O	5.66	126.07	118.38
1	A	6	HIS	CA-CB-CG	5.65	119.45	113.80
20	J	296	ARG	N-CA-CB	5.65	120.75	111.31
32	U	81	LYS	N-CA-C	-5.65	105.11	112.23
34	8	448	TYR	CA-C-N	5.65	131.44	122.62
34	8	448	TYR	C-N-CA	5.65	131.44	122.62
13	m	145	LEU	N-CA-C	-5.65	104.74	111.69
26	Z	387	ASN	CA-C-N	5.65	126.38	119.99
26	Z	387	ASN	C-N-CA	5.65	126.38	119.99
33	O	179	PHE	CA-CB-CG	-5.65	108.15	113.80
1	A	69	THR	CA-C-N	-5.65	115.67	122.90
1	A	69	THR	C-N-CA	-5.65	115.67	122.90
31	R	24	TYR	N-CA-C	5.65	118.37	111.82
9	2	182	LYS	CA-C-N	5.65	129.12	121.05
9	2	182	LYS	C-N-CA	5.65	129.12	121.05
14	7	223	LYS	N-CA-CB	5.65	119.61	110.40
17	K	106	ASN	CA-CB-CG	-5.65	106.95	112.60
22	V	277	LYS	N-CA-CB	5.65	118.20	110.01
23	T	144	TYR	CA-C-O	-5.65	113.43	118.63
13	m	65	VAL	CA-CB-CG1	5.65	120.00	110.40
5	E	63	ASP	CA-CB-CG	-5.65	106.95	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	24	ILE	N-CA-C	-5.65	105.02	110.72
29	P	161	CYS	CA-C-N	5.65	127.85	120.28
29	P	161	CYS	C-N-CA	5.65	127.85	120.28
31	R	347	THR	N-CA-CB	5.65	121.35	111.13
31	R	413	LYS	CA-C-N	5.65	128.31	120.29
31	R	413	LYS	C-N-CA	5.65	128.31	120.29
13	m	152	ASN	CA-C-O	5.64	126.40	120.42
17	K	332	GLY	O-C-N	5.64	129.02	122.30
27	N	130	ASP	CA-C-N	5.64	125.49	119.28
27	N	130	ASP	C-N-CA	5.64	125.49	119.28
27	N	422	TYR	CA-C-N	5.64	128.31	120.29
27	N	422	TYR	C-N-CA	5.64	128.31	120.29
27	N	726	ASP	O-C-N	5.64	129.70	122.93
28	S	153	GLU	CA-C-N	5.64	127.78	120.44
28	S	153	GLU	C-N-CA	5.64	127.78	120.44
34	8	261	LEU	N-CA-C	-5.64	100.50	109.59
34	8	379	PHE	CA-CB-CG	-5.64	108.16	113.80
9	i	222	ASP	N-CA-CB	5.64	118.95	109.92
12	l	30	THR	N-CA-C	-5.64	103.77	111.56
6	F	8	ASP	O-C-N	-5.64	116.34	123.17
23	T	82	PHE	CA-CB-CG	-5.64	108.16	113.80
26	Z	564	ARG	N-CA-C	-5.64	105.21	111.36
31	R	326	ALA	CA-C-N	5.64	127.84	120.28
31	R	326	ALA	C-N-CA	5.64	127.84	120.28
6	f	79	ASP	CA-C-N	5.64	127.84	120.28
6	f	79	ASP	C-N-CA	5.64	127.84	120.28
26	Z	60	ASP	CA-CB-CG	-5.64	106.96	112.60
26	Z	253	VAL	CA-C-N	5.64	125.31	119.56
26	Z	253	VAL	C-N-CA	5.64	125.31	119.56
4	d	170	ARG	NE-CZ-NH2	-5.64	114.12	119.20
7	g	106	PRO	N-CA-CB	5.64	109.50	103.52
1	A	52	ASP	CA-CB-CG	-5.64	106.96	112.60
1	A	89	LYS	CB-CA-C	-5.64	101.99	110.90
1	A	163	GLY	CA-C-N	5.64	125.34	119.64
1	A	163	GLY	C-N-CA	5.64	125.34	119.64
1	A	189	SER	O-C-N	5.64	129.94	122.95
3	C	208	ASP	CA-C-O	-5.64	111.72	119.05
26	Z	180	ASP	N-CA-C	-5.64	102.94	111.34
30	Q	29	SER	CA-C-N	5.64	128.15	120.54
30	Q	29	SER	C-N-CA	5.64	128.15	120.54
5	E	58	LYS	N-CA-C	-5.64	104.98	113.89
17	K	101	GLU	CA-C-O	5.64	126.22	120.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	415	MET	CA-C-N	5.64	127.77	120.44
26	Z	415	MET	C-N-CA	5.64	127.77	120.44
8	h	30	VAL	O-C-N	-5.64	114.81	122.14
26	Z	474	LEU	N-CA-C	5.64	120.00	113.18
27	N	506	GLN	N-CA-C	-5.64	104.76	111.69
29	P	358	SER	N-CA-C	-5.64	104.76	111.69
6	f	14	PRO	O-C-N	5.63	129.88	122.27
11	k	120	ASP	N-CA-C	-5.63	101.66	110.17
7	G	179	HIS	CG-CD2-NE2	5.63	112.83	107.20
16	I	364	ILE	O-C-N	5.63	127.76	121.90
26	Z	143	VAL	N-CA-C	-5.63	105.03	110.72
27	N	59	GLU	CB-CG-CD	-5.63	103.02	112.60
11	k	41	HIS	CB-CG-ND1	5.63	131.15	122.70
12	5	207	PHE	N-CA-CB	5.63	120.47	111.91
33	O	100	ASP	CA-C-O	5.63	126.45	119.97
6	f	210	LEU	CA-C-O	5.63	127.05	120.80
21	W	180	LEU	N-CA-CB	5.63	120.01	110.49
29	P	81	LEU	CA-C-N	5.63	127.76	120.44
29	P	81	LEU	C-N-CA	5.63	127.76	120.44
29	P	184	MET	CA-C-N	5.63	128.29	120.29
29	P	184	MET	C-N-CA	5.63	128.29	120.29
34	8	345	LEU	CA-C-N	5.63	128.22	120.39
34	8	345	LEU	C-N-CA	5.63	128.22	120.39
11	4	18	SER	CA-C-O	-5.63	115.58	121.55
29	P	210	ASN	CA-CB-CG	-5.63	106.97	112.60
9	i	138	LEU	O-C-N	-5.63	115.73	122.15
17	K	421	VAL	N-CA-C	5.63	121.05	109.34
28	S	266	SER	CA-C-N	5.63	127.82	120.28
28	S	266	SER	C-N-CA	5.63	127.82	120.28
4	d	134	ALA	CA-C-N	5.63	129.97	120.86
4	d	134	ALA	C-N-CA	5.63	129.97	120.86
5	E	149	HIS	ND1-CE1-NE2	5.63	114.03	108.40
9	2	38	SER	N-CA-C	-5.63	101.67	108.14
9	2	109	HIS	CA-CB-CG	5.63	119.43	113.80
2	b	47	THR	CA-C-O	-5.62	115.43	121.45
26	Z	935	THR	CA-CB-OG1	5.62	118.03	109.60
28	S	169	CYS	N-CA-C	-5.62	105.23	111.36
15	H	393	SER	CA-C-N	5.62	127.81	120.28
15	H	393	SER	C-N-CA	5.62	127.81	120.28
18	L	71	ASP	CB-CA-C	-5.62	101.29	110.85
24	X	71	GLY	CA-C-O	5.62	126.05	119.19
15	H	188	PRO	CA-C-N	5.62	125.90	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	188	PRO	C-N-CA	5.62	125.90	119.83
16	I	222	TYR	N-CA-CB	5.62	121.22	111.39
23	T	67	LEU	CA-C-N	5.62	128.37	120.28
23	T	67	LEU	C-N-CA	5.62	128.37	120.28
5	E	225	ASN	CA-CB-CG	-5.62	106.98	112.60
6	F	170	TYR	O-C-N	-5.62	116.16	122.12
12	5	166	HIS	CB-CG-CD2	-5.62	123.90	131.20
16	I	352	ASN	OD1-CG-ND2	-5.62	116.98	122.60
19	M	404	ARG	CA-C-N	5.62	127.81	120.28
19	M	404	ARG	C-N-CA	5.62	127.81	120.28
22	V	204	HIS	CA-CB-CG	-5.62	108.18	113.80
26	Z	706	LYS	CA-C-N	5.62	127.75	120.44
26	Z	706	LYS	C-N-CA	5.62	127.75	120.44
34	8	401	ASN	CA-C-O	-5.62	114.59	120.55
7	G	227	VAL	N-CA-CB	5.62	117.24	110.95
9	i	114	HIS	ND1-CE1-NE2	5.62	114.02	108.40
4	D	126	PRO	N-CA-CB	5.62	108.32	103.27
14	7	176	ALA	CA-C-O	-5.62	114.92	120.82
14	7	229	GLY	CA-C-O	-5.62	109.01	120.80
5	e	124	ARG	CA-C-O	5.61	126.50	120.32
1	A	50	VAL	N-CA-C	-5.61	102.59	108.15
18	L	232	ALA	CA-C-N	5.61	128.26	120.29
18	L	232	ALA	C-N-CA	5.61	128.26	120.29
18	L	310	THR	N-CA-C	5.61	117.40	111.28
20	J	156	GLN	N-CA-C	5.61	117.40	111.28
32	U	219	LEU	CA-C-N	5.61	125.94	119.93
32	U	219	LEU	C-N-CA	5.61	125.94	119.93
5	e	15	GLN	OE1-CD-NE2	-5.61	116.99	122.60
6	F	35	VAL	N-CA-C	-5.61	100.40	108.48
11	4	49	GLU	CA-C-N	5.61	131.68	121.97
11	4	49	GLU	C-N-CA	5.61	131.68	121.97
11	4	146	HIS	ND1-CE1-NE2	5.61	114.01	108.40
26	Z	286	VAL	N-CA-CB	5.61	117.12	110.55
34	8	137	ILE	CA-C-N	5.61	128.84	120.31
34	8	137	ILE	C-N-CA	5.61	128.84	120.31
8	h	29	ARG	CA-CB-CG	5.61	125.32	114.10
14	n	50	VAL	N-CA-C	-5.61	100.04	108.12
5	E	171	ALA	CA-C-N	5.61	128.84	120.31
5	E	171	ALA	C-N-CA	5.61	128.84	120.31
12	5	25	TRP	CB-CA-C	5.61	119.06	109.80
18	L	387	ASN	CA-C-N	5.61	127.35	120.22
18	L	387	ASN	C-N-CA	5.61	127.35	120.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	82	GLU	CA-C-O	5.61	126.00	119.32
26	Z	863	THR	O-C-N	5.61	128.93	122.25
1	a	187	GLU	N-CA-CB	5.61	118.27	109.69
2	b	247	LEU	N-CA-C	-5.61	105.94	112.89
29	P	188	ILE	CA-C-N	5.61	128.25	120.29
29	P	188	ILE	C-N-CA	5.61	128.25	120.29
11	k	89	ALA	O-C-N	-5.61	116.18	122.12
17	K	293	GLN	CA-C-N	5.61	128.25	120.29
17	K	293	GLN	C-N-CA	5.61	128.25	120.29
18	L	187	THR	CA-CB-OG1	5.61	118.01	109.60
26	Z	189	ALA	N-CA-C	-5.61	106.11	113.12
30	Q	354	PHE	CA-C-N	5.61	132.25	121.54
30	Q	354	PHE	C-N-CA	5.61	132.25	121.54
33	O	123	GLY	N-CA-C	-5.61	106.03	115.62
17	K	221	MET	O-C-N	5.61	128.06	122.12
8	l	41	ILE	O-C-N	-5.60	117.35	123.18
1	a	179	LYS	CA-C-N	5.60	128.83	120.31
1	a	179	LYS	C-N-CA	5.60	128.83	120.31
4	d	107	LEU	CA-C-O	-5.60	114.61	120.55
3	C	64	LYS	CB-CA-C	-5.60	101.49	110.79
7	G	123	ASN	CA-CB-CG	5.60	118.20	112.60
8	h	130	GLY	CA-C-N	5.60	127.78	120.28
8	h	130	GLY	C-N-CA	5.60	127.78	120.28
3	C	179	TYR	N-CA-CB	5.60	118.29	109.83
1	A	15	ARG	N-CA-C	-5.60	99.16	108.34
14	7	36	PHE	CA-CB-CG	-5.60	108.20	113.80
24	X	103	GLU	CA-C-O	5.60	127.30	120.92
26	Z	893	PHE	CA-CB-CG	5.60	119.40	113.80
27	N	552	ALA	CA-C-O	-5.60	114.61	120.55
4	d	91	ALA	CB-CA-C	-5.60	101.50	110.79
6	f	91	CYS	N-CA-C	5.60	117.46	111.36
8	h	121	LYS	CB-CA-C	-5.60	100.72	109.84
10	j	31	GLN	OE1-CD-NE2	5.60	128.20	122.60
13	m	80	ASN	CA-C-N	5.60	132.23	121.54
13	m	80	ASN	C-N-CA	5.60	132.23	121.54
27	N	545	SER	CA-C-N	5.60	127.72	120.44
27	N	545	SER	C-N-CA	5.60	127.72	120.44
29	P	271	SER	CA-C-N	5.60	125.61	119.90
29	P	271	SER	C-N-CA	5.60	125.61	119.90
5	e	67	GLY	CA-C-O	-5.60	115.33	121.77
18	L	159	LEU	CB-CA-C	-5.60	100.49	108.88
28	S	126	LYS	CB-CG-CD	5.60	124.17	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	218	GLU	O-C-N	-5.59	116.64	122.96
14	7	73	GLU	CA-C-N	5.59	127.78	120.28
14	7	73	GLU	C-N-CA	5.59	127.78	120.28
15	H	364	ALA	N-CA-C	-5.59	105.08	111.07
26	Z	823	ASN	CA-C-O	-5.59	115.62	120.88
3	C	63	GLU	CA-CB-CG	5.59	125.29	114.10
15	H	417	ALA	N-CA-C	5.59	117.06	111.07
5	e	216	LYS	N-CA-C	-5.59	105.19	111.28
5	E	149	HIS	CG-CD2-NE2	5.59	112.79	107.20
18	L	400	PHE	CA-C-N	5.59	128.04	120.38
18	L	400	PHE	C-N-CA	5.59	128.04	120.38
20	J	145	SER	N-CA-CB	5.59	119.94	110.49
23	T	175	ASP	N-CA-C	5.59	118.14	111.71
24	X	108	ASN	N-CA-C	5.59	117.05	111.07
2	b	123	GLN	CG-CD-NE2	5.59	124.78	116.40
14	n	123	GLY	N-CA-C	-5.59	107.48	115.64
8	1	89	ASN	OD1-CG-ND2	-5.59	117.01	122.60
32	U	187	SER	N-CA-CB	5.59	118.34	110.12
33	O	82	LEU	N-CA-C	-5.59	105.19	111.28
9	2	58	LEU	CA-C-N	5.59	128.35	120.42
9	2	58	LEU	C-N-CA	5.59	128.35	120.42
29	P	351	ARG	CA-C-O	-5.59	114.94	120.70
5	E	44	LYS	CA-C-N	5.59	131.37	122.93
5	E	44	LYS	C-N-CA	5.59	131.37	122.93
6	F	112	CYS	CA-C-O	5.59	126.69	120.82
17	K	421	VAL	CA-C-O	-5.59	113.80	120.78
30	Q	109	ASP	N-CA-CB	5.58	119.93	110.49
5	E	198	GLN	CA-C-O	-5.58	114.63	120.55
23	T	172	SER	N-CA-C	-5.58	98.91	110.80
32	U	52	PHE	CB-CA-C	5.58	119.29	109.80
32	U	218	GLU	N-CA-CB	5.58	120.20	111.71
9	i	149	GLU	CB-CG-CD	-5.58	103.11	112.60
11	k	108	ASP	CA-CB-CG	5.58	118.18	112.60
3	C	23	TYR	CB-CG-CD1	5.58	129.17	120.80
33	O	37	LEU	N-CA-CB	5.58	119.58	110.37
33	O	76	LEU	CA-C-O	5.58	126.47	120.55
7	g	179	HIS	O-C-N	-5.58	114.90	121.32
17	K	153	ASP	CA-C-O	-5.58	114.50	120.42
27	N	476	THR	N-CA-C	-5.58	107.02	113.88
15	H	81	LEU	N-CA-C	-5.58	105.20	112.23
18	L	375	ASP	CA-CB-CG	5.58	118.18	112.60
26	Z	194	GLU	CB-CG-CD	-5.58	103.12	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	936	VAL	CA-CB-CG2	-5.58	100.92	110.40
27	N	760	GLY	CA-C-O	-5.58	115.30	121.94
32	U	208	VAL	O-C-N	5.58	127.28	121.87
1	A	5	ARG	CA-C-O	5.58	126.37	119.79
14	7	56	ASP	CA-C-N	5.58	128.34	120.42
14	7	56	ASP	C-N-CA	5.58	128.34	120.42
15	H	156	VAL	N-CA-CB	5.58	116.80	110.72
25	Y	24	ILE	CA-C-N	5.58	128.21	120.29
25	Y	24	ILE	C-N-CA	5.58	128.21	120.29
7	G	178	HIS	CG-CD2-NE2	5.58	112.78	107.20
15	H	370	ARG	NE-CZ-NH2	5.58	124.22	119.20
23	T	164	LEU	N-CA-CB	5.58	118.10	110.01
27	N	352	ASN	N-CA-C	-5.58	103.91	111.55
3	c	124	HIS	CA-CB-CG	-5.57	108.23	113.80
8	1	160	SER	N-CA-C	-5.57	105.28	111.36
23	T	191	LYS	CA-C-N	5.57	127.75	120.28
23	T	191	LYS	C-N-CA	5.57	127.75	120.28
3	c	102	ASN	CA-CB-CG	-5.57	107.03	112.60
26	Z	149	TRP	CB-CA-C	-5.57	99.97	110.67
29	P	219	GLU	CA-C-N	5.57	128.20	120.29
29	P	219	GLU	C-N-CA	5.57	128.20	120.29
11	k	90	LYS	N-CA-CB	5.57	118.09	110.01
19	M	242	THR	CA-CB-OG1	5.57	117.96	109.60
26	Z	77	ASN	CA-CB-CG	-5.57	107.03	112.60
33	O	18	ALA	O-C-N	5.57	129.43	122.86
13	m	206	ILE	N-CA-CB	5.57	119.09	111.41
12	5	32	LYS	CA-C-O	5.57	126.83	120.54
18	L	172	SER	O-C-N	5.57	128.02	122.12
20	J	358	VAL	CB-CA-C	-5.57	104.62	112.14
30	Q	382	LEU	N-CA-C	-5.57	105.21	112.23
2	b	73	ALA	O-C-N	5.57	129.73	123.27
10	j	190	LYS	O-C-N	5.57	128.50	122.15
2	B	223	GLY	O-C-N	-5.57	115.36	122.43
17	K	258	PHE	CA-C-N	5.57	127.74	120.28
17	K	258	PHE	C-N-CA	5.57	127.74	120.28
19	M	418	GLY	O-C-N	-5.57	116.39	122.68
26	Z	623	ARG	CA-C-O	-5.57	114.65	120.55
4	d	57	ILE	N-CA-C	-5.57	104.50	112.35
5	e	95	TYR	N-CA-C	-5.57	107.49	114.56
6	f	171	LEU	CA-C-N	5.57	127.74	120.28
6	f	171	LEU	C-N-CA	5.57	127.74	120.28
3	C	171	ALA	N-CA-C	-5.57	105.29	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	178	PHE	N-CA-CB	5.57	118.87	110.30
12	5	71	LYS	CG-CD-CE	5.57	124.10	111.30
13	6	186	ASP	CA-CB-CG	5.57	118.17	112.60
23	T	101	LYS	CA-C-O	-5.57	113.57	119.97
26	Z	312	TYR	CA-C-N	5.57	127.68	120.56
26	Z	312	TYR	C-N-CA	5.57	127.68	120.56
28	S	295	ALA	CA-C-N	5.57	128.29	120.28
28	S	295	ALA	C-N-CA	5.57	128.29	120.28
31	R	194	VAL	CB-CA-C	-5.57	104.54	112.22
34	8	143	SER	CA-C-O	-5.57	114.65	120.55
34	8	244	THR	CA-C-O	-5.57	114.65	120.55
12	l	113	TYR	N-CA-CB	5.56	119.33	110.65
14	n	183	VAL	CA-CB-CG1	5.56	119.86	110.40
10	3	182	TRP	CD2-CE2-CZ2	-5.56	116.84	122.40
16	I	419	ALA	CA-C-N	5.56	127.74	120.28
16	I	419	ALA	C-N-CA	5.56	127.74	120.28
24	X	91	PHE	CB-CG-CD1	-5.56	111.24	120.70
4	d	101	PRO	CA-C-N	5.56	131.98	121.97
4	d	101	PRO	C-N-CA	5.56	131.98	121.97
5	e	217	GLN	OE1-CD-NE2	5.56	128.16	122.60
8	l	67	THR	CA-CB-OG1	5.56	117.94	109.60
15	H	98	GLN	CA-C-N	-5.56	116.29	123.19
15	H	98	GLN	C-N-CA	-5.56	116.29	123.19
20	J	170	HIS	CA-C-N	5.56	125.09	119.19
20	J	170	HIS	C-N-CA	5.56	125.09	119.19
23	T	97	SER	N-CA-CB	5.56	119.89	110.49
26	Z	321	PHE	CA-CB-CG	-5.56	108.24	113.80
29	P	378	THR	N-CA-C	-5.56	105.22	111.28
6	f	132	LEU	N-CA-CB	5.56	119.70	110.47
7	G	137	VAL	CA-CB-CG1	-5.56	100.95	110.40
18	L	191	ARG	N-CA-C	5.56	117.42	111.36
27	N	430	ASN	N-CA-C	-5.56	106.38	112.72
31	R	191	LEU	CA-C-N	5.56	127.73	120.28
31	R	191	LEU	C-N-CA	5.56	127.73	120.28
6	f	80	ALA	O-C-N	5.56	128.01	122.12
8	h	167	GLY	CA-C-N	5.56	127.67	120.44
8	h	167	GLY	C-N-CA	5.56	127.67	120.44
10	j	151	SER	CA-C-O	5.56	126.41	120.24
20	J	83	LYS	CG-CD-CE	5.56	124.08	111.30
28	S	286	TYR	N-CA-C	-5.56	106.39	114.12
28	S	337	ASN	OD1-CG-ND2	5.56	128.16	122.60
34	8	227	ASP	CA-CB-CG	-5.56	107.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	7	69	ASP	N-CA-CB	5.55	118.29	110.12
20	J	197	LEU	CA-C-N	5.55	127.72	120.28
20	J	197	LEU	C-N-CA	5.55	127.72	120.28
22	V	183	ALA	O-C-N	5.55	129.64	122.81
27	N	418	ASP	CA-C-O	5.55	126.31	120.42
8	h	82	PHE	N-CA-CB	5.55	118.28	110.12
10	j	31	GLN	N-CA-CB	5.55	119.88	110.49
10	3	178	ALA	O-C-N	5.55	128.09	122.09
18	L	283	VAL	CA-C-N	5.55	129.49	120.60
18	L	283	VAL	C-N-CA	5.55	129.49	120.60
27	N	747	HIS	CE1-NE2-CD2	-5.55	103.45	109.00
7	g	5	ASP	CB-CA-C	-5.55	101.41	110.85
17	K	216	GLY	N-CA-C	-5.55	107.12	114.95
3	c	236	ASP	CA-CB-CG	-5.55	107.05	112.60
5	E	9	PRO	CA-C-N	5.55	128.27	120.28
5	E	9	PRO	C-N-CA	5.55	128.27	120.28
29	P	120	GLU	O-C-N	-5.55	116.35	122.07
31	R	152	LYS	N-CA-CB	5.55	118.06	110.01
12	l	180	VAL	N-CA-CB	5.55	117.33	111.00
5	E	38	VAL	CA-C-N	-5.55	115.87	123.14
5	E	38	VAL	C-N-CA	-5.55	115.87	123.14
19	M	373	ASP	CA-CB-CG	-5.55	107.05	112.60
20	J	214	SER	CA-C-N	5.55	126.24	120.03
20	J	214	SER	C-N-CA	5.55	126.24	120.03
18	L	127	TYR	CA-C-O	5.55	127.67	121.40
33	O	267	ASP	CA-C-O	5.55	126.43	120.55
4	d	84	ILE	N-CA-C	-5.54	105.10	110.42
12	l	25	TRP	CE2-CD2-CE3	5.54	124.34	118.80
31	R	174	ILE	CB-CA-C	-5.54	104.65	112.14
11	4	93	ARG	NE-CZ-NH2	-5.54	114.21	119.20
13	6	63	ALA	N-CA-CB	5.54	118.36	110.16
21	W	34	GLU	CB-CA-C	-5.54	101.59	110.79
26	Z	450	GLY	CA-C-N	5.54	127.71	120.28
26	Z	450	GLY	C-N-CA	5.54	127.71	120.28
26	Z	619	ASP	N-CA-C	-5.54	106.72	112.93
27	N	373	VAL	N-CA-C	-5.54	105.44	110.82
5	e	129	PRO	CA-C-N	5.54	132.12	121.54
5	e	129	PRO	C-N-CA	5.54	132.12	121.54
11	k	146	HIS	O-C-N	5.54	128.07	122.09
2	B	99	ARG	O-C-N	5.54	127.97	122.10
14	7	226	LYS	CB-CA-C	-5.54	100.49	110.35
26	Z	327	GLN	N-CA-C	5.54	117.32	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Q	102	GLU	N-CA-C	5.54	117.76	111.11
34	8	111	PHE	N-CA-C	-5.54	99.38	108.41
1	a	112	MET	CA-C-O	-5.54	114.55	120.42
7	g	47	GLU	CA-C-N	-5.54	115.29	123.05
7	g	47	GLU	C-N-CA	-5.54	115.29	123.05
12	l	209	ASN	CA-CB-CG	-5.54	107.06	112.60
6	f	17	ARG	N-CA-C	-5.54	99.28	108.75
26	Z	25	PRO	N-CA-C	-5.54	105.33	114.75
10	j	57	THR	O-C-N	5.54	127.99	122.12
16	I	323	LYS	N-CA-CB	5.54	118.70	110.29
26	Z	625	THR	O-C-N	-5.54	115.55	120.48
3	C	90	ALA	CA-C-O	-5.53	115.01	120.82
5	E	217	GLN	OE1-CD-NE2	-5.53	117.07	122.60
11	4	97	PRO	CA-C-O	-5.53	115.00	122.08
20	J	16	GLU	CB-CA-C	-5.53	100.05	110.67
29	P	6	PRO	N-CA-CB	5.53	109.50	103.30
7	g	69	HIS	N-CA-C	-5.53	105.97	114.16
17	K	45	SER	N-CA-CB	5.53	118.35	110.16
4	d	79	ASP	CA-CB-CG	-5.53	107.07	112.60
12	5	33	LYS	CA-C-N	5.53	129.98	122.90
12	5	33	LYS	C-N-CA	5.53	129.98	122.90
26	Z	483	THR	CA-C-O	-5.53	114.69	120.55
28	S	30	GLN	CA-C-N	5.53	128.33	120.53
28	S	30	GLN	C-N-CA	5.53	128.33	120.53
31	R	308	LEU	N-CA-C	-5.53	105.33	111.36
11	4	168	LEU	CB-CA-C	-5.53	102.20	110.88
8	h	180	ALA	N-CA-C	-5.53	105.35	111.71
3	C	151	ASN	CA-C-O	-5.53	114.94	120.96
18	L	138	SER	CA-C-N	5.53	127.62	120.44
18	L	138	SER	C-N-CA	5.53	127.62	120.44
19	M	364	HIS	CE1-NE2-CD2	-5.53	103.47	109.00
21	W	160	ALA	O-C-N	5.53	127.98	122.12
29	P	26	SER	N-CA-C	5.53	117.39	111.36
32	U	109	LEU	O-C-N	5.53	128.45	122.15
11	k	45	SER	CB-CA-C	-5.53	100.16	109.50
11	k	69	ILE	CA-C-O	-5.53	115.31	121.17
6	F	138	LYS	CA-C-O	5.53	125.97	119.28
8	1	27	ALA	CB-CA-C	-5.53	101.51	110.79
23	T	80	ASN	CA-C-O	-5.53	114.99	120.90
23	T	187	ASP	CA-CB-CG	5.53	118.13	112.60
26	Z	39	SER	N-CA-C	-5.53	105.41	111.82
9	i	8	PHE	CA-CB-CG	-5.52	108.28	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	170	HIS	O-C-N	-5.52	114.97	121.32
29	P	339	GLU	CA-C-N	5.52	129.95	120.72
29	P	339	GLU	C-N-CA	5.52	129.95	120.72
14	7	60	MET	N-CA-C	-5.52	105.16	111.07
18	L	370	LYS	O-C-N	-5.52	117.51	123.42
22	V	239	ALA	CA-C-N	5.52	127.68	120.28
22	V	239	ALA	C-N-CA	5.52	127.68	120.28
26	Z	560	THR	N-CA-CB	5.52	118.33	110.16
28	S	133	GLU	CA-C-N	5.52	128.03	120.46
28	S	133	GLU	C-N-CA	5.52	128.03	120.46
34	8	418	PRO	N-CA-C	-5.52	107.24	114.03
2	b	128	ARG	NH1-CZ-NH2	-5.52	112.12	119.30
9	i	142	TRP	CB-CG-CD2	-5.52	119.07	126.80
7	G	79	PRO	CA-C-N	5.52	127.68	120.28
7	G	79	PRO	C-N-CA	5.52	127.68	120.28
34	8	186	ASN	CB-CG-OD1	5.52	131.84	120.80
27	N	202	PHE	CA-C-N	5.52	127.94	120.38
27	N	202	PHE	C-N-CA	5.52	127.94	120.38
29	P	337	HIS	N-CA-C	-5.52	106.71	113.50
31	R	346	LYS	N-CA-C	-5.52	105.34	111.36
2	B	92	VAL	CA-CB-CG2	-5.52	101.02	110.40
2	B	95	THR	N-CA-CB	5.52	118.23	110.12
16	I	70	LEU	N-CA-C	5.52	117.73	111.11
18	L	274	GLU	N-CA-CB	5.52	118.64	109.98
22	V	275	ASP	CA-C-N	5.52	125.04	119.19
22	V	275	ASP	C-N-CA	5.52	125.04	119.19
29	P	360	ILE	O-C-N	-5.52	116.71	123.00
1	a	10	PHE	CA-CB-CG	5.52	119.32	113.80
4	d	93	SER	CA-C-O	-5.52	115.03	120.82
13	m	46	CYS	N-CA-C	-5.52	105.91	113.30
13	m	86	ILE	N-CA-CB	5.52	118.85	110.58
1	a	102	ASP	N-CA-CB	5.51	118.74	109.92
2	B	65	SER	CA-C-O	5.51	126.31	120.36
10	3	182	TRP	CA-C-N	5.51	132.22	121.41
10	3	182	TRP	C-N-CA	5.51	132.22	121.41
13	6	75	TYR	CA-C-O	-5.51	115.03	120.82
13	6	109	THR	CA-C-O	5.51	126.92	120.80
34	8	442	ASN	OD1-CG-ND2	-5.51	117.09	122.60
5	e	217	GLN	N-CA-CB	5.51	118.15	109.94
26	Z	949	ILE	CA-C-O	-5.51	115.01	120.85
27	N	564	ASN	CA-C-N	5.51	128.12	120.29
27	N	564	ASN	C-N-CA	5.51	128.12	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	388	ILE	N-CA-C	-5.51	105.35	110.53
1	a	119	TYR	N-CA-CB	5.51	118.71	110.22
12	l	63	CYS	N-CA-CB	5.51	118.00	110.01
13	6	105	TYR	CA-CB-CG	-5.51	103.98	113.90
26	Z	458	SER	N-CA-C	5.51	117.09	111.14
2	b	160	LYS	N-CA-C	-5.51	105.19	111.14
4	d	15	ILE	CA-C-N	5.51	128.21	120.28
4	d	15	ILE	C-N-CA	5.51	128.21	120.28
7	g	122	TYR	CA-C-N	5.51	127.60	120.44
7	g	122	TYR	C-N-CA	5.51	127.60	120.44
14	n	154	LEU	CB-CA-C	-5.51	101.49	110.85
5	E	212	SER	CB-CA-C	-5.51	100.37	110.62
9	2	86	HIS	CB-CG-CD2	-5.51	124.04	131.20
17	K	73	ARG	CA-C-N	5.51	127.93	120.38
17	K	73	ARG	C-N-CA	5.51	127.93	120.38
19	M	356	SER	CB-CA-C	-5.51	101.64	110.79
21	W	127	ARG	CA-C-N	5.51	128.12	120.29
21	W	127	ARG	C-N-CA	5.51	128.12	120.29
27	N	344	THR	CA-C-O	-5.51	114.64	120.92
8	h	90	LYS	N-CA-C	5.51	117.36	111.36
12	5	208	ASN	N-CA-C	-5.51	106.72	113.50
14	7	74	ASN	CA-C-O	-5.51	114.71	120.55
14	7	190	ARG	O-C-N	5.51	127.74	122.07
29	P	335	LYS	CA-C-O	5.51	126.15	119.38
5	e	202	GLU	CA-C-O	5.51	127.03	120.70
12	l	116	ASP	O-C-N	-5.51	116.88	123.27
2	B	27	ALA	O-C-N	-5.51	115.87	122.15
3	C	91	ARG	CB-CA-C	-5.51	102.23	110.88
26	Z	898	HIS	CE1-NE2-CD2	-5.51	103.49	109.00
31	R	25	GLU	CA-C-N	5.51	127.50	120.56
31	R	25	GLU	C-N-CA	5.51	127.50	120.56
12	5	165	ALA	O-C-N	5.50	127.95	122.12
18	L	252	VAL	N-CA-C	5.50	116.80	109.37
1	a	227	LEU	CA-C-N	5.50	130.17	120.87
1	a	227	LEU	C-N-CA	5.50	130.17	120.87
2	b	90	ARG	NE-CZ-NH2	-5.50	114.25	119.20
4	d	98	LEU	CA-C-N	5.50	130.63	122.82
4	d	98	LEU	C-N-CA	5.50	130.63	122.82
8	h	70	TYR	CA-C-N	5.50	129.42	121.44
8	h	70	TYR	C-N-CA	5.50	129.42	121.44
11	k	115	GLU	CB-CA-C	-5.50	100.44	109.80
2	B	247	LEU	N-CA-CB	5.50	119.37	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	44	HIS	CG-CD2-NE2	5.50	112.70	107.20
17	K	142	HIS	CE1-NE2-CD2	-5.50	103.50	109.00
20	J	15	HIS	CG-CD2-NE2	5.50	112.70	107.20
23	T	239	SER	O-C-N	5.50	127.81	122.09
27	N	293	LEU	CA-C-O	-5.50	113.51	118.79
3	c	234	ILE	N-CA-C	-5.50	105.16	110.72
6	f	42	HIS	N-CA-CB	-5.50	102.12	111.69
14	n	169	THR	N-CA-CB	5.50	118.78	110.42
16	I	283	GLU	N-CA-C	-5.50	103.65	111.24
23	T	220	PHE	CA-C-N	5.50	127.65	120.28
23	T	220	PHE	C-N-CA	5.50	127.65	120.28
26	Z	151	HIS	ND1-CE1-NE2	5.50	113.90	108.40
28	S	261	HIS	ND1-CE1-NE2	5.50	113.90	108.40
12	l	93	ALA	N-CA-C	-5.50	103.92	110.41
6	F	153	THR	CA-C-N	5.50	129.69	121.72
6	F	153	THR	C-N-CA	5.50	129.69	121.72
12	5	141	ASP	CA-CB-CG	5.50	118.10	112.60
3	c	96	ASN	CA-C-O	-5.50	114.59	120.42
5	e	196	LEU	N-CA-CB	5.50	118.20	110.12
12	5	85	ASN	CA-C-N	5.50	127.59	120.44
12	5	85	ASN	C-N-CA	5.50	127.59	120.44
23	T	40	LEU	N-CA-C	-5.50	105.20	111.14
26	Z	79	THR	N-CA-C	-5.50	106.42	113.02
10	j	176	ARG	N-CA-C	-5.50	106.36	112.57
12	5	33	LYS	N-CA-C	-5.50	106.16	112.92
14	7	90	SER	CA-C-N	5.50	127.64	120.28
14	7	90	SER	C-N-CA	5.50	127.64	120.28
14	7	178	VAL	CA-C-N	5.50	127.92	120.44
14	7	178	VAL	C-N-CA	5.50	127.92	120.44
29	P	51	ASP	N-CA-C	-5.50	105.29	111.28
30	Q	164	GLU	N-CA-C	-5.50	106.53	113.18
12	5	152	ASP	CA-CB-CG	-5.50	107.11	112.60
15	H	55	ASP	N-CA-CB	5.50	117.98	110.01
15	H	339	GLN	CA-C-N	5.50	128.09	120.29
15	H	339	GLN	C-N-CA	5.50	128.09	120.29
3	c	88	ASN	O-C-N	-5.49	115.89	122.15
3	c	220	ASN	CA-C-N	5.49	130.37	122.40
3	c	220	ASN	C-N-CA	5.49	130.37	122.40
9	i	80	LEU	CA-C-O	-5.49	115.05	120.82
10	j	48	VAL	CA-C-O	5.49	127.08	120.65
12	5	159	ARG	N-CA-C	-5.49	105.37	111.36
20	J	63	ARG	CA-C-N	5.49	127.91	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	63	ARG	C-N-CA	5.49	127.91	120.44
20	J	132	PRO	CA-C-N	5.49	128.09	120.29
20	J	132	PRO	C-N-CA	5.49	128.09	120.29
26	Z	264	PHE	CA-CB-CG	5.49	119.29	113.80
26	Z	430	LEU	CB-CA-C	-5.49	101.51	110.85
6	f	40	ASN	N-CA-CB	5.49	118.19	110.12
11	k	110	LYS	O-C-N	-5.49	115.75	122.34
3	C	146	GLN	CA-C-O	5.49	127.19	120.60
8	l	4	MET	N-CA-CB	5.49	120.07	111.56
17	K	90	GLN	N-CA-CB	5.49	118.19	110.12
26	Z	959	HIS	N-CA-CB	5.49	120.23	111.66
28	S	298	ARG	CA-C-N	5.49	127.64	120.28
28	S	298	ARG	C-N-CA	5.49	127.64	120.28
32	U	156	HIS	CB-CG-CD2	-5.49	124.06	131.20
13	6	76	HIS	CA-C-O	-5.49	114.60	120.42
27	N	499	HIS	ND1-CE1-NE2	5.49	113.89	108.40
27	N	767	ALA	CA-C-N	-5.49	118.64	122.59
27	N	767	ALA	C-N-CA	-5.49	118.64	122.59
30	Q	147	GLN	CA-C-O	5.49	126.11	119.31
33	O	212	GLN	CA-C-N	5.49	128.08	120.29
33	O	212	GLN	C-N-CA	5.49	128.08	120.29
1	a	165	LYS	CA-C-N	5.49	127.63	120.28
1	a	165	LYS	C-N-CA	5.49	127.63	120.28
1	a	176	HIS	CG-CD2-NE2	5.49	112.69	107.20
29	P	41	VAL	CA-C-N	5.49	127.63	120.28
29	P	41	VAL	C-N-CA	5.49	127.63	120.28
4	d	34	VAL	N-CA-C	-5.49	100.16	108.17
8	h	67	THR	CA-C-O	-5.49	115.05	120.70
11	4	63	ASN	CA-CB-CG	5.49	118.09	112.60
34	8	424	GLU	CA-C-N	5.49	128.28	120.49
34	8	424	GLU	C-N-CA	5.49	128.28	120.49
3	C	22	GLU	N-CA-CB	5.48	118.18	110.12
7	G	22	TYR	CB-CG-CD2	-5.48	112.58	120.80
16	I	275	ALA	O-C-N	-5.48	115.29	121.43
21	W	4	GLU	CA-C-O	-5.48	114.02	120.60
28	S	142	VAL	CA-C-N	5.48	127.57	120.44
28	S	142	VAL	C-N-CA	5.48	127.57	120.44
28	S	345	TYR	CA-C-N	5.48	127.57	120.44
28	S	345	TYR	C-N-CA	5.48	127.57	120.44
29	P	198	VAL	CA-C-O	-5.48	115.36	121.17
4	d	212	VAL	N-CA-CB	5.48	118.12	110.56
7	G	223	LEU	O-C-N	-5.48	116.03	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	396	THR	N-CA-C	-5.48	104.95	111.69
32	U	30	ASN	N-CA-CB	5.48	119.75	110.49
7	G	22	TYR	CA-C-N	5.48	127.62	120.28
7	G	22	TYR	C-N-CA	5.48	127.62	120.28
26	Z	398	LYS	CA-C-N	5.48	128.07	120.29
26	Z	398	LYS	C-N-CA	5.48	128.07	120.29
14	n	3	GLN	O-C-N	-5.48	117.65	121.65
34	8	186	ASN	OD1-CG-ND2	-5.48	117.12	122.60
8	h	167	GLY	O-C-N	-5.48	116.88	122.19
7	G	180	PRO	CB-CA-C	-5.48	103.69	111.68
16	I	91	GLU	CA-C-N	5.48	127.56	120.44
16	I	91	GLU	C-N-CA	5.48	127.56	120.44
19	M	172	VAL	N-CA-CB	5.48	120.27	111.23
30	Q	106	GLN	CA-C-O	-5.48	115.07	120.82
9	i	142	TRP	CA-C-O	-5.47	115.75	121.55
7	G	189	VAL	CA-C-N	5.47	127.61	120.28
7	G	189	VAL	C-N-CA	5.47	127.61	120.28
17	K	294	ARG	CA-C-N	5.47	127.46	120.56
17	K	294	ARG	C-N-CA	5.47	127.46	120.56
21	W	31	ASP	N-CA-CB	5.47	118.17	110.12
26	Z	321	PHE	N-CA-CB	5.47	118.17	110.12
32	U	223	HIS	N-CA-C	-5.47	106.10	112.89
34	8	279	GLY	CA-C-O	-5.47	114.28	120.30
1	a	166	GLN	CA-C-O	-5.47	114.75	120.55
2	b	156	TYR	O-C-N	-5.47	116.51	123.24
28	S	61	SER	CB-CA-C	-5.47	101.70	110.79
30	Q	78	ILE	CA-CB-CG2	5.47	119.80	110.50
1	a	106	ASP	CA-CB-CG	-5.47	107.13	112.60
4	d	103	THR	N-CA-C	-5.47	100.78	109.59
13	m	36	ASN	CB-CA-C	-5.47	101.60	110.79
13	6	48	ASP	N-CA-CB	5.47	119.74	110.49
25	Y	74	THR	CA-C-O	-5.47	114.75	120.55
2	b	43	VAL	N-CA-C	-5.47	100.78	108.27
2	b	162	THR	O-C-N	-5.47	117.02	123.25
14	n	200	ILE	CA-C-O	5.47	126.08	120.39
1	A	114	ASN	N-CA-CB	5.47	118.16	110.12
2	B	50	LYS	CA-C-N	5.47	129.98	120.68
2	B	50	LYS	C-N-CA	5.47	129.98	120.68
7	G	220	THR	N-CA-C	-5.47	106.33	114.64
14	7	204	THR	CA-CB-OG1	5.47	117.80	109.60
20	J	119	SER	N-CA-CB	5.47	118.00	110.07
27	N	349	ILE	CA-C-N	5.47	127.61	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	349	ILE	C-N-CA	5.47	127.61	120.28
27	N	461	GLU	CA-C-N	5.47	128.19	120.42
27	N	461	GLU	C-N-CA	5.47	128.19	120.42
34	8	465	ASN	O-C-N	5.47	130.00	122.83
12	l	78	ALA	CA-C-N	5.47	127.55	120.44
12	l	78	ALA	C-N-CA	5.47	127.55	120.44
5	E	138	GLY	N-CA-C	5.47	118.51	110.80
12	5	66	HIS	CG-CD2-NE2	5.47	112.67	107.20
8	h	102	TYR	CA-C-O	5.47	126.03	120.24
3	C	57	GLU	CA-C-N	5.47	128.05	120.29
3	C	57	GLU	C-N-CA	5.47	128.05	120.29
14	7	221	PHE	CB-CG-CD2	-5.47	111.41	120.70
16	I	292	TYR	N-CA-C	-5.47	104.48	113.50
19	M	414	ASP	CA-C-N	5.47	127.61	120.28
19	M	414	ASP	C-N-CA	5.47	127.61	120.28
32	U	165	GLU	CA-C-N	5.47	127.61	120.28
32	U	165	GLU	C-N-CA	5.47	127.61	120.28
32	U	233	PHE	CA-CB-CG	-5.47	108.33	113.80
33	O	23	HIS	ND1-CE1-NE2	5.47	113.87	108.40
5	e	65	HIS	CE1-NE2-CD2	-5.46	103.53	109.00
8	l	38	HIS	CE1-NE2-CD2	-5.46	103.54	109.00
16	I	208	TYR	CA-CB-CG	-5.46	104.06	113.90
17	K	395	VAL	CB-CA-C	-5.46	104.68	112.22
20	J	230	VAL	CA-CB-CG1	-5.46	101.11	110.40
27	N	874	ILE	O-C-N	5.46	128.86	123.18
28	S	105	PRO	CA-C-O	-5.46	115.11	121.34
29	P	227	ILE	CA-C-N	5.46	127.87	120.44
29	P	227	ILE	C-N-CA	5.46	127.87	120.44
30	Q	147	GLN	O-C-N	-5.46	114.92	122.46
2	b	190	HIS	CG-CD2-NE2	5.46	112.66	107.20
19	M	136	ASP	CA-C-N	5.46	124.98	119.19
19	M	136	ASP	C-N-CA	5.46	124.98	119.19
5	e	71	SER	N-CA-CB	5.46	119.99	110.81
17	K	119	VAL	N-CA-C	-5.46	100.02	107.99
30	Q	86	MET	CA-C-N	5.46	128.14	120.28
30	Q	86	MET	C-N-CA	5.46	128.14	120.28
31	R	243	LEU	CB-CA-C	-5.46	100.16	110.16
6	f	98	PHE	CB-CA-C	-5.46	100.49	109.99
12	l	202	GLU	CA-C-N	5.46	127.87	120.44
12	l	202	GLU	C-N-CA	5.46	127.87	120.44
1	A	105	CYS	N-CA-CB	-5.46	102.09	110.12
16	I	391	ASP	CA-C-N	5.46	128.17	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	391	ASP	C-N-CA	5.46	128.17	120.42
18	L	328	ASN	N-CA-C	-5.46	108.40	114.62
26	Z	875	LYS	CA-C-N	5.46	128.17	120.42
26	Z	875	LYS	C-N-CA	5.46	128.17	120.42
34	8	123	THR	CA-C-O	5.46	126.21	120.42
2	b	48	GLU	N-CA-CB	5.46	119.53	110.52
2	b	241	GLN	CA-CB-CG	5.46	125.02	114.10
9	i	18	THR	CA-C-O	-5.46	113.04	119.48
10	j	49	PHE	CA-C-O	5.46	126.86	120.80
4	D	228	ASN	N-CA-C	-5.46	105.49	111.82
9	2	206	PRO	N-CA-CB	5.46	108.05	103.25
13	6	102	PHE	CA-CB-CG	-5.46	108.34	113.80
13	6	166	GLY	O-C-N	-5.46	116.20	122.42
24	X	76	VAL	CA-C-O	-5.46	115.67	119.38
26	Z	301	THR	CA-C-N	5.46	129.91	120.58
26	Z	301	THR	C-N-CA	5.46	129.91	120.58
31	R	361	VAL	N-CA-CB	5.46	117.96	110.54
34	8	264	HIS	ND1-CE1-NE2	5.46	113.86	108.40
7	g	149	PRO	CA-C-N	5.46	127.59	120.28
7	g	149	PRO	C-N-CA	5.46	127.59	120.28
6	F	142	HIS	CG-CD2-NE2	5.46	112.66	107.20
16	I	376	ASN	O-C-N	-5.46	116.31	123.02
19	M	301	VAL	CA-C-N	5.46	128.04	120.29
19	M	301	VAL	C-N-CA	5.46	128.04	120.29
34	8	181	PRO	CA-C-N	5.46	127.55	120.56
34	8	181	PRO	C-N-CA	5.46	127.55	120.56
2	b	106	PRO	N-CA-CB	5.46	107.90	103.32
29	P	225	VAL	CA-C-N	5.46	127.53	120.44
29	P	225	VAL	C-N-CA	5.46	127.53	120.44
11	k	188	GLY	N-CA-C	-5.45	105.54	111.21
14	7	137	TYR	N-CA-CB	5.45	120.01	111.56
17	K	110	VAL	CA-CB-CG1	5.45	119.67	110.40
27	N	432	GLY	CA-C-N	5.45	131.96	121.54
27	N	432	GLY	C-N-CA	5.45	131.96	121.54
27	N	780	ASP	CA-CB-CG	-5.45	107.15	112.60
33	O	337	LEU	N-CA-C	-5.45	100.78	109.23
2	B	216	ASP	CA-CB-CG	-5.45	107.15	112.60
7	G	108	PHE	CA-C-N	5.45	127.58	120.28
7	G	108	PHE	C-N-CA	5.45	127.58	120.28
20	J	29	GLU	CA-C-N	5.45	127.59	120.28
20	J	29	GLU	C-N-CA	5.45	127.59	120.28
20	J	382	PHE	N-CA-C	-5.45	105.42	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	142	ARG	N-CA-C	5.45	117.30	111.36
4	D	14	HIS	ND1-CE1-NE2	5.45	113.85	108.40
8	1	92	ASN	CA-CB-CG	-5.45	107.15	112.60
10	3	37	ASN	OD1-CG-ND2	5.45	128.05	122.60
11	4	8	ARG	NE-CZ-NH2	-5.45	114.29	119.20
16	I	85	PHE	O-C-N	5.45	126.92	121.85
2	b	107	THR	N-CA-C	-5.45	105.34	111.28
9	i	147	THR	N-CA-C	-5.45	102.45	110.52
4	D	177	TYR	N-CA-CB	-5.45	102.46	110.85
16	I	124	THR	CB-CA-C	-5.45	100.32	109.53
34	8	308	LYS	CB-CA-C	-5.45	101.42	110.68
34	8	403	SER	CB-CA-C	-5.45	101.75	110.79
5	e	65	HIS	CA-C-O	-5.45	113.84	119.51
26	Z	265	LEU	CA-C-O	-5.45	114.78	120.55
29	P	402	PHE	CA-CB-CG	-5.45	108.35	113.80
3	c	9	THR	O-C-N	-5.45	114.86	122.37
4	d	150	PRO	N-CA-CB	5.45	108.93	103.48
5	E	92	ASN	CB-CG-ND2	-5.45	108.23	116.40
22	V	96	LYS	CA-C-N	5.45	128.59	120.31
22	V	96	LYS	C-N-CA	5.45	128.59	120.31
34	8	438	HIS	CA-C-O	5.45	127.48	121.11
7	g	206	LYS	N-CA-C	-5.44	101.29	109.95
14	n	117	ALA	CA-C-O	5.44	126.24	120.36
20	J	35	ARG	N-CA-C	-5.44	105.26	111.14
3	C	44	VAL	CA-C-N	5.44	130.67	123.00
3	C	44	VAL	C-N-CA	5.44	130.67	123.00
5	E	77	ALA	CA-C-N	-5.44	113.36	120.44
5	E	77	ALA	C-N-CA	-5.44	113.36	120.44
27	N	10	LEU	N-CA-C	-5.44	105.43	111.36
9	2	205	PHE	CA-C-N	5.44	125.45	119.90
9	2	205	PHE	C-N-CA	5.44	125.45	119.90
16	I	119	ILE	N-CA-C	-5.44	100.29	108.12
17	K	52	LYS	N-CA-CB	5.44	118.12	110.12
17	K	248	GLY	CA-C-N	5.44	128.58	120.31
17	K	248	GLY	C-N-CA	5.44	128.58	120.31
18	L	138	SER	N-CA-CB	5.44	118.21	110.16
18	L	249	SER	N-CA-C	-5.44	106.48	113.23
18	L	403	ILE	CA-C-N	5.44	127.57	120.28
18	L	403	ILE	C-N-CA	5.44	127.57	120.28
19	M	316	SER	N-CA-C	-5.44	107.29	114.31
26	Z	773	ARG	N-CA-C	-5.44	104.52	113.50
8	h	60	GLN	N-CA-C	-5.44	105.35	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Q	59	LEU	CA-C-O	5.44	126.19	120.42
31	R	58	GLU	CA-C-O	5.44	128.29	120.51
6	f	47	ALA	CA-C-N	5.44	129.86	122.19
6	f	47	ALA	C-N-CA	5.44	129.86	122.19
10	3	134	ASP	O-C-N	5.44	127.67	122.07
18	L	112	LEU	N-CA-C	-5.44	107.30	114.04
18	L	161	ARG	CA-C-N	5.44	128.57	120.90
18	L	161	ARG	C-N-CA	5.44	128.57	120.90
27	N	450	ILE	O-C-N	-5.44	116.23	121.83
29	P	250	ILE	O-C-N	5.44	127.14	121.87
29	P	409	SER	CA-C-O	5.44	126.31	120.55
30	Q	299	MET	CG-SD-CE	-5.44	88.94	100.90
34	8	294	ASN	CA-C-N	5.44	128.81	120.82
34	8	294	ASN	C-N-CA	5.44	128.81	120.82
34	8	357	ARG	NE-CZ-NH2	-5.44	114.31	119.20
5	e	205	ASP	N-CA-CB	5.44	120.74	111.66
7	G	149	PRO	CA-C-N	5.44	127.56	120.28
7	G	149	PRO	C-N-CA	5.44	127.56	120.28
26	Z	705	GLU	O-C-N	5.44	128.35	122.15
33	O	245	ASP	N-CA-CB	5.44	118.68	110.42
5	e	144	GLY	CA-C-O	-5.43	115.16	122.33
9	i	145	ASP	CA-CB-CG	-5.43	107.17	112.60
14	7	39	VAL	O-C-N	5.43	129.51	122.77
18	L	399	GLY	CA-C-N	5.43	127.50	120.44
18	L	399	GLY	C-N-CA	5.43	127.50	120.44
19	M	410	VAL	N-CA-C	-5.43	100.65	108.53
21	W	88	ALA	O-C-N	5.43	127.96	122.09
24	X	17	TYR	CA-C-O	5.43	126.17	120.36
26	Z	308	LYS	O-C-N	5.43	127.67	122.07
27	N	18	ASP	O-C-N	5.43	127.67	122.07
1	A	17	TYR	CA-C-N	5.43	127.56	120.28
1	A	17	TYR	C-N-CA	5.43	127.56	120.28
1	A	87	ARG	NE-CZ-NH1	5.43	126.93	121.50
7	G	74	TYR	CA-CB-CG	-5.43	104.12	113.90
26	Z	22	LYS	CA-C-N	5.43	127.56	120.28
26	Z	22	LYS	C-N-CA	5.43	127.56	120.28
27	N	739	PHE	CA-CB-CG	5.43	119.23	113.80
31	R	148	ASP	O-C-N	-5.43	115.96	122.15
34	8	368	ASN	CB-CA-C	-5.43	98.64	109.99
27	N	650	ASP	CA-C-O	-5.43	114.79	120.55
14	n	40	GLU	CB-CG-CD	-5.43	103.37	112.60
6	F	131	LEU	O-C-N	5.43	129.98	123.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	73	GLN	N-CA-CB	5.43	118.10	110.12
28	S	187	ILE	CA-C-N	5.43	128.00	120.29
28	S	187	ILE	C-N-CA	5.43	128.00	120.29
2	b	183	LEU	CA-C-N	5.43	131.26	121.06
2	b	183	LEU	C-N-CA	5.43	131.26	121.06
6	f	208	ASP	CA-CB-CG	-5.43	107.17	112.60
8	h	82	PHE	CB-CA-C	-5.43	101.78	110.79
6	F	106	ARG	CA-C-O	-5.43	113.73	119.97
28	S	413	LEU	CA-C-O	-5.43	114.86	121.05
10	j	202	ARG	N-CA-C	-5.42	100.26	108.67
6	F	47	ALA	CB-CA-C	-5.42	98.37	109.38
9	2	182	LYS	O-C-N	5.42	129.46	123.33
26	Z	493	LEU	N-CA-C	-5.42	105.28	111.14
26	Z	549	ASN	N-CA-C	-5.42	105.28	111.14
10	3	28	LEU	CA-C-O	-5.42	114.50	120.36
12	5	25	TRP	CG-CD2-CE3	-5.42	128.48	133.90
16	I	291	ARG	N-CA-C	5.42	118.42	109.85
9	i	32	ALA	N-CA-CB	5.42	117.98	109.69
9	i	64	GLU	CA-C-N	5.42	127.49	120.44
9	i	64	GLU	C-N-CA	5.42	127.49	120.44
26	Z	956	LEU	N-CA-C	-5.42	99.68	108.52
29	P	336	HIS	CE1-NE2-CD2	-5.42	103.58	109.00
4	D	23	GLU	N-CA-C	-5.42	105.37	111.28
32	U	62	ASN	O-C-N	5.42	129.61	123.27
12	5	25	TRP	CZ3-CH2-CZ2	-5.42	114.46	121.50
13	6	98	TYR	CA-C-N	5.42	126.10	120.03
13	6	98	TYR	C-N-CA	5.42	126.10	120.03
16	I	381	VAL	O-C-N	-5.42	116.62	121.87
18	L	175	GLN	CB-CA-C	-5.42	110.35	116.63
31	R	68	GLU	O-C-N	5.42	127.66	122.03
6	f	184	ASN	N-CA-CB	5.42	120.24	110.17
8	h	13	ILE	N-CA-CB	5.42	118.68	111.64
8	h	121	LYS	N-CA-CB	5.42	118.34	109.95
11	k	172	MET	N-CA-C	-5.42	101.81	110.10
14	7	95	TYR	CB-CG-CD1	-5.42	112.68	120.80
32	U	167	GLU	CB-CG-CD	-5.42	103.39	112.60
4	D	220	VAL	N-CA-C	-5.41	101.20	108.35
11	4	111	LYS	CA-C-N	5.41	130.51	122.82
11	4	111	LYS	C-N-CA	5.41	130.51	122.82
26	Z	125	THR	N-CA-CB	5.41	118.08	110.12
27	N	325	PHE	CA-CB-CG	5.41	119.21	113.80
10	j	39	PHE	N-CA-CB	5.41	118.69	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	88	ASN	N-CA-C	5.41	117.26	111.36
16	I	280	PHE	CB-CG-CD2	-5.41	111.50	120.70
22	V	160	ASP	CA-C-N	5.41	127.98	120.29
22	V	160	ASP	C-N-CA	5.41	127.98	120.29
26	Z	258	PRO	N-CA-C	5.41	117.30	110.70
26	Z	334	LYS	CA-C-N	5.41	127.80	120.44
26	Z	334	LYS	C-N-CA	5.41	127.80	120.44
14	n	137	TYR	N-CA-CB	5.41	120.86	111.39
1	A	67	SER	CA-C-O	5.41	127.15	121.25
15	H	223	GLU	CA-C-N	5.41	127.49	120.56
15	H	223	GLU	C-N-CA	5.41	127.49	120.56
26	Z	297	VAL	CB-CA-C	-5.41	105.04	111.97
26	Z	502	ASN	CA-CB-CG	-5.41	107.19	112.60
27	N	440	ASP	N-CA-C	5.41	116.86	111.07
28	S	351	ALA	CA-C-N	5.41	127.87	120.46
28	S	351	ALA	C-N-CA	5.41	127.87	120.46
31	R	178	GLY	CA-C-N	5.41	128.53	120.31
31	R	178	GLY	C-N-CA	5.41	128.53	120.31
34	8	255	ASN	N-CA-C	-5.41	106.35	113.17
5	e	215	THR	CA-CB-CG2	-5.41	101.31	110.50
11	4	133	HIS	CA-C-O	-5.41	115.11	121.44
32	U	106	ILE	N-CA-C	-5.41	105.10	110.62
5	E	216	LYS	N-CA-C	-5.41	105.47	111.36
30	Q	335	PHE	N-CA-CB	5.41	118.63	110.30
33	O	137	TYR	O-C-N	-5.41	115.99	122.15
2	b	43	VAL	CA-C-O	5.41	126.42	120.64
4	d	105	GLU	CA-C-N	5.41	127.47	120.44
4	d	105	GLU	C-N-CA	5.41	127.47	120.44
3	C	236	ASP	N-CA-CB	5.41	118.07	110.12
14	7	218	LYS	CA-C-N	5.41	128.50	120.17
14	7	218	LYS	C-N-CA	5.41	128.50	120.17
17	K	393	ARG	CA-C-N	5.41	129.75	120.72
17	K	393	ARG	C-N-CA	5.41	129.75	120.72
23	T	235	PHE	CA-C-N	5.41	128.53	120.31
23	T	235	PHE	C-N-CA	5.41	128.53	120.31
26	Z	949	ILE	N-CA-C	5.41	116.18	110.72
26	Z	954	PRO	N-CA-C	-5.41	102.70	111.19
30	Q	248	ASN	CA-CB-CG	-5.41	107.19	112.60
1	a	121	GLN	CA-C-N	5.40	129.02	121.02
1	a	121	GLN	C-N-CA	5.40	129.02	121.02
2	b	94	HIS	CG-CD2-NE2	5.40	112.60	107.20
3	C	157	THR	CA-CB-OG1	5.40	117.71	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	290	SER	CA-C-N	5.40	127.52	120.28
31	R	290	SER	C-N-CA	5.40	127.52	120.28
1	a	49	LYS	N-CA-C	-5.40	102.39	110.23
4	d	11	PRO	N-CA-C	-5.40	106.98	114.27
13	6	72	VAL	CA-CB-CG2	-5.40	101.21	110.40
16	I	110	GLU	O-C-N	5.40	129.59	122.30
27	N	805	SER	CA-C-O	-5.40	114.82	120.55
28	S	56	SER	CA-C-N	5.40	127.78	120.38
28	S	56	SER	C-N-CA	5.40	127.78	120.38
28	S	215	MET	CA-C-O	-5.40	114.69	120.42
28	S	483	GLU	N-CA-C	5.40	117.92	111.71
33	O	143	LEU	CA-C-N	5.40	127.47	120.56
33	O	143	LEU	C-N-CA	5.40	127.47	120.56
5	e	124	ARG	N-CA-CB	5.40	119.03	110.55
2	B	182	GLU	CA-C-O	-5.40	114.00	120.10
19	M	310	ASN	OD1-CG-ND2	-5.40	117.20	122.60
31	R	60	ALA	O-C-N	-5.40	115.35	120.70
31	R	351	LYS	O-C-N	5.40	128.31	122.15
32	U	58	GLU	CA-CB-CG	-5.40	103.30	114.10
33	O	314	SER	CA-C-N	5.40	127.96	120.29
33	O	314	SER	C-N-CA	5.40	127.96	120.29
9	i	137	VAL	CA-C-O	5.40	126.56	120.95
14	n	110	LEU	CA-C-O	5.40	126.70	120.60
3	C	93	HIS	CE1-NE2-CD2	-5.40	103.60	109.00
21	W	123	ASP	CB-CA-C	-5.40	101.83	110.79
6	f	60	LYS	N-CA-CB	5.40	117.89	109.85
10	j	82	GLU	CA-C-O	-5.40	115.30	120.97
12	l	84	SER	O-C-N	5.40	128.30	122.15
4	D	68	HIS	CE1-NE2-CD2	-5.40	103.60	109.00
20	J	128	ASN	OD1-CG-ND2	-5.40	117.20	122.60
28	S	346	TYR	CA-C-O	5.40	126.49	120.82
29	P	142	ASP	CA-C-N	5.40	127.95	120.29
29	P	142	ASP	C-N-CA	5.40	127.95	120.29
29	P	230	HIS	O-C-N	5.40	127.84	122.12
4	d	12	ASP	N-CA-CB	5.40	118.57	110.53
7	g	89	ARG	NE-CZ-NH2	5.40	124.06	119.20
13	6	195	HIS	CA-CB-CG	5.40	119.20	113.80
21	W	155	ASP	CA-C-N	5.40	127.51	120.28
21	W	155	ASP	C-N-CA	5.40	127.51	120.28
26	Z	44	LYS	CA-C-N	5.40	127.51	120.28
26	Z	44	LYS	C-N-CA	5.40	127.51	120.28
34	8	183	VAL	CA-C-N	5.40	127.45	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	8	183	VAL	C-N-CA	5.40	127.45	120.44
34	8	213	LEU	CB-CA-C	-5.40	101.83	110.79
9	2	165	ASN	OD1-CG-ND2	5.39	127.99	122.60
18	L	82	ARG	N-CA-C	5.39	117.16	111.28
9	2	76	VAL	CA-C-N	5.39	129.14	120.30
9	2	76	VAL	C-N-CA	5.39	129.14	120.30
19	M	429	SER	N-CA-CB	5.39	117.94	109.69
26	Z	779	ALA	CA-C-O	5.39	126.27	120.55
28	S	425	ARG	CB-CA-C	-5.39	101.84	110.79
29	P	39	LEU	CA-C-N	5.39	127.50	120.28
29	P	39	LEU	C-N-CA	5.39	127.50	120.28
31	R	250	ALA	CA-C-N	5.39	127.45	120.44
31	R	250	ALA	C-N-CA	5.39	127.45	120.44
30	Q	201	ALA	O-C-N	5.39	127.62	122.07
14	n	97	ALA	N-CA-C	-5.39	105.48	111.36
5	E	149	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
9	2	190	TYR	O-C-N	-5.39	116.52	122.07
12	5	205	GLY	N-CA-C	-5.39	107.83	115.43
14	7	86	ALA	N-CA-C	-5.39	103.02	110.35
22	V	114	PHE	N-CA-CB	-5.39	102.86	111.43
27	N	329	HIS	N-CA-CB	5.39	118.63	110.28
27	N	896	PHE	CA-C-N	5.39	127.45	120.44
27	N	896	PHE	C-N-CA	5.39	127.45	120.44
28	S	144	LEU	N-CA-CB	5.39	117.83	110.01
33	O	361	ASP	CA-C-N	5.39	128.04	120.28
33	O	361	ASP	C-N-CA	5.39	128.04	120.28
6	F	186	ASP	CA-CB-CG	-5.39	107.21	112.60
9	2	133	ALA	CB-CA-C	-5.39	102.42	110.88
30	Q	219	ASP	CA-C-N	5.39	128.04	120.28
30	Q	219	ASP	C-N-CA	5.39	128.04	120.28
2	b	139	HIS	CE1-NE2-CD2	-5.39	103.61	109.00
9	i	73	GLU	CA-C-O	-5.39	114.23	119.51
28	S	213	THR	N-CA-C	5.39	117.23	111.36
2	b	26	THR	O-C-N	5.38	127.83	122.12
13	m	79	HIS	CE1-NE2-CD2	-5.38	103.62	109.00
9	2	79	ALA	CA-C-N	5.38	127.81	120.54
9	2	79	ALA	C-N-CA	5.38	127.81	120.54
11	4	57	ALA	CA-C-N	5.38	128.49	120.31
11	4	57	ALA	C-N-CA	5.38	128.49	120.31
15	H	230	LEU	CB-CA-C	-5.38	100.85	110.70
17	K	178	ASP	N-CA-C	-5.38	106.21	112.89
20	J	88	VAL	N-CA-CB	5.38	116.80	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	396	THR	CA-CB-OG1	5.38	117.68	109.60
22	V	135	ARG	NE-CZ-NH1	5.38	126.88	121.50
22	V	250	GLN	CA-C-N	5.38	127.50	120.28
22	V	250	GLN	C-N-CA	5.38	127.50	120.28
10	3	47	HIS	CE1-NE2-CD2	-5.38	103.62	109.00
20	J	192	GLY	CA-C-O	5.38	125.70	119.13
22	V	152	VAL	CA-C-O	5.38	127.51	120.78
31	R	184	GLN	OE1-CD-NE2	5.38	127.98	122.60
1	a	74	VAL	CA-C-N	5.38	131.03	122.74
1	a	74	VAL	C-N-CA	5.38	131.03	122.74
18	L	87	LEU	N-CA-C	5.38	117.14	111.28
22	V	52	LEU	N-CA-CB	5.38	119.14	110.85
25	Y	68	GLU	N-CA-C	-5.38	100.89	109.07
30	Q	52	ASN	CA-C-N	5.38	127.80	120.54
30	Q	52	ASN	C-N-CA	5.38	127.80	120.54
4	d	14	HIS	CE1-NE2-CD2	-5.38	103.62	109.00
17	K	212	TYR	CB-CG-CD1	-5.38	112.73	120.80
8	h	115	LEU	CA-C-N	5.38	127.12	120.34
8	h	115	LEU	C-N-CA	5.38	127.12	120.34
3	C	58	GLN	CA-C-N	5.38	127.49	120.28
3	C	58	GLN	C-N-CA	5.38	127.49	120.28
14	7	69	ASP	CB-CA-C	-5.38	101.86	110.79
16	I	141	LEU	CB-CA-C	-5.38	101.47	110.29
18	L	55	LYS	CA-C-N	5.38	127.49	120.28
18	L	55	LYS	C-N-CA	5.38	127.49	120.28
23	T	61	ILE	N-CA-C	5.38	115.58	110.42
26	Z	219	ASP	CA-C-N	5.38	127.49	120.28
26	Z	219	ASP	C-N-CA	5.38	127.49	120.28
2	b	80	PRO	N-CD-CG	5.38	111.26	103.20
6	f	196	ILE	CA-CB-CG1	5.38	119.54	110.40
12	5	198	TRP	CE2-CD2-CE3	5.38	124.18	118.80
26	Z	716	THR	O-C-N	-5.38	116.53	122.07
30	Q	89	ALA	CA-C-O	-5.38	115.47	122.14
33	O	65	PHE	CA-C-O	-5.38	114.85	120.55
34	8	352	GLU	CB-CA-C	-5.38	101.86	110.79
28	S	156	VAL	N-CA-C	5.38	115.58	110.42
29	P	166	GLU	CA-C-O	-5.38	114.79	120.92
31	R	298	ALA	N-CA-C	-5.38	106.68	113.18
5	e	153	SER	CA-C-O	-5.37	113.31	119.60
1	A	19	VAL	CA-C-N	5.37	127.48	120.28
1	A	19	VAL	C-N-CA	5.37	127.48	120.28
16	I	333	THR	N-CA-C	-5.37	106.73	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	373	GLU	N-CA-C	-5.37	99.92	109.06
21	W	184	ASN	N-CA-C	-5.37	105.50	111.36
26	Z	332	ASN	OD1-CG-ND2	5.37	127.97	122.60
27	N	598	ASP	CA-CB-CG	-5.37	107.23	112.60
31	R	162	ILE	CA-C-N	5.37	128.34	120.71
31	R	162	ILE	C-N-CA	5.37	128.34	120.71
4	d	96	LEU	O-C-N	5.37	127.60	122.07
4	D	75	GLY	CA-C-N	5.37	131.80	121.54
4	D	75	GLY	C-N-CA	5.37	131.80	121.54
26	Z	105	LYS	CA-C-O	-5.37	114.86	120.55
27	N	619	CYS	CA-C-N	5.37	130.35	120.79
27	N	619	CYS	C-N-CA	5.37	130.35	120.79
31	R	347	THR	CA-C-O	5.37	127.15	120.54
33	O	235	HIS	CG-CD2-NE2	5.37	112.57	107.20
4	D	201	VAL	CA-C-N	5.37	129.80	122.34
4	D	201	VAL	C-N-CA	5.37	129.80	122.34
10	3	199	LEU	N-CA-C	-5.37	102.80	110.59
17	K	315	ILE	CA-CB-CG1	5.37	119.53	110.40
29	P	52	LEU	CA-C-O	-5.37	115.18	120.82
31	R	96	GLN	N-CA-C	-5.37	105.99	112.54
33	O	23	HIS	CG-CD2-NE2	5.37	112.57	107.20
6	f	114	LYS	CA-C-N	5.37	127.42	120.44
6	f	114	LYS	C-N-CA	5.37	127.42	120.44
12	l	65	LEU	N-CA-CB	5.37	117.94	109.94
1	A	143	PRO	CA-C-O	5.37	127.17	121.32
8	1	143	ARG	CB-CA-C	-5.37	100.67	109.80
16	I	132	ILE	N-CA-C	-5.37	100.02	108.23
17	K	220	THR	O-C-N	5.37	128.87	122.27
18	L	384	ASP	N-CA-CB	5.37	117.90	110.17
19	M	273	LYS	CA-C-N	5.37	128.84	120.68
19	M	273	LYS	C-N-CA	5.37	128.84	120.68
27	N	501	MET	CA-C-N	5.37	127.42	120.44
27	N	501	MET	C-N-CA	5.37	127.42	120.44
27	N	786	ARG	NE-CZ-NH1	-5.37	116.13	121.50
34	8	128	TYR	CB-CG-CD2	-5.37	112.75	120.80
34	8	257	SER	O-C-N	5.37	129.16	123.42
4	d	54	ASP	CA-C-N	5.37	127.47	120.28
4	d	54	ASP	C-N-CA	5.37	127.47	120.28
12	l	122	LEU	CA-C-O	5.37	125.93	120.24
14	n	76	TYR	CA-C-O	-5.37	115.71	121.56
9	2	208	GLY	CA-C-N	5.37	127.47	120.28
9	2	208	GLY	C-N-CA	5.37	127.47	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	187	TYR	N-CA-CB	5.37	119.17	110.42
22	V	182	LYS	N-CA-C	-5.37	108.50	114.62
26	Z	502	ASN	OD1-CG-ND2	5.37	127.97	122.60
34	8	313	GLN	CA-C-N	5.37	128.39	120.82
34	8	313	GLN	C-N-CA	5.37	128.39	120.82
7	g	51	THR	O-C-N	5.37	127.89	122.09
1	A	106	ASP	N-CA-C	-5.37	105.35	111.14
4	D	215	PRO	N-CD-CG	5.37	111.25	103.20
5	E	18	TYR	N-CA-CB	5.37	118.48	110.22
5	E	128	ARG	N-CA-CB	5.37	119.92	110.37
10	3	129	ILE	N-CA-C	-5.37	98.75	107.28
23	T	168	SER	N-CA-C	-5.37	106.41	113.17
23	T	250	MET	CG-SD-CE	-5.37	89.09	100.90
26	Z	593	HIS	CB-CG-CD2	-5.37	124.22	131.20
6	f	47	ALA	N-CA-CB	5.36	121.51	111.53
1	A	62	TYR	CA-CB-CG	-5.36	104.25	113.90
27	N	700	CYS	CA-C-O	-5.36	114.86	120.55
29	P	137	ALA	CA-C-N	5.36	127.47	120.28
29	P	137	ALA	C-N-CA	5.36	127.47	120.28
33	O	65	PHE	N-CA-CB	5.36	118.00	110.12
10	j	79	ARG	CD-NE-CZ	5.36	131.91	124.40
16	I	369	MET	N-CA-CB	5.36	117.92	110.04
7	g	224	HIS	CA-C-O	5.36	126.27	120.43
8	l	63	LEU	O-C-N	-5.36	115.25	122.43
19	M	177	THR	N-CA-C	-5.36	99.78	108.41
33	O	103	LYS	CA-C-N	5.36	127.46	120.28
33	O	103	LYS	C-N-CA	5.36	127.46	120.28
2	b	53	SER	CA-C-N	5.36	125.83	120.04
2	b	53	SER	C-N-CA	5.36	125.83	120.04
14	n	36	PHE	CA-C-N	-5.36	114.26	122.62
14	n	36	PHE	C-N-CA	-5.36	114.26	122.62
18	L	332	THR	N-CA-CB	5.36	118.53	110.65
23	T	9	LYS	N-CA-C	-5.36	106.25	112.89
28	S	334	HIS	CG-CD2-NE2	5.36	112.56	107.20
7	G	77	LEU	CA-C-N	5.36	124.62	120.33
7	G	77	LEU	C-N-CA	5.36	124.62	120.33
10	3	2	ASP	CA-CB-CG	-5.36	107.24	112.60
11	4	138	PHE	CA-CB-CG	5.36	119.16	113.80
27	N	660	LEU	N-CA-C	-5.36	105.44	111.28
28	S	352	VAL	CA-C-N	5.36	127.40	120.44
28	S	352	VAL	C-N-CA	5.36	127.40	120.44
29	P	77	GLU	N-CA-C	5.36	117.12	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	88	ALA	N-CA-C	-5.36	105.10	111.69
19	M	248	ALA	CA-C-O	-5.36	112.82	120.16
33	O	259	THR	N-CA-CB	5.36	117.99	110.12
17	K	81	ARG	CA-C-N	5.35	127.89	120.29
17	K	81	ARG	C-N-CA	5.35	127.89	120.29
3	c	236	ASP	N-CA-CB	5.35	117.99	110.12
11	k	20	ALA	CB-CA-C	-5.35	100.50	109.65
12	l	106	ARG	CA-C-N	5.35	127.40	120.44
12	l	106	ARG	C-N-CA	5.35	127.40	120.44
2	B	142	PHE	CA-CB-CG	-5.35	108.45	113.80
6	F	184	ASN	CA-CB-CG	-5.35	107.25	112.60
7	G	17	ASN	CA-C-N	5.35	127.89	120.29
7	G	17	ASN	C-N-CA	5.35	127.89	120.29
10	3	192	ASP	CA-CB-CG	-5.35	107.25	112.60
21	W	147	ILE	N-CA-C	-5.35	107.26	112.29
23	T	83	ASN	N-CA-C	5.35	117.53	111.11
26	Z	451	ALA	CA-C-N	5.35	127.45	120.28
26	Z	451	ALA	C-N-CA	5.35	127.45	120.28
28	S	22	GLU	CB-CA-C	-5.35	102.44	110.90
29	P	367	GLU	CA-C-N	5.35	127.89	120.29
29	P	367	GLU	C-N-CA	5.35	127.89	120.29
30	Q	351	ILE	CA-C-O	-5.35	113.12	119.54
32	U	65	VAL	N-CA-C	-5.35	100.62	108.11
33	O	317	THR	CA-C-O	-5.35	113.05	119.15
15	H	297	MET	CA-C-N	5.35	127.40	120.44
15	H	297	MET	C-N-CA	5.35	127.40	120.44
18	L	242	ASN	N-CA-CB	5.35	117.91	110.04
31	R	149	ASN	N-CA-C	-5.35	106.59	113.23
33	O	259	THR	O-C-N	-5.35	116.45	122.12
6	f	25	LEU	CB-CA-C	-5.35	100.73	110.63
11	k	67	TYR	CA-C-O	5.35	126.22	120.55
13	m	77	PHE	CB-CA-C	-5.35	101.91	110.79
3	C	219	ALA	N-CA-C	-5.35	100.98	109.59
4	D	2	TYR	N-CA-C	-5.35	106.62	112.72
20	J	19	ILE	CA-C-N	5.35	127.64	120.58
20	J	19	ILE	C-N-CA	5.35	127.64	120.58
28	S	322	LEU	O-C-N	5.35	127.79	122.12
32	U	68	LEU	N-CA-C	-5.35	100.94	109.23
33	O	108	GLU	CA-C-N	5.35	127.98	120.28
33	O	108	GLU	C-N-CA	5.35	127.98	120.28
8	h	172	VAL	CB-CA-C	5.35	120.33	111.51
5	E	58	LYS	CA-CB-CG	-5.35	103.41	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	701	ILE	CA-C-N	5.35	127.88	120.29
26	Z	701	ILE	C-N-CA	5.35	127.88	120.29
2	b	111	VAL	CB-CA-C	-5.35	104.92	112.14
3	c	185	VAL	N-CA-CB	5.34	117.15	110.47
9	i	93	HIS	N-CA-CB	5.34	117.82	110.07
3	C	97	TYR	CA-C-N	5.34	127.88	120.29
3	C	97	TYR	C-N-CA	5.34	127.88	120.29
3	C	152	PRO	CA-C-N	5.34	127.39	120.44
3	C	152	PRO	C-N-CA	5.34	127.39	120.44
7	G	162	GLY	CA-C-N	5.34	127.71	120.44
7	G	162	GLY	C-N-CA	5.34	127.71	120.44
10	3	169	ALA	CB-CA-C	-5.34	101.92	110.79
15	H	383	GLU	N-CA-C	5.34	117.19	111.36
28	S	134	ILE	CA-C-N	5.34	127.39	120.44
28	S	134	ILE	C-N-CA	5.34	127.39	120.44
30	Q	162	LEU	CA-C-N	5.34	127.44	120.28
30	Q	162	LEU	C-N-CA	5.34	127.44	120.28
3	c	69	ASN	N-CA-CB	5.34	119.66	111.22
27	N	330	THR	CA-C-O	-5.34	115.20	120.70
29	P	366	ASN	N-CA-C	5.34	117.85	111.71
30	Q	328	ASP	O-C-N	5.34	129.52	123.27
9	2	86	HIS	CB-CG-ND1	5.34	130.71	122.70
12	5	34	VAL	N-CA-CB	5.34	117.46	111.21
15	H	91	LEU	N-CA-C	-5.34	105.54	111.36
18	L	111	GLU	CA-C-N	-5.34	112.97	122.42
18	L	111	GLU	C-N-CA	-5.34	112.97	122.42
27	N	764	SER	N-CA-C	-5.34	106.07	112.59
30	Q	183	LYS	O-C-N	5.34	127.78	122.12
32	U	69	ASP	CA-C-N	5.34	127.44	120.28
32	U	69	ASP	C-N-CA	5.34	127.44	120.28
2	b	164	ILE	N-CA-C	-5.34	100.91	108.65
1	A	105	CYS	CA-C-N	5.34	127.70	120.44
1	A	105	CYS	C-N-CA	5.34	127.70	120.44
4	D	59	PRO	N-CA-CB	5.34	108.00	103.19
6	F	114	LYS	CA-C-N	5.34	127.44	120.28
6	F	114	LYS	C-N-CA	5.34	127.44	120.28
8	1	186	LEU	CA-C-N	-5.34	115.02	122.71
8	1	186	LEU	C-N-CA	-5.34	115.02	122.71
18	L	317	ASN	CA-CB-CG	-5.34	107.26	112.60
31	R	97	GLU	CA-C-O	-5.34	115.19	120.90
10	j	44	HIS	ND1-CE1-NE2	5.34	113.74	108.40
4	D	21	ALA	N-CA-C	-5.34	105.54	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	P	283	LYS	CB-CG-CD	5.34	123.58	111.30
30	Q	297	ASP	CA-CB-CG	-5.34	107.26	112.60
34	8	467	ASP	CA-CB-CG	-5.34	107.26	112.60
3	c	142	ARG	NH1-CZ-NH2	5.34	126.24	119.30
7	g	89	ARG	N-CA-CB	5.34	117.97	110.12
2	B	170	ALA	O-C-N	5.34	127.85	122.09
6	F	219	THR	CA-C-O	-5.34	114.49	120.25
8	1	161	GLN	CB-CA-C	-5.34	100.42	110.67
26	Z	253	VAL	CG1-CB-CG2	-5.34	99.06	110.80
26	Z	574	TYR	N-CA-C	5.34	119.05	112.54
27	N	315	ASN	CA-CB-CG	-5.34	107.26	112.60
29	P	361	THR	CA-C-O	-5.34	114.97	121.05
34	8	158	LYS	CB-CA-C	-5.34	101.78	110.85
34	8	186	ASN	CA-C-N	5.34	127.96	120.28
34	8	186	ASN	C-N-CA	5.34	127.96	120.28
34	8	330	LEU	CA-C-O	5.34	125.53	119.18
2	b	70	ASP	CA-C-N	5.33	130.41	122.99
2	b	70	ASP	C-N-CA	5.33	130.41	122.99
34	8	250	ILE	N-CA-C	-5.33	98.24	109.34
5	e	234	GLU	N-CA-C	-5.33	105.55	111.36
6	f	142	HIS	CE1-NE2-CD2	-5.33	103.67	109.00
7	G	99	TYR	CA-C-N	5.33	129.71	122.19
7	G	99	TYR	C-N-CA	5.33	129.71	122.19
18	L	288	GLY	O-C-N	5.33	128.82	123.11
20	J	352	GLY	N-CA-C	-5.33	100.54	113.18
22	V	65	VAL	O-C-N	5.33	130.09	122.62
23	T	269	SER	N-CA-C	-5.33	105.55	111.36
29	P	230	HIS	ND1-CE1-NE2	5.33	113.73	108.40
30	Q	109	ASP	CA-CB-CG	5.33	117.93	112.60
1	a	103	MET	CB-CA-C	-5.33	101.10	109.52
5	E	180	HIS	CG-CD2-NE2	5.33	112.53	107.20
12	5	89	GLN	CB-CA-C	-5.33	101.94	110.79
20	J	164	ILE	CA-C-O	-5.33	114.46	120.32
27	N	533	ASP	CA-C-N	5.33	127.37	120.44
27	N	533	ASP	C-N-CA	5.33	127.37	120.44
27	N	757	THR	O-C-N	-5.33	117.91	123.56
14	n	167	LYS	CB-CA-C	-5.33	102.51	110.88
13	m	59	ALA	CA-C-N	5.33	128.41	120.31
13	m	59	ALA	C-N-CA	5.33	128.41	120.31
14	n	153	PRO	N-CA-C	5.33	121.69	113.75
7	G	83	HIS	CA-CB-CG	-5.33	108.47	113.80
8	1	176	VAL	N-CA-C	-5.33	99.97	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	86	HIS	N-CA-C	-5.33	98.53	107.32
27	N	270	LEU	O-C-N	5.33	127.77	122.12
29	P	74	ASP	CA-C-N	5.33	127.37	120.44
29	P	74	ASP	C-N-CA	5.33	127.37	120.44
1	a	144	SER	CA-C-N	5.33	130.47	122.75
1	a	144	SER	C-N-CA	5.33	130.47	122.75
2	b	105	PRO	CA-C-O	-5.33	112.84	120.56
3	c	13	SER	CA-C-O	-5.33	114.50	120.25
3	c	101	TYR	CB-CG-CD1	5.33	128.79	120.80
21	W	196	SER	N-CA-C	-5.33	105.43	112.94
27	N	69	TYR	CA-C-O	5.33	126.07	120.42
29	P	414	GLU	CB-CG-CD	-5.33	103.54	112.60
33	O	225	ASP	N-CA-C	-5.33	105.75	113.21
10	j	45	TYR	CB-CG-CD2	-5.33	112.81	120.80
7	G	167	SER	N-CA-CB	5.33	117.73	110.01
16	I	285	ASP	CA-C-N	5.33	127.42	120.28
16	I	285	ASP	C-N-CA	5.33	127.42	120.28
19	M	231	LEU	O-C-N	5.33	127.84	122.09
27	N	68	VAL	CB-CA-C	-5.33	104.87	112.22
2	b	17	LYS	CA-CB-CG	5.32	124.75	114.10
9	i	98	LEU	N-CA-CB	5.32	121.06	111.37
9	2	160	GLN	CB-CA-C	-5.32	101.63	110.68
13	6	195	HIS	CA-C-N	5.32	129.19	121.52
13	6	195	HIS	C-N-CA	5.32	129.19	121.52
15	H	151	GLN	CA-C-N	5.32	131.55	121.97
15	H	151	GLN	C-N-CA	5.32	131.55	121.97
16	I	123	PRO	N-CA-CB	-5.32	98.16	103.48
18	L	234	ALA	CA-C-N	5.32	127.75	120.46
18	L	234	ALA	C-N-CA	5.32	127.75	120.46
27	N	811	LYS	CB-CA-C	-5.32	99.82	110.42
31	R	51	LEU	CA-C-N	5.32	127.41	120.28
31	R	51	LEU	C-N-CA	5.32	127.41	120.28
13	m	103	PHE	CA-C-O	-5.32	115.05	121.22
20	J	105	LYS	CA-C-N	5.32	128.40	120.31
20	J	105	LYS	C-N-CA	5.32	128.40	120.31
13	m	173	LYS	CA-C-N	5.32	128.78	120.75
13	m	173	LYS	C-N-CA	5.32	128.78	120.75
15	H	93	GLU	O-C-N	5.32	129.85	123.36
17	K	209	VAL	N-CA-C	-5.32	100.40	108.17
27	N	589	ILE	CA-C-O	5.32	126.48	120.95
27	N	683	LEU	CA-C-O	-5.32	114.09	120.10
27	N	747	HIS	CG-CD2-NE2	5.32	112.52	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Q	313	ASP	CA-C-N	5.32	127.41	120.28
30	Q	313	ASP	C-N-CA	5.32	127.41	120.28
20	J	394	GLN	N-CA-C	5.32	117.99	111.82
6	f	104	VAL	CA-C-N	5.32	127.84	120.29
6	f	104	VAL	C-N-CA	5.32	127.84	120.29
4	D	184	ALA	CA-C-O	5.32	126.09	119.97
15	H	88	ARG	CD-NE-CZ	-5.32	116.95	124.40
16	I	393	GLN	CA-C-N	5.32	127.41	120.28
16	I	393	GLN	C-N-CA	5.32	127.41	120.28
19	M	310	ASN	CB-CA-C	-5.32	101.96	110.79
27	N	616	HIS	ND1-CE1-NE2	5.32	113.72	108.40
34	8	253	LYS	N-CA-C	-5.32	100.73	109.40
13	6	173	LYS	CA-C-O	5.32	125.87	120.24
20	J	328	LEU	O-C-N	5.32	128.21	122.15
26	Z	95	THR	CA-C-N	5.32	126.37	119.78
26	Z	95	THR	C-N-CA	5.32	126.37	119.78
28	S	37	VAL	CA-C-N	5.32	127.35	120.44
28	S	37	VAL	C-N-CA	5.32	127.35	120.44
29	P	325	ASP	N-CA-CB	5.32	117.78	109.97
33	O	121	ASP	CA-C-O	-5.32	115.92	121.55
1	a	135	VAL	N-CA-CB	5.31	120.17	111.45
2	b	182	GLU	CB-CG-CD	-5.31	103.57	112.60
7	g	161	THR	CA-C-N	5.31	129.15	121.44
7	g	161	THR	C-N-CA	5.31	129.15	121.44
12	l	191	HIS	CG-CD2-NE2	5.31	112.51	107.20
6	F	231	LYS	CB-CA-C	-5.31	102.54	110.88
28	S	33	GLU	CA-C-O	-5.31	115.21	120.90
33	O	230	PHE	CA-C-O	-5.31	113.86	119.97
1	a	116	SER	N-CA-CB	5.31	117.93	110.12
5	E	179	TRP	N-CA-CB	5.31	117.85	109.83
17	K	427	TYR	N-CA-CB	5.31	118.96	110.73
18	L	332	THR	CA-C-O	5.31	124.89	119.05
23	T	224	ARG	NE-CZ-NH1	-5.31	116.19	121.50
26	Z	572	ILE	CA-C-N	5.31	127.40	120.28
26	Z	572	ILE	C-N-CA	5.31	127.40	120.28
9	i	223	ILE	CA-CB-CG2	-5.31	101.47	110.50
7	G	113	GLY	O-C-N	5.31	127.34	122.19
9	i	26	VAL	N-CA-C	-5.31	101.01	108.12
9	i	31	CYS	CA-C-N	5.31	128.31	120.82
9	i	31	CYS	C-N-CA	5.31	128.31	120.82
10	3	25	ASP	O-C-N	-5.31	116.12	122.65
14	7	175	GLU	O-C-N	5.31	127.75	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	8	292	GLY	CA-C-N	5.31	131.68	121.54
34	8	292	GLY	C-N-CA	5.31	131.68	121.54
5	e	3	GLY	CA-C-N	5.31	129.01	120.30
5	e	3	GLY	C-N-CA	5.31	129.01	120.30
13	m	92	ASN	CB-CA-C	-5.31	101.98	110.79
7	G	113	GLY	N-CA-C	-5.31	105.98	112.77
24	X	91	PHE	CA-CB-CG	-5.31	108.49	113.80
24	X	102	GLN	N-CA-C	-5.31	104.60	111.71
28	S	137	PHE	N-CA-CB	5.31	118.01	110.16
34	8	239	THR	O-C-N	5.31	129.55	123.29
9	i	54	ALA	CA-C-N	5.31	127.95	120.42
9	i	54	ALA	C-N-CA	5.31	127.95	120.42
4	D	35	LYS	N-CA-CB	5.31	120.06	110.83
29	P	370	ASP	CB-CA-C	-5.31	104.36	112.11
2	b	208	THR	N-CA-CB	5.30	119.46	110.49
10	j	41	LYS	N-CA-C	-5.30	108.07	114.75
11	k	87	GLU	CA-C-N	5.30	128.37	120.31
11	k	87	GLU	C-N-CA	5.30	128.37	120.31
3	C	203	SER	N-CA-CB	5.30	118.56	110.44
4	D	34	VAL	N-CA-C	-5.30	100.43	108.17
11	4	124	THR	N-CA-CB	5.30	119.14	110.39
18	L	241	ALA	CA-C-O	-5.30	115.36	121.19
20	J	310	ILE	CA-CB-CG1	5.30	119.42	110.40
26	Z	926	ASN	CA-C-O	5.30	128.10	120.51
31	R	204	TRP	CA-C-O	-5.30	113.53	119.79
11	k	60	ILE	N-CA-C	-5.30	105.36	110.72
12	5	39	PRO	N-CA-CB	5.30	108.82	103.25
18	L	426	LYS	CA-C-O	-5.30	114.93	120.55
19	M	63	LYS	CB-CA-C	-5.30	101.83	110.85
4	d	68	HIS	CE1-NE2-CD2	-5.30	103.70	109.00
10	j	161	ASP	CA-CB-CG	-5.30	107.30	112.60
12	l	88	TYR	CB-CG-CD1	-5.30	112.85	120.80
5	E	21	GLU	O-C-N	5.30	128.19	122.15
7	G	148	GLU	O-C-N	-5.30	115.59	121.53
14	7	169	THR	O-C-N	5.30	128.88	122.94
4	d	44	CYS	CA-C-O	5.30	126.96	120.60
3	C	194	LYS	CB-CA-C	5.30	119.20	110.88
15	H	265	ASN	OD1-CG-ND2	-5.30	117.30	122.60
17	K	70	ASP	CA-CB-CG	-5.30	107.30	112.60
17	K	388	GLN	OE1-CD-NE2	5.30	127.90	122.60
18	L	367	LYS	CB-CA-C	-5.30	102.56	110.88
19	M	385	GLU	CB-CA-C	-5.30	104.37	112.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	270	ARG	CA-C-O	-5.30	115.24	120.70
21	W	15	TYR	N-CA-C	-5.30	106.04	112.88
28	S	308	GLY	CA-C-N	5.30	127.65	120.44
28	S	308	GLY	C-N-CA	5.30	127.65	120.44
12	l	188	HIS	CE1-NE2-CD2	-5.30	103.70	109.00
12	5	31	VAL	CA-C-N	-5.30	114.72	122.19
12	5	31	VAL	C-N-CA	-5.30	114.72	122.19
27	N	390	LEU	CA-C-N	5.30	125.24	119.78
27	N	390	LEU	C-N-CA	5.30	125.24	119.78
3	c	220	ASN	N-CA-C	5.30	118.48	110.64
9	i	207	ARG	CB-CG-CD	5.30	123.48	111.30
12	l	161	ILE	N-CA-CB	5.30	118.53	110.58
4	D	15	ILE	CA-C-N	5.30	127.91	120.28
4	D	15	ILE	C-N-CA	5.30	127.91	120.28
9	2	76	VAL	N-CA-CB	5.30	119.41	110.56
20	J	292	MET	N-CA-CB	5.30	118.82	110.56
27	N	543	ASP	N-CA-C	-5.29	106.82	113.28
2	b	204	PHE	CA-CB-CG	-5.29	108.51	113.80
7	g	176	VAL	CB-CA-C	-5.29	104.91	112.22
17	K	250	GLY	CA-C-O	-5.29	113.95	121.52
19	M	270	ALA	N-CA-C	5.29	117.13	111.36
23	T	102	LYS	CA-C-O	-5.29	115.24	120.90
11	k	127	GLU	CB-CA-C	-5.29	101.22	109.84
1	A	132	LEU	CA-C-O	5.29	125.96	120.30
6	F	89	GLN	OE1-CD-NE2	5.29	127.89	122.60
7	G	65	VAL	CA-C-N	5.29	130.29	122.94
7	G	65	VAL	C-N-CA	5.29	130.29	122.94
8	l	153	ASP	CA-C-N	5.29	127.37	120.28
8	l	153	ASP	C-N-CA	5.29	127.37	120.28
19	M	305	MET	CA-C-N	5.29	127.37	120.28
19	M	305	MET	C-N-CA	5.29	127.37	120.28
1	a	38	GLY	O-C-N	-5.29	117.85	122.88
3	c	156	TYR	O-C-N	5.29	129.41	123.27
19	M	44	PHE	CA-C-O	5.29	126.16	120.55
22	V	107	TRP	CA-C-O	5.29	126.92	120.99
26	Z	471	LEU	CA-C-N	5.29	127.68	120.54
26	Z	471	LEU	C-N-CA	5.29	127.68	120.54
3	C	191	LEU	CA-C-N	5.29	127.36	120.28
3	C	191	LEU	C-N-CA	5.29	127.36	120.28
20	J	271	THR	CA-C-N	5.29	127.31	120.44
20	J	271	THR	C-N-CA	5.29	127.31	120.44
30	Q	77	PHE	N-CA-C	5.29	117.12	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Q	405	GLN	OE1-CD-NE2	5.29	127.89	122.60
7	g	62	LYS	CB-CA-C	-5.29	102.55	110.90
8	h	53	GLN	N-CA-CB	5.29	117.68	110.01
4	D	229	GLN	O-C-N	-5.29	116.12	122.15
31	R	65	TYR	N-CA-C	-5.29	105.60	111.36
1	A	202	ILE	CA-C-O	-5.29	115.45	120.95
23	T	245	TYR	CB-CA-C	-5.29	102.02	110.79
26	Z	17	GLN	CB-CG-CD	-5.29	103.61	112.60
31	R	138	GLY	CA-C-O	-5.29	113.26	119.50
14	7	3	GLN	CA-C-N	5.28	125.58	119.93
14	7	3	GLN	C-N-CA	5.28	125.58	119.93
19	M	201	MET	CG-SD-CE	-5.28	89.28	100.90
20	J	390	MET	CA-C-O	5.28	126.17	119.78
23	T	186	ARG	NE-CZ-NH1	5.28	126.78	121.50
12	l	186	ILE	CA-C-N	5.28	129.05	121.50
12	l	186	ILE	C-N-CA	5.28	129.05	121.50
9	2	93	HIS	CE1-NE2-CD2	-5.28	103.72	109.00
14	7	10	SER	CA-C-N	5.28	130.33	122.99
14	7	10	SER	C-N-CA	5.28	130.33	122.99
30	Q	172	PRO	CA-C-N	5.28	130.38	121.14
30	Q	172	PRO	C-N-CA	5.28	130.38	121.14
8	h	109	GLU	N-CA-C	-5.28	100.08	109.06
13	m	35	ILE	N-CA-C	-5.28	100.28	107.99
1	A	242	GLN	OE1-CD-NE2	5.28	127.88	122.60
3	C	178	ASP	O-C-N	5.28	128.68	122.34
12	5	133	GLN	CA-C-N	5.28	127.79	120.29
12	5	133	GLN	C-N-CA	5.28	127.79	120.29
17	K	416	LYS	CA-C-N	5.28	129.64	122.19
17	K	416	LYS	C-N-CA	5.28	129.64	122.19
27	N	434	SER	O-C-N	-5.28	116.94	121.85
31	R	56	GLU	N-CA-CB	5.28	117.88	110.12
1	a	91	GLU	O-C-N	5.28	128.76	122.27
4	D	58	THR	CA-C-N	5.28	125.58	119.93
4	D	58	THR	C-N-CA	5.28	125.58	119.93
18	L	169	ASN	CB-CA-C	-5.28	102.03	110.79
22	V	229	ASP	CA-CB-CG	5.28	117.88	112.60
23	T	158	GLN	CA-C-O	5.28	126.55	120.90
26	Z	31	LYS	CB-CA-C	-5.28	102.56	110.90
6	F	88	ARG	CA-C-N	5.28	127.67	120.54
6	F	88	ARG	C-N-CA	5.28	127.67	120.54
26	Z	241	THR	CA-C-N	5.28	127.35	120.28
26	Z	241	THR	C-N-CA	5.28	127.35	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	417	SER	CA-C-N	5.28	127.35	120.28
26	Z	417	SER	C-N-CA	5.28	127.35	120.28
26	Z	421	SER	CA-C-N	5.28	128.95	120.30
26	Z	421	SER	C-N-CA	5.28	128.95	120.30
27	N	159	GLU	O-C-N	5.28	127.71	122.12
27	N	165	ILE	O-C-N	5.28	127.27	121.83
30	Q	131	VAL	CA-C-N	5.28	127.30	120.44
30	Q	131	VAL	C-N-CA	5.28	127.30	120.44
31	R	148	ASP	CA-CB-CG	-5.28	107.32	112.60
7	g	8	ASN	N-CA-C	-5.28	103.56	110.53
9	i	72	ARG	N-CA-C	-5.28	99.73	108.75
11	4	25	ILE	CA-C-O	-5.28	114.79	119.38
15	H	171	GLY	CA-C-O	5.28	125.04	119.03
22	V	22	ASP	CA-C-N	5.28	128.57	120.82
22	V	22	ASP	C-N-CA	5.28	128.57	120.82
26	Z	119	LEU	N-CA-C	5.28	117.03	111.28
11	k	96	ARG	NH1-CZ-NH2	-5.27	112.44	119.30
9	2	116	HIS	ND1-CE1-NE2	5.27	113.67	108.40
26	Z	276	ASN	CA-CB-CG	5.27	117.87	112.60
26	Z	528	LEU	N-CA-C	-5.27	105.70	111.82
6	f	50	ARG	N-CA-CB	5.27	120.00	110.83
7	g	29	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	A	49	LYS	N-CA-CB	5.27	117.79	110.04
2	B	230	ASP	CA-CB-CG	5.27	117.87	112.60
8	1	122	LEU	CB-CA-C	-5.27	100.21	108.91
14	7	93	PHE	O-C-N	5.27	127.71	122.12
16	I	364	ILE	N-CA-C	-5.27	105.57	110.53
27	N	103	SER	N-CA-CB	5.27	117.87	110.12
27	N	176	GLN	N-CA-CB	5.27	119.40	110.49
27	N	257	ILE	N-CA-CB	5.27	117.71	110.54
27	N	548	ARG	CA-C-N	5.27	127.34	120.28
27	N	548	ARG	C-N-CA	5.27	127.34	120.28
27	N	727	THR	CA-C-N	5.27	127.78	120.29
27	N	727	THR	C-N-CA	5.27	127.78	120.29
34	8	477	ILE	N-CA-C	-5.27	105.39	110.72
6	f	99	ASN	OD1-CG-ND2	-5.27	117.33	122.60
5	E	218	ASP	CA-C-O	5.27	125.81	119.59
12	5	33	LYS	CB-CG-CD	5.27	123.42	111.30
29	P	276	LEU	CA-C-O	5.27	126.36	120.82
31	R	199	GLU	N-CA-C	-5.27	106.87	113.72
1	a	68	ARG	N-CA-C	-5.27	102.25	110.10
5	E	130	PHE	CA-CB-CG	5.27	119.07	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	116	MET	N-CA-CB	5.27	117.83	109.51
20	J	294	THR	N-CA-C	-5.27	100.73	108.79
22	V	304	ALA	CA-C-N	5.27	127.31	120.56
22	V	304	ALA	C-N-CA	5.27	127.31	120.56
26	Z	413	ASP	CA-CB-CG	-5.27	107.33	112.60
34	8	337	PHE	CB-CG-CD2	5.27	129.66	120.70
34	8	435	VAL	CA-C-N	5.27	129.07	122.43
34	8	435	VAL	C-N-CA	5.27	129.07	122.43
9	i	156	SER	CA-C-N	5.27	127.29	120.44
9	i	156	SER	C-N-CA	5.27	127.29	120.44
12	l	115	VAL	N-CA-CB	5.27	120.56	111.39
14	n	101	TYR	N-CA-C	-5.27	105.62	111.36
1	A	87	ARG	NE-CZ-NH2	-5.27	114.46	119.20
3	C	180	LYS	N-CA-C	-5.27	99.82	108.41
6	F	42	HIS	CB-CG-ND1	5.27	130.60	122.70
6	F	51	ASN	CA-CB-CG	-5.27	107.33	112.60
13	6	32	ASP	CA-CB-CG	-5.27	107.33	112.60
15	H	80	HIS	CA-C-O	5.27	124.61	118.97
16	I	335	ASP	N-CA-CB	5.27	117.80	110.11
30	Q	186	HIS	CE1-NE2-CD2	-5.27	103.73	109.00
11	k	107	TYR	N-CA-CB	5.27	119.06	110.37
22	V	171	ARG	NE-CZ-NH1	5.27	126.77	121.50
23	T	148	LEU	CA-C-O	-5.27	115.29	120.82
28	S	185	PHE	O-C-N	5.27	128.15	122.15
10	j	147	GLY	O-C-N	5.26	129.54	122.70
15	H	362	ASP	CA-C-O	-5.26	114.70	120.17
19	M	30	LEU	CA-C-O	-5.26	114.84	120.42
27	N	96	GLN	CA-C-O	5.26	126.00	120.42
27	N	509	GLN	CA-C-N	5.26	129.41	122.30
27	N	509	GLN	C-N-CA	5.26	129.41	122.30
28	S	423	VAL	N-CA-C	5.26	116.04	110.72
32	U	238	ASN	OD1-CG-ND2	5.26	127.86	122.60
3	c	114	LEU	CA-C-N	5.26	127.33	120.28
3	c	114	LEU	C-N-CA	5.26	127.33	120.28
4	d	78	ALA	CA-C-N	5.26	127.64	120.54
4	d	78	ALA	C-N-CA	5.26	127.64	120.54
7	g	242	GLU	CA-C-O	5.26	125.76	119.60
7	G	101	THR	CA-C-O	5.26	125.08	119.50
12	5	170	TYR	CA-CB-CG	-5.26	104.43	113.90
20	J	58	ILE	N-CA-C	-5.26	105.41	110.72
26	Z	516	THR	CA-CB-OG1	5.26	117.49	109.60
34	8	186	ASN	CA-CB-CG	-5.26	107.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	120	ILE	N-CA-C	-5.26	100.17	108.90
13	6	214	LYS	N-CA-CB	5.26	119.98	110.83
19	M	133	GLY	CA-C-N	5.26	128.31	120.31
19	M	133	GLY	C-N-CA	5.26	128.31	120.31
20	J	386	VAL	N-CA-CB	5.26	117.70	110.54
23	T	212	ASN	N-CA-C	-5.26	106.91	113.38
9	i	66	HIS	ND1-CE1-NE2	5.26	113.66	108.40
10	j	134	ASP	CB-CA-C	-5.26	102.59	110.90
4	D	108	THR	CA-C-O	5.26	126.34	120.82
14	7	60	MET	CG-SD-CE	-5.26	89.33	100.90
14	7	132	LEU	N-CA-C	5.26	117.09	111.36
17	K	361	SER	N-CA-CB	5.26	117.77	109.83
23	T	77	SER	N-CA-C	5.26	117.69	111.33
1	a	149	ASP	CA-C-N	5.26	125.06	119.28
1	a	149	ASP	C-N-CA	5.26	125.06	119.28
14	7	90	SER	CB-CA-C	-5.26	100.57	110.67
26	Z	128	GLU	CA-C-N	5.26	128.30	120.31
26	Z	128	GLU	C-N-CA	5.26	128.30	120.31
28	S	317	HIS	CA-CB-CG	5.26	119.06	113.80
33	O	214	ALA	N-CA-C	5.26	117.92	111.82
5	e	28	THR	CA-C-O	5.26	126.32	120.43
5	e	179	TRP	N-CA-CB	5.26	117.81	109.71
7	g	196	ILE	N-CA-C	-5.26	105.59	110.53
9	i	101	ALA	N-CA-C	-5.26	101.30	109.24
4	D	94	HIS	CG-CD2-NE2	5.26	112.46	107.20
9	2	141	HIS	ND1-CE1-NE2	5.26	113.66	108.40
22	V	245	VAL	CB-CA-C	-5.26	104.97	112.22
29	P	10	ASP	CA-C-O	-5.26	114.95	120.63
30	Q	344	GLU	CA-C-O	-5.26	114.85	120.42
1	a	21	TYR	CA-C-O	-5.25	114.85	120.42
5	e	2	ARG	NE-CZ-NH2	-5.25	114.47	119.20
6	f	11	THR	CA-C-O	5.25	126.74	120.28
14	n	45	VAL	CA-CB-CG2	-5.25	101.47	110.40
1	A	190	TRP	CA-C-N	5.25	127.75	120.29
1	A	190	TRP	C-N-CA	5.25	127.75	120.29
11	4	149	ARG	N-CA-C	-5.25	99.94	108.82
1	a	82	ARG	N-CA-CB	5.25	117.94	110.16
7	g	124	SER	N-CA-CB	-5.25	102.13	110.22
3	C	170	ALA	N-CA-CB	5.25	117.69	110.07
17	K	101	GLU	O-C-N	-5.25	117.45	121.55
17	K	193	VAL	N-CA-CB	5.25	118.46	110.58
24	X	109	LEU	O-C-N	5.25	125.97	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	105	GLY	N-CA-C	-5.25	100.73	113.18
11	k	108	ASP	CA-C-O	5.25	126.65	120.98
12	l	104	TYR	CA-CB-CG	5.25	123.35	113.90
15	H	158	GLY	CA-C-N	5.25	129.19	120.94
15	H	158	GLY	C-N-CA	5.25	129.19	120.94
27	N	46	ILE	N-CA-C	-5.25	105.42	110.72
25	Y	38	PHE	CA-C-O	-5.25	113.25	118.34
26	Z	232	LYS	N-CA-C	5.25	117.00	111.28
6	f	142	HIS	ND1-CE1-NE2	5.25	113.65	108.40
10	j	45	TYR	CB-CG-CD1	5.25	128.67	120.80
16	I	365	HIS	ND1-CG-CD2	-5.25	100.85	106.10
33	O	38	TRP	N-CA-C	-5.25	106.88	113.28
34	8	289	ASP	CA-CB-CG	-5.25	107.35	112.60
3	c	239	VAL	CA-C-N	5.25	127.26	120.44
3	c	239	VAL	C-N-CA	5.25	127.26	120.44
8	h	134	ILE	N-CA-C	-5.25	106.32	111.88
3	C	10	THR	CA-CB-CG2	5.25	119.42	110.50
14	7	62	HIS	CB-CG-ND1	5.25	130.57	122.70
15	H	165	PRO	CA-N-CD	-5.25	104.66	112.00
16	I	78	ASN	O-C-N	5.25	127.68	122.12
18	L	423	ALA	O-C-N	5.25	127.68	122.12
30	Q	83	GLU	N-CA-C	-5.25	105.24	111.69
30	Q	172	PRO	N-CA-C	-5.25	106.57	113.65
32	U	236	LEU	CA-C-N	5.25	126.40	119.84
32	U	236	LEU	C-N-CA	5.25	126.40	119.84
4	D	228	ASN	CA-CB-CG	-5.25	107.36	112.60
6	F	217	LYS	N-CA-C	-5.24	106.72	113.01
34	8	294	ASN	CB-CA-C	-5.24	101.70	110.56
12	5	106	ARG	N-CA-C	-5.24	106.28	113.30
26	Z	305	VAL	CB-CA-C	5.24	117.50	110.42
29	P	428	THR	CA-C-N	5.24	127.92	120.53
29	P	428	THR	C-N-CA	5.24	127.92	120.53
3	c	128	ARG	CA-C-O	-5.24	115.24	120.64
12	l	175	VAL	N-CA-CB	5.24	118.38	111.25
10	3	43	PHE	N-CA-C	-5.24	101.40	109.52
18	L	60	PHE	CB-CG-CD2	-5.24	111.79	120.70
21	W	84	LYS	O-C-N	-5.24	117.28	123.41
23	T	224	ARG	NH1-CZ-NH2	5.24	126.11	119.30
27	N	32	VAL	CA-C-N	5.24	127.73	120.29
27	N	32	VAL	C-N-CA	5.24	127.73	120.29
30	Q	112	ASP	N-CA-C	5.24	117.41	111.02
9	2	114	HIS	CA-CB-CG	-5.24	108.56	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	209	GLU	CA-C-O	-5.24	114.87	120.42
31	R	381	ILE	CA-C-O	5.24	125.56	120.27
33	O	258	LEU	CA-C-N	5.24	127.30	120.28
33	O	258	LEU	C-N-CA	5.24	127.30	120.28
34	8	192	TYR	CB-CG-CD2	5.24	128.66	120.80
4	d	57	ILE	CA-C-N	5.24	134.58	121.80
4	d	57	ILE	C-N-CA	5.24	134.58	121.80
30	Q	122	ILE	CA-CB-CG2	-5.24	101.60	110.50
3	c	97	TYR	CA-C-N	5.24	127.30	120.28
3	c	97	TYR	C-N-CA	5.24	127.30	120.28
14	n	1	THR	CA-CB-CG2	5.24	119.40	110.50
12	5	49	ALA	CA-C-N	5.24	127.72	120.29
12	5	49	ALA	C-N-CA	5.24	127.72	120.29
18	L	421	LYS	O-C-N	5.24	127.67	122.12
19	M	305	MET	N-CA-C	-5.24	105.49	111.14
24	X	111	LEU	N-CA-CB	5.24	119.40	110.87
27	N	149	GLU	CA-C-O	-5.24	114.71	120.36
28	S	489	GLN	CA-C-O	5.24	127.10	121.55
30	Q	406	ASP	CA-C-N	5.24	128.27	120.31
30	Q	406	ASP	C-N-CA	5.24	128.27	120.31
33	O	168	THR	N-CA-CB	5.24	118.93	110.40
5	e	80	MET	N-CA-CB	5.23	117.81	110.12
13	m	160	TYR	N-CA-C	-5.23	103.62	110.53
14	7	219	TRP	CG-CD2-CE3	-5.23	128.67	133.90
15	H	306	ILE	CB-CA-C	5.23	118.20	110.77
26	Z	372	ALA	N-CA-C	-5.23	101.34	109.24
5	e	25	LEU	N-CA-CB	5.23	117.91	110.16
10	3	71	ASN	CA-CB-CG	-5.23	107.37	112.60
34	8	236	GLN	N-CA-CB	5.23	118.94	110.41
34	8	281	ASN	N-CA-CB	5.23	117.04	110.45
1	A	64	PHE	CA-CB-CG	-5.23	108.57	113.80
13	6	186	ASP	N-CA-CB	5.23	117.90	110.16
26	Z	63	LEU	N-CA-C	-5.23	106.49	112.92
28	S	131	THR	N-CA-C	-5.23	105.64	112.23
32	U	199	GLY	CA-C-N	5.23	127.29	120.28
32	U	199	GLY	C-N-CA	5.23	127.29	120.28
33	O	317	THR	CA-CB-OG1	5.23	117.44	109.60
4	D	179	ARG	N-CA-C	-5.23	105.58	111.28
19	M	183	VAL	CA-C-N	5.23	125.64	120.31
19	M	183	VAL	C-N-CA	5.23	125.64	120.31
26	Z	857	LEU	CA-C-N	5.23	125.31	120.34
26	Z	857	LEU	C-N-CA	5.23	125.31	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	164	GLU	CA-C-N	5.23	127.24	120.44
10	j	164	GLU	C-N-CA	5.23	127.24	120.44
12	l	135	PHE	CA-CB-CG	-5.23	108.57	113.80
12	l	188	HIS	CB-CG-CD2	-5.23	124.40	131.20
2	B	12	PHE	CA-CB-CG	-5.23	108.57	113.80
3	C	83	ALA	CA-C-N	5.23	127.81	120.28
3	C	83	ALA	C-N-CA	5.23	127.81	120.28
4	D	79	ASP	CA-CB-CG	5.23	117.83	112.60
15	H	95	HIS	ND1-CE1-NE2	5.23	113.63	108.40
17	K	342	SER	N-CA-C	-5.23	107.57	114.31
26	Z	565	PHE	O-C-N	5.23	127.66	122.12
5	e	183	LEU	N-CA-C	-5.23	101.25	109.25
7	g	33	SER	N-CA-C	-5.23	101.24	109.50
10	j	96	GLU	CB-CG-CD	-5.23	103.72	112.60
5	E	180	HIS	CA-CB-CG	5.23	119.03	113.80
8	h	94	THR	N-CA-C	-5.22	100.00	108.52
5	E	61	GLU	N-CA-CB	5.22	118.39	109.87
6	F	24	ALA	N-CA-C	-5.22	105.67	111.36
12	5	209	ASN	OD1-CG-ND2	5.22	127.82	122.60
17	K	179	MET	N-CA-C	-5.22	105.19	112.45
18	L	359	GLU	CB-CG-CD	-5.22	103.72	112.60
22	V	159	ILE	CA-C-O	5.22	126.52	120.67
25	Y	72	ASP	CA-CB-CG	-5.22	107.38	112.60
27	N	232	LEU	N-CA-C	-5.22	105.65	112.23
27	N	606	VAL	CA-C-N	5.22	127.23	120.44
27	N	606	VAL	C-N-CA	5.22	127.23	120.44
29	P	95	TYR	N-CA-C	-5.22	105.67	111.36
29	P	230	HIS	CE1-NE2-CD2	-5.22	103.78	109.00
1	a	78	ILE	CA-C-O	-5.22	114.41	118.85
2	b	5	TYR	CA-C-N	5.22	130.59	122.49
2	b	5	TYR	C-N-CA	5.22	130.59	122.49
2	b	198	GLU	CB-CG-CD	-5.22	103.72	112.60
16	I	286	ALA	CA-C-N	5.22	127.25	120.56
16	I	286	ALA	C-N-CA	5.22	127.25	120.56
34	8	214	PHE	CB-CG-CD1	5.22	129.58	120.70
6	F	186	ASP	CB-CA-C	-5.22	102.12	110.79
18	L	93	ASN	CA-C-N	5.22	127.54	120.44
18	L	93	ASN	C-N-CA	5.22	127.54	120.44
23	T	157	TYR	CA-C-N	5.22	127.59	120.54
23	T	157	TYR	C-N-CA	5.22	127.59	120.54
26	Z	312	TYR	CB-CG-CD1	5.22	128.63	120.80
28	S	317	HIS	ND1-CE1-NE2	5.22	113.62	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	74	TRP	CG-CD2-CE3	-5.22	128.68	133.90
3	C	45	LEU	CA-C-O	5.22	125.89	120.30
26	Z	256	LEU	CA-C-N	5.22	125.76	120.38
26	Z	256	LEU	C-N-CA	5.22	125.76	120.38
26	Z	380	ASN	OD1-CG-ND2	5.22	127.82	122.60
26	Z	814	ALA	CB-CA-C	-5.22	102.86	110.95
8	h	17	ASP	CA-C-O	-5.22	115.32	121.16
13	m	170	LYS	CA-C-N	5.22	125.12	119.85
13	m	170	LYS	C-N-CA	5.22	125.12	119.85
9	2	82	MET	N-CA-CB	5.22	117.88	110.16
21	W	75	GLY	O-C-N	-5.22	117.13	122.19
26	Z	548	ASP	CA-CB-CG	-5.22	107.38	112.60
26	Z	957	LEU	CA-C-N	5.22	130.05	121.39
26	Z	957	LEU	C-N-CA	5.22	130.05	121.39
5	e	84	ALA	CA-C-N	5.22	127.27	120.28
5	e	84	ALA	C-N-CA	5.22	127.27	120.28
4	D	211	THR	CA-C-O	5.22	125.99	120.36
21	W	53	SER	CA-C-N	5.22	131.63	121.41
21	W	53	SER	C-N-CA	5.22	131.63	121.41
26	Z	893	PHE	O-C-N	-5.22	116.91	123.27
27	N	322	ASP	N-CA-C	-5.22	99.91	108.41
29	P	364	ARG	CA-C-O	5.22	126.08	120.55
6	f	20	GLN	N-CA-C	5.21	116.96	111.28
27	N	487	LEU	N-CA-C	-5.21	105.68	111.36
4	d	29	THR	N-CA-C	5.21	117.26	110.43
7	g	184	SER	N-CA-CB	5.21	118.26	109.92
27	N	204	SER	CA-C-O	-5.21	115.35	120.82
27	N	768	ILE	O-C-N	5.21	126.11	121.57
32	U	84	ASN	CA-C-O	5.21	126.34	119.98
32	U	282	VAL	O-C-N	-5.21	116.81	121.87
3	c	182	ASP	N-CA-C	-5.21	106.23	112.59
14	7	103	ARG	CA-C-N	5.21	127.69	120.29
14	7	103	ARG	C-N-CA	5.21	127.69	120.29
16	I	194	ILE	N-CA-C	-5.21	105.32	111.00
18	L	416	MET	CG-SD-CE	-5.21	89.44	100.90
22	V	95	LEU	N-CA-C	-5.21	106.18	112.54
30	Q	195	LYS	N-CA-C	5.21	116.96	111.28
30	Q	416	VAL	CA-C-N	5.21	125.76	119.98
30	Q	416	VAL	C-N-CA	5.21	125.76	119.98
34	8	241	ILE	N-CA-CB	5.21	118.46	112.15
11	k	158	LEU	N-CA-CB	5.21	117.87	110.16
26	Z	102	ILE	CA-C-O	5.21	124.72	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	110	VAL	O-C-N	-5.21	117.58	123.20
1	A	223	LYS	N-CA-CB	5.21	120.51	111.39
6	F	8	ASP	N-CA-C	-5.21	101.38	109.24
15	H	80	HIS	ND1-CE1-NE2	5.21	113.61	108.40
19	M	130	PRO	N-CD-CG	5.21	111.01	103.20
24	X	19	GLU	N-CA-C	-5.21	105.66	113.89
28	S	174	ARG	N-CA-C	5.21	121.90	110.80
33	O	13	THR	CA-CB-OG1	5.21	117.41	109.60
13	m	215	GLU	N-CA-CB	5.21	119.56	110.81
12	5	141	ASP	O-C-N	-5.21	116.60	122.12
15	H	65	GLU	CA-C-N	5.21	127.21	120.44
15	H	65	GLU	C-N-CA	5.21	127.21	120.44
18	L	384	ASP	N-CA-C	-5.21	103.16	110.50
27	N	653	ARG	CA-C-O	5.21	126.07	120.55
30	Q	191	LEU	N-CA-C	-5.21	106.32	113.30
34	8	116	ASN	CA-CB-CG	-5.21	107.39	112.60
34	8	428	CYS	N-CA-C	-5.21	106.95	113.72
2	b	227	ILE	CA-CB-CG2	-5.21	101.65	110.50
11	k	110	LYS	N-CA-CB	5.21	118.16	110.56
14	n	117	ALA	O-C-N	-5.21	117.11	123.30
1	A	200	HIS	CE1-NE2-CD2	-5.21	103.80	109.00
27	N	405	LEU	CA-C-O	5.21	126.02	120.24
5	e	120	SER	N-CA-C	-5.20	105.67	113.89
8	h	70	TYR	CB-CA-C	-5.20	101.69	110.64
21	W	196	SER	CA-C-N	5.20	131.06	121.70
21	W	196	SER	C-N-CA	5.20	131.06	121.70
29	P	289	ASN	N-CA-C	5.20	117.03	111.36
30	Q	113	ASP	CA-C-O	5.20	126.47	120.90
32	U	77	ASN	CA-C-O	-5.20	115.03	120.55
34	8	165	LYS	N-CA-CB	5.20	117.77	110.12
11	4	166	GLN	CA-C-N	5.20	127.68	120.29
11	4	166	GLN	C-N-CA	5.20	127.68	120.29
30	Q	251	THR	CA-C-N	5.20	127.68	120.29
30	Q	251	THR	C-N-CA	5.20	127.68	120.29
31	R	149	ASN	CA-C-N	5.20	127.20	120.44
31	R	149	ASN	C-N-CA	5.20	127.20	120.44
31	R	204	TRP	CB-CG-CD2	-5.20	119.52	126.80
2	b	246	ARG	N-CA-C	-5.20	106.89	113.18
8	h	27	ALA	CA-C-O	5.20	126.01	120.24
10	j	202	ARG	NE-CZ-NH2	5.20	123.88	119.20
10	3	144	GLN	CA-C-O	5.20	126.28	120.82
15	H	217	GLN	CB-CA-C	-5.20	102.16	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	317	ALA	N-CA-C	5.20	117.98	110.28
21	W	191	ILE	N-CA-CB	5.20	119.81	111.23
26	Z	597	SER	CA-C-N	5.20	127.67	120.29
26	Z	597	SER	C-N-CA	5.20	127.67	120.29
26	Z	744	ALA	N-CA-C	-5.20	105.61	111.28
28	S	148	ASP	CA-CB-CG	-5.20	107.40	112.60
29	P	173	MET	N-CA-CB	5.20	117.86	110.16
33	O	117	ASN	N-CA-C	-5.20	105.29	111.69
3	c	98	LEU	O-C-N	-5.20	116.61	122.12
7	g	221	ASN	N-CA-CB	5.20	119.28	110.49
10	j	39	PHE	N-CA-C	-5.20	101.30	109.25
13	6	48	ASP	CA-CB-CG	-5.20	107.40	112.60
14	7	64	GLU	N-CA-C	-5.20	105.61	111.28
18	L	235	VAL	N-CA-C	5.20	115.92	110.62
33	O	168	THR	N-CA-C	-5.20	106.44	112.89
4	D	230	TYR	N-CA-CB	5.20	117.85	110.16
5	E	61	GLU	CA-C-O	5.20	126.52	120.49
15	H	344	ASP	CA-CB-CG	5.20	117.80	112.60
15	H	380	PRO	O-C-N	5.20	129.66	122.64
16	I	356	SER	CB-CA-C	-5.20	100.69	110.67
30	Q	398	TYR	CB-CG-CD2	5.20	128.59	120.80
3	c	124	HIS	CB-CA-C	-5.20	99.45	109.37
1	A	91	GLU	CA-C-O	5.20	125.94	119.97
4	D	63	SER	CA-C-O	5.20	125.75	120.24
13	6	161	GLU	O-C-N	-5.20	114.57	121.64
4	d	89	VAL	N-CA-C	-5.19	105.43	110.42
5	e	147	LEU	CB-CA-C	-5.19	100.56	109.65
6	f	171	LEU	N-CA-CB	5.19	117.76	110.12
6	f	178	PHE	N-CA-CB	5.19	118.30	110.30
12	5	66	HIS	CE1-NE2-CD2	-5.19	103.81	109.00
15	H	343	PHE	CA-CB-CG	5.19	118.99	113.80
26	Z	298	PHE	CA-CB-CG	-5.19	108.61	113.80
6	f	196	ILE	CA-C-N	5.19	127.76	120.28
6	f	196	ILE	C-N-CA	5.19	127.76	120.28
12	l	202	GLU	CB-CG-CD	-5.19	103.77	112.60
5	E	8	SER	N-CA-CB	5.19	117.87	110.03
6	F	190	LYS	O-C-N	-5.19	116.69	122.09
8	1	157	HIS	CB-CA-C	-5.19	102.73	110.88
26	Z	247	GLN	CA-C-N	5.19	127.50	120.44
26	Z	247	GLN	C-N-CA	5.19	127.50	120.44
28	S	37	VAL	N-CA-CB	5.19	120.17	110.77
28	S	71	ALA	N-CA-C	-5.19	106.70	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	O	334	LEU	N-CA-C	-5.19	105.70	111.36
5	e	180	HIS	CB-CG-CD2	-5.19	124.45	131.20
10	j	69	LYS	N-CA-C	5.19	117.02	111.36
14	n	93	PHE	CA-CB-CG	-5.19	108.61	113.80
14	n	172	VAL	CB-CA-C	-5.19	105.06	112.22
1	A	38	GLY	N-CA-C	-5.19	104.06	112.31
1	A	224	PHE	CA-CB-CG	-5.19	108.61	113.80
20	J	332	SER	N-CA-CB	5.19	117.75	110.12
27	N	674	GLN	CA-C-N	5.19	127.57	120.46
27	N	674	GLN	C-N-CA	5.19	127.57	120.46
33	O	70	TYR	CA-C-N	5.19	127.24	120.28
33	O	70	TYR	C-N-CA	5.19	127.24	120.28
33	O	85	SER	CB-CA-C	-5.19	102.02	110.85
33	O	266	PHE	CA-C-N	5.19	127.23	120.28
33	O	266	PHE	C-N-CA	5.19	127.23	120.28
12	l	114	TYR	CA-C-O	5.19	126.61	120.69
14	n	125	GLN	CG-CD-NE2	-5.19	108.62	116.40
2	B	20	GLN	CB-CG-CD	-5.19	103.78	112.60
16	I	71	LEU	CA-C-N	5.19	127.19	120.44
16	I	71	LEU	C-N-CA	5.19	127.19	120.44
17	K	225	ALA	N-CA-CB	5.19	117.53	110.01
19	M	305	MET	CA-C-O	-5.19	115.36	120.70
2	b	218	ASN	CA-CB-CG	-5.19	107.41	112.60
13	m	110	ILE	N-CA-C	-5.19	100.65	108.12
3	C	40	SER	N-CA-C	-5.19	106.90	113.18
13	6	132	GLU	CB-CA-C	-5.19	99.30	110.45
15	H	202	GLU	CA-C-N	5.19	134.46	121.80
15	H	202	GLU	C-N-CA	5.19	134.46	121.80
18	L	222	GLY	N-CA-C	-5.19	101.76	112.34
18	L	282	GLU	CA-C-N	5.19	128.66	120.47
18	L	282	GLU	C-N-CA	5.19	128.66	120.47
30	Q	208	ILE	CA-CB-CG1	5.19	119.22	110.40
30	Q	410	ASP	N-CA-C	-5.19	105.70	111.36
14	n	67	LEU	N-CA-CB	5.19	117.84	110.16
16	I	317	ASP	O-C-N	-5.19	117.67	123.48
6	F	77	ALA	CA-C-O	-5.18	113.31	118.34
20	J	255	SER	CB-CA-C	-5.18	102.18	110.79
26	Z	141	SER	N-CA-C	-5.18	106.95	113.28
32	U	254	ARG	NH1-CZ-NH2	5.18	126.04	119.30
33	O	286	PHE	CA-C-N	5.18	127.18	120.44
33	O	286	PHE	C-N-CA	5.18	127.18	120.44
7	g	179	HIS	CG-CD2-NE2	5.18	112.38	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	156	LYS	N-CA-C	-5.18	105.53	111.07
2	B	40	THR	CA-C-N	5.18	130.35	122.37
2	B	40	THR	C-N-CA	5.18	130.35	122.37
2	B	128	ARG	CA-C-N	5.18	126.32	119.84
2	B	128	ARG	C-N-CA	5.18	126.32	119.84
11	4	65	GLN	CA-C-N	5.18	127.22	120.28
11	4	65	GLN	C-N-CA	5.18	127.22	120.28
17	K	398	ASN	N-CA-CB	5.18	119.25	110.49
26	Z	151	HIS	CE1-NE2-CD2	-5.18	103.82	109.00
27	N	483	LEU	N-CA-CB	5.18	117.53	110.01
2	B	109	LEU	O-C-N	-5.18	116.24	122.15
16	I	114	ASP	N-CA-CB	5.18	117.75	110.24
27	N	467	LYS	N-CA-C	-5.18	105.63	111.28
30	Q	88	PHE	CA-C-O	-5.18	114.93	120.42
34	8	107	LEU	N-CA-CB	5.18	118.11	109.98
18	L	164	ASP	CA-CB-CG	-5.18	107.42	112.60
21	W	186	ALA	CB-CA-C	-5.18	102.05	110.85
24	X	127	GLY	CA-C-O	-5.18	115.10	120.90
26	Z	796	LEU	CA-C-N	5.18	127.74	120.28
26	Z	796	LEU	C-N-CA	5.18	127.74	120.28
29	P	245	TYR	CA-C-O	-5.18	115.06	120.55
31	R	188	LYS	CA-C-N	5.18	127.64	120.29
31	R	188	LYS	C-N-CA	5.18	127.64	120.29
32	U	297	GLN	N-CA-CB	5.18	117.82	110.16
34	8	263	CYS	N-CA-CB	-5.18	101.83	110.37
34	8	436	ILE	N-CA-C	-5.18	99.65	107.73
1	A	141	LEU	N-CA-C	-5.18	107.13	113.50
2	B	163	ALA	N-CA-C	-5.18	101.20	109.07
3	C	53	SER	O-C-N	5.18	129.21	122.89
14	7	169	THR	N-CA-C	-5.18	102.86	110.52
19	M	230	LEU	N-CA-C	5.18	121.83	110.80
24	X	79	LYS	CB-CA-C	-5.18	102.48	109.16
11	4	180	ILE	N-CA-C	-5.18	100.96	108.36
17	K	151	PRO	CA-C-O	-5.18	113.05	120.56
18	L	135	VAL	N-CA-C	-5.18	100.19	107.75
28	S	473	ASP	N-CA-C	-5.18	105.72	111.36
30	Q	253	ASN	N-CA-CB	5.18	119.24	110.49
1	A	146	TYR	CA-C-N	5.17	130.14	123.00
1	A	146	TYR	C-N-CA	5.17	130.14	123.00
1	A	240	ALA	N-CA-C	5.17	118.37	111.75
18	L	258	GLU	O-C-N	5.17	128.63	122.27
20	J	199	ALA	N-CA-CB	5.17	117.82	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	812	ALA	N-CA-C	5.17	117.00	111.36
28	S	361	THR	N-CA-CB	5.17	117.51	110.01
31	R	41	GLU	N-CA-C	5.17	116.61	111.07
34	8	331	ARG	N-CA-CB	5.17	117.64	109.83
8	h	153	ASP	CA-C-N	5.17	127.48	120.44
8	h	153	ASP	C-N-CA	5.17	127.48	120.44
9	i	86	HIS	ND1-CE1-NE2	5.17	113.57	108.40
9	i	210	THR	CA-C-N	5.17	128.82	121.42
9	i	210	THR	C-N-CA	5.17	128.82	121.42
17	K	386	ILE	N-CA-C	-5.17	105.50	110.72
23	T	74	ASN	N-CA-C	-5.17	99.95	108.49
27	N	596	LEU	N-CA-C	-5.17	105.72	111.36
14	n	9	THR	N-CA-CB	5.17	119.50	110.81
5	E	22	ALA	N-CA-C	-5.17	105.72	111.36
14	7	98	THR	N-CA-C	-5.17	105.56	111.14
16	I	178	THR	CA-C-N	5.17	129.48	122.19
16	I	178	THR	C-N-CA	5.17	129.48	122.19
16	I	209	GLU	N-CA-CB	5.17	117.57	110.07
18	L	86	LYS	O-C-N	-5.17	116.74	122.07
20	J	323	ALA	CB-CA-C	-5.17	102.06	110.85
26	Z	801	HIS	N-CA-C	-5.17	106.12	112.90
29	P	14	SER	N-CA-C	-5.17	105.72	111.36
3	c	112	ARG	CD-NE-CZ	5.17	131.64	124.40
25	Y	76	GLU	O-C-N	5.17	127.47	122.09
3	c	188	ALA	N-CA-C	5.17	117.65	111.71
8	h	131	SER	CA-C-N	5.17	127.21	120.28
8	h	131	SER	C-N-CA	5.17	127.21	120.28
9	i	116	HIS	CE1-NE2-CD2	-5.17	103.83	109.00
3	C	117	ILE	N-CA-C	-5.17	105.50	110.72
11	4	97	PRO	O-C-N	5.17	129.31	123.00
15	H	344	ASP	N-CA-C	-5.17	98.39	109.81
27	N	768	ILE	CA-C-O	-5.17	116.10	119.15
29	P	434	THR	CA-C-N	5.17	127.16	120.44
29	P	434	THR	C-N-CA	5.17	127.16	120.44
32	U	112	LYS	N-CA-C	-5.17	105.73	111.36
8	h	177	VAL	CB-CA-C	-5.17	103.90	110.98
11	4	62	ALA	N-CA-C	5.17	116.91	111.28
15	H	254	THR	N-CA-CB	5.17	118.29	110.28
16	I	303	GLN	CB-CA-C	-5.17	102.54	110.81
20	J	112	ARG	CA-C-O	-5.17	115.16	121.05
27	N	499	HIS	CG-CD2-NE2	5.17	112.37	107.20
31	R	103	CYS	CB-CA-C	5.17	119.46	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	61	SER	CA-C-N	5.17	127.62	120.29
12	5	61	SER	C-N-CA	5.17	127.62	120.29
16	I	303	GLN	N-CA-CB	5.17	117.64	109.94
31	R	215	GLY	O-C-N	5.17	127.14	122.18
1	A	158	LYS	CA-C-N	5.16	130.68	121.75
1	A	158	LYS	C-N-CA	5.16	130.68	121.75
17	K	230	THR	CA-CB-OG1	-5.16	101.85	109.60
31	R	351	LYS	N-CA-C	-5.16	105.73	111.36
4	d	109	ARG	CA-C-O	-5.16	115.08	120.55
5	e	10	GLU	CA-C-O	-5.16	115.39	120.70
11	k	111	LYS	CA-C-N	5.16	129.51	122.34
11	k	111	LYS	C-N-CA	5.16	129.51	122.34
9	2	52	THR	CA-C-O	-5.16	115.40	120.82
11	4	116	LEU	CB-CA-C	-5.16	101.59	110.16
18	L	233	LYS	CB-CG-CD	5.16	123.17	111.30
28	S	251	SER	CA-C-N	5.16	127.62	120.29
28	S	251	SER	C-N-CA	5.16	127.62	120.29
30	Q	10	GLU	O-C-N	-5.16	116.65	122.12
30	Q	246	TYR	CA-C-N	5.16	127.19	120.28
30	Q	246	TYR	C-N-CA	5.16	127.19	120.28
6	f	204	SER	CA-C-O	5.16	126.86	121.19
9	i	138	LEU	N-CA-C	5.16	116.98	111.36
1	A	80	ASP	CB-CA-C	-5.16	100.77	110.67
11	4	141	PHE	CA-C-N	5.16	127.45	120.44
11	4	141	PHE	C-N-CA	5.16	127.45	120.44
15	H	315	GLY	N-CA-C	-5.16	108.50	115.36
30	Q	227	CYS	N-CA-CB	5.16	117.70	110.12
33	O	258	LEU	O-C-N	5.16	127.38	122.07
1	a	109	ALA	CB-CA-C	-5.16	102.23	110.79
28	S	489	GLN	CA-CB-CG	-5.16	103.79	114.10
2	b	111	VAL	CA-CB-CG2	-5.16	101.64	110.40
5	e	180	HIS	ND1-CE1-NE2	5.16	113.56	108.40
1	A	187	GLU	CA-C-N	5.16	127.19	120.28
1	A	187	GLU	C-N-CA	5.16	127.19	120.28
4	D	171	GLU	N-CA-CB	5.16	117.70	110.12
5	E	223	TYR	N-CA-CB	5.16	117.85	110.06
7	G	104	PRO	CA-C-N	5.16	123.49	120.24
7	G	104	PRO	C-N-CA	5.16	123.49	120.24
9	2	89	LYS	CB-CA-C	-5.16	102.78	110.88
14	7	203	ASN	CA-C-O	-5.16	113.58	119.41
20	J	179	ILE	N-CA-C	-5.16	101.54	108.35
26	Z	232	LYS	N-CA-CB	5.16	117.70	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	374	ASP	CA-C-N	5.16	130.16	122.74
28	S	374	ASP	C-N-CA	5.16	130.16	122.74
3	c	24	ALA	CA-C-O	-5.15	115.09	120.55
13	6	102	PHE	N-CA-CB	5.15	117.54	110.07
7	g	99	TYR	CA-CB-CG	-5.15	104.63	113.90
9	i	3	ILE	CB-CA-C	-5.15	101.80	110.71
1	A	6	HIS	CE1-NE2-CD2	-5.15	103.85	109.00
6	F	218	ASP	CA-CB-CG	-5.15	107.45	112.60
26	Z	88	PRO	CA-C-N	5.15	127.18	120.28
26	Z	88	PRO	C-N-CA	5.15	127.18	120.28
27	N	338	PHE	CA-C-N	5.15	127.50	120.54
27	N	338	PHE	C-N-CA	5.15	127.50	120.54
28	S	291	GLU	CA-C-N	5.15	128.14	120.31
28	S	291	GLU	C-N-CA	5.15	128.14	120.31
34	8	173	ASN	CA-CB-CG	-5.15	107.45	112.60
9	i	204	LYS	CB-CG-CD	5.15	123.14	111.30
7	G	187	GLU	CB-CG-CD	-5.15	103.84	112.60
14	7	106	LYS	N-CA-C	-5.15	106.85	112.72
21	W	110	ILE	CA-C-O	-5.15	114.98	120.39
24	X	91	PHE	CB-CG-CD2	5.15	129.46	120.70
30	Q	78	ILE	O-C-N	-5.15	115.23	121.10
2	b	206	GLY	N-CA-C	-5.15	107.54	115.73
10	j	18	ASP	N-CA-CB	5.15	120.30	112.47
5	e	191	LEU	N-CA-CB	5.15	117.69	110.12
11	k	6	GLY	CA-C-O	5.15	126.10	121.47
14	n	41	ARG	CA-C-N	5.15	129.18	121.72
14	n	41	ARG	C-N-CA	5.15	129.18	121.72
2	B	93	ALA	O-C-N	-5.15	115.94	122.27
16	I	189	SER	CA-C-O	-5.15	114.97	120.42
18	L	264	ARG	CA-C-N	5.15	127.18	120.28
18	L	264	ARG	C-N-CA	5.15	127.18	120.28
26	Z	312	TYR	CB-CG-CD2	-5.15	113.08	120.80
28	S	300	ALA	CA-C-N	5.15	126.27	119.84
28	S	300	ALA	C-N-CA	5.15	126.27	119.84
7	G	221	ASN	N-CA-CB	5.15	120.92	112.63
8	1	180	ALA	CA-C-N	5.15	127.43	120.38
8	1	180	ALA	C-N-CA	5.15	127.43	120.38
20	J	62	LEU	N-CA-C	5.15	116.89	111.28
29	P	183	GLN	CA-C-N	5.15	127.69	120.28
29	P	183	GLN	C-N-CA	5.15	127.69	120.28
30	Q	93	THR	CA-C-N	5.15	127.04	120.56
30	Q	93	THR	C-N-CA	5.15	127.04	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	203	ASP	CA-C-N	5.14	127.17	120.28
1	a	203	ASP	C-N-CA	5.14	127.17	120.28
3	c	66	TYR	CB-CG-CD2	-5.14	113.08	120.80
26	Z	394	TYR	N-CA-CB	5.14	117.92	109.95
33	O	70	TYR	O-C-N	5.14	128.92	122.23
1	a	37	ARG	CA-C-N	5.14	127.36	122.27
1	a	37	ARG	C-N-CA	5.14	127.36	122.27
6	f	211	SER	CA-C-O	-5.14	113.95	120.28
7	g	138	ASP	CA-CB-CG	-5.14	107.46	112.60
11	k	124	THR	O-C-N	-5.14	117.11	123.44
8	1	71	GLY	O-C-N	5.14	128.15	122.70
8	1	120	HIS	ND1-CE1-NE2	5.14	113.54	108.40
8	1	138	CYS	N-CA-CB	5.14	117.77	110.16
11	4	91	SER	O-C-N	-5.14	116.67	122.12
12	5	80	SER	CA-C-N	5.14	129.38	120.58
12	5	80	SER	C-N-CA	5.14	129.38	120.58
26	Z	729	GLU	O-C-N	-5.14	114.92	122.43
27	N	792	SER	CB-CA-C	-5.14	102.81	110.88
31	R	422	ARG	CA-C-N	5.14	127.17	120.28
31	R	422	ARG	C-N-CA	5.14	127.17	120.28
13	6	114	LEU	CA-C-O	-5.14	115.15	120.70
18	L	187	THR	CA-C-N	5.14	131.36	121.54
18	L	187	THR	C-N-CA	5.14	131.36	121.54
20	J	317	PRO	CA-C-N	5.14	123.41	119.66
20	J	317	PRO	C-N-CA	5.14	123.41	119.66
28	S	73	THR	N-CA-C	-5.14	105.57	111.07
34	8	414	LYS	CB-CA-C	-5.14	100.80	110.67
4	d	230	TYR	N-CA-CB	5.14	117.77	110.16
5	e	76	ASP	CA-CB-CG	-5.14	107.46	112.60
6	f	170	TYR	CA-C-O	-5.14	115.42	120.82
12	5	86	LEU	N-CA-C	-5.14	105.57	111.07
13	6	216	PHE	CA-C-N	5.14	131.21	122.37
13	6	216	PHE	C-N-CA	5.14	131.21	122.37
15	H	310	GLU	N-CA-C	5.14	121.75	110.80
20	J	18	GLY	N-CA-C	5.14	119.35	112.77
27	N	774	ASN	CA-C-N	5.14	130.16	122.86
27	N	774	ASN	C-N-CA	5.14	130.16	122.86
31	R	227	ALA	CA-C-O	5.14	126.00	120.55
34	8	400	LEU	N-CA-C	-5.14	105.57	111.07
5	E	19	SER	CB-CA-C	-5.14	102.12	110.85
8	1	33	LYS	CB-CA-C	-5.14	102.46	110.37
10	3	35	VAL	CA-C-O	-5.14	115.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	125	ARG	CA-C-N	5.14	125.05	119.76
4	d	125	ARG	C-N-CA	5.14	125.05	119.76
6	F	225	ASP	O-C-N	5.14	128.65	123.26
19	M	309	LEU	N-CA-C	5.14	116.96	111.36
27	N	178	SER	O-C-N	-5.14	117.62	123.48
32	U	157	LEU	N-CA-C	-5.14	99.19	108.85
34	8	365	LYS	CA-C-O	-5.14	115.10	120.55
14	n	74	ASN	O-C-N	-5.13	116.68	122.12
14	7	192	SER	CA-C-N	5.13	127.58	120.29
14	7	192	SER	C-N-CA	5.13	127.58	120.29
17	K	240	SER	N-CA-CB	5.13	117.67	110.12
26	Z	15	GLN	CB-CG-CD	-5.13	103.87	112.60
26	Z	158	ALA	N-CA-C	-5.13	105.68	111.28
12	l	126	ILE	CA-C-O	5.13	125.45	120.27
15	H	434	ARG	N-CA-CB	5.13	119.17	110.49
26	Z	288	LEU	CB-CA-C	-5.13	102.79	110.90
8	h	154	PHE	CA-C-O	-5.13	115.42	120.70
13	m	41	PRO	N-CD-CG	5.13	110.90	103.20
11	4	39	SER	CA-C-O	-5.13	116.25	120.71
13	m	218	GLU	CB-CA-C	-5.13	101.20	109.72
26	Z	473	LEU	CA-C-O	5.13	125.98	120.70
7	g	148	GLU	CA-C-O	-5.13	115.11	120.70
9	i	99	ILE	CB-CA-C	-5.13	103.95	110.98
9	i	144	GLN	N-CA-C	-5.13	102.46	110.10
2	B	49	LYS	CA-C-O	5.13	126.96	121.16
6	F	62	ILE	N-CA-C	-5.13	100.99	108.17
12	5	210	VAL	N-CA-C	5.13	116.29	109.37
18	L	57	LEU	CB-CA-C	-5.13	101.14	110.63
5	E	15	GLN	OE1-CD-NE2	5.13	127.73	122.60
6	F	131	LEU	N-CA-CB	5.13	119.42	110.81
9	2	56	THR	CA-C-O	-5.13	115.11	120.55
14	7	2	GLN	OE1-CD-NE2	5.13	127.73	122.60
15	H	360	THR	N-CA-CB	5.13	118.11	110.22
28	S	165	PRO	N-CD-CG	5.13	110.89	103.20
32	U	116	ASN	N-CA-C	-5.13	102.57	109.95
33	O	62	TYR	O-C-N	5.13	127.36	122.03
34	8	386	ASN	O-C-N	-5.13	115.77	122.59
34	8	493	MET	N-CA-CB	5.13	119.29	110.68
7	G	26	ALA	N-CA-C	5.12	118.63	112.38
13	6	31	THR	N-CA-CB	5.12	119.42	110.81
20	J	140	GLU	N-CA-C	5.12	116.95	111.36
33	O	15	ARG	CA-C-N	5.12	127.57	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	O	15	ARG	C-N-CA	5.12	127.57	120.29
7	g	97	LYS	N-CA-CB	5.12	117.41	109.98
13	m	81	ASP	N-CA-CB	5.12	119.15	110.49
12	5	27	ALA	N-CA-CB	5.12	117.74	110.16
29	P	114	THR	CA-C-N	5.12	127.57	120.29
29	P	114	THR	C-N-CA	5.12	127.57	120.29
30	Q	214	THR	CA-C-N	5.12	127.69	120.42
30	Q	214	THR	C-N-CA	5.12	127.69	120.42
12	l	208	ASN	N-CA-C	-5.12	105.88	111.82
1	A	175	ASN	OD1-CG-ND2	5.12	127.72	122.60
20	J	283	GLU	CB-CA-C	-5.12	102.81	110.90
27	N	796	VAL	N-CA-C	-5.12	105.50	110.42
12	l	199	LYS	CB-CG-CD	5.12	123.07	111.30
1	A	115	LEU	N-CA-CB	5.12	117.65	110.12
4	D	21	ALA	CA-C-N	5.12	127.14	120.28
4	D	21	ALA	C-N-CA	5.12	127.14	120.28
4	D	226	GLU	CB-CA-C	-5.12	102.29	110.79
10	3	11	VAL	N-CA-CB	5.12	119.84	111.45
12	5	102	CYS	N-CA-CB	5.12	119.28	110.68
18	L	429	GLU	CB-CG-CD	-5.12	103.90	112.60
27	N	464	GLU	CA-CB-CG	5.12	124.34	114.10
34	8	472	VAL	N-CA-CB	5.12	118.18	112.45
5	e	198	GLN	CB-CA-C	-5.12	102.15	110.85
13	m	1	GLN	CA-CB-CG	5.12	124.33	114.10
15	H	206	VAL	N-CA-C	-5.12	101.60	108.35
17	K	155	ASP	CA-CB-CG	-5.12	107.48	112.60
19	M	68	LYS	N-CA-CB	5.12	117.64	110.12
29	P	272	PRO	N-CA-CB	5.12	107.75	103.25
31	R	357	PHE	CA-CB-CG	-5.12	108.68	113.80
3	c	38	MET	N-CA-CB	5.12	118.96	110.52
8	h	168	SER	N-CA-CB	5.12	117.43	110.01
1	A	124	TYR	O-C-N	5.12	127.54	122.12
8	l	92	ASN	CB-CA-C	-5.12	102.15	110.85
28	S	304	SER	N-CA-CB	-5.12	103.05	110.47
31	R	216	ILE	N-CA-CB	5.12	117.50	110.54
10	j	102	TYR	CB-CA-C	-5.11	100.89	109.53
13	m	135	GLN	CA-CB-CG	5.11	124.33	114.10
6	F	127	TYR	CA-CB-CG	-5.11	104.70	113.90
20	J	207	ASP	N-CA-CB	5.11	119.13	110.49
22	V	100	ARG	N-CA-C	-5.11	106.82	113.16
27	N	808	ALA	CA-C-O	-5.11	115.44	121.07
31	R	152	LYS	CB-CG-CD	5.11	123.06	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	222	ILE	CB-CG1-CD1	5.11	124.53	113.80
7	g	160	ALA	CA-C-N	5.11	130.54	122.36
7	g	160	ALA	C-N-CA	5.11	130.54	122.36
6	F	168	LYS	N-CA-C	-5.11	105.71	111.28
13	6	47	GLY	CA-C-N	5.11	131.30	121.54
13	6	47	GLY	C-N-CA	5.11	131.30	121.54
22	V	301	ASN	CA-C-O	-5.11	115.45	120.82
6	f	18	LEU	CA-C-N	5.11	128.08	120.31
6	f	18	LEU	C-N-CA	5.11	128.08	120.31
6	f	109	HIS	CA-CB-CG	-5.11	108.69	113.80
4	D	12	ASP	CA-C-N	5.11	131.84	121.93
4	D	12	ASP	C-N-CA	5.11	131.84	121.93
16	I	124	THR	N-CA-CB	5.11	117.78	110.06
22	V	249	GLU	N-CA-C	-5.11	105.79	111.36
33	O	366	MET	O-C-N	-5.11	116.70	122.12
13	m	127	PRO	N-CA-C	-5.11	106.88	113.57
4	D	228	ASN	CB-CG-ND2	-5.11	108.74	116.40
27	N	361	ASN	N-CA-C	5.11	116.08	108.31
28	S	401	LYS	N-CA-C	-5.11	100.08	108.41
30	Q	341	THR	CA-C-N	5.11	127.13	120.28
30	Q	341	THR	C-N-CA	5.11	127.13	120.28
12	l	8	PHE	N-CA-CB	5.11	119.74	111.21
12	l	108	GLU	N-CA-C	-5.11	107.10	113.38
14	n	62	HIS	CG-CD2-NE2	5.11	112.31	107.20
6	F	79	ASP	CB-CA-C	-5.11	102.86	110.88
33	O	138	LEU	CB-CA-C	-5.11	102.31	110.79
2	b	193	LEU	O-C-N	5.11	127.53	122.12
7	g	12	SER	CA-C-N	5.11	125.18	119.87
7	g	12	SER	C-N-CA	5.11	125.18	119.87
15	H	268	ASP	CA-CB-CG	-5.11	107.49	112.60
26	Z	551	LEU	O-C-N	5.11	127.33	122.07
27	N	203	ARG	N-CA-C	5.11	117.51	111.33
27	N	616	HIS	CA-CB-CG	-5.11	108.69	113.80
29	P	42	LEU	N-CA-CB	5.11	117.62	110.12
5	e	240	ALA	N-CA-C	-5.10	106.74	113.17
26	Z	223	LEU	N-CA-C	-5.10	105.80	111.36
1	A	97	TYR	CA-C-N	5.10	127.53	120.29
1	A	97	TYR	C-N-CA	5.10	127.53	120.29
1	A	110	LYS	CA-C-O	-5.10	115.14	120.55
6	F	142	HIS	CE1-NE2-CD2	-5.10	103.90	109.00
27	N	684	SER	CA-C-N	5.10	127.67	120.42
27	N	684	SER	C-N-CA	5.10	127.67	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	33	GLU	CA-C-N	5.10	127.07	120.44
28	S	33	GLU	C-N-CA	5.10	127.07	120.44
28	S	235	ASN	CA-C-N	5.10	127.53	120.29
28	S	235	ASN	C-N-CA	5.10	127.53	120.29
28	S	465	ILE	N-CA-C	-5.10	105.42	110.62
13	m	66	LYS	N-CA-C	-5.10	105.61	111.07
2	B	159	TRP	CB-CG-CD2	-5.10	119.66	126.80
15	H	185	LEU	N-CA-C	-5.10	102.44	110.14
17	K	389	GLU	CA-C-O	5.10	125.83	120.42
20	J	192	GLY	O-C-N	-5.10	116.03	122.41
29	P	296	GLN	N-CA-CB	5.10	117.71	110.16
4	d	4	ARG	N-CA-CB	5.10	118.18	109.87
13	m	77	PHE	O-C-N	5.10	127.53	122.12
10	3	171	LEU	O-C-N	5.10	127.32	122.07
11	4	126	VAL	O-C-N	5.10	128.81	123.00
19	M	28	GLN	OE1-CD-NE2	5.10	127.70	122.60
27	N	157	ALA	CB-CA-C	-5.10	102.18	110.85
27	N	318	LYS	N-CA-CB	5.10	117.41	110.01
33	O	83	LEU	CA-C-N	5.10	127.53	120.29
33	O	83	LEU	C-N-CA	5.10	127.53	120.29
34	8	210	ALA	N-CA-C	-5.10	105.91	111.82
20	J	243	SER	O-C-N	-5.10	117.57	123.33
27	N	908	ARG	O-C-N	5.10	127.60	122.09
32	U	191	THR	CA-C-N	5.10	127.62	120.28
32	U	191	THR	C-N-CA	5.10	127.62	120.28
33	O	58	ARG	CA-C-N	5.10	129.22	120.71
33	O	58	ARG	C-N-CA	5.10	129.22	120.71
4	d	157	TRP	CG-CD2-CE3	-5.10	128.80	133.90
6	F	105	GLU	N-CA-C	-5.10	105.64	111.14
10	3	89	LEU	CA-C-N	5.10	127.44	120.46
10	3	89	LEU	C-N-CA	5.10	127.44	120.46
14	7	137	TYR	CA-CB-CG	-5.10	104.73	113.90
17	K	64	GLN	O-C-N	5.10	127.52	122.12
20	J	150	VAL	CA-CB-CG1	-5.10	101.74	110.40
21	W	103	ASN	CB-CA-C	-5.10	101.14	110.62
22	V	83	VAL	CA-CB-CG2	5.10	119.06	110.40
26	Z	348	LEU	CA-C-N	5.10	127.53	120.29
26	Z	348	LEU	C-N-CA	5.10	127.53	120.29
26	Z	361	HIS	CA-CB-CG	5.10	118.90	113.80
3	c	14	PRO	N-CA-CB	5.09	108.60	103.25
1	A	20	GLU	N-CA-CB	5.09	117.61	110.12
4	D	196	SER	CA-C-N	5.09	127.11	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	196	SER	C-N-CA	5.09	127.11	120.28
12	5	66	HIS	CA-C-N	5.09	127.11	120.28
12	5	66	HIS	C-N-CA	5.09	127.11	120.28
23	T	9	LYS	CA-C-N	5.09	127.53	120.29
23	T	9	LYS	C-N-CA	5.09	127.53	120.29
27	N	176	GLN	OE1-CD-NE2	5.09	127.69	122.60
28	S	378	GLN	CA-C-N	5.09	128.05	120.31
28	S	378	GLN	C-N-CA	5.09	128.05	120.31
29	P	269	VAL	N-CA-C	-5.09	105.57	110.72
29	P	336	HIS	ND1-CE1-NE2	5.09	113.50	108.40
30	Q	245	SER	N-CA-C	5.09	116.52	111.07
31	R	252	TYR	CA-C-N	5.09	127.11	120.28
31	R	252	TYR	C-N-CA	5.09	127.11	120.28
7	g	116	VAL	CA-CB-CG2	-5.09	101.74	110.40
2	B	180	ASN	CA-C-N	5.09	127.36	120.38
2	B	180	ASN	C-N-CA	5.09	127.36	120.38
3	C	93	HIS	CA-C-O	-5.09	115.15	120.55
5	E	7	PHE	N-CA-C	-5.09	101.01	109.46
23	T	234	TYR	CA-C-N	5.09	131.27	121.54
23	T	234	TYR	C-N-CA	5.09	131.27	121.54
29	P	313	ILE	CA-C-N	5.09	127.44	120.46
29	P	313	ILE	C-N-CA	5.09	127.44	120.46
14	n	106	LYS	CA-C-O	5.09	125.80	119.79
8	1	106	ASN	CB-CA-C	-5.09	102.77	111.02
31	R	349	SER	CA-C-O	-5.09	115.71	121.72
2	B	217	GLU	CA-CB-CG	5.09	124.28	114.10
8	1	80	SER	N-CA-CB	5.09	117.69	110.16
14	7	85	GLU	O-C-N	5.09	129.92	122.39
15	H	395	SER	N-CA-CB	5.09	118.17	110.28
18	L	434	TYR	N-CA-CB	5.09	118.59	110.65
21	W	122	ARG	CA-C-N	5.09	127.10	120.28
21	W	122	ARG	C-N-CA	5.09	127.10	120.28
29	P	143	LEU	N-CA-CB	5.09	117.69	110.16
29	P	379	TYR	CB-CG-CD2	-5.09	113.17	120.80
6	F	185	PRO	CA-C-N	5.09	127.10	120.28
6	F	185	PRO	C-N-CA	5.09	127.10	120.28
8	1	77	THR	O-C-N	5.09	127.51	122.12
9	2	4	VAL	N-CA-CB	5.09	120.99	112.44
28	S	426	ALA	CA-C-O	5.09	125.81	120.42
29	P	233	GLU	CA-C-N	5.09	128.04	120.31
29	P	233	GLU	C-N-CA	5.09	128.04	120.31
4	d	120	GLN	OE1-CD-NE2	5.09	127.69	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	g	165	ARG	N-CA-CB	5.09	118.05	110.22
12	l	198	TRP	CB-CG-CD1	5.09	134.53	126.90
2	B	32	VAL	CA-C-O	-5.09	116.98	121.97
4	D	205	ALA	N-CA-CB	5.09	117.66	110.13
19	M	56	ASN	CA-C-O	-5.09	115.46	120.70
20	J	278	GLN	N-CA-C	-5.09	105.38	112.45
22	V	233	LYS	CA-C-N	5.09	127.05	120.44
22	V	233	LYS	C-N-CA	5.09	127.05	120.44
7	g	171	GLU	CB-CA-C	5.08	119.23	110.79
11	4	9	VAL	CB-CA-C	5.08	119.63	111.29
28	S	480	ARG	O-C-N	-5.08	116.02	122.27
30	Q	425	GLN	N-CA-C	5.08	116.82	111.28
1	a	148	THR	CA-C-O	5.08	125.85	120.36
13	m	58	ALA	O-C-N	5.08	127.51	122.12
6	F	132	LEU	N-CA-CB	5.08	118.76	110.37
12	5	65	LEU	CB-CA-C	-5.08	102.21	110.85
18	L	159	LEU	N-CA-C	-5.08	102.46	110.14
21	W	102	GLN	O-C-N	-5.08	116.73	122.12
26	Z	516	THR	N-CA-C	-5.08	106.59	112.89
34	8	248	ASN	CA-CB-CG	-5.08	107.52	112.60
2	b	23	TYR	CB-CG-CD2	-5.08	113.18	120.80
2	b	94	HIS	CA-C-N	5.08	127.09	120.28
2	b	94	HIS	C-N-CA	5.08	127.09	120.28
7	G	138	ASP	CA-C-O	5.08	126.16	120.77
18	L	215	PRO	CA-C-O	-5.08	115.73	121.98
20	J	207	ASP	CA-CB-CG	-5.08	107.52	112.60
22	V	78	VAL	N-CA-C	-5.08	100.25	107.77
34	8	196	ALA	N-CA-C	-5.08	106.59	112.89
34	8	475	GLU	CA-C-N	5.08	127.09	120.28
34	8	475	GLU	C-N-CA	5.08	127.09	120.28
1	a	63	ILE	N-CA-C	-5.08	101.10	108.36
4	d	233	GLN	OE1-CD-NE2	-5.08	117.52	122.60
5	E	160	ASN	N-CA-C	-5.08	107.21	113.41
9	2	93	HIS	CA-CB-CG	5.08	118.88	113.80
14	7	91	TYR	CA-C-N	5.08	127.06	120.56
14	7	91	TYR	C-N-CA	5.08	127.06	120.56
30	Q	132	PHE	CA-C-N	5.08	127.09	120.28
30	Q	132	PHE	C-N-CA	5.08	127.09	120.28
34	8	113	ASN	CA-C-N	5.08	127.88	119.35
34	8	113	ASN	C-N-CA	5.08	127.88	119.35
2	b	126	GLY	N-CA-C	-5.08	101.14	113.18
2	b	229	THR	CA-CB-CG2	5.08	119.13	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	78	ARG	CB-CA-C	5.08	118.85	110.88
6	F	26	GLU	CB-CG-CD	-5.08	103.97	112.60
11	4	2	ASP	O-C-N	-5.08	115.84	122.59
17	K	142	HIS	ND1-CE1-NE2	5.08	113.48	108.40
18	L	162	GLU	N-CA-CB	5.08	117.77	109.69
27	N	507	GLU	CB-CG-CD	5.08	121.23	112.60
33	O	52	ALA	N-CA-C	-5.08	107.24	112.93
6	f	41	THR	N-CA-C	5.08	117.94	111.69
8	h	92	ASN	CB-CA-C	-5.08	102.22	110.85
1	A	112	MET	CA-C-O	-5.08	114.13	119.97
19	M	345	ARG	CA-C-N	5.08	129.93	122.77
19	M	345	ARG	C-N-CA	5.08	129.93	122.77
29	P	253	ASP	CA-C-N	5.08	127.85	120.79
29	P	253	ASP	C-N-CA	5.08	127.85	120.79
2	b	95	THR	N-CA-CB	5.08	117.58	110.12
3	c	101	TYR	CB-CA-C	-5.08	101.59	110.17
4	D	46	ARG	N-CA-C	-5.08	100.02	108.34
6	F	84	SER	N-CA-CB	5.08	117.76	110.20
8	1	192	GLU	CB-CG-CD	-5.08	103.97	112.60
15	H	177	ASP	CA-C-N	5.08	127.39	120.54
15	H	177	ASP	C-N-CA	5.08	127.39	120.54
18	L	127	TYR	O-C-N	-5.08	117.03	123.17
26	Z	318	LYS	O-C-N	5.08	127.50	122.12
1	a	141	LEU	N-CA-C	-5.07	107.12	113.72
3	C	180	LYS	O-C-N	-5.07	117.38	123.27
10	3	98	ARG	NE-CZ-NH2	5.07	123.77	119.20
28	S	30	GLN	N-CA-C	5.07	116.50	111.07
28	S	337	ASN	N-CA-C	-5.07	106.93	113.02
29	P	284	ILE	CA-C-N	5.07	127.08	120.28
29	P	284	ILE	C-N-CA	5.07	127.08	120.28
1	a	29	THR	CA-C-O	5.07	125.60	119.31
13	m	23	LEU	CA-C-N	5.07	130.77	122.81
13	m	23	LEU	C-N-CA	5.07	130.77	122.81
13	m	78	ASP	O-C-N	-5.07	115.46	122.46
13	m	149	PHE	O-C-N	5.07	127.29	122.07
2	B	166	LYS	O-C-N	-5.07	116.74	122.12
7	G	178	HIS	CB-CA-C	-5.07	100.93	110.67
9	2	190	TYR	CA-C-O	5.07	126.15	120.82
27	N	459	ASN	N-CA-CB	5.07	118.27	110.21
34	8	439	GLN	N-CA-CB	5.07	120.21	111.13
1	a	210	SER	O-C-N	-5.07	115.74	122.74
3	c	108	GLU	CA-C-N	5.07	126.95	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	108	GLU	C-N-CA	5.07	126.95	120.56
3	c	174	LEU	CA-C-O	5.07	125.79	120.42
4	d	229	GLN	CA-C-O	5.07	125.92	120.55
5	e	73	LEU	CB-CA-C	-5.07	102.52	110.79
10	3	56	ALA	N-CA-C	5.07	116.81	111.28
23	T	131	LYS	O-C-N	5.07	127.50	122.12
29	P	419	VAL	CA-C-N	5.07	127.49	120.29
29	P	419	VAL	C-N-CA	5.07	127.49	120.29
30	Q	389	VAL	CA-C-O	5.07	126.33	120.90
31	R	239	THR	CA-C-N	5.07	127.33	120.44
31	R	239	THR	C-N-CA	5.07	127.33	120.44
33	O	71	ASP	CB-CA-C	-5.07	102.37	110.79
6	f	137	ASP	CA-C-O	5.07	127.76	120.51
1	A	78	ILE	O-C-N	5.07	123.67	120.07
17	K	234	PHE	N-CA-C	-5.07	99.72	108.69
19	M	413	GLU	CA-C-N	5.07	127.03	120.44
19	M	413	GLU	C-N-CA	5.07	127.03	120.44
26	Z	831	LEU	N-CA-CB	5.07	117.57	110.12
33	O	49	PHE	CA-C-N	5.07	127.49	120.29
33	O	49	PHE	C-N-CA	5.07	127.49	120.29
3	c	13	SER	CA-C-N	5.07	126.17	119.84
3	c	13	SER	C-N-CA	5.07	126.17	119.84
4	D	114	VAL	CB-CA-C	-5.07	105.45	112.24
18	L	321	THR	N-CA-C	-5.07	100.91	109.07
19	M	300	GLU	O-C-N	-5.07	116.75	122.12
22	V	22	ASP	CA-CB-CG	-5.07	107.53	112.60
26	Z	280	ASP	N-CA-C	-5.07	105.84	111.36
4	D	231	VAL	N-CA-CB	5.07	116.48	110.55
8	1	57	ASP	CA-CB-CG	5.07	117.67	112.60
8	1	74	SER	N-CA-CB	5.07	118.25	110.70
20	J	390	MET	CA-C-N	5.07	127.07	120.28
20	J	390	MET	C-N-CA	5.07	127.07	120.28
21	W	127	ARG	N-CA-CB	5.07	117.66	110.16
23	T	110	LEU	N-CA-C	-5.07	105.65	111.07
24	X	131	ASN	CA-C-N	5.07	128.40	120.75
24	X	131	ASN	C-N-CA	5.07	128.40	120.75
30	Q	170	ASP	CA-CB-CG	5.07	117.67	112.60
3	C	190	GLU	N-CA-CB	5.06	117.35	110.01
2	b	151	ASP	N-CA-C	-5.06	103.77	110.40
6	f	94	SER	N-CA-C	-5.06	105.76	111.28
17	K	80	LYS	CB-CA-C	-5.06	102.24	110.85
24	X	113	GLU	N-CA-CB	5.06	119.61	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	593	HIS	CG-CD2-NE2	5.06	112.26	107.20
31	R	196	SER	N-CA-CB	5.06	117.65	110.16
14	7	157	LYS	N-CA-C	-5.06	105.89	111.71
4	d	234	ILE	O-C-N	5.06	126.78	121.87
5	e	81	ILE	O-C-N	5.06	127.16	121.90
15	H	201	GLU	CA-C-N	5.06	129.58	122.09
15	H	201	GLU	C-N-CA	5.06	129.58	122.09
16	I	395	MET	CA-C-O	-5.06	115.06	120.42
18	L	62	ARG	NH1-CZ-NH2	-5.06	112.72	119.30
28	S	186	TYR	CB-CG-CD1	5.06	128.39	120.80
30	Q	342	LEU	CA-C-N	5.06	127.06	120.28
30	Q	342	LEU	C-N-CA	5.06	127.06	120.28
33	O	307	MET	N-CA-C	-5.06	100.46	109.06
2	b	128	ARG	NE-CZ-NH2	5.06	123.75	119.20
6	f	118	ASN	CB-CG-ND2	-5.06	108.81	116.40
11	4	67	TYR	N-CA-CB	5.06	117.40	110.07
18	L	53	HIS	CE1-NE2-CD2	-5.06	103.94	109.00
19	M	156	LEU	CA-C-N	5.06	130.45	121.80
19	M	156	LEU	C-N-CA	5.06	130.45	121.80
27	N	164	ASP	CA-C-O	-5.06	115.19	120.55
33	O	276	LYS	N-CA-C	5.06	116.87	111.36
5	E	57	GLU	N-CA-CB	5.06	119.94	110.99
19	M	160	PRO	N-CA-C	-5.06	103.25	111.19
26	Z	377	ALA	CB-CA-C	-5.06	110.72	116.54
28	S	428	ARG	N-CA-C	-5.06	105.77	111.28
4	D	138	PRO	N-CA-CB	5.05	107.74	103.19
5	E	82	GLU	N-CA-CB	5.05	117.55	110.12
9	2	176	CYS	CB-CA-C	5.05	118.23	110.14
12	5	209	ASN	N-CA-C	-5.05	105.77	111.28
19	M	328	ASN	CA-C-N	5.05	128.03	120.95
19	M	328	ASN	C-N-CA	5.05	128.03	120.95
22	V	74	SER	N-CA-C	-5.05	101.05	108.99
26	Z	290	GLU	CA-C-N	5.05	127.05	120.28
26	Z	290	GLU	C-N-CA	5.05	127.05	120.28
27	N	355	TRP	CA-C-N	5.05	127.05	120.28
27	N	355	TRP	C-N-CA	5.05	127.05	120.28
28	S	109	GLU	N-CA-C	-5.05	98.81	107.61
2	b	88	LYS	CA-C-O	5.05	125.91	120.55
12	l	58	TRP	CB-CG-CD1	5.05	134.48	126.90
14	n	164	ASP	CA-CB-CG	-5.05	107.55	112.60
2	B	98	LYS	N-CA-C	-5.05	106.81	113.17
12	5	2	THR	CA-C-N	5.05	131.06	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	2	THR	C-N-CA	5.05	131.06	122.37
14	7	50	VAL	N-CA-C	-5.05	100.25	107.78
20	J	141	LYS	CA-C-O	5.05	127.73	120.51
22	V	99	GLY	N-CA-C	-5.05	108.28	115.30
24	X	45	PHE	CA-CB-CG	5.05	118.85	113.80
28	S	282	ILE	N-CA-C	-5.05	105.63	113.16
30	Q	175	VAL	N-CA-C	-5.05	105.62	110.72
10	j	33	LEU	N-CA-CB	5.05	117.88	109.60
10	j	190	LYS	CA-C-O	-5.05	115.07	120.42
12	5	8	PHE	O-C-N	-5.05	116.22	122.73
16	I	365	HIS	ND1-CE1-NE2	5.05	113.45	108.40
16	I	394	ALA	O-C-N	5.05	127.47	122.12
22	V	173	THR	CA-CB-CG2	-5.05	101.92	110.50
27	N	739	PHE	CA-C-N	5.05	127.05	120.28
27	N	739	PHE	C-N-CA	5.05	127.05	120.28
5	E	201	GLU	N-CA-CB	5.05	117.54	110.12
5	E	238	LYS	CA-C-O	-5.05	114.17	119.97
13	6	199	GLY	O-C-N	-5.05	118.88	123.78
18	L	187	THR	N-CA-CB	5.05	117.28	109.91
20	J	147	TYR	N-CA-CB	5.05	117.54	110.12
30	Q	307	ASN	N-CA-C	5.05	116.86	111.36
2	b	115	ALA	CA-C-O	5.05	125.90	120.55
5	e	205	ASP	CA-CB-CG	-5.05	107.55	112.60
12	l	14	VAL	CA-C-O	5.05	125.69	120.39
8	1	68	SER	CB-CA-C	-5.05	102.27	110.85
14	7	41	ARG	N-CA-C	-5.05	107.17	113.38
18	L	55	LYS	N-CA-CB	5.05	117.63	110.16
21	W	8	LEU	N-CA-C	-5.05	101.08	109.46
4	D	229	GLN	CG-CD-NE2	-5.04	108.83	116.40
5	e	176	LEU	CA-C-O	-5.04	115.07	120.42
13	m	21	ALA	CA-C-N	-5.04	116.10	123.06
13	m	21	ALA	C-N-CA	-5.04	116.10	123.06
5	E	32	ILE	CA-C-N	5.04	129.30	122.19
5	E	32	ILE	C-N-CA	5.04	129.30	122.19
18	L	374	PHE	N-CA-C	-5.04	106.15	113.21
26	Z	929	VAL	CA-C-O	5.04	127.13	121.28
29	P	413	ASN	N-CA-C	-5.04	105.49	111.69
30	Q	251	THR	CA-CB-OG1	5.04	117.17	109.60
5	e	134	LEU	N-CA-C	-5.04	101.53	109.50
5	e	159	TYR	CA-CB-CG	-5.04	104.83	113.90
7	g	34	ILE	CA-C-N	5.04	125.49	121.61
7	g	34	ILE	C-N-CA	5.04	125.49	121.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	170	TYR	N-CA-C	-5.04	106.91	113.16
12	l	209	ASN	N-CA-C	-5.04	105.78	111.28
4	D	116	GLN	N-CA-C	5.04	116.46	111.07
11	4	146	HIS	CE1-NE2-CD2	-5.04	103.96	109.00
23	T	266	TYR	CA-CB-CG	-5.04	104.83	113.90
27	N	902	VAL	CA-C-O	5.04	126.60	120.85
31	R	229	LYS	CA-C-N	5.04	127.45	120.29
31	R	229	LYS	C-N-CA	5.04	127.45	120.29
3	c	61	SER	CA-C-N	5.04	129.75	122.44
3	c	61	SER	C-N-CA	5.04	129.75	122.44
12	5	207	PHE	CB-CA-C	-5.04	105.11	111.86
15	H	270	THR	N-CA-CB	5.04	119.01	110.49
26	Z	556	ILE	N-CA-C	-5.04	100.31	107.77
1	a	105	CYS	CA-C-N	5.04	127.29	120.44
1	a	105	CYS	C-N-CA	5.04	127.29	120.44
3	C	49	ARG	NE-CZ-NH1	5.04	126.54	121.50
3	C	149	THR	N-CA-C	-5.04	101.71	109.52
12	5	85	ASN	N-CA-CB	5.04	117.31	110.01
17	K	314	VAL	N-CA-C	5.04	119.82	109.34
18	L	407	ARG	N-CA-C	-5.04	101.41	109.07
25	Y	21	ASN	CA-CB-CG	-5.04	107.56	112.60
31	R	206	ARG	CB-CG-CD	5.04	122.89	111.30
33	O	80	LYS	CA-C-O	5.04	125.76	120.42
34	8	473	GLU	CA-C-N	5.04	127.03	120.28
34	8	473	GLU	C-N-CA	5.04	127.03	120.28
26	Z	784	SER	CA-C-N	-5.04	113.56	120.46
26	Z	784	SER	C-N-CA	-5.04	113.56	120.46
31	R	411	LEU	CA-C-N	5.04	126.99	120.44
31	R	411	LEU	C-N-CA	5.04	126.99	120.44
33	O	256	ASN	CA-C-N	5.04	127.03	120.28
33	O	256	ASN	C-N-CA	5.04	127.03	120.28
2	B	186	GLU	CA-CB-CG	5.04	124.17	114.10
5	E	142	ASP	CA-C-N	5.04	130.13	122.37
5	E	142	ASP	C-N-CA	5.04	130.13	122.37
7	G	19	GLN	N-CA-C	5.04	116.77	111.28
8	1	71	GLY	CA-C-N	5.04	127.81	120.51
8	1	71	GLY	C-N-CA	5.04	127.81	120.51
15	H	352	MET	N-CA-CB	5.04	119.59	110.83
15	H	414	SER	N-CA-C	-5.04	101.46	108.96
26	Z	275	GLN	CB-CG-CD	-5.04	104.04	112.60
28	S	196	ARG	N-CA-C	-5.04	106.65	112.89
33	O	165	LEU	CA-C-N	5.04	127.03	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	O	165	LEU	C-N-CA	5.04	127.03	120.28
33	O	295	THR	CA-C-N	5.04	127.29	120.44
33	O	295	THR	C-N-CA	5.04	127.29	120.44
1	A	62	TYR	CA-C-O	5.03	124.72	118.43
3	C	201	ASP	CA-CB-CG	-5.03	107.57	112.60
20	J	138	MET	CA-C-N	5.03	127.36	120.46
20	J	138	MET	C-N-CA	5.03	127.36	120.46
23	T	21	ALA	N-CA-CB	5.03	117.61	110.16
34	8	217	LEU	N-CA-CB	5.03	117.52	110.12
34	8	259	SER	N-CA-C	-5.03	105.89	112.23
2	b	174	PHE	CA-C-N	5.03	127.02	120.28
2	b	174	PHE	C-N-CA	5.03	127.02	120.28
4	d	237	GLU	CA-C-N	5.03	127.96	120.31
4	d	237	GLU	C-N-CA	5.03	127.96	120.31
18	L	53	HIS	ND1-CE1-NE2	5.03	113.43	108.40
18	L	327	THR	CA-CB-OG1	5.03	117.15	109.60
29	P	222	ASN	CA-CB-CG	-5.03	107.57	112.60
31	R	138	GLY	O-C-N	5.03	128.37	122.68
1	a	186	ASN	OD1-CG-ND2	5.03	127.63	122.60
3	C	185	VAL	CA-C-O	-5.03	115.52	120.85
8	1	90	LYS	CA-C-O	5.03	125.75	120.42
19	M	61	LYS	N-CA-C	5.03	117.49	111.71
22	V	183	ALA	CA-C-N	5.03	131.15	121.54
22	V	183	ALA	C-N-CA	5.03	131.15	121.54
26	Z	871	HIS	CG-CD2-NE2	5.03	112.23	107.20
27	N	820	GLU	N-CA-C	-5.03	107.27	113.41
27	N	903	VAL	CB-CA-C	5.03	117.67	110.33
28	S	205	ASN	N-CA-C	-5.03	105.80	111.28
32	U	283	ARG	N-CA-C	-5.03	105.92	111.71
33	O	289	GLN	O-C-N	5.03	127.89	122.15
14	7	190	ARG	N-CA-C	-5.03	105.69	111.07
17	K	194	GLN	CB-CA-C	-5.03	103.03	110.62
32	U	177	ASP	CA-CB-CG	-5.03	107.57	112.60
4	d	14	HIS	CB-CG-ND1	5.03	130.24	122.70
4	D	143	PRO	N-CA-CB	5.03	107.72	103.35
15	H	162	ARG	N-CA-CB	5.03	118.99	110.49
18	L	384	ASP	CA-CB-CG	5.03	117.63	112.60
19	M	277	ILE	N-CA-CB	5.03	119.43	111.99
22	V	294	SER	CA-C-N	5.03	127.35	120.46
22	V	294	SER	C-N-CA	5.03	127.35	120.46
28	S	148	ASP	N-CA-CB	5.03	117.30	110.01
8	1	52	THR	CA-C-O	-5.03	115.22	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	86	HIS	ND1-CE1-NE2	5.03	113.43	108.40
14	7	161	ARG	CA-C-N	5.03	127.02	120.28
14	7	161	ARG	C-N-CA	5.03	127.02	120.28
27	N	452	LEU	N-CA-CB	5.03	117.60	110.16
29	P	310	ARG	CA-C-N	5.03	126.99	120.26
29	P	310	ARG	C-N-CA	5.03	126.99	120.26
7	g	225	LYS	CA-C-N	5.02	129.73	121.39
7	g	225	LYS	C-N-CA	5.02	129.73	121.39
13	6	199	GLY	CA-C-N	5.02	131.14	121.54
13	6	199	GLY	C-N-CA	5.02	131.14	121.54
29	P	231	LYS	CA-C-N	5.02	129.69	122.40
29	P	231	LYS	C-N-CA	5.02	129.69	122.40
33	O	31	LYS	CB-CA-C	-5.02	102.31	110.85
8	h	98	ILE	N-CA-CB	5.02	117.69	111.41
11	k	41	HIS	N-CA-C	-5.02	104.96	112.54
11	k	142	SER	CA-C-O	-5.02	115.53	120.70
13	m	216	PHE	CA-CB-CG	-5.02	108.78	113.80
3	C	188	ALA	CA-C-N	5.02	127.55	120.42
3	C	188	ALA	C-N-CA	5.02	127.55	120.42
4	D	53	GLN	CA-C-O	-5.02	114.93	120.30
11	4	50	ALA	N-CA-C	5.02	118.07	110.64
16	I	154	MET	N-CA-CB	5.02	117.84	109.60
19	M	323	VAL	N-CA-CB	5.02	119.72	111.58
27	N	333	SER	CA-C-N	5.02	126.99	120.56
27	N	333	SER	C-N-CA	5.02	126.99	120.56
29	P	382	ASP	CA-CB-CG	-5.02	107.58	112.60
30	Q	247	HIS	ND1-CE1-NE2	5.02	113.42	108.40
3	c	234	ILE	CA-C-N	5.02	126.97	120.44
3	c	234	ILE	C-N-CA	5.02	126.97	120.44
11	4	86	GLN	N-CA-C	5.02	116.44	111.07
32	U	183	ALA	CA-C-N	5.02	131.25	121.41
32	U	183	ALA	C-N-CA	5.02	131.25	121.41
7	g	214	TRP	CB-CG-CD1	5.02	134.43	126.90
4	D	226	GLU	CA-C-N	5.02	127.34	120.46
4	D	226	GLU	C-N-CA	5.02	127.34	120.46
17	K	398	ASN	CB-CG-ND2	5.02	123.93	116.40
19	M	55	ASN	CA-CB-CG	-5.02	107.58	112.60
26	Z	718	ASP	CA-C-O	5.02	125.74	120.42
27	N	105	SER	CA-C-O	5.02	125.74	120.42
32	U	13	LEU	N-CA-C	-5.02	105.89	111.36
33	O	276	LYS	CA-C-O	5.02	125.74	120.42
34	8	234	ARG	N-CA-CB	5.02	118.44	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	238	PHE	N-CA-CB	-5.02	102.73	110.01
11	4	158	LEU	CD1-CG-CD2	-5.02	99.76	110.80
15	H	339	GLN	OE1-CD-NE2	5.02	127.62	122.60
18	L	67	HIS	ND1-CE1-NE2	5.02	113.42	108.40
23	T	21	ALA	N-CA-C	-5.02	105.89	111.36
27	N	69	TYR	CA-C-N	5.02	127.31	120.54
27	N	69	TYR	C-N-CA	5.02	127.31	120.54
30	Q	356	CYS	O-C-N	-5.02	118.88	123.50
8	1	58	ILE	CA-C-N	5.02	127.33	120.46
8	1	58	ILE	C-N-CA	5.02	127.33	120.46
12	5	51	ASP	O-C-N	-5.02	116.80	122.12
27	N	514	THR	O-C-N	5.02	127.44	122.12
2	b	229	THR	CB-CA-C	-5.01	102.33	110.85
3	c	96	ASN	N-CA-C	-5.01	105.89	111.36
2	B	248	GLU	CA-C-O	-5.01	113.21	119.18
14	7	155	LEU	CA-C-O	-5.01	115.23	120.55
17	K	242	PHE	CA-CB-CG	-5.01	108.79	113.80
17	K	347	ARG	NE-CZ-NH1	5.01	126.51	121.50
22	V	197	TYR	N-CA-C	-5.01	101.06	109.24
26	Z	12	ILE	CA-C-O	5.01	126.48	121.27
30	Q	186	HIS	CG-CD2-NE2	5.01	112.21	107.20
3	c	165	GLY	CA-C-N	5.01	128.81	120.94
3	c	165	GLY	C-N-CA	5.01	128.81	120.94
11	k	13	VAL	O-C-N	5.01	128.67	123.26
2	B	245	ASP	O-C-N	5.01	127.43	122.12
11	4	101	ASN	N-CA-C	-5.01	101.54	109.76
27	N	65	ALA	CA-C-N	5.01	127.00	120.28
27	N	65	ALA	C-N-CA	5.01	127.00	120.28
28	S	316	LEU	CA-C-N	5.01	127.50	120.28
28	S	316	LEU	C-N-CA	5.01	127.50	120.28
33	O	47	LYS	N-CA-C	-5.01	105.82	111.28
9	i	94	ILE	CA-CB-CG1	5.01	118.92	110.40
9	i	157	ASP	O-C-N	5.01	127.23	122.07
10	j	125	LEU	CB-CA-C	-5.01	102.98	110.90
12	l	144	TYR	CA-C-N	5.01	130.55	122.29
12	l	144	TYR	C-N-CA	5.01	130.55	122.29
5	E	161	ALA	N-CA-C	-5.01	101.13	108.99
18	L	161	ARG	NE-CZ-NH2	5.01	123.71	119.20
26	Z	67	SER	N-CA-CB	5.01	117.33	110.07
26	Z	912	PHE	CA-C-N	5.01	130.99	121.97
26	Z	912	PHE	C-N-CA	5.01	130.99	121.97
4	d	189	CYS	CA-CB-SG	-5.01	102.88	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	353	PHE	CB-CG-CD1	5.01	129.21	120.70
21	W	107	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
9	i	183	ASP	N-CA-CB	5.01	117.24	109.48
11	k	146	HIS	N-CA-C	5.01	116.55	111.14
2	B	90	ARG	CA-C-O	5.01	125.73	120.42
7	G	186	ARG	NE-CZ-NH1	5.01	126.51	121.50
8	l	25	TYR	CA-C-O	-5.01	115.34	121.05
23	T	153	MET	CA-C-N	5.01	126.99	120.28
23	T	153	MET	C-N-CA	5.01	126.99	120.28
27	N	146	LYS	N-CA-C	-5.01	105.90	111.36
33	O	120	LYS	O-C-N	5.01	129.25	122.59
12	l	41	LEU	N-CA-CB	5.00	119.46	110.80
19	M	343	LEU	CB-CA-C	5.00	118.80	110.74
2	b	230	ASP	CA-C-O	-5.00	115.65	121.15
3	c	98	LEU	N-CA-C	-5.00	105.83	111.28
5	e	55	SER	O-C-N	5.00	127.42	122.12
7	g	178	HIS	N-CA-CB	5.00	118.04	110.28
9	i	151	ALA	CA-C-N	5.00	126.86	120.56
9	i	151	ALA	C-N-CA	5.00	126.86	120.56
11	k	57	ALA	CA-C-N	5.00	127.39	120.29
11	k	57	ALA	C-N-CA	5.00	127.39	120.29
4	D	49	THR	N-CA-C	-5.00	107.12	113.18
4	D	128	GLY	CA-C-N	5.00	129.89	122.94
4	D	128	GLY	C-N-CA	5.00	129.89	122.94
6	F	17	ARG	N-CA-C	-5.00	100.26	108.41
10	3	38	LYS	O-C-N	-5.00	117.37	123.27
13	6	205	LEU	N-CA-CB	5.00	118.58	110.42
16	I	119	ILE	N-CA-CB	5.00	118.83	111.52
27	N	22	THR	CA-C-N	5.00	126.98	120.28
27	N	22	THR	C-N-CA	5.00	126.98	120.28
34	8	192	TYR	CB-CG-CD1	-5.00	113.29	120.80
4	d	215	PRO	O-C-N	5.00	129.39	122.64
9	i	142	TRP	N-CA-C	5.00	117.15	110.35
10	j	62	LEU	N-CA-C	5.00	117.62	111.82
12	l	27	ALA	CB-CA-C	-5.00	103.03	110.88
12	l	193	VAL	CA-C-O	-5.00	115.75	120.95
14	n	158	VAL	N-CA-C	-5.00	106.80	111.45
26	Z	407	VAL	CA-CB-CG2	-5.00	101.90	110.40
28	S	130	VAL	O-C-N	-5.00	116.32	122.57
29	P	48	GLN	N-CA-C	-5.00	101.25	109.40

There are no chirality outliers.

All (347) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	193	TYR	Sidechain
8	1	25	TYR	Sidechain
8	1	70	TYR	Sidechain
8	1	87	TYR	Sidechain
9	2	123	TYR	Sidechain
9	2	124	TYR	Sidechain
9	2	19	ARG	Sidechain
9	2	69	TYR	Sidechain
9	2	72	ARG	Sidechain
9	2	75	ARG	Sidechain
10	3	197	ARG	Sidechain
11	4	146	HIS	Sidechain
11	4	148	TYR	Sidechain
11	4	149	ARG	Sidechain
11	4	176	PHE	Sidechain
11	4	36	ARG	Sidechain
12	5	144	TYR	Sidechain
12	5	167	ARG	Sidechain
12	5	187	TYR	Sidechain
12	5	88	TYR	Sidechain
13	6	108	HIS	Sidechain
13	6	137	ARG	Sidechain
13	6	160	TYR	Sidechain
13	6	174	TYR	Sidechain
13	6	2	PHE	Sidechain
13	6	5	TYR	Sidechain
13	6	68	PHE	Sidechain
13	6	75	TYR	Sidechain
14	7	101	TYR	Sidechain
14	7	103	ARG	Sidechain
14	7	128	ARG	Sidechain
14	7	129	TYR	Sidechain
14	7	16	TYR	Sidechain
14	7	193	ARG	Sidechain
14	7	195	PHE	Sidechain
14	7	76	TYR	Sidechain
14	7	91	TYR	Sidechain
14	7	93	PHE	Sidechain
34	8	128	TYR	Sidechain
34	8	205	TYR	Sidechain
34	8	218	PHE	Sidechain
34	8	229	PHE	Sidechain

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Mol	Chain	Res	Type	Group
34	8	273	ARG	Sidechain
34	8	321	ARG	Sidechain
34	8	372	ARG	Sidechain
34	8	385	GLU	Peptide
34	8	394	TYR	Sidechain
34	8	430	TYR	Sidechain
34	8	494	TYR	Sidechain
1	A	101	TYR	Sidechain
1	A	153	TYR	Sidechain
1	A	21	TYR	Sidechain
1	A	62	TYR	Sidechain
1	A	96	ARG	Sidechain
2	B	105	PRO	Peptide
2	B	134	LEU	Peptide
2	B	156	TYR	Sidechain
2	B	235	PHE	Sidechain
2	B	82	TYR	Sidechain
2	B	90	ARG	Sidechain
3	C	101	TYR	Sidechain
3	C	112	ARG	Sidechain
3	C	134	PHE	Sidechain
3	C	139	TYR	Sidechain
3	C	148	TYR	Sidechain
3	C	156	TYR	Sidechain
3	C	225	TYR	Sidechain
3	C	23	TYR	Sidechain
3	C	8	ARG	Sidechain
3	C	97	TYR	Sidechain
4	D	109	ARG	Sidechain
4	D	117	ARG	Sidechain
4	D	16	PHE	Sidechain
4	D	2	TYR	Sidechain
4	D	56	ARG	Sidechain
4	D	95	ARG	Sidechain
5	E	114	ARG	Sidechain
5	E	115	PHE	Sidechain
5	E	128	ARG	Peptide
5	E	14	PHE	Sidechain
5	E	145	TYR	Sidechain
5	E	157	TYR	Sidechain
5	E	158	ARG	Sidechain
5	E	159	TYR	Sidechain

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Mol	Chain	Res	Type	Group
5	E	7	PHE	Sidechain
5	E	94	TYR	Sidechain
5	E	95	TYR	Sidechain
6	F	125	ARG	Sidechain
6	F	170	TYR	Sidechain
6	F	173	ARG	Sidechain
6	F	38	ARG	Sidechain
6	F	58	TYR	Sidechain
6	F	86	TYR	Sidechain
6	F	88	ARG	Sidechain
7	G	134	PHE	Sidechain
7	G	186	ARG	Sidechain
7	G	87	ARG	Sidechain
7	G	89	ARG	Sidechain
15	H	145	TYR	Sidechain
15	H	178	ARG	Sidechain
15	H	367	ARG	Peptide
15	H	390	ARG	Sidechain
15	H	400	ARG	Sidechain
15	H	420	ARG	Sidechain
16	I	100	ARG	Peptide
16	I	128	TYR	Sidechain
16	I	179	GLU	Peptide
16	I	199	GLU	Peptide
16	I	223	GLY	Peptide
16	I	291	ARG	Sidechain
16	I	319	ARG	Sidechain
20	J	144	ASP	Peptide
20	J	154	THR	Peptide
20	J	231	ARG	Sidechain
20	J	368	TYR	Sidechain
20	J	71	TYR	Peptide
20	J	94	TYR	Sidechain
17	K	103	ILE	Peptide
17	K	118	TYR	Sidechain
17	K	121	ARG	Sidechain
17	K	212	TYR	Peptide
17	K	231	LYS	Peptide
17	K	255	ARG	Sidechain
17	K	262	ARG	Sidechain
17	K	329	LEU	Peptide
17	K	333	ARG	Sidechain,Peptide

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Mol	Chain	Res	Type	Group
17	K	346	ARG	Sidechain
17	K	426	PHE	Sidechain
17	K	67	TYR	Sidechain
18	L	191	ARG	Sidechain
18	L	207	PHE	Sidechain
18	L	290	ARG	Sidechain
18	L	342	ARG	Sidechain,Peptide
18	L	345	ARG	Sidechain
18	L	361	PHE	Sidechain
18	L	400	PHE	Sidechain
18	L	407	ARG	Sidechain
18	L	420	ARG	Sidechain
18	L	62	ARG	Sidechain
18	L	78	ARG	Sidechain
19	M	128	PHE	Sidechain
19	M	166	ARG	Sidechain
19	M	175	LYS	Peptide
19	M	229	THR	Peptide
19	M	279	PHE	Sidechain
19	M	281	ASP	Peptide
19	M	303	ARG	Sidechain
19	M	42	ARG	Sidechain
19	M	433	TYR	Sidechain
19	M	44	PHE	Sidechain
19	M	45	ARG	Sidechain
19	M	50	ARG	Sidechain
19	M	73	ARG	Sidechain
27	N	117	TYR	Sidechain
27	N	412	TYR	Sidechain
27	N	422	TYR	Sidechain
27	N	548	ARG	Sidechain
27	N	580	ASN	Peptide
27	N	599	TYR	Sidechain
27	N	75	TYR	Sidechain
27	N	786	ARG	Sidechain
27	N	866	TYR	Sidechain
27	N	908	ARG	Sidechain
33	O	115	ARG	Sidechain
33	O	210	ARG	Sidechain
33	O	248	TYR	Sidechain
33	O	283	HIS	Sidechain
33	O	310	PHE	Sidechain

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Mol	Chain	Res	Type	Group
33	O	48	PHE	Sidechain
33	O	62	TYR	Sidechain
29	P	109	SER	Peptide
29	P	21	PHE	Sidechain
29	P	221	TYR	Sidechain
29	P	234	TYR	Sidechain
29	P	273	TYR	Sidechain
29	P	274	GLY	Peptide
29	P	286	ASN	Peptide
29	P	390	TYR	Sidechain
29	P	79	LEU	Mainchain,Peptide
30	Q	146	TYR	Sidechain
30	Q	161	LEU	Peptide
30	Q	240	PHE	Sidechain
30	Q	246	TYR	Sidechain
30	Q	255	TYR	Sidechain
30	Q	50	ARG	Sidechain
31	R	123	ASP	Peptide
31	R	186	TYR	Sidechain
31	R	213	TYR	Sidechain
31	R	217	HIS	Sidechain
31	R	24	TYR	Sidechain
31	R	246	TYR	Sidechain
31	R	305	PHE	Sidechain
31	R	307	TYR	Sidechain
31	R	338	TYR	Sidechain
31	R	345	TYR	Sidechain
31	R	62	TYR	Sidechain
31	R	63	TYR	Sidechain
31	R	65	TYR	Sidechain
31	R	68	GLU	Peptide
31	R	70	TYR	Sidechain
31	R	99	TYR	Sidechain
28	S	111	ARG	Sidechain
28	S	170	TYR	Sidechain
28	S	173	LEU	Peptide
28	S	174	ARG	Sidechain
28	S	185	PHE	Sidechain
28	S	259	TYR	Sidechain
28	S	292	TYR	Sidechain
28	S	377	TYR	Sidechain
28	S	399	TYR	Sidechain

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Mol	Chain	Res	Type	Group
28	S	428	ARG	Sidechain
23	T	129	LEU	Peptide
23	T	197	TYR	Sidechain
23	T	199	PHE	Sidechain
23	T	233	VAL	Peptide
23	T	251	HIS	Peptide
23	T	266	TYR	Sidechain
23	T	91	SER	Mainchain,Peptide
23	T	96	LEU	Peptide
32	U	179	ARG	Sidechain
32	U	72	TYR	Sidechain
22	V	100	ARG	Sidechain
22	V	157	ARG	Sidechain
22	V	254	ARG	Sidechain
22	V	270	TYR	Sidechain
21	W	101	ARG	Sidechain
21	W	25	ARG	Sidechain
21	W	26	PHE	Sidechain
21	W	65	PHE	Sidechain
24	X	22	ARG	Sidechain
24	X	27	ILE	Peptide
24	X	48	PHE	Sidechain
24	X	85	ARG	Sidechain
26	Z	394	TYR	Sidechain
26	Z	408	TYR	Sidechain
26	Z	426	TYR	Sidechain
1	a	15	ARG	Sidechain
1	a	157	TYR	Sidechain
1	a	235	ARG	Sidechain
1	a	3	TYR	Sidechain
1	a	62	TYR	Sidechain
1	a	82	ARG	Sidechain
1	a	96	ARG	Sidechain
2	b	148	TYR	Sidechain
2	b	178	ARG	Sidechain
2	b	23	TYR	Sidechain
2	b	4	ARG	Sidechain
2	b	83	ARG	Sidechain
3	c	101	TYR	Sidechain
3	c	112	ARG	Sidechain
3	c	113	ARG	Sidechain
3	c	128	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	c	142	ARG	Sidechain
3	c	179	TYR	Sidechain
3	c	216	ARG	Sidechain
3	c	5	TYR	Sidechain
3	c	66	TYR	Sidechain
3	c	97	TYR	Sidechain
4	d	106	TYR	Sidechain
4	d	110	TYR	Sidechain
4	d	164	ARG	Sidechain
4	d	170	ARG	Sidechain
4	d	177	TYR	Sidechain
4	d	195	ARG	Sidechain
4	d	73	PHE	Sidechain
4	d	95	ARG	Sidechain
5	e	124	ARG	Sidechain
5	e	128	ARG	Peptide
5	e	2	ARG	Sidechain
5	e	95	TYR	Sidechain
6	f	100	ARG	Sidechain
6	f	125	ARG	Sidechain
6	f	146	PHE	Sidechain
6	f	156	TYR	Sidechain
6	f	163	ARG	Sidechain
6	f	50	ARG	Sidechain
6	f	58	TYR	Sidechain
7	g	108	PHE	Sidechain
7	g	156	TYR	Sidechain
7	g	16	ARG	Sidechain
7	g	197	TYR	Sidechain
7	g	69	HIS	Sidechain
8	h	185	ARG	Sidechain
8	h	189	TYR	Sidechain
8	h	36	ARG	Sidechain
8	h	45	ARG	Sidechain
8	h	70	TYR	Sidechain
8	h	8	PHE	Sidechain
8	h	82	PHE	Sidechain
8	h	87	TYR	Sidechain
9	i	111	PHE	Sidechain
9	i	123	TYR	Sidechain
9	i	124	TYR	Sidechain
9	i	141	HIS	Sidechain

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Mol	Chain	Res	Type	Group
9	i	186	TYR	Sidechain
9	i	75	ARG	Sidechain
9	i	8	PHE	Sidechain
9	i	97	TYR	Sidechain
10	j	103	PHE	Sidechain
10	j	146	PHE	Sidechain
10	j	27	ARG	Sidechain
10	j	73	TYR	Sidechain
10	j	79	ARG	Sidechain
10	j	99	PHE	Sidechain
11	k	107	TYR	Sidechain
11	k	121	TYR	Sidechain
11	k	59	TYR	Sidechain
11	k	67	TYR	Sidechain
11	k	70	ARG	Sidechain
11	k	73	TYR	Sidechain
11	k	93	ARG	Sidechain
12	l	114	TYR	Sidechain
12	l	121	ARG	Sidechain
12	l	135	PHE	Sidechain
12	l	144	TYR	Sidechain
12	l	170	TYR	Sidechain
12	l	188	HIS	Sidechain
12	l	40	PHE	Sidechain
12	l	54	PHE	Sidechain
12	l	6	PHE	Sidechain
12	l	7	ARG	Sidechain
12	l	73	ARG	Sidechain
12	l	88	TYR	Sidechain
13	m	106	TYR	Sidechain
13	m	133	ARG	Sidechain
13	m	174	TYR	Sidechain
13	m	194	ARG	Sidechain
13	m	213	ARG	Sidechain
13	m	221	ARG	Sidechain
13	m	39	TYR	Sidechain
13	m	75	TYR	Sidechain
13	m	98	TYR	Sidechain
14	n	103	ARG	Sidechain
14	n	126	PHE	Sidechain
14	n	146	PHE	Sidechain
14	n	182	ARG	Sidechain

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Mol	Chain	Res	Type	Group
14	n	185	TYR	Sidechain
14	n	190	ARG	Sidechain
14	n	228	TYR	Sidechain
14	n	35	ARG	Sidechain
14	n	41	ARG	Sidechain
14	n	91	TYR	Sidechain
14	n	95	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1907	0	1901	12	0
1	a	1907	0	1901	3	0
2	B	1915	0	1929	8	0
2	b	1915	0	1929	2	0
3	C	1904	0	1904	10	0
3	c	1904	0	1904	3	0
4	D	1881	0	1895	3	0
4	d	1881	0	1895	1	0
5	E	1861	0	1839	13	0
5	e	1861	0	1839	1	0
6	F	1795	0	1800	8	0
6	f	1773	0	1775	4	0
7	G	1892	0	1883	5	0
7	g	1892	0	1883	5	0
8	1	1512	0	1481	10	0
8	h	1512	0	1481	21	0
9	2	1719	0	1719	6	0
9	i	1719	0	1719	3	0
10	3	1581	0	1574	5	0
10	j	1581	0	1574	5	0
11	4	1561	0	1569	13	0
11	k	1561	0	1569	1	0
12	5	1644	0	1595	7	0
12	l	1644	0	1595	1	0
13	6	1757	0	1711	18	0
13	m	1757	0	1711	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	7	1790	0	1793	26	0
14	n	1815	0	1821	2	0
15	H	2967	0	3051	25	0
16	I	3022	0	3092	10	0
17	K	3078	0	3141	13	0
18	L	3082	0	3156	8	0
19	M	2986	0	3055	8	0
20	J	3089	0	3221	25	0
21	W	1534	0	1542	6	0
22	V	2274	0	2273	12	0
23	T	2192	0	2161	7	0
24	X	1032	0	1017	5	0
25	Y	435	0	394	0	0
26	Z	7005	0	6932	42	0
27	N	6882	0	6958	62	0
28	S	3894	0	3938	28	0
29	P	3608	0	3694	20	0
30	Q	3499	0	3524	11	0
31	R	3060	0	3083	59	0
32	U	2373	0	2403	6	0
33	O	3186	0	3213	10	0
34	8	3219	0	3184	17	0
35	H	31	0	12	6	0
35	I	31	0	12	5	0
35	J	31	0	12	0	0
35	M	31	0	12	1	0
36	H	1	0	0	0	0
36	I	1	0	0	0	0
36	J	1	0	0	0	0
36	K	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
37	K	27	0	12	2	0
37	L	27	0	12	0	0
All	All	112042	0	112293	507	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (507) 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)
15:H:388:ILE:HD11	35:H:501:ATP:C2	1.24	1.63
8:h:30:VAL:CB	14:7:225:ILE:HD11	1.27	1.58
20:J:17:SER:CA	28:S:171:TYR:CE1	1.88	1.54
20:J:17:SER:CA	28:S:171:TYR:HE1	0.97	1.52
8:h:30:VAL:HB	14:7:225:ILE:CD1	1.39	1.51
20:J:17:SER:HA	28:S:171:TYR:CE1	1.38	1.51
27:N:861:TYR:CB	27:N:861:TYR:CA	1.88	1.51
15:H:388:ILE:CD1	35:H:501:ATP:C2	2.04	1.40
8:h:30:VAL:CG2	14:7:225:ILE:HD13	1.63	1.28
8:h:30:VAL:CB	14:7:225:ILE:CD1	2.00	1.27
20:J:17:SER:OG	28:S:171:TYR:CE1	1.86	1.25
15:H:388:ILE:CD1	35:H:501:ATP:N1	2.02	1.22
8:h:30:VAL:CG2	14:7:225:ILE:CD1	2.19	1.19
15:H:388:ILE:HD13	35:H:501:ATP:N1	1.58	1.18
27:N:778:LYS:N	27:N:861:TYR:HA	1.59	1.17
20:J:17:SER:CB	28:S:171:TYR:CE1	2.27	1.16
34:8:136:MET:HE3	34:8:225:PHE:CE2	1.80	1.15
5:E:214:ILE:HG12	5:E:220:PHE:CD1	1.83	1.14
20:J:13:GLU:O	28:S:171:TYR:OH	1.65	1.12
5:E:214:ILE:HG12	5:E:220:PHE:HD1	1.00	1.12
27:N:778:LYS:H	27:N:861:TYR:HA	0.95	1.11
27:N:777:ALA:C	27:N:861:TYR:O	1.93	1.10
27:N:861:TYR:CB	27:N:861:TYR:N	2.14	1.10
31:R:107:GLU:OE2	31:R:111:LYS:HD2	1.50	1.09
15:H:77:ALA:CB	15:H:78:PRO:HD3	1.83	1.08
20:J:17:SER:N	28:S:171:TYR:CE1	2.22	1.07
20:J:17:SER:CB	28:S:171:TYR:HE1	1.66	1.05
20:J:17:SER:HA	28:S:171:TYR:CD1	1.90	1.05
27:N:861:TYR:O	27:N:862:SER:O	1.76	1.04
20:J:17:SER:N	28:S:171:TYR:HE1	1.54	1.03
15:H:77:ALA:HB3	15:H:78:PRO:HD3	1.38	1.03
27:N:777:ALA:HA	27:N:861:TYR:CA	1.86	1.03
27:N:777:ALA:CA	27:N:861:TYR:O	2.11	0.97
31:R:107:GLU:OE2	31:R:111:LYS:CD	2.14	0.95
17:K:221:MET:HE1	37:K:501:ADP:H2'	1.49	0.94
35:I:501:ATP:O1G	20:J:308:GLY:O	1.86	0.94
8:h:30:VAL:HG21	14:7:225:ILE:HD13	1.49	0.93
1:A:242:GLN:C	29:P:86:HIS:CA	2.42	0.93
5:E:214:ILE:CG1	5:E:220:PHE:CD1	2.52	0.91
8:h:30:VAL:HG23	14:7:225:ILE:CD1	1.99	0.91
27:N:104:LYS:HE2	27:N:104:LYS:HA	1.53	0.90
15:H:75:GLY:O	15:H:80:HIS:CD2	2.26	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:77:ALA:HB3	15:H:78:PRO:CD	2.04	0.87
8:h:30:VAL:O	14:7:225:ILE:HD12	1.73	0.86
34:8:136:MET:HG2	34:8:225:PHE:CE1	2.10	0.86
13:6:50:ILE:HG12	13:6:86:ILE:HD13	1.56	0.85
31:R:103:CYS:O	31:R:106:ASN:HB2	1.77	0.85
31:R:106:ASN:O	31:R:110:ILE:HB	1.76	0.84
34:8:136:MET:HE3	34:8:225:PHE:CZ	2.13	0.83
13:6:154:VAL:HG22	13:6:175:LEU:HD11	1.60	0.83
31:R:109:LYS:HB2	31:R:140:TYR:CD1	2.14	0.83
22:V:196:TYR:CD1	22:V:196:TYR:C	2.57	0.82
24:X:78:ILE:CG2	24:X:81:SER:HA	2.08	0.82
15:H:77:ALA:CB	15:H:78:PRO:CD	2.57	0.82
20:J:16:GLU:HB2	28:S:171:TYR:OH	1.79	0.82
28:S:459:GLN:N	28:S:459:GLN:OE1	2.12	0.82
27:N:855:GLU:O	27:N:857:TYR:N	2.12	0.81
31:R:107:GLU:O	31:R:111:LYS:HB3	1.80	0.81
30:Q:377:LEU:HD21	30:Q:397:LEU:HD13	1.63	0.81
31:R:107:GLU:O	31:R:111:LYS:CB	2.29	0.80
5:E:214:ILE:CG1	5:E:220:PHE:HD1	1.86	0.80
15:H:388:ILE:CD1	35:H:501:ATP:H2	1.71	0.80
31:R:109:LYS:HB2	31:R:140:TYR:CE1	2.17	0.78
27:N:777:ALA:C	27:N:861:TYR:C	2.53	0.77
13:6:86:ILE:HG13	13:6:114:LEU:O	1.85	0.77
13:6:50:ILE:HG13	13:6:86:ILE:CD1	2.15	0.77
27:N:777:ALA:HA	27:N:861:TYR:C	2.10	0.76
13:6:50:ILE:CG1	13:6:86:ILE:HD13	2.15	0.76
26:Z:464:ASP:O	26:Z:464:ASP:OD1	2.05	0.75
27:N:777:ALA:HA	27:N:861:TYR:CB	2.17	0.75
15:H:77:ALA:HB1	15:H:78:PRO:HD3	1.68	0.74
8:h:30:VAL:HG23	14:7:225:ILE:HD13	1.53	0.74
8:h:30:VAL:CA	14:7:225:ILE:HD11	2.16	0.73
27:N:777:ALA:CA	27:N:861:TYR:CA	2.63	0.73
27:N:778:LYS:N	27:N:861:TYR:CA	2.48	0.73
31:R:58:GLU:CD	31:R:102:LEU:HA	2.13	0.72
27:N:777:ALA:HA	27:N:861:TYR:O	1.89	0.72
27:N:861:TYR:C	27:N:862:SER:O	2.28	0.71
17:K:89:ILE:CG2	17:K:147:VAL:HG11	2.20	0.71
13:6:50:ILE:CG1	13:6:86:ILE:CD1	2.69	0.71
31:R:33:LEU:HB3	31:R:70:TYR:CE2	2.26	0.70
5:E:214:ILE:CG1	5:E:220:PHE:CE1	2.75	0.70
33:O:163:ILE:HD13	33:O:163:ILE:H	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:856:PHE:O	27:N:858:LYS:O	2.07	0.70
31:R:103:CYS:HA	31:R:106:ASN:HB2	1.74	0.69
3:C:106:PRO:HD2	3:C:109:ILE:HD12	1.73	0.69
16:I:227:THR:O	35:I:501:ATP:C6	2.45	0.69
34:8:136:MET:HE3	34:8:225:PHE:CD2	2.27	0.69
27:N:777:ALA:HA	27:N:861:TYR:HB3	1.75	0.68
27:N:778:LYS:N	27:N:861:TYR:C	2.51	0.68
27:N:871:MET:HG3	27:N:871:MET:O	1.93	0.68
6:F:233:ILE:OXT	6:F:233:ILE:HG22	1.93	0.67
22:V:196:TYR:CD1	22:V:196:TYR:O	2.47	0.67
27:N:375:HIS:CG	27:N:375:HIS:O	2.48	0.67
13:6:50:ILE:HG13	13:6:86:ILE:HD11	1.75	0.67
31:R:61:PRO:HD3	31:R:102:LEU:HD13	1.76	0.67
9:2:99:ILE:HD11	9:2:127:LEU:HB2	1.77	0.66
20:J:17:SER:N	28:S:171:TYR:CZ	2.63	0.66
31:R:279:LEU:O	31:R:280:ILE:HG12	1.95	0.66
14:7:152:ASN:N	14:7:153:PRO:CD	2.59	0.65
27:N:777:ALA:CA	27:N:861:TYR:C	2.68	0.65
1:A:242:GLN:C	29:P:86:HIS:N	2.54	0.65
22:V:117:TRP:CD2	22:V:187:ALA:HB1	2.32	0.64
31:R:61:PRO:CD	31:R:102:LEU:HD13	2.28	0.64
20:J:273:LEU:HD22	20:J:309:ARG:HH22	1.62	0.64
26:Z:579:GLU:OE1	26:Z:579:GLU:N	2.31	0.64
8:h:30:VAL:O	14:7:225:ILE:CD1	2.44	0.64
31:R:312:TYR:CE1	31:R:330:VAL:HG12	2.32	0.64
14:7:16:TYR:CE2	14:7:21:ILE:HG13	2.34	0.63
31:R:331:ARG:HH12	31:R:370:LYS:HD2	1.63	0.63
16:I:227:THR:O	35:I:501:ATP:C5	2.52	0.63
31:R:103:CYS:C	31:R:106:ASN:HB2	2.23	0.63
31:R:279:LEU:O	31:R:280:ILE:CG1	2.46	0.63
31:R:107:GLU:O	31:R:111:LYS:HB2	1.98	0.63
5:E:214:ILE:HG13	5:E:220:PHE:CE1	2.34	0.63
26:Z:82:MET:O	26:Z:83:THR:O	2.16	0.63
1:A:242:GLN:HB2	29:P:86:HIS:HA	1.80	0.62
1:A:18:GLN:HE22	7:G:11:PHE:H	1.46	0.62
27:N:860:LYS:C	27:N:861:TYR:CB	2.72	0.62
11:4:4:ILE:HG13	11:4:103:LEU:HD12	1.81	0.62
27:N:598:ASP:OD1	27:N:600:THR:OG1	2.18	0.62
34:8:136:MET:CE	34:8:225:PHE:CE2	2.71	0.62
13:6:22:VAL:HG12	13:6:206:ILE:HG12	1.82	0.61
26:Z:376:SER:HB3	34:8:388:MET:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:J:17:SER:N	28:S:171:TYR:OH	2.33	0.61
30:Q:54:GLN:HA	30:Q:54:GLN:OE1	2.01	0.61
31:R:106:ASN:O	31:R:110:ILE:CA	2.48	0.60
6:F:233:ILE:OXT	6:F:233:ILE:CG2	2.49	0.60
31:R:103:CYS:O	31:R:106:ASN:CB	2.49	0.60
8:1:173:ILE:HG12	8:1:193:TYR:CE2	2.37	0.60
15:H:100:ALA:HB2	15:H:149:LEU:HD23	1.82	0.59
27:N:776:TYR:O	27:N:881:TYR:CD2	2.55	0.59
8:1:13:ILE:HD12	8:1:151:THR:HB	1.84	0.59
5:E:65:HIS:CD2	5:E:66:ILE:HG13	2.38	0.59
31:R:60:ALA:HB3	31:R:102:LEU:HB2	1.84	0.58
33:O:132:GLU:OE1	33:O:132:GLU:HA	2.03	0.58
27:N:104:LYS:HE2	27:N:104:LYS:CA	2.29	0.58
16:I:307:LEU:HD12	16:I:310:LEU:HD23	1.85	0.58
17:K:89:ILE:HG22	17:K:147:VAL:HG11	1.84	0.58
30:Q:67:THR:H	30:Q:68:MET:HB2	1.68	0.58
8:h:134:ILE:HG21	8:h:158:SER:O	2.04	0.57
34:8:136:MET:SD	34:8:225:PHE:CD1	2.96	0.57
24:X:78:ILE:HG23	24:X:81:SER:HA	1.86	0.57
34:8:136:MET:CE	34:8:225:PHE:CD2	2.87	0.57
8:1:13:ILE:HD12	8:1:151:THR:CG2	2.34	0.57
27:N:860:LYS:C	27:N:861:TYR:CG	2.82	0.57
31:R:58:GLU:OE1	31:R:102:LEU:HA	2.05	0.57
31:R:58:GLU:OE2	31:R:102:LEU:HD12	2.05	0.57
26:Z:82:MET:O	26:Z:82:MET:HG3	2.04	0.56
26:Z:518:LEU:HB3	26:Z:520:ILE:HG22	1.87	0.56
3:C:3:ARG:HB3	3:C:5:TYR:CE2	2.40	0.56
29:P:243:GLU:HA	29:P:243:GLU:OE1	2.05	0.56
11:4:120:ASP:HA	11:4:133:HIS:CE1	2.40	0.56
16:I:221:LEU:HD13	16:I:325:ILE:HG23	1.87	0.56
13:6:147:MET:HE3	13:6:151:ASP:OD2	2.06	0.56
27:N:314:LEU:HD23	27:N:348:PHE:CD1	2.40	0.56
27:N:777:ALA:C	27:N:861:TYR:HA	2.26	0.56
26:Z:809:MET:O	26:Z:812:ILE:HG22	2.06	0.55
11:4:40:PRO:O	11:4:189:ILE:HG13	2.06	0.55
31:R:113:LEU:HD13	31:R:137:LEU:HD21	1.87	0.55
31:R:59:MET:H	31:R:98:LEU:HD11	1.70	0.55
31:R:106:ASN:O	31:R:110:ILE:CB	2.51	0.55
3:c:193:LEU:HD22	3:c:237:ILE:HG22	1.88	0.55
29:P:392:LYS:HB3	30:Q:355:GLU:HB2	1.88	0.55
17:K:101:GLU:O	17:K:109:ILE:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:69:PHE:CD1	21:W:69:PHE:C	2.85	0.55
26:Z:428:TRP:CD1	26:Z:428:TRP:O	2.60	0.55
29:P:94:GLN:N	29:P:94:GLN:OE1	2.39	0.55
6:f:136:TYR:CZ	6:f:217:LYS:HA	2.42	0.54
11:4:192:VAL:O	11:4:195:PHE:O	2.25	0.54
26:Z:508:LEU:C	26:Z:508:LEU:HD23	2.32	0.54
31:R:103:CYS:CA	31:R:106:ASN:HB2	2.38	0.54
31:R:109:LYS:CB	31:R:140:TYR:CD1	2.88	0.54
15:H:157:VAL:C	19:M:75:LEU:HD13	2.33	0.54
9:i:159:ILE:HG21	9:i:173:VAL:HG22	1.89	0.54
10:j:172:ASN:ND2	13:6:152:ASN:HB2	2.22	0.54
12:5:6:PHE:HB3	12:5:126:ILE:HD12	1.88	0.54
29:P:86:HIS:O	29:P:86:HIS:ND1	2.40	0.54
31:R:168:ILE:HG23	31:R:194:VAL:HG13	1.90	0.54
2:B:12:PHE:CZ	3:C:24:ALA:HA	2.43	0.53
15:H:388:ILE:HD11	35:H:501:ATP:H2	0.74	0.53
33:O:163:ILE:HD13	33:O:163:ILE:N	2.21	0.53
33:O:186:ASN:HD22	33:O:227:ILE:HD11	1.72	0.53
10:j:49:PHE:CE1	10:j:189:ILE:HD11	2.43	0.53
26:Z:377:ALA:HA	34:8:387:VAL:HA	1.90	0.53
26:Z:617:ILE:HD12	26:Z:617:ILE:N	2.22	0.53
31:R:50:VAL:O	31:R:54:ILE:HG13	2.08	0.53
34:8:136:MET:CG	34:8:225:PHE:CE1	2.87	0.53
4:D:210:ILE:HG21	4:D:222:LEU:HD12	1.91	0.53
31:R:107:GLU:OE2	31:R:111:LYS:HD3	2.03	0.53
26:Z:894:MET:HA	26:Z:965:LEU:HB2	1.91	0.53
29:P:88:GLN:O	29:P:88:GLN:HG2	2.09	0.53
31:R:60:ALA:O	31:R:99:TYR:CZ	2.62	0.53
30:Q:78:ILE:N	30:Q:79:PRO:HD2	2.24	0.52
4:D:43:GLY:HA2	4:D:210:ILE:HD13	1.91	0.52
14:7:115:ILE:HD11	14:7:144:THR:HG23	1.91	0.52
12:5:6:PHE:CB	12:5:126:ILE:CD1	2.87	0.52
4:D:2:TYR:H	4:D:16:PHE:HE2	1.58	0.52
11:4:4:ILE:HG12	11:4:45:SER:OG	2.09	0.52
12:5:6:PHE:HA	12:5:126:ILE:HD13	1.91	0.52
18:L:403:ILE:HG21	19:M:207:PHE:CE1	2.45	0.52
29:P:163:LEU:HD23	29:P:163:LEU:C	2.35	0.52
30:Q:386:PHE:CD1	30:Q:386:PHE:C	2.88	0.52
34:8:136:MET:SD	34:8:225:PHE:CE1	3.03	0.52
5:e:206:GLU:CD	5:e:206:GLU:H	2.18	0.52
6:f:71:LEU:C	6:f:71:LEU:HD22	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:78:ILE:HG21	24:X:81:SER:HA	1.88	0.51
28:S:464:ARG:HH22	31:R:404:VAL:HB	1.75	0.51
1:A:7:ILE:HG13	1:A:7:ILE:O	2.09	0.51
14:7:21:ILE:HG21	14:7:177:ILE:HG13	1.92	0.51
16:I:339:ILE:HD12	16:I:343:ARG:HH11	1.75	0.51
8:h:38:HIS:CG	8:h:39:ASP:H	2.29	0.51
27:N:50:TYR:O	27:N:58:ARG:HG3	2.11	0.51
31:R:109:LYS:HD2	31:R:140:TYR:HD1	1.76	0.51
5:E:65:HIS:C	5:E:66:ILE:HG13	2.35	0.51
26:Z:83:THR:OG1	26:Z:84:ALA:N	2.43	0.51
26:Z:617:ILE:N	26:Z:617:ILE:CD1	2.74	0.51
5:E:159:TYR:CE2	6:F:56:SER:HB2	2.46	0.50
26:Z:903:MET:SD	26:Z:906:ALA:HB3	2.52	0.50
27:N:860:LYS:C	27:N:861:TYR:CD2	2.89	0.50
9:2:3:ILE:HG12	9:2:16:ALA:HB2	1.91	0.50
31:R:109:LYS:HD2	31:R:140:TYR:CD1	2.46	0.50
9:2:160:GLN:HA	9:2:163:ILE:HD12	1.92	0.50
8:h:14:LEU:HD12	8:h:14:LEU:N	2.26	0.50
2:B:37:ILE:CD1	2:B:175:LEU:HD22	2.42	0.50
14:7:151:ALA:O	14:7:155:LEU:HG	2.12	0.50
9:i:167:LEU:HD21	13:6:35:ILE:HD11	1.93	0.50
7:G:119:HIS:CG	7:G:125:VAL:HG11	2.47	0.50
16:I:220:ILE:HD11	16:I:344:ILE:HB	1.94	0.50
17:K:422:ASP:HA	17:K:425:ASP:OD2	2.11	0.50
31:R:43:ARG:NH2	31:R:70:TYR:CE1	2.79	0.50
27:N:648:PRO:O	27:N:653:ARG:NH1	2.45	0.50
14:7:16:TYR:HE2	14:7:21:ILE:HG13	1.75	0.50
26:Z:389:PHE:O	26:Z:392:LEU:HG	2.12	0.50
7:G:47:GLU:HG3	7:G:208:PHE:CD2	2.47	0.49
8:1:126:ILE:HD12	8:1:131:SER:HB2	1.92	0.49
2:b:75:TYR:CE1	2:b:82:TYR:CD2	2.99	0.49
8:h:102:TYR:CE1	8:h:107:LYS:HA	2.47	0.49
23:T:205:ILE:HD11	23:T:233:VAL:HG21	1.94	0.49
27:N:777:ALA:CA	27:N:861:TYR:HA	2.39	0.49
30:Q:356:CYS:SG	30:Q:396:TRP:HB3	2.53	0.49
14:n:217:MET:HE2	14:n:217:MET:H	1.78	0.49
21:W:33:VAL:HG11	21:W:76:LEU:HD11	1.95	0.49
3:C:106:PRO:CD	3:C:109:ILE:HD12	2.42	0.49
15:H:388:ILE:HG13	15:H:392:HIS:CE1	2.47	0.49
32:U:197:LEU:HD22	33:O:381:GLY:HA3	1.93	0.49
1:A:12:PRO:HA	2:B:23:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1:13:ILE:HD12	8:1:151:THR:CB	2.43	0.49
27:N:104:LYS:HA	27:N:104:LYS:CE	2.35	0.49
27:N:884:PHE:CD1	27:N:884:PHE:N	2.78	0.49
15:H:75:GLY:O	15:H:80:HIS:NE2	2.44	0.49
20:J:17:SER:OG	28:S:171:TYR:CZ	2.39	0.49
1:A:242:GLN:HA	29:P:85:LYS:C	2.38	0.48
26:Z:256:LEU:HD22	26:Z:264:PHE:CE2	2.48	0.48
29:P:350:LEU:HD23	29:P:383:LEU:HD22	1.95	0.48
31:R:60:ALA:HB1	31:R:99:TYR:CD2	2.48	0.48
31:R:99:TYR:CD1	31:R:99:TYR:N	2.81	0.48
5:E:214:ILE:HD11	5:E:220:PHE:CE1	2.48	0.48
22:V:29:ILE:HB	22:V:203:TYR:CE2	2.48	0.48
31:R:51:LEU:HA	31:R:54:ILE:HD12	1.94	0.48
27:N:777:ALA:CA	27:N:861:TYR:HB3	2.41	0.48
26:Z:201:LEU:HD22	26:Z:244:ARG:CD	2.44	0.48
11:k:15:LEU:HD12	11:k:43:LEU:HD23	1.95	0.48
32:U:6:GLU:N	32:U:6:GLU:OE1	2.46	0.48
27:N:154:LEU:HD13	27:N:189:LEU:HD21	1.95	0.48
27:N:777:ALA:C	27:N:861:TYR:CA	2.86	0.48
8:1:159:LEU:HD13	8:1:173:ILE:HD12	1.95	0.48
26:Z:553:ARG:C	26:Z:553:ARG:HD2	2.39	0.48
10:j:148:MET:HE3	10:j:152:LEU:HD11	1.96	0.48
35:I:501:ATP:O1G	20:J:308:GLY:C	2.55	0.48
27:N:104:LYS:CA	27:N:104:LYS:CE	2.91	0.48
22:V:73:GLN:OE1	22:V:73:GLN:N	2.32	0.47
11:4:4:ILE:HD12	11:4:16:ALA:O	2.14	0.47
29:P:427:GLU:HA	32:U:203:LYS:HE2	1.96	0.47
10:3:37:ASN:HA	10:3:182:TRP:CE3	2.49	0.47
14:7:137:TYR:HE1	14:7:142:LEU:CD2	2.27	0.47
28:S:356:ASP:OD1	28:S:356:ASP:C	2.57	0.47
31:R:279:LEU:C	31:R:280:ILE:HG12	2.38	0.47
31:R:106:ASN:O	31:R:110:ILE:N	2.48	0.47
5:E:16:VAL:HG11	19:M:432:PHE:CE1	2.50	0.47
34:8:136:MET:HG2	34:8:225:PHE:CZ	2.49	0.47
2:B:37:ILE:HD11	2:B:175:LEU:HD22	1.96	0.47
35:I:501:ATP:O1G	20:J:308:GLY:HA2	2.15	0.47
27:N:38:GLU:H	27:N:38:GLU:CD	2.23	0.47
1:A:232:ILE:HG22	1:A:236:LEU:HD12	1.96	0.47
2:B:37:ILE:HD11	2:B:175:LEU:CD2	2.45	0.47
12:5:67:GLU:O	12:5:71:LYS:HA	2.15	0.47
11:4:130:TYR:HE2	11:4:148:TYR:CD2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:5:35:ILE:HD11	12:5:45:MET:SD	2.55	0.46
21:W:37:PHE:CD2	21:W:37:PHE:C	2.91	0.46
29:P:86:HIS:HB2	29:P:88:GLN:H	1.80	0.46
31:R:58:GLU:OE1	31:R:102:LEU:CB	2.64	0.46
9:2:84:LYS:HA	9:2:113:ILE:HD11	1.97	0.46
22:V:108:TYR:C	22:V:108:TYR:CD1	2.94	0.46
31:R:120:LEU:CD1	31:R:133:ALA:HB2	2.46	0.46
3:C:4:ARG:H	3:C:4:ARG:HG3	1.49	0.46
28:S:51:ARG:HD3	28:S:178:LEU:HD22	1.98	0.46
9:2:225:GLU:C	9:2:226:GLU:O	2.56	0.46
22:V:109:HIS:CE1	22:V:140:VAL:HG22	2.51	0.46
22:V:117:TRP:CE3	22:V:187:ALA:HB1	2.49	0.46
26:Z:894:MET:H	26:Z:903:MET:HA	1.81	0.46
6:f:64:LYS:HG3	6:f:221:PHE:CD2	2.50	0.46
14:7:119:VAL:HG23	14:7:200:ILE:HG22	1.98	0.46
20:J:275:LEU:HA	20:J:278:GLN:HE21	1.80	0.46
26:Z:743:ILE:HG12	26:Z:761:PHE:CE2	2.51	0.46
3:C:3:ARG:HD2	3:C:3:ARG:HA	1.41	0.46
6:F:151:ASN:OD1	7:G:78:ILE:CG2	2.64	0.46
34:8:116:ASN:HB3	34:8:206:LYS:HA	1.98	0.46
27:N:464:GLU:O	27:N:467:LYS:HB3	2.15	0.46
29:P:239:GLN:C	29:P:239:GLN:CD	2.83	0.46
8:h:52:THR:HG22	8:h:95:ALA:HB1	1.99	0.45
22:V:196:TYR:C	22:V:196:TYR:HD1	2.20	0.45
27:N:81:TYR:C	27:N:81:TYR:CD1	2.93	0.45
31:R:219:LEU:CD2	31:R:252:TYR:CD2	2.99	0.45
5:E:91:HIS:CE1	5:E:95:TYR:CD2	3.05	0.45
17:K:420:THR:O	17:K:424:PHE:HB2	2.16	0.45
28:S:126:LYS:HE3	28:S:129:GLU:CG	2.46	0.45
5:E:136:ILE:HD12	5:E:150:ALA:HB2	1.97	0.45
16:I:130:VAL:HG12	16:I:154:MET:HB2	1.99	0.45
8:h:30:VAL:HB	14:7:225:ILE:HD11	0.49	0.45
8:h:38:HIS:CG	8:h:39:ASP:N	2.85	0.45
6:F:189:ILE:HG21	6:F:232:TYR:CE2	2.51	0.45
17:K:67:TYR:CD1	27:N:572:LEU:HB3	2.51	0.45
26:Z:922:PRO:O	26:Z:924:LYS:HG3	2.16	0.45
6:F:200:LEU:C	6:F:202:ASP:H	2.24	0.45
26:Z:100:CYS:HB3	26:Z:155:ARG:HD2	1.98	0.45
26:Z:253:VAL:O	26:Z:253:VAL:CG1	2.64	0.45
29:P:2:SER:O	29:P:3:ARG:HB2	2.16	0.45
9:2:3:ILE:HG12	9:2:16:ALA:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:417:THR:HG22	17:K:417:THR:O	2.17	0.45
26:Z:104:ASP:OD1	26:Z:105:LYS:N	2.49	0.45
31:R:33:LEU:HD23	31:R:43:ARG:O	2.17	0.45
3:C:27:SER:HA	3:C:30:HIS:CD2	2.52	0.45
12:5:6:PHE:HB3	12:5:126:ILE:CD1	2.47	0.45
22:V:196:TYR:CD2	22:V:196:TYR:N	2.81	0.45
27:N:777:ALA:CB	27:N:861:TYR:HB3	2.47	0.45
26:Z:256:LEU:HA	26:Z:257:PRO:HD3	1.91	0.45
1:A:242:GLN:C	29:P:86:HIS:HA	2.38	0.44
10:j:62:LEU:HD21	10:j:102:TYR:CE1	2.52	0.44
26:Z:812:ILE:HG23	26:Z:813:PHE:N	2.32	0.44
27:N:70:TYR:CE2	27:N:98:VAL:HG22	2.52	0.44
27:N:775:CYS:SG	27:N:882:ILE:HG12	2.57	0.44
31:R:238:PHE:CZ	31:R:240:SER:HA	2.52	0.44
31:R:312:TYR:CD1	31:R:330:VAL:HG12	2.53	0.44
3:c:121:TYR:CE2	3:c:130:PHE:CD1	3.06	0.44
30:Q:389:VAL:O	30:Q:389:VAL:HG23	2.17	0.44
31:R:60:ALA:CB	31:R:99:TYR:HA	2.48	0.44
6:f:68:HIS:H	6:f:68:HIS:CD2	2.35	0.44
14:7:142:LEU:HD23	14:7:142:LEU:HA	1.89	0.44
21:W:18:ASN:OD1	33:O:38:TRP:N	2.50	0.44
27:N:880:ARG:NH2	27:N:881:TYR:CE2	2.85	0.44
31:R:113:LEU:HD13	31:R:137:LEU:CD2	2.48	0.44
15:H:341:ASP:OD2	35:M:501:ATP:O2A	2.36	0.44
18:L:233:LYS:HG2	18:L:245:PHE:CZ	2.53	0.44
27:N:4:THR:OG1	27:N:5:THR:N	2.51	0.44
33:O:32:PHE:CD2	33:O:40:GLN:HB3	2.52	0.44
17:K:221:MET:CE	37:K:501:ADP:H2'	2.34	0.44
17:K:418:ASP:HA	17:K:422:ASP:OD1	2.18	0.44
34:8:206:LYS:HG2	34:8:207:GLN:H	1.83	0.44
12:5:54:PHE:CD2	13:6:98:TYR:CE2	3.06	0.44
21:W:143:ASN:HD21	21:W:147:ILE:HG23	1.83	0.44
27:N:861:TYR:N	27:N:861:TYR:HB2	2.20	0.44
34:8:148:ASN:ND2	34:8:226:GLY:HA2	2.33	0.44
18:L:178:ILE:HD13	18:L:230:LEU:HD12	2.00	0.43
20:J:16:GLU:HB2	28:S:171:TYR:CZ	2.52	0.43
33:O:303:LYS:HB3	33:O:305:ILE:HG22	2.00	0.43
10:3:120:ILE:HD12	10:3:136:ILE:HG12	1.99	0.43
11:4:4:ILE:HD11	11:4:45:SER:CB	2.47	0.43
20:J:16:GLU:HA	20:J:19:ILE:HG12	2.00	0.43
28:S:170:TYR:CZ	28:S:176:LEU:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:SER:OG	17:K:420:THR:HB	2.18	0.43
6:F:71:LEU:HD23	6:F:131:LEU:HD22	2.01	0.43
13:6:5:TYR:CE2	13:6:103:PHE:CZ	3.06	0.43
20:J:277:ASN:HD22	20:J:283:GLU:HG2	1.83	0.43
8:1:38:HIS:CG	8:1:39:ASP:H	2.36	0.43
11:4:88:LEU:O	11:4:92:ILE:HG23	2.18	0.43
13:6:154:VAL:HG22	13:6:175:LEU:CD1	2.42	0.43
27:N:856:PHE:HB3	27:N:858:LYS:O	2.17	0.43
1:A:116:SER:HA	1:A:119:TYR:CD2	2.53	0.43
13:6:141:ALA:HB3	13:6:197:GLN:HE22	1.83	0.43
27:N:9:LEU:HD21	27:N:28:ILE:HA	2.00	0.43
29:P:40:LEU:O	29:P:44:LYS:HG3	2.19	0.43
3:c:2:SER:O	3:c:3:ARG:C	2.61	0.43
17:K:201:ILE:HG12	20:J:375:ILE:HA	2.01	0.43
26:Z:927:VAL:O	26:Z:927:VAL:HG13	2.18	0.43
18:L:105:ILE:HG23	19:M:128:PHE:HB3	1.99	0.43
31:R:33:LEU:O	31:R:70:TYR:CD1	2.72	0.43
1:A:167:GLN:CD	1:A:167:GLN:H	2.27	0.43
10:3:50:LEU:HD21	10:3:52:ILE:HD11	2.00	0.43
10:j:12:VAL:HG23	10:j:137:VAL:HG12	2.00	0.43
26:Z:120:SER:HA	26:Z:159:LEU:HD21	2.01	0.43
15:H:424:THR:HA	16:I:213:ILE:HD11	2.01	0.42
19:M:243:PHE:CE1	19:M:279:PHE:HB2	2.54	0.42
21:W:133:LYS:HE3	21:W:163:ASN:HB2	2.00	0.42
26:Z:931:GLN:OE1	26:Z:931:GLN:N	2.44	0.42
33:O:213:LEU:O	33:O:217:LEU:HD13	2.19	0.42
7:g:83:HIS:CD2	7:g:83:HIS:C	2.97	0.42
14:7:152:ASN:H	14:7:153:PRO:CD	2.30	0.42
15:H:75:GLY:O	15:H:80:HIS:CG	2.68	0.42
16:I:268:PHE:CE1	16:I:312:GLN:HB3	2.54	0.42
26:Z:212:LEU:HD23	26:Z:220:ALA:HB1	2.01	0.42
31:R:105:LYS:C	31:R:140:TYR:OH	2.62	0.42
19:M:216:LYS:H	19:M:344:ASP:HB3	1.84	0.42
8:h:135:TYR:HB3	8:1:165:TRP:CE2	2.54	0.42
8:1:5:ALA:C	8:1:6:VAL:HG23	2.45	0.42
8:1:173:ILE:HG12	8:1:193:TYR:CZ	2.54	0.42
18:L:361:PHE:CZ	18:L:415:LEU:HD21	2.55	0.42
26:Z:508:LEU:HD23	26:Z:508:LEU:O	2.19	0.42
2:B:94:HIS:CD2	2:B:98:LYS:HD2	2.54	0.42
24:X:89:LEU:HD12	24:X:89:LEU:N	2.34	0.42
27:N:788:TYR:N	27:N:788:TYR:CD1	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:78:ALA:O	8:h:81:VAL:HG22	2.20	0.42
1:A:242:GLN:CA	29:P:86:HIS:N	2.82	0.42
11:4:175:ASP:CG	11:4:177:LYS:H	2.28	0.42
13:6:86:ILE:CG1	13:6:114:LEU:O	2.62	0.42
15:H:144:LYS:HA	15:H:158:GLY:HA2	2.01	0.42
23:T:11:LEU:HD22	23:T:30:ILE:HG21	2.01	0.42
23:T:82:PHE:O	23:T:85:LEU:HB3	2.19	0.42
26:Z:377:ALA:H	34:8:388:MET:H	1.68	0.42
31:R:381:ILE:CG1	31:R:388:VAL:HG22	2.50	0.42
27:N:517:LEU:HD23	27:N:517:LEU:HA	1.95	0.42
31:R:61:PRO:HD3	31:R:102:LEU:CD1	2.47	0.42
6:F:71:LEU:HD22	6:F:71:LEU:C	2.45	0.42
14:7:21:ILE:HD12	14:7:173:ALA:HB1	2.01	0.42
15:H:157:VAL:O	19:M:75:LEU:HD13	2.19	0.42
20:J:16:GLU:C	28:S:171:TYR:CE1	2.96	0.42
22:V:45:VAL:HG21	22:V:144:ILE:CG2	2.49	0.42
26:Z:738:TYR:CD1	26:Z:738:TYR:C	2.97	0.42
29:P:51:ASP:OD2	29:P:92:SER:OG	2.38	0.42
2:B:1:MET:HE2	2:B:1:MET:HA	2.01	0.42
11:4:4:ILE:CD1	11:4:45:SER:HB2	2.50	0.42
13:6:48:ASP:C	13:6:50:ILE:HD12	2.45	0.42
16:I:220:ILE:HD12	16:I:220:ILE:N	2.35	0.42
17:K:113:THR:HG21	18:L:126:ARG:H	1.85	0.42
30:Q:50:ARG:HE	30:Q:51:ARG:N	2.17	0.42
12:l:54:PHE:CE2	12:l:55:TRP:CZ2	3.07	0.41
26:Z:201:LEU:HD22	26:Z:244:ARG:HD3	2.01	0.41
26:Z:573:LEU:HD23	26:Z:573:LEU:C	2.45	0.41
27:N:7:ALA:HB3	27:N:8:PRO:HD3	2.01	0.41
27:N:855:GLU:C	27:N:857:TYR:N	2.76	0.41
27:N:860:LYS:O	27:N:861:TYR:CG	2.73	0.41
28:S:51:ARG:CG	28:S:178:LEU:HD13	2.50	0.41
31:R:113:LEU:H	31:R:113:LEU:HG	1.74	0.41
8:h:59:VAL:HG11	8:h:82:PHE:CE2	2.56	0.41
10:3:50:LEU:CD2	10:3:52:ILE:HD11	2.50	0.41
11:4:120:ASP:CA	11:4:133:HIS:CE1	3.03	0.41
31:R:33:LEU:O	31:R:70:TYR:CE1	2.73	0.41
20:J:17:SER:OG	28:S:171:TYR:CD1	2.50	0.41
27:N:556:ALA:HB1	27:N:593:PHE:HB2	2.03	0.41
18:L:173:PHE:O	18:L:174:GLU:HB2	2.21	0.41
32:U:1:MET:SD	32:U:115:GLN:HA	2.60	0.41
34:8:367:LYS:HG3	34:8:408:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:771:HIS:HD1	26:Z:912:PHE:HE2	1.67	0.41
27:N:861:TYR:OH	27:N:877:GLN:HB3	2.20	0.41
30:Q:44:ALA:O	30:Q:53:GLU:HG2	2.21	0.41
1:a:95:PHE:HE2	1:a:101:TYR:CE2	2.39	0.41
7:g:8:ASN:HA	7:g:17:ASN:OD1	2.21	0.41
7:g:31:THR:HG22	7:g:203:ASN:ND2	2.34	0.41
23:T:86:LYS:N	23:T:87:PRO:HD2	2.35	0.41
23:T:86:LYS:HB2	23:T:87:PRO:CD	2.51	0.41
26:Z:428:TRP:O	26:Z:428:TRP:CG	2.71	0.41
29:P:395:ARG:N	29:P:396:PRO:HD2	2.36	0.41
2:b:190:HIS:CE1	2:b:246:ARG:HD2	2.56	0.41
9:i:127:LEU:HD12	9:i:128:GLY:H	1.86	0.41
3:C:3:ARG:HG3	3:C:5:TYR:CZ	2.56	0.41
10:3:71:ASN:HD22	10:3:71:ASN:HA	1.84	0.41
28:S:51:ARG:HA	28:S:54:TRP:CE3	2.56	0.41
28:S:51:ARG:HG3	28:S:178:LEU:HD13	2.03	0.41
31:R:58:GLU:OE1	31:R:102:LEU:CA	2.69	0.41
31:R:60:ALA:HB1	31:R:99:TYR:CG	2.55	0.41
14:n:93:PHE:CE1	14:n:130:VAL:HB	2.56	0.41
7:G:63:ILE:HD13	7:G:73:VAL:CG2	2.51	0.41
28:S:201:ILE:HG13	28:S:202:ASN:N	2.35	0.41
30:Q:434:TYR:CD1	30:Q:434:TYR:N	2.88	0.41
31:R:117:ILE:CD1	31:R:137:LEU:HD12	2.51	0.41
1:a:45:ILE:HG23	1:a:216:VAL:HG22	2.03	0.41
7:g:205:GLU:CD	7:g:205:GLU:H	2.28	0.41
11:4:129:PRO:HB2	11:4:130:TYR:CD2	2.55	0.41
14:7:152:ASN:N	14:7:153:PRO:HD2	2.34	0.41
15:H:102:CYS:SG	15:H:105:ILE:CD1	3.09	0.41
18:L:67:HIS:HE1	19:M:41:ILE:HG13	1.86	0.41
22:V:188:LEU:O	22:V:188:LEU:HG	2.21	0.41
23:T:19:ASP:OD1	23:T:19:ASP:C	2.62	0.41
23:T:55:LEU:HG	23:T:59:LYS:HD2	2.03	0.41
27:N:43:LEU:N	27:N:44:PRO:HD2	2.36	0.41
32:U:28:LYS:H	32:U:31:LYS:HB2	1.85	0.41
3:C:159:TRP:CE2	3:C:162:ILE:HD13	2.56	0.41
32:U:197:LEU:C	32:U:197:LEU:HD23	2.46	0.41
1:a:34:LEU:HD23	1:a:34:LEU:C	2.46	0.40
15:H:157:VAL:HG23	15:H:158:GLY:N	2.37	0.40
24:X:48:PHE:CZ	24:X:87:PHE:CE2	3.09	0.40
28:S:167:LEU:O	28:S:170:TYR:CD1	2.74	0.40
4:d:66:ASP:CG	4:d:67:SER:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4:ARG:HB3	3:C:19:TYR:HE2	1.87	0.40
13:6:108:HIS:CD2	13:6:108:HIS:C	2.99	0.40
14:7:127:LEU:HG	14:7:142:LEU:HD12	2.04	0.40
26:Z:87:LYS:N	26:Z:88:PRO:HD2	2.36	0.40
27:N:777:ALA:N	27:N:861:TYR:O	2.52	0.40
33:O:26:PHE:HA	33:O:29:PHE:CD2	2.56	0.40
7:g:134:PHE:CD1	7:g:134:PHE:N	2.89	0.40
26:Z:85:VAL:O	26:Z:85:VAL:HG12	2.20	0.40
15:H:76:LEU:O	15:H:78:PRO:N	2.55	0.40
26:Z:518:LEU:C	26:Z:520:ILE:H	2.30	0.40
26:Z:632:GLU:HG2	27:N:803:VAL:HG11	2.02	0.40
13:m:172:LEU:HD12	13:m:172:LEU:H	1.86	0.40
14:7:137:TYR:HE1	14:7:142:LEU:HD22	1.86	0.40
15:H:76:LEU:HD23	15:H:76:LEU:HA	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/252 (95%)	227 (95%)	11 (5%)	1 (0%)	30	67
1	a	239/252 (95%)	231 (97%)	8 (3%)	0	100	100
2	B	248/250 (99%)	236 (95%)	11 (4%)	1 (0%)	30	67
2	b	248/250 (99%)	234 (94%)	11 (4%)	3 (1%)	10	44
3	C	242/258 (94%)	228 (94%)	11 (4%)	3 (1%)	10	44
3	c	242/258 (94%)	227 (94%)	12 (5%)	3 (1%)	10	44
4	D	238/254 (94%)	222 (93%)	12 (5%)	4 (2%)	7	36
4	d	238/254 (94%)	219 (92%)	16 (7%)	3 (1%)	9	42
5	E	240/260 (92%)	227 (95%)	11 (5%)	2 (1%)	16	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	240/260 (92%)	228 (95%)	10 (4%)	2 (1%)	16	54
6	F	231/234 (99%)	220 (95%)	9 (4%)	2 (1%)	14	51
6	f	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
7	G	241/288 (84%)	228 (95%)	12 (5%)	1 (0%)	30	67
7	g	241/288 (84%)	230 (95%)	10 (4%)	1 (0%)	30	67
8	1	194/215 (90%)	184 (95%)	8 (4%)	2 (1%)	12	48
8	h	194/215 (90%)	189 (97%)	5 (3%)	0	100	100
9	2	224/261 (86%)	213 (95%)	9 (4%)	2 (1%)	14	51
9	i	224/261 (86%)	214 (96%)	10 (4%)	0	100	100
10	3	202/205 (98%)	190 (94%)	10 (5%)	2 (1%)	12	48
10	j	202/205 (98%)	187 (93%)	12 (6%)	3 (2%)	8	40
11	4	193/198 (98%)	187 (97%)	6 (3%)	0	100	100
11	k	193/198 (98%)	188 (97%)	4 (2%)	1 (0%)	24	63
12	5	210/287 (73%)	201 (96%)	9 (4%)	0	100	100
12	l	210/287 (73%)	202 (96%)	7 (3%)	1 (0%)	24	63
13	6	220/241 (91%)	205 (93%)	13 (6%)	2 (1%)	14	51
13	m	220/241 (91%)	203 (92%)	17 (8%)	0	100	100
14	7	227/266 (85%)	209 (92%)	16 (7%)	2 (1%)	14	51
14	n	230/266 (86%)	214 (93%)	14 (6%)	2 (1%)	14	51
15	H	376/467 (80%)	340 (90%)	23 (6%)	13 (4%)	3	20
16	I	383/437 (88%)	346 (90%)	27 (7%)	10 (3%)	4	25
17	K	387/428 (90%)	351 (91%)	24 (6%)	12 (3%)	3	22
18	L	386/437 (88%)	353 (92%)	26 (7%)	7 (2%)	6	34
19	M	377/434 (87%)	350 (93%)	19 (5%)	8 (2%)	5	30
20	J	391/405 (96%)	360 (92%)	21 (5%)	10 (3%)	4	25
21	W	195/268 (73%)	180 (92%)	11 (6%)	4 (2%)	5	30
22	V	287/306 (94%)	263 (92%)	20 (7%)	4 (1%)	9	40
23	T	264/274 (96%)	240 (91%)	19 (7%)	5 (2%)	6	32
24	X	125/156 (80%)	101 (81%)	15 (12%)	9 (7%)	1	11
25	Y	47/89 (53%)	44 (94%)	1 (2%)	2 (4%)	2	17
26	Z	902/993 (91%)	824 (91%)	52 (6%)	26 (3%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	N	886/945 (94%)	850 (96%)	25 (3%)	11 (1%)	10	44
28	S	473/523 (90%)	435 (92%)	18 (4%)	20 (4%)	2	17
29	P	438/445 (98%)	417 (95%)	13 (3%)	8 (2%)	6	34
30	Q	432/434 (100%)	387 (90%)	28 (6%)	17 (4%)	2	19
31	R	377/429 (88%)	355 (94%)	18 (5%)	4 (1%)	11	46
32	U	296/338 (88%)	284 (96%)	9 (3%)	3 (1%)	12	48
33	O	386/393 (98%)	368 (95%)	16 (4%)	2 (0%)	24	63
34	8	393/499 (79%)	366 (93%)	21 (5%)	6 (2%)	8	40
All	All	14100/15638 (90%)	13178 (94%)	698 (5%)	224 (2%)	10	38

All (224) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	e	129	PRO
10	j	182	TRP
5	E	128	ARG
5	E	129	PRO
6	F	162	ALA
15	H	77	ALA
16	I	79	SER
16	I	115	ASP
16	I	224	ALA
16	I	330	LYS
17	K	244	HIS
17	K	334	LEU
18	L	174	GLU
19	M	229	THR
19	M	230	LEU
19	M	296	SER
19	M	345	ARG
20	J	72	VAL
20	J	145	SER
23	T	92	ASN
23	T	234	TYR
25	Y	31	GLU
26	Z	19	SER
26	Z	83	THR
26	Z	939	ALA
27	N	856	PHE

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Mol	Chain	Res	Type
27	N	857	TYR
27	N	862	SER
28	S	44	THR
28	S	47	THR
28	S	102	SER
28	S	150	LYS
28	S	174	ARG
29	P	110	LEU
29	P	397	ALA
30	Q	68	MET
30	Q	170	ASP
30	Q	354	PHE
30	Q	387	TYR
31	R	245	SER
31	R	280	ILE
33	O	199	LEU
2	b	20	GLN
2	b	200	VAL
4	d	52	LEU
4	D	203	THR
15	H	78	PRO
15	H	94	GLU
15	H	280	VAL
15	H	344	ASP
15	H	434	ARG
15	H	456	LYS
17	K	127	ASP
17	K	232	ALA
17	K	274	VAL
17	K	314	VAL
17	K	398	ASN
18	L	101	ILE
18	L	188	GLU
20	J	117	SER
20	J	353	CYS
22	V	143	PRO
23	T	97	SER
23	T	138	ASP
24	X	29	VAL
24	X	38	ASN
24	X	44	GLY
24	X	59	ARG

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Mol	Chain	Res	Type
24	X	110	PRO
26	Z	8	LYS
26	Z	237	VAL
26	Z	825	ALA
26	Z	887	GLY
27	N	666	GLN
27	N	895	LYS
28	S	132	ALA
29	P	130	ILE
29	P	327	LEU
29	P	328	ALA
30	Q	40	ALA
30	Q	44	ALA
30	Q	286	TYR
30	Q	309	ARG
34	8	383	SER
2	b	19	GLY
10	j	156	ASN
10	j	191	LYS
14	n	81	ALA
1	A	187	GLU
4	D	29	THR
4	D	102	VAL
6	F	4	ASN
8	1	107	LYS
9	2	171	SER
13	6	130	SER
13	6	200	ASP
16	I	136	VAL
17	K	248	GLY
17	K	344	ARG
17	K	419	ASN
18	L	291	PHE
18	L	343	LEU
20	J	207	ASP
21	W	179	ARG
22	V	61	TYR
22	V	215	ASN
22	V	259	LYS
24	X	42	GLU
24	X	114	LEU
26	Z	82	MET

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Mol	Chain	Res	Type
26	Z	84	ALA
26	Z	174	GLU
26	Z	309	GLN
26	Z	463	HIS
26	Z	728	LYS
26	Z	913	ILE
27	N	739	PHE
28	S	69	LEU
28	S	83	PRO
28	S	97	THR
28	S	117	SER
28	S	153	GLU
29	P	79	LEU
30	Q	45	SER
30	Q	51	ARG
30	Q	75	ARG
30	Q	355	GLU
31	R	102	LEU
32	U	30	ASN
34	8	205	TYR
34	8	385	GLU
3	c	53	SER
3	c	205	LEU
3	c	206	THR
4	d	203	THR
5	e	27	SER
12	l	95	LEU
2	B	225	THR
3	C	6	ASP
3	C	183	MET
4	D	10	SER
7	G	69	HIS
15	H	415	THR
16	I	175	LYS
16	I	339	ILE
16	I	411	VAL
17	K	104	ASP
17	K	421	VAL
18	L	221	TYR
19	M	151	ASP
20	J	152	GLY
20	J	155	LYS

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Mol	Chain	Res	Type
20	J	309	ARG
21	W	3	LEU
21	W	136	ASN
21	W	144	PHE
23	T	96	LEU
24	X	22	ARG
25	Y	69	VAL
26	Z	70	ALA
26	Z	76	LYS
26	Z	142	ASP
26	Z	429	ASN
26	Z	444	GLU
26	Z	926	ASN
26	Z	963	ALA
27	N	395	ALA
27	N	790	GLU
28	S	101	LYS
28	S	126	LYS
28	S	263	ASP
30	Q	18	LYS
30	Q	46	VAL
30	Q	384	LYS
31	R	58	GLU
34	8	206	LYS
34	8	316	ARG
34	8	386	ASN
7	g	221	ASN
11	k	178	GLY
14	n	10	SER
3	C	220	ASN
9	2	193	PRO
10	3	156	ASN
14	7	77	ASP
14	7	83	ALA
15	H	190	ARG
15	H	203	LYS
15	H	314	VAL
16	I	340	ARG
19	M	124	ARG
19	M	186	LEU
20	J	335	MET
24	X	28	PRO

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Mol	Chain	Res	Type
26	Z	789	GLN
26	Z	940	GLY
27	N	631	GLY
28	S	65	ASN
28	S	118	PHE
28	S	152	LEU
28	S	198	SER
29	P	3	ARG
29	P	92	SER
30	Q	110	SER
30	Q	253	ASN
32	U	146	ASP
33	O	243	VAL
8	1	172	VAL
15	H	152	ILE
18	L	179	THR
19	M	172	VAL
26	Z	366	LYS
27	N	176	GLN
32	U	5	HIS
4	d	36	GLY
10	3	183	GLY
16	I	176	SER
20	J	308	GLY
15	H	412	PRO
26	Z	233	LEU
26	Z	85	VAL
27	N	432	GLY
28	S	301	PRO
28	S	96	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	206/210 (98%)	201 (98%)	5 (2%)	43 64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	206/210 (98%)	194 (94%)	12 (6%)	18	40
2	B	209/209 (100%)	202 (97%)	7 (3%)	33	55
2	b	209/209 (100%)	198 (95%)	11 (5%)	20	41
3	C	203/216 (94%)	194 (96%)	9 (4%)	25	47
3	c	203/216 (94%)	195 (96%)	8 (4%)	28	49
4	D	212/226 (94%)	204 (96%)	8 (4%)	29	50
4	d	212/226 (94%)	204 (96%)	8 (4%)	29	50
5	E	198/215 (92%)	190 (96%)	8 (4%)	28	49
5	e	198/215 (92%)	189 (96%)	9 (4%)	24	46
6	F	192/193 (100%)	188 (98%)	4 (2%)	47	65
6	f	190/193 (98%)	182 (96%)	8 (4%)	26	48
7	G	201/239 (84%)	196 (98%)	5 (2%)	42	63
7	g	201/239 (84%)	200 (100%)	1 (0%)	81	83
8	1	162/178 (91%)	161 (99%)	1 (1%)	78	83
8	h	162/178 (91%)	160 (99%)	2 (1%)	63	75
9	2	185/214 (86%)	185 (100%)	0	100	100
9	i	185/214 (86%)	179 (97%)	6 (3%)	34	55
10	3	172/173 (99%)	166 (96%)	6 (4%)	32	53
10	j	172/173 (99%)	169 (98%)	3 (2%)	53	69
11	4	173/175 (99%)	168 (97%)	5 (3%)	37	58
11	k	173/175 (99%)	168 (97%)	5 (3%)	37	58
12	5	169/235 (72%)	164 (97%)	5 (3%)	36	57
12	l	169/235 (72%)	163 (96%)	6 (4%)	31	52
13	6	185/201 (92%)	181 (98%)	4 (2%)	45	64
13	m	185/201 (92%)	182 (98%)	3 (2%)	55	70
14	7	195/224 (87%)	188 (96%)	7 (4%)	31	52
14	n	198/224 (88%)	194 (98%)	4 (2%)	48	66
15	H	320/399 (80%)	310 (97%)	10 (3%)	35	56
16	I	342/385 (89%)	325 (95%)	17 (5%)	22	43
17	K	342/374 (91%)	334 (98%)	8 (2%)	44	64
18	L	332/377 (88%)	325 (98%)	7 (2%)	47	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	M	329/375 (88%)	323 (98%)	6 (2%)	51	68
20	J	342/352 (97%)	326 (95%)	16 (5%)	23	45
21	W	171/230 (74%)	169 (99%)	2 (1%)	63	75
22	V	253/268 (94%)	251 (99%)	2 (1%)	73	80
23	T	249/256 (97%)	245 (98%)	4 (2%)	55	70
24	X	116/144 (81%)	111 (96%)	5 (4%)	26	47
25	Y	50/81 (62%)	49 (98%)	1 (2%)	48	66
26	Z	773/850 (91%)	767 (99%)	6 (1%)	73	80
27	N	745/797 (94%)	741 (100%)	4 (0%)	81	83
28	S	447/489 (91%)	439 (98%)	8 (2%)	51	68
29	P	412/415 (99%)	409 (99%)	3 (1%)	76	81
30	Q	391/391 (100%)	382 (98%)	9 (2%)	44	64
31	R	333/379 (88%)	325 (98%)	8 (2%)	43	64
32	U	271/308 (88%)	270 (100%)	1 (0%)	84	84
33	O	363/368 (99%)	361 (99%)	2 (1%)	78	83
34	8	359/449 (80%)	351 (98%)	8 (2%)	45	64
All	All	12265/13503 (91%)	11978 (98%)	287 (2%)	44	64

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	10	PHE
1	a	16	LEU
1	a	96	ARG
1	a	114	ASN
1	a	135	VAL
1	a	150	PRO
1	a	160	THR
1	a	162	THR
1	a	176	HIS
1	a	200	HIS
1	a	231	ASN
1	a	235	ARG
2	b	12	PHE
2	b	23	TYR
2	b	33	THR

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Mol	Chain	Res	Type
2	b	35	LEU
2	b	80	PRO
2	b	86	VAL
2	b	92	VAL
2	b	98	LYS
2	b	181	ASP
2	b	204	PHE
2	b	233	PRO
3	c	18	LEU
3	c	48	GLU
3	c	65	LEU
3	c	80	THR
3	c	113	ARG
3	c	141	ASP
3	c	157	THR
3	c	210	LEU
4	d	4	ARG
4	d	53	GLN
4	d	63	SER
4	d	76	LEU
4	d	92	GLN
4	d	200	VAL
4	d	213	VAL
4	d	222	LEU
5	e	16	VAL
5	e	17	GLU
5	e	70	MET
5	e	80	MET
5	e	94	TYR
5	e	128	ARG
5	e	187	GLU
5	e	201	GLU
5	e	215	THR
6	f	15	THR
6	f	44	VAL
6	f	66	ASP
6	f	71	LEU
6	f	73	LEU
6	f	178	PHE
6	f	188	LEU
6	f	204	SER
7	g	214	TRP

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Mol	Chain	Res	Type
8	h	31	THR
8	h	118	SER
9	i	14	ILE
9	i	179	GLU
9	i	195	VAL
9	i	204	LYS
9	i	215	GLU
9	i	218	VAL
10	j	12	VAL
10	j	88	GLN
10	j	158	GLU
11	k	4	ILE
11	k	7	ILE
11	k	37	GLN
11	k	40	PRO
11	k	118	GLN
12	l	4	LEU
12	l	8	PHE
12	l	34	VAL
12	l	86	LEU
12	l	90	TYR
12	l	129	VAL
13	m	18	GLU
13	m	19	ASP
13	m	35	ILE
14	n	9	THR
14	n	102	GLN
14	n	127	LEU
14	n	132	LEU
1	A	19	VAL
1	A	139	GLU
1	A	143	PRO
1	A	221	LYS
1	A	223	LYS
2	B	44	VAL
2	B	65	SER
2	B	84	VAL
2	B	109	LEU
2	B	119	GLN
2	B	179	TRP
2	B	186	GLU
3	C	3	ARG

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Mol	Chain	Res	Type
3	C	4	ARG
3	C	22	GLU
3	C	33	THR
3	C	63	GLU
3	C	88	ASN
3	C	194	LYS
3	C	231	PRO
3	C	235	LYS
4	D	40	VAL
4	D	50	LEU
4	D	103	THR
4	D	107	LEU
4	D	147	GLN
4	D	161	THR
4	D	220	VAL
4	D	229	GLN
5	E	1	ASP
5	E	9	PRO
5	E	63	ASP
5	E	104	LEU
5	E	110	ASP
5	E	125	LEU
5	E	201	GLU
5	E	224	ASP
6	F	71	LEU
6	F	152	VAL
6	F	165	GLN
6	F	188	LEU
7	G	11	PHE
7	G	64	GLN
7	G	127	PRO
7	G	175	LEU
7	G	220	THR
8	1	74	SER
10	3	12	VAL
10	3	25	ASP
10	3	85	THR
10	3	135	PHE
10	3	146	PHE
10	3	165	THR
11	4	13	VAL
11	4	29	LYS

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Mol	Chain	Res	Type
11	4	68	SER
11	4	126	VAL
11	4	191	GLN
12	5	1	THR
12	5	4	LEU
12	5	72	GLU
12	5	106	ARG
12	5	181	THR
13	6	3	ASN
13	6	107	VAL
13	6	207	VAL
13	6	222	ASP
14	7	47	ASP
14	7	49	THR
14	7	104	ARG
14	7	140	PRO
14	7	187	ARG
14	7	188	ASP
14	7	221	PHE
15	H	93	GLU
15	H	94	GLU
15	H	103	THR
15	H	172	MET
15	H	191	ILE
15	H	208	TYR
15	H	267	THR
15	H	300	THR
15	H	367	ARG
15	H	419	LEU
16	I	69	LEU
16	I	80	GLU
16	I	85	PHE
16	I	86	GLU
16	I	105	SER
16	I	123	PRO
16	I	155	SER
16	I	206	GLU
16	I	216	PRO
16	I	230	THR
16	I	261	PRO
16	I	310	LEU
16	I	324	VAL

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Mol	Chain	Res	Type
16	I	339	ILE
16	I	341	PRO
16	I	379	THR
16	I	416	PHE
17	K	121	ARG
17	K	159	SER
17	K	281	ARG
17	K	323	THR
17	K	324	LEU
17	K	330	ARG
17	K	360	MET
17	K	415	VAL
18	L	174	GLU
18	L	177	GLU
18	L	192	GLU
18	L	228	LYS
18	L	243	PHE
18	L	309	LEU
18	L	426	LYS
19	M	83	VAL
19	M	315	PHE
19	M	340	SER
19	M	343	LEU
19	M	403	LEU
19	M	431	SER
20	J	37	LYS
20	J	62	LEU
20	J	84	VAL
20	J	131	ASP
20	J	153	LEU
20	J	170	HIS
20	J	218	LEU
20	J	230	VAL
20	J	240	HIS
20	J	243	SER
20	J	288	ILE
20	J	309	ARG
20	J	312	ARG
20	J	343	LEU
20	J	354	SER
20	J	403	LEU
21	W	59	PRO

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Mol	Chain	Res	Type
21	W	116	SER
22	V	29	ILE
22	V	156	PHE
23	T	163	LEU
23	T	197	TYR
23	T	213	ASN
23	T	257	THR
24	X	17	TYR
24	X	53	THR
24	X	81	SER
24	X	111	LEU
24	X	115	SER
25	Y	32	ASP
26	Z	1	MET
26	Z	185	ASP
26	Z	354	PRO
26	Z	367	SER
26	Z	473	LEU
26	Z	577	GLN
27	N	343	THR
27	N	509	GLN
27	N	603	PRO
27	N	739	PHE
28	S	46	LEU
28	S	72	GLU
28	S	81	LEU
28	S	82	TYR
28	S	103	SER
28	S	207	ASN
28	S	247	VAL
28	S	401	LYS
29	P	277	GLN
29	P	285	GLN
29	P	362	LEU
30	Q	2	SER
30	Q	29	SER
30	Q	50	ARG
30	Q	94	VAL
30	Q	111	LEU
30	Q	207	SER
30	Q	302	VAL
30	Q	318	LEU

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Mol	Chain	Res	Type
30	Q	422	VAL
31	R	70	TYR
31	R	99	TYR
31	R	109	LYS
31	R	113	LEU
31	R	117	ILE
31	R	122	GLU
31	R	137	LEU
31	R	199	GLU
32	U	115	GLN
33	O	127	LEU
33	O	163	ILE
34	8	128	TYR
34	8	183	VAL
34	8	201	GLN
34	8	284	ILE
34	8	335	PHE
34	8	405	LYS
34	8	415	HIS
34	8	433	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (304) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	6	HIS
1	a	121	GLN
1	a	167	GLN
1	a	200	HIS
2	b	94	HIS
2	b	180	ASN
2	b	190	HIS
3	c	88	ASN
3	c	93	HIS
3	c	102	ASN
3	c	123	GLN
3	c	155	ASN
4	d	77	ASN
4	d	92	GLN
4	d	160	GLN
4	d	202	GLN
4	d	207	ASN
4	d	228	ASN

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Mol	Chain	Res	Type
4	d	239	GLN
5	e	65	HIS
5	e	139	HIS
5	e	149	HIS
5	e	208	ASN
6	f	40	ASN
6	f	59	GLN
6	f	68	HIS
6	f	92	ASN
6	f	109	HIS
6	f	116	GLN
6	f	209	ASN
7	g	69	HIS
7	g	83	HIS
7	g	114	GLN
7	g	117	GLN
7	g	119	HIS
7	g	143	HIS
7	g	203	ASN
7	g	240	GLN
8	h	38	HIS
8	h	53	GLN
8	h	62	HIS
8	h	106	ASN
8	h	157	HIS
9	i	10	ASN
9	i	57	GLN
9	i	81	GLN
9	i	91	GLN
9	i	114	HIS
9	i	172	ASN
9	i	189	ASN
10	j	31	GLN
10	j	71	ASN
10	j	172	ASN
10	j	203	GLN
11	k	86	GLN
11	k	99	GLN
11	k	118	GLN
12	l	29	GLN
12	l	62	GLN
12	l	66	HIS

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Mol	Chain	Res	Type
12	l	85	ASN
12	l	89	GLN
12	l	179	HIS
12	l	188	HIS
12	l	191	HIS
13	m	8	ASN
13	m	55	ASN
13	m	76	HIS
13	m	79	HIS
13	m	87	ASN
13	m	152	ASN
13	m	155	ASN
13	m	158	ASN
13	m	195	HIS
14	n	62	HIS
14	n	74	ASN
14	n	112	ASN
14	n	122	ASN
14	n	194	ASN
14	n	213	GLN
1	A	18	GLN
1	A	27	ASN
1	A	30	ASN
1	A	75	ASN
1	A	83	ASN
1	A	114	ASN
2	B	94	HIS
2	B	139	HIS
2	B	180	ASN
2	B	190	HIS
2	B	205	ASN
3	C	124	HIS
3	C	155	ASN
3	C	167	ASN
4	D	38	ASN
4	D	68	HIS
4	D	115	GLN
4	D	116	GLN
4	D	120	GLN
4	D	176	ASN
5	E	65	HIS
5	E	83	HIS

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Mol	Chain	Res	Type
5	E	91	HIS
5	E	149	HIS
5	E	160	ASN
5	E	180	HIS
6	F	20	GLN
6	F	59	GLN
6	F	92	ASN
6	F	142	HIS
6	F	184	ASN
7	G	83	HIS
7	G	123	ASN
7	G	203	ASN
7	G	224	HIS
7	G	244	ASN
8	1	161	GLN
9	2	30	ASN
9	2	62	ASN
9	2	66	HIS
9	2	81	GLN
9	2	189	ASN
9	2	224	GLN
10	3	7	ASN
10	3	31	GLN
10	3	47	HIS
10	3	71	ASN
10	3	88	GLN
10	3	112	ASN
10	3	168	GLN
11	4	61	GLN
11	4	78	GLN
11	4	86	GLN
11	4	118	GLN
11	4	133	HIS
11	4	146	HIS
11	4	147	HIS
12	5	38	ASN
12	5	89	GLN
12	5	191	HIS
12	5	208	ASN
12	5	209	ASN
13	6	79	HIS
13	6	108	HIS

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Mol	Chain	Res	Type
13	6	135	GLN
13	6	152	ASN
13	6	153	GLN
13	6	159	GLN
13	6	165	ASN
13	6	197	GLN
14	7	18	ASN
14	7	48	ASN
14	7	62	HIS
14	7	194	ASN
14	7	203	ASN
14	7	213	GLN
15	H	80	HIS
15	H	98	GLN
15	H	182	ASN
15	H	217	GLN
15	H	392	HIS
16	I	68	HIS
16	I	95	GLN
16	I	117	HIS
16	I	150	HIS
16	I	204	HIS
16	I	239	GLN
16	I	352	ASN
16	I	393	GLN
17	K	64	GLN
17	K	83	GLN
17	K	98	GLN
17	K	106	ASN
17	K	140	HIS
17	K	164	ASN
17	K	264	ASN
17	K	285	GLN
17	K	308	GLN
18	L	50	GLN
18	L	67	HIS
18	L	80	ASN
18	L	208	GLN
18	L	302	GLN
18	L	435	GLN
19	M	31	GLN
19	M	53	HIS

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Mol	Chain	Res	Type
19	M	81	ASN
19	M	143	ASN
19	M	189	GLN
19	M	240	ASN
19	M	250	GLN
19	M	359	GLN
19	M	405	ASN
20	J	28	GLN
20	J	181	GLN
20	J	277	ASN
20	J	278	GLN
20	J	342	ASN
21	W	42	ASN
21	W	77	HIS
21	W	95	GLN
21	W	100	HIS
21	W	102	GLN
21	W	103	ASN
21	W	135	ASN
21	W	143	ASN
22	V	111	HIS
22	V	172	GLN
22	V	204	HIS
22	V	222	GLN
23	T	71	GLN
23	T	118	ASN
23	T	135	ASN
23	T	170	ASN
23	T	225	ASN
23	T	236	ASN
23	T	251	HIS
24	X	18	ASN
26	Z	132	HIS
26	Z	166	ASN
26	Z	214	HIS
26	Z	235	GLN
26	Z	275	GLN
26	Z	309	GLN
26	Z	475	GLN
26	Z	480	ASN
26	Z	532	HIS
26	Z	593	HIS

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Mol	Chain	Res	Type
26	Z	618	GLN
26	Z	833	GLN
26	Z	897	HIS
27	N	29	ASN
27	N	96	GLN
27	N	122	GLN
27	N	216	ASN
27	N	233	ASN
27	N	288	ASN
27	N	315	ASN
27	N	430	ASN
27	N	506	GLN
27	N	510	HIS
27	N	580	ASN
27	N	613	HIS
27	N	654	GLN
27	N	679	ASN
27	N	703	GLN
27	N	707	ASN
27	N	859	ASN
27	N	877	GLN
27	N	878	GLN
27	N	900	ASN
28	S	30	GLN
28	S	65	ASN
28	S	191	HIS
28	S	225	HIS
28	S	321	GLN
29	P	242	GLN
29	P	282	HIS
29	P	334	ASN
29	P	337	HIS
29	P	348	HIS
30	Q	19	GLN
30	Q	37	GLN
30	Q	135	HIS
30	Q	307	ASN
30	Q	394	ASN
30	Q	420	ASN
31	R	132	GLN
31	R	136	ASN
31	R	323	ASN

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Mol	Chain	Res	Type
31	R	397	ASN
32	U	5	HIS
32	U	84	ASN
32	U	156	HIS
32	U	216	ASN
32	U	234	ASN
32	U	238	ASN
32	U	262	GLN
33	O	117	ASN
33	O	186	ASN
33	O	235	HIS
33	O	236	HIS
33	O	247	ASN
33	O	354	GLN
34	8	113	ASN
34	8	148	ASN
34	8	157	HIS
34	8	170	ASN
34	8	186	ASN
34	8	201	GLN
34	8	262	GLN
34	8	264	HIS
34	8	274	ASN
34	8	294	ASN
34	8	324	ASN
34	8	338	GLN
34	8	368	ASN
34	8	386	ASN
34	8	393	GLN
34	8	407	GLN
34	8	415	HIS
34	8	439	GLN
34	8	447	HIS
34	8	465	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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
37	ADP	K	501	36	28,29,29	2.65	5 (17%)	43,45,45	1.87	10 (23%)
35	ATP	M	501	36	32,33,33	3.35	5 (15%)	48,52,52	1.33	7 (14%)
35	ATP	J	501	36	32,33,33	4.30	3 (9%)	48,52,52	1.29	5 (10%)
35	ATP	H	501	36	32,33,33	3.90	5 (15%)	48,52,52	1.20	4 (8%)
35	ATP	I	501	36	32,33,33	4.52	7 (21%)	48,52,52	1.49	8 (16%)
37	ADP	L	501	36	28,29,29	2.02	3 (10%)	43,45,45	1.55	8 (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
37	ADP	K	501	36	-	3/16/32/32	0/3/3/3
35	ATP	M	501	36	-	6/22/38/38	0/3/3/3
35	ATP	J	501	36	-	6/22/38/38	0/3/3/3
35	ATP	H	501	36	-	6/22/38/38	0/3/3/3
35	ATP	I	501	36	-	6/22/38/38	0/3/3/3
37	ADP	L	501	36	-	2/16/32/32	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	I	501	ATP	PB-O3B	19.41	1.80	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	J	501	ATP	PB-O3B	18.66	1.79	1.59
35	H	501	ATP	PB-O3A	16.60	1.77	1.59
35	J	501	ATP	PB-O3A	14.59	1.75	1.59
35	M	501	ATP	PB-O3B	13.40	1.74	1.59
35	I	501	ATP	PB-O3A	13.00	1.73	1.59
37	K	501	ADP	PA-O3A	12.19	1.72	1.59
35	H	501	ATP	PB-O3B	11.51	1.71	1.59
35	M	501	ATP	PB-O3A	11.39	1.71	1.59
37	L	501	ADP	PA-O3A	8.10	1.68	1.59
35	I	501	ATP	PA-O3A	7.22	1.67	1.59
35	H	501	ATP	PA-O3A	5.76	1.65	1.59
35	M	501	ATP	C8-N9	3.80	1.44	1.37
37	L	501	ADP	C5-C4	3.63	1.45	1.39
35	H	501	ATP	C5-N7	-3.18	1.33	1.39
37	K	501	ADP	C5-N7	-3.10	1.33	1.39
35	I	501	ATP	O4'-C4'	3.04	1.51	1.45
37	L	501	ADP	O4'-C4'	-2.99	1.38	1.45
35	M	501	ATP	PA-O3A	2.87	1.62	1.59
35	J	501	ATP	C5-N7	-2.66	1.34	1.39
35	I	501	ATP	C5-N7	-2.57	1.34	1.39
37	K	501	ADP	C6-N6	2.48	1.40	1.34
35	M	501	ATP	C8-N7	-2.37	1.27	1.31
37	K	501	ADP	C3'-C4'	2.35	1.58	1.53
35	I	501	ATP	C1'-N9	2.30	1.52	1.46
35	I	501	ATP	C6-N6	2.26	1.40	1.34
35	H	501	ATP	C2'-C3'	2.24	1.59	1.53
37	K	501	ADP	C5-C4	2.21	1.43	1.39

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	K	501	ADP	C6-C5-C4	4.44	123.24	117.18
37	K	501	ADP	C5-C4-N3	-4.28	120.82	126.72
35	I	501	ATP	O4'-C1'-N9	4.21	116.17	108.09
37	L	501	ADP	N3-C2-N1	3.82	134.36	128.58
37	K	501	ADP	C4-N9-C8	-3.77	101.78	105.74
35	M	501	ATP	N6-C6-N1	3.73	126.69	118.38
35	J	501	ATP	N6-C6-N1	3.73	126.69	118.38
37	K	501	ADP	N3-C2-N1	3.65	134.11	128.58
35	J	501	ATP	C5-N7-C8	3.47	108.91	103.45
37	L	501	ADP	C5-C4-N9	-3.31	102.20	105.81
37	K	501	ADP	O3B-PB-O2B	3.29	120.15	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	K	501	ADP	O4'-C1'-N9	3.22	114.27	108.09
35	I	501	ATP	C4-N9-C1'	3.10	133.89	126.63
37	L	501	ADP	O4'-C1'-N9	3.09	114.03	108.09
35	H	501	ATP	C5-C4-N9	-3.03	102.51	105.81
37	K	501	ADP	N3-C4-N9	2.95	132.19	127.17
35	I	501	ATP	C4-N9-C8	-2.72	102.88	105.74
35	I	501	ATP	O2A-PA-O1A	2.71	125.06	112.44
37	L	501	ADP	N3-C4-N9	2.69	131.75	127.17
37	K	501	ADP	N6-C6-N1	2.65	124.29	118.38
35	J	501	ATP	N9-C8-N7	-2.61	110.24	113.94
35	J	501	ATP	C5-C6-N6	-2.57	116.92	123.29
35	J	501	ATP	O2B-PB-O3A	2.46	113.91	107.27
37	L	501	ADP	O5'-C5'-C4'	2.44	117.29	108.99
37	L	501	ADP	C2-N1-C6	-2.38	114.82	118.73
35	H	501	ATP	N6-C6-N1	2.28	123.46	118.38
35	M	501	ATP	O4'-C1'-N9	2.25	112.41	108.09
35	H	501	ATP	N3-C4-N9	2.24	130.97	127.17
37	L	501	ADP	C1'-N9-C8	2.24	132.06	127.09
37	K	501	ADP	C2'-C3'-C4'	2.23	106.91	102.61
35	M	501	ATP	C2'-C1'-N9	-2.19	107.85	113.30
37	K	501	ADP	C6-C5-N7	-2.17	127.92	132.09
35	I	501	ATP	O5'-C5'-C4'	2.16	116.36	108.99
35	M	501	ATP	O3'-C3'-C2'	2.14	118.67	111.82
35	M	501	ATP	C6-C5-C4	2.13	120.08	117.18
35	I	501	ATP	C5-C4-N3	-2.11	123.81	126.72
37	L	501	ADP	N9-C8-N7	2.10	116.91	113.94
35	I	501	ATP	O2B-PB-O1B	2.09	122.18	112.44
35	I	501	ATP	C1'-N9-C8	-2.08	122.48	127.09
35	M	501	ATP	O2A-PA-O3A	2.07	112.86	107.27
35	M	501	ATP	C6-C5-N7	-2.02	128.19	132.09
35	H	501	ATP	O4'-C1'-N9	2.02	111.97	108.09

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	H	501	ATP	PB-O3B-PG-O2G
35	I	501	ATP	C5'-O5'-PA-O1A
35	M	501	ATP	PB-O3B-PG-O2G
35	M	501	ATP	PB-O3B-PG-O3G
35	J	501	ATP	C5'-O5'-PA-O3A
37	K	501	ADP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
37	L	501	ADP	C5'-O5'-PA-O2A
35	I	501	ATP	C2'-C1'-N9-C4
37	K	501	ADP	PB-O3A-PA-O5'
35	M	501	ATP	PG-O3B-PB-O1B
37	L	501	ADP	PB-O3A-PA-O1A
35	J	501	ATP	C5'-O5'-PA-O1A
35	M	501	ATP	PG-O3B-PB-O2B
35	J	501	ATP	PG-O3B-PB-O2B
35	I	501	ATP	PA-O3A-PB-O3B
35	I	501	ATP	C2'-C1'-N9-C8
35	H	501	ATP	PB-O3B-PG-O1G
35	I	501	ATP	O4'-C1'-N9-C8
35	J	501	ATP	PB-O3B-PG-O1G
35	J	501	ATP	PB-O3B-PG-O2G
35	J	501	ATP	PB-O3B-PG-O3G
35	H	501	ATP	PG-O3B-PB-O1B
35	H	501	ATP	PG-O3B-PB-O2B
35	H	501	ATP	PA-O3A-PB-O1B
35	H	501	ATP	PA-O3A-PB-O2B
35	I	501	ATP	PA-O3A-PB-O1B
35	M	501	ATP	PB-O3A-PA-O2A
37	K	501	ADP	PA-O3A-PB-O1B
35	M	501	ATP	PB-O3A-PA-O1A

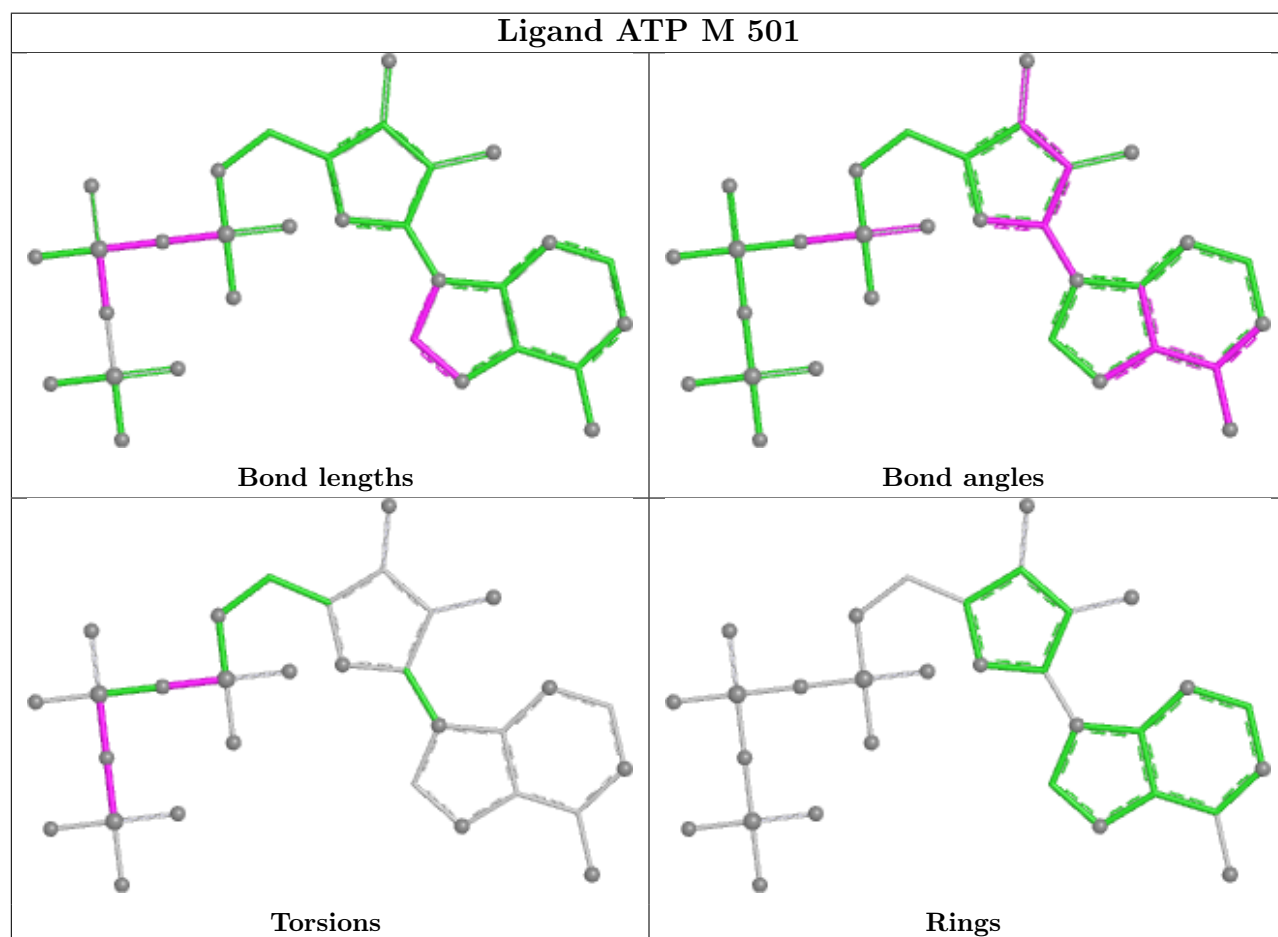
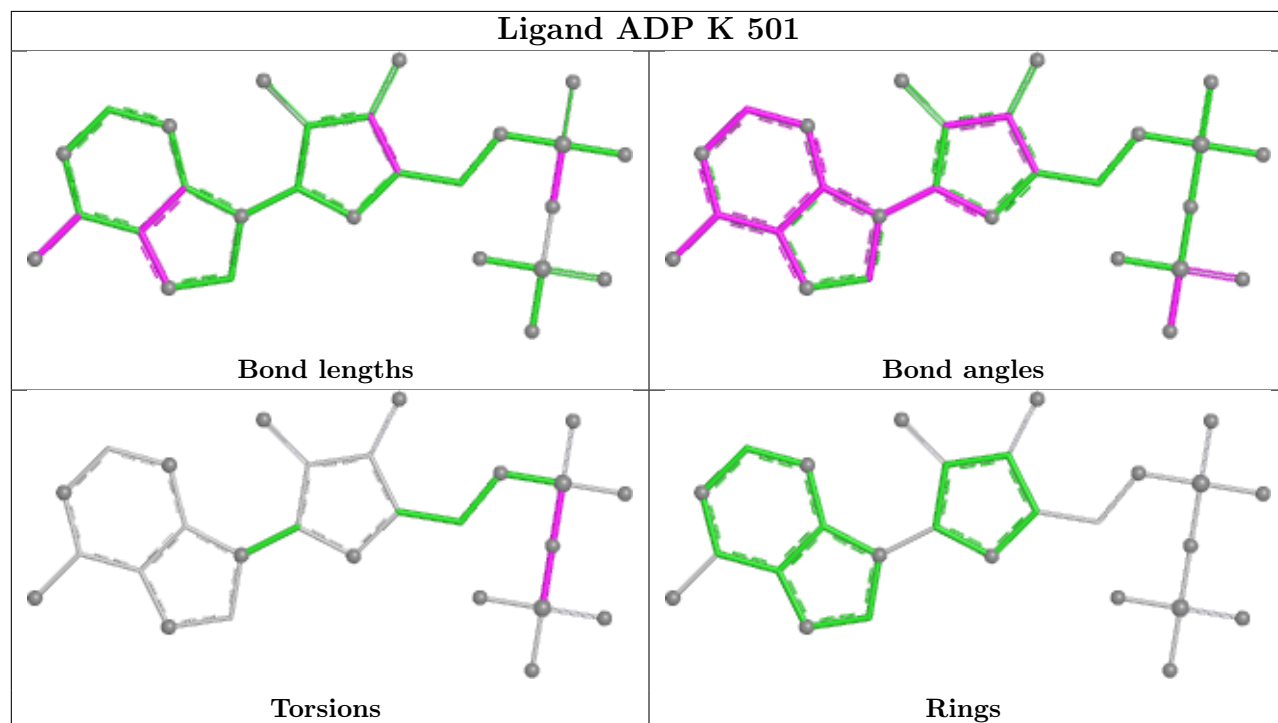
There are no ring outliers.

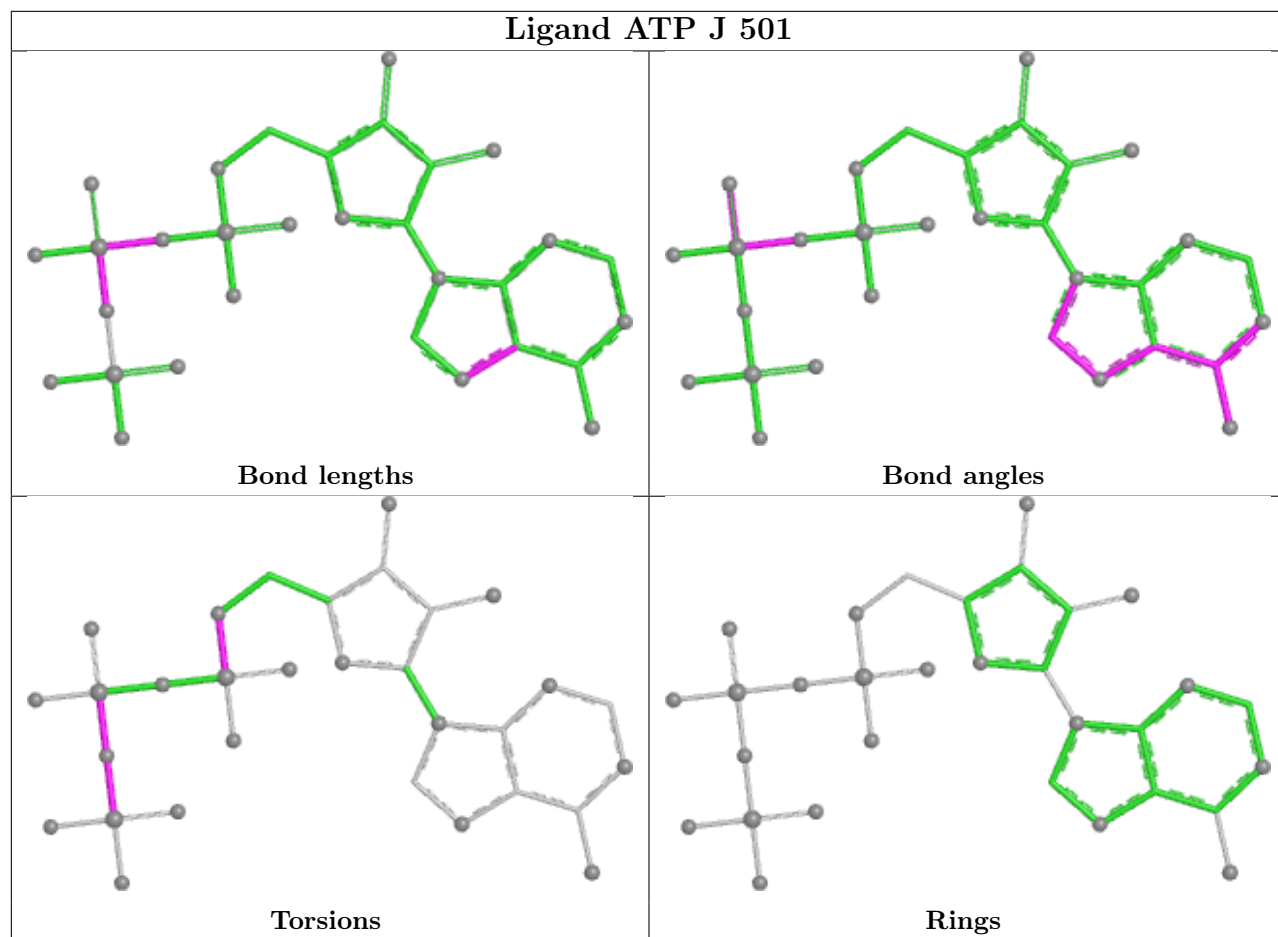
4 monomers are involved in 14 short contacts:

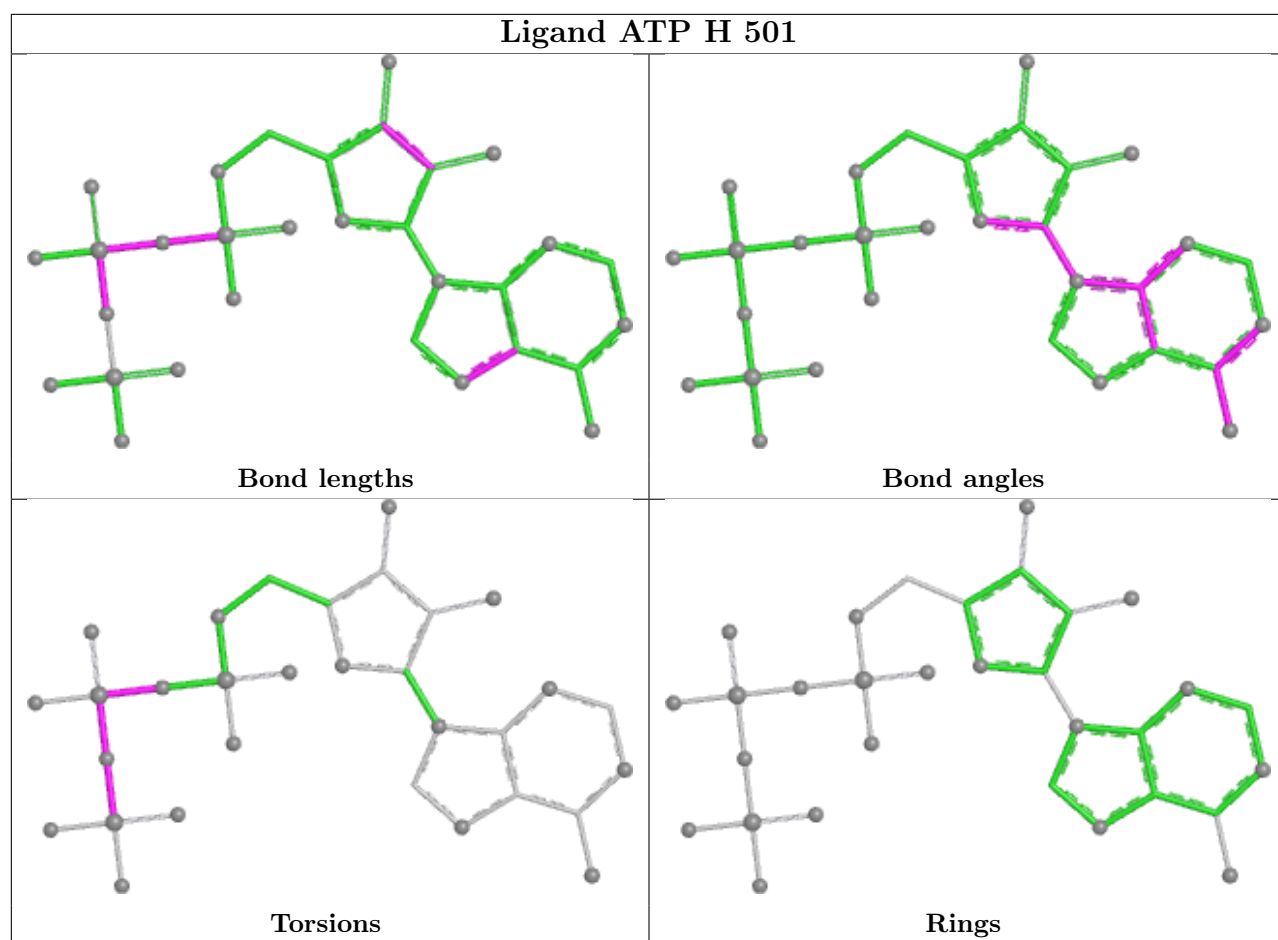
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	K	501	ADP	2	0
35	M	501	ATP	1	0
35	H	501	ATP	6	0
35	I	501	ATP	5	0

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

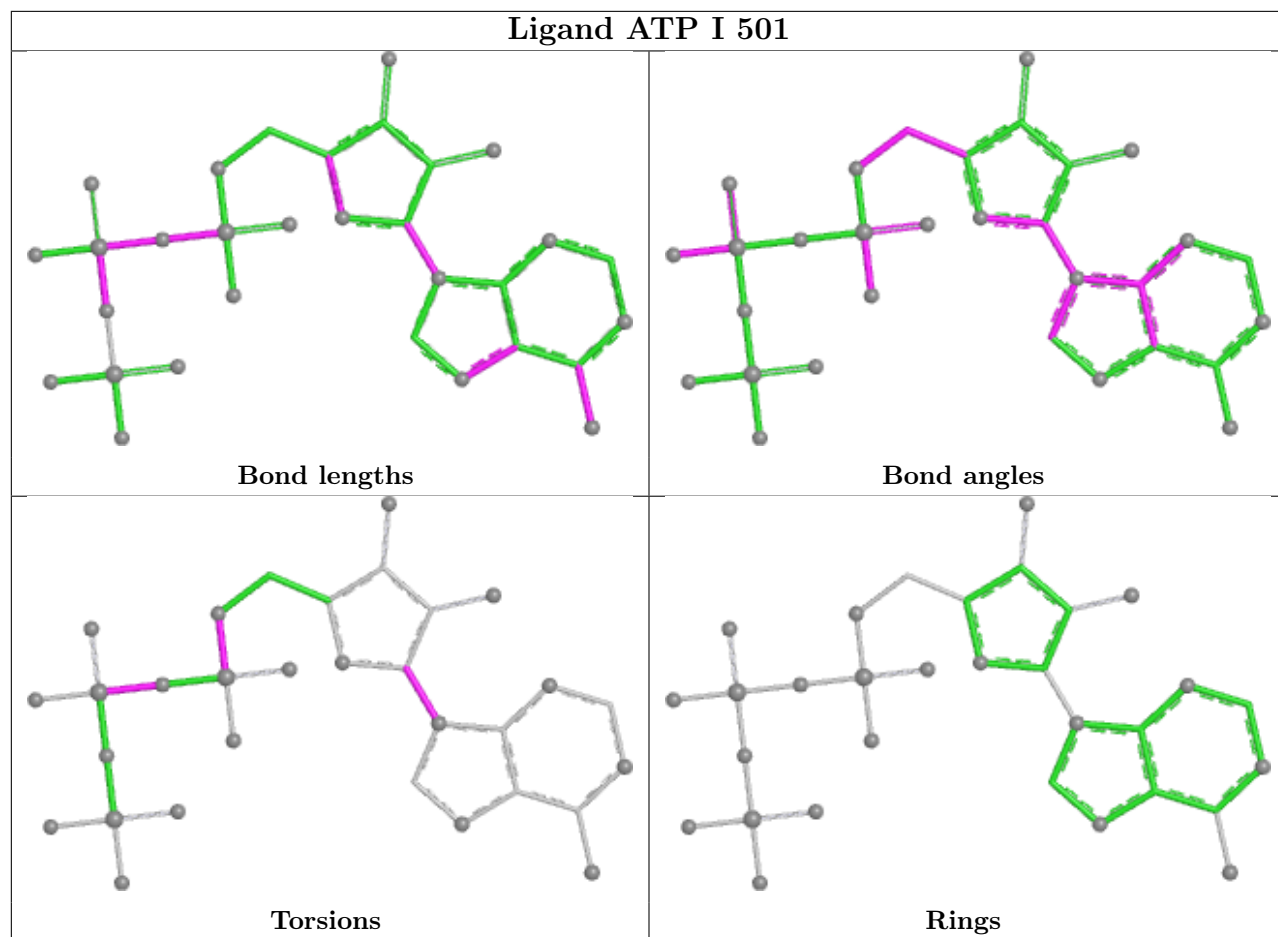
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



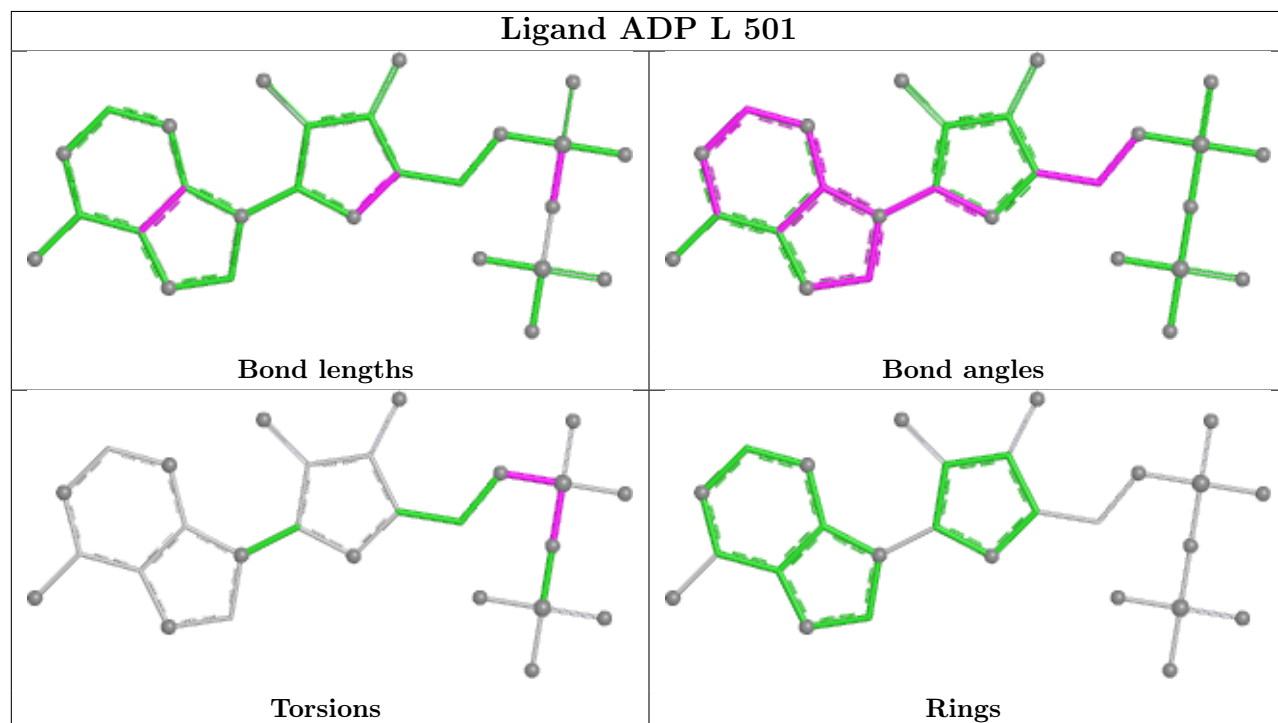




Ligand ATP I 501



Ligand ADP L 501



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

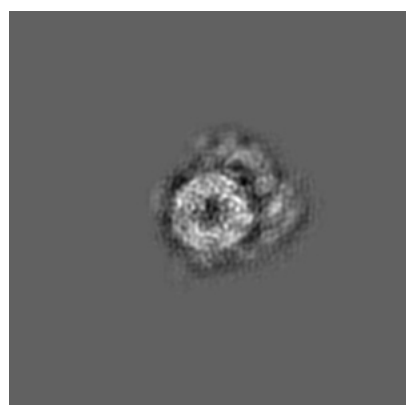
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3537. These allow visual inspection of the internal detail of the map and identification of artifacts.

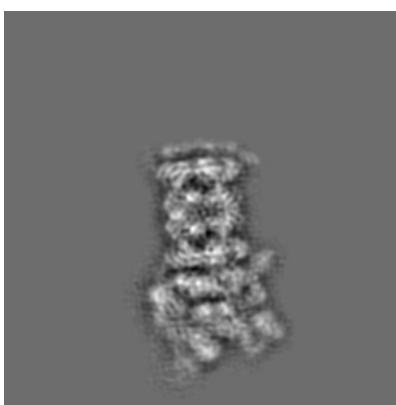
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

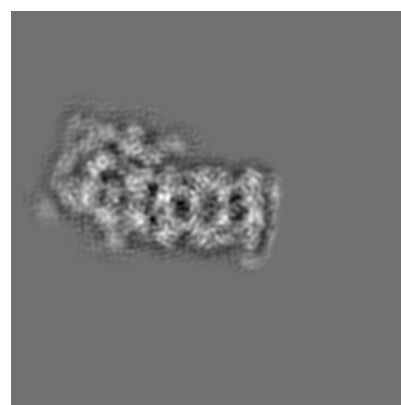
6.1.1 Primary map



X



Y

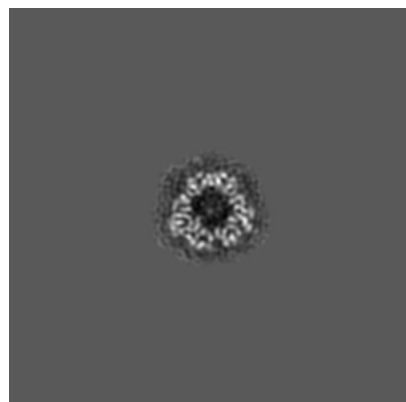


Z

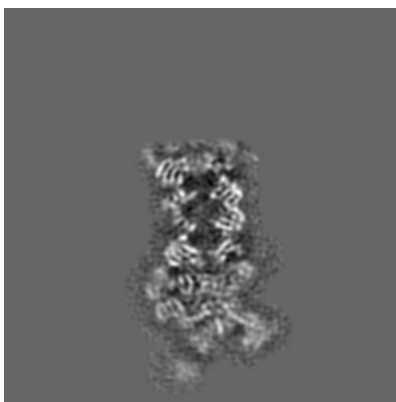
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

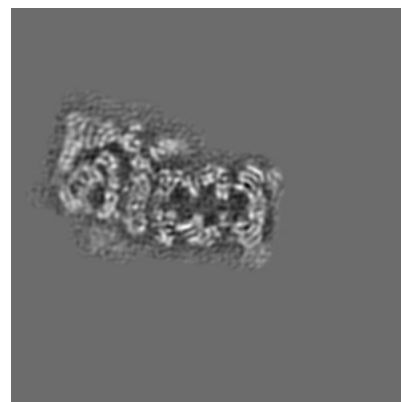
6.2.1 Primary map



X Index: 208



Y Index: 208

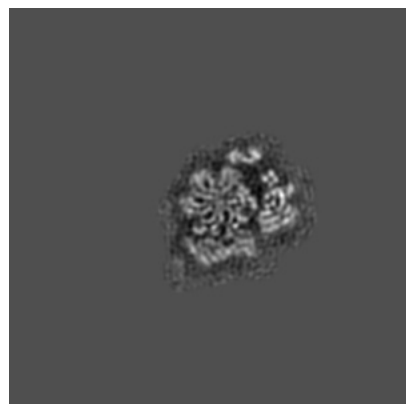


Z Index: 208

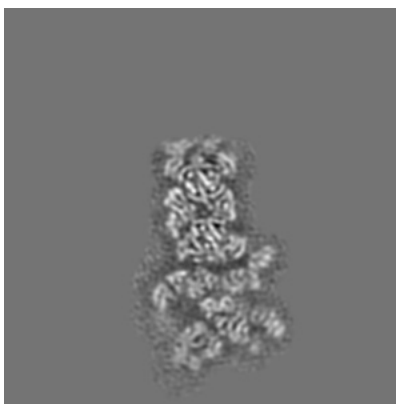
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

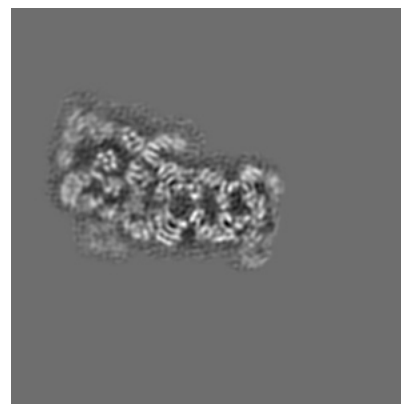
6.3.1 Primary map



X Index: 126



Y Index: 230

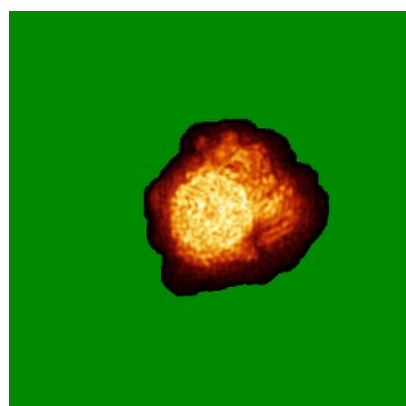


Z Index: 216

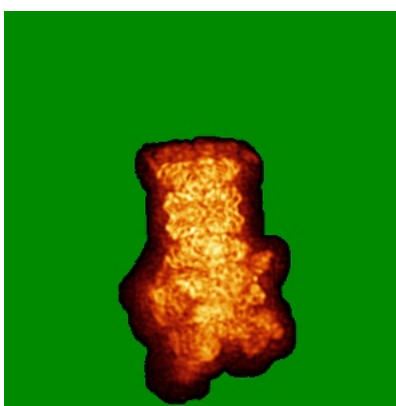
The images above show the largest variance slices of the map in three orthogonal directions.

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

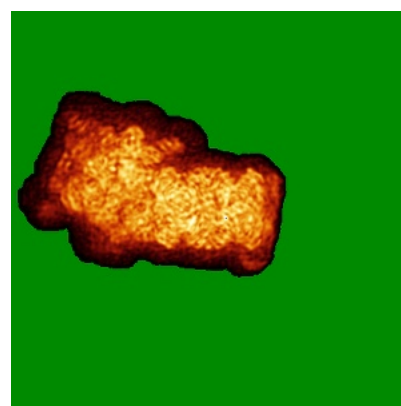
6.4.1 Primary map



X



Y

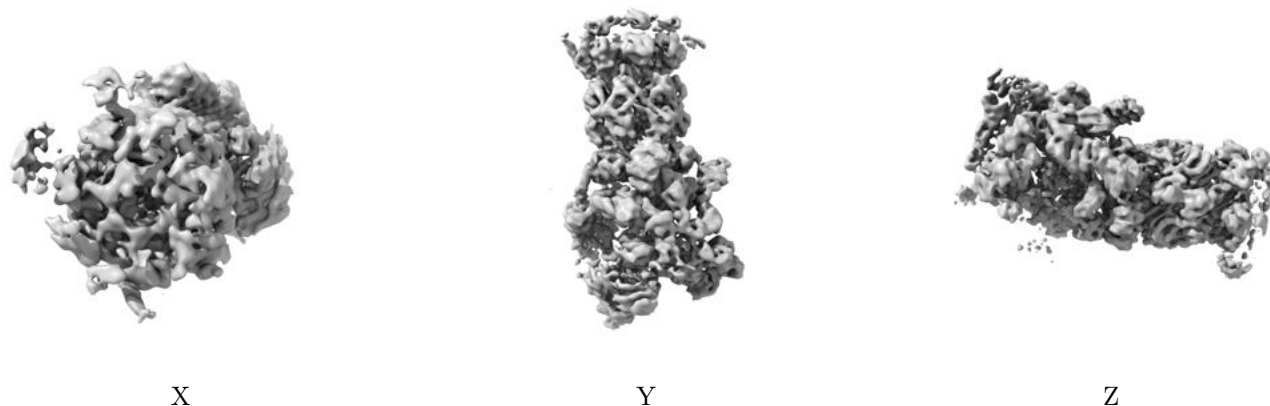


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

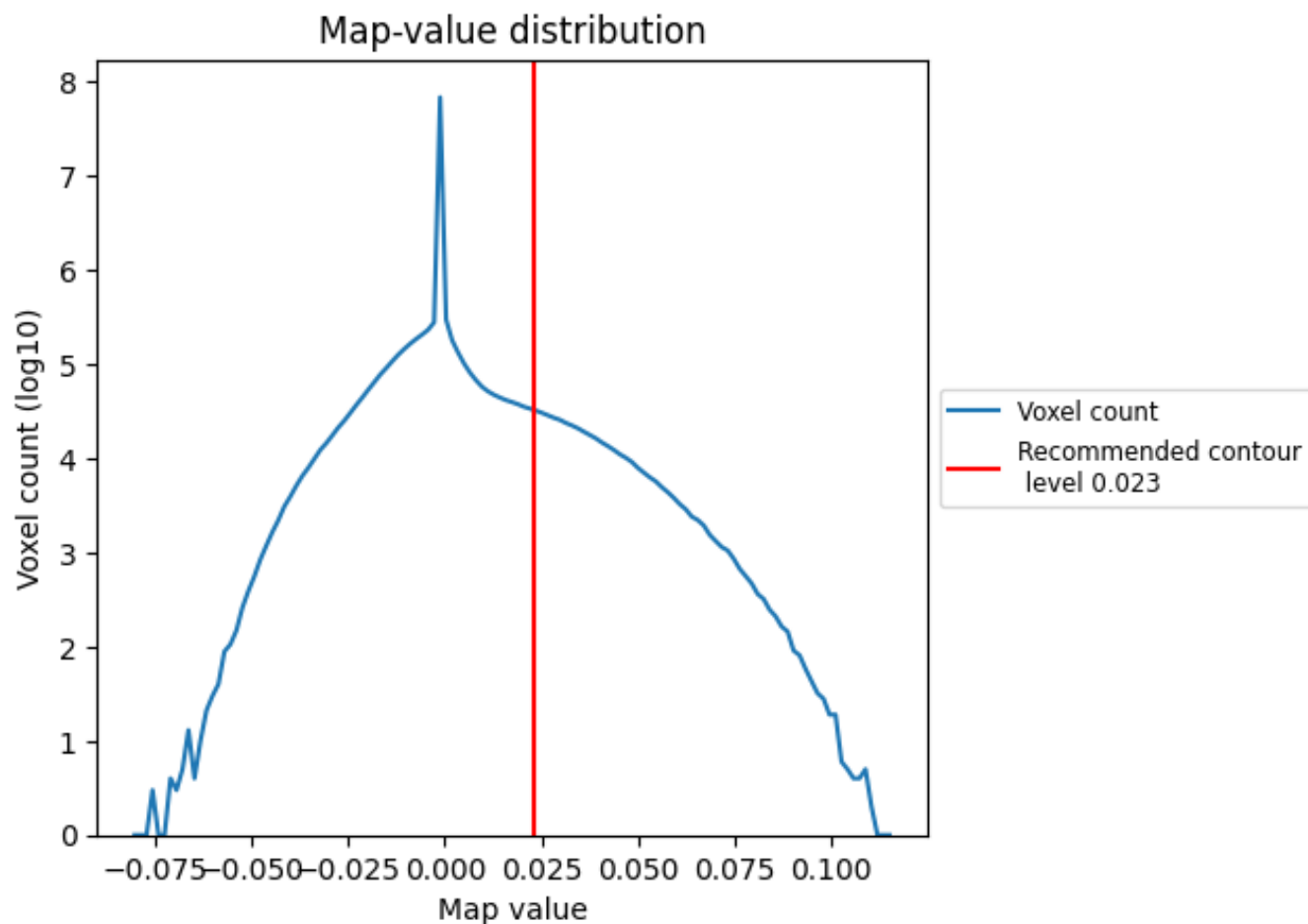
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

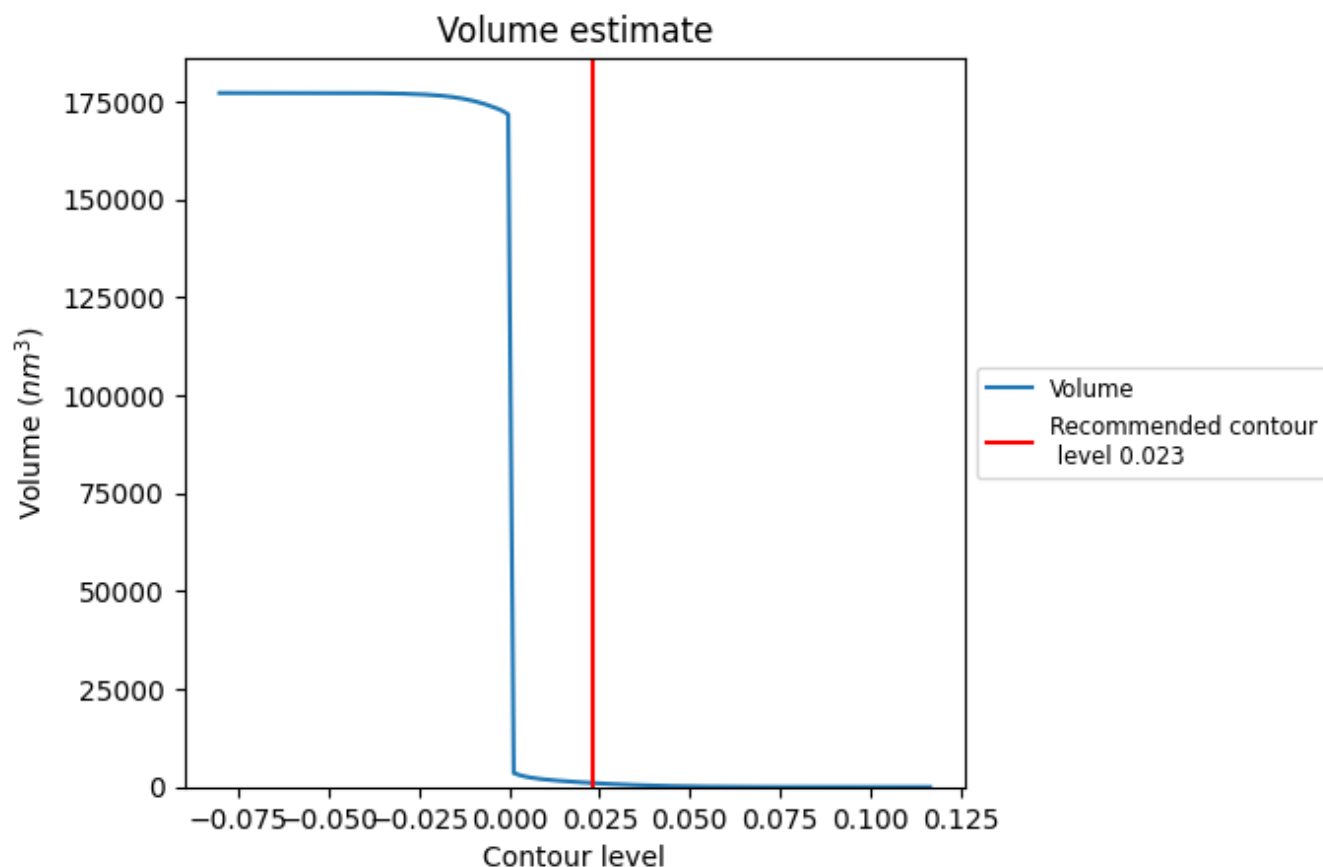
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

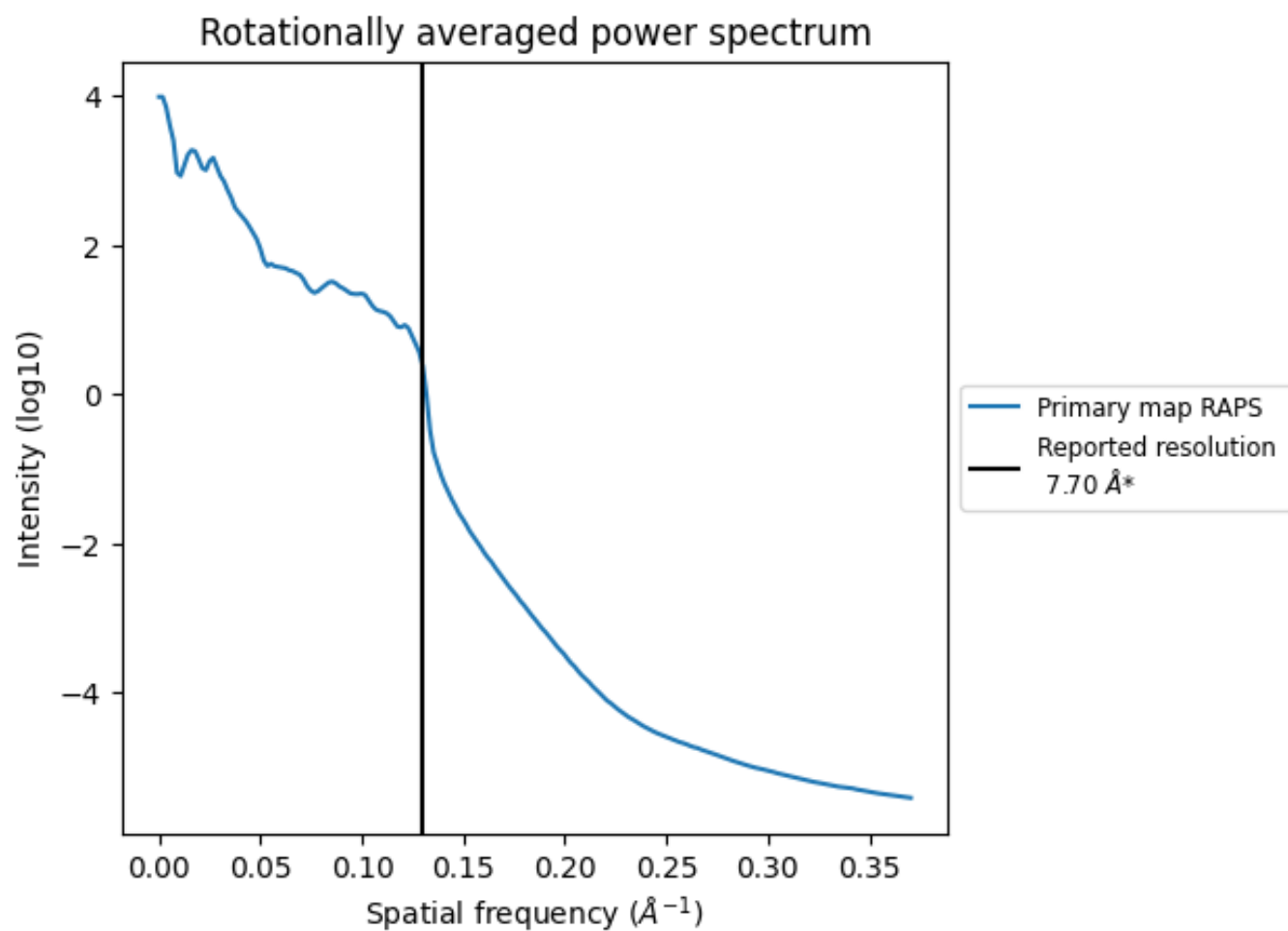
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1008 nm^3 ; this corresponds to an approximate mass of 911 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 0.130 Å⁻¹

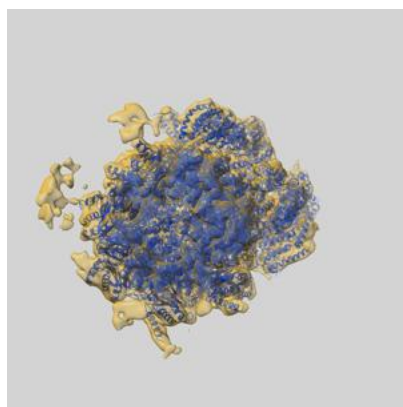
8 Fourier-Shell correlation

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

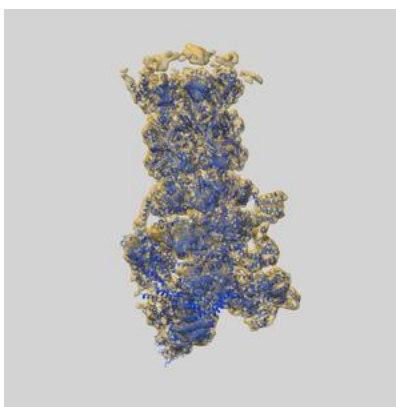
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3537 and PDB model 5MPC. Per-residue inclusion information can be found in section [3](#) on page [13](#).

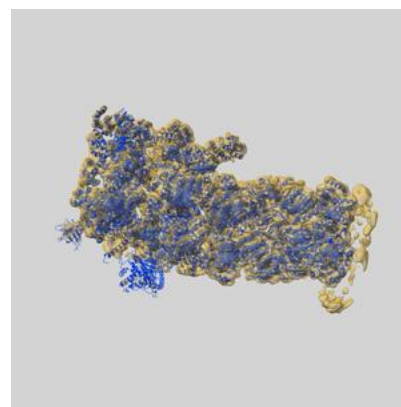
9.1 Map-model overlay [i](#)



X



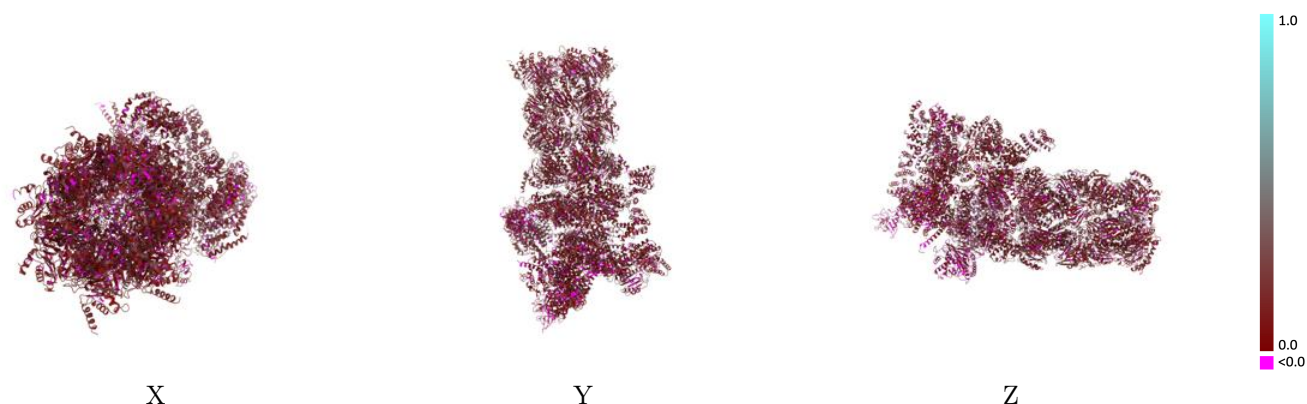
Y



Z

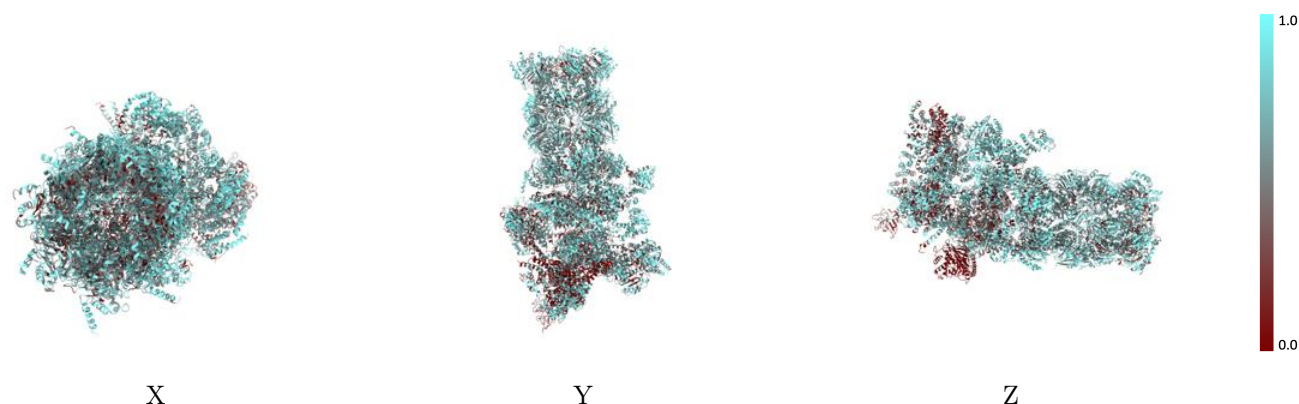
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



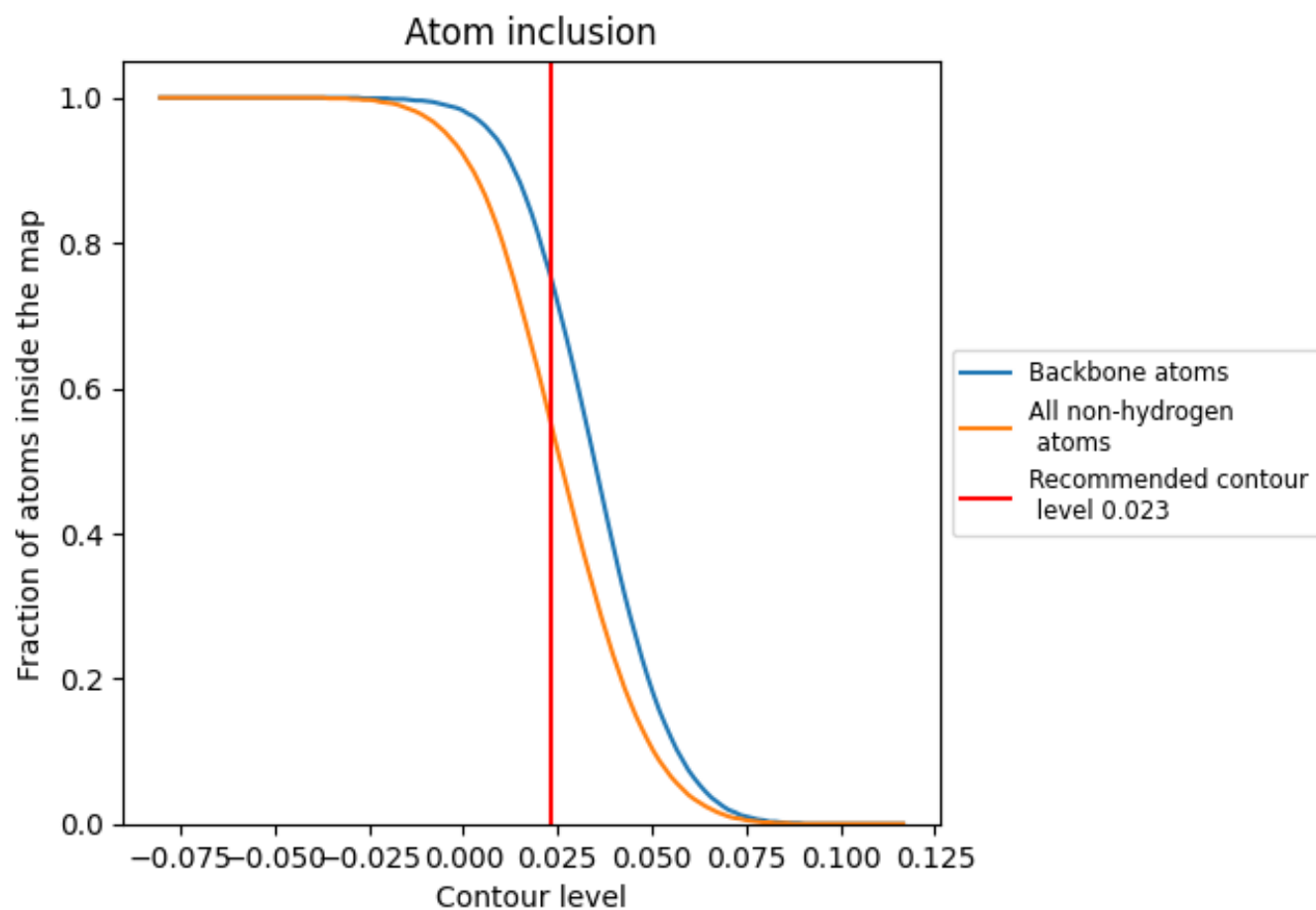
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.023).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 56% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5570	 0.1350
1	 0.6670	 0.1510
2	 0.6500	 0.1520
3	 0.5710	 0.1440
4	 0.6580	 0.1530
5	 0.6910	 0.1510
6	 0.6630	 0.1460
7	 0.6780	 0.1580
8	 0.0200	 0.0730
A	 0.6410	 0.1500
B	 0.5860	 0.1460
C	 0.5730	 0.1450
D	 0.6100	 0.1450
E	 0.6030	 0.1480
F	 0.6420	 0.1480
G	 0.6630	 0.1450
H	 0.5290	 0.1280
I	 0.4630	 0.1340
J	 0.4630	 0.1230
K	 0.4850	 0.1240
L	 0.4990	 0.1200
M	 0.5330	 0.1350
N	 0.5010	 0.1310
O	 0.6040	 0.1470
P	 0.7570	 0.1490
Q	 0.7040	 0.1430
R	 0.6900	 0.1460
S	 0.4410	 0.1290
T	 0.3330	 0.1250
U	 0.5110	 0.1410
V	 0.5200	 0.1350
W	 0.5480	 0.1110
X	 0.1510	 0.0710
Y	 0.4120	 0.0880
Z	 0.5140	 0.1040



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Chain	Atom inclusion	Q-score
a	 0.6210	 0.1460
b	 0.5430	 0.1380
c	 0.5560	 0.1380
d	 0.6150	 0.1420
e	 0.5990	 0.1440
f	 0.6200	 0.1400
g	 0.6440	 0.1500
h	 0.6510	 0.1420
i	 0.6260	 0.1470
j	 0.5850	 0.1390
k	 0.6480	 0.1410
l	 0.6780	 0.1490
m	 0.6550	 0.1510
n	 0.6390	 0.1430